Supporting Information

Structural Properties of Gas Phase Molybdenum Sulfide Clusters [Mo$_3$S$_{13}$]$^{2-}$, [HMo$_3$S$_{13}$]$^-$, and [H$_3$Mo$_3$S$_{13}$]$^+$ as Model Systems of a Promising Hydrogen Evolution Catalyst

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Table S1: Overview of all measured fragment ions, sorted by parent ion.

| $[Mo_3S_{13}]^{2-}$ Fragment	Measured m/z	Exact m/z	$[HMo_3S_{13}]^{-}$ Fragment	Measured m/z	Exact m/z	$[H_3Mo_3S_{13}]^{+}$ Fragment	Measured m/z	Exact m/z
$Mo_3S_{11}^{--}$	313.707	313.707	$HMo_3S_{11}^{-}$	628.425	628.422	$H_2Mo_3S_{12}^{+}$	661.402	661.400
$Mo_3S_9^{--}$	281.735	281.735	$Mo_3S_{11}^{-}$	627.417	627.414	$HMo_3S_{12}^{+}$	660.394	660.393
$Mo_3S_7^{--}$	249.763	249.763	$HMo_3S_{10}^{-}$	596.453	596.450	$H_5Mo_3S_{11}O^{+}$	648.448	648.447
$Mo_3S_{10}^{-}$	595.442	595.442	$Mo_3S_{10}^{-}$	595.444	595.442	$H_3Mo_3S_{11}^{+}$	630.438	630.436
$Mo_3S_9^{-}$	563.470	563.470	$HMo_3S_9^{-}$	564.481	564.477	$H_2Mo_3S_{11}^{+}$	629.430	629.428
$Mo_3S_8^{-}$	531.491	531.498	$Mo_3S_9^{-}$	563.473	563.470	$H_3Mo_3S_{10}O^{+}$	614.461	614.459
$Mo_3S_7^{-}$	499.526	499.525	$HMo_3S_8^{-}$	532.508	532.505	$H_2Mo_3S_{10}^{+}$	597.458	597.456
$Mo_2S_6^{-}$	375.644	375.647	$Mo_3S_8^{-}$	531.501	531.498	$HMo_3S_{10}^{+}$	596.450	596.448
			$Mo_3S_7O^{-}$	515.524	515.520	$Mo_3S_{10}^{+}$	595.442	595.441
			$HMo_3S_7^{-}$	500.536	500.533	$H_5Mo_3S_9O^{+}$	584.504	584.503
			$Mo_3S_7^{-}$	499.528	499.525	$H_4Mo_3S_9O^{+}$	583.496	583.495
			$Mo_3S_5O_2^{-}$	467.575	467.571	$H_5Mo_3S_8O_2^{+}$	568.527	568.525
						$H_4Mo_3S_8O_2^{+}$	567.519	567.518
						$H_3Mo_3S_9^{+}$	566.494	566.492
						$H_2Mo_3S_9^{+}$	565.485	565.484
						$Mo_3S_9^{+}$	563.470	563.469
						$H_3Mo_3S_8O^{+}$	550.516	550.515
						$H_2Mo_3S_8O^{+}$	549.508	549.507
						$HMo_3S_8O^{+}$	548.500	548.499
						$HMo_3S_8^{+}$	532.506	532.504
						$Mo_3S_8^{+}$	531.498	531.496
						$H_2Mo_3S_7O^{+}$	517.541	517.535
						$HMo_3S_7O^{+}$	516.529	516.527
						$H_4Mo_3S_5O_4^{+}$	503.592	503.591
						$H_2Mo_3S_6O_2^{+}$	501.559	501.558
						$HMo_3S_6O_2^{+}$	500.551	500.550
						$Mo_3S_7^{+}$	499.526	499.524
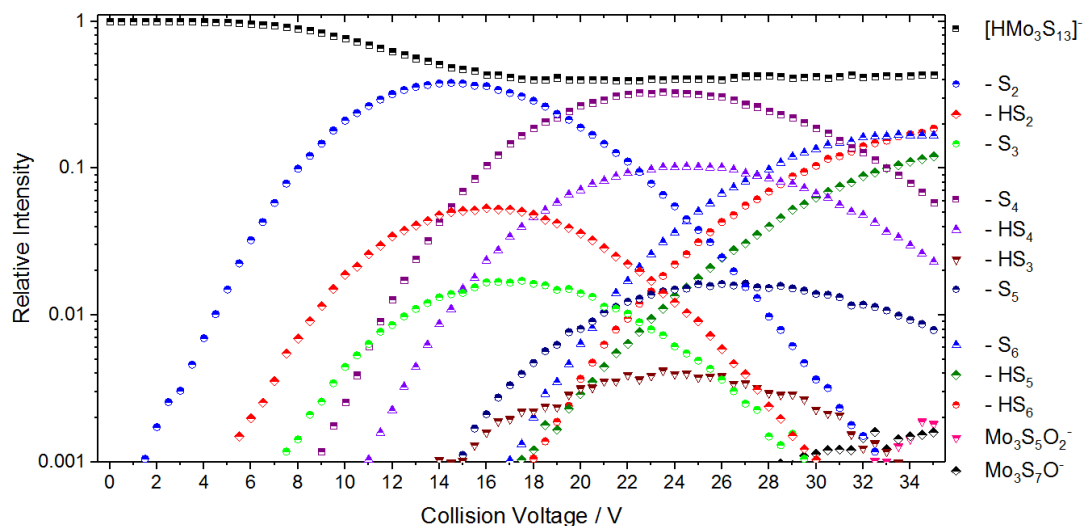
Figure S1: Qualitative breakdown curves of protonated thiomolybdate $[HMo_3S_{13}]^-$ from collision cell CID. The first fragmentation channel to open is the elimination of S_2. Elimination of S2 and $2S_2$ are the most effective channels. The formation of oxide $[Mo_3S_7O]^-$ and $[Mo_3S_5O_2]^-$ is admitted to water contamination in the argon inlet system of the collision cell. Oxo-Species in below 2‰ at Vc > 30 V.
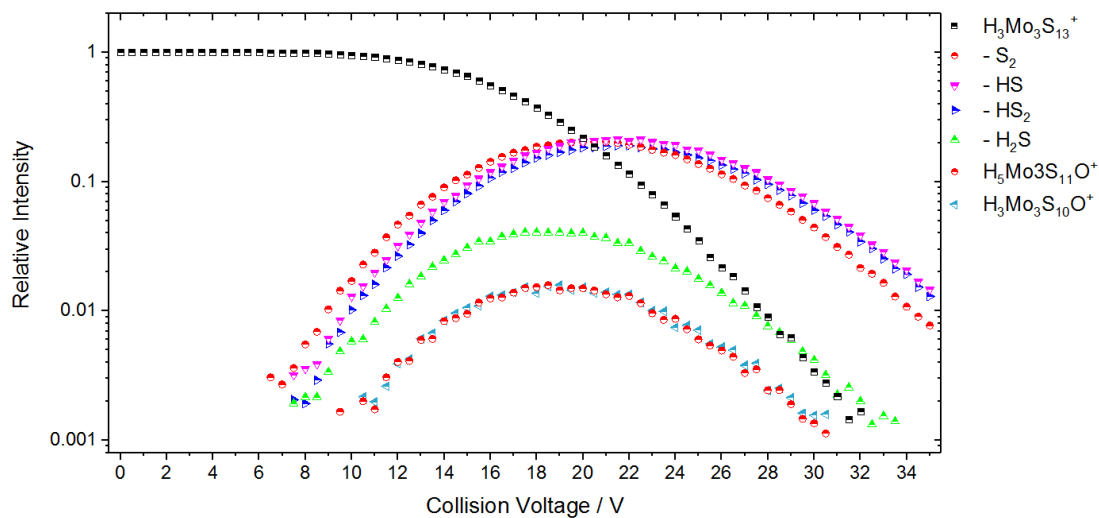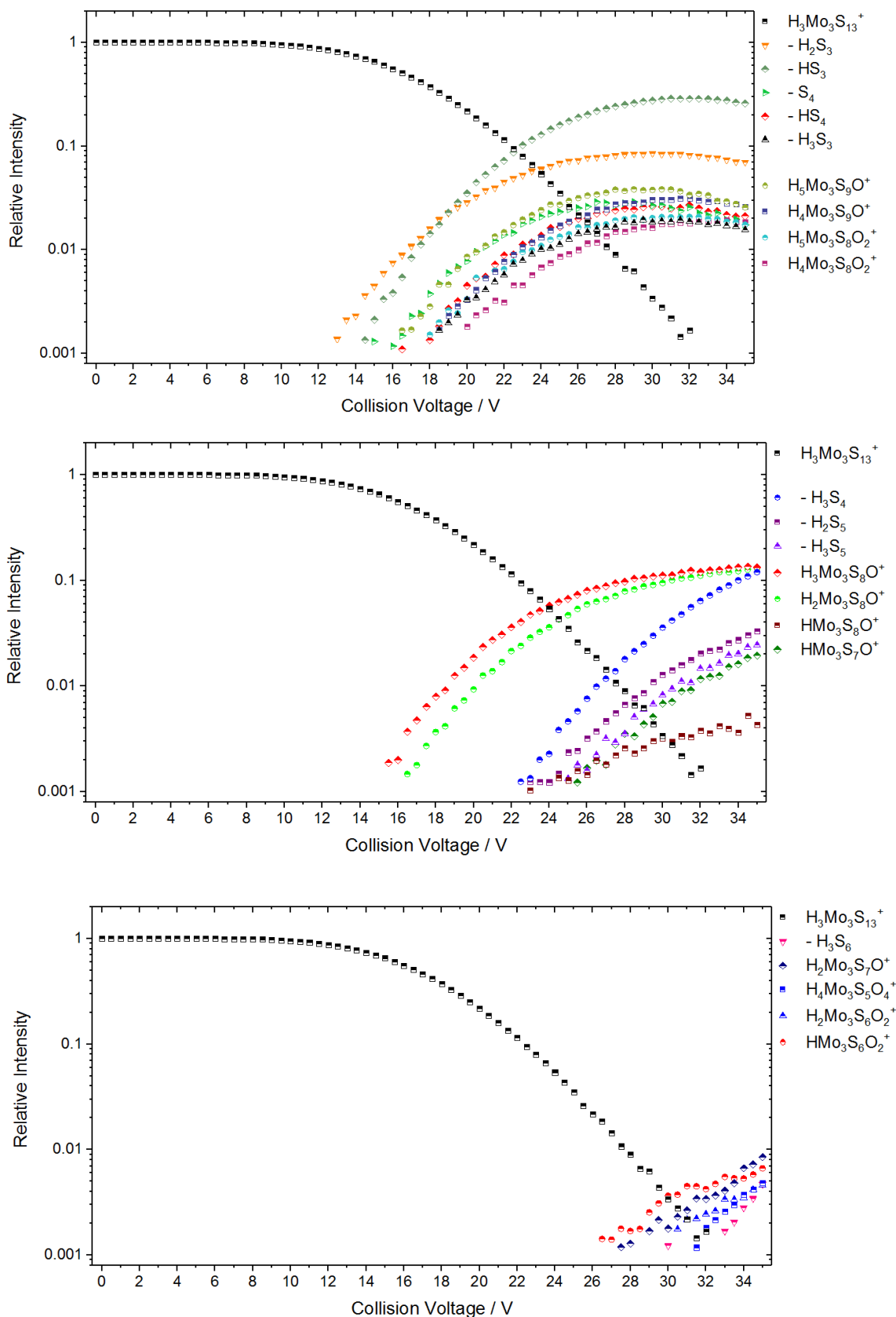
Figure S2: Qualitative breakdown curves of triply protonated thiomolybdate $[H_3Mo_3S_{13}]^+$ split up into four graphs for better view. The formation of protonated thio-oxo-molybdates may be admitted to water/oxygen contamination inside the argon inlet system of the collision cell.

Figure S3: Calculated structures of $[Mo_3S_{13}]^{2-}$ in the lowest spin multiplicity.

Figure S4: Calculated structures of $[Mo_3S_{11}]^{2-}$ in the lowest spin multiplicity.

Figure S5: Calculated structures of $[Mo_3S_{11}]^-$ in the lowest spin multiplicity.

Figure S6: Calculated structures of $[Mo_3S_{10}]^-$ in the lowest spin multiplicity.

Figure S7: Calculated structures of $[Mo_3S_9]^{2-}$ in the lowest spin multiplicity.

Figure S8: Calculated structures of $[Mo_3S_9]^-$ in the lowest spin multiplicity.

Figure S9: Calculated structures of $[Mo_3S_8]^-$ in the lowest spin multiplicity.
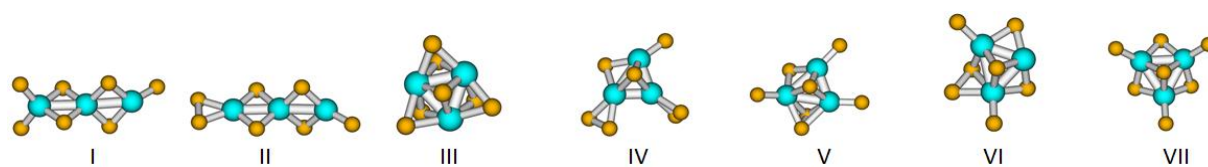
Figure S10: Calculated structures of $[Mo_3S_7]^{2-}$ in the lowest spin multiplicity.
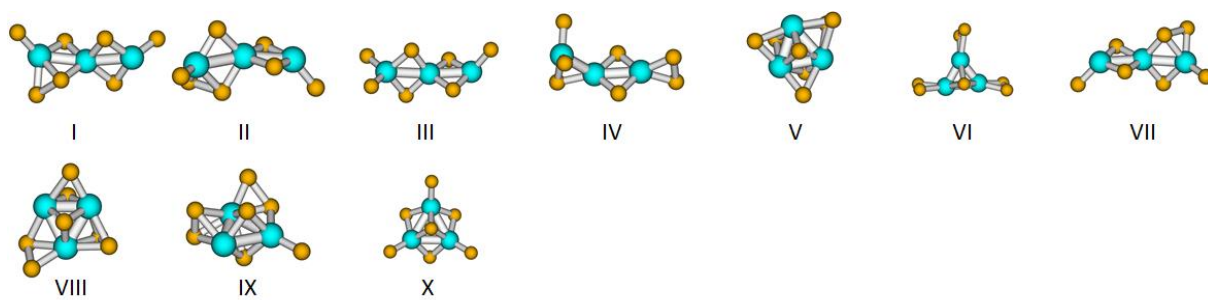
Figure S11: Calculated structures of $[Mo_3S_7]^-$ in the lowest spin multiplicity.
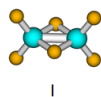
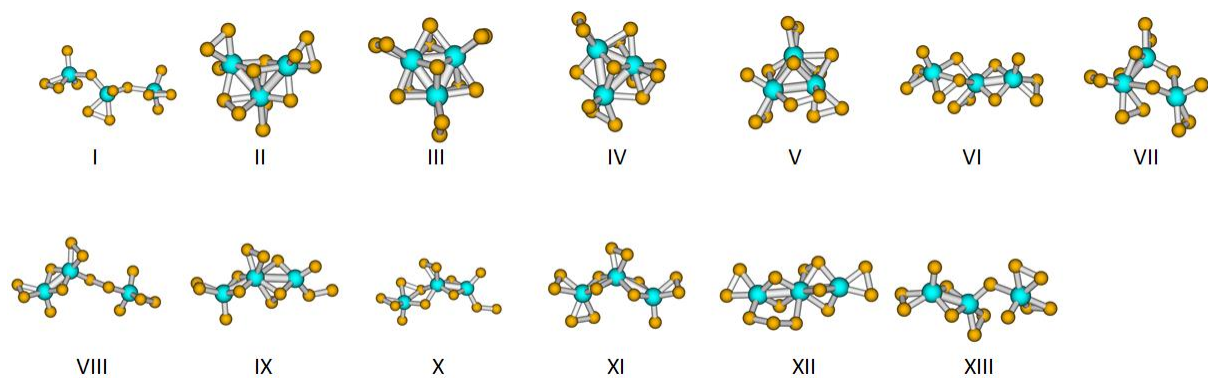**Figure S12**: Calculated structure of $[Mo_2S_6]^-$ in the lowest spin multiplicity.
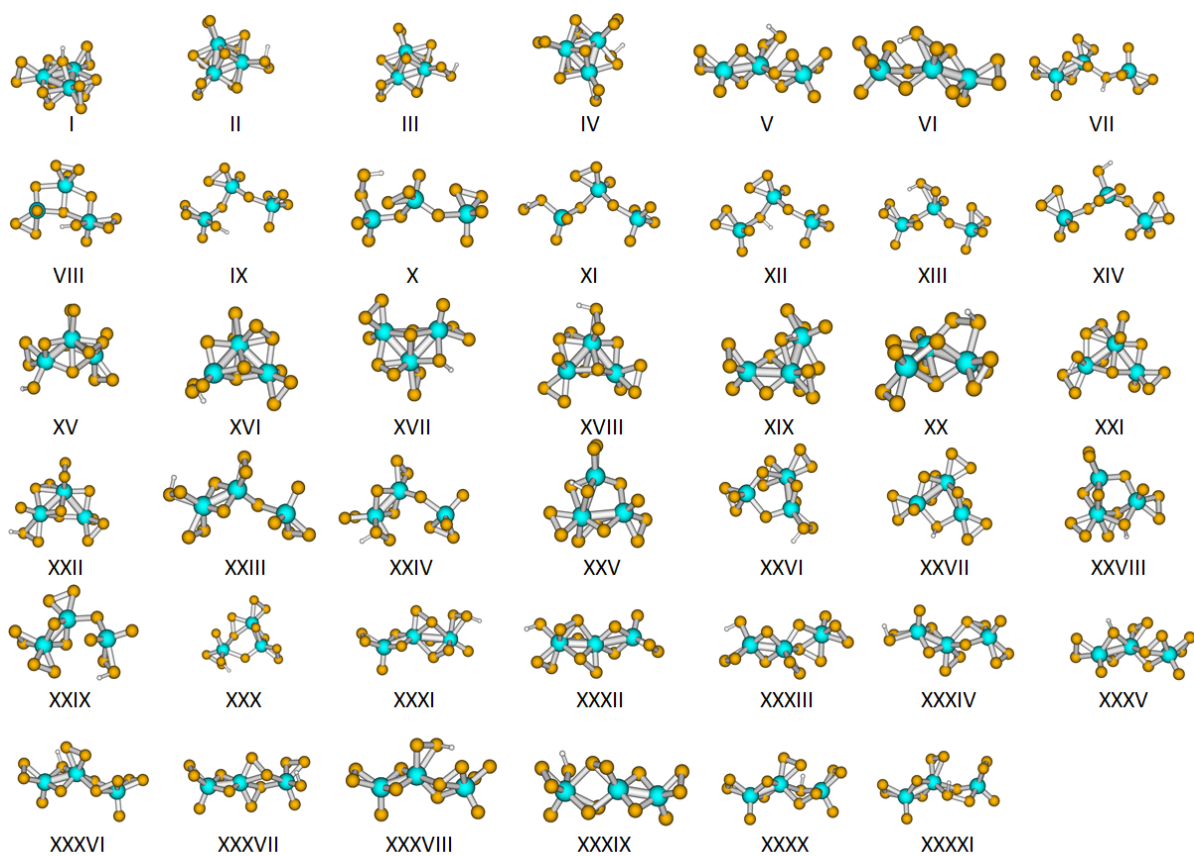
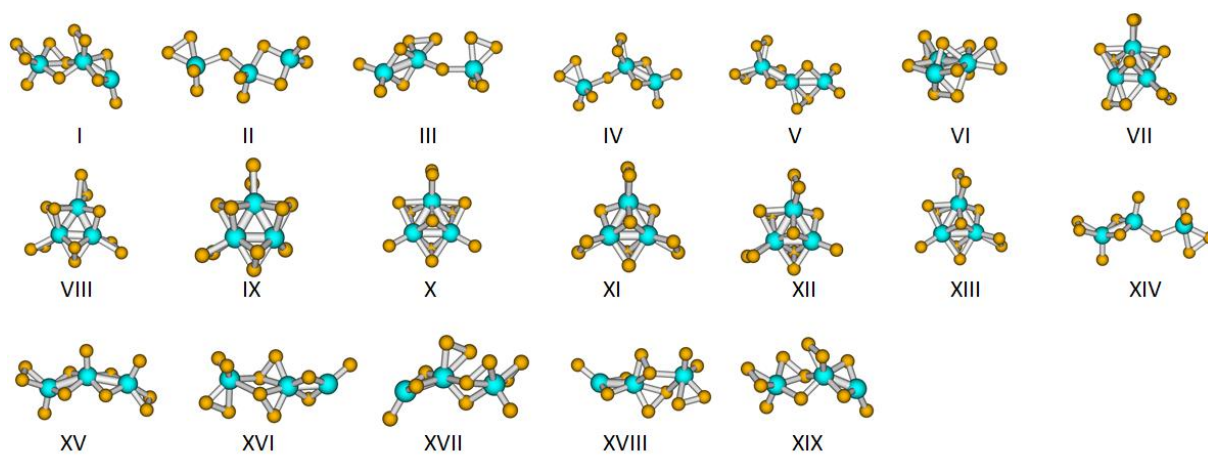**Figure S13**: Calculated structures of $[HMo_3S_{13}]^-$ in the lowest spin multiplicity.
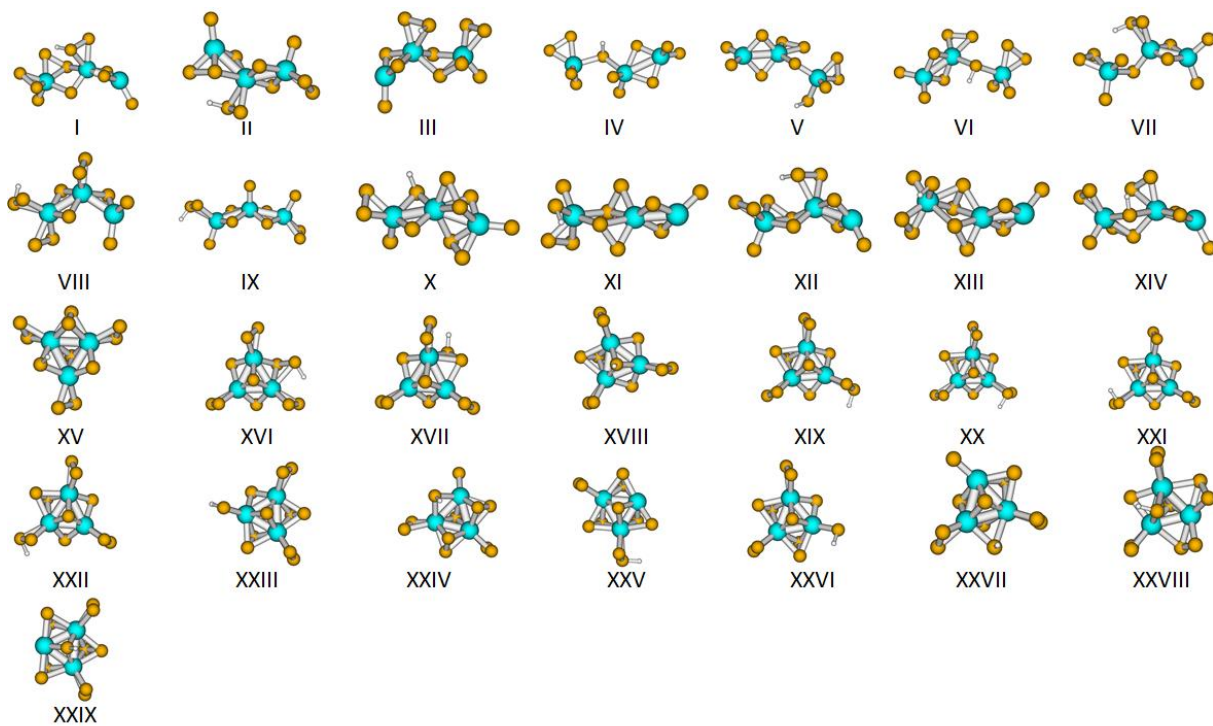
Figure S14: Calculated structures of $[HMo_3S_{11}]^-$ in the lowest spin multiplicity.
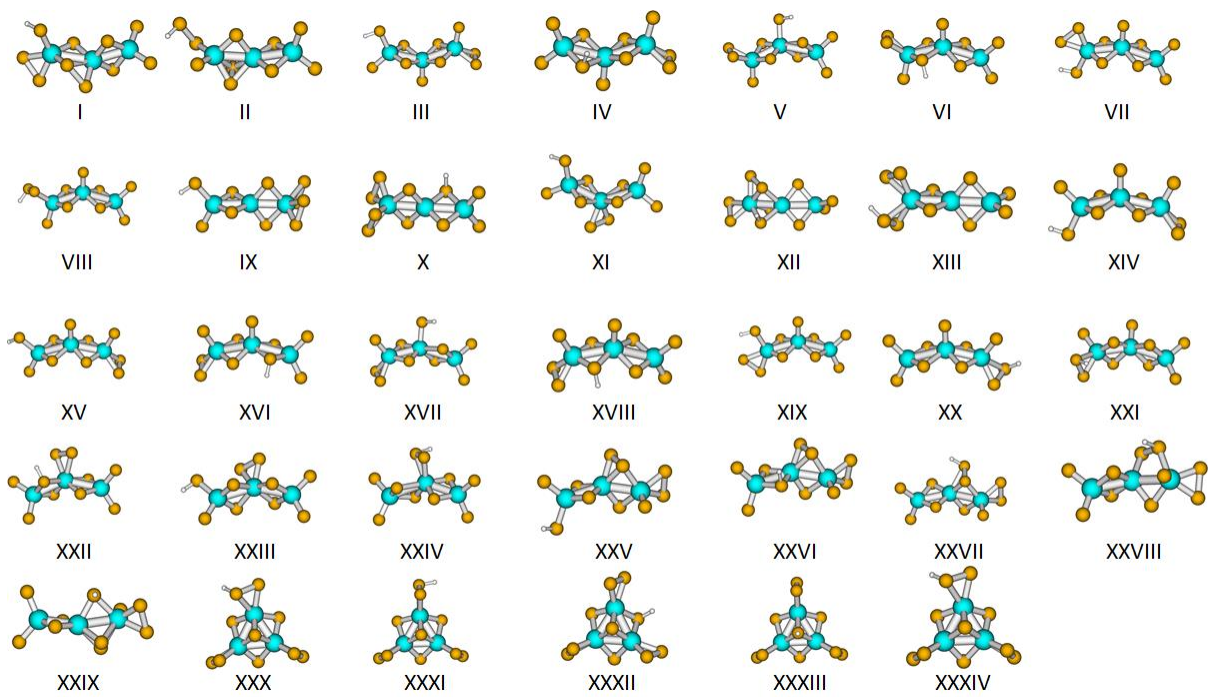
Figure S15: Calculated structures of [HMo$_3$S$_{10}$]$^-$ in the lowest spin multiplicity.
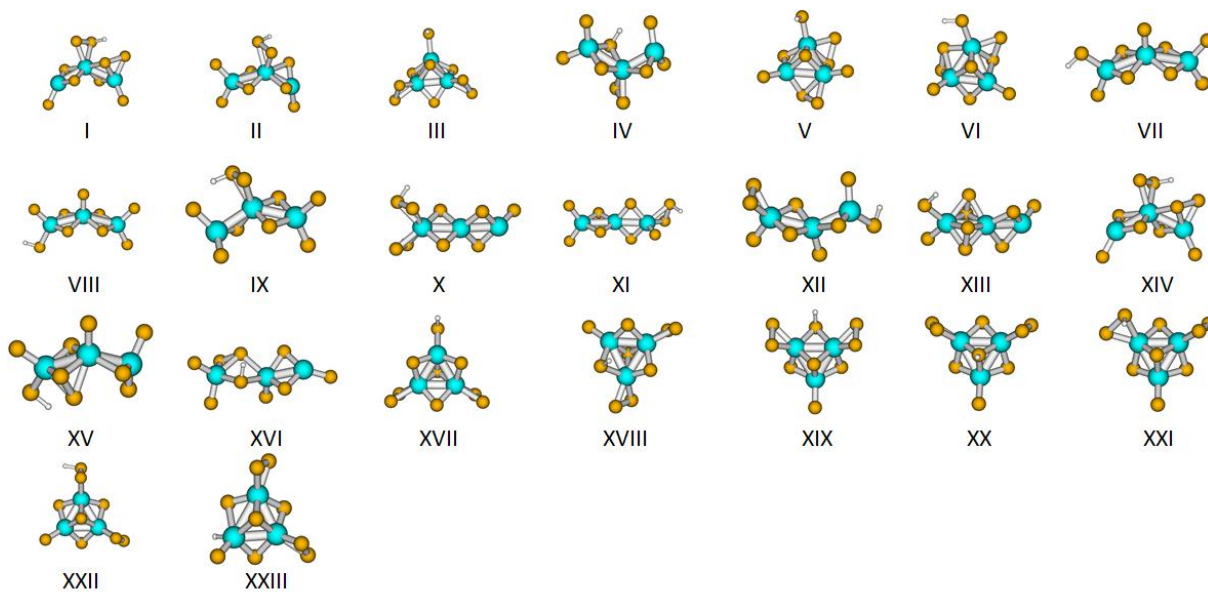
Figure S16: Calculated structures of [HMo$_3$S$_9$]$^-$ in the lowest spin multiplicity.
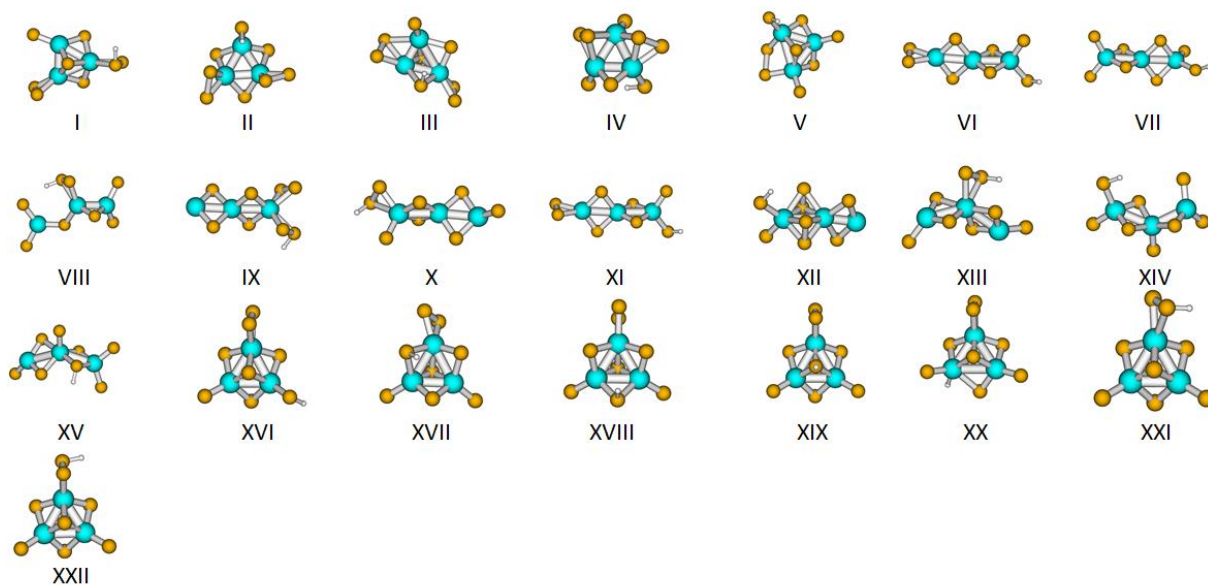
Figure S17: Calculated structures of $[HMo_3S_8]^-$ in the lowest spin multiplicity.
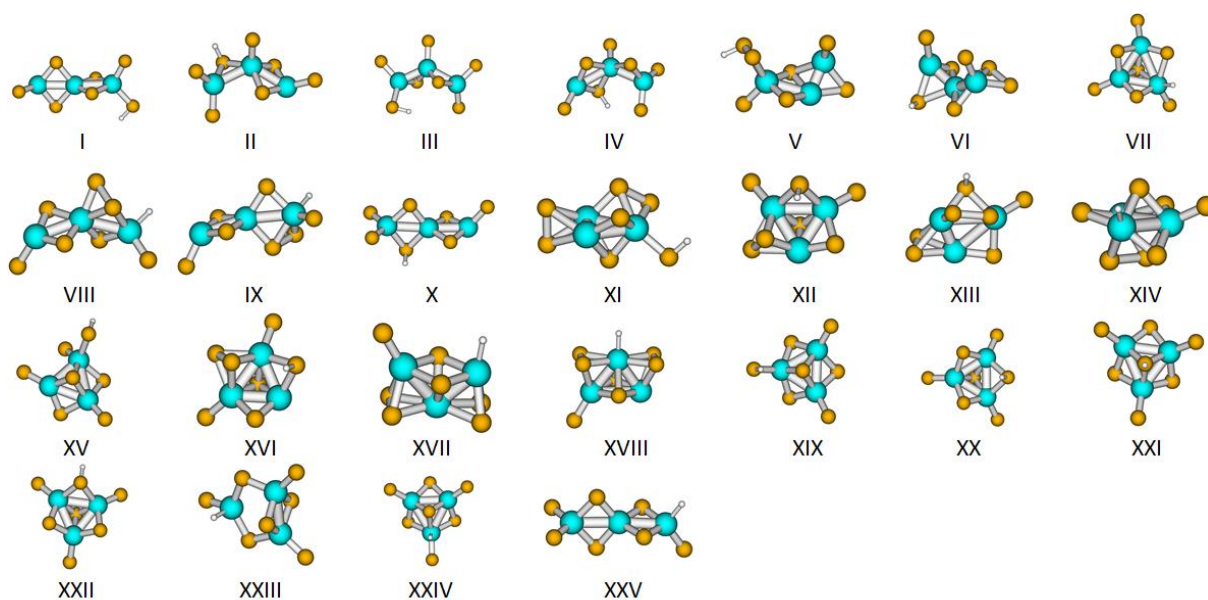
Figure S18: Calculated structures of $[HMo_3S_7]^-$ in the lowest spin multiplicity.
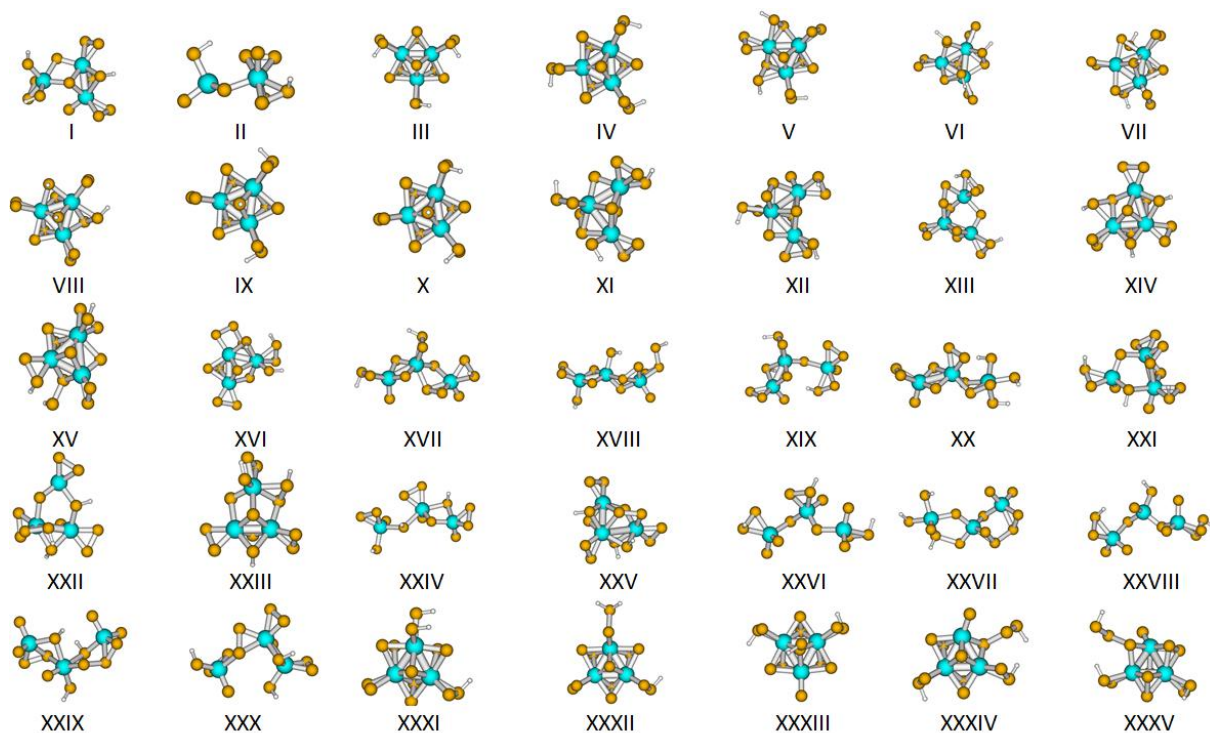
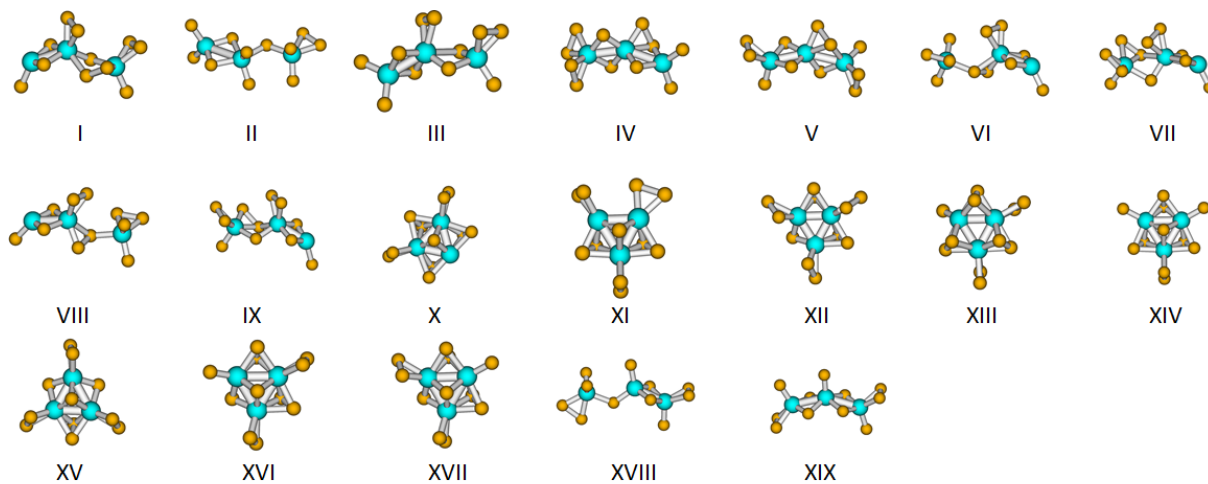**Figure S19**: Calculated structures of $[H_3Mo_3S_{13}]^+$ in the lowest spin multiplicity.
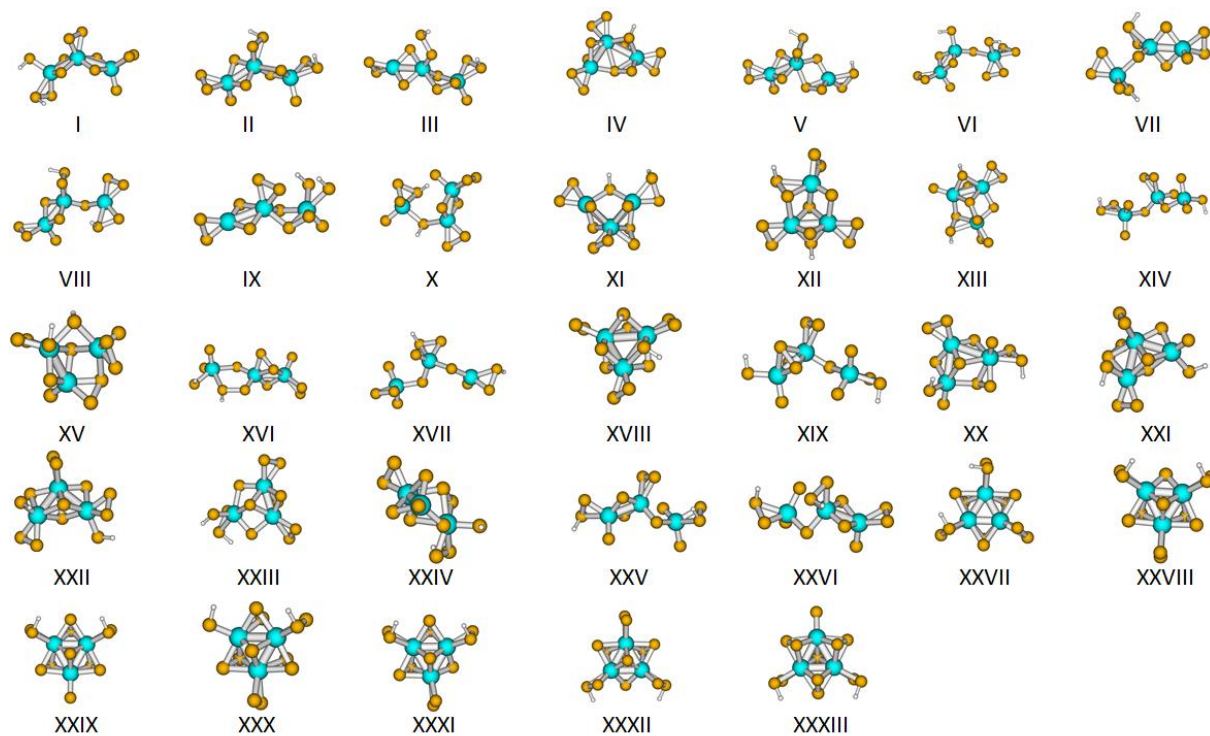
Figure S20: Calculated structures of $[H_2Mo_3S_{12}]^+$ in the lowest spin multiplicity.
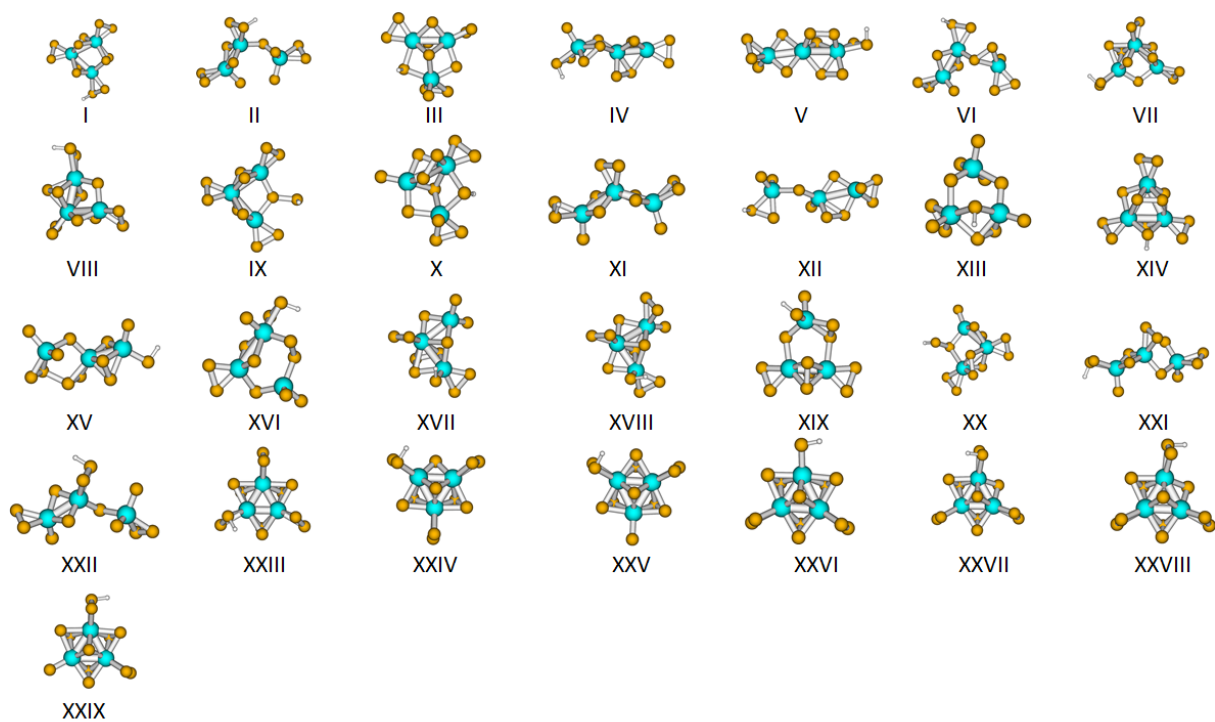
Figure S21: Calculated structures of $[HMo_3S_{12}]^+$ in the lowest spin multiplicity.
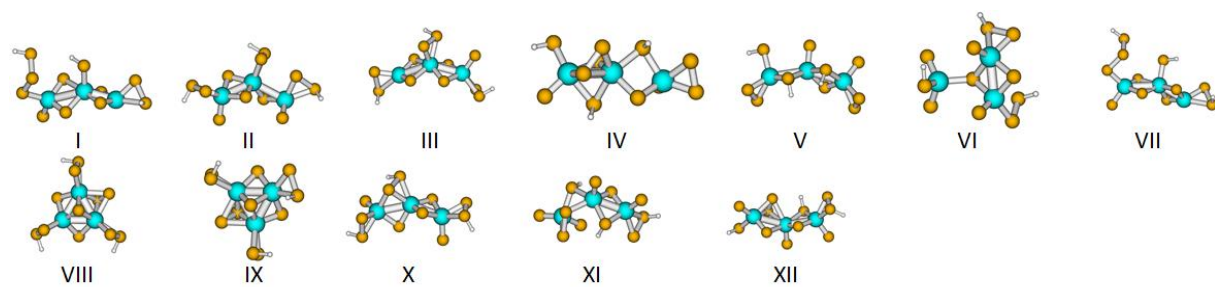
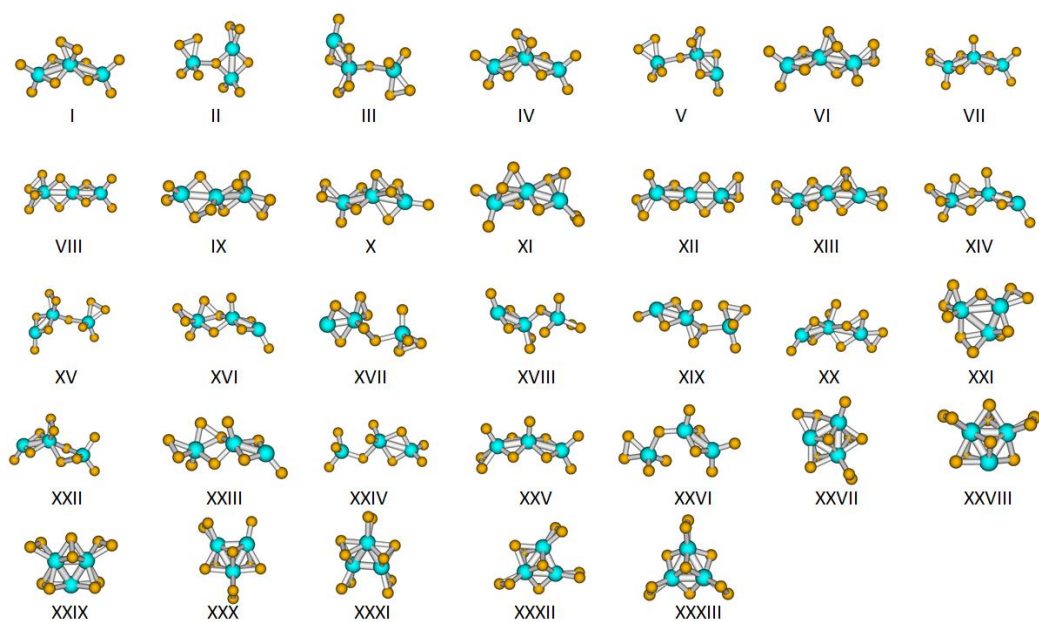**Figure S22**: Calculated structures of $[H_3Mo_3S_{11}]^+$ in the lowest spin multiplicity.
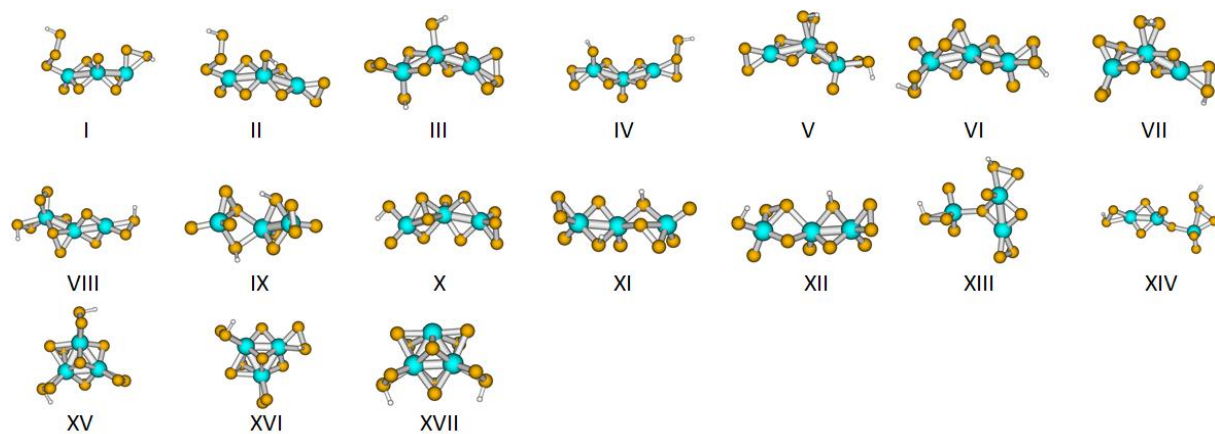
Figure S23: Calculated structures of $[H_2Mo_3S_{11}]^+$ in the lowest spin multiplicity.
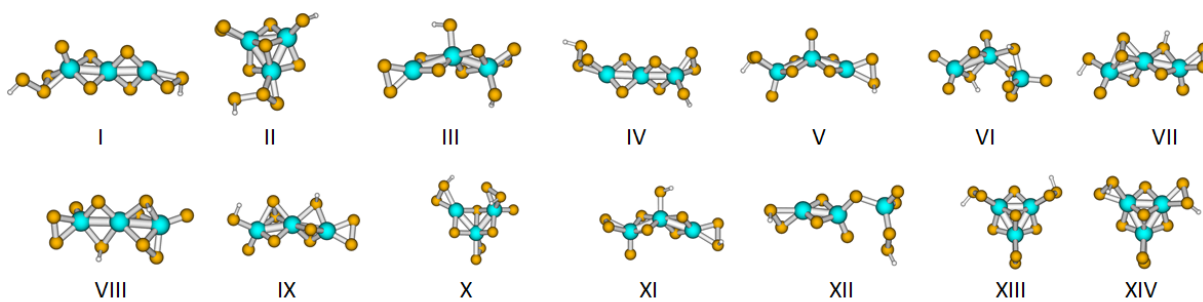
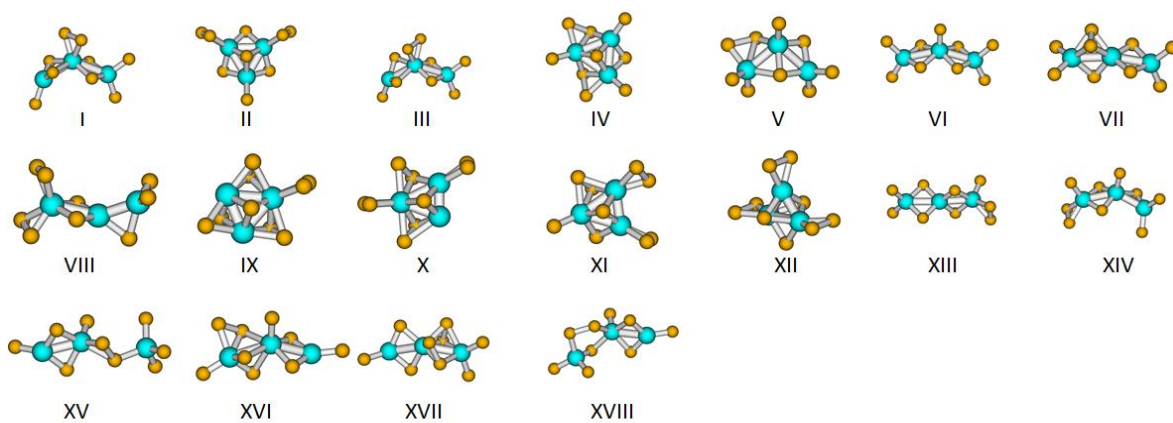**Figure S24**: Calculated structures of $[H_2Mo_3S_{10}]^+$ in the lowest spin multiplicity.
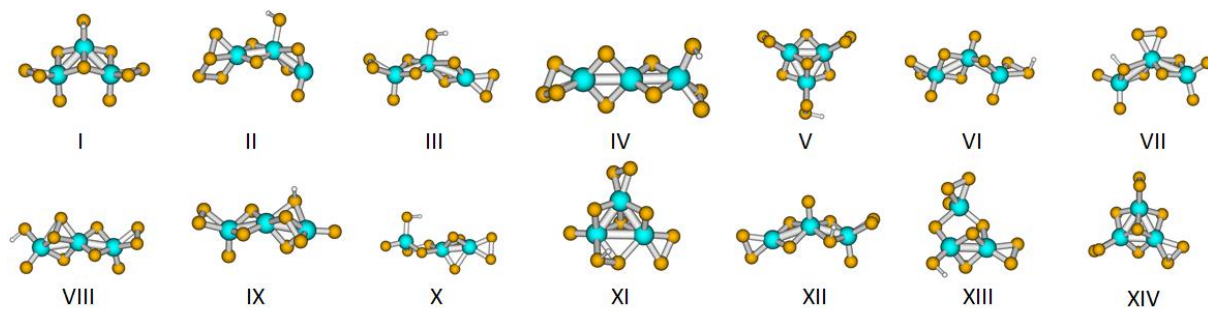
Figure S25: Calculated structures of $[HMo_3S_{10}]^+$ in the lowest spin multiplicity.
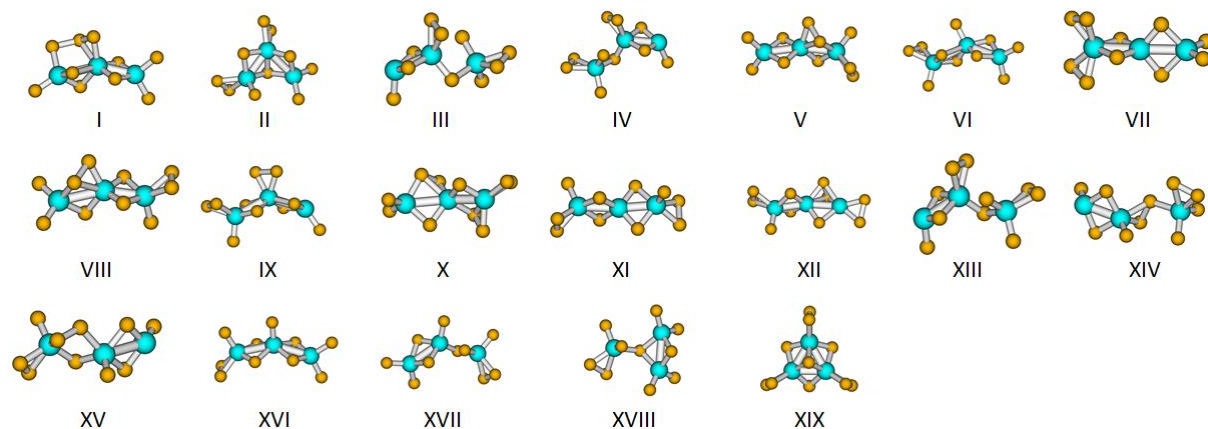
Figure S26: Calculated structures of $[Mo_3S_{10}]^+$ in the lowest spin multiplicity.
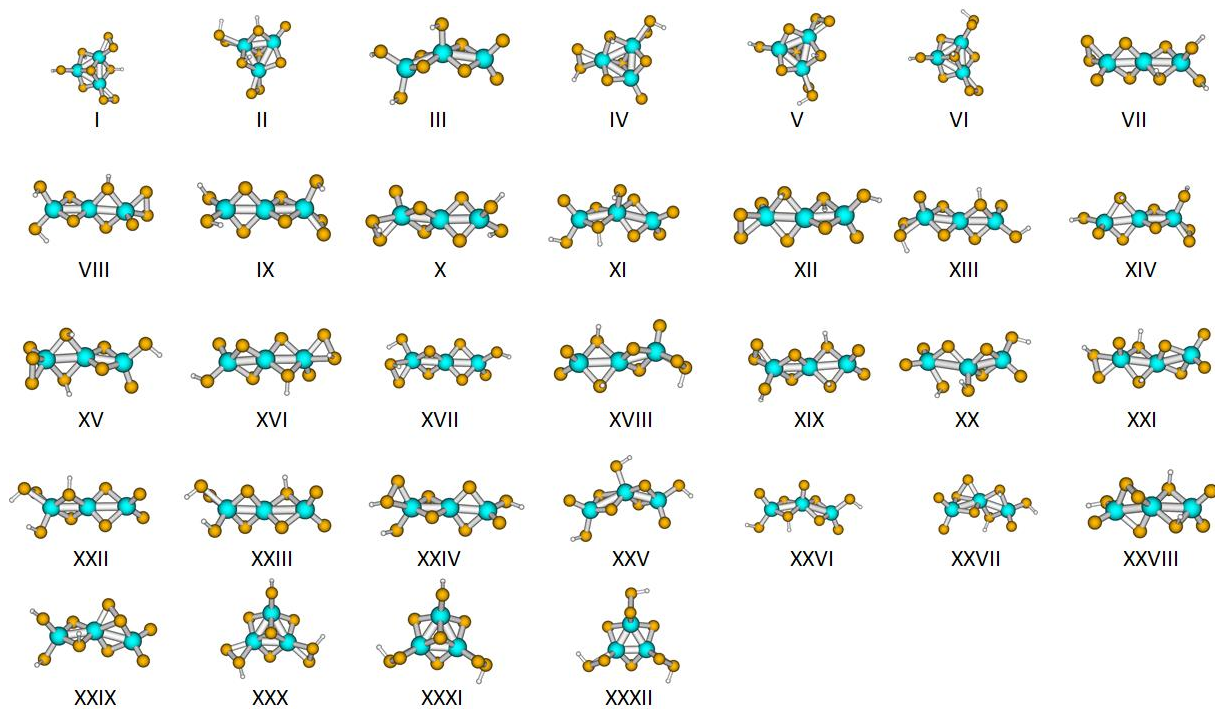
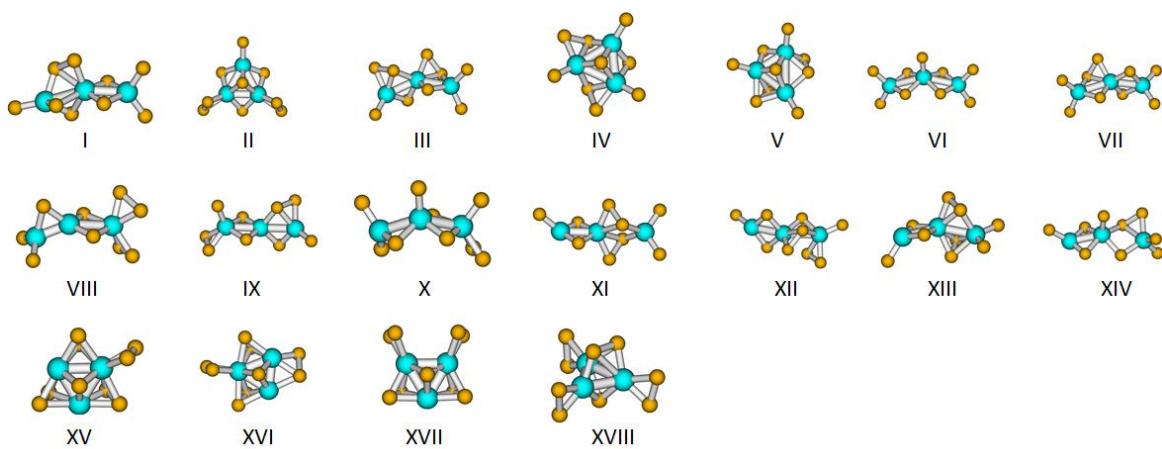**Figure S27**: Calculated structures of $[H_3Mo_3S_9]^+$ in the lowest spin multiplicity.
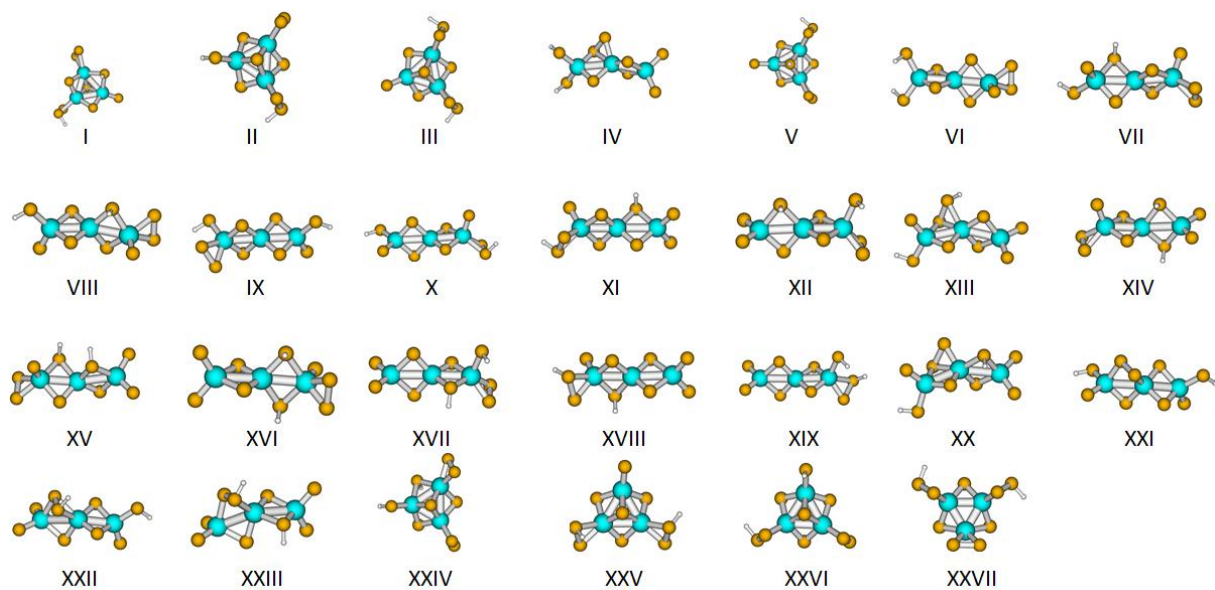
Figure S28: Calculated structures of $[H_2Mo_3S_9]^+$ in the lowest spin multiplicity.
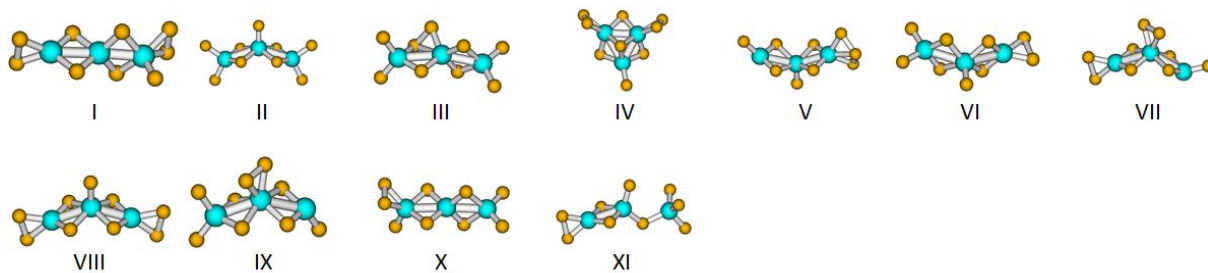
Figure S29: Calculated structures of $[Mo_3S_9]^+$ in the lowest spin multiplicity.
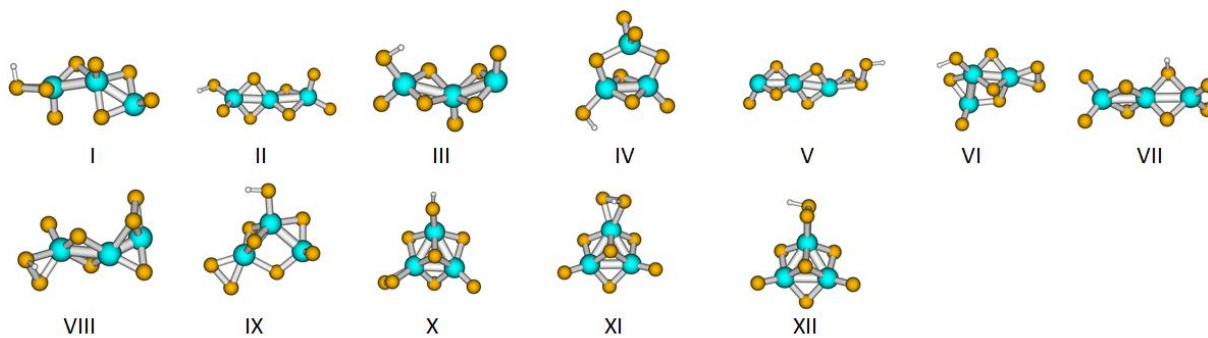
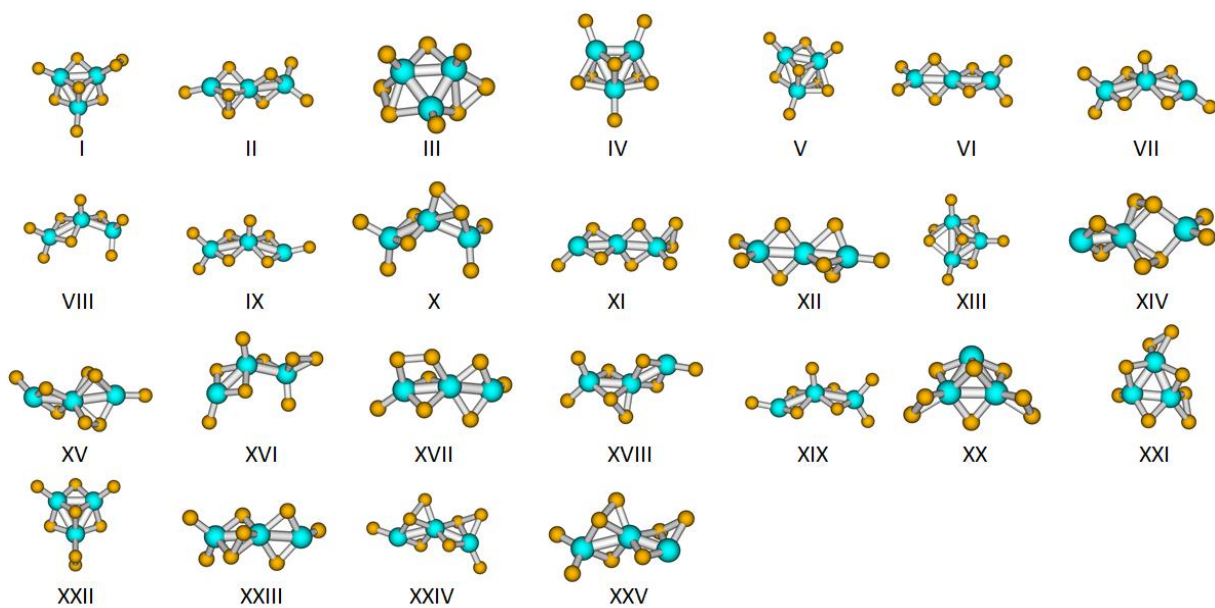**Figure S30**: Calculated structures of $[HMo_3S_8]^+$ in the lowest spin multiplicity.
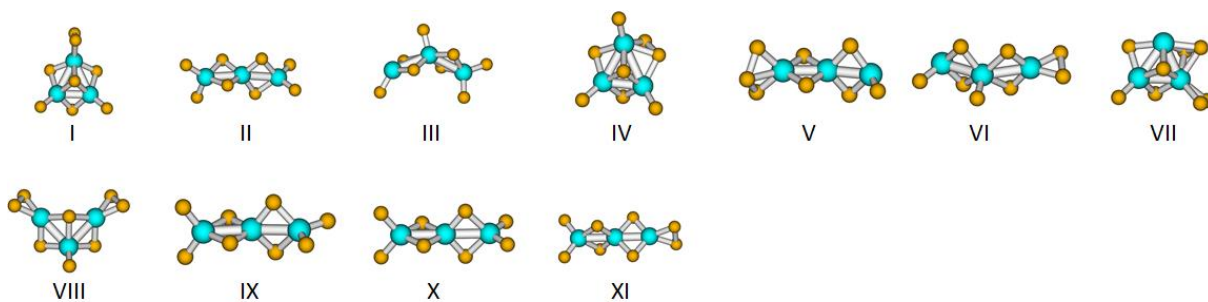
Figure S31: Calculated structures of $[Mo_3S_8]^+$ in the lowest spin multiplicity.
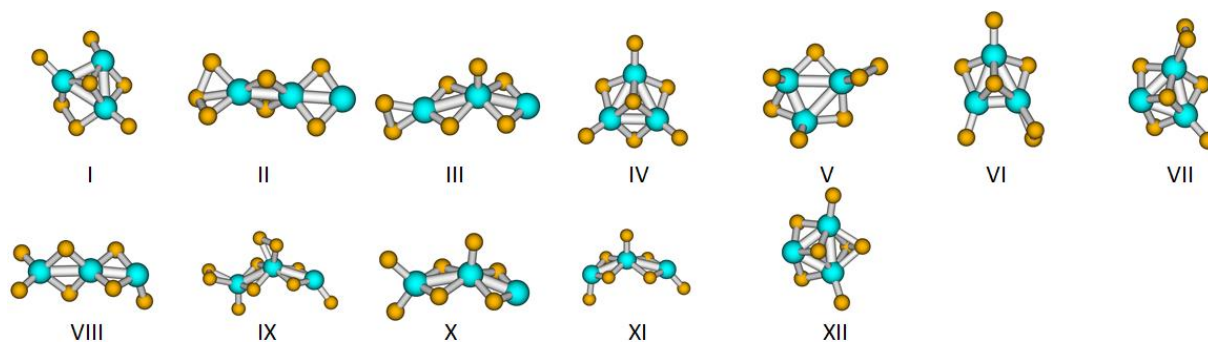
Figure S32: Calculated structures of $[Mo_3S_7]^+$ in the lowest spin multiplicity.

**Table S2**: Absolute energy difference ΔE_{opt} between structures optimized at the B3LYP/def2TZVP and ωB97XD/def2TZVP level of theory; relative isomer energy $\Delta E_{iso,B3LYP}$ and $\Delta E_{iso,ωB97XD}$ in the respective two structures. Energies were calculated at the ωB97XD/def2TZVP level and are given in eV. Zero-point energy correction is included in $\Delta E_{iso,B3LYP}$ and $\Delta E_{iso,ωB97XD}$ values, calculated at the B3LYP/def2TZVP and ωB97XD/def2TZVP level of theory, respectively.

isomer	ΔE_{opt}	$\Delta E_{iso,B3LYP}$	$\Delta E_{iso,ωB97XD}$
Ia	−0.10	0.00	0.00
Ib	−0.11	0.89	0.87
Ic	−0.09	0.96	0.97
Id	−0.14	1.00	0.96
IIa	−0.07	0.00	0.00
IIb	−0.08	0.06	0.04
IIc	−0.07	0.42	0.39
IId	−0.08	0.52	0.52
IIe	−0.09	2.23	2.21
IIIa	−0.08	0.00	0.00
IIIb	−0.07	0.05	0.08
IIIc	−0.06	0.07	0.11
IIId	−0.08	1.57	1.61
IVa	−0.06	0.00	0.00
IVb	−0.06	0.20	0.21
IVc	−0.05	0.64	0.65
Va	−0.05	0.00	0.00
Vb	−0.05	0.12	0.12
Vc	−0.17	0.13	0.02
VIa	−0.08	0.00	0.00
VIb	−0.05	0.25	0.28
VIIa	−0.05	0.00	0.00
VIIb	−0.04	1.30	1.30
VIIIa	−0.04	0.00	0.00
VIIIb	−0.04	1.21	1.21
IX	−0.03	-	-
Xa	−0.11	0.00	0.00
Xb	−0.09	0.98	0.99
Xc	−0.11	1.29	1.29
Xd	−0.11	1.53	1.53
XIa	−0.07	0.00	0.00
XIb	−0.08	0.35	0.34
XIc	−0.08	0.59	0.58
XIIa	−0.11	0.00	0.00
XIIb	−0.06	0.18	0.23
XIIIa	−0.06	0.00	0.00
XIIIb	−0.07	0.23	0.21
XIVa	−0.06	0.00	0.00
XIVb	−0.05	0.17	0.18

XVa	−0.05	0.00	0.00
XVb	−0.05	0.14	0.19
XVc	−0.05	0.17	0.22
XVIa	−0.04	0.00	0.00
XVIb	−0.04	0.78	0.78
XVIc	−0.05	0.90	0.89
XVId	−0.04	1.81	1.81
XVIIa	−0.10	0.00	0.00
XVIIb	−0.10	1.11	1.10
XVIIc	−0.11	1.58	1.57
XVIId	−0.12	1.97	1.95
XVIIe	−0.10	1.98	1.97
XVIIf	−0.11	2.69	2.67
XVIIg	−0.12	2.74	2.71
XVIIIa	−0.08	0.00	0.00
XVIIIb	−0.08	2.16	2.15
XIXa	−0.09	0.00	0.00
XIXb	−0.09	1.95	1.95
XXa	−0.07	0.00	0.00
XXb	−0.07	1.77	1.75
XXIa	−0.07	0.00	0.00
XXIb	−0.06	1.24	1.24
XXIIa	−0.06	0.00	0.00
XXIIb	−0.07	1.50	1.49
XXIIIa	−0.06	0.00	0.00
XXIIIb	−0.07	1.29	1.28
XXIVa	−0.06	0.00	0.00
XXIVb	−0.06	0.88	0.87
XXVa	−0.05	0.00	0.00
XXVb	−0.06	1.32	1.30
XXVIa	−0.05	0.00	0.00
XXVIb	−0.05	0.96	0.95
XXVIIa	−0.06	0.00	0.00
XXVIIb	−0.07	0.86	0.84
XXVIIIa	−0.05	0.00	0.00
XXVIIIb	−0.05	0.66	0.65
XXIXa	−0.05	0.00	0.00
XXIXb	−0.06	0.92	0.91
XXXa	−0.05	0.00	0.00
XXXb	−0.06	0.05	0.03
XXXc	−0.05	0.85	0.85

Table S3: Energies of calculated structures in the $[Mo_3S_{13}]^{2-}$ dissociation series (in eV). See Figures S3–12 for the respective structures.

ion	isomer	singlet/doublet	triplet/quartet	pentet/hextet
$[Mo_3S_{13}]^{2-}$	I	1.77	2.04	-
	II	2.15	2.82	-
	III	0.00	1.74	-
	IV	2.56	2.91	-
	V	3.25	1.78	-
	VI	0.96	1.53	-
	VII	2.35	2.27	-
	VIII	1.00	1.44	-
	IX	2.07	2.17	-
	X	1.92	2.32	-
	XI	1.63	1.45	-
	XII	2.26	1.84	-
	XIII	0.89	1.53	-
$[Mo_3S_{11}]^{-2}$	I	3.17	3.09	3.43
	II	1.23	2.83	2.74
	III	0.96	1.30	2.39
	IV	0.74	3.01	1.87
	V	0.84	1.49	2.14
	VI	3.04	2.84	4.53
	VII	2.23	3.11	3.37
	VIII	3.46	4.03	4.78
	IX	3.87	4.33	4.61
	X	1.77	2.45	3.63
	XI	0.00	0.85	2.06
	XII	0.52	1.42	2.42
	XIII	0.89	2.01	2.85
	XIV	0.42	0.72	2.75
	XV	0.06	0.72	2.10
	XVI	3.42	3.26	4.24
	XVII	2.99	2.90	3.20
	XVIII	3.42	3.26	4.09
	XIX	3.17	3.09	3.43
$[Mo_3S_{10}]^-$	I	0.52	0.91	-
	II	2.05	1.27	-
	III	2.53	2.44	-
	IV	0.52	0.91	-
	V	2.53	2.50	-
	VI	0.28	1.01	-
	VII	0.85	1.41	-
	VIII	0.43	1.31	-
	IX	0.24	1.19	-
	X	1.20	2.50	-
	XI	0.95	1.69	-
	XII	0.05	1.02	-
	XIII	0.66	1.64	-
	XIV	2.16	2.42	-
	XV	2.53	2.45	-
	XVI	2.16	2.42	-
	XVII	4.97	3.38	-
	XVIII	2.53	4.10	-
	XIX	2.17	2.61	-
	XX	4.05	2.75	-
	XXI	2.40	5.00	-
	XXII	2.50	2.57	-
	XXIII	2.16	2.42	-
	XXIV	2.05	1.67	-
	XXV	0.07	1.10	-
	XXVI	0.95	2.99	-
	XXVII	1.71	2.87	-
	XXVIII	1.57	2.94	-

	XXIX	3.95	4.22	-
	XXX	2.27	2.57	-
	XXXI	4.97	5.10	-
	XXXII	2.05	2.56	-
	XXXIII	0.00	0.93	-
$[Mo_3S_9]^{2-}$	I	3.09	1.38	-
	II	0.64	1.77	-
	III	3.09	2.00	-
	IV	2.71	2.93	-
	V	2.15	2.08	-
	VI	0.00	1.27	-
	VII	0.77	4.98	-
	VIII	3.90	4.14	-
	IX	5.55	5.78	6.42
	X	6.46	6.36	6.86
	XI	3.70	5.78	6.14
	XII	3.91	3.80	4.12
	XIII	0.20	1.17	-
	XIV	2.24	4.50	-
	XV	3.10	4.03	-
	XVI	3.65	4.26	-
	XVII	3.90	3.90	-
	XVIII	3.17	2.98	-
$[Mo_3S_9]^{-}$	I	1.06	2.24	-
	II	0.13	1.06	-
	III	1.00	2.15	-
	IV	1.60	1.72	-
	V	0.99	1.78	-
	VI	0.00	1.04	-
	VII	0.12	1.04	-
	VIII	3.34	3.77	-
	IX	1.31	2.54	-
	X	1.77	2.24	-
	XI	2.72	2.65	-
	XII	2.96	2.32	-
	XIII	2.39	2.65	-
	XIV	1.87	2.04	-
	XV	3.63	3.53	-
	XVI	3.21	4.78	-
	XVII	3.35	4.03	-
	XVIII	4.29	4.75	-
$[Mo_3S_8]^{-}$	I	0.25	1.11	-
	II	1.28	1.76	-
	III	3.16	3.42	-
	IV	2.98	2.98	-
	V	0.82	1.19	-
	VI	0.00	0.56	-
	VII	1.20	1.84	-
	VIII	1.80	0.56	-
	IX	1.18	2.01	-
	X	2.46	2.93	-
	XI	1.61	1.77	-
	XII	0.80	1.34	-
	XIII	0.88	1.87	-
	XIV	5.18	5.32	-
	XV	4.02	2.72	-
	XVI	2.85	2.49	-
	XVII	2.29	1.77	-
	XVIII	1.68	2.92	-
	XIX	1.18	2.01	-
	XX	1.56	2.67	-
	XXI	2.91	3.15	-
	XXII	0.25	1.11	-
	XXIII	1.64	2.11	-

	XXIV	3.38	3.11	-
	XXV	3.71	3.71	-
[Mo$_3$S$_7$]$^{2-}$	I	1.49	1.30	1.97
	II	3.76	3.31	4.14
	III	7.53	4.71	7.25
	IV	4.78	8.58	8.62
	V	3.15	7.54	5.81
	VI	3.61	5.69	6.87
	VII	0.00	0.98	1.37
[Mo$_3$S$_7$]$^{-}$	I	3.00	2.89	-
	II	3.00	3.00	3.89
	III	1.21	1.32	2.07
	IV	4.00	2.60	4.09
	V	5.23	5.58	-
	VI	8.02	8.23	-
	VII	2.92	2.89	3.20
	VIII	5.21	4.19	6.24
	IX	4.89	4.58	4.97
	X	0.00	0.75	1.46
[Mo$_2$S$_6$]$^{-}$	I	0	2.09	3.26

Table S4: Energies of calculated structures in the [HMo$_3$S$_{13}$]$^-$ dissociation series (in eV). See Figures S13–18 for the respective structures.

ion	isomer	singlet/doublet	triplet/quartet	pentet/hextet
[Mo$_3$S$_{13}$H]$^-$	I	1.29	2.38	2.33
	II	0.09	1.31	2.44
	III	0.00	1.21	2.69
	IV	1.53	1.53	2.94
	V	1.33	2.79	-
	VI	1.25	1.94	-
	VII	1.54	1.98	-
	VIII	2.47	2.58	-
	IX	2.36	2.82	-
	X	2.49	3.87	-
	XI	2.63	3.02	-
	XII	2.33	2.80	-
	XIII	2.46	2.80	-
	XIV	2.85	2.84	-
	XV	2.41	2.42	-
	XVI	2.24	2.51	-
	XVII	2.22	2.55	-
	XVIII	2.43	2.83	-
	XIX	2.25	2.56	-
	XX	2.51	2.99	-
	XXI	2.48	2.73	-
	XXII	2.65	3.28	-
	XXIII	1.90	2.35	-
	XXIV	2.01	2.67	-
	XXV	2.61	2.85	-
	XXVI	2.99	2.13	-
	XXVII	2.70	2.22	-
	XXVIII	2.34	2.45	-
	XXIX	2.21	3.00	-
	XXX	2.39	2.96	-
	XXXI	1.74	1.88	-
	XXXII	1.72	1.71	-
	XXXIII	1.69	1.74	-
	XXXIV	1.41	2.21	-
	XXXV	1.58	2.04	-
	XXXVI	1.45	1.67	-
	XXXVII	1.23	3.03	-
	XXXVIII	0.98	1.84	-
	XXXIX	1.20	2.40	-
	XXXX	1.15	1.70	-
	XXXXI	2.08	2.36	-
[Mo$_3$S$_{11}$H]-	I	2.89	2.83	-
	II	1.90	1.97	-
	III	3.19	3.26	3.59
	IV	1.51	3.53	2.89
	V	1.43	3.36	2.27
	VI	1.37	1.75	2.84
	VII	0.96	1.23	1.94
	VIII	3.04	3.39	3.87
	IX	0.59	1.03	3.18
	X	2.17	1.12	2.84
	XI	3.22	3.13	3.68
	XII	2.89	2.83	3.29
	XIII	3.04	3.00	3.42
	XIV	2.95	2.89	3.22
	XV	0.82	1.29	-
	XVI	0.96	1.56	-
	XVII	1.55	1.68	-
	XVIII	1.37	2.05	-
	XIX	0.00	0.86	-

	XX	0.52	1.05	-
	XXI	0.43	0.83	-
	XXII	0.06	1.40	-
	XXIII	0.35	0.95	2.06
	XXIV	0.94	2.39	3.65
	XXV	2.21	2.38	3.69
	XXVI	0.33	2.82	3.71
	XXVII	1.58	2.54	3.24
	XXVIII	2.70	2.92	3.66
	XXIX	3.33	3.28	3.75
$[Mo_3S_{11}]-$	I	2.47	2.55	3.45
	II	1.81	3.02	2.90
	III	0.93	1.67	2.35
	IV	0.87	3.41	2.37
	V	0.18	0.89	3.04
	VI	2.50	3.44	3.53
	VII	2.42	2.67	3.20
	VIII	2.50	2.99	4.07
	IX	2.47	2.55	3.45
	X	1.12	2.29	-
	XI	2.12	2.22	-
	XII	3.85	3.60	-
	XIII	3.40	3.94	-
	XIV	1.10	1.93	-
	XV	0.00	0.98	-
	XVI	0.17	1.07	-
	XVII	0.57	1.80	-
	XVIII	1.38	0.89	-
	XIX	0.64	0.89	-
$[Mo_3S_{10}H]-$	I	1.32	1.18	-
	II	0.69	1.35	-
	III	0.47	1.82	-
	IV	0.77	1.58	-
	V	0.59	0.81	-
	VI	0.57	1.11	-
	VII	0.40	1.17	-
	VIII	0.42	1.27	-
	IX	0.84	1.31	-
	X	1.45	1.78	-
	XI	0.96	1.45	-
	XII	0.93	1.49	-
	XIII	0.87	1.18	-
	XIV	0.34	1.78	-
	XV	0.36	1.77	-
	XVI	0.61	1.34	-
	XVII	0.61	0.85	-
	XVIII	0.43	1.14	-
	XIX	0.45	0.97	-
	XX	0.25	1.26	-
	XXI	0.23	1.22	-
	XXII	1.19	1.16	-
	XXIII	0.94	1.05	-
	XXIV	0.87	1.08	-
	XXV	0.36	1.20	-
	XXVI	0.90	1.66	-
	XXVII	1.07	0.81	-
	XXVIII	1.60	1.48	-
	XXIX	0.96	1.29	-
	XXX	0.51	1.07	-
	XXXI	0.00	1.12	-
	XXXII	0.81	1.35	-
	XXXIII	1.30	2.11	-
	XXXIV	0.51	1.07	-
$[Mo_3S_9H]-$	I	3.37	3.39	-

	II	2.74	3.99	4.15
	III	0.22	1.23	2.10
	IV	2.77	3.16	3.89
	V	1.63	1.87	2.85
	VI	1.81	1.87	2.55
	VII	0.07	1.00	1.89
	VIII	0.00	1.23	2.30
	IX	2.36	4.88	2.59
	X	3.06	4.03	4.56
	XI	0.29	2.23	3.05
	XII	2.40	2.57	3.41
	XIII	2.99	2.46	3.52
	XIV	3.37	3.39	4.05
	XV	2.39	2.46	3.51
	XVI	3.12	3.26	4.33
	XVII	0.17	1.11	-
	XVIII	0.98	1.50	-
	XIX	0.93	1.53	-
	XX	1.52	2.31	-
	XXI	0.65	1.24	-
	XXII	0.18	1.28	-
	XXIII	1.21	1.90	-
$[Mo_3S_8H]-$	I	3.20	4.02	-
	II	2.70	2.91	-
	III	3.77	3.72	-
	IV	3.36	4.16	-
	V	1.09	1.66	-
	VI	1.61	1.53	-
	VII	0.00	0.56	-
	VIII	5.05	4.97	-
	IX	5.56	5.59	-
	X	2.39	2.20	-
	XI	1.61	1.53	-
	XII	5.75	5.65	-
	XIII	3.97	3.97	-
	XIV	1.52	0.60	-
	XV	2.18	1.99	-
	XVI	0.14	1.04	-
	XVII	0.93	1.64	-
	XVIII	1.00	1.55	-
	XIX	1.52	2.24	-
	XX	1.01	1.66	-
	XXI	0.68	1.20	-
	XXII	0.17	1.17	-
$[Mo_3S_7H]-$	I	1.81	4.06	3.47
	II	3.38	3.59	4.17
	III	3.71	2.37	2.71
	IV	3.93	4.26	4.27
	V	4.16	4.90	5.32
	VI	4.14	4.09	4.11
	VII	0.78	3.73	4.68
	VIII	3.00	2.80	3.58
	IX	3.01	3.00	2.83
	X	2.29	4.27	3.19
	XI	4.43	3.33	4.13
	XII	3.07	3.75	4.78
	XIII	4.65	5.41	6.95
	XIV	3.89	4.13	3.02
	XV	2.12	2.45	4.13
	XVI	3.49	6.72	6.32
	XVII	5.32	4.66	4.22
	XVIII	5.14	4.73	4.78
	XIX	0.00	0.90	1.50
	XX	0.85	1.50	1.84

XXI	1.35	2.37	2.76
XXII	0.95	1.50	1.84
XXIII	1.54	1.27	1.86
XXIV	1.15	1.25	2.04
XXV	0.90	1.26	-

Table S5: Energies of calculated structures in the $[Mo_3S_{13}]^+$ dissociation series (in eV). See Figures S19–32 for the respective structures.

ion	isomer	singlet/doublet	triplet/quartet	pentet/hextet
$[Mo_3S_{13}H_3]^+$	I	4.18	3.56	-
	II	4.73	3.54	-
	III	0.31	1.84	3.37
	IV	0.00	1.62	2.77
	V	2.90	2.68	2.90
	VI	4.62	4.38	4.17
	VII	5.49	6.31	4.61
	VIII	4.11	4.12	4.24
	IX	1.97	2.02	2.83
	X	2.20	2.24	3.56
	XI	3.80	3.66	-
	XII	3.49	3.47	-
	XIII	4.34	3.92	-
	XIV	3.74	4.29	-
	XV	3.21	3.07	-
	XVI	3.77	3.32	-
	XVII	2.69	3.21	-
	XVIII	2.95	3.98	-
	XIX	3.82	3.68	-
	XX	4.14	4.14	-
	XXI	4.18	4.30	-
	XXII	4.89	4.41	-
	XXIII	4.24	4.14	-
	XXIV	4.07	4.84	-
	XXV	4.40	5.27	-
	XXVI	3.83	4.13	-
	XXVII	4.63	4.73	-
	XXVIII	3.95	5.13	-
	XXIX	4.46	5.09	-
	XXX	4.10	4.39	-
	XXXI	1.11	1.11	-
	XXXII	1.58	1.58	-
	XXXIII	2.74	2.95	-
	XXXIV	2.04	2.56	-
	XXXV	1.98	2.53	-
$[Mo_3S_{12}H_2]^+$	I	2.77	4.07	-
	II	2.16	2.84	-
	III	3.39	3.67	-
	IV	4.45	2.97	-
	V	3.84	3.53	-
	VI	2.97	2.92	-
	VII	2.51	2.58	-
	VIII	3.40	3.33	-
	IX	4.30	4.30	-
	X	2.87	4.08	-
	XI	3.62	3.55	-
	XII	3.39	3.77	-
	XIII	4.37	4.37	-
	XIV	3.55	3.08	-
	XV	3.10	3.72	-
	XVI	3.76	5.35	-
	XVII	4.58	4.57	-
	XVIII	2.90	3.98	-
	XIX	2.93	2.87	-
	XX	3.58	3.92	-
	XXI	3.47	3.62	-
	XXII	3.47	3.36	-
	XXIII	3.52	3.73	-
	XXIV	3.87	4.41	-
	XXV	2.26	2.82	-

	XXVI	2.16	3.29	-
	XXVII	3.33	3.86	-
	XXVIII	1.00	1.54	-
	XXIX	1.08	2.21	-
	XXX	0.26	1.60	-
	XXXI	0.78	1.45	-
	XXXII	0.00	1.30	-
	XXXIII	0.90	2.19	-
$[Mo_3S_{12}H]^+$	I	2.71	3.23	-
	II	2.01	1.95	-
	III	3.36	3.50	-
	IV	2.58	3.06	-
	V	2.71	1.97	-
	VI	3.08	3.18	-
	VII	2.61	2.61	-
	VIII	2.84	3.18	-
	IX	3.16	3.89	-
	X	3.89	3.17	-
	XI	2.24	4.05	-
	XII	3.01	4.22	-
	XIII	3.39	4.16	-
	XIV	2.74	3.06	-
	XV	2.21	2.59	-
	XVI	3.38	3.57	-
	XVII	3.17	3.14	-
	XVIII	3.06	3.05	-
	XIX	2.27	2.66	-
	XX	3.22	2.84	-
	XXI	2.08	2.09	-
	XXII	1.95	1.95	-
	XXIII	2.95	2.95	-
	XXIV	0.53	0.53	-
	XXV	0.81	0.81	-
	XXVI	0.00	0.00	-
	XXVII	0.52	0.52	-
	XXVIII	0.03	0.03	-
	XXIX	0.72	0.73	-
$[Mo_3S_{11}H_3]^+$	I	3.65	3.12	-
	II	2.94	3.25	-
	III	3.50	4.18	-
	IV	3.50	3.62	-
	V	3.16	3.50	-
	VI	2.62	3.56	-
	VII	3.65	3.44	-
	VIII	0.00	1.35	-
	IX	1.51	1.89	-
	X	1.77	2.56	-
	XI	1.94	2.87	-
	XII	2.05	2.95	-
$[Mo_3S_{11}H_2]^+$	I	3.41	3.35	-
	II	3.03	3.15	-
	III	2.17	5.04	-
	IV	3.16	3.16	-
	V	2.37	3.21	-
	VI	1.24	3.12	-
	VII	3.62	3.26	-
	VIII	2.77	3.18	-
	IX	1.78	2.70	-
	X	1.90	2.20	-
	XI	2.17	3.16	-
	XII	2.30	2.67	-
	XIII	3.18	3.27	-
	XIV	3.57	3.34	-
	XV	0.00	1.21	-

	XVI	0.96	1.41	-
	XVII	0.80	2.28	-
[Mo$_3$S$_{10}$H$_2$]$^+$	I	2.68	3.07	-
	II	1.25	4.17	-
	III	3.10	3.10	-
	IV	3.23	3.39	-
	V	2.46	3.23	-
	VI	2.83	3.37	-
	VII	1.50	2.41	-
	VIII	2.95	2.76	-
	IX	2.11	3.43	-
	X	3.05	2.47	-
	XI	2.99	3.00	-
	XII	3.77	4.12	-
	XIII	0.00	1.45	-
	XIV	1.04	1.74	-
[Mo$_3$S$_{10}$H]$^+$	I	1.45	4.84	-
	II	3.22	3.88	-
	III	2.32	2.32	-
	IV	1.79	2.17	-
	V	0.00	0.00	-
	VI	2.98	2.30	-
	VII	3.15	3.08	-
	VIII	1.29	1.29	-
	IX	1.99	2.29	-
	X	2.72	3.44	-
	XI	2.63	1.94	-
	XII	4.05	2.55	-
	XIII	2.59	2.81	-
	XIV	0.52	0.52	-
[Mo$_3$S$_{10}$]$^+$	I	2.19	3.34	-
	II	1.44	1.52	-
	III	3.46	2.86	-
	IV	3.46	2.86	-
	V	1.88	3.31	-
	VI	2.69	2.30	-
	VII	1.90	1.90	-
	VIII	1.02	1.73	-
	IX	3.05	3.04	-
	X	2.08	3.70	-
	XI	0.88	0.88	-
	XII	1.97	1.75	-
	XIII	3.46	2.86	-
	XIV	3.17	3.42	-
	XV	2.95	2.99	-
	XVI	2.23	2.24	-
	XVII	2.71	2.24	-
	XVIII	2.93	4.52	-
	XIX	0.00	0.00	-
[Mo$_3$S$_9$H$_3$]$^+$	I	2.60	2.80	-
	II	2.42	2.49	-
	III	2.68	3.01	-
	IV	1.62	2.33	-
	V	1.42	2.81	-
	VI	2.14	2.43	-
	VII	2.16	2.19	-
	VIII	2.07	2.06	-
	IX	1.93	2.11	-
	X	1.32	1.76	-
	XI	2.77	3.18	-
	XII	2.36	2.40	-
	XIII	1.54	2.25	-
	XIV	2.17	2.33	-

	XV	2.58	2.64	-
	XVI	1.62	2.06	-
	XVII	1.38	1.74	-
	XVIII	2.24	3.00	-
	XIX	2.87	3.06	-
	XX	2.20	2.70	-
	XXI	2.96	3.11	-
	XXII	2.81	2.81	-
	XXIII	2.52	2.44	-
	XXIV	1.43	1.73	-
	XXV	1.75	1.90	-
	XXVI	1.47	2.67	-
	XXVII	2.80	3.25	-
	XXVIII	2.42	3.12	-
	XXIX	2.64	2.74	-
	XXX	1.03	1.69	-
	XXXI	0.00	1.27	-
	XXXII	2.97	3.55	-
$[Mo_3S_9H_2]^+$	I	1.06	2.45	-
	II	0.00	1.96	-
	III	0.42	2.13	-
	IV	2.49	2.60	-
	V	1.58	2.41	-
	VI	1.12	1.51	-
	VII	1.35	2.07	-
	VIII	1.37	1.78	-
	IX	1.46	1.74	-
	X	0.96	1.74	-
	XI	1.72	2.32	-
	XII	2.29	2.44	-
	XIII	2.44	2.42	-
	XIV	2.05	2.74	-
	XV	2.63	2.51	-
	XVI	2.83	2.94	-
	XVII	2.45	2.83	-
	XVIII	1.74	2.51	-
	XIX	1.70	2.86	-
	XX	1.90	2.63	-
	XXI	1.40	2.15	-
	XXII	1.93	2.84	-
	XXIII	2.75	3.36	-
	XXIV	1.35	1.66	-
	XXV	1.29	2.00	-
	XXVI	0.08	1.28	-
	XXVII	2.98	3.64	-
$[Mo_3S_9]^+$	I	0.90	0.90	-
	II	1.94	1.96	-
	III	1.16	2.96	-
	IV	0.00	0.07	-
	V	1.41	3.25	-
	VI	1.93	1.90	-
	VII	2.75	2.75	-
	VIII	1.88	2.28	-
	IX	2.85	1.32	-
	X	0.86	0.99	-
	XI	2.75	2.75	-
$[Mo_3S_8H]^+$	I	2.29	2.82	-
	II	0.80	0.66	-
	III	1.22	1.37	-
	IV	0.35	0.93	-
	V	2.63	2.49	-
	VI	2.23	2.41	-
	VII	1.50	1.44	-

	VIII	3.75	1.07	-
	IX	2.17	2.41	-
	X	0.07	0.07	-
	XI	0.48	0.53	-
	XII	0.00	0.20	-
$[Mo_3S_8]^+$	I	0.00	0.05	-
	II	1.06	1.08	-
	III	2.15	1.75	-
	IV	0.14	1.25	-
	V	0.92	1.53	-
	VI	1.32	2.15	-
	VII	0.60	0.62	-
	VIII	1.79	1.68	-
	IX	1.06	1.08	-
	X	1.47	1.08	-
	XI	1.16	0.96	-
$[Mo_3S_7]^+$	I	2.19	1.40	-
	II	2.09	1.97	-
	III	2.59	2.28	-
	IV	0.05	0.14	-
	V	1.72	1.87	-
	VI	1.86	1.89	-
	VII	0.00	0.40	-
	VIII	0.85	1.43	-
	IX	3.45	1.43	-
	X	2.62	2.31	-
	XI	1.76	1.92	-
	XII	0.57	1.41	-

Cartesian coordinates (in Ångstrom) of species optimized at the ωB97XD/def2TZVP level of theory along the respective ZPE-corrected energy (in Hartree)

S E=-398.107641067
S 0.000000 0.000000 0.000000

S2 E=-796.381098
S 0.000000 0.000000 0.942032
S 0.000000 0.000000 -0.942032

S2- E=-796.434976
S 0.000000 0.000000 1.002206
S 0.000000 0.000000 -1.002206

S3 E=-1194.574630
S 1.623483 -0.328824 0.000000
S 0.000000 0.657634 0.000000
S -1.623483 -0.328810 0.000000

S3- E=-1194.667431
S 1.677581 -0.355070 0.000000
S 0.000000 0.710158 0.000000
S -1.677581 -0.355088 -0.000000

MoS3- E=-1263.027450
Mo -0.000023 0.000003 -0.000555
S 1.821533 -1.144666 0.000485
S -1.902291 -1.004754 0.000485
S 0.080818 2.149413 0.000485

MoS5- E=-2059.471044
Mo -0.309782 -0.000107 0.034880
S 1.917100 1.010892 0.102691
S -1.223577 -0.000661 1.958638
S -0.897318 -1.748331 -1.127609
S -0.902126 1.745593 -1.128527
S 1.919099 -1.007213 0.103247

HS E=-398.743957
S 0.000000 0.000000 0.079004
H 0.000000 0.000000 -1.264071

H2S E=-399.387999
S 0.000000 -0.000000 0.102698
H -0.000000 0.968973 -0.821583
H -0.000000 -0.968973 -0.821583

HS2 E=-796.972776
H -1.281812 -1.218008 0.000000
S 0.040057 -0.942466 0.000000
S 0.040057 1.018592 0.000000

[MoS13]2-

E=-5382.010687
S -0.000455 0.000058 1.796715
Mo -0.990231 1.214131 0.010962
S -2.210402 2.709276 1.453115
S -2.517158 3.087778 -0.555099
Mo 1.546923 0.249688 0.011104
S 3.932506 0.635697 -0.556549
S 3.453803 0.556717 1.452304
Mo -0.557247 -1.463892 0.011343
S -1.418761 -3.722184 -0.554629
S -1.241642 -3.267665 1.453559
S 1.817296 -2.230357 0.123950
S 1.203802 -1.473930 -1.648714
S 0.677557 1.777957 -1.648578
S 1.023573 2.688554 0.123983
S -2.840344 -0.458516 0.122443
S -1.878321 -0.303191 -1.650196

E=-5381.978698
S -2.237026 -0.442132 2.045276
Mo -3.027182 -0.439087 0.119142
S -4.617871 -2.240046 0.037437
Mo 0.721431 0.962608 -0.202478
S -0.886299 -0.213206 -1.200254
S 0.217218 2.682578 1.257815
S 0.189310 3.297855 -0.719833

Mo 3.004216 -0.676334 -0.074089
S 2.566521 -2.510619 -1.016690
S 1.462945 -0.269943 1.594682
S 2.509243 1.047054 -1.569260
S -4.990183 0.946577 0.189945
S -3.298552 1.751259 -0.651548
S 5.319433 -0.109021 -0.241511
S 4.735056 -0.973406 1.550183
S -2.803265 -2.565816 -0.862997

E=-5381.975444
Mo -0.985847 0.802235 -0.052582
Mo -3.390295 -0.651604 -0.057342
S -1.880128 -0.357640 1.685095
S -5.187697 -0.663029 1.516529
S -5.619296 0.131163 -0.347870
S -2.648820 0.929392 -1.599732
S -3.106715 -2.562186 -0.897599
S 0.188575 2.233911 1.411764
S -0.586951 3.100459 -0.296497
Mo 3.869458 -0.186478 -0.206227
S 1.722609 -1.158095 0.248565
S 3.543747 1.888006 0.033001
S 5.904330 -0.616661 0.932039
S 4.301353 -1.689979 1.651143
S 4.226853 -0.679154 -2.246053
S 0.472188 -0.462090 -1.260108

E=-5381.974973
S 1.070504 -1.447931 0.896608
Mo -3.093163 -0.407691 -0.104658
Mo -0.410480 0.472530 -0.064789
Mo 2.982029 -0.502189 -0.138233
S 2.550880 -0.911036 2.203316
S 1.125050 -0.274243 -1.694552
S -3.142930 -2.472650 -0.566370
S 4.009937 -2.182077 -0.865304
S -1.729336 -0.119880 1.730084
S -1.927249 0.653037 -1.788580
S -5.119162 0.667595 -0.782397
S -4.972970 0.222697 1.238494
S -0.119378 2.746180 -0.062111
S 1.119136 1.846378 1.308576
S 3.777503 1.380406 -1.300106
S 4.727254 1.039568 0.490003

[MoS3S11]2-

E=-4585.575129
Mo 0.686374 1.352915 0.005882
Mo -1.662789 -0.000004 -0.069525
Mo 0.686380 -1.352912 0.005882
S -0.136307 0.000000 1.734719
S -3.493613 -0.000004 1.349435
S -4.133254 -0.000013 -0.627622
S 1.265424 3.076764 1.452235
S 1.866235 3.521794 -0.476548
S 2.812835 0.000006 0.046344
S 1.751559 0.000004 -1.705015
S 1.265440 -3.076757 1.452236
S 1.866261 -3.521788 -0.476546
S -1.151617 1.851082 -1.298809
S -1.151609 -1.851088 -1.298809

E=-4585.573535
Mo 2.840456 -0.509033 -0.000036
S 1.503117 -0.103886 1.772781
S 1.503147 -0.103503 -1.772796
S 3.267857 -2.582260 -0.000268
Mo 0.015134 0.546329 0.000047
S -1.477924 -0.138964 1.745755
S -4.382801 -1.535319 1.036486
S -3.804254 1.953962 0.000147
Mo -2.902318 0.041093 -0.000011
S 4.652029 0.668116 1.036399
S 4.652007 0.668419 -1.036161
S 0.070133 2.641474 0.000258

S -1.477901 -0.138635 -1.745799
S -4.382748 -1.535172 -1.036801

E=-4585.560673
Mo 0.486085 -0.677260 -0.329885
S 1.360271 0.109687 1.593100
Mo 3.024366 0.519116 0.015690
S 2.092309 -0.485568 -1.882139
S 3.045184 2.597109 -0.363712
S -1.270575 0.575664 -1.091184
S -3.925417 2.110674 -0.722072
Mo -3.287115 -0.027887 0.153678
S -5.341036 1.149569 0.425416
S -3.870886 -1.858951 -0.741643
S -2.598440 -0.327609 2.134847
S 0.081313 -2.746967 -0.078319
S 4.715226 -0.120700 1.569904
S 5.125791 -0.514575 -0.422839

E=-4585.556159
S 0.088650 0.359138 -1.727732
Mo -0.047420 1.851477 0.051989
S -1.600653 1.003132 1.723722
S -2.519994 1.521037 -0.020344
Mo -1.227040 -0.633508 -0.022461
S 0.295824 -2.610443 -0.246385
S 0.211181 -1.725880 1.583155
Mo 1.492192 -0.410632 0.002983
S 1.719111 1.324888 1.484697
S -2.808664 -1.611046 -1.556537
S -3.242191 -2.004360 0.427456
S 3.732647 -1.456868 0.491996
S 3.311376 -0.737475 -1.404209
S 0.241169 3.818615 -0.841159

E=-4585.493921
S 0.030784 -0.104743 1.944615
Mo -1.207250 -0.724328 0.003427
S -2.980870 -1.885086 1.146673
S -3.127745 -1.973676 -0.914946
Mo -0.375424 1.614724 0.320659
S -2.747855 1.353534 0.353183
S -2.017895 2.892541 -0.882551
Mo 1.446525 -0.264413 0.003650
S 3.723607 -0.924430 -0.769066
S 3.305485 -1.163969 1.241717
S 1.378023 1.776024 -1.313011
S 2.079975 2.117856 0.566348
S 0.479787 -2.533272 -0.356148
S 0.234096 -1.197982 -1.877122

[Mo3S10]-
E=-4187.338822
S -2.902223 -1.757701 1.409351
Mo -1.438977 -0.797796 -0.103680
S -0.002091 -2.127890 -1.289631
Mo 1.437451 -0.800381 -0.104214
S 3.621890 -1.701873 -0.526231
S 2.898927 -1.762818 1.409044
S -1.862064 1.117759 -1.281664
Mo 0.001317 1.516242 -0.046303
S 0.002816 3.973287 -0.399928
S 0.004393 3.191289 1.519277
S 0.000159 -0.135025 1.635769
S 1.863312 1.114589 -1.282394
S -3.624573 -1.696539 -0.526324

E=-4187.335763
Mo 0.081437 -0.039266 -0.006534
Mo -2.932674 0.254617 0.040700
S -1.286202 0.822963 -1.573326
S -1.346729 -0.881103 1.476578
S -4.304581 -1.644076 0.193826
S -4.641673 -0.395690 -1.421517
S -3.552459 1.957826 1.080670
S 1.386477 -1.596670 -0.906869
S 1.385308 1.545782 0.843930

Mo 2.864093 -0.143322 0.179920
S 3.494715 -1.113828 1.933871
S 4.417082 -0.348035 -1.590640
S 4.414313 1.463755 -0.598500

E=-4187.334776
S -1.243058 -0.121633 -1.767499
Mo 0.163243 0.537981 -0.000044
S -1.243127 -0.121316 1.767488
Mo -2.635826 0.053462 -0.000041
S -4.063297 -1.687291 0.984502
S -4.063128 -1.687632 -0.984204
S -3.634080 1.898787 -0.000252
S 0.255704 2.616642 -0.000201
S 1.754365 -0.179626 1.738796
Mo 3.154164 -0.374169 0.000060
S 4.086357 -2.288063 0.000176
S 1.754441 -0.179811 -1.738751
S 4.606671 1.179601 0.000014

E=-4187.279577
S -0.083573 0.225954 1.883091
Mo 0.076073 1.909676 0.258968
S 1.774643 1.503313 -1.370801
S 2.572787 1.653501 0.506641
Mo 1.203217 -0.440622 -0.011653
S -0.356842 -2.344416 -0.284279
S -0.242014 -1.068857 -1.861296
Mo -1.500308 -0.155710 0.014053
S -1.905390 2.009048 -0.848500
S 2.669398 -1.796668 1.289197
S 3.135598 -1.767304 -0.717016
S -3.729156 -1.060883 -0.630781
S -3.255278 -0.801212 1.347656

[Mo3S9]2-
E=-3789.160634
S -1.514966 -0.145686 -1.757599
Mo 0.000000 0.514941 -0.000062
S -1.514841 -0.145437 1.757651
Mo -2.899886 -0.293066 0.000081
S -4.339646 1.296629 0.000025
S -3.856918 -2.216859 0.000247
S 1.514963 0.145293 1.757630
S -0.000017 2.609562 -0.000296
S 3.856924 -2.216857 0.000248
Mo 2.899889 -0.293063 -0.000010
S 4.339646 1.296635 -0.000305
S 1.514847 -0.145825 -1.757621

E=-3789.153047
Mo 0.241955 0.000135 -0.030563
S -1.105911 1.785710 -0.048781
Mo -2.599048 0.000010 0.247258
S -1.105680 -1.785583 -0.048422
S -3.208582 0.000156 2.274227
S 1.625576 -0.000111 -1.825655
S 1.644396 0.000298 1.736356
Mo 3.116818 -0.000042 -0.056330
S 4.270455 1.811769 -0.062174
S 4.270138 -1.812051 -0.061665
S -4.192444 1.036599 -1.192458
S -4.192229 -1.037058 -1.192386

E=-3789.136696
S -0.000380 3.771064 0.852574
Mo -0.000178 1.811065 -0.096698
S 1.836129 1.260917 -1.363373
Mo 1.367145 -0.560279 -0.050196
S 0.000003 0.300389 1.644068
Mo -1.366960 -0.560579 -0.050196
S -1.836342 1.260471 -1.363382
S -2.902681 -1.401681 1.467068
S 0.000268 -1.960199 -1.234887
S 2.902597 -1.401697 1.467157
S 3.517964 -1.820231 -0.475879
S -3.517576 -1.820824 -0.475985

[Mo3S9]-
E=-3789.117522
S 1.556800 -0.157565 1.719850
Mo -0.000006 0.526253 0.000042

S 1.556889 -0.157259 -1.719893
Mo 3.006715 -0.306353 -0.000014
S 4.387615 1.302556 0.000164
S 4.009550 -2.174003 -0.000143
S -1.556774 -0.157481 -1.719851
S -0.000014 2.599506 0.000092
S -1.556895 -0.157363 1.719891
Mo -3.006713 -0.306355 -0.000021
S -4.009550 -2.174004 -0.000003
S -4.387608 1.302558 -0.000123

E=-3789.116621
S -0.830669 3.648035 0.864475
Mo -0.307492 1.807126 -0.087566
S 1.636086 1.593202 -1.273927
Mo 1.518085 -0.392005 -0.084126
S 0.035679 0.286312 1.624855
Mo -1.257522 -0.730256 -0.059990
S -1.998656 0.978583 -1.375303
S -2.579555 -1.794747 1.482391
S 0.278217 -1.946553 -1.216398
S 3.154768 -0.979802 1.456445
S 3.641598 -1.390576 -0.501450
S -3.214280 -2.192225 -0.452921

E=-3789.113110
S -1.713029 0.810833 -1.678640
Mo -0.096045 0.311470 -0.136611
S -1.248078 -0.535092 1.627740
Mo -2.877608 -0.207683 0.026297
S -4.338554 1.133761 0.798909
S -3.682295 -2.058698 -0.636990
S 1.694707 1.220011 1.397534
S 0.839188 2.443474 -0.035016
S 1.089018 -1.246828 -1.279883
Mo 2.794697 -0.328921 -0.007876
S 3.562325 -1.762670 1.340827
S 4.266480 0.586186 -1.224235

[Mo3S8]-
E=-3390.903267
Mo -0.068797 0.000094 -0.000122
Mo -2.889217 -0.000020 0.000032
S -4.030444 0.001972 -1.793919
S -4.030123 -0.002113 1.794186
S -1.405430 -1.788631 -0.002198
S -1.405571 1.788713 0.002028
Mo 2.936568 -0.000016 0.000022
S 1.363549 -0.001711 1.747962
S 1.363743 0.002037 -1.748107
S 4.100586 1.764770 0.001888
S 4.099984 -1.765190 -0.001693

E=-3390.893082
S 2.178788 2.882804 0.929195
Mo 1.058952 1.360798 -0.079470
S -0.841884 1.903906 -1.230161
Mo -1.452467 -0.001036 -0.072500
S -3.798854 -0.000909 -0.457745
S -3.160501 -0.001203 1.502074
S 2.302099 0.001606 -1.434648
Mo 1.061259 -1.359767 -0.079546
S 2.184296 -2.879535 0.928835
S 0.222855 -0.000254 1.600100
S -0.839175 -1.905402 -1.229865

[Mo3S7]2-
E=-2992.674498
Mo 0.433116 -1.542223 0.068673
Mo -1.553373 0.396596 0.069820
Mo 1.120065 1.145993 0.068506
S 2.446562 2.503551 -1.008240
S -3.390912 0.865318 -1.010117
S 0.946503 -3.369441 -1.008278
S -1.482064 -1.515654 1.356817
S 2.054101 -0.525200 1.356582
S -0.001293 -0.000141 -1.587030
S -0.572393 2.040606 1.356891

E=-2992.626790
Mo 0.228754 -0.000134 -0.159624
Mo 3.087709 0.000021 -0.216361

S 1.633302 1.782630 -0.340741
S 1.633514 -1.782774 -0.340554
S 4.902761 0.000214 0.976150
S -0.988249 -0.000000 1.740393
S -3.797691 -1.815051 0.227655
Mo -2.648567 0.000038 0.113306
S -1.339587 -0.000217 -1.800780
S -3.797276 1.815394 0.227408

[Mo3S7]-
E=-2992.667836
Mo 0.000726 1.601080 0.052638
Mo 1.426136 -0.826530 0.055098
Mo -1.427450 -0.824868 0.055490
S -3.118499 -1.626666 -0.965403
S 3.116896 -1.630942 -0.964208
S 0.003536 3.514240 -0.901974
S 1.805914 1.032789 1.355526
S -1.805142 1.035307 1.355701
S -0.000079 -0.009284 -1.578139
S -0.001084 -2.183358 1.270029

-2992.623262
S -0.840229 -0.000037 1.701023
Mo 0.246129 -0.000024 -0.231942
S -1.313276 0.000083 -1.816115
Mo -2.576606 0.000020 0.141835
S -3.693852 -1.806416 0.290596
S -3.693997 1.806363 0.290724
S 1.684569 1.799900 -0.436920
Mo 3.024141 -0.000018 -0.278487
S 4.351340 0.000129 1.375038
S 1.684577 -1.799965 -0.436786

[Mo2S6]-
E=-2526.101800
S -0.000023 -0.000320 1.748753
Mo -1.513100 -0.000011 -0.000020
S -2.696768 1.761392 0.000175
Mo 1.513100 -0.000012 0.000021
S 2.696787 1.761380 0.000248
S 0.000022 0.000123 -1.748753
S -2.697018 -1.761251 -0.000248
S 2.696999 -1.761264 -0.000176

[HMo3S13]-
E=-5382.592498
S -0.015106 -0.004397 1.790676
Mo 1.518073 -0.263382 0.002665
S 0.647305 -1.790015 -1.650105
S 0.992230 -2.706161 0.123669
Mo -1.018455 -1.201876 0.006168
S -2.834201 0.476039 0.105930
S -1.889655 0.313507 -1.669329
Mo -0.567641 1.457475 0.008497
S 1.197649 1.461758 -1.651591
S 1.836355 2.214594 0.119720
S -2.243263 -2.645873 1.462090
S -2.572499 -3.018511 -0.535546
S -1.438052 3.686280 -0.527709
S -1.238355 3.221297 1.467953
S 4.008605 -0.658398 -0.502078
S 3.455352 -0.568860 1.466127
H 4.355170 0.626659 -0.724749

E=-5382.556022
S 0.863398 -1.395240 -0.719697
Mo 3.005965 -0.550546 0.116985
S 4.605468 0.843363 -1.010787
S 3.308036 -0.216926 -2.194508
S 1.465656 -0.101668 1.877860
S 3.087321 1.140455 1.807375
Mo -0.447129 0.334816 0.048906
S -0.193061 2.617125 0.700397
S 0.909055 2.307340 -0.999942
Mo -3.107983 -0.475905 -0.118290
S -4.966692 0.231112 1.166196
S -5.005088 0.750473 -0.833045
S -3.240148 -2.501057 -0.647251
S -1.747908 -0.347312 1.757570
S -1.829884 0.592769 -1.722746

S 4.051812 -2.243193 0.720816
H 2.135728 2.212830 -0.435064

E=-5382.545054
S -0.000045 -0.001274 1.761089
Mo 0.892649 1.317055 0.032157
S 1.880516 -0.134524 -1.614284
S 2.882752 -0.207493 0.130644
Mo 0.694273 -1.431229 0.031695
S -1.620930 -2.393485 0.131330
S -1.059148 -1.559885 -1.613182
Mo -1.587193 0.114444 0.032357
S -0.823935 1.697716 -1.612710
S -1.261983 2.600479 0.133054
S 1.559931 -3.213524 1.382999
S 1.720426 -3.543813 -0.637488
S -3.928507 0.283959 -0.638069
S -3.563890 0.255287 1.382999
S 2.210980 3.260308 -0.636798
S 2.004713 2.955808 1.383896
H -0.002731 -0.004296 3.103519

E=-5382.536329
S -0.098036 0.028064 -1.822483
Mo 1.355167 -0.694251 -0.045567
S 2.160123 0.634620 1.957174
S 2.324834 1.623277 0.155644
Mo -0.170318 1.598706 -0.094627
S -2.615397 1.310290 0.123274
S -1.518273 0.828121 1.773738
Mo -1.340583 -0.829422 0.017200
S 0.099641 -2.000137 1.553121
S 0.114038 -2.839168 -0.279036
S -0.039972 3.433468 -1.497054
S -0.310850 3.966677 0.433868
S -3.325658 -2.125363 0.629024
S -3.036779 -1.768367 -1.378588
S 3.503441 -1.899895 0.227108
S 2.940104 -1.392112 -1.676825
H 3.385311 0.057013 1.982326

[HMo3S11]-
E=-4586.157259
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Mo 0.843635 -1.277115 0.009058
S -0.956169 -1.957357 -1.290137
Mo -1.609478 -0.171517 -0.053156
S -1.330281 1.710575 -1.291116
Mo 0.568050 1.408067 0.010049
S 1.742716 0.171474 -1.726649
S 2.790896 0.280022 0.023133
S 0.965361 3.156966 1.444420
S 1.524322 3.652996 -0.473443
S -3.498574 -0.332358 1.349676
S -4.155079 -0.419011 -0.607408
S 1.588791 -2.911425 1.440209
S 2.231428 -3.282262 -0.479735
H -4.459536 0.876371 -0.811429

E=-4586.144750
S 0.084425 0.426832 1.692140
Mo -1.247426 -0.586502 0.033566
S -2.793418 -1.446305 1.638668
S -3.238189 -1.948141 -0.308030
Mo 0.010590 1.775510 -0.213336
S -2.490165 1.610529 -0.068782
S -1.613438 0.959160 -1.794343
Mo 1.463775 -0.454531 -0.011918
S 3.630888 -1.588597 -0.440792
S 3.245755 -0.750473 1.398597
S 1.758753 1.243166 -1.574027
S 0.428156 3.655228 1.166191
S 0.211091 -2.571092 0.329898
S 0.137322 -1.796582 -1.543183
H 0.689739 4.452343 0.109449

E=-4586.136115
Mo 0.009519 0.572024 -0.027086
S 1.437024 -0.055859 -1.849197
Mo 2.734995 -0.501871 -0.111622
S 1.522329 -0.093681 1.702941
S 3.271466 -2.547520 -0.227652

S -1.460348 -0.115138 1.752949
S -4.373830 -1.526205 1.119992
Mo -2.927268 0.026088 0.038397
S -4.392662 -1.567513 -0.946861
S -3.825371 1.926604 0.023516
S -1.523393 -0.161083 -1.728700
S 0.063354 2.655306 -0.039391
S 4.450955 0.983564 -0.737267
S 4.951474 0.295313 1.142795
H 5.739690 -0.742716 0.803020

[Mo3S11]-
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Mo 0.072327 1.454983 0.026441
S 1.880061 1.090978 -1.325692
Mo 1.529813 -0.823484 -0.125362
S 0.135171 -2.134793 -1.307356
Mo -1.374720 -0.857951 -0.018173
S -1.547802 0.891757 -1.710254
S -2.413069 1.367500 0.079518
S -2.690054 -2.078388 1.417496
S -3.442090 -2.001867 -0.499130
S 3.035687 -1.826376 1.331450
S 3.770799 -1.544057 -0.579437
S 0.447389 3.138426 1.538156
S 0.092753 3.913152 -0.334269

E=-4585.543575
Mo -2.804348 -0.395410 -0.102142
S -1.756390 1.134846 -1.507412
S -1.172117 -0.690402 1.534608
S -3.010050 -1.692342 -1.154744
Mo -0.134042 0.413940 -0.119055
S 1.100887 -0.953388 -1.417887
S 3.926316 -2.134746 0.044261
S 3.992066 1.269540 -1.375273
Mo 2.873240 -0.038914 -0.182925
S -4.783237 0.901031 -0.150543
S -4.445661 -0.160288 1.589859
S 0.621334 2.569227 0.328640
S 1.692456 1.215077 1.475251
S 4.005414 -0.898488 1.694057

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E=-4187.945030
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Mo 1.027195 -1.203114 -0.057926
S 2.120783 0.376472 -1.284729
Mo 0.545133 1.473903 -0.057874
S 0.045459 0.003341 1.692708
Mo -1.498588 -0.276058 -0.036783
S -4.024151 -0.726526 -0.500292
S -3.312898 -0.578407 1.435441
S -1.381134 1.621771 -1.295529
S 2.591195 -3.073671 -0.561146
S 2.210919 -2.520672 1.400453
S 1.364835 3.772581 -0.554643
S 1.194819 3.118293 1.404372
H -4.442826 0.537710 -0.697592

E=-4187.937220
S 1.279611 -0.191885 -1.706801
Mo -0.189368 0.558676 -0.019308
S -1.815552 -0.009438 1.738040
Mo -3.167832 -0.383832 -0.008006
S -4.638767 1.141942 -0.187182
Mo 2.608481 0.060815 0.085237
S 4.375021 -1.516131 -0.975786
S 3.753363 -1.818272 0.966115
S 3.698221 1.862967 0.060287
S 1.178527 0.060648 1.826686
S -1.726540 -0.328364 -1.724193
S -0.284034 2.629741 -0.192569
S -4.075360 -2.303665 0.145370
H 3.534358 -2.338388 -1.632277

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E=-3789.727556
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Mo 0.047033 -0.534334 -0.000102
S -1.519304 0.142612 -1.742195

Mo -2.925438 0.307951 -0.000064
S -4.347375 -1.272186 -0.000368
S -3.884868 2.207133 0.000212
S 1.497523 0.104591 -1.771131
S 0.059148 -2.615552 -0.000466
S 3.810521 2.358015 0.000623
Mo 2.813019 0.229940 0.000154
S 4.261494 -1.297639 -0.000059
S 1.497376 0.103956 1.771277
H 5.064817 1.883262 0.000495

E=-3789.720846
S -0.000055 3.618454 1.165973
Mo 0.000010 1.743647 -0.253377
S -1.827495 1.185143 -1.486111
Mo -1.364724 -0.548178 -0.047006
S -3.465022 -1.815525 -0.408211
S -2.849601 -1.339832 1.511359
S 1.827523 1.185067 -1.486094
Mo 1.364697 -0.548210 -0.047005
S 3.464900 -1.815705 -0.408272
S 2.849855 -1.339478 1.511289
S -0.000004 0.370779 1.615379
S -0.000050 -2.028994 -1.112139
H -0.000102 4.496592 0.139547

[HMo3S8]-
E=-3391.503462
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Mo -0.029418 -0.063967 0.000295
S 1.388781 -0.106369 1.784904
Mo 2.794537 0.089520 -0.000079
S 4.339711 -1.652343 0.000717
Mo -2.873449 0.000635 -0.000016
S -4.005191 0.026473 1.803749
S -4.004500 0.024358 -1.804229
S -1.412746 -1.810282 0.001041
S 1.388402 -0.108499 -1.784528
S 3.705463 1.980773 -0.001249
H 3.425956 -2.638612 0.001190

E=-3391.496304
S 0.329547 0.087397 1.593877
Mo -1.338966 -0.012686 -0.045185
Mo 0.974386 1.350360 -0.247272
Mo 1.070085 -1.345621 -0.048528
S 2.293843 -0.037178 -1.496400
S 1.854707 2.940836 1.241273
H 2.238584 3.783366 0.257471
S -0.909897 1.758466 -1.451113
S -0.837053 -1.929456 -1.178771
S 2.072015 -2.926044 1.001761
S -3.798687 -0.091466 -0.370273
S -2.996339 -0.018155 1.538639

E=-3391.495206
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Mo -1.305657 -0.046781 -0.036672
Mo 1.015805 1.405386 -0.076739
Mo 1.098111 -1.358283 -0.078717
S 2.316709 0.062410 -1.411547
S 1.977356 3.057086 0.910409
S -0.896368 1.822446 -1.292507
S -0.785544 -1.886867 -1.292199
S 2.152589 -2.954092 0.905614
S -3.891177 -0.107899 -0.403520
S -3.084025 -0.070850 1.501844
H -4.124577 1.204917 -0.588842

[HMo3S7]-
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Mo -3.059350 0.009425 -0.287185
S -1.771876 -1.821097 -0.343471
S -4.571131 0.067762 1.215709
S 1.338011 -0.176961 -1.797776
S 4.096657 -1.644120 0.345243
H 3.200671 -2.643450 0.278274
S 0.956370 -0.056753 1.734331
Mo 2.534966 0.094608 0.103247
S 3.492439 1.975232 0.142300

E=-2993.270159
S 3.013709 -1.664287 1.059150
Mo 1.390244 -0.781421 -0.032428
S 0.007157 -2.190074 -1.208478
Mo -1.385008 -0.790309 -0.032505
S -0.000289 0.118562 1.568760
Mo -0.004935 1.547353 -0.266242
S -1.851762 0.947083 -1.473436
S -0.011873 3.395491 1.185700
S -3.003182 -1.683349 1.058660
S 1.846130 0.959009 -1.473094
H -0.010872 2.905200 2.433204

E=-2993.241482
S 0.680725 -2.232489 1.075746
Mo 1.648654 -0.545212 0.001217
S 3.561749 -0.748753 -0.916545
S 1.565936 1.307192 1.375554
Mo -0.321096 1.484060 0.092669
S -1.986360 0.661450 1.422853
Mo -1.383451 -1.098259 0.108885
S 0.083260 -0.060249 -1.571735
S -0.684705 3.359992 -0.876290
S -2.966431 -1.738615 -1.132479
H -1.719249 -2.081152 1.449994

E=-2993.237419
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Mo -3.037755 0.000026 -0.296406
S -4.348571 -0.000036 1.355727
Mo -0.220983 -0.000007 -0.190928
Mo 2.607329 -0.000001 0.120905
S 3.726729 1.806856 0.242159
S -1.677859 -1.783877 -0.338101
S 1.296374 -0.000116 -1.808453
S 0.908005 0.000067 1.718532
S 3.726751 -1.806834 0.242326
H -3.898882 -0.000198 -1.795654

[H3Mo3S13]+
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Mo -1.043391 -1.142885 -0.010215
S -1.851312 0.408824 -1.665370
S -2.806686 0.622810 0.109189
Mo -0.462253 1.473541 -0.008056
S 1.949249 2.112985 0.111454
S 1.290751 1.397585 -1.664592
Mo 1.514422 -0.339098 -0.011000
S 0.574393 -1.816795 -1.668045
S 0.863694 -2.742231 0.107526
S -1.034628 3.270926 1.489100
S -1.177079 3.873946 -0.452917
S 3.949165 -0.923668 -0.456764
S 3.360264 -0.742399 1.485918
S -2.702626 -3.017247 -0.452199
S -2.324403 -2.526714 1.489447
H -3.813731 -2.289559 -0.693257
H 4.436785 0.311662 -0.699052
H -2.492099 3.680188 -0.689742

E=-5383.399198
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Mo -0.880811 -1.277533 -0.004411
S -2.009368 -2.965271 1.358565
S -2.282989 -3.270676 -0.547760
Mo -0.658766 1.392848 0.023616
S -1.567561 2.960565 1.729157
S -1.755805 3.477199 -0.884005
Mo 1.544098 -0.137781 -0.007825
S 4.032745 -0.381478 -0.485214
S 3.441168 -0.308145 1.464429
S 1.072674 1.576384 -1.633791
S 1.623700 2.359226 0.151142
S -1.946787 0.164700 -1.598080
S -2.848172 0.240748 0.207593
S 1.216609 -2.607491 0.074246
S 0.786250 -1.705980 -1.682889
H -0.717948 4.320915 -0.779469
H 4.351819 0.910747 -0.708855
H -0.513139 3.779618 1.855382

E=-5383.381781
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Mo -1.340516 -0.782417 -0.023586
S -3.063174 -1.881073 1.316529
S -3.426537 -2.025141 -0.593748
Mo -0.037056 1.569972 0.100748
S -0.030669 2.822834 2.087502
S 0.016298 4.019452 -0.848560
Mo 1.348700 -0.732754 -0.031237
S 3.510740 -1.961734 -0.550640
S 3.021184 -1.695219 1.409529
S 1.598668 1.036156 -1.632878
S 2.473453 1.486006 0.140591
S -1.703004 0.985954 -1.589906
S -2.532973 1.393220 0.210755
S 0.032107 -2.858835 0.036175
S 0.009590 -1.838822 -1.707893
H -0.613024 3.953594 -2.033624
H 4.322430 -0.903815 -0.761657
H -1.042546 4.548098 -0.215548

E=-5383.367813
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S -0.000007 -2.891043 0.139794
Mo -1.368851 -0.779496 0.021555
S -2.499534 1.448353 0.127385
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Mo 0.000003 1.597627 0.036164
S 1.628636 0.958775 -1.622810
S 2.499543 1.448339 0.127386
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S 0.000003 3.907380 -0.611487
S 0.000006 3.537727 1.395397
S 3.499892 -1.978366 -0.585768
S 3.105256 -1.752276 1.394102
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H 4.307220 -0.919877 -0.815267
H -4.307223 -0.919877 -0.815273

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S 0.664164 -0.071234 1.856777
Mo 1.816431 0.137710 -0.207531
S 4.145488 0.503601 -1.134918
S 3.919908 0.548518 0.891814
S -1.780706 -0.612654 -1.077440
Mo -0.673177 1.055749 0.293794
S -1.892194 2.062016 1.959759
S -2.544242 2.802112 0.149627
S 2.148164 -2.314878 0.035157
S 1.197918 -1.731515 -1.657691
S -3.668040 -0.901625 -0.154020
S -4.981672 -0.318330 -1.577469
S 0.586050 1.569974 -1.726824
S 1.217268 2.554206 -0.061615
H 4.074155 1.818617 -1.429825
H -3.604374 1.990150 -0.048946
H -5.081294 -1.480411 -2.247871

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Mo 2.885158 -0.680088 -0.186469
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S 3.973508 1.398196 -0.334122
S 0.718461 -1.511957 0.209204
S 1.964195 -1.756791 1.826734
Mo -0.339573 0.752924 -0.139475
S 0.292102 2.408067 1.340785
S 0.289917 3.219913 -0.548071
Mo -2.874600 -0.490204 -0.032591
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S -2.682419 -2.439890 -0.740555
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S -2.090990 1.059732 -1.536184
S 3.887678 -2.125974 -1.260560
H -0.910385 3.831425 -0.504825

H 4.151837 0.711159 2.218794
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E=-5383.339791
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Mo 0.023329 1.853548 -0.094089
Mo 1.378636 -0.646579 -0.140473
S 3.516927 -1.823681 -0.762716
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S -0.238565 -0.030944 3.565280
Mo -1.383582 -0.592424 -0.174156
S -3.146938 -1.566470 1.155452
S -3.558461 -1.696759 -0.833400
S -1.571523 1.236181 -1.752175
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S -0.049533 -2.721989 -0.051476
S -0.003062 -1.700169 -1.800550
S 1.658631 1.191935 -1.695708
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H 4.339063 -0.763949 -0.930761

[H2Mo3S12]+
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S 0.910227 1.639866 -1.646501
S 1.357982 2.491786 0.143218
Mo 1.475862 -0.000070 0.012330
S 1.357739 -2.491915 0.143208
S 0.910059 -1.639943 -1.646506
Mo -0.847352 -1.335237 -0.012407
S -2.087460 0.000103 -1.406501
S 3.460811 -0.000172 1.440497
S 3.917850 -0.000196 -0.455785
S -2.158244 -2.648508 1.398826
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H -3.350147 -2.900705 -0.961769
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E=-4984.536037
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Mo -0.280381 0.705547 -0.052866
S -1.912742 1.090318 -1.538822
Mo -2.731011 -0.571045 -0.153072
S -1.210507 -0.552038 1.574672
Mo 2.722906 -0.663518 0.124332
S 2.910423 -2.682888 0.592604
S 5.146992 -0.021362 0.341723
S 4.228693 0.222921 -1.471437
S 1.965172 0.500234 1.759794
S -0.268502 2.736193 1.157725
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S -4.978361 0.328968 -0.316108
S -2.577953 -2.380893 -1.135602
H -0.264661 3.493444 -1.375146
H 5.013966 1.216296 0.863385

[HMo3S12]+
E=-4984.007629
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S 0.211558 3.906054 -0.750231
Mo -1.358435 -0.574079 -0.011901
S -3.135018 -1.532376 -1.393901
S -3.492876 -1.756791 0.509390
Mo 1.330037 -0.621048 -0.011047
S 3.416255 -1.885038 0.510516
S 3.071894 -1.640768 -1.392805
S -0.035201 -1.770523 1.604462
S -0.051865 -2.683547 -0.196346
S -2.439771 1.665770 -0.161270
S -1.651597 1.164067 1.633585
S 2.495668 1.577059 -0.145934
S 1.678109 1.098023 1.640391
H -1.073701 4.264860 -0.899033

S33

E=-4983.936020
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Mo 3.040081 -0.248565 0.187864
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S 1.088461 -0.453000 -1.263600
Mo -0.457563 0.772199 -0.210927
S 0.462404 3.085585 -0.866131
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Mo -2.807968 -0.664294 -0.093177
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S -2.198883 1.016780 -1.582526
S 5.037406 -1.569305 0.285672
S 3.831074 -2.186620 -1.122426
S -2.522796 -2.498964 -0.998331
H -0.666896 3.681308 -1.300626

[H3Mo3S11]+
E=-4586.997348
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Mo -0.541562 1.406350 -0.002894
Mo 1.615698 -0.183586 -0.057050
Mo -0.841011 -1.251216 -0.004856
S 0.928645 -1.950882 -1.300208
S -0.901452 3.170203 1.478814
S -1.449735 3.748906 -0.415051
H -0.331052 4.386466 -0.813414
S -1.583660 -2.895360 1.472547
S -2.242041 -3.337052 -0.423022
H -1.290541 -4.205289 -0.819598
S 3.429031 -0.401421 1.364067
S 4.100202 -0.510659 -0.579081
H 4.496853 0.764010 -0.764293
S -1.721358 0.193903 -1.731486
S -2.789075 0.314135 0.011787
S 1.339713 1.695230 -1.298799

E=-4586.932901
S -0.927739 -1.031021 -1.237311
Mo 0.072660 0.540761 -0.010026
S 1.709651 1.403882 -1.307804
Mo 2.689921 -0.357458 -0.173985
S 4.690767 -0.641684 1.355462
S 4.699467 0.839791 -0.061743
Mo -2.711737 -0.083698 -0.140172
S -3.783506 -1.180877 1.635704
S -3.844319 -2.319347 -0.067465
S -3.874425 1.092475 -1.402594
S -1.684654 1.368159 1.515542
S -0.953426 2.858970 0.253537
S 1.191137 -0.573920 1.584532
S 2.750688 -2.039822 -1.389293
H -5.054152 -1.958225 -0.544984
H 5.334625 -1.626030 0.693137
H -1.994146 2.975190 -0.589539

[H2Mo3S11]+
E=-4586.388029
S -0.000002 0.126327 1.740419
Mo -1.335547 -0.687264 0.003992
Mo -0.000010 1.643877 -0.071308
Mo 1.335556 -0.687246 0.003993
S 1.818545 1.140510 -1.314447
S -3.058174 -1.219507 1.480896
S -3.569540 -1.837213 -0.411102
H -4.320937 -0.794835 -0.818514
S 3.058192 -1.219458 1.480901
S 3.569565 -1.837164 -0.411099
H 4.320953 -0.794764 -0.818514
S -0.000037 3.586028 1.307764
S -0.000025 4.049424 -0.607707
S 0.000012 -1.740726 -1.718008
S 0.000022 -2.796441 0.035366
S -1.818556 1.140481 -1.314449

E=-4586.342374
S -1.083872 -1.081535 -1.229826
Mo -2.825705 0.006704 -0.145755
S -3.910268 1.253595 -1.389214
Mo 0.124697 0.429041 -0.065701
S -1.691206 1.291101 1.508660

S -0.697513 2.575594 0.240347
S -1.271039 -0.525386 1.614573
Mo 2.767432 -0.372237 -0.144336
S 2.942142 -2.168481 -1.168103
S 1.678588 1.134503 -1.527504
S 4.688187 0.966088 -0.159425
S 4.775423 -0.359629 1.402094
S -4.138676 -2.125763 -0.017828
S -4.019933 -0.936523 1.641903
H -5.299794 -1.685204 -0.548079
H 5.487395 -1.359174 0.840483

[H2Mo3S10]+
E=-4188.177097
S -0.001244 0.028611 1.699607
Mo 0.091917 1.565542 -0.063828
Mo 1.290923 -0.843023 -0.038627
Mo -1.382245 -0.684596 -0.042988
S -2.993293 -1.470122 1.417976
S -3.654957 -1.760148 -0.510918
S 0.231482 3.975197 -0.541481
S 0.181706 3.469680 1.364017
H -3.300777 -3.048027 -0.691910
S 2.791898 -1.815084 1.426613
S 3.376087 -2.254119 -0.499705
H 4.304351 -1.295329 -0.690315
S 1.889271 0.953985 -1.306169
S -0.125529 -2.127580 -1.273681
S -1.759706 1.171495 -1.308085

E=-4188.122505
S -3.644030 -1.966176 0.919876
Mo -0.160664 0.362271 0.119150
S -1.102282 -1.046456 -1.308458
Mo -2.850868 -0.286820 -0.007312
S -4.468460 0.790972 -1.231817
S -1.814464 0.763788 1.816999
S -1.744268 2.162814 0.355367
S 1.170859 -0.736114 1.577442
Mo 2.552925 -0.265997 -0.210279
S 4.452350 -0.293147 1.279424
S 4.530532 1.133493 -0.061843
S 1.338488 1.422150 -1.437821
S 2.707600 -1.873579 -1.489605
H -5.243315 -0.288179 -1.443886
H 1.683612 2.567152 -0.818968

[HMo3S10]+
E=-4187.567170
S 0.964958 -1.881968 -1.290338
Mo -0.848511 -1.311640 -0.056947
S -2.098037 0.098572 -1.323071
Mo 1.532231 -0.071142 -0.033077
S 1.132844 1.787968 -1.287850
Mo -0.725319 1.383761 -0.053874
S -1.615167 3.063283 1.378283
S -1.846992 3.521982 -0.526275
S -0.030356 0.000307 1.701022
S 4.043617 -0.235262 -0.496446
S 3.318391 -0.168791 1.430674
S -2.154029 -3.340748 -0.536115
S -1.878664 -2.914349 1.369948
H 4.362149 1.062500 -0.673581

E=-4187.520311
S 4.174140 1.637076 0.880211
Mo 2.984531 0.201617 -0.016956
S 4.271524 -1.072649 -1.415524
Mo 0.080350 -0.184918 0.073275
S -1.289420 -1.146453 -1.416386
Mo -2.633360 0.274543 -0.163033
S -2.917354 2.045589 -1.185572
S 1.272626 1.367504 -1.045611
S 1.898592 -0.777264 1.802422
S 1.475271 -2.071088 0.259926
S -1.263608 0.644676 1.673192
S -4.536991 -0.188571 1.257068
S -4.547736 -1.190372 -0.429095
H 5.283401 -0.207329 -1.608118

[Mo3S10]+
E=-4186.957364

S 0.000011 0.001843 1.705589
Mo -0.496662 1.471418 -0.047722
Mo 1.523750 -0.306043 -0.047432
Mo -1.026050 -1.166777 -0.046709
S -2.289220 -2.589076 1.382312
S -2.622326 -2.978718 -0.522786
S -1.272016 3.760473 -0.522579
S -1.099659 3.275067 1.381708
S 3.387816 -0.684417 1.382411
S 3.893249 -0.779475 -0.522017
S 1.388002 1.576965 -1.304893
S 0.672253 -1.991478 -1.303757
S -2.060834 0.412497 -1.303597

E=-4186.925390
Mo 0.081959 -0.072209 -0.031379
Mo -2.903393 0.275284 -0.002076
S -1.328877 0.226143 -1.756066
S -1.350216 -0.392421 1.656718
S -4.590486 -1.304040 0.696781
S -4.599861 -0.919249 -1.228826
S -3.500419 2.212570 0.347521
S 1.412036 -1.804053 -0.414842
S 1.364092 1.717902 0.223194
Mo 2.844695 -0.082990 0.236465
S 3.399784 -0.429961 2.195035
S 4.579674 -0.775547 -1.303490
S 4.553213 1.153433 -0.948927

[H3Mo3S9]+
E=-3790.549082
S -0.014124 3.588876 1.121536
Mo -0.009703 1.764491 -0.267647
S 0.000039 0.414643 1.615445
Mo 1.352443 -0.519321 -0.042579
S 0.012847 -2.010270 -1.123631
Mo -1.342769 -0.537183 -0.039302
S -2.872694 -1.286903 1.523541
S -3.475727 -1.899126 -0.347140
S -1.844134 1.150907 -1.476370
S 1.827541 1.176521 -1.478958
S 3.541190 -1.781988 -0.367856
S 2.904310 -1.239252 1.512797
H -0.011445 4.432818 0.061342
H -4.360465 -0.925577 -0.641656
H 3.105178 -3.057179 -0.409358

E=-3790.501304
S -1.635407 -0.692500 1.595520
Mo -3.001464 0.049855 -0.018067
S -4.026015 1.999669 0.490329
Mo -0.223049 -0.029681 -0.078158
S 1.062594 1.676102 0.462477
Mo 2.548671 -0.122535 0.229985
S 3.068638 -0.865363 2.088546
S 1.071445 -1.694787 -0.696624
S -1.708108 0.601223 -1.735083
S 4.125650 -0.463549 -1.470179
S 4.488331 1.293105 -0.477484
S -4.402907 -1.645109 -0.579538
H -4.697981 1.415179 1.510636
H -3.508141 -2.645797 -0.690502
H 3.883976 2.189118 -1.285465

[H2Mo3S9]+
E=-3789.939432
S 0.072580 3.577990 1.140446
Mo 0.031824 1.759165 -0.254387
S -1.820108 1.195146 -1.457551
Mo -1.343200 -0.511229 -0.033824
S -3.495333 -1.844442 -0.343775
S -2.878228 -1.250060 1.528019
S 1.843260 1.124652 -1.487513
Mo 1.359107 -0.559302 -0.054923
S 3.417112 -1.847464 -0.393751
S 2.985331 -1.390009 1.474602
S 0.032817 0.397311 1.618628
S -0.015940 -1.993825 -1.144240
H -4.367606 -0.857170 -0.629934
H 0.099070 4.425755 0.083688

E=-3789.904499

S 1.674204 -0.199459 1.680203
Mo 3.162851 0.081686 -0.048034
S 4.568496 -1.695015 -0.276034
Mo 0.174977 -0.019740 -0.018758
S -1.093678 -1.799528 -0.286264
Mo -2.589543 -0.078849 0.235938
S -3.167728 -0.397292 2.198058
S -1.144848 1.750123 0.120529
S 1.639938 0.191541 -1.756716
S -4.500694 1.135699 -0.879734
S -4.114169 -0.814009 -1.379123
S 4.155719 1.875909 0.142803
H 5.734099 -1.027515 -0.201796
H -5.437960 0.969940 0.078100

[Mo3S9]+
E=-3788.706852
S -1.262940 3.533754 0.825737
Mo -0.475342 1.824990 -0.082685
S 1.541652 1.736107 -1.212860
Mo 1.550045 -0.251555 -0.096040
S 0.027079 0.337406 1.620675
Mo -1.151689 -0.815662 -0.066179
S -2.046165 0.785738 -1.368118
S -2.576166 -1.975013 1.441670
S 0.455746 -1.863325 -1.269643
S 3.252895 -0.827010 1.457701
S 3.722245 -1.228879 -0.418162
S -2.912257 -2.487929 -0.434126

E=-3788.675813
S 1.646053 1.685870 -0.033295
Mo 0.278217 -0.043867 0.000911
S -1.125896 -0.081706 -1.732895
Mo -2.711492 0.268257 -0.005019
S -4.360996 -1.205442 -0.959336
S -4.363179 -1.165950 1.004275
Mo 3.267883 -0.050693 0.001005
S 1.636387 -1.779951 0.035096
S 4.432106 -0.088938 -1.728705
S 4.432052 -0.021230 1.730915
S -1.126235 -0.015567 1.734809
S -3.361138 2.216961 -0.042717

[HMo3S8]+
E=-3391.077369

S 1.550988 3.244838 0.877595
Mo 1.087186 1.474360 -0.099713
S -0.784598 1.802888 -1.354387
Mo -1.247275 0.009273 -0.057628
S -3.762799 0.054267 -0.440588
S -2.980762 0.034087 1.466608
S 2.642618 -0.016554 -0.999620
Mo 1.077058 -1.480514 -0.089177
S 1.538878 -3.253823 0.884609
S 0.435653 0.002147 1.596854
S -0.795382 -1.797396 -1.346246
H -4.026230 -1.258275 -0.603427

E=-3391.053304
S -1.400419 1.718796 -0.000181
Mo -3.031094 -0.013650 -0.000068
S -4.193542 -0.021145 -1.730365
Mo -0.041332 -0.011585 -0.000005
S 1.438603 -0.006741 -1.727228
Mo 2.945503 0.051494 0.000064
S 3.969281 1.835087 -0.000029
S -1.392766 -1.743063 0.000109
S 1.438496 -0.006449 1.727292
S -4.193608 -0.020853 1.730187
S 4.323091 -1.755140 0.000266
H 5.504574 -1.110783 -0.000420

[Mo3S8]+
E=-3390.461359
S 2.337850 -0.000011 -1.426510
Mo 1.130991 1.370687 -0.079748
S 2.307961 2.742093 0.948071
Mo 1.130972 -1.370696 -0.079751
S 0.141610 0.000001 1.528359
S 2.307919 -2.742121 0.948069
S -0.853987 1.933153 -1.140643
Mo -1.578994 0.000012 -0.156050
S -3.263516 0.000006 1.492349
S -3.916617 0.000008 -0.380728
S -0.854012 -1.933135 -1.140649

E=-3390.427882
Mo 2.104490 -0.080732 0.000018
S 3.735397 -0.007591 1.610354
S 4.240542 1.191143 -0.000193
S 0.921479 -2.000414 0.000294

S 0.511821 1.531289 -0.000224
S 3.735392 -0.008128 -1.610341
Mo -0.650370 -0.387413 0.000050
S -2.073595 -0.538088 -1.774841
Mo -3.396217 -0.110761 0.000013
S -3.899435 1.889057 -0.000236
S -2.073600 -0.537640 1.774975

[Mo3S7]+
E=-2992.229507
S -2.312229 1.236744 -0.931444
Mo -0.659834 1.705946 0.499307
S 1.154254 2.064941 -0.769476
Mo 1.202486 -0.098383 -0.034501
S 3.501666 -0.583661 -0.699346
S 3.002525 -1.131279 1.127167
Mo -1.462220 -0.765763 -0.158781
S 0.187404 -1.315624 -1.646834
S -2.803189 -2.293856 0.345072
S -0.316565 -0.186989 1.771547

E=-2992.228241
S -2.014853 -0.000012 -1.470617
Mo -0.888538 1.399234 -0.081310
S 1.125222 2.011989 -1.031138
Mo 1.857752 0.000013 -0.110545
S 3.658669 0.000008 0.890084
Mo -0.888518 -1.399241 -0.081309
S 1.125242 -2.011969 -1.031144
S -2.116876 -2.723357 0.928513
S 0.127683 0.000003 1.502839
S -2.116917 2.723323 0.928519

E=-2992.198347
S 1.231768 -0.000052 -1.810150
Mo -0.356850 -0.000024 -0.294613
S -1.756860 -1.784517 -0.563353
Mo -3.099870 0.000000 -0.238759
S -3.671996 0.000052 1.735888
Mo 2.597356 0.000005 0.145007
S 3.746113 -1.732965 0.301086
S 3.746060 1.733017 0.301012
S 0.717568 0.000014 1.618402
S -1.756821 1.784485 -0.563427

Cartesian coordinates (in Ångstrom) of species optimized at the B3LYP/def2TZVP level of theory along the respective ZPE-corrected energy (in Hartree)

[Mo3S13]2- I
E= -5382.242356
S 1.529877 -0.684312 0.223797
Mo -3.886433 -0.846104 -0.051868
Mo 0.016270 0.979183 -0.207300
Mo 3.982312 -0.751502 0.169266
S 4.218045 -2.761683 -0.555832
S 4.415589 -0.641676 2.265706
S -3.297459 -1.678679 1.824072
S -4.435078 -2.397611 -1.430728
S -1.757164 -0.210343 -1.069770
S 0.719842 2.118232 -1.853465
S -5.904719 0.327713 0.430869
S -4.413637 1.476893 -0.449298
S 0.527434 2.263559 1.715815
S -1.498119 2.163925 1.213290
S 5.751845 0.424976 -0.890342
S 3.849154 1.222366 -1.188121

E= -5382.230031
S -1.744932 1.058643 -0.478985
Mo 4.086189 0.592709 0.001921
Mo -0.000125 -0.447341 -0.217380
Mo -4.085948 0.592839 0.001356
S -4.996884 2.114186 -1.217785
S -4.213513 1.086822 2.086055
S 4.212558 1.083470 2.087444
S 4.996070 2.116797 -1.214620
S 1.744741 1.057998 -0.478449
S -0.000439 -1.807310 -1.857661
S 5.540485 -1.290419 -0.230197
S 3.561460 -1.632966 -0.754193
S -1.004853 -1.398332 1.800043
S 1.003936 -1.400957 1.799211
S -5.539017 -1.291764 -0.227724
S -3.559918 -1.633964 -0.751119

[Mo3S13]2- II
E= -5382.199820
S 0.071660 -0.801116 1.459461
Mo 1.812979 -0.969628 -0.330704
Mo -2.078706 -0.551953 0.309986
Mo 0.165907 1.378652 0.165653
S -3.049137 -1.599850 1.931348
S -2.000667 1.733882 0.928100
S 1.427284 1.826171 2.309455
S 2.573375 1.211133 0.716089
S -0.294993 -0.522242 -1.425048
S 3.039032 -0.317067 -1.990021
S 3.062801 -2.566171 0.956616
S 1.664561 -3.352592 -0.364358
S -3.577534 0.199654 -1.398040
S -3.414085 -1.854097 -1.367373
S 0.287936 2.536769 -1.835540
S 0.471796 3.880713 -0.301142

E= -5382.177434
S 0.122281 -0.711395 1.515643
Mo 1.779102 -1.014365 -0.361447
Mo -2.105133 -0.481937 0.344806
Mo 0.270455 1.379534 0.220580
S -3.007322 -1.701212 1.882923
S -2.000128 1.748864 1.035400
S 1.702983 1.853154 2.251764
S 2.717857 1.140015 0.600901
S -0.363993 -0.510708 -1.368538
S 2.937895 -0.427035 -2.097386
S 3.014143 -2.654478 0.875482
S 1.511515 -3.385003 -0.360435
S -3.710121 0.298031 -1.203439
S -3.484231 -1.735579 -1.425199
S 0.071214 2.661299 -1.915172
S 0.633797 3.730562 -0.327283

[Mo3S13]2- III
E= -5382.244404

S -0.000154 0.000071 1.805048
Mo -0.799400 -1.373590 0.010708
S -1.770796 -3.040216 1.475741
S -2.029843 -3.483647 -0.545464
Mo -0.789616 1.379163 0.010778
S -2.003993 3.498100 -0.545781
S -1.747853 3.053958 1.475620
Mo 1.589505 -0.005748 0.010752
S 4.031316 -0.015236 -0.546487
S 3.519421 -0.013153 1.475007
S 1.463051 2.513116 0.115630
S 0.970142 1.666806 -1.674210
S -1.927124 0.006951 -1.674912
S -2.908025 0.010621 0.114034
S 1.444392 -2.523640 0.115449
S 0.958181 -1.673272 -1.674301

E= -5382.203157
S -0.000130 -0.009024 -1.827916
Mo -0.002369 -1.585134 -0.029178
S -0.005541 -3.526473 -1.485703
S -0.005951 -4.029831 0.538238
Mo 1.343532 0.807093 -0.011791
S 3.483747 2.019284 0.648826
S 3.152529 1.829968 -1.348469
Mo -1.341100 0.811063 -0.011638
S -3.477834 2.029666 0.648612
S -3.146944 1.839083 -1.348600
S 0.004204 2.847479 -0.461866
S 0.002717 1.749861 1.808459
S 1.675014 -0.960888 1.637484
S 2.517647 -1.464180 -0.154640
S -2.522081 -1.456624 -0.154128
S -1.677543 -0.955407 1.637796

[Mo3S13]2- IV
E= -5382.175152
S -0.397723 -0.519553 1.704786
Mo -1.753990 -0.534184 -0.203704
Mo 0.143450 1.399460 0.229025
Mo 1.333301 -1.295295 0.154660
S 1.133315 1.999951 2.479721
S 2.327688 0.924073 1.210996
S 1.546080 -3.058267 1.397356
S -0.649119 -2.081319 -1.323915
S -2.312443 1.987820 0.483774
S -1.613465 1.550136 -1.412705
S -4.112191 -0.853941 -0.809632
S -3.504154 -1.514788 1.067454
S 1.421477 1.818828 -1.861027
S 0.954590 3.520314 -0.777240
S 2.319293 -1.691378 -2.018905
S 3.614404 -0.953077 -0.613113

E= -5382.162372
S -0.302981 -0.549526 1.566705
Mo -1.912272 -0.610215 -0.183948
Mo -0.021031 1.469469 0.229559
Mo 1.596963 -1.244699 0.179849
S 1.036670 2.091554 2.418660
S 2.305164 1.111092 1.132011
S 1.970342 -2.954291 1.398476
S -0.361970 -2.081744 -1.304462
S -2.479746 1.826592 0.750838
S -1.945444 1.574102 -1.235554
S -4.202197 -1.281075 -0.873860
S -3.484496 -1.905033 0.994540
S 1.042779 1.747777 -1.971617
S 0.874750 3.498016 -0.891222
S 2.590957 -1.615901 -1.957705
S 3.839065 -0.685742 -0.618643

[Mo3S13]2- V
E= -5382.158212
S -0.301326 -0.473706 1.639210
Mo -1.775285 -0.680054 -0.185476

Mo -0.087527 1.502091 0.244497
Mo 1.483499 -1.095406 0.132789
S 1.513255 2.102432 2.012541
S 2.708810 0.471169 1.451454
S 1.518170 -3.176496 0.791946
S -0.580369 -1.942852 -1.498837
S -2.595494 1.752746 0.600764
S -1.962808 1.421219 -1.342552
S -4.104133 -1.256331 -0.600369
S -3.265323 -1.946026 1.177626
S 1.307807 2.212486 -1.438268
S 0.312318 3.844834 -0.667663
S 2.492383 -0.909871 -1.992690
S 3.952409 -1.382012 -0.636664

E= -5382.211572
S 0.434307 -0.070518 -0.859181
Mo -1.429334 -1.509168 -0.321875
Mo -1.278326 1.331999 0.050042
Mo 2.679726 0.038329 0.145290
S 0.366033 2.857102 0.771408
S 2.402154 2.325754 0.465956
S 2.631870 -1.046031 1.972842
S -2.259884 -1.843872 -2.263230
S -1.635550 -0.121542 2.024954
S -3.177974 -0.131159 0.637364
S -2.036101 -3.464201 0.983658
S -0.039874 -3.269777 0.437549
S -2.519748 2.377649 -1.627587
S -2.726762 3.400124 0.181121
S 3.707497 -0.969712 -1.756668
S 4.927359 0.320638 -0.636011

[Mo3S13]2- VI
E= -5382.246093
S 1.141403 -1.389943 1.002260
Mo -3.164131 -0.427588 -0.100676
Mo -0.439565 0.462412 -0.069789
Mo 3.058715 -0.496996 -0.129067
S 2.667553 -0.773876 2.252632
S 1.160074 -0.296844 -1.672663
S -3.283972 -2.520647 -0.504998
S 4.052900 -2.248157 -0.798329
S -1.770368 -0.130022 1.734088
S -1.939226 0.523074 -1.834719
S -5.163217 0.703034 -0.818888
S -5.044955 0.295511 1.233077
S -0.215619 2.757905 -0.099251
S 1.088996 1.925712 1.281906
S 3.874538 1.323612 -1.396580
S 4.862464 1.043843 0.407737

E= -5382.229289
S 1.305250 -0.392319 1.720885
Mo -3.264494 -0.605393 -0.109905
Mo -0.291142 0.907961 0.005941
Mo 3.036958 -0.697656 0.011719
S 3.193917 0.380167 2.117575
S 0.992095 -0.522943 -1.318554
S -2.866187 -2.694236 -0.338059
S 3.448602 -2.772837 0.140033
S -1.803038 0.205464 1.614659
S -2.133904 0.652549 -1.645358
S -5.513768 -0.176398 -0.818153
S -5.155865 0.040014 1.237979
S -0.414380 3.137791 -0.721439
S 1.106000 2.758914 0.640282
S 3.922224 0.185949 -1.979914
S 5.280586 0.234991 -0.407795

[Mo3S13]2- VII
E= -5382.198536
S -0.917418 0.919984 -1.639427
Mo 1.576005 -1.384630 -0.131100
Mo 0.939925 1.428850 -0.063596
Mo -2.390381 -0.495279 0.407874

S36

S -0.678384 2.878765 -1.069108
S -1.249519 0.991394 1.586017
S -0.565961 -2.094015 -0.128898
S -3.334476 -1.733228 1.886480
S 2.230988 0.125332 -1.655873
S 1.579326 0.010288 1.706680
S 3.236595 -2.711957 0.912875
S 2.841738 -3.223714 -1.081777
S 1.547870 3.449408 1.368258
S 2.786037 2.829559 -0.157498
S -4.149564 0.723159 -0.605013
S -3.656799 -0.980944 -1.682306

E= -5382.202690
S -0.730378 -1.309899 1.220743
Mo 1.415421 1.620231 -0.086546
Mo 1.472052 -1.470773 -0.262820
Mo -2.560137 0.077997 0.285359
S -2.470922 -2.256832 0.549689
S 0.210205 -2.270892 -1.803450
S -3.389393 1.012982 1.995629
S -0.856680 1.791652 -0.394044
S 1.681736 0.120988 1.655069
S 2.381452 0.366243 -1.662605
S 1.785267 3.996105 -0.614998
S 2.649700 3.227467 1.126404
S 3.619491 -2.466712 -0.287160
S 2.278622 -3.325683 1.054251
S -3.383535 0.993487 -1.714487
S -4.634821 -0.475975 -0.957022

 [Mo3S13]2- VIII
E= -5382.260080
Mo -1.342145 -1.130749 0.106514
Mo -3.267634 0.941485 -0.042069
S -2.113991 -0.127332 -1.788235
S -5.235786 1.038367 -1.425230
S -5.566253 0.839192 0.626885
S -2.674337 -0.372550 1.812226
S -2.417609 2.865393 0.247481
S -0.727806 -3.117474 -1.072846
S -1.518208 -3.383222 0.842490
Mo 4.100005 0.448029 0.235745
S 2.028182 -0.314762 -0.733933
S 4.397871 -0.871793 1.896657
S 6.206712 0.594948 -0.848918
S 4.687735 -0.067724 -2.102827
S 3.656173 2.418614 0.940174
S 0.615473 -0.180916 0.818076

E= -5382.242929
Mo -1.223740 0.739724 -0.126048
Mo -3.696646 -0.661462 0.102213
S -2.448984 0.439616 1.771162
S -5.730319 0.015831 1.190055
S -5.860855 -0.269145 -0.880037
S -2.639663 0.095179 -1.842849
S -3.345472 -2.749699 0.307504
S 0.132648 2.719068 0.690232
S -0.746503 2.914148 -1.102153
Mo 4.242574 -0.480100 -0.210250
S 2.191212 0.102150 0.916227
S 4.099787 0.519715 -2.097395
S 6.465568 -0.113507 0.552267
S 5.015039 0.609582 1.853179
S 4.058257 -2.598290 -0.477851
S 0.588540 -0.629521 -0.265867

[Mo3S13]2- IX
E= -5382.215750
Mo 0.403293 0.634896 -0.057211
Mo 2.953295 -0.721419 -0.028145
S 1.998655 0.630937 -1.683431
S 5.049098 0.358614 -0.492289
S 4.895844 -0.537193 1.394037
S 1.494667 -0.627945 1.733198
S 2.870640 -2.722768 -0.765025
S -0.115927 3.072132 -0.598704
S 0.893578 2.577739 1.111065
Mo -2.860066 0.107333 -0.004423
S -1.320492 0.148238 -1.841910
S -1.743707 0.632576 1.811662

S -4.400783 1.509940 -0.474723
S -4.054342 -1.830973 0.178406
S -0.846988 -1.509103 -0.704679
S -6.023612 -1.856820 0.568064

E= -5382.212461
Mo 0.136518 0.644693 -0.000337
Mo 2.923916 -0.700861 -0.069093
S 2.009314 0.661019 -1.638211
S 5.099769 0.328801 -0.317058
S 4.654693 -0.415959 1.587218
S 1.342201 -0.767747 1.593168
S 3.047854 -2.667681 -0.889295
S -0.109404 3.063708 -0.332557
S 1.062792 2.567058 1.209611
Mo -2.808927 0.057798 -0.143726
S -1.333841 0.373588 -1.985889
S -1.715483 0.646585 1.712853
S -4.372326 1.462173 -0.625582
S -3.867286 -1.965162 0.125387
S -0.912877 -1.427101 -1.085852
S -5.565612 -1.863547 1.205739

[Mo3S13]2- X
E= -5382.222300
S 1.084803 -0.633191 -1.294686
Mo 3.118423 -0.772261 0.037938
S 5.327204 0.165974 -0.439904
S 4.031025 -0.106746 -2.041668
S 1.347082 -0.348687 1.669052
S 3.199813 0.516504 2.022247
Mo -0.330425 0.783823 -0.046048
S 0.736179 2.795668 0.902037
S -0.418214 2.976286 -0.816938
Mo -3.137320 0.045738 -0.084243
S -4.684034 1.517686 -0.008719
S -3.900102 -2.083268 -0.145340
S -1.722058 0.260810 1.730487
S -1.789115 0.282839 -1.890185
S 3.505369 -2.828004 0.368021
S -5.800984 -2.666282 0.188020

E= -5382.202400
S 1.038825 0.812180 1.143945
Mo 3.115421 0.699138 -0.113301
S 5.314224 -0.072421 0.642534
S 3.951986 0.524719 2.095515
S 1.417726 -0.082752 -1.713349
S 3.277378 -1.014494 -1.725257
Mo -0.380029 -0.759148 0.098101
S 0.667209 -2.934863 -0.335685
S -0.697399 -2.785044 1.230020
Mo -3.177945 -0.095281 -0.075002
S -4.807229 -1.506959 0.004798
S -4.034084 2.026864 -0.828414
S -1.649417 -0.396042 -1.804502
S -1.886880 0.163881 1.764845
S 3.506970 2.635182 -0.883302
S -4.937606 3.037422 0.645634

[Mo3S13]2- XI
E= -5382.226128
S -1.403513 -0.318620 -1.668896
Mo -2.678610 0.390480 0.020759
S -3.588760 2.529582 -0.409966
Mo 0.058807 -0.882307 0.158761
S -1.525204 -0.518298 1.869277
S 1.053837 -2.900861 -0.914599
S -0.315049 -3.088676 0.627632
Mo 2.952571 0.701978 -0.086690
S 3.028827 2.817976 0.207394
S 1.589125 0.189084 -1.744144
S 1.626715 -0.080643 1.676905
S -4.776678 -0.281707 -1.275068
S -4.470030 -0.947738 0.669695
S 4.731925 -0.627945 0.876204
S 5.103705 0.172014 -1.015347
S -1.928418 2.503958 0.857235

E= -5382.230756
S -1.685638 0.496264 1.649233
Mo -2.824720 -0.396811 0.031276

S -4.045168 -2.249642 1.010170
Mo 0.337878 0.642415 -0.039122
S -0.944441 -0.323235 -1.623822
S 0.758245 2.861479 1.317810
S -0.440499 3.031809 -0.262462
Mo 2.943189 -0.566690 -0.194522
S 2.939029 -2.243277 -1.510419
S 1.278824 -0.904668 1.394869
S 2.172303 1.279167 -1.355527
S -4.977713 0.756253 0.088211
S -3.659632 1.251248 -1.439859
S 5.157258 0.407714 -0.106782
S 4.626394 -0.812790 1.508380
S -2.376871 -2.707469 -0.138587

[Mo3S13]2- XII
E= -5382.195743
S -1.341200 -0.288264 -1.655326
Mo -2.877567 -0.253046 0.053577
S -3.523199 1.994932 -0.191226
Mo 0.216787 -0.103229 0.062462
S -0.280024 2.354985 0.639761
S -1.590476 -0.382833 1.840083
S 1.748296 -1.819305 -0.866796
S 0.521435 -2.442589 0.669234
Mo 3.106444 0.040080 -0.054345
S 1.869096 1.200723 -1.482754
S 1.949255 0.531192 1.819937
S -4.066792 -2.219023 -0.603819
S -5.226013 -0.753770 0.358358
S 5.138289 -1.149177 -0.487375
S 5.368514 0.736770 0.420104
S -1.737051 3.066368 -0.622127

E= -5382.209877
S -1.325212 0.066736 1.842461
Mo -2.945178 -0.041295 0.070744
S -4.687197 -1.572831 -0.390878
Mo 0.115299 0.020156 0.047186
S 0.512543 -2.285912 -0.691638
S -1.648236 0.322911 -1.675676
S 2.866005 2.231532 -0.550765
S 0.781755 2.236469 -0.725306
Mo 3.175704 0.017982 0.101415
S 1.867209 -0.145761 1.856909
S 1.786623 -0.922833 -1.618663
S -3.786190 1.884860 1.076904
S -4.717722 1.588831 -0.754508
S 5.513993 0.394872 0.648084
S 5.021961 -1.423102 -0.287886
S -3.093319 -2.367485 0.695182

[Mo3S11]2- I
E= -4585.696986
S 0.541714 -0.403643 -1.534041
Mo 2.482846 -0.649820 -0.069029
S 4.559537 0.650843 0.040744
S 3.432489 0.763117 -1.702592
S 0.550594 -0.947050 1.348549
S 2.246503 -0.190516 2.270496
Mo -0.960323 0.687418 -0.084967
S 0.290693 2.492577 1.137166
S -0.906117 2.969986 -0.479568
Mo -3.324262 -0.462154 -0.044607
S -4.057455 -2.511211 -0.116093
S -2.475907 0.380196 1.837505
S -2.615805 0.545758 -1.907034
S 3.163319 -2.635601 -0.373800

E= -4585.700087
S -0.795247 -0.854437 1.163941
Mo -2.792336 -0.441396 -0.130722
S -4.902581 0.544372 0.628344
S -3.700875 -0.360182 2.065720
S -0.982164 0.209399 -1.716084
S -2.667331 1.427165 -1.541035
Mo 0.890552 0.399980 0.090101
S 0.366950 2.754504 -0.261901
S 1.817257 2.293630 1.165775
Mo 3.544998 -0.750254 -0.062311
S 5.712314 -0.468612 -0.126966
S 2.024902 -0.368922 -1.792757

S 2.213473 -0.857091 1.768715
S -3.400135 -2.241691 -1.083552

E= -4585.689944
S 0.584277 -0.448959 -1.388591
Mo 2.607321 -0.729114 -0.063154
S 4.877826 0.271627 -0.317421
S 3.497345 0.488021 -1.856775
S 0.839564 -0.675320 1.610754
S 2.692981 0.091269 2.158707
Mo -0.763879 0.816736 0.071883
S 0.509459 2.685315 0.904738
S -0.962121 3.096727 -0.514144
Mo -3.655176 -0.617400 -0.102950
S -5.518643 -1.754910 -0.081188
S -2.320518 -0.002930 1.693879
S -2.561376 0.434567 -1.747132
S 3.117005 -2.794738 -0.215496

[Mo3S11]2- II
E= -4585.790449
S -1.145342 0.950489 -0.001147
Mo -3.408970 0.066946 -0.000462
S -3.452277 -1.160108 1.756431
S -3.452954 -1.154175 -1.761652
Mo 0.617624 -0.693740 0.000358
S 0.107059 -1.823201 1.729492
S 3.068562 -1.648993 -0.022385
Mo 3.754631 0.461259 -0.000907
S 1.775564 1.538524 0.011929
S 4.903222 0.916200 1.771509
S 0.094445 -1.828933 -1.722104
S 4.900673 0.951847 -1.765446
S -3.823863 2.464343 0.004548
S -5.503713 1.228537 0.001481

E= -4585.711252
S 1.237889 1.255027 -0.231087
Mo 2.877884 -0.558333 0.075660
S 1.964581 -2.233202 -0.904016
S 2.897045 -0.817495 2.205407
Mo -1.065467 1.084385 0.091230
S -0.743349 -1.218106 1.054431
S -2.233439 -0.073784 1.913344
Mo -2.861921 -1.202144 -0.195351
S -2.287340 0.449014 -1.743589
S -4.437678 -2.601011 -0.797063
S -1.081894 3.507493 -0.796009
S -1.918120 3.071538 1.025540
S 4.182492 1.121809 -1.085066
S 5.174763 -0.632541 -0.567184

E= -4585.709365
S 0.975322 -0.257198 -1.736469
Mo 2.486991 -0.632245 -0.049758
S 2.611692 -2.752233 0.209095
S 1.461470 0.246809 1.780831
Mo -0.320365 0.645835 0.120500
S -1.322563 -1.736990 0.636989
S -1.954452 -0.175140 1.863409
Mo -3.268609 -0.497107 -0.164190
S -2.276192 0.939430 -1.594247
S -5.342496 -1.063616 -0.560217
S 0.511941 2.806321 -0.556269
S -0.700429 2.852361 1.071422
S 4.298689 0.104746 -1.463684
S 4.629721 0.304740 0.594439

[Mo3S11]2- III
E= -4585.791937
S 2.055149 -0.377204 1.704576
Mo 0.856597 0.649005 0.037874
S 2.161368 0.244126 -1.776707
Mo 3.505618 -0.602999 -0.080993
S 5.275847 0.608685 0.169494
S 3.917871 -2.696044 -0.423453
S -0.667147 2.527948 0.040360
S 1.335469 2.876336 0.545051
S -0.957862 -0.748874 -0.250243
Mo -3.352618 -0.587161 0.156235
S -3.891140 -2.629069 -0.241413
S -3.283867 1.086531 -1.571495

S -5.154733 0.697736 -0.747986
S -3.441146 -0.169639 2.254890

E= -4585.781212
S 2.489148 0.449675 1.722290
Mo 0.772233 0.836559 0.039586
S 1.836350 -0.372087 -1.630926
Mo 3.421141 -0.719585 0.024023
S 5.331242 0.111072 -0.548346
S 3.601456 -2.814676 0.498414
S -0.460048 2.593251 -1.013383
S 1.150837 3.166151 0.165756
S -0.994263 -0.263930 0.927344
Mo -3.369110 -0.279678 0.226801
S -4.256618 -0.755503 2.129437
S -2.561370 -1.917873 -1.338009
S -4.609274 -1.539094 -1.378804
S -3.691153 1.770115 -0.296096

E= -4585.745947
S 2.456077 -0.003173 -1.792621
Mo 0.747828 -0.649786 -0.230020
S 2.108529 -0.158955 1.682078
Mo 3.628893 0.495582 0.107862
S 5.442065 -0.672103 0.255128
S 4.059653 2.608333 0.234150
S -0.549076 -2.540757 0.782224
S -0.212128 -2.669368 -1.220574
S -0.992143 0.836405 -0.672991
Mo -3.285413 0.622214 -0.165127
S -3.952549 2.668056 -0.144438
S -2.543058 -0.487453 1.872260
S -4.579980 -0.389879 1.629244
S -4.102072 -0.419633 -1.870334

[Mo3S11]2- IV
E= -4585.795854
S 1.555372 -0.406974 1.619959
Mo 0.771471 0.865862 -0.163936
S 2.490038 0.677523 -1.704564
Mo 3.184287 -0.691040 0.020340
S 5.072503 0.044899 0.788561
S 3.294956 -2.747496 -0.629561
S 0.513368 3.218902 -0.674825
S 0.132697 2.590605 1.279827
S -0.890407 -0.304758 -1.130796
Mo -3.025938 -0.710753 0.066263
S -3.581404 -2.520638 -0.943061
S -3.581541 1.471538 -0.774324
S -5.064465 0.501412 0.314692
S -2.381895 -1.118551 2.057090

E= -4585.725994
S -2.327273 -0.370153 -0.666138
Mo -0.388845 0.956326 0.014135
S -0.729178 1.569374 2.019289
Mo -4.410193 -0.703477 0.060722
S -5.786871 -1.672587 -1.285426
S -5.153355 -0.060261 1.970121
S 0.976252 2.528806 -1.081773
S -1.017408 2.512013 -1.712163
S 1.069644 -0.828091 -0.024969
Mo 3.512595 -0.864076 -0.060889
S 3.840248 -2.819859 0.776337
S 3.326758 1.123751 1.276100
S 5.260067 0.476192 0.860091
S 3.918029 -0.854717 -2.168137

E= -4585.757848
S -1.651074 -1.048753 -1.524619
Mo -0.315380 0.362855 -0.221458
S -2.176988 0.742853 1.457962
Mo -3.252597 -0.645892 0.090301
S -4.983861 0.295336 -0.793200
S -3.808611 -2.479555 1.081795
S -0.980901 4.032443 0.538297
S -0.154737 2.739897 -0.727236
S 1.043080 -0.512664 1.396051
Mo 2.987634 -0.653966 -0.033618
S 3.417949 -2.718376 -0.377020
S 4.386239 0.460268 1.562182
S 4.868665 0.766195 -0.459261

S 1.563638 0.181987 -1.722418

[Mo3S11]2- V
E= -4585.777950
Mo -3.157750 0.375668 0.010612
S -4.673290 -0.101850 -1.456295
S -3.845125 1.574663 1.661582
S -1.317685 1.393945 -0.981323
Mo -0.365078 -0.450449 -0.077610
S 1.348001 -0.894594 -1.626682
S 0.758849 0.135469 1.795574
Mo 2.455880 0.138536 0.084222
S 3.535151 -1.399556 1.446166
S 4.583085 -1.105582 -0.332577
S -2.221204 -1.579997 1.050824
S -1.480180 -2.532233 -0.657089
S 3.459750 1.913302 -1.397813
S 2.653388 2.429077 0.452420

E= -4585.759408
Mo -3.331253 0.331418 -0.000750
S -4.858558 -0.362071 -1.382751
S -4.192348 1.562784 1.566805
S -1.518066 1.403214 -0.986792
Mo -0.272809 -0.346189 -0.126269
S 1.386410 -0.634854 -1.739909
S 0.816992 0.120305 1.792377
Mo 2.521784 0.136421 0.105197
S 3.483084 -1.570055 1.352647
S 4.617717 -1.124804 -0.339244
S -2.299931 -1.506660 0.973569
S -1.092421 -2.530215 -0.494879
S 3.628006 1.949636 -1.286062
S 2.870095 2.373389 0.601524

E= -4585.739175
Mo -3.469205 0.358231 0.017111
S -5.016217 -0.386640 -1.306503
S -4.243426 1.768218 1.468207
S -1.601582 1.269173 -1.040983
Mo -0.330772 -0.420781 -0.095814
S 1.329256 -1.003896 -1.626687
S 0.909685 0.187362 1.669257
Mo 2.674942 0.072196 -0.015782
S 4.090130 -1.212476 1.390982
S 4.831095 -0.964075 -0.544054
S -2.475780 -1.434551 1.153224
S -1.265271 -2.587337 -0.170641
S 2.768155 2.090788 -1.299470
S 3.627173 2.248112 0.554695

[Mo3S11]2- VI
E= -4585.679275
S -0.000002 0.195058 -1.883749
Mo 0.000297 1.860677 -0.243240
S -1.096084 1.391957 1.815760
S -2.348758 1.918221 -0.747051
Mo -1.399550 -0.356461 -0.029755
S -0.000026 -2.488188 -0.171982
S -0.000004 -1.544314 1.617693
Mo 1.399511 -0.356588 -0.029670
S 1.095590 1.391421 1.816676
S 2.348853 1.918390 -0.747395
S -3.197599 -1.465681 -1.256201
S -3.493030 -1.431738 0.803353
S 3.492924 -1.431825 0.803471
S 3.197544 -1.465823 -1.256080

E= -4585.676984
S -0.000001 0.100203 -1.906545
Mo 0.000006 1.876761 -0.287784
S -1.746597 1.625718 1.385399
S -2.497515 1.870721 -0.524273
Mo -1.397067 -0.406303 -0.009504
S -0.000019 -2.490871 0.264597
S -0.000004 -1.203641 1.853742
Mo 1.397063 -0.406312 -0.009503
S 1.746600 1.625707 1.385407
S 2.497528 1.870689 -0.524264
S -3.063200 -1.594428 -1.296974
S -3.541170 -1.501529 0.732612
S 3.541179 -1.501519 0.732604

S 3.063194 -1.594434 -1.296977

E= -4585.634148
S -0.000003 0.085779 -1.917315
Mo -0.000002 1.867173 -0.314450
S -1.779162 1.652720 1.317914
S -2.519709 1.855537 -0.597068
Mo -1.361712 -0.422766 0.008074
S 0.000007 -2.500191 -0.067054
S -0.000006 -0.988385 1.971519
Mo 1.361710 -0.422765 0.008074
S 1.779161 1.652718 1.317915
S 2.519696 1.855533 -0.597086
S -3.159825 -1.661081 -1.158308
S -3.528735 -1.486693 0.835404
S 3.528728 -1.486664 0.835416
S 3.159861 -1.661081 -1.158294

[Mo3S11]2- VII
E= -4585.702894
S 0.052159 -0.120946 1.958279
Mo -1.171386 -0.771674 -0.000430
S -2.987148 -1.917776 1.127615
S -3.086917 -2.053748 -0.948643
Mo -0.467865 1.558704 0.294996
S -2.840357 1.309582 0.369431
S -2.141881 2.944681 -0.803221
Mo 1.490503 -0.230150 0.012194
S 3.818722 -0.795239 -0.752314
S 3.395179 -1.014512 1.279728
S 1.277419 1.793884 -1.364523
S 2.009114 2.235905 0.501563
S 0.583915 -2.569901 -0.301155
S 0.310256 -1.273737 -1.872006

E= -4585.679702
S -0.066403 -0.000266 1.871070
Mo -0.915433 1.251027 0.003407
S 0.824293 1.595806 -1.670718
S 1.337019 2.549012 0.094274
Mo 1.512184 0.000223 0.054024
S 1.336065 -2.548768 0.090233
S 0.822687 -1.592312 -1.672883
Mo -0.915475 -1.250010 0.003193
S 3.440381 -0.001661 1.511659
S 3.954897 -0.000656 -0.512297
S -2.606550 -2.668814 -0.988554
S -2.797429 -2.296996 1.054562
S -2.607716 2.666461 -0.989744
S -2.800595 2.294937 1.053261

E= -4585.660815
S 0.001254 0.404531 1.669256
Mo 1.755682 0.838007 0.045071
S 1.694454 -0.897453 -1.694289
S 2.504318 -1.488905 0.101860
Mo -0.004480 -1.388411 0.031403
S -2.514030 -1.473577 0.102416
S -1.700750 -0.887273 -1.693917
Mo -1.750679 0.848733 0.045259
S -0.009553 -3.176956 1.666676
S -0.012014 -3.891957 -0.295414
S -3.506059 2.324565 -0.866769
S -2.376039 3.008581 0.778659
S 3.520045 2.302438 -0.867764
S 2.397001 2.992893 0.779735

[Mo3S11]2- VIII
E= -4585.669329
Mo 0.774741 -1.303514 0.108356
Mo -1.415305 0.063348 0.070768
Mo 0.888398 1.229053 0.108266
S 2.149376 2.064717 -1.625948
S 2.424962 3.414536 -0.048077
S -1.218319 2.514606 -0.161111
S -0.914999 1.806530 1.747334
S -2.749983 0.122841 -1.949511
S -3.973949 0.178154 -0.251754
S -1.438017 -2.396139 -0.160728
S -1.073063 -1.717907 1.747693
S 2.110705 -3.617486 -0.048912
S 1.955817 -2.247762 -1.626024

S 2.076906 -0.092918 1.622640

E= -4585.645383
S 0.744385 -2.242686 -1.159379
Mo -1.053808 -1.212852 -0.102759
S -1.824622 0.310585 -1.928580
S -2.826211 0.503243 -0.132584
Mo -0.504990 1.267965 -0.057671
S 1.454647 1.523884 -1.572919
S 1.783369 2.025789 0.405376
Mo 1.731897 -0.430198 -0.071408
S 3.243999 -1.088551 1.585986
S 4.216646 -0.810426 -0.255071
S -1.192306 2.593756 1.850023
S -1.384325 3.690966 0.076776
S -1.864272 -2.370735 1.720853
S -2.805695 -3.151228 0.018091

E= -4585.616211
Mo -1.500398 -0.959811 0.042645
Mo 0.004818 1.481541 -0.004430
Mo 1.493968 -0.967333 0.042694
S 2.753488 -2.087452 -1.570149
S 3.739354 -2.065819 0.288734
S 2.444705 1.322295 -0.339340
S 1.829825 0.927870 1.594752
S 0.009834 3.255073 -1.685397
S 0.012125 3.955866 0.288406
S -2.435685 1.335793 -0.339974
S -1.823850 0.938029 1.594396
S -3.752175 -2.044381 0.289502
S -2.766878 -2.072843 -1.569676
S -0.006512 -2.294723 1.236413

[Mo3S11]2- IX
E= -4585.652789
Mo -1.302324 -0.504512 0.059858
Mo 1.302371 -0.504433 0.059839
Mo -0.000053 1.742753 -0.021022
S 2.519605 1.646862 -0.059512
S 1.696834 1.256035 1.785947
S 2.673481 -1.282446 -1.765268
S 3.493555 -1.842712 0.077189
S 0.000074 -2.584808 -0.130038
S 0.000079 -1.758690 1.737005
S -3.493536 -1.842751 0.077180
S -2.673403 -1.282544 -1.765269
S -2.519654 1.646713 -0.059541
S -1.696941 1.255936 1.785952
S -0.000078 2.862158 -1.942668

E= -4585.631369
Mo -1.089195 -0.863193 0.028116
Mo 1.496455 -0.277785 0.065022
Mo -0.554384 1.862325 0.027527
S 1.885369 2.065152 -0.497088
S 1.434702 1.803482 1.508194
S 3.047883 -0.877669 -1.712673
S 3.872797 -1.104038 0.198874
S 0.668072 -2.572799 -0.035553
S 0.427250 -1.691556 1.808886
S -2.873581 -2.695973 0.051060
S -2.150943 -2.039943 -1.800226
S -2.795926 0.883252 -0.236965
S -2.044599 0.746360 1.684027
S -1.084827 3.590197 -1.285282

E= -4585.619968
Mo -1.760495 -0.178641 -0.012409
Mo 1.088784 -1.031518 0.101840
Mo 0.912503 1.740053 0.131236
S 2.911038 0.433844 0.990976
S 1.198790 0.349518 2.153422
S 2.504965 -1.520523 -1.790454
S 2.565268 -3.007218 -0.306755
S -0.858906 -2.264299 -0.917209
S -0.798478 -2.181511 1.147422
S -3.950395 -0.683138 0.903814
S -3.975296 0.169202 -1.003317
S -0.941072 1.686392 -1.422510
S -1.451544 2.351989 0.487245
S 2.163553 3.273830 -0.821884

[Mo3S11]2- X
E= -4585.724673
S -0.229202 -0.000151 -1.761644
Mo -1.010840 -1.429793 -0.048729
S 0.726583 -1.685009 1.628624
S 1.294509 -2.533065 -0.145151
Mo 1.420448 0.000217 -0.018554
S 1.293800 2.533396 -0.145591
S 0.726062 1.685531 1.628334
Mo -1.011311 1.429450 -0.048861
S -2.114300 -0.000265 1.568486
S -3.187959 -0.000347 -0.175468
S 3.363625 0.000261 -1.462564
S 3.852389 0.000431 0.569165
S -2.073514 3.285845 -0.699478
S -2.072520 -3.286296 -0.699835

E= -4585.706397
S -0.187559 0.000583 -1.797302
Mo -1.058205 -1.441795 -0.068452
S 0.689841 -1.702194 1.586892
S 1.306276 -2.530755 -0.181993
Mo 1.395064 -0.000263 -0.021048
S 1.306736 2.529994 -0.181106
S 0.690632 1.701342 1.587638
Mo -1.057864 1.442237 -0.067717
S -1.936441 -0.000447 1.712412
S -2.981553 0.000751 -0.610722
S 3.363426 -0.000219 -1.449532
S 3.812060 -0.000837 0.591213
S -2.084188 3.376610 -0.422700
S -2.086593 -3.375299 -0.422104

E= -4585.663175
S -0.073938 -0.000180 -1.868515
Mo -1.045065 -1.449550 -0.170681
S 0.639106 -1.691263 1.599174
S 1.291237 -2.473855 -0.213064
Mo 1.516851 -0.000279 0.003422
S 1.292506 2.473330 -0.213885
S 0.640451 1.691746 1.598719
Mo -1.044243 1.449846 -0.170725
S -2.342025 0.000498 1.358473
S -3.020378 0.000721 -0.653567
S 3.582134 -0.001163 -1.309997
S 3.834031 -0.000861 0.765778
S -2.169229 3.397203 -0.087821
S -2.171196 -3.396220 -0.088086

[Mo3S11]2- XI
E= -4585.788395
Mo -0.694222 -1.366268 0.008007
Mo 1.676716 0.000135 -0.069153
Mo -0.694438 1.366164 0.008011
S 0.135409 0.000010 1.752699
S 3.525367 0.000233 1.350355
S 4.179225 0.000326 -0.643027
S -1.258358 -3.110109 1.456557
S -1.882810 -3.567817 -0.479318
S -2.852134 -0.000227 0.051195
S -1.781338 -0.000137 -1.716821
S -1.258846 3.109918 1.456564
S -1.883380 3.567525 -0.479309
S 1.160504 -1.866182 -1.304711
S 1.160211 1.866378 -1.304707

E= -4585.760013
Mo -1.514190 -0.680448 -0.019040
Mo 1.441049 -0.986488 -0.146107
Mo 0.219645 1.477019 0.022965
S 0.104857 -0.247739 1.691994
S 2.917411 -2.080848 1.333762
S 3.678792 -1.928757 -0.613178
S -2.917489 -2.160838 1.351693
S -3.649189 -1.672458 -0.540628
S -2.296054 1.718144 0.171262
S -1.531449 1.149905 -1.671328
S 0.837115 3.113393 1.567289
S 0.564643 3.988262 -0.304843
S -0.028083 -2.280917 -1.208127
S 1.935583 0.900387 -1.404666

E= -4585.718749
Mo -0.819221 -1.446314 -0.035027
Mo 2.044913 -0.000157 -0.036639
Mo -0.818106 1.446659 -0.034932
S 0.204733 -0.000063 1.654428
S 4.007841 -0.003748 1.293146
S 4.372730 -0.000887 -0.785189
S -1.427620 -3.123673 1.480569
S -2.115822 -3.514963 -0.458014
S -2.921237 0.000784 0.117757
S -1.916147 0.000575 -1.695020
S -1.422948 3.125069 1.480774
S -2.113329 3.516407 -0.456953
S 1.130586 -1.858683 -1.175575
S 1.131301 1.858687 -1.176102

[Mo3S11]2- XII
E= -4585.767915
S 0.084842 0.363077 -1.739808
Mo -0.025098 1.868999 0.055457
S -1.607824 1.029902 1.748050
S -2.533896 1.571586 -0.008012
Mo -1.253742 -0.634469 -0.023921
S 0.271502 -2.646700 -0.240837
S 0.198652 -1.748013 1.603828
Mo 1.501481 -0.427795 0.000791
S 1.763890 1.333394 1.476599
S -2.846837 -1.598496 -1.575520
S -3.299635 -1.999582 0.422807
S 3.767396 -1.502689 0.492399
S 3.330445 -0.765258 -1.410691
S 0.287036 3.845102 -0.853693

E= -4585.737139
S 0.025108 0.479813 -1.705318
Mo -0.948836 1.814623 -0.001086
S -1.890086 0.361503 1.705906
S -3.008568 0.270972 -0.024709
Mo -0.838861 -1.033588 -0.013255
S 1.289464 -2.370944 -0.126387
S 0.878404 -1.475707 1.682629
Mo 1.705203 0.125945 0.024329
S 1.140524 2.178628 1.022733
S -1.849087 -2.589021 -1.583586
S -2.145521 -3.113659 0.414724
S 4.103132 -0.108554 0.591306
S 3.580196 0.294224 -1.405968
S -1.907020 3.691924 -0.597549

E= -4585.705949
S 0.127458 0.368657 -1.694162
Mo 0.724652 1.964125 -0.047276
S -1.157738 1.756602 1.354485
S -2.673208 1.879160 -0.051061
Mo -1.493040 -0.333140 0.027147
S -0.476429 -2.627845 -0.118928
S -0.291426 -1.672865 1.703853
Mo 1.329300 -0.916979 0.002929
S 2.234964 0.948518 1.328482
S -3.262257 -1.075371 -1.506160
S -3.613821 -1.474128 0.500572
S 3.132485 -2.456792 0.449632
S 3.229408 -1.537761 -1.410603
S 1.278167 4.017561 -0.510962

[Mo3S11]2- XIII
E= -4585.757241
Mo -1.365181 -0.713374 0.007360
S 0.000036 0.089013 -1.774044
Mo -0.000060 1.724342 -0.079413
Mo 1.365280 -0.713272 0.007373
S 0.000088 -1.967380 1.396414
S 2.726036 -2.024462 -1.362459
S 3.485216 -2.024730 0.581771
S 2.576130 1.543776 -0.166443
S -2.576268 1.543520 -0.166598
S -1.629103 1.132236 1.611506
S 1.628918 1.132329 1.611606
S -2.725977 -2.024630 -1.362397
S -3.485060 -2.024819 0.581870
S -0.000120 3.843695 -0.781443

E= -4585.719150
Mo -1.351007 -0.722326 0.021122
S -0.000009 -0.036408 -1.835681
Mo -0.000002 1.754880 -0.224733
Mo 1.351023 -0.722316 0.021103
S 0.000017 -1.788542 1.572816
S 2.649316 -2.197209 -1.234251
S 3.446813 -2.032347 0.689350
S 2.502177 1.476092 -0.423060
S -2.502170 1.476086 -0.423064
S -1.686919 1.242942 1.489508
S 1.686890 1.242960 1.489502
S -2.649362 -2.197138 -1.234269
S -3.446805 -2.032364 0.689361
S 0.000016 4.031556 -0.301130

E= -4585.689987
Mo -1.585449 -0.607493 0.038844
S -0.002260 -0.200272 -1.753315
Mo 0.135203 1.709177 -0.247186
Mo 1.381460 -0.845040 0.100126
S -0.063571 -1.853725 1.509409
S 2.667297 -2.316489 -1.222798
S 3.512501 -1.978733 0.658775
S 2.622742 1.323509 -0.431941
S -2.397841 1.696077 -0.556907
S -1.711071 1.475295 1.406563
S 1.785181 1.165575 1.465145
S -2.854622 -2.375636 -1.072501
S -3.712976 -1.580121 0.652494
S 0.335187 3.970724 -0.370855

[Mo3S11]2- XIV
E= -4585.808376
Mo 0.578235 -0.608465 -0.000414
S 1.870695 -0.152527 1.810626
Mo 3.219936 0.503272 0.000068
S 1.871413 -0.152689 -1.810983
S 3.253570 2.635044 -0.000022
S -1.247638 0.781695 -0.000864
S -3.951192 2.326316 -0.001063
Mo -3.559356 -0.066237 0.000196
S -5.638344 1.111708 0.000377
S -3.652730 -1.275704 -1.760435
S -3.651604 -1.273937 1.762103
S 0.169731 -2.705652 -0.000389
S 5.174387 -0.422066 1.046957
S 5.174821 -0.422183 -1.045914

E= -4585.784099
Mo -0.255304 0.514164 -0.031109
S -1.259701 -0.943039 1.397468
Mo -2.940113 -0.376065 -0.163065
S -2.001306 1.506397 -1.182604
S -3.062176 -1.965388 -1.579785
S 1.204234 -0.450644 -1.524573
S 3.907353 -2.304334 -0.175533
Mo 3.136264 -0.054614 -0.205129
S 4.073485 -1.284873 1.328482
S 4.454087 1.305840 -1.196199
S 1.881686 1.143482 1.503806
S 0.649255 2.594148 0.619324
S -4.618501 -0.576597 1.547043
S -5.073139 0.755860 -0.005589

E= -4585.713681
Mo 0.229446 1.016431 -0.202762
S -1.116175 0.298724 1.532180
Mo -2.727416 -0.704428 0.035274
S -1.763493 0.501624 -1.647734
S -2.247090 -2.785875 -0.100699
S 1.456508 -0.432280 -1.624404
S 1.968288 0.160885 1.656025
Mo 3.216562 -0.887152 -0.170054
S 3.971303 0.787104 1.311064
S 4.188411 -2.806672 -0.386156
S 1.439307 3.050170 0.148614
S -0.238431 3.153018 -1.076267
S -4.491802 -0.016921 1.529868
S -5.053130 -0.400012 -0.456445

[Mo3S11]2- XV
E= -4585.815454
Mo 2.888239 -0.507830 0.000022
S 1.532510 -0.080038 1.776447
S 1.532638 -0.079380 -1.776365
S 3.287467 -2.606581 -0.000063
Mo 0.013373 0.564465 0.000083
S -1.505713 -0.113383 1.754548
S -4.431122 -1.571265 1.047676
S -3.883337 1.950684 0.000003
Mo -2.952272 0.030694 0.000069
S 4.742221 0.637572 1.047434
S 4.741915 0.638234 -1.047425
S 0.052786 2.679396 0.000099
S -1.505574 -0.113294 -1.754320
S -4.430806 -1.571184 -1.048184

E= -4585.784097
Mo -2.939107 -0.376409 -0.163870
S -2.002608 1.509683 -1.179148
S -1.257572 -0.944700 1.394960
S -3.059873 -1.962774 -1.584011
Mo -0.255308 0.517535 -0.030041
S 1.203534 -0.442810 -1.526925
S 3.902966 -2.306758 -0.178652
S 4.458879 1.303831 -1.190718
Mo 3.135909 -0.055637 -0.205192
S -5.073258 0.753271 -0.003138
S -4.616055 -0.581333 1.546875
S 0.652911 2.597180 0.619800
S 1.879696 1.141825 1.503856
S 4.064958 -1.291825 1.644747

E= -4585.738391
Mo -2.937784 0.353628 0.251167
S -2.130948 -1.818206 0.567014
S -1.154853 1.348783 -0.934188
S -3.077605 1.335393 2.138998
Mo -0.289059 -0.578307 -0.088947
S 1.118488 -0.298121 1.707682
S 3.619977 2.092866 0.443723
S 4.644188 -1.528489 0.936524
Mo 3.015667 -0.244392 0.312197
S -5.098929 -0.526799 -0.383411
S -4.510097 1.246513 -1.332040
S 0.524983 -2.312534 -1.464235
S 1.908815 -0.732525 -1.724245
S 4.710319 2.424430 -1.201167

[Mo3S11]2- XVI
E= -4585.693231
S -3.176369 1.088348 2.109888
Mo -2.967692 0.400703 0.050377
S -3.677481 2.040620 -1.158204
S -0.815598 0.596507 -1.415914
Mo 1.107725 -0.230964 0.068964
S 2.568109 -0.967646 -1.623035
Mo 3.884115 -0.151316 0.046882
S 2.548722 0.146910 1.873878
S 0.327341 1.949239 -0.338962
S -4.674241 -1.203838 -0.013229
S -3.092415 -1.720333 -1.256359
S -0.902295 -0.880669 1.475289
S 0.057553 -2.300963 0.295623
S 5.523287 1.203467 -0.385310

E= -4585.699766
S 3.229572 -1.081051 2.099679
Mo 2.996928 -0.380641 0.046438
S 3.737822 -1.995422 -1.178497
S 0.838604 -0.625603 -1.402587
Mo -1.094362 0.201232 0.067560
S -2.517717 0.805253 -1.668866
Mo -3.929682 0.163117 0.023037
S -2.560767 -0.204202 1.823359
S -0.267219 -1.980853 -0.289532
S 4.665188 1.263641 -0.013746
S 3.071864 1.747022 -1.255620
S 0.923628 0.848904 1.491847
S -0.071427 2.281419 0.352862
S -5.728369 -1.016342 -0.318618

E= -4585.661657
S 3.581791 -1.740244 1.533530
Mo 2.878898 -0.211818 -0.022348
S 3.498201 -1.939851 -1.323461
S 0.840891 0.006947 -1.607017
Mo -1.093681 0.147245 0.108211
S -2.539206 1.417817 -1.179167
Mo -3.923373 0.138197 0.138117
S -2.512495 -0.917604 1.604391
S -0.288337 -1.670927 -1.130453
S 4.661460 1.250287 0.149651
S 3.103087 2.157806 -0.898012
S 1.006782 0.142137 1.675882
S -0.004811 1.905116 1.198553
S -5.734703 -0.804746 -0.611844

[Mo3S11]2- XVII
E= -4585.701778
S -0.230056 -1.589410 0.305698
Mo 0.893638 0.406534 0.040876
S 2.387430 0.417516 1.876534
Mo 3.581852 -0.154792 0.043300
S 2.426725 0.534108 -1.783300
Mo -2.441404 -0.527830 -0.200717
S -3.386337 -2.166081 -1.191715
S -4.233380 0.340600 1.201164
S -2.853941 -0.894421 2.128286
S -1.009494 0.303955 -1.951408
S -2.737146 1.387304 -1.638622
S 0.225702 2.688349 0.027357
S -0.895809 1.537178 1.334688
S 4.966832 -1.834365 -0.002762

E= -4585.706130
S 0.314883 -1.501109 -0.688165
Mo -0.874024 0.366270 0.028376
S -2.352900 0.684854 -1.732184
Mo -3.692223 -0.110762 -0.050416
S -2.343919 -0.066303 1.806461
Mo 2.492005 -0.546182 0.083389
S 3.470913 -2.349648 0.678209
S 4.283379 0.648723 -1.063461
S 2.925970 -0.356355 -2.261295
S 1.042907 -0.152420 1.965900
S 2.756685 0.994750 1.921147
S -0.246108 2.600728 0.536229
S 0.924438 1.779089 -0.966861
S -5.331364 -1.519286 -0.357023

E= -4585.696044
S -0.800060 -0.861369 1.355988
Mo 0.757748 0.272903 -0.039377
S 2.415430 0.190382 1.885756
Mo 3.730665 -0.481474 0.185265
S 2.205991 -1.038550 -1.455572
Mo -2.780112 -0.500531 -0.023708
S -3.600290 -2.428806 -0.371934
S -4.849491 0.780541 0.487831
S -3.502178 0.388203 2.021161
S -1.035746 -0.344357 -1.763670
S -2.721103 0.876917 -1.932236
S 1.482643 2.390839 -1.029145
S 0.014847 2.498628 0.418075
S 5.905668 -0.591036 0.063023

[Mo3S11]2- XVIII
E= -4585.693231
S -3.176293 1.088795 2.109622
Mo -2.967684 0.400687 0.050284
S -3.678362 2.039914 -1.158729
S -0.815212 0.597808 -1.415152
Mo 1.107929 -0.230930 0.069339
S 2.567270 -0.966804 -1.623532
Mo 3.884081 -0.151857 0.046523
S 2.549122 0.146071 1.874015
S 0.327329 1.949750 -0.336687
S -4.672999 -1.205001 -0.013120
S -3.091645 -1.720109 -1.257360
S -0.902555 -0.881022 1.475383
S 0.057758 -2.300867 0.295591
S 5.521734 1.204479 -0.386163

E= -4585.699761
S 3.229050 -1.082350 2.098983
Mo 2.997084 -0.380232 0.046219
S 3.738813 -1.993610 -1.180056
S 0.838694 -0.625943 -1.403382
Mo -1.094274 0.200339 0.067009
S -2.518019 0.805125 -1.668806
Mo -3.929719 0.163272 0.023492
S -2.560223 -0.205554 1.823078
S -0.266258 -1.981473 -0.289856
S 4.664726 1.264700 -0.011043
S 3.072382 1.747917 -1.254257
S 0.923374 0.847997 1.491387
S -0.071897 2.280687 0.353006
S -5.730006 -1.013867 -0.317945

E= -4585.669509
S 3.228025 -1.728326 1.763887
Mo 2.919772 -0.447792 0.047528
S 4.172049 -1.232762 -1.635180
S 0.851916 -0.800847 -1.426078
Mo -1.094624 0.128865 0.076774
S -2.460694 0.816967 -1.674479
Mo -3.920471 0.223709 -0.003803
S -2.584427 -0.182381 1.818609
S -0.345290 -2.055651 -0.279608
S 4.409244 1.416441 0.412479
S 3.043041 2.047325 -0.899605
S 0.910929 0.698582 1.569188
S 0.023884 2.170755 0.403823
S -5.748454 -0.900153 -0.369344

[Mo3S11]2- XIX
E= -4585.696986
S 0.541689 -0.402458 -1.534618
Mo -0.960426 0.687499 -0.084805
S -2.616393 0.547206 -1.906653
Mo -3.324132 -0.461897 -0.044555
S -2.476057 0.379987 1.837876
Mo 2.482515 -0.649982 -0.069372
S 3.163261 -2.635387 -0.376141
S 4.559149 0.650839 0.041968
S 3.431904 0.765127 -1.701053
S 0.549883 -0.948518 1.347367
S 2.245577 -0.192979 2.270555
S 0.292288 2.491303 1.137666
S -0.904756 2.970218 -0.478359
S -4.056183 -2.511338 -0.116937

E= -4585.700087
S -0.795393 -0.855692 1.163096
Mo 0.890565 0.399715 0.090345
S 2.213406 -0.858934 1.767978
Mo 3.545018 -0.750165 -0.062876
S 2.024863 -0.367635 -1.793080
Mo -2.792464 -0.441030 -0.131021
S -3.400655 -2.240076 -1.085929
S -4.902265 0.544468 0.629342
S -3.701186 -0.362801 2.065542
S -0.982190 0.210831 -1.763670
S -2.667171 1.428684 -1.539816
S 0.367296 2.754579 -0.259679
S 1.817822 2.292341 1.167375
S 5.712286 -0.468131 -0.127037

E= -4585.689943
S 0.584264 -0.448885 -1.388612
Mo -0.763907 0.816569 0.072008
S -2.561441 0.434624 -1.747100
Mo -3.655310 -0.617248 -0.102928
S -2.320496 -0.003403 1.693970
Mo 2.607415 -0.729091 -0.063227
S 3.117230 -2.794659 -0.215982
S 4.877708 0.272036 -0.317335
S 3.497262 0.488380 -1.856727
S 0.839603 -0.675604 1.610487
S 2.692941 0.090785 2.158906
S 0.509737 2.684937 0.904929
S -0.961710 3.096627 -0.513914
S -5.519119 -1.754192 -0.081483

[Mo3S10]- I

E= -4187.552526
S 1.746554 0.000770 1.797439
Mo 2.947205 -0.529886 -0.015520
S 3.680353 -2.533937 0.108083
Mo 0.000062 0.588912 0.000112
S -1.746715 0.000836 -1.797614
Mo -2.947116 -0.529947 0.015447
S -1.334298 -0.376551 1.659332
S 1.334361 -0.376435 -1.659345
S -0.785870 2.687994 -0.655622
S 0.785359 2.688401 0.655700
S 4.553043 0.839639 -0.377592
S -3.680156 -2.534029 -0.108074
S -4.553028 0.839477 0.377588

E= -4187.536963
S 1.229261 -0.689790 1.553334
Mo 2.889293 -0.576731 -0.036572
S 3.384689 -2.537480 -0.727779
Mo -0.000090 0.574238 0.000092
S -1.228876 -0.690289 -1.553031
Mo -2.889202 -0.576872 0.036541
S -1.876792 0.666888 1.619691
S 1.877005 0.667726 -1.619241
S -0.625187 2.895649 -0.767295
S 0.624708 2.895647 0.767352
S 4.617113 0.424466 0.734320
S -3.385808 -2.537472 0.727336
S -4.616118 0.425485 -0.734846

[Mo3S10]- II
E= -4187.492880
S 3.408633 0.256023 -0.000236
Mo 1.880479 -1.510685 -0.015307
S 2.093770 -2.651228 1.779575
Mo 1.478525 1.412396 0.006481
S -0.077986 -0.238500 -0.017365
Mo -2.574689 -0.459310 0.019398
S -2.755400 -1.514693 1.863508
S 1.348985 3.475151 1.074620
S 1.350090 3.501717 -1.009490
S 2.105041 -2.630756 -1.821999
S -2.786919 -1.783979 -1.637378
S -2.425768 1.944255 -0.181456
S -4.319274 1.105706 -0.077531

E= -4187.516650
S -2.597316 0.736014 -1.153814
Mo -2.117906 -1.101647 0.177017
S -2.031409 -2.856803 -1.024334
Mo -0.556595 1.424461 -0.343674
S -0.074036 -0.512248 1.156622
Mo 2.086630 -0.718650 -0.146981
S 1.247841 0.908055 -1.654685
S -0.631347 3.812737 -0.601010
S -0.398990 3.073742 1.311334
S -3.576425 -1.278088 1.724747
S 2.130319 -2.657357 -0.987879
S 3.226690 -0.340884 1.902212
S 4.247834 0.153902 0.150107

[Mo3S10]- III
E= -4187.474560
S 1.735465 -0.453741 1.729190
Mo 3.285582 -0.696162 0.142272
S 3.775900 -2.698828 -0.421500
Mo 1.007391 0.895986 -0.081584
S -0.556437 -0.193386 -1.189291
Mo -2.696433 -0.708230 0.031333
S -2.067713 -0.839914 2.064218
S 2.877665 0.744588 -1.521069
S 0.924408 3.242192 -0.458971
S 0.287035 2.559829 1.389778
S -2.959282 -2.657093 -0.800168
S -3.390750 1.313980 -1.078893
S -4.817237 0.316938 0.045152

E= -4187.473804
S -1.567427 -1.037462 -1.430871
Mo -3.047008 -0.748681 0.193160
S -5.147231 -1.049712 -0.106797
Mo -0.286888 0.537608 -0.018780

S41

S 0.807304 -0.375287 1.743193
Mo 2.314004 -0.614249 -0.033283
S 1.345080 0.593986 -1.741672
S -2.312239 0.711287 1.628886
S 0.044003 2.940623 0.312841
S -1.325537 2.639840 -1.097510
S 2.317131 -2.666145 -0.575942
S 4.101037 -0.023833 1.446410
S 4.415096 0.433173 -0.548920

[Mo3S10]- IV
E= -4187.552526
S 1.746542 0.000731 1.797436
Mo 2.947211 -0.529881 -0.015523
S 3.680372 -2.533929 0.108049
Mo 0.000060 0.588902 0.000117
S -1.746691 0.000809 -1.797610
Mo -2.947119 -0.529945 0.015445
S -1.334317 -0.376543 1.659343
S 1.334378 -0.376400 -1.659354
S -0.785875 2.687983 -0.655610
S 0.785345 2.688390 0.655721
S 4.553044 0.839662 -0.377558
S -3.680173 -2.534022 -0.108069
S -4.553025 0.839495 0.377553

E= -4187.536963
S 1.229262 -0.689789 1.553335
Mo 2.889293 -0.576729 -0.036572
S 3.384691 -2.537478 -0.727779
Mo -0.000090 0.574237 0.000093
S -1.228874 -0.690292 -1.553030
Mo -2.889200 -0.576872 0.036541
S -1.876789 0.666884 1.619693
S 1.877004 0.667725 -1.619242
S -0.625191 2.895645 -0.767297
S 0.624703 2.895648 0.767351
S 4.617113 0.424469 0.734319
S -3.385814 -2.537471 0.727334
S -4.616113 0.425491 -0.734847

[Mo3S10]- V
E= -4187.474560
S 1.734956 -0.454510 1.728837
Mo 3.285401 -0.696467 0.142177
S 3.776542 -2.698835 -0.422055
Mo 1.007423 0.896170 -0.081494
S -0.556743 -0.192411 -1.189491
Mo -2.696546 -0.708246 0.031126
S -2.067645 -0.840882 2.063889
S 2.877901 0.744898 -1.520705
S 0.924999 3.242539 -0.458275
S 0.287687 2.559808 1.390374
S -2.959163 -2.656737 -0.801333
S -3.391283 1.314464 -1.077963
S -4.817478 0.316594 0.045723

E= -4187.473554
S -1.848176 -0.891823 -1.553171
Mo -3.307607 -0.349262 0.020330
S -4.993892 -1.604048 0.413130
Mo -0.388147 0.481622 -0.072384
S 0.837199 -0.425475 1.642345
Mo 2.474032 -0.632284 -0.052059
S 1.316065 0.124399 -1.826280
S -2.270782 0.620050 1.675538
S 0.125083 2.786312 0.313111
S -1.217939 2.523648 -1.174246
S 2.769734 -2.726956 -0.236648
S 3.899597 0.541386 1.486988
S 4.590133 0.364409 -0.467473

[Mo3S10]- VI
E= -4187.552459
S -1.898494 0.509488 -1.821711
Mo -3.151595 -0.178908 -0.002164
S -4.021160 -2.092183 -0.414078
Mo -0.302931 0.276171 -0.161838
S 0.898063 -1.418902 -1.059816
Mo 2.573976 -0.357177 0.215290
S -1.555575 -0.291016 1.676584
S 1.393103 1.459535 1.280560

S 0.597553 2.442023 -0.373626
S -4.607791 1.300476 0.533502
S 2.937924 -1.543818 1.927309
S 4.404516 1.018560 -0.367816
S 4.163302 -0.701889 -1.515540

E= -4187.525770
S 1.868062 -0.423574 1.633523
Mo 3.429774 -0.192441 -0.075460
S 4.265546 -2.080229 -0.625237
Mo 0.406359 0.313241 0.000001
S -0.982349 -1.255028 -0.912199
Mo -2.960630 -0.441391 0.136546
S 2.065841 0.648123 -1.693379
S -0.564831 2.424904 0.068603
S -1.526228 1.163748 1.443206
S 4.964758 1.192034 0.470361
S -3.580723 -1.711562 1.719002
S -4.432346 -0.433074 -1.705312
S -4.375924 1.316209 -0.562119

[Mo3S10]- VII
E= -4187.560121
S -1.759185 0.042506 1.746465
Mo -3.171435 0.271932 0.000024
S -4.076279 2.217122 0.000070
Mo -0.148625 -0.620159 0.000001
S 1.283272 -0.017076 -1.799893
Mo 2.556877 0.516237 -0.000091
S 1.283184 -0.016591 1.799783
S -1.759122 0.042556 -1.746398
S -0.123120 -2.726704 0.000169
S -4.667087 -1.265613 -0.000114
S 2.869511 2.612258 -0.000439
S 4.476020 -0.665089 -1.000211
S 4.476160 -0.664394 1.000742

E= -4187.522020
S -1.478057 -0.770434 -1.484258
Mo -3.156233 -0.321899 0.024082
S -3.851674 -2.099629 0.989727
Mo -0.203424 0.543884 -0.020322
S 1.031463 -0.479796 1.596427
Mo 2.652892 -0.410717 -0.132225
S 1.540276 0.958066 -1.596630
S -2.070896 1.005292 1.516727
S -0.365198 2.813494 -0.048088
S -4.765029 0.717621 -0.926080
S 2.755866 -2.383314 -0.890942
S 4.200311 0.292736 1.562631
S 4.858196 0.441385 -0.382293

[Mo3S10]- VIII
E= -4187.546043
Mo 0.488288 -0.049416 0.037287
Mo -2.516095 0.038368 0.031410
S -0.994458 -0.542237 -1.630795
S -0.799822 0.358006 1.805627
S -2.791148 2.349054 0.297692
S -4.166237 1.420362 -0.925527
S -3.413301 -1.628237 1.309461
S -4.047974 -1.813553 -0.658460
S 1.891194 -1.782509 0.404338
Mo 3.350182 -0.015533 -0.058445
S 4.485318 -0.438398 -1.826280
S 4.543639 0.441474 1.661166
S 1.821554 1.705815 -0.463993

E= -4187.521942
Mo 0.412610 -0.000762 -0.001718
Mo -2.475125 -0.000113 0.000393
S -0.944151 0.727185 -1.633632
S -0.942143 -0.728783 1.631828
S -3.416849 1.743450 1.307206
S -4.120649 1.713520 -0.611906
S -4.120920 -1.712415 0.614680
S -3.421966 -1.741390 -1.306286
S 1.926955 -1.580548 -0.713227
Mo 3.489401 0.000106 0.000444
S 4.685925 0.719255 -1.616037
S 4.683271 -0.718646 1.619054
S 1.924954 1.580392 0.710632

[Mo3S10]- IX
E= -4187.554071
S -3.848113 -1.810452 1.284209
Mo -3.073474 -0.294632 -0.000269
S -1.975240 1.203235 1.473726
S -1.035764 2.500763 0.127251
Mo -0.109795 0.351657 -0.113147
Mo 2.625140 -0.351376 -0.102548
S 2.927517 -2.245488 -1.001357
S -4.566869 0.673616 -1.179178
S -1.352122 -1.137559 -1.322078
S 1.021627 -0.605905 1.596017
S 1.467310 0.990361 -1.634668
S 4.529700 1.071765 -0.309634
S 4.297043 0.132338 1.532620

E= -4187.519279
S -4.006300 -1.847895 1.224402
Mo -3.175006 -0.295292 -0.009671
S -2.090845 1.274597 1.358021
S -0.902806 2.543554 0.107490
Mo -0.081787 0.357003 -0.076642
Mo 2.613927 -0.375057 -0.102558
S 2.845430 -2.293638 -0.965030
S -4.674889 0.709066 -1.177678
S -1.364217 -1.148613 -1.221883
S 1.105042 -0.518201 1.667180
S 1.573066 1.053338 -1.571957
S 4.760780 0.851521 -0.389575
S 4.442261 0.198803 1.464815

[Mo3S10]- X
E= -4187.517838
S -1.104054 -0.029085 -1.794588
Mo 0.186291 -0.284259 0.049583
S 1.497178 1.798033 -0.646017
Mo 3.074965 0.332471 -0.028774
S 2.198493 -0.288871 1.908572
Mo -2.541882 0.408036 -0.008005
S -2.961236 2.485050 -0.036633
S -4.249416 -0.884091 1.034111
S -4.252624 -0.888071 -1.046518
S -1.130805 0.061614 1.833644
S 0.724704 -2.546524 0.005947
S 2.180633 -1.501600 -1.182087
S 5.208771 0.595893 -0.110043

E= -4187.473553
S 1.316243 0.125666 -1.826265
Mo -0.388238 0.481601 -0.072364
S -1.847908 -0.892037 -1.553037
Mo -3.307549 -0.349063 0.020170
S -2.270939 0.620375 1.675446
Mo 2.474031 -0.632176 -0.052298
S 2.769782 -2.726753 -0.237874
S 3.899080 0.540819 1.487896
S 4.590194 0.364713 -0.466384
S 0.836849 -0.426203 1.641973
S 0.124578 2.786477 0.313095
S -1.218238 2.523806 -1.174308
S -4.992531 -1.605311 0.413750

[Mo3S10]- XI
E= -4187.517101
S 3.212019 -2.500064 -0.566841
Mo 2.821502 -0.543044 0.189916
S 2.104126 0.744092 -1.697233
S 1.344611 2.463670 -0.747585
Mo 0.179704 0.536373 -0.133480
Mo -2.532877 -0.112537 -0.083159
S -3.844749 -1.398834 1.322460
S -4.266175 -1.695463 -0.718013
S 4.506276 0.410380 1.102428
S 1.040709 -0.542436 1.682428
S -0.961765 -0.894196 -1.541699
S -1.478293 1.541117 1.337142
S -2.886123 2.184655 -0.102939

E= -4187.492867
S 3.553710 -2.467135 -0.385737
Mo 3.048354 -0.469964 0.188838

S 2.123314 0.462635 -1.813948
S 1.296868 2.262220 -1.103778
Mo 0.345246 0.372808 -0.093943
Mo -2.876898 -0.089276 -0.097764
S -4.267899 -1.443539 1.158759
S -4.902590 -1.131843 -0.823690
S 4.708844 0.714341 0.839994
S 1.376361 -0.456510 1.789998
S -1.114520 -0.979860 -1.298121
S -1.311310 1.334053 1.436368
S -2.819122 2.195023 0.207684

[Mo3S10]- XII
E= -4187.559999
Mo 0.065457 -0.010969 0.029330
Mo -2.937104 0.258629 -0.005503
S -1.312113 0.528338 -1.700331
S -1.384524 -0.534942 1.668526
S -4.206326 -1.715925 0.396793
S -4.719393 -0.633767 -1.283792
S -3.612972 2.134951 0.692576
S 1.360410 -1.740642 -0.573600
S 1.412291 1.697796 0.567710
Mo 2.886919 -0.109654 0.192810
S 3.552487 -0.746918 2.102565
S 4.419777 -0.666574 -1.542001
S 4.450273 1.315418 -0.897118

E= -4187.526657
Mo -0.000294 0.005302 0.025567
Mo -3.033904 -0.151684 0.162940
S -1.435975 1.245697 1.272070
S -1.501774 -1.147998 -1.281705
S -4.909337 0.108348 -1.277546
S -4.275195 1.826207 -0.316555
S -3.726752 -1.529772 1.617391
S 1.456319 1.274746 -1.225144
S 1.475273 -1.271664 1.178898
Mo 3.036526 -0.118386 -0.228660
S 3.749069 -1.564492 -1.606989
S 4.871499 1.373906 0.011916
S 4.290762 0.380036 1.733066

[Mo3S10]- XIII
E= -4187.524031
S -1.348678 -0.323331 -1.796104
Mo -2.725636 0.351717 -0.000054
S -4.592191 -0.709607 1.043514
S -4.592350 -0.709603 -1.043496
Mo 0.022475 -0.320838 -0.000008
S 1.746563 -1.813062 1.037388
S 1.746735 -1.813550 -1.036473
Mo 2.837687 0.109179 0.000179
S -1.348558 -0.322688 1.796152
S 1.194242 1.661562 -0.000314
S -2.907725 2.463277 -0.000179
S 4.874582 0.600369 1.054468
S 4.874247 0.598983 -1.055264

E= -4187.495224
S 1.156945 0.076658 1.736804
Mo 2.740240 0.380794 0.020086
S 4.691108 -0.836176 -0.616697
S 4.441902 -0.523836 1.429470
Mo 0.006278 -0.294885 -0.175537
S -0.922522 -2.426978 -0.617919
S -1.887971 -1.548013 1.034104
Mo -2.988121 0.237052 0.021697
S 1.580240 -0.485282 -1.824521
S -1.258307 1.507018 -0.833501
S 2.985332 2.465297 -0.273830
S -5.189761 -0.048764 -0.753164
S -4.962760 0.972304 1.070358

[Mo3S10]- XIV
E= -4187.483783
S 0.554905 -1.454579 -0.092910
Mo 2.617162 -0.242818 0.403438
S 2.593633 2.109145 0.243677
S 0.890365 1.351742 1.166950
Mo -0.888693 0.375167 -0.438847
S -0.522087 1.647711 -2.091532

S -2.379842 -1.286904 -1.357029
Mo -3.666114 -0.069092 -0.023512
S -4.975898 -1.238079 1.197837
S -2.392971 1.382684 1.107353
S 3.318762 -0.959499 2.258474
S 4.646811 -0.075260 -0.934906
S 3.352640 -1.643012 -1.343246

E= -4187.475694
S 0.679492 1.108730 -1.071225
Mo 2.697534 -0.152415 -0.429820
S 2.589595 -1.748503 1.305211
S 0.904360 -1.768962 0.095806
Mo -0.774830 0.183024 0.479269
S -0.233027 0.579032 2.491278
S -2.433551 1.820827 -0.144427
Mo -3.805469 0.006262 -0.223006
S -5.874409 -0.152611 -0.774707
S -2.289807 -1.660550 0.205972
S 3.443372 -0.950191 -2.230720
S 4.695003 0.621741 0.714017
S 3.461232 2.053703 -0.135616

[Mo3S10]- XV
E= -4187.474560
Mo -1.007746 0.896353 -0.081584
S -1.735161 -0.453062 1.729641
Mo -3.285004 -0.696893 0.142570
S -2.877876 0.743839 -1.520982
S -0.925752 3.242494 -0.459671
S -0.287393 2.560882 1.389014
S 0.556267 -0.192897 -1.189209
Mo 2.696293 -0.708205 0.031196
S 3.391139 1.314235 -1.078280
S 4.816893 0.317292 0.046815
S 2.959310 -2.656538 -0.801561
S 2.066640 -0.840834 2.063688
S -3.773371 -2.699957 -0.421432

E= -4187.473856
Mo 0.285061 0.577573 -0.023094
S 1.614735 -0.809774 -1.574481
Mo 3.150410 -0.451584 -0.014644
S 2.312944 0.700245 1.630704
S -0.168343 2.924840 0.459365
S 1.204778 2.794679 -0.977130
S -0.714222 -0.514378 1.694603
Mo -2.274557 -0.670540 -0.042254
S -4.026589 -0.201804 1.523026
S -4.409238 0.369728 -0.427488
S -2.261903 -2.685621 -0.704323
S -1.385877 0.650554 -1.708547
S 4.786318 -1.799021 0.294250

[Mo3S10]- XVI
E= -4187.483783
S 0.554905 -1.454579 -0.092910
Mo 2.617162 -0.242818 0.403438
S 2.593633 2.109145 0.243677
S 0.890365 1.351742 1.166950
Mo -0.888693 0.375167 -0.438847
S -0.522087 1.647711 -2.091532
S -2.379842 -1.286904 -1.357029
Mo -3.666114 -0.069092 -0.023512
S -4.975898 -1.238079 1.197837
S -2.392971 1.382684 1.107353
S 3.318762 -0.959499 2.258474
S 4.646811 -0.075260 -0.934906
S 3.352640 -1.643012 -1.343246

E= -4187.475694
S 0.679492 1.108730 -1.071225
Mo 2.697534 -0.152415 -0.429820
S 2.589595 -1.748503 1.305211
S 0.904360 -1.768962 0.095806
Mo -0.774830 0.183024 0.479269
S -0.233027 0.579032 2.491278
S -2.433551 1.820827 -0.144427
Mo -3.805469 0.006262 -0.223006
S -5.874409 -0.152611 -0.774707
S -2.289807 -1.660550 0.205972
S 3.443372 -0.950191 -2.230720

S 4.695003 0.621741 0.714017
S 3.461232 2.053703 -0.135616

[Mo3S10]- XVII
E= -4187.383309
S -2.428344 0.400584 2.097777
Mo -2.936908 0.310030 0.033634
S -2.937513 -1.746558 -1.276243
S -4.656451 -1.275580 -0.220392
S -3.673561 2.194903 -0.660696
S -0.732073 0.315742 -1.118484
S 0.427267 1.903693 -0.475560
Mo 1.521852 -0.022871 0.242393
S 0.659408 -2.104590 1.183967
S 1.525338 -0.728695 2.447008
S 2.320785 -1.295158 -1.762253
Mo 3.745258 0.026861 -0.707766
S 3.378364 1.511357 0.918191

E= -4187.438164
S 2.215878 -0.551570 -2.123441
Mo 3.044955 -0.018471 -0.231769
S 2.868100 -1.396788 1.772257
S 4.428927 -1.786346 0.466801
S 4.262864 1.729162 -0.394473
S 1.122269 0.970252 1.011222
S 0.121867 2.411825 -0.111395
Mo -1.244218 0.504291 0.148517
S -1.192255 -1.390059 -1.111592
S -3.256184 -2.053279 -1.109589
S -2.372079 -0.184264 2.085432
Mo -3.741552 -0.257214 0.219408
S -3.104745 1.650975 -0.842630

[Mo3S10]- XVIII
E= -4187.474560
S 2.067079 -0.841979 -2.063610
Mo 2.696421 -0.708276 -0.031049
S 4.817381 0.316473 -0.046619
S 3.391565 1.314833 1.077114
S 2.959186 -2.656338 0.802340
S 0.556798 -0.191770 1.189687
Mo -1.007675 0.896437 0.081793
S -0.287457 2.560111 -1.389731
S -0.925508 3.242806 0.458719
S -1.734901 -0.453609 -1.729035
Mo -3.285217 -0.696736 -0.142425
S -3.775250 -2.699644 0.420803
S -2.878157 0.744126 1.521000

E= -4187.414414
S 3.582768 1.936206 -0.565774
Mo 3.330916 -0.149612 -0.203443
S 5.037821 -1.671914 -0.733629
S 4.684390 -1.342180 1.321421
S 1.086838 -0.895592 -0.325583
S 0.063375 -0.837784 1.565806
Mo -1.117731 0.589754 0.246050
S -0.018855 2.480462 -0.837276
S -1.209837 2.812543 0.815577
S -2.001652 -0.121132 -1.821792
Mo -3.621540 -0.505269 -0.321535
S -4.498970 -2.455359 -0.363176
S -3.028947 0.265710 1.676414

[Mo3S10]- XIX
E= -4187.486848
S 3.117365 -1.595843 1.267383
Mo 3.204895 -0.034472 -0.176245
S 2.617195 2.276048 0.312079
S 4.568982 1.681702 0.673118
S 4.106906 -0.724919 -1.986869
S 0.869396 0.164223 -1.067479
S -0.052079 -1.672670 -1.364293
Mo -1.118616 -0.478399 0.363389
S -0.529300 -0.942583 2.328907
S -1.973843 1.733160 0.314175
Mo -3.782350 0.427732 0.150574
S -5.147413 1.007777 -1.389585
S -3.125022 -1.703403 0.026053

E= -4187.472660

S 3.178747 -1.352267 1.562014
Mo 3.335379 -0.036567 -0.103539
S 2.788320 2.334543 0.007170
S 4.717802 1.764976 0.499738
S 4.246740 -1.019945 -1.767776
S 1.028183 0.094098 -1.060478
S 0.112274 -1.769110 -1.221107
Mo -1.059409 -0.431675 0.307504
S -0.363993 -0.513038 2.293550
S -2.079504 1.625376 -0.219284
Mo -4.005530 0.341651 -0.141332
S -6.057138 0.899690 -0.417577
S -3.031337 -1.732021 0.159336

[Mo3S10]- XX
E= -4187.408869
S -0.482000 -1.630999 -0.208168
Mo 0.632221 0.260913 0.450991
S 2.246534 -1.269760 1.414822
Mo 3.365554 -0.165149 -0.136541
S 2.095508 1.451243 -1.004359
Mo -2.508848 -0.341261 -0.419805
S -4.773920 -0.559816 0.122743
S -3.601565 -2.216172 0.536354
S -1.083415 0.972350 -1.754714
S -2.868819 1.862182 -1.244190
S -0.310995 2.378473 1.257801
S 0.281625 0.961388 2.633795
S 4.588613 -1.304457 -1.477526

E= -4187.457104
S -0.300236 -0.129850 -1.697506
Mo 0.812308 -0.599796 0.151572
S 2.723281 -1.775322 -0.563168
Mo 3.462370 0.211954 0.175109
S 1.757403 1.254520 1.213454
Mo -2.294909 0.254823 -0.204046
S -4.499580 -0.432547 -0.263917
S -3.237651 -1.646600 -1.379472
S -1.929225 2.521767 -0.607329
S -2.977911 2.194107 1.149271
S -1.225550 -0.631997 1.690207
S -0.138578 -2.406740 1.303297
S 4.631153 1.401837 -1.166751

[Mo3S10]- XXI
E= -4187.470672
S -0.128680 -1.915884 -1.377999
Mo 1.489598 -0.728830 -0.433485
S 2.026909 1.250511 -1.525319
Mo 0.603300 1.486165 0.307851
S 1.664228 1.940019 2.101046
Mo -1.736872 -0.511486 -0.190999
S -2.983777 -0.170752 -1.863846
S -2.963166 -0.715169 1.829216
S -2.268803 -2.473004 0.986633
S -0.883351 2.962053 -0.909277
S -1.741309 1.840084 0.620099
S 2.541077 -2.000957 1.238584
S 3.802304 -1.362255 -0.267973

E= -4187.375736
S 0.335780 -0.141663 -1.640356
Mo -1.180725 0.389556 0.042970
S -2.807452 0.692227 -1.745857
Mo -3.648851 -0.858565 -0.319357
S -2.598208 -0.669838 1.684613
Mo 2.321007 -0.465930 -0.214206
S 3.289873 -2.139806 -1.054967
S 4.072960 1.081484 0.368163
S 3.020503 1.468861 -1.373945
S 0.467206 -1.449230 0.969841
S 2.038258 -0.848018 2.158354
S 0.018356 1.780436 1.638068
S -1.252280 2.679781 0.283895

[Mo3S10]- XXII
E= -4187.472188
S 0.680697 -0.930870 -1.291593
Mo -0.662336 0.564803 -0.113232
S -2.252320 0.018878 -1.863546
Mo -3.319792 -0.341769 0.039368

S -2.030589 0.204373 1.787336
Mo 2.773622 -0.569066 -0.157393
S 3.885367 -2.382450 -0.212423
S 3.656906 0.893209 -1.445103
S 1.110292 -0.475177 1.645349
S 2.919369 0.463606 1.979816
S 0.238405 2.636136 0.834951
S -0.687351 2.694278 -1.008372
S -4.348451 -2.213649 0.180635

E= -4187.470376
S 0.799644 -0.791840 -1.369605
Mo -0.480845 0.531909 0.027959
S -2.240355 -0.008321 -1.823835
Mo -3.461842 -0.524544 -0.021688
S -1.848546 -0.380882 1.667173
Mo 2.882611 -0.547688 -0.201061
S 3.862472 -2.431113 -0.157500
S 3.916566 0.779270 -1.520129
S 1.245856 -0.400996 1.716470
S 3.073463 0.572645 1.873885
S 0.511199 2.573702 0.651768
S -1.038694 2.690927 -0.698558
S -5.498906 -1.185041 0.171658

[Mo3S10]- XXIII
E= -4187.483783
S 0.555658 -1.454819 -0.091238
Mo -0.888733 0.373923 -0.439860
S -2.379845 -1.290614 -1.353433
Mo -3.666249 -0.069147 -0.023376
S -2.393090 1.385249 1.103973
Mo 2.617353 -0.241874 0.403792
S 3.318196 -0.954953 2.260482
S 4.647160 -0.075689 -0.934105
S 3.354638 -1.645613 -1.339436
S 0.889893 1.353623 1.164540
S 2.593058 2.109894 0.240336
S -0.522800 1.642407 -2.095784
S -4.976592 -1.234655 1.200705

E= -4187.475695
S 0.679527 1.110354 -1.068827
Mo -0.774908 0.182373 0.480359
S -2.433484 1.821150 -0.142552
Mo -3.805370 0.006793 -0.223580
S -2.289999 -1.660570 0.204715
Mo 2.697484 -0.151965 -0.430117
S 3.441740 -0.949203 -2.231909
S 4.695913 0.620506 0.713019
S 3.462717 2.053652 -0.135475
S 0.904162 -1.768865 0.095214
S 2.589764 -1.748786 1.304121
S -0.233977 0.576367 2.492988
S -5.874029 -0.152261 -0.776281

[Mo3S10]- XXIV
E= -4187.512575
S 1.357417 -1.185710 0.000565
Mo 3.489404 -0.417876 0.004975
S 3.904311 0.824298 -1.742276
Mo -0.389319 0.660535 -0.008421
S -1.583569 -1.547221 0.052738
Mo -3.511052 -0.374735 -0.002614
S -4.654315 -0.657727 1.785799
S 0.398011 1.668335 -1.700474
S 0.295207 1.653653 1.730748
S -2.648584 1.699640 -0.138267
S 4.807336 -2.113099 0.031136
S 3.890022 0.869498 1.719642
S -4.687047 -0.864970 -1.723704

E= -4187.517148
S 1.300335 -0.821073 -1.052431
Mo -0.364975 0.457618 -0.011692
S -0.081280 2.497437 -0.448262
Mo 3.448646 -0.293665 -0.258876
S 4.677411 -2.046250 -0.217163
S 2.853241 0.221365 1.996041
S 4.339736 1.436047 -1.156906
S 0.846777 0.301455 2.205264
S -2.071447 0.148448 1.693117

Mo -3.400517 -0.311724 -0.098370
S -4.808812 1.255888 -0.458036
S -1.828127 -0.416543 -1.728568
S -4.396114 -2.188874 0.135405

[Mo3S10]- XXV
E= -4187.565482
S -1.267426 -0.094510 -1.779907
Mo 0.166576 0.560159 -0.000057
S -1.267645 -0.094260 1.779926
Mo -2.672070 0.051111 -0.000026
S -4.073150 -1.737901 0.995918
S -4.072955 -1.738606 -0.995621
S -3.712397 1.893636 -0.000222
S 0.244057 2.660041 -0.000094
S 1.778432 -0.149157 1.742731
Mo 3.192474 -0.382843 0.000023
S 4.089224 -2.332519 0.000183
S 1.778532 -0.149452 -1.742803
S 4.700006 1.143106 0.000046

E= -4187.531893
S -1.378223 -0.421616 1.613272
Mo 0.381464 -0.882627 -0.000042
S -1.377789 -0.420923 -1.613357
Mo -2.976953 -0.008942 -0.000048
S -3.642538 2.164300 -0.998091
S -3.642822 2.163791 0.998332
S -4.475225 -1.513563 -0.000058
S 0.679256 -2.964713 -0.000277
S 1.791087 0.080808 -1.731819
Mo 3.190353 0.522410 0.000073
S 3.799078 2.575467 0.000712
S 1.791770 0.079385 1.732071
S 4.893891 -0.773895 -0.000738

[Mo3S10]- XXVI
E= -4187.539422
S -1.381844 1.624767 0.032933
Mo 0.841175 1.456506 0.023899
S 1.714630 0.187199 1.721965
Mo -2.730967 -0.479032 0.126965
S -4.974490 -0.852434 -0.491951
S -4.314902 1.081355 -0.831646
S -2.574316 -0.907163 2.211696
S -1.542728 -1.833660 -1.005855
S 1.611570 3.427793 0.092569
S 4.905845 -0.435818 -0.054417
Mo 2.813815 -0.848743 -0.064457
S 1.711029 0.307744 -1.768054
S 2.419647 -2.937701 -0.134058

E= -4187.467351
S 0.958947 -1.128335 -0.384896
Mo -1.004724 0.204067 0.243967
S 0.220279 2.123914 -0.531156
Mo 2.968054 -0.203121 0.207369
S 4.842260 0.284407 -1.244751
S 4.424878 -1.697927 -1.026210
S 3.236900 -0.243639 2.315158
S 2.274505 1.947632 -0.504897
S -1.015039 0.234182 2.349811
S -2.773521 1.724476 -0.460358
Mo -3.680927 -0.290996 -0.611043
S -2.104828 -1.842482 -0.457424
S -5.555691 -0.640845 0.363953

[Mo3S10]- XXVII
E= -4187.470902
S 0.224471 0.127416 -1.818067
Mo 0.885710 -1.505705 -0.271446
S 2.419414 -0.466102 1.323407
S 3.222842 -1.732548 -0.233299
Mo 1.209561 1.207085 0.026106
S -0.878807 2.491881 0.328987
S -0.381361 1.298905 1.927226
Mo -1.337385 0.044941 0.005493
S -0.860912 -1.986310 1.337018
S -1.410534 -2.444932 -0.597930
S 2.621928 2.574894 -0.874450
S -3.724520 0.259337 0.615271
S -3.221970 0.543166 -1.378564

E= -4187.430901
S 0.216189 0.024983 -1.879384
Mo 0.384182 -1.764768 -0.272709
S 2.127756 -1.235441 1.345061
S 2.827335 -1.365644 -0.627320
Mo 1.553557 0.792462 -0.043704
S -0.232266 2.544232 0.156151
S 0.057485 1.342235 1.794562
Mo -1.284685 0.277447 -0.008229
S -1.313702 -1.712639 1.459529
S -2.051757 -2.145690 -0.420700
S 3.248437 2.172094 -0.309953
S -3.522829 1.041662 0.678951
S -3.070915 1.158216 -1.344712

[Mo3S10]- XXVIII
E= -4187.475038
S 0.079803 0.229629 -1.899919
Mo -0.070300 1.919904 -0.259494
S -1.778204 1.533926 1.392636
S -2.601233 1.688450 1.469160
Mo -1.224269 -0.452654 0.008120
S 0.357527 -2.367770 0.285135
S 0.246204 -1.089212 1.884150
Mo 1.516450 -0.162979 -0.015205
S 1.924291 2.040014 0.839031
S -2.699059 -1.799098 -1.307335
S -3.172802 -1.785981 0.716148
S 3.768025 -1.079068 0.635948
S 3.293011 -0.794770 -1.351863

E= -4187.441855
S 0.132713 0.198094 -1.917139
Mo -0.042529 1.954522 -0.306586
S -1.774952 1.578748 1.390461
S -2.590016 1.666464 -0.507096
Mo -1.211437 -0.407982 0.001995
S 0.318259 -2.407698 0.198750
S 0.236846 -1.143699 1.818828
Mo 1.536163 -0.176058 -0.028246
S 1.874711 1.900804 1.022702
S -2.879761 -1.821098 -1.208745
S -3.227207 -1.734357 0.749405
S 3.802650 -1.074317 0.660107
S 3.365991 -0.760455 -1.333577

[Mo3S10]- XXIX
E= -4187.391959
Mo -1.301405 -0.345858 0.073793
Mo -0.000049 1.769269 -0.392204
Mo 1.301411 -0.345825 0.073737
S 2.448629 -1.675657 -1.548216
S 3.466163 -1.623518 0.269667
S 0.000043 -2.339047 0.604019
S 0.000047 -0.964595 2.117521
S -1.934048 1.830988 1.126873
S -2.392932 1.705697 -0.887799
S -2.448482 -1.675681 -1.548269
S -3.466143 -1.623663 0.269553
S 2.392825 1.705810 -0.887884
S 1.934009 1.831043 1.126801

E= -4187.379177
Mo -1.675764 -0.233341 0.005187
Mo 0.526814 1.716912 -0.145172
Mo 1.343216 -0.496432 0.041133
S 2.534643 -1.391043 -1.835487
S 3.338818 -2.015472 -0.009322
S -0.326494 -2.276103 -0.278233
S -0.264386 -1.519813 1.644396
S -1.832171 2.217855 0.512646
S -1.491154 1.781289 -1.509445
S -3.773615 -0.756458 -1.016230
S -3.602686 -1.291003 0.981477
S 2.912798 1.491512 -0.036871
S 1.994300 1.167994 1.806556

[Mo3S10]- XXX
E= -4187.455429
S -0.111993 0.188528 1.881715
Mo -0.575050 1.698232 0.086825

Mo -1.293508 -0.811901 0.047582
Mo 1.377756 -0.226681 0.022905
S -3.313804 -1.509503 -0.949775
S -3.380697 -1.130082 1.081770
S 0.432025 -2.573314 0.066642
S 0.239506 -1.550739 -1.714014
S 3.208731 -0.801690 1.439076
S 3.677044 -0.920658 -0.580412
S 1.905250 2.222711 0.146975
S 1.094664 1.609629 -1.643656
S -2.462373 2.733535 -0.141262

E= -4187.443438
S -0.163813 0.296370 1.833816
Mo -0.695560 1.740626 0.046257
Mo -1.248705 -0.998260 0.088914
Mo 1.413736 -0.200075 0.003386
S -3.224971 -1.695406 -1.003600
S -3.424560 -1.127303 1.013577
S 0.655329 -2.548376 0.296520
S 0.381491 -1.757972 -1.585841
S 3.367916 -0.488808 1.469544
S 3.676384 -0.776382 -0.532508
S 1.765213 2.324177 -0.092303
S 0.876393 1.472622 -1.755482
S -2.516742 2.867557 -0.007434

[Mo3S10]- XXXI
E= -4187.364109
Mo 0.795766 -1.244480 0.038461
Mo 0.794637 1.268541 0.183564
Mo -1.501867 0.005351 -0.077863
S -1.357940 2.394062 0.412277
S -0.867375 1.862861 -1.532421
S 2.912281 1.587480 1.128136
S 2.709249 2.187983 -0.852499
S -3.998865 -0.016976 -0.045773
S -3.027900 -0.173721 1.787674
S -1.338031 -2.419041 0.004820
S -0.821093 -1.592625 -1.829701
S 2.631152 -1.983596 1.315510
S 2.926117 -1.923636 -0.766449

E= -4187.355683
Mo -0.906196 1.269032 0.118226
Mo -0.752921 -1.300308 -0.108400
Mo 1.460344 0.068005 -0.090971
S 1.460756 -2.386402 -0.238999
S 0.893233 -1.412989 -1.985628
S -2.162275 -2.362094 1.450259
S -3.012340 -1.951234 -0.435014
S 4.044610 0.130835 0.080222
S 3.080546 -0.210200 1.788076
S 1.197255 2.389177 0.636014
S 0.915281 2.076957 -1.393495
S -2.965279 1.634589 1.188585
S -2.930005 1.994946 -0.877014

[Mo3S10]- XXXII
E= -4187.468609
Mo 1.579896 0.204144 0.008336
Mo -0.687314 -1.268791 0.122534
Mo -0.916642 1.283514 -0.148124
S 0.022872 0.282612 1.818546
S -2.705717 -1.949321 1.126344
S -2.416978 -2.559704 -0.841246
S 1.570478 -2.304409 0.203619
S 0.992946 -1.540081 -1.637059
S 3.334201 0.785210 1.395982
S 4.036485 0.374534 -0.506403
S -2.708479 2.428727 0.925805
S -2.955083 1.924859 -1.087311
S 0.892431 1.983046 -1.352987

E= -4187.451975
Mo 1.675774 0.254815 0.006347
Mo -0.694347 -1.238186 0.072185
Mo -1.043252 1.212251 -0.108262
S 0.062745 0.306915 1.818591
S -2.621486 -2.145155 1.114861
S -2.315281 -2.693382 -0.865193
S 1.575058 -2.222139 0.270482

S 1.065569 -1.515877 -1.615728
S 3.423049 0.944605 1.393042
S 4.033707 0.396696 -0.516644
S -2.875911 2.221173 0.999109
S -2.945528 2.263788 -1.083008
S 0.760371 1.842566 -1.437469

[Mo3S10]- XXXIII
E= -4187.549584
S -3.460747 -0.022171 1.392262
Mo -1.645165 -0.009219 -0.088141
S -1.038923 -1.871188 -1.296933
Mo 0.821968 -1.353110 -0.061035
S 2.240617 -3.336332 -0.460052
S 1.572620 -2.949298 1.470180
S -1.060906 1.860551 -1.295070
Mo 0.805621 1.361487 -0.059595
S 2.197236 3.364826 -0.459498
S 1.537835 2.965614 1.471400
S -0.068558 -0.002150 1.671673
S 2.159282 0.013295 -1.339303
S -4.032316 -0.020938 -0.606635

E= -4187.517323
S -3.876766 -1.039752 0.353936
Mo -1.789733 0.001177 -0.108970
S -0.943046 -1.889736 -1.339633
Mo 0.851983 -1.397141 -0.095961
S 2.326060 -3.297056 -0.335485
S 1.555616 -2.942146 1.551833
S -0.939699 1.891175 -1.339278
Mo 0.854476 1.395933 -0.095715
S 2.332809 3.292457 -0.335951
S 1.560469 2.940241 1.551305
S -0.192430 0.000086 1.574897
S 2.269930 -0.001886 -1.246304
S -3.874348 1.046701 0.353878

[Mo3S9]2- I
E= -3789.256847
Mo 0.295484 0.742634 0.101963
Mo 2.723206 -0.602562 -0.040499
S 2.031565 0.183410 1.901404
S 2.064009 0.594200 -1.751329
S 3.538839 -2.599300 -0.274577
S -1.063960 -0.242568 -1.714259
S -4.250082 0.537007 -0.069374
Mo -2.451954 -0.666329 -0.001576
S -1.113756 -0.134196 1.770928
S 0.712905 2.934088 0.807308
S -0.463493 2.880927 -0.900472
S -2.943712 -2.772145 0.073166

E= -3789.320055
Mo -0.147518 0.316692 -0.135287
Mo -2.963798 -0.225948 0.022948
S -1.816289 0.785752 -1.697416
S -4.463738 1.128352 0.812327
S -3.794379 -2.119834 -0.619507
S -1.321594 -0.553983 1.628806
S 3.760864 -1.858928 1.277907
Mo 2.920513 -0.325731 -0.014534
S 1.177050 -1.188532 -1.290596
S 0.656570 2.515507 0.049552
S 1.821667 1.227051 1.319065
S 4.480706 0.681458 -1.147097

[Mo3S9]2- II
E= -3789.323470
S -0.000358 3.814377 0.845400
Mo -0.000402 1.829883 -0.095032
S 1.844749 1.270519 -1.372325
Mo 1.380266 -0.565455 -0.046176
S 0.000413 0.308951 1.660619
Mo -1.379725 -0.566188 -0.045687
S -1.845669 1.269441 -1.371641
S -2.930198 -1.418511 1.472920
S 0.000382 -1.969598 -1.243805
S 2.929473 -1.418486 1.473119
S 3.556068 -1.844548 -0.486462
S -3.555226 -1.845026 -0.487227

E= -3789.286557
S -0.003330 3.664154 0.979985
Mo -0.001215 1.750204 -0.085619
S 1.846797 1.330661 -1.387638
Mo 1.552568 -0.576584 -0.065343
S 0.000590 0.154996 1.647768
Mo -1.551487 -0.578091 -0.065018
S -1.847658 1.328066 -1.388487
S -3.163174 -1.359772 1.451692
S 0.001272 -1.970001 -1.073543
S 3.164270 -1.357091 1.451773
S 3.714216 -1.676099 -0.557144
S -3.712632 -1.678176 -0.557458

[Mo3S9]2- III
E= -3789.256847
S 1.063887 -0.242604 -1.714242
Mo 2.451943 -0.666325 -0.001588
S 2.943548 -2.772168 0.073392
S 4.250167 0.536855 -0.069671
Mo -0.295448 0.742699 0.101971
S 1.113952 -0.133828 1.770966
S -2.031438 0.183302 1.901395
Mo -2.723184 -0.602641 -0.040490
S -2.064080 0.594190 -1.751288
S -3.538723 -2.599419 -0.274606
S 0.463498 2.880262 -0.900363
S -0.713252 2.934199 0.807198

E= -3789.292302
S 1.469559 -0.095490 -1.821165
Mo 2.859559 -0.179002 0.030189
S 3.951238 -2.054712 0.009258
S 4.187633 1.534758 0.042692
Mo -0.023001 0.142823 -0.090148
S 1.420338 -0.129455 1.792077
S -1.372051 -1.853204 0.687901
Mo -2.910578 -0.357291 -0.012695
S -1.963056 0.193507 -1.950242
S -5.081714 -0.487047 0.199063
S -0.515957 2.499500 0.039519
S -1.901687 1.425000 1.191615

[Mo3S9]2- IV
E= -3789.259932
S -3.566118 0.748189 -0.969083
Mo -1.744038 0.083536 0.053554
S -0.630364 -1.684186 1.552026
Mo 0.998477 -1.250700 -0.158975
S -0.148762 0.117935 -1.649792
Mo 0.631252 1.605657 -0.019127
S -1.092606 1.814633 1.471306
S 1.440410 3.431190 -0.919567
S 1.997547 0.411771 1.490878
S 1.340067 -3.052201 -1.363997
S -2.346264 -2.237381 0.462103
S 3.306154 -0.700993 0.253064

E= -3789.249448
S 0.661402 3.445243 -0.957483
Mo 0.196718 1.580296 0.085818
S -1.439023 0.688944 1.797933
Mo -1.683076 -0.650701 -0.177309
S 0.156158 -0.110725 -1.562778
Mo 1.871847 -0.701514 -0.002344
S 1.976971 1.028820 1.499053
S 3.741355 -1.054182 -1.059475
S 0.869059 -2.570650 0.984688
S -3.643384 -1.055464 -1.061130
S -2.245100 1.966381 0.357802
S -1.089349 -2.937080 0.247706

[Mo3S9]2- V
E= -3789.293852
S -3.043818 -0.964226 2.080711
Mo -1.975330 -0.721172 0.219733
S -1.478823 1.078679 -1.815866
Mo 0.017103 1.305941 -0.064004
S 0.332070 -0.573883 1.299239
Mo 2.321571 -0.478285 0.021034
S -1.696620 -2.580859 -0.831385
S 3.965921 -0.000702 1.343528

S 1.896068 1.220725 -1.470621
S -0.120110 3.177695 0.985077
S -3.445362 0.661750 -0.956147
S 2.636894 -2.298700 -1.098538

E= -3789.306004
S 2.650222 -2.365356 -1.525941
Mo 2.112444 -0.972317 0.033007
S 3.611815 -0.779601 1.574713
S 1.762769 1.146594 -1.008355
Mo -0.130921 2.115115 -0.143405
S -0.223635 4.054801 -1.057774
S 0.090250 -1.606277 1.025629
Mo -1.986375 -1.160973 0.047709
S -3.496136 -1.376823 1.575206
S -0.009461 2.355984 1.984522
S -2.082712 1.080367 -0.758581
S -2.290377 -2.461980 -1.644860

[Mo3S9]2- VI
E= -3789.374849
S -1.542602 -0.116162 -1.763210
Mo -0.000005 0.538668 -0.000004
S -1.542361 -0.116291 1.763150
Mo -2.941821 -0.304057 0.000011
S -4.436406 1.259896 0.000163
S -3.866832 -2.262744 -0.000019
S 1.542602 -0.115756 1.763300
S 0.000341 2.653187 -0.000216
S 3.866991 -2.262693 0.000353
Mo 2.941736 -0.304094 0.000034
S 4.436276 1.259899 -0.000542
S 1.542225 -0.116944 -1.763085

E= -3789.332084
S -1.692559 -0.100236 -1.737300
Mo -0.086912 0.619422 0.000018
S -1.692633 -0.100020 1.737334
Mo -3.105300 -0.345234 -0.000004
S -4.645739 1.167790 -0.000126
S -3.992583 -2.313743 0.000078
S 1.541707 -0.125414 1.583342
S -0.038834 2.746070 -0.000116
S 1.541663 -0.125693 -1.583267
Mo 3.256863 -0.338113 0.000023
S 4.162280 -2.307613 0.000147
S 4.646988 1.326662 -0.000189

[Mo3S9]2- VII
E= -3789.336676
S -1.546535 -0.189959 1.787573
Mo -0.087714 -0.197099 0.000417
S -1.546950 -0.197575 -1.786738
Mo -2.980442 0.146155 -0.000248
S -4.467988 -1.435347 0.002531
S -3.821231 2.137827 -0.003972
S 1.523123 -1.756242 -1.029542
S 1.523310 -1.751846 1.036451
S 1.059880 1.742302 -0.003430
Mo 2.794850 0.184364 -0.000409
S 3.996984 0.546384 -1.782629
S 3.996834 0.554228 1.780383

E= -3789.210108
S -1.636237 -0.018558 -0.328879
Mo 0.008694 1.568819 0.244309
S -0.505451 2.392225 2.134604
Mo -3.554960 -1.101611 -0.078765
S -4.355687 -2.182441 -1.769427
S -4.721059 -0.972537 1.730636
S 1.443180 2.979021 -1.028146
S -0.577454 3.020291 -1.557004
S 1.709507 0.002295 0.692570
Mo 3.479846 -1.175672 0.046613
S 4.724559 -2.053666 1.582229
S 4.092996 -1.307814 -2.013495

[Mo3S9]2- VIII
E= -3789.221421
Mo 3.065863 0.171210 -0.039342
S 3.650445 1.245623 -1.827620
S 3.803450 0.695529 1.930688

S 2.442957 -2.076241 -0.360282
Mo 0.638296 -0.619390 -0.087137
S -0.737177 -0.071342 -1.780812
S -0.517307 -0.599738 1.808170
Mo -2.112897 0.107725 0.123220
S -2.389315 2.072879 1.301561
S -3.018735 2.328689 -0.666340
S -4.038076 -0.967312 -1.108520
S -3.373303 -1.734392 0.711706

E= -3789.210191
Mo 3.313436 0.107189 -0.049494
S 3.761866 1.553515 -1.593919
S 4.054814 0.353351 1.970295
S 2.364252 -1.960807 -0.629339
Mo 0.540720 -0.613104 -0.165459
S -0.848278 0.090040 -1.792489
S -0.532033 -0.563232 1.778537
Mo -2.188113 0.115401 0.142994
S -2.415777 2.071568 1.341457
S -3.290944 2.280317 -0.537373
S -4.043083 -1.064411 -1.109787
S -3.424178 -1.735243 0.761509

[Mo3S9]2- IX
E= -3789.135730
S 0.283528 0.000559 -1.948678
Mo 1.274395 1.237487 -0.136206
S -0.378514 1.787458 1.569638
S -0.919457 2.524076 -0.300773
Mo -1.139934 0.000453 -0.010842
S -0.922208 -2.523142 -0.303109
S -0.380274 -1.788654 1.567974
Mo 1.273040 -1.238306 -0.136775
S 2.130195 -0.002555 1.816441
S 3.232889 0.000891 -1.063044
S -3.192549 0.001880 -1.324508
S -3.548303 0.000447 0.731094

E= -3789.133305
S 0.295934 0.000384 -1.924194
Mo 1.284474 1.284537 -0.173562
S -0.333293 1.766449 1.538589
S -0.965056 2.546940 -0.276110
Mo -1.126987 0.000384 -0.020470
S -0.967230 -2.546261 -0.276473
S -0.333731 -1.766054 1.538227
Mo 1.283464 -1.285296 -0.174147
S 2.040250 -0.001395 1.793911
S 3.208300 0.000074 -0.907614
S -3.206884 0.000789 -1.291461
S -3.520790 0.000058 0.771592

E= -3789.103199
S 0.259412 -0.000086 -1.981055
Mo 1.213019 1.313551 -0.186912
S -0.376121 1.692649 1.614574
S -0.974610 2.564300 -0.164909
Mo -1.180535 -0.000033 -0.031013
S -0.974470 -2.564427 -0.165064
S -0.376340 -1.692833 1.614536
Mo 1.213048 -1.313520 -0.186733
S 2.686266 0.000167 1.306218
S 3.320773 0.000012 -0.689050
S -3.254294 0.000053 -1.268323
S -3.580139 0.000167 0.795299

[Mo3S9]2- X
E= -3789.110343
Mo -0.556057 1.735829 0.022231
Mo 1.233237 -0.255938 0.066772
Mo -1.543537 -0.249764 0.024920
S -0.202572 0.398271 1.936105
S 2.244608 2.180856 0.019064
S 1.153655 1.543547 -1.632481
S 3.083461 -1.037329 1.418689
S 3.401764 -1.267397 -0.631013
S 0.219294 -2.628658 0.082515
S -0.129925 -1.443787 -1.573996
S -3.744645 -0.331898 1.081372
S -3.751452 -0.642688 -0.999303

E= -3789.111442
Mo -0.427126 1.771879 -0.010123
Mo 1.213866 -0.277754 0.047382
Mo -1.527711 -0.308864 0.051308
S -0.200757 0.400230 1.951606
S 2.181002 2.092732 0.089051
S 1.310190 1.526901 -1.719864
S 2.980599 -1.131955 1.466702
S 3.382278 -1.382515 -0.565082
S -0.084562 -2.462563 0.129352
S -0.160318 -1.415681 -1.649247
S -3.720201 -0.035741 1.034882
S -3.743180 -0.702721 -0.969890

E= -3789.089033
Mo -0.281489 1.919268 0.023901
Mo 1.185587 -0.290298 0.043082
Mo -1.613887 -0.524228 0.120594
S -0.279404 0.423654 1.902746
S 2.244742 2.046895 0.018968
S 1.317478 1.456999 -1.770317
S 2.948880 -1.126651 1.477386
S 3.364339 -1.397754 -0.551886
S -0.059375 -2.474070 0.182268
S -0.180547 -1.474735 -1.625395
S -3.766231 0.193023 0.931048
S -3.726686 -0.547886 -1.057208

[Mo3S9]2- XI
E= -3789.215464
S -0.310702 0.003522 1.773291
Mo 0.445464 1.268515 -0.118111
Mo -1.858899 -0.362926 0.030961
Mo 0.760354 -1.148915 -0.026897
S 2.757633 -2.184022 -0.895008
S 2.599934 -2.130500 1.204122
S -0.922789 -2.068569 -1.302279
S -3.643327 -1.106651 1.070030
S -1.218068 1.190639 -1.824429
S -2.084542 2.120034 -0.155670
S 2.624684 1.862307 -0.616087
S 1.911516 2.951970 1.045402

E= -3789.134407
S -0.001238 0.177972 1.973402
Mo 1.210374 -0.468646 -0.011300
Mo -0.001361 1.868560 0.264483
Mo -1.210430 -0.470271 -0.012536
S -2.393176 -2.209329 -1.201872
S -2.308205 -2.447713 0.890962
S -1.691326 1.486037 -1.453537
S -2.479100 1.855486 0.459484
S 1.689510 1.487175 -1.452744
S 2.476454 1.858434 0.460331
S 2.403374 -2.202207 -1.199761
S 2.307427 -2.446167 0.892035

E= -3789.117198
S 0.000256 0.031449 1.906989
Mo 1.422834 -0.446831 0.013570
Mo 0.000382 1.821904 0.292230
Mo -1.422680 -0.446392 0.013734
S -2.620320 -2.101952 -1.257063
S -2.431402 -2.486068 0.817648
S -1.704745 1.554583 -1.441046
S -2.452558 1.800652 0.508217
S 1.705498 1.554244 -1.440977
S 2.453266 1.800065 0.508370
S 2.617217 -2.103811 -1.258045
S 2.431382 -2.486950 0.817132

[Mo3S9]2- XII
E= -3789.211742
Mo -1.434058 -0.790534 0.000410
Mo 0.000111 1.193793 -0.000128
Mo 1.433978 -0.790515 -0.000333
S 0.000548 -0.212517 1.957499
S 0.000567 3.363697 1.054681
S -0.000161 3.363938 -1.054679
S 3.573203 -0.666254 1.059975
S 3.573477 -0.665119 -1.060011
S -3.573463 -0.664464 1.060007

S -0.000165 -2.623669 0.000194
S -3.573192 -0.666226 -1.059981
S -0.000896 -0.212840 -1.957550

E= -3789.211709
Mo 1.263230 0.920652 -0.000029
Mo 0.126323 -1.395940 0.000082
Mo -1.452472 0.740807 -0.000025
S -0.075108 0.042368 1.894707
S 0.487183 -3.519203 1.049455
S 0.487007 -3.519342 -1.049032
S -3.590755 0.546623 1.054604
S -3.590731 0.546124 -1.054625
S 3.395794 1.226206 1.057881
S -0.268927 2.713484 -0.000300
S 3.395724 1.224736 -1.058017
S -0.075024 0.042013 -1.894744

E= -3789.195366
S 0.088874 0.040441 1.801962
Mo 1.755814 -0.038276 0.010642
S 0.136455 0.136922 -1.723398
Mo -0.979794 1.309512 0.069717
S -1.899732 3.268656 -1.078081
S -2.758878 2.730338 0.784916
Mo -0.602946 -1.448290 -0.002537
S -2.454269 -2.485119 -1.086515
S -2.415295 -2.620113 1.013569
S 1.458114 -2.432523 -0.092284
S 3.299181 1.741973 0.610420
S 4.091232 0.084192 -0.434874

[Mo3S9]2- XIII
E= -3789.356465
Mo 0.243269 0.000327 -0.018096
S -1.126670 1.794580 -0.020574
Mo -2.639210 -0.001460 0.242170
S -1.125796 -1.794254 -0.038975
S -3.274333 -0.013800 2.280371
S 1.644150 0.009251 -1.824015
S 1.683473 -0.008336 1.743875
Mo 3.162846 0.000526 -0.060631
S 4.334951 1.820664 -0.063068
S 4.332759 -1.820761 -0.081805
S -4.241906 1.054179 -1.205711
S -4.239753 -1.039928 -1.219134

E= -3789.324475
Mo -0.171365 -0.000291 0.007556
S 1.222518 -1.810359 -0.086647
Mo 2.689249 -0.000084 0.221444
S 1.222368 1.810079 -0.085641
S 3.281124 -0.001167 2.277324
S -1.705968 0.000682 -1.757359
S -1.765356 0.000036 1.700478
Mo -3.273548 0.000086 -0.062197
S -4.501152 -1.783900 -0.085344
S -4.501380 1.783915 -0.083975
S 4.365509 -1.048128 -1.159056
S 4.365954 1.049673 -1.157637

[Mo3S9]2- XIV
E= -3789.288317
Mo 2.886423 0.555348 0.067764
S 4.318030 -0.708436 -0.936711
S 2.048209 -0.025329 2.041072
S 2.810853 2.630360 -0.508660
Mo 0.428270 -0.729111 0.124479
S -0.589592 0.376708 -1.599282
S -3.462372 1.976109 -0.850662
S -3.396266 -1.769413 -0.809341
Mo -2.353535 -0.036138 -0.128278
S 0.788119 -2.747032 -0.427625
S -1.179981 -0.565917 1.803014
S -3.860037 1.383940 1.120284

E= -3789.200558
Mo 3.227655 0.227281 -0.206915
S 1.934813 -1.324198 -1.310062
S 1.710277 1.511800 0.878811
S 5.370560 0.034051 0.210831
Mo 0.340559 -0.240259 -0.019586

S -1.476362 -1.686906 -1.180974
S -1.141249 1.390573 -1.302818
S -4.820947 -0.477568 -0.061545
Mo -2.689457 -0.043877 -0.154669
S -0.136280 -1.698885 1.877141
S -1.406858 -0.049075 1.851333
S -2.340692 2.449455 0.037852

[Mo3S9]2- XV
E= -3789.261150
S 4.758297 -1.276142 -1.069607
Mo 3.534386 0.166430 -0.024061
S 4.158741 2.189099 -0.437235
S 3.483125 -0.226409 2.085176
Mo -1.022463 -0.204873 0.226719
S -2.733188 -1.831122 0.318581
Mo -3.730995 0.081740 -0.413932
S -2.021665 1.428729 -1.130973
S -0.614329 0.474232 2.202315
S 1.331038 0.088838 -1.050109
S 0.471052 -1.784450 -0.702851
S -5.633010 0.823569 0.339298

E= -3789.215177
S -4.382752 -1.462088 -0.870331
Mo -3.153804 0.097473 -0.029384
S -4.244397 1.782350 0.755549
S -1.395766 0.822357 -1.525524
Mo 0.654973 -0.108007 0.036385
S 2.078303 -0.688822 -1.699668
Mo 3.511952 -0.182959 0.031888
S 2.109933 0.177541 1.820327
S -0.233238 2.074411 -0.302740
S -1.556011 -0.790517 1.548759
S -0.505420 -2.174410 0.375554
S 5.469908 0.767096 -0.204010

[Mo3S9]2- XVI
E= -3789.234121
S -0.913365 -1.576583 -1.198449
Mo 0.340999 0.394520 0.265541
S 1.734266 -1.259986 1.326583
Mo 3.122923 -0.372388 -0.221688
S 1.780872 0.754962 -1.642883
Mo -2.533658 -0.444646 -0.081529
S -4.396087 -1.558461 -0.213937
S -1.585791 1.395857 -1.285784
S -3.223017 1.910439 -0.098670
S 0.430297 2.200663 1.405149
S -1.562081 -0.543656 1.881537
S 5.292963 -0.214139 -0.074648

E= -3789.209551
S -0.935275 -1.341215 -1.515384
Mo 0.312206 0.056277 0.038440
S 1.869710 -1.718489 0.584371
Mo 3.275544 -0.112323 -0.140006
S 1.870243 1.595235 -0.801735
Mo -2.628963 -0.292018 -0.283855
S -4.565172 -1.291471 -0.405484
S -1.445518 1.715255 -0.980769
S -3.037575 2.020109 0.334989
S -0.315012 0.834247 2.260722
S -1.424284 -0.839115 1.701899
S 5.466068 -0.060889 -0.166880

[Mo3S9]2- XVII
E= -3789.215536
S -2.998859 2.403668 0.038232
Mo -2.517845 0.291977 -0.007448
S -4.285136 -0.932769 0.377984
S -1.365937 -1.534283 -1.447477
Mo 0.356383 -0.320224 -0.036271
S 2.178434 -1.635288 -0.933934
Mo 3.064864 0.313043 -0.244739
S 1.424000 1.822289 0.081136
S -0.933684 0.423650 -1.918965
S -1.037929 0.142119 1.891728
S -0.288970 -1.804695 1.793432
S 4.936651 0.367720 0.875066

E= -3789.218935

S -2.689895 -2.497314 -0.690417
Mo -2.509082 -0.472736 0.099684
S -4.471380 0.306284 0.653497
S -1.205507 0.941790 1.861224
Mo 0.371915 0.555697 -0.130414
S 2.207796 1.558934 1.009330
Mo 3.146465 -0.149380 -0.168364
S 1.455468 -0.946650 -1.520800
S -0.535043 -0.982904 1.517096
S -1.645179 0.727352 -1.736164
S -0.536491 2.471688 -1.158474
S 4.770825 -1.404832 0.587332

[Mo3S9]2- XVIII
E= -3789.259085
S -1.430273 -0.106421 -1.556746
Mo 0.631846 0.708253 -0.332240
S 1.597762 -1.330483 -1.195544
Mo 3.217227 -0.611146 0.207404
S 2.206066 0.881769 1.550961
Mo -2.982525 -0.457967 0.006019
S -2.530562 -2.123293 1.299457
S -2.859853 1.523135 1.172531
S -0.744158 1.371658 1.496894
S 1.061197 2.357888 -1.604800
S -4.933263 -0.646044 -0.886785
S 5.358395 -0.980950 0.035927

E= -3789.249271
S -0.354750 -0.689448 -1.554805
Mo 0.458648 0.604137 0.096936
S 2.389136 1.565828 -0.972921
Mo 3.204840 -0.262213 0.140033
S 1.525652 -0.703279 1.698882
Mo -2.279304 -0.189898 -0.296761
S -3.520477 1.065458 -1.505834
S -3.459988 -1.417223 1.394248
S -2.942580 -2.487397 -0.324461
S -0.521877 2.766509 0.499993
S -1.442313 1.182179 1.529859
S 4.693715 -1.681694 -0.608008

[Mo3S9]- I
E= -3789.289398
Mo -0.005779 0.261965 0.068914
Mo -2.846157 -0.369241 -0.025683
S -1.324454 -1.806116 -0.794459
S -1.875499 0.139161 1.917772
S -4.980949 -0.635478 -0.035456
S 1.398718 -0.083639 1.815339
S 4.166151 1.453721 -0.059564
Mo 2.824011 -0.214165 -0.014099
S 1.329949 -0.135181 -1.769445
S -2.006501 1.514543 -1.141580
S -0.446827 2.511295 -0.020645
S 3.812715 -2.114524 0.011567

E= -3789.241810
Mo -0.710197 0.511539 0.002151
Mo -3.396130 -0.205908 0.181126
S -2.487910 1.398227 -1.159372
S -1.701697 -0.840961 1.577922
S -4.702365 -1.697275 -0.638024
S 3.382981 -2.302276 -0.422790
S 3.708104 -1.320517 1.390351
Mo 2.543894 -0.098036 -0.294932
S 0.549623 -0.588639 -1.528752
S 0.182962 2.479392 0.831050
S 1.466196 0.994196 1.585510
S 3.703493 1.332917 -1.342800

[Mo3S9]- II
E= -3789.310762
S -0.000173 3.859759 0.734392
Mo -0.000277 1.864802 -0.100555
S 1.831650 1.254276 -1.355456
Mo 1.361793 -0.585608 -0.048662
S 0.000109 0.357237 1.652668
Mo -1.361424 -0.586193 -0.048483
S -1.832055 1.253419 -1.355331
S -2.993713 -1.308622 1.485822
S 0.000400 -1.974567 -1.277526

S 2.993463 -1.308356 1.485862
S 3.381998 -1.976252 -0.425580
S -3.381921 -1.976021 -0.425887

E= -3789.276967
S -0.427514 3.742749 0.859586
Mo -0.148107 1.809802 -0.047091
S 1.657937 1.508861 -1.353625
Mo 1.580854 -0.532831 -0.073360
S 0.003680 0.201112 1.644671
Mo -1.408996 -0.713757 -0.085694
S -1.994433 1.198004 -1.261669
S -2.828437 -1.734880 1.492995
S 0.081066 -1.914393 -1.282825
S 3.313338 -1.097832 1.450037
S 3.657699 -1.569802 -0.553102
S -3.525683 -1.812256 -0.454938

[Mo3S9]- III
E= -3789.281824
S -0.780569 -0.746007 -1.582849
Mo -2.610702 0.401745 -0.193456
S -4.147909 0.624095 -1.274170
S -3.236958 -2.221282 0.733084
Mo 0.099077 0.440922 0.153024
S 1.899638 1.169527 -1.359785
S 3.461410 1.788958 -0.079504
Mo 2.738753 -0.452637 0.143884
S 1.150977 -0.858958 1.746254
S 3.769568 -2.176813 -0.604756
S -1.831879 0.977989 1.604416
S -0.880490 2.527823 0.545749

E= -3789.241662
S -1.131630 0.200084 1.767608
Mo -2.799622 0.354870 0.175082
S -4.384236 -1.034188 0.551067
S -3.457409 2.383136 0.006530
Mo 0.196809 -0.403089 -0.029775
S 1.873056 -0.984331 1.736466
S 2.151339 -1.973288 -0.052827
Mo 3.056210 0.347251 0.036148
S 1.252454 1.400967 -0.982551
S 4.977423 1.317068 -0.154032
S -1.692239 -0.119783 -1.862511
S -0.778928 -1.974625 -1.486071

[Mo3S9]- IV
E= -3789.261710
S -3.654197 -0.063457 -0.857007
Mo -1.716384 -0.309038 0.052594
S -0.216470 -1.760481 1.545217
Mo 1.319700 -1.044602 -0.164746
S -0.167160 0.048052 -1.641473
Mo 0.248587 1.731552 -0.053607
S -1.429177 1.521162 1.464833
S 0.391695 3.688357 -0.930510
S 1.863860 0.932989 1.475232
S 1.979168 -2.742449 -1.300601
S -1.727635 -2.692975 0.437646
S 3.348668 0.076784 0.241782

E= -3789.258831
S 1.197904 3.166766 -1.260509
Mo 0.417745 1.602985 -0.050980
S -1.864395 0.541952 1.811052
Mo -1.834710 -0.539542 -0.263112
S 0.164355 -0.249030 -1.513092
Mo 1.776437 -0.903666 0.087958
S 1.985452 0.917906 1.484138
S 3.606525 -1.473214 -0.865860
S 0.510751 -2.608512 1.018950
S -3.650926 -0.386952 -1.380680
S -1.437030 2.479357 1.100542
S -1.456249 -2.807687 0.199062

[Mo3S9]- V
E= -3789.272934
S 3.468206 -1.705144 -0.897164
Mo 1.695058 -0.729363 -0.175664
S 1.352007 0.566887 1.860410
Mo -0.130195 1.621994 0.106821

S 0.056051 0.131270 -1.699181
Mo -1.604132 -0.694950 -0.143697
S -0.020281 -2.567701 0.028610
S -3.349207 -0.843409 -1.358095
S -1.959979 1.012036 1.383012
S -0.474467 3.568932 -0.767249
S 2.356602 1.604766 0.370668
S -1.325850 -2.286548 1.636905

E= -3789.266899
S 2.066646 -3.102038 -0.881005
Mo 1.061025 -1.381429 -0.047119
S 0.988461 0.454815 1.857668
Mo 1.026490 1.559047 -0.216925
S 1.128776 0.022469 -1.928661
Mo -2.119111 -0.033945 0.038197
S -1.076533 -2.134282 0.316738
S -3.196266 -0.189679 -1.798058
S -1.186915 2.153445 0.052285
S 2.302347 3.273964 -0.351869
S 2.575203 -0.903109 1.683505
S -3.518781 0.047275 1.642247

[Mo3S9]- VI
E= -3789.336134
S 1.577632 -0.133466 1.725268
Mo -0.000095 0.549281 0.000168
S 1.577724 -0.132932 -1.725330
Mo 3.039770 -0.316671 -0.000064
S 4.471058 1.272226 0.000145
S 4.017309 -2.218152 -0.000189
S -1.577451 -0.133440 -1.725185
S -0.000305 2.645892 0.000045
S -1.577613 -0.133256 1.725302
Mo -3.039733 -0.316694 -0.000036
S -4.017076 -2.218267 0.000041
S -4.471128 1.272114 -0.000272

E= -3789.294100
S -1.765451 0.376758 -1.746634
Mo -0.061210 0.228686 -0.125728
S -1.441957 -0.394651 1.613721
Mo -3.123710 -0.176493 0.025822
S -4.491082 1.384042 0.539755
S -4.136862 -2.028702 -0.312638
S 1.894326 1.283421 1.338248
S 0.781012 2.413904 -0.064137
S 1.292511 -1.350441 -1.151431
Mo 3.000913 -0.308936 -0.010511
S 3.925475 -1.686573 1.343532
S 4.425048 0.676192 -1.270573

[Mo3S9]- VII
E= -3789.324641
S -1.729400 0.756273 -1.708219
Mo -0.094774 0.311034 -0.140027
S -1.273970 -0.519986 1.636142
Mo -2.919422 -0.207318 0.028095
S -4.381854 1.168733 0.782864
S -3.764250 -2.073093 -0.599977
S 1.738270 1.248449 1.392773
S 0.831376 2.462532 -0.047256
S 1.118586 -1.255311 -1.275988
Mo 2.833634 -0.328402 -0.004647
S 3.609385 -1.762270 1.369144
S 4.325832 0.564475 -1.243465

E= -3789.294100
S -1.765657 0.378965 -1.746211
Mo -0.061079 0.229246 -0.125612
S -1.441398 -0.395709 1.613431
Mo -3.123300 -0.176722 0.025848
S -4.491264 1.382777 0.541348
S -4.135676 -2.029003 -0.314500
S 1.893778 1.283008 1.338130
S 0.780864 2.414649 -0.063849
S 1.292092 -1.349659 -1.152299
Mo 3.000565 -0.309135 -0.010508
S 3.924495 -1.687564 1.343204
S 4.425279 0.676140 -1.269792

[Mo3S9]- VIII

S48

E= -3789.206808
Mo -3.128547 0.154179 0.003017
S -3.850200 0.308957 2.025383
S -3.627253 1.573050 -1.537000
S -2.397575 -1.965110 -0.751364
Mo -0.757363 -0.454378 -0.184108
S 0.434545 -0.812726 1.629990
S 0.690811 0.441106 -1.682453
Mo 2.213787 0.060330 0.076380
S 3.281939 2.272796 -0.341474
S 2.636185 1.743379 1.558961
S 3.022933 -2.125154 0.226159
S 4.197937 -0.806645 -0.853333

E= -3789.193151
Mo 3.154957 0.147540 0.019343
S 3.359699 1.604961 -1.535136
S 3.396530 0.803081 2.043012
S 2.661978 -2.086397 -0.453953
Mo 0.741946 -0.769886 -0.137866
S -0.581866 -0.006631 -1.795711
S -0.589114 -0.703158 1.692991
Mo -2.093020 0.088388 0.037639
S -2.165439 2.241524 0.928802
S -3.270889 2.049237 -0.797028
S -3.563526 -1.490208 -0.921486
S -3.982566 -1.010769 1.050830

[Mo3S9]- IX
E= -3789.271590
Mo -0.281203 -0.053787 0.236158
S 1.209699 0.809153 1.667005
Mo 2.524242 0.198367 -0.197623
S 0.840401 -0.894488 -1.479407
S 3.033121 1.948296 -1.283746
S -1.674009 -1.578418 1.289439
S -1.776937 1.546225 -0.769898
Mo -3.110094 -0.265361 0.097656
S -3.185911 1.993344 0.748199
S -4.436784 -1.301618 -1.228836
S 4.264252 -0.570719 1.233005
S 4.002188 -1.634723 -0.533261

E= -3789.230358
Mo -0.244826 0.065211 -0.020615
S 1.206891 -1.769408 -0.171304
Mo 2.620134 0.014699 0.229517
S 1.183045 1.848096 0.070803
S 3.246268 -0.083913 2.256982
S -2.007167 1.877444 -0.042079
S -2.010254 -1.559511 1.000870
Mo -3.362709 0.141969 -0.043622
S -2.015584 -1.555900 -1.086112
S -5.495097 0.389594 -0.103630
S 4.288321 -0.905475 -1.216491
S 4.195506 1.176640 -1.142899

[Mo3S9]- X
E= -3789.264446
Mo 2.853422 0.604241 0.114579
S 4.148331 -0.600473 -1.088764
S 1.984507 -0.150969 2.048699
S 2.534314 2.631456 -0.498393
Mo 0.452369 -0.774829 0.187792
S -0.486165 0.454036 -1.524161
S -3.283569 2.110354 -0.693433
S -3.350452 -1.712469 -1.000550
Mo -2.274776 -0.087952 -0.174616
S 0.792413 -2.749925 -0.467707
S -1.251770 -0.697996 1.790233
S -3.794024 1.394654 1.098721

E= -3789.241811
Mo -3.396298 -0.205984 0.180891
S -2.488008 1.397797 -1.159709
S -1.702205 -0.840626 1.578232
S -4.702820 -1.697282 -0.637977
Mo -0.710361 0.511710 0.002572
S 0.549471 -0.588939 -1.528053
S 3.383124 -2.302352 -0.422375
S 3.703657 1.332449 -1.343518
Mo 2.544176 -0.098151 -0.295064

S 0.182894 2.479757 0.830780
S 1.466438 0.994270 1.585206
S 3.708963 -1.319957 1.390368

[Mo3S9]- XI
E= -3789.227830
S -4.259277 -1.418094 -0.882901
Mo -3.040006 0.122388 -0.044660
S -4.096343 1.817816 0.707635
S -1.235406 0.741481 -1.575855
Mo 0.605218 -0.143348 0.057254
S 2.012783 -0.890361 -1.619642
Mo 3.395440 -0.247654 0.066983
S 2.048504 0.298896 1.808852
S -0.143929 2.054103 -0.365821
S -1.433036 -0.701757 1.601374
S -0.506854 -2.196711 0.474255
S 5.091848 0.999739 -0.356522

E= -3789.225510
S -4.325659 -1.368499 -0.890050
Mo -3.075082 0.134750 -0.032220
S -4.084846 1.829668 0.784162
S -1.260373 0.781769 -1.548916
Mo 0.634354 -0.158908 0.039602
S 2.038044 -0.758162 -1.685955
Mo 3.426429 -0.240877 0.052771
S 2.055386 0.123198 1.832706
S -0.155770 2.035640 -0.295760
S -1.455837 -0.795345 1.557958
S -0.508903 -2.206586 0.348449
S 5.110492 1.054035 -0.260491

[Mo3S9]- XII
E= -3789.219809
S -0.630886 -1.499284 -1.142541
Mo 0.421216 0.083875 0.216941
S 1.962767 -1.245403 1.329070
Mo 3.260747 0.067591 0.010235
S 1.821993 1.538477 -0.950688
Mo -2.569712 -0.411965 -0.263419
S -4.307575 -1.620301 -0.560781
S -1.639828 1.429466 -1.393029
S -3.166025 1.932883 -0.091905
S -0.536803 1.340383 2.002924
S -1.453770 -0.531634 1.874598
S 5.030469 -0.660775 -0.972512

E= -3789.238126
S -0.538894 -0.988454 -1.227925
Mo 0.712813 0.392778 0.082990
S 2.018882 -0.671616 1.646764
Mo 3.469082 0.011041 0.017511
S 2.247595 1.351614 -1.352836
Mo -2.549838 -0.513417 -0.021732
S -3.145506 -2.218420 1.090786
S -3.943577 -0.064568 -1.880269
S -4.109100 1.244739 -0.260500
S -0.366982 2.316567 0.806704
S -1.320337 0.715139 1.758806
S 4.873770 -1.397307 -0.788299

[Mo3S9]- XIII
E= -3789.232611
S -2.876166 -2.313564 -0.827099
Mo -2.426768 -0.441059 0.136546
S -4.233972 0.578939 0.736245
S -0.986888 0.596464 1.986148
Mo 0.333691 0.488058 -0.145429
S 2.182176 1.611026 0.920783
Mo 3.089811 -0.044356 -0.251669
S 1.503561 -0.994472 -1.542660
S -0.406772 -1.272925 1.344198
S -1.487462 0.688738 -1.740521
S -0.765628 2.471187 -0.931988
S 4.454722 -1.372332 0.738847

E= -3789.225511
S -4.085126 1.828772 0.785090
Mo -3.075018 0.134502 -0.032114
S -4.325758 -1.368107 -0.890803
S -1.260323 0.783350 -1.548149

Mo 0.634195 -0.158607 0.039453
S 2.037844 -0.755814 -1.686923
Mo 3.426291 -0.241105 0.052402
S 2.055501 0.121355 1.832745
S -0.155551 2.036370 -0.294151
S -1.455603 -0.796313 1.557593
S -0.508883 -2.206765 0.347023
S 5.111045 1.053329 -0.259247

[Mo3S9]- XIV
E= -3789.261849
S 0.968855 -1.488875 -0.620420
Mo -0.669798 0.013073 0.240763
S -2.101752 -1.924249 -0.029313
Mo -3.328003 -0.155743 -0.564829
S -2.011274 1.628244 -0.892173
Mo 2.883555 -0.182911 -0.152270
S 4.176140 -0.175574 -1.843771
S 2.728670 1.935847 0.852827
S 1.163151 1.681363 -0.496595
S -0.646885 0.344213 2.323147
S 3.802360 -1.280674 1.443079
S -5.154369 0.134355 0.513602

E= -3789.245282
S -0.696208 -0.359309 -1.768670
Mo 0.371877 0.396970 0.063222
S 2.277316 1.391984 -1.107689
Mo 3.374346 -0.342407 -0.112793
S 1.600393 -1.277917 1.103708
Mo -2.425112 -0.034970 -0.222681
S -3.622415 1.567507 -0.923832
S -3.547190 -1.543813 1.228272
S -3.330691 -2.170360 -0.743884
S -0.308678 2.415617 1.085389
S -1.311283 0.711031 1.793154
S 5.470838 -0.786169 0.048211

[Mo3S9]- XV
E= -3789.162776
S 0.237780 0.020501 -1.966482
Mo 1.204322 1.269516 -0.162517
S -0.357108 1.711120 1.664938
S -0.933649 2.554684 -0.132876
Mo -1.169505 0.015761 -0.007495
S -1.023825 -2.530342 -0.151790
S -0.414345 -1.701989 1.639149
Mo 1.163719 -1.304104 -0.165250
S 2.792793 -0.028474 1.230739
S 3.260889 -0.020586 -0.801784
S -3.166040 0.049360 -1.320528
S -3.542650 -0.004851 0.718698

E= -3789.165138
S 0.259553 0.000154 -1.947693
Mo 1.189768 1.315410 -0.178836
S -0.382237 1.723320 1.635523
S -0.998477 2.548466 -0.149799
Mo -1.154957 0.000098 0.000799
S -0.998972 -2.548174 -0.149660
S -0.382212 -1.723099 1.635534
Mo 1.189552 -1.315502 -0.179084
S 2.718191 -0.000360 1.259973
S 3.254214 -0.000181 -0.753019
S -3.155502 0.000061 -1.317274
S -3.528512 -0.000204 0.723857

[Mo3S9]- XVI
E= -3789.178063
Mo -0.882164 1.485950 0.098009
Mo 1.202386 -0.111409 -0.002594
Mo -1.328606 -0.848112 0.301064
S -0.093624 0.343457 2.051280
S 1.442028 2.391836 -0.178049
S 0.603631 1.523234 -1.866138
S 3.243667 -0.320249 1.223910
S 3.481356 -0.645826 -0.809285
S 0.556713 -2.529609 0.413089
S 0.073812 -1.791401 -1.435956
S -3.240720 0.656953 0.449167
S -3.419856 -1.010269 -0.888777

E= -3789.129028
Mo -0.324743 1.838806 0.007326
Mo 1.194564 -0.304198 0.038264
Mo -1.564593 -0.360578 0.060610
S -0.232517 0.367292 1.912160
S 2.209460 2.024292 0.170123
S 1.406241 1.545980 -1.684050
S 2.871244 -1.223740 1.474381
S 3.310102 -1.433659 -0.544473
S -0.152354 -2.437047 0.053174
S -0.195989 -1.355593 -1.706669
S -3.702708 -0.056295 1.035497
S -3.689700 -0.513061 -0.988917

[Mo3S9]- XVIII
E= -3789.173164
S -0.001745 0.140032 1.978888
Mo 1.326231 -0.395785 0.014718
Mo -0.039688 1.824650 0.268310
Mo -1.308402 -0.449852 0.010350
S -2.279412 -2.193791 -1.254368
S -2.012782 -2.573416 0.803568
S -1.783529 1.552061 -1.438992
S -2.499068 1.682922 0.516883
S 1.703176 1.609849 -1.448462
S 2.423070 1.790606 0.502620
S 2.391184 -2.090313 -1.241855
S 2.116488 -2.487859 0.811603

E= -3789.159505
S 0.000024 0.131240 1.965183
Mo 1.256566 -0.462517 -0.008020
Mo 0.000115 1.846862 0.290467
Mo -1.256543 -0.462391 -0.008028
S -2.547480 -2.089218 -1.193917
S -2.186059 -2.483701 0.808706
S -1.694535 1.518884 -1.440225
S -2.465455 1.778981 0.482661
S 1.694803 1.518759 -1.440184
S 2.465678 1.778626 0.482748
S 2.547080 -2.089623 -1.193972
S 2.185582 -2.484079 0.808650

[Mo3S9]- XVIII
E= -3789.157469
Mo -1.074696 -1.018418 0.122710
Mo -0.442640 1.363069 -0.088722
Mo 1.626351 -0.408197 0.114176
S 0.128832 0.099641 1.884054
S -1.225472 3.347050 0.858270
S -1.211809 3.313252 -1.220801
S 3.570678 -0.005664 1.297736
S 3.903202 -0.567380 -0.688766
S -2.801256 -1.789877 1.465499
S 0.616980 -1.936453 -1.396477
S -3.060525 -2.277253 -0.550678
S -0.206795 -0.016508 -2.037769

E= -3789.140774
Mo 1.382463 0.752569 0.121968
Mo 0.000044 -1.361607 -0.166897
Mo -1.382623 0.752532 0.122025
S -0.000056 -0.113681 1.907892
S 0.000419 -3.604668 0.599590
S 0.000315 -3.333596 -1.467409
S -3.484749 0.186763 1.038572
S -3.504328 0.850420 -0.939110
S 3.484744 0.187519 1.038682
S -0.000090 2.813252 0.187132
S 3.504173 0.850666 -0.939140
S -0.000122 1.786653 -1.628584

[Mo3S8]- I
E= -3391.074105
S -2.177038 -2.929087 0.936182
Mo -1.066817 -1.376951 -0.077538
S 0.845184 -1.897399 -1.258405
Mo 1.453476 0.001814 -0.072186
S 3.836531 0.001869 -0.453271
S 3.193233 0.002721 1.513232
S -2.325125 -0.002488 -1.431280
Mo -1.070511 1.375207 -0.077490

S -2.185495 2.923992 0.936091
S -0.232867 0.000295 1.611925
S 0.840690 1.899914 -1.258033

E= -3391.043333
S -0.404571 -3.614392 0.909013
Mo -0.404356 -1.691211 -0.049789
S 1.417117 -1.436379 -1.418164
Mo 1.368959 0.473330 -0.114232
S 3.697962 0.954867 -0.487422
S 2.957419 1.212967 1.442956
S -2.274967 -0.976271 -1.113623
Mo -1.689453 1.036344 0.073589
S -3.359759 2.346153 0.428342
S -0.232682 -0.038968 1.631870
S 0.102213 2.028558 -1.155591

[Mo3S8]- II
E= -3391.039657
S -1.457452 -0.590835 -1.709665
Mo 0.105439 -0.211363 -0.091756
Mo -2.754255 0.133906 0.080416
S -1.143735 0.174234 1.764751
S -4.194788 -1.387048 0.560555
S -3.598116 2.071026 -0.278626
S 1.253245 1.730485 -0.628689
S 1.823301 -1.546069 0.987549
S 1.977689 -1.838863 -1.054981
Mo 2.890148 0.251672 -0.152256
S 4.706355 0.929770 0.788544

E= -3391.026909
S 1.414614 0.851221 -1.498271
Mo -0.143320 -0.162325 -0.121970
Mo 2.898666 -0.004212 0.088531
S 1.279905 -0.936545 1.502970
S 3.987192 1.560137 1.063218
S 4.193656 -1.493595 -0.732717
S -1.554493 -1.694856 -1.100010
S -1.532948 1.587196 0.677225
S -2.928281 2.036667 -0.886319
Mo -2.942429 -0.177428 -0.085309
S -4.368555 -1.007317 1.285620

[Mo3S8]- III
E= -3390.972407
S -1.897529 -1.670893 1.822002
Mo -1.372048 -0.898824 -0.077197
S -3.138736 -0.024541 -1.295588
S -1.557894 1.419010 -1.581959
Mo -0.161747 1.435499 0.287855
S 2.169552 1.699439 -0.481342
S 2.676935 0.147294 -1.831817
Mo 1.464632 -0.658639 0.003080
S 2.320677 -1.453621 1.776648
S 0.184563 -2.265587 -1.081540
S -0.576015 2.469054 2.112535

E= -3390.959460
S 1.886657 -1.431565 -2.180789
Mo 1.068667 -1.209286 -0.222646
S 2.597951 -1.473321 1.503765
S 1.310683 0.102884 2.114624
Mo 0.834546 1.266938 0.045213
S -1.248152 1.815414 -1.467409
S -1.404879 1.956363 0.946718
Mo -2.082952 -0.212251 0.008057
S -4.182715 -0.676199 0.050523
S -0.955055 -2.266863 -0.063977
S 2.467325 2.379378 -0.785452

[Mo3S8]- IV
E= -3390.967597
S 3.040600 2.010540 -0.010455
Mo 1.028553 1.254188 -0.028091
S -1.191293 2.476584 -0.224001
S -0.751044 1.610364 1.598803
Mo -1.575224 -0.010185 -0.063857
S -1.156544 -2.493717 -0.226633
S -0.731281 -1.625698 1.598044
Mo 1.047955 -1.243743 -0.030378
S 3.067400 -1.974776 -0.013414

S 0.120727 0.002423 -1.854034
S -3.714433 -0.006401 -0.547206

E= -3390.968562
S -0.959190 -2.512224 0.316174
Mo 0.961921 -1.417198 -0.279464
S 3.300606 -1.486652 0.094189
S 2.202808 -0.214186 1.400407
Mo 0.777884 1.182559 -0.029344
S -1.443884 2.276026 0.224963
S -0.904946 1.057683 1.824334
Mo -1.796443 -0.266288 -0.020225
S -3.947381 -0.388147 -0.272247
S -0.210435 -0.058815 -1.821945
S 2.111096 2.641246 -0.902165

[Mo3S8]- V
E= -3391.050190
S 1.568059 3.090861 -1.002200
Mo 0.561600 1.462848 -0.000792
S -1.882030 1.955595 -0.092358
S -1.224202 1.189833 1.718255
Mo -1.647842 -0.520159 -0.030370
S -3.456476 -1.313737 -0.893612
S -0.443724 -2.244029 1.159864
Mo 1.270802 -1.184692 0.085316
S 2.841041 -2.311309 -0.867399
S 0.050389 -0.155527 -1.648191
S 2.062472 0.423569 1.483487

E= -3391.046723
S -3.694201 -0.818644 -1.245029
Mo -1.918641 -0.583734 -0.072536
S -1.112496 -2.547964 0.777520
S 1.110000 -2.550062 0.776241
Mo 1.917811 -0.585353 -0.072460
S 3.693170 -0.819720 -1.245244
S 1.905066 1.147375 1.457133
Mo 0.001208 1.600150 0.219123
S 0.000829 3.473745 -0.804943
S -0.000091 -0.165778 -1.367625
S -1.903268 1.149508 1.457364

[Mo3S8]- VI
E= -3391.099068
Mo -0.000171 -0.000267 -0.000504
Mo -2.915051 0.000081 0.000087
S -4.092326 -1.282498 -1.238382
S -4.091170 1.283053 1.239229
S -1.390020 -1.244827 1.289061
S -1.390257 1.244620 -1.289542
Mo 2.915112 0.000053 0.000019
S 1.389609 1.289477 1.244005
S 1.390274 -1.289467 -1.244797
S 4.092852 1.238827 -1.281852
S 4.091108 -1.238833 1.283323

E= -3391.077788
S 1.537892 1.203647 -1.245601
Mo 3.078087 0.000030 0.000085
S 4.285406 1.269428 1.226436
Mo -0.000020 -0.000273 -0.000166
Mo -3.078000 0.000089 0.000045
S -4.286574 -1.225143 1.269424
S 1.538334 -1.204208 1.245075
S -1.538190 1.245864 1.203216
S -1.538418 -1.246766 -1.202792
S 4.286826 -1.268422 -1.225930
S -4.285453 1.226004 -1.269730

[Mo3S8]- VII
E= -3391.054299
S -1.243094 -0.149904 -1.759955
Mo -2.655282 -0.421838 -0.000012
S -3.447725 -2.416542 -0.000029
Mo 0.188390 0.635805 0.000020
Mo 3.099635 -0.116735 0.000005
S -1.243137 -0.149921 1.759963
S 1.841141 0.092702 1.784827
S 0.083482 2.739129 0.000055
S 1.841173 0.092860 -1.784817
S -4.213159 1.051241 -0.000028

S 4.720368 -1.514801 -0.000049

E= -3391.031748
S -1.355514 -0.142613 -1.726237
Mo -2.801023 -0.396290 -0.000015
S -3.682897 -2.346604 -0.000037
Mo 0.200369 0.606967 0.000026
Mo 3.251057 -0.323189 -0.000013
S -1.355580 -0.142615 1.726253
S 1.808325 0.014642 1.736918
S 0.071491 2.705544 0.000091
S 1.808370 0.014843 -1.736928
S -4.312433 1.119266 -0.000043
S 5.310929 -0.927118 -0.000011

[Mo3S8]- VIII
E= -3391.034912
S -1.565333 -0.702297 1.696023
Mo -2.587553 0.286433 -0.097187
S -3.437988 2.180464 0.419984
Mo 0.279762 -0.776349 0.200945
Mo 2.759389 0.540147 0.120967
S 3.874044 -0.666188 -1.240554
S -0.727974 0.558318 -1.430936
S 0.539113 -2.729385 -0.539563
S 1.811511 -0.315842 2.003032
S -4.042264 -0.996637 -0.996245
S 2.363446 2.539710 -0.501645

E= -3391.077808
S 1.538116 -1.445588 0.954456
Mo 3.077905 0.000177 0.000114
S 4.286167 -0.972184 -1.472218
Mo 0.000083 -0.000515 -0.000532
Mo -3.077904 0.000213 0.000080
S -4.285817 -1.471900 0.973216
S 1.537705 1.445339 -0.954662
S -1.537549 0.954587 1.445132
S -1.538495 -0.955348 -1.445195
S 4.285671 0.972851 1.472647
S -4.286018 1.472573 -0.972490

[Mo3S8]- IX
E= -3391.055643
S 1.299642 -0.115256 1.754481
Mo 2.730008 -0.255766 0.000089
S 3.721091 -2.159477 0.000679
Mo -0.253531 0.478095 -0.000085
Mo -3.008107 -0.605391 0.000266
S -5.078401 -0.059190 -0.000483
S 1.299491 -0.116177 -1.754242
S -1.783413 -0.240756 -1.790669
S -0.417850 2.575222 -0.000966
S -1.783901 -0.238544 1.791166
S 4.138868 1.359713 -0.000674

E= -3391.019337
S 1.406834 -0.019487 1.847869
Mo 2.751795 -0.144268 -0.030611
S 3.632447 -2.089106 -0.223769
Mo -0.103311 0.168210 0.112970
Mo -3.020578 -0.393009 -0.276792
S -5.040096 -0.511739 0.439247
S 1.229274 0.256334 -1.740996
S -1.992714 1.616240 -0.977375
S -1.176484 2.094388 0.906302
S -1.283837 -1.816778 0.245339
S 4.201325 1.438948 0.013769

[Mo3S8]- X
E= -3391.006549
S 1.132979 0.260244 1.846529
Mo 2.492991 -0.340502 0.035878
S 2.924857 -2.436947 0.061902
Mo -0.101046 0.756554 0.036331
Mo -2.486829 -0.553165 -0.005429
S -3.155583 -0.772781 2.009975
S 1.047192 0.103695 -1.761307
S -2.416154 1.636097 -0.974969
S -0.915146 2.866829 0.006945
S 4.217758 0.929460 -0.033122
S -2.586832 -2.226675 -1.331251

E= -3390.989789
S 1.007444 0.034469 1.733475
Mo 2.585372 -0.279120 0.045060
S 3.184495 -2.325961 -0.078008
Mo -0.237980 0.854456 -0.007870
Mo -2.459567 -0.643496 -0.004048
S -3.251669 -1.048303 1.942544
S 1.220652 0.334171 -1.725407
S -2.560476 1.553529 -0.983550
S -1.290327 2.858444 0.180855
S 4.270530 1.020173 0.252857
S -2.286190 -2.247636 -1.409764

[Mo3S8]- XI
E= -3391.030267
S 0.632493 -0.084291 1.708785
Mo 2.343891 0.246303 0.106073
S 3.993470 -1.188288 -0.845096
S 3.757837 -1.314478 1.219377
Mo -0.484741 -0.005400 -0.216815
Mo -3.307521 -0.060686 -0.291104
S 1.028902 0.090345 -1.851875
S -1.919787 -1.828477 -0.499625
S -1.982322 1.772956 -0.300455
S -4.689617 -0.182835 1.334162
S 2.980998 2.261998 0.289575

E= -3391.025708
S 0.854073 -0.041789 1.780631
Mo 2.435044 0.228177 0.047134
S 4.036669 -1.216619 -0.962702
S 3.944365 -1.269503 1.118704
Mo -0.392548 0.024840 -0.079975
Mo -3.442841 -0.080674 -0.122214
S 1.011899 0.046462 -1.828350
S -1.823329 -1.778442 -0.196545
S -1.930802 1.726205 -0.112034
S -5.500555 -0.165143 0.481439
S 3.083586 2.246427 0.125877

[Mo3S8]- XII
E= -3391.067504
Mo -0.107890 -0.109016 -0.000155
Mo -2.839025 0.045978 -0.000190
S -1.917688 -1.065076 -1.668959
S -1.413790 1.862734 -0.005788
S -4.974707 0.321607 -0.000816
S -1.918794 -1.054144 1.675800
S 1.346652 -0.189668 1.789383
S 1.347451 -0.200425 -1.788527
Mo 2.793615 0.041057 0.000054
S 3.736814 1.961162 -0.005542
S 4.196475 -1.578488 0.005209

E= -3391.048297
Mo 0.153912 -0.002231 0.090115
Mo 2.975689 0.000641 -0.031667
S 2.101934 -0.075173 1.992111
S 1.771200 1.707404 -0.842958
S 5.113052 0.007477 -0.222605
S 1.768863 -1.638773 -0.968590
S -1.423620 0.068893 -1.716951
S -1.493514 -0.067292 1.757473
Mo -2.947405 0.000820 -0.027217
S -4.160491 1.763305 0.027341
S -4.155687 -1.763910 -0.108462

[Mo3S8]- XIII
E= -3391.048014
S -3.273890 -1.760193 -0.922480
Mo -1.505708 -1.005749 0.020223
Mo -0.363292 1.610604 0.165023
S 1.601003 1.468148 1.313442
Mo 1.617192 -0.357798 -0.163370
S 1.557198 -1.927404 1.626788
S 0.452334 -2.579113 -0.017134
S -1.902511 0.630151 1.587248
S -0.221219 0.110136 -1.623951
S -0.903769 3.541510 -0.638724
S 3.351851 -0.131761 -1.382617

E= -3391.019689
S -3.946007 -1.979234 -0.679483
Mo -2.207229 -0.953550 0.040072
Mo -0.440639 1.470841 0.202909
S 1.508840 1.436620 1.368585
Mo 1.815064 -0.285497 -0.193801
S 3.018648 -1.576299 1.402731
S 1.818379 -2.643344 0.072328
S -2.212325 0.794774 1.551653
S -0.331791 -0.368274 -1.292598
S -0.762364 3.311857 -0.823760
S 3.092732 0.415441 -1.728554

[Mo3S8]- XIV
E= -3390.898948
S -3.795647 -1.751628 -0.436437
Mo -2.650845 0.000580 -0.000043
S -0.937043 -0.363837 1.699653
S 0.069659 -2.024790 0.938443
Mo 0.977827 -0.000567 0.000890
S 0.071848 2.023038 -0.940418
S -0.935917 0.361707 -1.699282
S -3.793401 1.754333 0.436043
S 2.384175 -1.031106 -1.700262
Mo 3.406934 0.000649 -0.000418
S 2.384795 1.030546 1.701137

E= -3390.899344
S -3.863140 -1.741364 -0.471502
Mo -2.714372 -0.000046 0.000110
S -0.983817 -0.406917 1.685058
S -0.012081 -2.037225 0.819430
Mo 0.941400 0.000101 0.000178
S -0.011837 2.037495 -0.819406
S -0.983688 0.406986 -1.684597
S -3.863427 1.741301 0.470831
S 2.367277 -0.953382 -1.609808
Mo 3.671217 -0.000094 -0.000227
S 2.367823 0.953207 1.609836

[Mo3S8]- XV
E= -3390.948395
S -4.666129 -1.010009 -0.586641
Mo -2.631198 -0.467943 -0.101442
S -1.698531 1.438963 -1.147179
S -0.834096 2.597838 0.384622
Mo 0.214544 0.469199 0.102423
S -0.660072 -1.774213 0.532765
S -1.291555 -0.427650 1.973268
S 2.038459 0.741966 1.631122
Mo 2.955745 0.027650 -0.270137
S 4.349011 -1.610832 -0.215522
S 1.347796 -0.031942 -1.865899

E= -3390.992897
S -4.609876 0.864342 0.034356
Mo -2.691275 0.032357 -0.425317
S -1.167523 1.404870 -1.328412
S -0.205350 1.085970 2.346999
Mo 0.105949 0.298638 0.396686
S -2.353384 -2.268449 -0.841949
S -1.626808 -1.510891 0.974015
S 1.535962 -1.626210 0.401837
Mo 3.107296 -0.074552 -0.168116
S 5.214824 -0.365894 -0.503088
S 1.841985 1.743099 -0.567301

[Mo3S8]- XVI
E= -3390.989449
S -1.556127 -2.679398 0.134820
Mo -2.119091 -0.645698 0.381613
S -1.044845 0.350339 2.091865
S -0.057154 2.913570 -0.524817
Mo 0.245826 0.923419 0.140245
S 1.040733 -0.361643 -1.676947
Mo 2.827832 -0.146059 -0.359211
S 3.975688 -1.932739 -0.053686
S 2.208927 0.962963 1.475568
S -2.751450 0.590477 -1.486558
S -4.321512 -0.189181 -0.387194

E= -3391.000897

S -1.264180 0.032848 -1.778075
Mo -2.547910 -0.241891 0.001322
S -1.263908 0.048845 1.778062
S 0.280884 2.748175 -0.011913
Mo 0.272640 0.634511 -0.002740
S 1.827730 -0.096888 -1.759170
Mo 3.216127 -0.400067 0.001589
S 5.264301 -1.071066 0.004537
S 1.828396 -0.080014 1.759895
S -4.839767 0.231865 -0.001109
S -4.303206 -1.794216 0.007324

[Mo3S8]- XVII
E= -3391.008487
Mo 0.270846 0.281461 0.290861
Mo 2.961297 -0.117912 0.166679
S 4.134071 -0.971444 -1.415489
S 1.613447 -1.383008 1.427379
S -1.504948 -0.297336 1.866320
Mo -2.381316 -0.403847 -0.194631
S -0.583388 -0.679277 -1.592947
S 2.022096 1.901338 -0.094090
S -3.065308 1.761921 -0.458935
S -1.072656 2.322245 -0.037966
S -3.776736 -2.023658 -0.384409

E= -3391.025708
Mo 0.392500 0.024832 -0.080470
Mo 3.442705 -0.080100 -0.122019
S 5.500433 -0.166437 0.481621
S 1.930497 1.726487 -0.111513
S -1.012302 0.047145 -1.828607
Mo -2.435075 0.228150 0.047254
S -0.853739 -0.042601 1.780299
S 1.823908 -1.778085 -0.197336
S -4.036825 -1.216481 -0.962634
S -3.943818 -1.270243 1.118719
S -3.083496 2.246402 0.126943

[Mo3S8]- XVIII
E= -3391.029284
S -0.999917 0.015883 -1.849480
Mo -2.532302 0.291649 -0.111785
S -1.349999 -0.386270 1.858437
S -0.462316 -2.194376 1.244746
Mo 0.274817 -0.391223 -0.027874
S 1.318058 1.548926 0.765280
Mo 2.948436 0.446276 -0.332187
S -4.182772 -1.032611 -0.447075
S 2.093529 -1.408577 -1.205532
S -3.053059 2.342397 0.187700
S 4.822730 0.204537 0.684520

E= -3390.983884
S -1.250270 -1.702533 -1.013119
Mo -2.682770 -0.257659 -0.055369
S -1.588681 1.660318 -0.903789
S -0.111846 2.381249 0.428201
Mo 0.220865 0.064792 0.080796
S 1.608984 0.029488 -1.825253
Mo 2.971351 -0.485282 -0.119350
S -1.672786 -0.105476 1.921310
S 1.655528 -0.747373 1.705155
S -4.837177 -0.251319 -0.153444
S 4.858952 0.515787 0.087489

[Mo3S8]- XIX
E= -3391.055642
S -1.783606 -0.237897 1.791016
Mo -3.007934 -0.605475 0.000411
S -1.783625 -0.240745 -1.790823
S -0.417912 2.575688 -0.001761
Mo -0.253716 0.478517 -0.000428
S 1.299589 -0.116809 -1.754248
Mo 2.729978 -0.255892 0.000212
S 3.720470 -2.159881 0.001448
S 1.299384 -0.114012 1.754310
S -5.078452 -0.060105 0.000240
S 4.139790 1.358745 -0.000694

E= -3391.019337
S -1.283994 -1.817023 0.243916

Mo -3.020859 -0.392813 -0.276514
S -1.992916 1.616056 -0.978098
S -1.177641 2.093085 0.906249
Mo -0.103070 0.167959 0.112508
S 1.229975 0.256598 -1.741031
Mo 2.752098 -0.144134 -0.030334
S 3.633311 -2.088688 -0.223839
S 1.406464 -0.019696 1.847740
S -5.040126 -0.511374 0.440242
S 4.200981 1.439634 0.014961

[Mo3S8]- XX
E= -3391.015616
S 0.000000 0.099993 1.847453
Mo 1.373438 -0.298596 -0.068325
Mo -0.000000 1.918135 0.392651
Mo -1.373437 -0.298593 -0.068325
S -1.932160 1.848007 -0.828508
S 1.932153 1.848005 -0.828517
S 2.868168 -1.551099 1.168929
S 3.507274 -1.400008 -0.813575
S 0.000003 -1.361273 -1.573121
S -2.868190 -1.551065 1.168930
S -3.507251 -1.400044 -0.813592

E= -3390.979366
S 0.053440 0.303874 1.785989
Mo 1.481735 -0.277990 -0.095422
Mo -0.309148 2.060880 0.293010
Mo -1.310083 -0.390927 -0.077518
S -2.236757 1.595892 -0.857908
S 1.660522 1.921816 -0.902769
S 3.136280 -1.184072 1.282580
S 3.563296 -1.333983 -0.752018
S 0.132037 -1.472802 -1.512545
S -2.675965 -1.625193 1.313493
S -3.271924 -1.859436 -0.672005

[Mo3S8]- XXI
E= -3390.981778
S 0.486340 2.239149 2.139011
Mo 0.381547 1.705641 0.063986
Mo 1.124880 -0.706083 -0.406300
S -0.309398 -1.542166 -1.952050
Mo -1.418521 -0.163891 -0.364702
S -2.431710 -0.442647 1.679152
S -3.115353 -1.807406 0.262139
S -1.582547 1.968442 -1.200707
S 2.304194 1.213540 -1.126200
S 3.128839 -1.772406 0.586946
S 1.288883 -2.050132 1.467623

E= -3390.969879
S 1.267233 2.126033 1.972039
Mo 0.621796 1.603947 -0.002522
S -1.564616 2.091647 -0.629221
Mo -1.733008 -0.169414 -0.193780
S -4.065843 -0.827049 -0.204849
S -2.986349 -0.857084 1.600753
S 2.183305 1.235033 -1.825252
Mo 1.250737 -0.759612 -0.351980
S 3.420908 -1.684751 0.164303
S 1.885877 -1.938575 1.539807
S -0.506770 -1.735856 -1.425242

[Mo3S8]- XXII
E= -3391.074105
S -2.176987 2.929121 0.936181
Mo -1.066791 1.376963 -0.077534
S -2.325122 0.002524 -1.431278
Mo -1.070534 -1.375199 -0.077489
S -2.185552 -2.923970 0.936079
S 0.845212 1.897390 -1.258404
Mo 1.453474 -0.001832 -0.072186
S 3.836530 -0.001894 -0.453273
S 3.193236 -0.002774 1.513231
S -0.232867 -0.000301 1.611927
S 0.840659 -1.899917 -1.258041

E= -3391.043333
S -0.404545 3.614386 0.909017
Mo -0.404348 1.691207 -0.049790

S -2.274967 0.976273 -1.113619
Mo -1.689460 -1.036336 0.073595
S -3.359793 -2.346114 0.428336
S 1.417117 1.436372 -1.418171
Mo 1.368962 -0.473339 -0.114234
S 3.697963 -0.954865 -0.487420
S 2.957423 -1.212983 1.442956
S -0.232679 0.038967 1.631869
S 0.102200 -2.028556 -1.155592

[Mo3S8]- XXIII
E= -3391.030163
S -0.584747 -0.686698 -1.600897
Mo 0.273895 0.537097 0.086866
S -0.877975 2.543599 0.529089
S -1.624987 0.906627 1.601210
Mo -2.422234 -0.484255 -0.178220
S -2.902937 -2.350401 0.746046
S -4.037643 0.462608 -1.221075
S 2.102915 1.475668 -1.172180
Mo 2.998643 -0.058818 0.165349
S 4.265073 -1.557994 -0.699888
S 1.428252 -0.777721 1.623457

E= -3391.013238
S 0.948721 0.299827 -1.794025
Mo -0.165714 -0.298597 0.081427
S 0.700760 -2.160842 1.249460
S 1.538476 -0.333772 1.844907
Mo 2.633192 0.301261 -0.190125
S 3.298209 2.295804 0.199001
S 4.181702 -1.077701 -0.727288
S -1.968631 -1.486342 -1.056703
Mo -3.188953 0.227035 -0.172560
S -5.310722 0.466391 0.071581
S -1.494643 1.393678 0.951371

[Mo3S8]- XXIV
E= -3390.960648
S -0.928784 -1.436253 -1.094561
Mo -0.107505 0.390589 0.093524
S -1.186155 2.441780 -0.131115
S -2.106329 1.185205 1.340497
Mo -2.718922 -0.713634 0.105770
S -4.665629 -0.587357 -0.789393
S 1.568607 0.655894 -1.673554
Mo 2.587024 -0.306275 0.227636
S 3.692238 -2.138713 0.053590
S 1.091543 -0.212047 1.970507
S 3.162941 1.743456 -0.796662

E= -3390.969940
S -0.941253 -1.434065 -1.076956
Mo -0.081276 0.382141 0.088439
S -1.178835 2.418438 -0.174532
S -2.078056 1.225005 1.346313
Mo -2.761824 -0.648195 0.068008
S -4.776592 -0.683010 -0.687139
S 1.598377 0.627868 -1.675948
Mo 2.607745 -0.313495 0.237182
S 3.703918 -2.151186 0.069026
S 1.105352 -0.212181 1.974429
S 3.184893 1.730450 -0.808467

[Mo3S8]- XXV
E= -3390.949815
S 0.769812 0.022523 -1.813924
Mo -0.458023 -0.182617 0.102171
S 0.110298 -2.100959 1.339983
S 1.274637 -0.425188 1.841522
Mo 0.440190 0.110732 -0.196051
S 3.231486 2.079033 0.084353
S 3.887636 -1.411634 -0.626785
S -2.325680 -1.238980 -1.162241
Mo -2.696532 0.894635 -0.196358
S -1.098309 1.977122 0.945366
S -3.974672 -1.061635 0.153600

E= -3390.949761
S 0.679985 0.231411 -1.772481
Mo -0.401318 -0.176446 0.201561
S 0.218350 -2.121684 1.333266

S 1.423558 -0.473667 1.861030
Mo 2.420054 0.136905 -0.232275
S 3.286820 2.064855 0.093297
S 3.808105 -1.382351 -0.827996
S -2.195486 -1.189918 -1.213432
Mo -2.818820 0.905370 -0.223479
S -1.207999 1.785846 1.165237
S -3.913111 -1.187291 0.028336

[Mo3S7]2- I
E= -2992.789920
Mo -0.243677 -0.000015 -0.161622
Mo -3.117471 -0.000000 -0.227961
S -1.679794 -1.791277 -0.368114
S -1.679776 1.791256 -0.368142
S -4.884227 0.000033 1.047043
S 3.843710 1.824734 0.230891
S 1.348496 -0.000022 -1.798687
Mo 2.679336 0.000005 0.116658
S 0.997602 0.000002 1.742517
S 3.843745 -1.824699 0.230919

E= -2992.797388
Mo 0.241270 -0.002755 -0.160698
Mo 3.132735 0.000896 -0.228775
S 1.664792 1.786045 -0.349461
S 1.669634 -1.788438 -0.346538
S 4.925690 0.003788 1.019478
S -1.008475 -0.001100 1.742672
S -3.854610 -1.821248 0.230878
Mo -2.683959 0.000872 0.113582
S -1.359072 -0.002968 -1.800960
S -3.849327 1.826511 0.228141

E= -2992.772622
Mo -0.147327 -0.000086 0.123209
Mo -3.254058 0.000038 0.109621
S -1.725369 -1.765669 0.281105
S -1.725631 1.765440 0.281191
S -5.299860 0.000030 -0.643958
S 1.415473 -0.000337 1.810617
S 3.945724 1.815271 -0.171781
Mo 2.749236 0.000029 -0.086075
S 1.154516 -0.000303 -1.770524
S 3.947036 -1.814381 -0.171882

[Mo3S7]2- II
E= -2992.700476
Mo -3.234407 -0.216241 0.000166
S -1.795174 -0.362049 -1.786615
S -4.990027 1.073555 0.000759
S -1.794309 -0.364267 1.786100
Mo -0.346708 -0.164827 -0.000463
S 0.886931 1.758824 0.000440
S 1.234037 -1.854470 -0.000737
Mo 2.504218 0.074939 0.000173
S 4.518902 1.323213 0.000463
S 4.766495 -0.771216 -0.000084

E= -2992.717135
Mo -3.261849 -0.009523 -0.194631
S -1.826678 1.771854 -0.451068
S -5.054274 0.044846 1.052589
S -1.836935 -1.800740 -0.231834
Mo -0.375035 -0.001321 -0.171770
S 0.924332 0.126024 1.702034
S 1.230590 -0.144849 -1.806743
Mo 2.552790 0.001129 0.069726
S 4.707511 -1.040850 0.330168
S 4.701202 1.069215 0.183625

E= -2992.692688
Mo 2.784639 0.000178 -0.275465
S 3.365141 1.906954 -1.164409
S 3.365318 -1.906593 -1.164245
S 2.343464 -0.000387 2.072634
Mo 0.524872 -0.000177 0.643062
S -0.971489 -1.757805 0.235783
S -0.971489 1.757620 0.236819
Mo -2.505769 -0.000034 -0.083191
S -4.828310 0.000302 0.555576
S -4.412459 -0.000006 -1.518721

[Mo3S7]2- III
E= -2992.567281
S -0.001945 -0.000344 -1.911273
Mo -1.497291 -0.123262 -0.099810
S -0.736792 -1.561821 1.740511
S -1.185468 -2.504712 -0.832468
Mo 0.854010 -1.235244 -0.101920
S 2.760074 0.227094 -0.836583
S 1.734452 0.143424 1.731527
Mo 0.640413 1.357838 -0.102350
S -0.983264 1.421773 1.740298
S -1.579527 2.276339 -0.833802

E= -2992.667356
S 0.112261 -1.230280 -0.653346
Mo -2.137010 -0.685939 -0.123834
S -3.530087 -2.372632 0.168765
S 3.886208 -1.865940 -0.071922
Mo 2.315159 -0.309828 0.047108
S 1.951398 1.468684 -1.407071
S 1.434705 0.666840 1.976086
Mo 0.033862 1.078309 0.058338
S -2.228375 1.465813 1.067904
S -2.182638 1.650841 -1.032149

E= -2992.565368
S -0.001034 0.156530 -1.920833
Mo 0.010070 -1.474405 -0.217365
S 1.973407 -1.144984 1.307741
S 2.504410 -1.356995 -0.694605
Mo 1.270684 0.883834 -0.011346
S -0.020037 2.884816 -0.671740
S -0.007146 1.291177 1.994772
Mo -1.283101 0.867265 -0.011271
S -1.957533 -1.171453 1.308140
S -2.485905 -1.385412 -0.693523

[Mo3S7]2- IV
E= -2992.665923
Mo -0.414280 0.953065 -0.006491
Mo 1.290683 -0.608675 0.233211
S -0.417956 -0.354142 2.031472
Mo -1.457685 -1.204126 0.021658
S -3.551927 -1.014827 -0.574223
S 0.258242 -2.581249 -0.689825
S -0.569040 2.879359 -1.460481
S -0.810392 3.318901 0.597584
S 3.490406 -0.808479 -0.916599
S 3.126533 0.817245 0.360079

E= -2992.532292
Mo -1.264616 -0.737935 -0.063281
Mo -0.000495 1.315706 -0.033051
S 0.000148 -0.197713 1.908812
Mo 1.265166 -0.737143 -0.063306
S 3.200267 -1.437273 -1.337496
S 3.339920 -1.766809 0.749466
S -3.199529 -1.438846 -1.337337
S -3.339009 -1.768179 0.749659
S -0.001444 3.441436 -1.217596
S -0.000499 3.585736 0.903544

E= -2992.527760
Mo -0.823594 -1.124648 0.022141
Mo -0.834454 1.118572 0.021837
S 0.139597 0.002200 1.912509
Mo 1.596395 0.007104 -0.109398
S 3.641731 0.014104 -1.402579
S 3.889827 0.012503 0.707404
S -2.033877 -2.746831 -1.263296
S -1.692575 -3.300660 0.740837
S -2.060282 2.729092 -1.263430
S -1.722583 3.286894 0.740280

[Mo3S7]2- V
E= -2992.721355
Mo 0.963510 -1.239701 0.027199
Mo -1.617425 -0.218934 0.021598
Mo 0.887137 1.203328 -0.080952
S -1.497595 2.278067 -0.069030
S -0.720989 1.487649 1.688580

S -0.695603 -1.842905 1.503397
S 2.902760 2.030812 -0.251642
S -0.061216 -0.165681 -1.804554
S -3.482413 -0.914511 -0.915470
S 2.942849 -2.203251 -0.066873

E= -2992.561597
Mo 0.025884 -1.025155 -0.899655
Mo 1.468459 0.227397 0.231240
Mo -1.668405 0.018166 0.275928
S -0.163488 1.955445 1.086275
S 1.158653 2.580349 -0.430477
S 3.638999 0.228696 -0.914944
S -3.734086 1.030710 -0.628321
S 0.000656 -1.462281 1.450868
S 3.375856 -1.266555 0.530916
S -3.819679 -1.019937 -0.064038

E= -2992.620645
Mo 0.692094 -1.687679 -0.034937
Mo 1.067819 0.720489 -0.123362
Mo -1.773125 -0.022601 0.149883
S -0.164258 2.951444 -0.338105
S -0.772331 1.335770 -1.571926
S 2.978969 -0.687316 -0.526927
S -3.857630 0.417620 0.712396
S -0.074233 -0.146864 1.778217
S 3.353645 0.896165 0.886876
S -1.429479 -2.168617 -0.918441

[Mo3S7]2- VI
E= -2992.704081
Mo 0.355238 -1.796093 0.185405
Mo 1.423868 0.570353 0.047365
Mo -1.498234 0.211993 -0.005924
S -1.293623 2.601011 -0.647514
S 0.004492 1.302082 -1.708351
S 2.477017 -1.501440 -0.640664
S -3.446790 0.334438 1.023394
S -0.035223 -0.127585 1.803413
S 3.025086 1.931801 0.745457
S -1.468245 -1.879223 -1.171207

E= -2992.627153
Mo -0.036913 -1.775903 -0.074478
Mo -1.203126 0.208222 0.052160
Mo 1.580374 0.335963 0.007226
S 0.075549 1.352088 -1.673342
S 0.285419 2.517737 0.045306
S -3.351461 -0.015748 1.182510
S 3.505614 0.828761 0.979535
S 1.804462 -1.515436 -1.503292
S -3.483071 0.524970 -0.855385
S 0.270108 -0.459113 1.864283

E= -2992.575708
Mo 0.324760 2.320930 -0.000099
Mo -1.149571 -0.313831 -0.000140
Mo 1.553122 -0.471051 0.000242
S 0.142138 -2.200397 1.036044
S 0.141004 -2.199806 -1.035080
S -3.309929 -0.260129 -1.059698
S 3.744505 -0.703937 -0.000811
S 0.340540 0.794849 1.732795
S -3.309982 -0.257369 1.059859
S 0.339906 0.794662 -1.733115

[Mo3S7]2- VII
E= -2992.834242
Mo -0.956867 -1.308050 0.068447
Mo -0.654821 1.482246 0.067798
Mo 1.611217 -0.174438 0.068145
S 3.518025 -0.378404 -1.011166
S -1.429087 3.236686 -1.011195
S -2.087758 -2.855884 -1.012184
S -2.120168 0.230264 1.365381
S 0.861847 -1.952062 1.364302
S 0.000106 -0.000591 -1.597386
S 1.258270 1.720625 1.365726

E= -2992.800005
Mo -1.598677 -0.796557 0.063770

Mo 0.000058 1.551335 0.049816
Mo 1.598252 -0.797335 0.064236
S 3.454144 -1.550524 -0.816603
S 0.001028 3.452215 -1.048680
S -3.455210 -1.549358 -0.816048
S -1.815331 1.099443 1.410481
S -0.000417 -2.277741 0.965315
S 0.000279 -0.161112 -1.571434
S 1.816471 1.098787 1.410187

E= -2992.788128
Mo -1.994226 -0.001284 -0.007311
Mo 0.979133 1.402868 0.061597
Mo 0.980563 -1.402175 0.061169
S 2.302093 -2.903346 -0.804368
S 2.297856 2.906650 -0.803983
S -4.127355 -0.000833 -0.483439
S -1.126488 2.057416 0.855613
S -1.124242 -2.058912 0.855610
S -0.080031 0.000076 -1.540059
S 1.948807 0.000502 1.617557

[Mo3S7]- I
E= -2992.730703
S -0.982101 -0.896793 1.760331
Mo 0.186044 0.203003 0.123298
S 1.315382 -1.126977 -1.357826
Mo 2.968952 0.086078 -0.367740
S 4.591483 -0.985119 0.539132
Mo -2.596721 -0.273365 0.247363
S -3.858262 -1.849906 -0.483444
S -2.886535 2.059091 -0.022152
S -1.486442 1.136195 -1.328056
S 1.841001 1.622253 0.884348

E= -2992.726999
S -0.985377 -0.937526 1.724748
Mo 0.190908 0.184276 0.115422
S 1.354601 -1.213678 -1.308307
Mo 2.975743 0.071757 -0.387939
S 4.593628 -0.901229 0.624091
Mo -2.621047 -0.251958 0.249077
S -3.921973 -1.785556 -0.502279
S -2.909660 2.050671 0.020117
S -1.443389 1.138108 -1.298013
S 1.879957 1.638515 0.801175

[Mo3S7]- II
E= -2992.724566
Mo 0.170082 -0.104261 0.427025
Mo 2.970269 -0.290113 0.083825
S 1.388779 -1.633624 -0.808188
S 1.876527 1.104477 1.479096
S 4.370522 0.534158 -1.318264
S -0.953471 1.165499 -1.195187
S -2.449331 2.288433 -0.093943
Mo -2.648500 -0.033068 0.004513
S -1.491535 -1.088978 1.684127
S -4.032600 -1.247932 -1.100466

E= -2992.724352
Mo 0.120433 0.109197 0.107685
Mo 2.954296 -0.357468 0.172276
S 1.338637 -1.486155 -1.002174
S 1.753587 1.226261 1.303929
S 4.817176 0.181256 -0.763950
S -1.377532 0.729117 -1.666108
S -1.684946 2.164958 -0.191273
Mo -2.707672 -0.042791 0.146632
S -1.278646 -0.997456 1.606729
S -4.531802 -1.053943 -0.406962

E= -2992.698757
Mo 0.096552 0.021380 0.008251
Mo 3.141281 -0.042132 -0.216914
S 1.784087 -1.818878 -0.064771
S 1.755945 1.737031 -0.273438
S 5.229249 0.017515 0.295110
S -1.625371 1.708246 -0.617483
S -3.069613 1.910998 0.931504
Mo -2.744822 -0.260398 0.098662
S -1.277975 -1.532722 1.236825

S -4.090475 -1.284173 -1.218995

[Mo3S7]- III
E= -2992.796074
S -0.876799 0.000993 1.712217
Mo 0.254329 -0.099040 -0.221911
S -1.324965 -0.001482 -1.816554
Mo -2.615931 -0.000070 0.137788
S -3.752324 -1.814587 0.279317
S -3.751137 1.815359 0.277029
S 1.709516 1.804755 -0.419048
Mo 3.070949 0.000083 -0.288705
S 4.423461 -0.000018 1.364528
S 1.710211 -1.804819 -0.418815

E= -2992.793904
S -1.113824 -0.000735 -1.779621
Mo 0.162202 0.000528 0.083971
S -1.303219 0.000294 1.805579
Mo -2.703846 -0.000233 -0.065608
S -3.866091 1.800711 -0.126216
S -3.864722 -1.801999 -0.126063
S 1.622397 -1.761666 0.175454
Mo 3.185748 0.000747 0.146952
S 5.212718 -0.002420 -0.556403
S 1.621970 1.763080 0.173319

E= -2992.766536
S -1.229018 0.000662 -1.712030
Mo 0.223498 -0.000089 0.088908
S -1.394762 -0.000524 1.741876
Mo -2.857266 -0.000015 -0.059656
S -4.063642 1.767128 -0.116038
S -4.063819 -1.767062 -0.117145
S 1.774839 -1.757511 0.183796
Mo 3.321775 0.000095 0.087020
S 5.395494 -0.000173 -0.469474
S 1.774940 1.757507 0.183804

[Mo3S7]- IV
E= -2992.704074
Mo 2.774555 0.309905 0.006216
S 2.882047 1.363916 1.870532
S 2.881339 1.439314 -1.813529
S 2.510431 -1.988822 -0.040644
Mo 0.429818 -0.824243 -0.016415
S -0.982416 -0.389828 -1.787785
S -0.984291 -0.465148 1.770419
Mo -2.317134 0.022161 0.000213
S -4.637839 -0.327496 -0.009540
S -3.998275 1.660028 0.036761

E= -2992.742338
Mo -3.225731 0.001017 -0.242292
S -1.820555 1.789696 -0.357304
S -4.752224 -0.006575 1.269876
S -1.820008 -1.785962 -0.377238
Mo -0.391610 0.001365 -0.215863
S 0.886871 -0.010795 1.689392
S 1.270298 0.011851 -1.823227
Mo 2.496820 -0.000274 0.079079
S 4.588470 -1.048390 0.288898
S 4.588514 1.044644 0.304678

E= -2992.691496
Mo 3.002612 0.000250 -0.236945
S 3.329375 1.868031 -1.249938
S 3.329431 -1.864681 -1.255140
S 2.284550 -0.003014 2.021650
Mo 0.398333 -0.000631 0.746168
S -1.053801 -1.729970 0.268423
S -1.054631 1.729488 0.272517
Mo -2.524738 -0.000053 -0.095195
S -4.801053 -0.001438 0.451404
S -4.333914 0.002723 -1.595740

[Mo3S7]- V
E= -2992.635897
S 0.267842 0.001357 -1.877697
Mo -0.652431 -1.316388 -0.149250
S 0.397011 -1.356300 1.908463
S 1.752405 -2.215912 -0.675520

Mo 1.525310 0.002185 0.103599
S 1.743303 2.222907 -0.672083
S 0.394946 1.351653 1.911264
Mo -0.655921 1.314732 -0.147233
S -2.467561 -0.004344 0.988732
S -2.657462 -0.000748 -1.076841

E= -2992.610079
S 0.000043 0.001525 -1.999834
Mo 0.001846 -1.493743 -0.103140
S 1.888257 -1.062198 1.456283
S 2.515138 -1.471422 -0.484297
Mo 1.317536 0.761044 -0.133696
S -0.003561 2.907650 -0.446182
S -0.002686 2.102824 1.474890
Mo -1.319430 0.757823 -0.133811
S -1.885576 -1.066691 1.456316
S -2.511491 -1.477637 -0.484226

[Mo3S7]- VI
E= -2992.554158
Mo 0.097724 -1.072440 0.192277
Mo -1.314455 0.761784 -0.177541
S 0.048030 0.886059 1.788834
Mo 1.305473 0.942481 -0.237850
S 3.388230 0.620540 -1.272341
S 3.503899 1.155001 0.740779
S -0.055410 -3.068413 -1.044825
S -0.258174 -3.454127 0.972538
S -3.389495 0.774264 -1.289083
S -3.470028 1.428137 0.689774

E= -2992.548229
Mo -1.406622 -0.285744 -0.095114
Mo 0.453252 1.355053 -0.097158
S -0.001804 -0.001962 1.834038
Mo 0.945533 -1.074506 -0.097110
S 2.340048 -2.640841 -1.224092
S 2.403951 -2.702920 0.866342
S -3.461667 -0.694870 -1.224949
S -3.552242 -0.709005 0.866034
S 1.128656 3.340688 -1.224070
S 1.163628 3.422553 0.866325

[Mo3S7]- VII
E= -2992.726999
S -0.984661 -0.937498 1.724431
Mo 0.190961 0.184740 0.115041
S 1.880181 1.637948 0.802375
Mo 2.975849 0.071813 -0.387700
S 1.354599 -1.212386 -1.309605
Mo -2.620972 -0.252192 0.249220
S -3.922702 -1.785398 -0.501585
S -1.443769 1.137886 -1.298434
S -2.909825 2.050204 0.020393
S 4.593353 -0.902202 0.623953

E= -2992.730702
S -0.981701 -0.897494 1.759660
Mo 0.186193 0.203159 0.122981
S 1.841167 1.622177 0.884637
Mo 2.968838 0.086280 -0.367896
S 1.315552 -1.126273 -1.358861
Mo -2.596502 -0.273532 0.247225
S -3.857885 -1.850316 -0.483353
S -1.486684 1.137068 -1.327531
S -2.886369 2.059242 -0.020889
S 4.589783 -0.986158 0.540273

E= -2992.716311
S 1.018062 -1.795777 -0.002398
Mo -0.109762 0.168726 -0.000077
S -1.585063 0.282184 -1.799890
Mo -3.025238 -0.013512 0.000012
S -1.584699 0.277401 1.800300
Mo 2.816457 -0.237225 -0.000523
S 4.823573 -1.034602 -0.000278
S 1.594320 1.652313 1.048111
S 1.594026 1.655357 -1.044102
S -5.024043 -0.821596 -0.000201

[Mo3S7]- VIII

E= -2992.641379
S 2.559309 -1.376052 -0.870777
Mo 1.486829 0.566039 -0.193899
S 1.318685 -0.860990 1.886817
Mo 0.137657 -1.548510 0.022344
S -0.050494 -0.104902 -1.889860
Mo -1.180168 0.682257 0.012374
S -3.299365 -0.284247 -0.630189
S -2.229951 -1.326702 0.914151
S 0.204987 2.768090 -0.464743
S 0.330494 1.972863 1.472451

E= -2992.669499
Mo -0.790817 1.594249 -0.043612
Mo -1.039076 -0.767194 -0.178826
Mo 1.691299 -0.008549 0.113803
S 0.894340 -2.434389 -0.041190
S 0.764776 -1.244471 -1.760604
S -3.097240 0.445395 -0.525733
S 3.780502 -0.282640 0.624767
S -0.073518 0.222804 1.767537
S -3.224907 -1.174386 0.847444
S 1.319856 2.319109 -0.627054

E= -2992.593096
Mo 0.368938 -1.663901 -0.153301
Mo 1.167146 0.603040 -0.066784
Mo -1.586677 0.655265 0.148565
S -0.320829 2.786927 0.117378
S -0.285070 1.694936 -1.688482
S 2.799636 -1.070180 -0.710872
S -3.335405 -0.880695 0.637587
S -0.103944 -0.071760 1.833559
S 3.366997 0.214429 0.902370
S -1.988579 -1.608965 -0.903801

[Mo3S7]- IX
E= -2992.652837
Mo 0.810759 -1.592981 -0.265926
Mo 0.798239 0.854143 0.288470
Mo -1.727012 -0.209882 -0.011100
S -1.250726 2.134262 0.660487
S 0.311146 3.066982 -0.504332
S 2.815372 -0.140323 -0.961566
S -3.711721 -1.063502 -0.253666
S -0.327119 -0.886014 1.758674
S 2.684328 -0.555772 1.063878
S -0.211493 -0.065242 -1.793515

E= -2992.651798
Mo 0.804249 -1.585563 -0.274068
Mo 0.797005 0.849436 0.294831
Mo -1.720290 -0.206124 0.001151
S -1.259905 2.128218 0.645898
S 0.339048 3.060547 -0.493388
S 2.802589 -0.136353 -0.966522
S -3.708595 -1.042070 -0.265655
S -0.331494 -0.907814 1.758210
S 2.695551 -0.562168 1.057779
S -0.224725 -0.066951 -1.793848

E= -2992.634864
Mo -1.722791 -1.375159 -0.000035
Mo -0.561707 0.926632 0.000109
Mo 1.866190 -0.269183 0.000075
S 1.486857 1.976199 -1.034865
S 1.487439 1.976907 1.034086
S -2.860598 0.616511 1.047674
S 3.606557 -1.575130 0.000161
S 0.118958 -0.863723 -1.561865
S -2.860120 0.616404 -1.047701
S 0.118962 -0.863180 1.562117

[Mo3S7]- X
E= -2992.834759
Mo -1.357087 -0.939511 0.053175
Mo -0.135144 1.644858 0.053130
Mo 1.492254 -0.705477 0.053225
S 3.213140 -1.518044 -0.949206
S -0.291223 3.541778 -0.948987
S -2.922278 -2.022323 -0.949062
S -1.920598 0.908160 1.337647

S 0.174095 -2.118398 1.336744
S 0.000099 -0.000240 -1.583532
S 1.746705 1.209409 1.337628

E= -2992.807564
Mo -1.859173 -0.000580 -0.102798
Mo 0.891903 1.401351 0.077922
Mo 0.894178 -1.400427 0.078327
S 2.128582 -2.905529 -0.828539
S 2.124916 2.907086 -0.830072
S -3.979583 -0.002476 -0.479189
S -1.076702 1.965462 1.061276
S -1.074972 -1.966318 1.059770
S 0.015657 -0.000758 -1.613190
S 2.053967 0.001631 1.489634

E= -2992.782939
Mo -1.923127 -0.000705 -0.025257
Mo 0.968786 -1.525022 -0.008597
Mo 0.967279 1.525450 -0.007402
S 2.031334 3.269437 0.637471
S 2.033972 -3.267316 0.639024
S -4.009888 -0.001442 0.465165
S -1.092733 -2.019135 -0.929330
S -1.094518 2.018544 -0.928340
S -0.006773 -0.000725 1.572375
S 2.104646 0.001363 -1.348068

[Mo3S6]- I
E= -2526.252181
S -0.000068 -0.000426 1.748862
Mo -1.533109 -0.000028 0.000035
S -2.732013 1.773970 0.000043
Mo 1.533121 -0.000009 0.000001
S 2.732044 1.773038 0.000160
S 0.000063 0.000227 -1.748717
S -2.732411 -1.772906 -0.000229
S 2.732353 -1.772932 -0.000212

E= -2526.177396
S -0.000139 -0.669391 1.496516
Mo 1.742248 -0.017841 0.000112
S 3.406813 -1.366673 0.000328
Mo -1.742176 -0.017950 -0.000142
S -3.406835 -1.366634 -0.000230
S 0.000302 -0.669832 -1.496338
S 2.203395 2.083331 -0.000643
S -2.203723 2.083149 0.000446

E= -2526.134307
S 0.135982 -0.000446 1.738204
Mo 1.681340 0.000008 -0.000180
S 2.883695 -1.777071 -0.001109
Mo -1.406886 -0.000426 0.001144
S -3.378858 -1.293236 -0.000523
S 0.134244 -0.000529 -1.737145
S 2.882150 1.778143 -0.000531
S -3.377654 1.294235 -0.001427

[Mo3S13H]- I
E= -5382.779589
S -0.000607 0.000130 1.762748
Mo 1.571866 -0.396672 0.033280
S 0.522808 -1.840376 -1.634315
S 0.798143 -2.813127 0.126937
Mo -1.129907 -1.162571 0.032482
S -2.835460 0.716062 0.122612
S -1.853096 0.468185 -1.637528
Mo -0.442424 1.558961 0.032009
S 1.332696 1.371329 -1.635614
S 2.037291 2.097620 0.125183
S -2.509326 -2.580558 1.404838
S -2.778674 -2.860186 -0.631928
S -1.087135 3.835952 -0.630904
S -0.982934 3.461675 1.405995
S 3.865499 -0.975442 -0.633382
S 3.492518 -0.880796 1.404029
H -0.008051 0.004287 3.114914

E= -5382.758971
S 0.414542 0.000113 2.039656
Mo 0.794016 -1.357917 0.023260

S -1.045271 -1.823831 -1.556746
S -1.434354 -2.465817 0.340533
Mo -1.648654 -0.000459 -0.045926
S -1.435773 2.465036 0.340422
S -1.046276 1.823171 -1.556821
Mo 0.793223 1.358370 0.023261
S 1.738122 0.000494 -1.764957
S 2.916364 0.000844 -0.108985
S -3.629083 -0.001098 1.376814
S -4.141852 -0.001059 -0.570358
S 1.971767 3.432417 -0.686491
S 1.887007 3.080530 1.334594
S 1.973791 -3.431271 -0.686574
S 1.888806 -3.079545 1.334492
H 1.654725 0.000503 2.605727

E= -5382.742799
S 1.008826 -0.007372 1.998270
Mo 0.975614 1.443348 -0.024329
S 2.455892 3.019244 1.068291
S 2.042229 3.395662 -0.930158
Mo 0.847820 -1.508348 0.025972
S 2.178309 -3.174247 1.194713
S 1.680221 -3.609084 -0.766818
S -1.279437 -1.980355 -1.092073
Mo -1.988067 0.094031 0.001576
S -4.177561 -0.380791 -0.847106
S -4.114161 0.684393 0.928320
S -1.380793 -2.195606 0.953416
S 1.293090 -0.080679 -1.921408
S 2.879367 -0.136280 -0.645932
S -1.115542 2.246443 0.983894
S -1.183748 2.146481 -1.073501
H 2.327537 -0.064256 2.266298

[Mo3S13H]- II
E= -5382.822378
S -0.025332 0.001972 1.807742
Mo 1.548497 0.003626 -0.003839
S 0.978019 -1.688449 -1.646715
S 1.456709 -2.503965 0.158894
Mo -0.816156 -1.372182 0.012738
S -2.909917 -0.005761 0.063815
S -1.916606 -0.004420 -1.713375
Mo -0.822932 1.369066 0.012857
S 0.964089 1.688049 -1.650313
S 1.448448 2.510947 0.152995
S -1.787245 -2.997532 1.481873
S -2.035676 -3.453111 -0.529040
S -2.051163 3.445840 -0.526549
S -1.799093 2.989534 1.483929
S 4.020596 0.024054 -0.634577
S 3.660971 -0.084480 1.384356
H 3.743978 1.215759 1.757656

E= -5382.787381
S -0.037730 0.001147 1.792241
Mo 1.465843 -0.038475 -0.058890
S 0.857094 -1.801702 -1.635732
S 1.333269 -2.530488 0.221816
Mo -0.895382 -1.364350 0.021294
S -2.984305 0.072269 0.098946
S -1.955911 0.044255 -1.668198
Mo -0.827441 1.403398 0.018753
S 0.943537 1.747227 -1.642859
S 1.455400 2.461433 0.211522
S -1.927844 -3.032471 1.506369
S -2.163532 -3.449996 -0.463339
S -1.989487 3.546181 -0.469351
S -1.772171 3.115762 1.504433
S 3.891962 -0.086886 -0.708255
S 4.728179 -0.160502 1.207914
H 4.737783 1.156292 1.503253

E= -5382.746646
S 0.004002 -0.000334 1.703906
Mo 1.613665 -0.115265 -0.123678
S 0.764140 -1.810819 -1.679445
S 1.217258 -2.586015 0.173905
Mo -1.032945 -1.441444 0.012754
S -2.951545 0.188827 0.201054
S -2.029561 0.118242 -1.623494

Mo -0.837497 1.548660 -0.001094
S 0.987045 1.661659 -1.698316
S 1.547940 2.393122 0.143667
S -2.043608 -2.984723 1.586894
S -2.378033 -3.367499 -0.418941
S -1.923770 3.629928 -0.445960
S -1.630309 3.221472 1.562703
S 3.989900 -0.276883 -0.616889
S 4.819148 -0.234557 1.310796
H 4.822896 1.099357 1.506658

[Mo3S13H]- III
E= -5382.825844
S -0.017462 -0.005101 1.798055
Mo 1.537137 -0.239521 0.000812
S 0.690929 -1.798945 -1.674089
S 1.051716 -2.717577 0.115021
Mo -1.014795 -1.237973 0.005960
S -2.869923 0.433880 0.091666
S -1.917050 0.286878 -1.701512
Mo -0.603371 1.471541 0.009477
S 1.190279 1.500718 -1.672270
S 1.826486 2.267803 0.113653
S -2.207513 -2.700296 1.485744
S -2.551696 -3.096187 -0.523351
S -1.518016 3.704350 -0.516614
S -1.301754 3.219539 1.491121
S 4.075263 -0.605450 -0.491102
S 3.485516 -0.517139 1.485530
H 4.414845 0.687238 -0.712033

E= -5382.783318
S 0.021400 -0.086853 1.726737
Mo -0.190484 1.527623 -0.008368
S 1.588887 1.196736 -1.663437
S 2.331946 1.784437 0.150932
Mo 1.659862 -0.628330 -0.011767
S 0.362645 -2.840138 0.091302
S 0.241536 -1.826071 -1.670637
Mo -1.429937 -1.022316 -0.008757
S -1.825260 0.753300 -1.665252
S -2.697506 1.157729 0.144068
S 3.369970 -1.414441 1.478246
S 3.842160 -1.508481 -0.545640
S -3.325420 -2.421892 -0.535727
S -2.887614 -2.203206 1.486285
S -0.556072 4.055250 -0.422394
S -0.451609 3.423697 1.540135
H -1.897531 4.045871 -0.620404

E= -5382.743009
S 0.017305 -0.043379 1.768778
Mo -0.279058 1.542476 0.021974
S 1.503535 1.254971 -1.615635
S 2.239683 1.899643 0.184874
Mo 1.625405 -0.580767 -0.011323
S 0.508066 -2.734628 0.462530
S 0.315675 -1.660870 -1.798479
Mo -1.293628 -1.116215 -0.009111
S -1.828332 0.629354 -1.625511
S -2.762233 1.002150 0.163056
S 3.528193 -1.347135 1.333569
S 3.904053 -1.254120 -0.657057
S -3.187224 -2.552955 -0.644263
S -2.799797 -2.488096 1.348659
S -0.789257 4.009980 -0.432499
S -0.654920 3.444793 1.547258
H -2.130146 3.932592 -0.629160

[Mo3S13H]- IV
E= -5382.778791
S 0.107488 0.027438 1.832839
Mo -1.348979 -0.750063 0.051685
S -2.256422 0.562839 -1.987641
S -2.376412 1.579196 -0.167623
Mo 0.121881 1.619727 0.097629
S 2.601794 1.404263 -0.111568
S 1.518655 0.900967 -1.786998
Mo 1.389003 -0.802568 -0.019574
S -0.040537 -2.008975 -1.593737
S -0.024425 -2.880583 0.244327
S -0.090093 3.480146 1.502940

S 0.195851 4.019703 -0.436654
S 3.431211 -2.043036 -0.629175
S 3.108729 -1.695827 1.394134
S -3.489177 -2.032235 -0.190576
S -2.894987 -1.486420 1.711145
H -3.466776 -0.057607 -1.951707

E= -5382.785706
S -0.316100 -0.005652 1.946606
Mo 0.755015 1.306268 0.282641
S 2.462889 -0.065969 -2.781492
S 2.533003 -0.047901 -0.588055
Mo 0.697630 -1.343548 0.266103
S -1.589683 -2.492691 0.066866
S -0.812175 -1.632479 -1.631635
Mo -1.630158 0.032659 -0.054145
S -0.743510 1.688412 -1.602831
S -1.500387 2.553404 0.103001
S 1.891982 -2.709366 1.748446
S 2.014108 -3.475643 -0.143123
S -3.970179 0.079004 -0.933790
S -3.876418 0.068257 1.055302
S 2.164290 3.377194 -0.124184
S 2.025744 2.600860 1.767299
H 2.918508 1.195205 -2.891692

E= -5382.768081
S -0.134333 -0.005175 1.892918
Mo 0.768188 1.458520 0.229329
S 2.446061 -0.105306 -2.751004
S 2.465199 -0.069218 -0.596473
Mo 0.682566 -1.505136 0.213335
S -1.668799 -2.460466 0.099235
S -0.912455 -1.659961 -1.645237
Mo -1.589210 0.046044 -0.040093
S -0.815254 1.728706 -1.624677
S -1.532932 2.553231 0.125356
S 2.053204 -2.740181 1.732929
S 1.804200 -3.603346 -0.146186
S -4.018071 0.118097 -0.768947
S -3.764305 0.100892 1.196703
S 2.027520 3.480840 -0.134573
S 2.231856 2.643038 1.743467
H 2.904877 1.153431 -2.884124

[Mo3S13H]- V
E= -5382.813666
S 1.036560 -1.443565 0.809338
Mo -3.121834 -0.466928 -0.018500
Mo -0.443384 0.456945 -0.230106
Mo 3.061078 -0.558564 -0.112282
S 2.446075 -0.897618 2.214608
S 1.259585 -0.194651 -1.744156
S -3.199431 -2.579251 -0.180119
S 4.102998 -2.241984 -0.822312
S -1.668059 0.063385 1.707761
S -1.940652 0.263567 -1.910248
S -5.088847 0.591915 -0.847486
S -4.984438 0.360469 1.224458
S -0.351472 2.798486 -0.307970
S 1.054500 2.261231 1.113444
S 3.904071 1.391618 -1.150976
S 4.736006 0.978204 0.702715
H 0.263551 2.250060 2.212395

E= -5382.756334
S -0.600313 0.331318 1.905315
Mo 1.961341 -1.122326 -0.020302
Mo 0.650890 1.400999 -0.093723
Mo -2.190446 -0.415373 0.065833
S -1.440411 1.775998 -0.811799
S -2.617261 0.663573 2.141935
S -0.297962 -1.863272 -0.760422
S -1.536141 -2.691408 0.654198
S 1.695689 0.383039 -1.847726
S 2.311396 0.435053 1.539116
S 2.673471 -3.324485 0.551770
S 3.872304 -2.219425 -0.771259
S 1.727813 3.321535 0.540691
S 1.016174 4.836678 -0.770091
S -4.470493 -0.525336 -0.275629
S -3.428695 -1.075841 -1.955747

H -0.204121 4.982595 -0.221527

[Mo3S13H]- VI
E= -5382.816184
S 1.273911 -0.082605 -1.751127
Mo 3.041401 -0.584465 -0.125415
S 4.732057 0.862583 0.825018
S 3.929403 1.451178 -0.995142
S 0.987673 -1.469624 0.714815
S 2.400510 -1.045912 2.159945
Mo -0.449942 0.512304 -0.218051
S 1.002093 2.309540 1.167196
S -0.371041 2.854653 -0.288790
Mo -3.102529 -0.474286 -0.019324
S -4.982197 0.256306 1.258871
S -5.108875 0.542965 -0.804794
S -3.110246 -2.583505 -0.237615
S -1.663374 0.069319 1.712596
S -1.952784 0.348788 -1.893686
S 4.071865 -2.225199 -0.938901
H 2.120990 2.334970 0.383017

E= -5382.790287
S 1.250705 0.088676 -1.757194
Mo 2.952244 -0.632784 -0.144943
S 4.621614 0.698251 0.993549
S 3.959723 1.432216 -0.829264
S 0.864037 -1.574359 0.541510
S 2.247820 -1.301965 2.059958
Mo -0.418285 0.678956 -0.159841
S 1.020257 2.489901 1.122292
S -0.387655 3.037143 -0.311203
Mo -2.946664 -0.526450 -0.034871
S -4.960462 0.121019 1.223422
S -5.173685 0.260485 -0.760621
S -2.777964 -2.628223 -0.235933
S -1.661615 0.177625 1.759760
S -2.049729 0.516725 -1.867802
S 3.996444 -2.211543 -1.067851
H 2.141752 2.476451 0.335572

[Mo3S13H]- VII
E= -5382.810549
S 0.122787 -1.022122 -1.572319
Mo -3.621174 -0.261055 -0.197589
Mo 0.674854 0.706766 -0.091091
Mo 3.097632 -0.720191 0.215125
S 1.744177 0.264794 1.845906
S 2.023136 -0.196158 -1.888284
S -3.067069 -1.890493 -1.466647
S 2.995072 -2.818712 0.465452
S -1.490357 0.029675 1.144064
S -3.505887 1.608769 -1.210802
S -5.840161 -0.629649 0.479260
S -4.476741 -0.530042 2.038735
S 1.230648 2.812823 -0.838225
S -0.160225 2.899237 0.685089
S 5.098563 0.025117 -0.818565
S 5.006167 0.247168 1.246255
H -1.236884 -1.278368 1.330577

E= -5382.792078
S -0.994390 -0.987007 -1.081771
Mo -3.097829 -0.704164 0.143406
Mo 0.277402 0.942205 0.035491
Mo 2.956832 -0.777680 -0.138077
S 1.455843 -0.207095 1.614868
S 1.882600 0.210383 -1.831464
S -3.186500 -2.522337 1.243069
S 2.714690 -2.883056 -0.278127
S -1.706565 0.706497 1.713715
S -1.655397 0.905072 -1.573479
S -4.917612 -0.500136 -1.336710
S -4.945381 0.790623 0.297378
S 1.339430 2.941507 -0.613460
S -0.115979 3.164261 0.798643
S 5.240877 -0.405156 -0.542451
S 4.607747 0.221210 1.327326
H -1.238787 -0.291375 2.484928

[Mo3S13H]- VIII
E= -5382.786160

S -0.191228 -0.489836 -0.696897
Mo -2.349387 -1.017087 0.222322
Mo -0.604122 1.848887 -0.332942
Mo 2.403011 -0.765678 -0.095398
S 1.863027 1.461131 -0.697452
S -0.934717 2.793751 -2.188425
S 1.725566 -1.503071 2.060872
S 2.362351 -2.330896 -1.523680
S -1.972018 -1.207685 2.307493
S -3.132150 0.985517 -0.269947
S -3.998700 -2.584269 -0.302679
S -2.206617 -2.893816 -1.282802
S -1.579761 3.114291 1.416377
S 0.448710 3.311624 1.155820
S 4.575687 0.193752 -0.642013
S 4.454572 -0.903143 1.094616
H 0.485352 -1.934749 1.752271

E= -5382.770087
S 0.018770 -1.949290 0.425632
Mo 2.302896 -0.716410 0.165683
Mo -2.202395 -0.942841 -0.055959
Mo -0.609494 1.692450 -0.060701
S -1.804780 0.609851 1.652409
S -2.192592 0.513295 -1.687971
S 1.418332 1.266262 1.538707
S 0.999854 1.004167 -1.437075
S 2.950200 -1.729882 1.923675
S 1.262006 -2.456974 -1.123500
S 4.016406 -0.892049 -1.457425
S 4.148788 0.774077 -0.256817
S -3.175093 -3.088111 -0.420277
S -4.301186 -1.697323 0.665434
S -1.717192 3.596379 -0.811852
S -0.341128 3.922640 0.698520
H 0.859535 0.637001 2.589663

[Mo3S13H]- IX
E= -5382.799652
S -1.386419 0.340578 -0.955695
Mo -3.548761 -0.753541 -0.317919
S -3.276960 0.286863 1.821714
S -5.010376 -0.813374 1.514655
Mo 0.039573 1.638224 0.134364
S 2.180165 2.390065 -0.642577
S 0.501107 3.381371 -1.341346
S 1.277723 -0.140432 1.277192
Mo 3.065631 -1.072485 0.266191
S 4.745330 0.528143 0.544424
S 4.806294 -0.433730 -1.288166
S 2.157377 -1.952529 -1.732974
S 3.542468 -2.713376 1.505451
S -0.869294 2.500422 1.832435
S -2.906153 -2.751100 -0.720709
S -4.670310 0.036646 -1.959845
H 1.174160 -2.665085 -1.143730

E= -5382.788896
S 1.379104 -0.718956 -0.920458
Mo 3.596764 -0.858907 0.036359
S 3.595309 1.596226 -0.052612
S 5.306431 0.730022 0.613120
Mo 0.026469 1.124445 -0.503106
S -1.016816 2.023217 1.480235
S 0.887096 1.321083 1.712225
S -1.951207 0.304945 -1.495849
Mo -3.619334 -0.606612 -0.246732
S -4.492806 1.328868 0.767578
S -4.532703 -0.372754 1.958020
S -2.559192 -2.463918 0.775991
S -5.009237 -1.328132 -1.664850
S 0.708217 2.675808 -1.771127
S 4.554785 -2.136217 -1.379004
S 3.248749 -1.877478 1.871628
H -2.047440 -2.998336 -0.352224

[Mo3S13H]- X
E= -5382.799804
S -1.875690 0.511776 -1.047854
Mo -3.963500 -0.579044 -0.185893
S -2.928537 -0.533643 1.972136
S -4.859619 -1.287741 1.861384

Mo -0.025568 1.247667 -0.082627
S 1.846968 2.315104 -1.109237
S 0.115967 3.434243 -0.871401
S 1.260257 -0.843483 -0.227176
Mo 3.507088 -1.052028 -0.363177
S 4.118382 1.021993 2.249874
S 4.499265 -0.973211 1.765179
S 4.395073 0.357931 -1.686698
S 3.929534 -3.037274 -0.980975
S -0.248437 1.351314 2.018832
S -3.862082 -2.269932 -1.486800
S -5.301107 0.902750 -0.956862
H 2.803560 0.905777 2.524800

E= -5382.758049
S 1.252276 -0.568318 -1.010519
Mo 3.395836 -0.930954 0.008836
S 3.583629 1.515090 0.062938
S 5.215463 0.498494 0.694942
Mo -0.077200 1.300705 -0.501475
S -0.762867 2.429517 1.492115
S 0.855162 1.212147 1.720687
S -2.041564 0.759909 -1.390532
Mo -3.412426 -0.855782 -0.013324
S -4.522991 1.444910 0.472645
S -5.530286 -1.005926 0.772236
S -2.085515 -1.466181 1.529839
S -3.362918 -2.272784 -1.621540
S 0.733419 2.835283 -1.709808
S 4.299494 -2.217983 -1.431294
S 2.928811 -1.987835 1.793478
H -5.054677 1.592171 -0.752551

[Mo3S13H]- XI
E= -5382.794286
S -1.431843 0.200044 -0.894413
Mo -3.661388 -0.819181 -0.360094
S -3.389081 0.083688 1.841061
S -5.166624 -0.908245 1.436405
Mo -0.103490 1.604763 0.174632
S 1.956575 2.580790 -0.559110
S 0.208282 3.379537 -1.317489
S 1.354344 0.013389 1.375705
Mo 2.968293 -1.283891 0.207336
S 4.851424 0.389001 0.463705
S 6.356972 -0.587976 -0.604081
S 2.528708 -1.283093 -1.857331
S 3.341520 -2.900858 1.153401
S -1.088071 2.396490 1.860718
S -3.100919 -2.816036 -0.862364
S -4.704127 0.115343 -1.978528
H 5.982013 -0.206211 -1.841563

E= -5382.785372
S 1.380348 -0.689617 -0.894426
Mo 3.557393 -0.936902 0.119496
S 3.694832 1.516040 0.017141
S 5.334540 0.565517 0.737794
Mo 0.122284 1.229576 -0.539660
S -0.903341 2.268767 1.389346
S 0.929072 1.422439 1.694673
S -1.914024 0.573497 -1.594382
Mo -3.333977 -0.708901 -0.393754
S -4.736156 0.922589 0.599153
S -6.086266 -0.202316 1.733849
S -2.352649 -1.835081 1.121140
S -4.454376 -1.944412 -1.721156
S 0.923511 2.714060 -1.815207
S 4.491086 -2.269922 -1.259024
S 3.116247 -1.921523 1.953169
H -5.284572 -0.439053 2.791464

[Mo3S13H]- XII
E= -5382.799129
S -1.395037 0.361590 -0.967463
Mo -3.523961 -0.800438 -0.310334
S -3.164891 0.102424 1.881626
S -4.893077 -1.007872 1.582133
Mo -0.028654 1.725310 0.096658
S 2.103217 2.528748 -0.671644
S 0.381826 3.519458 -1.296377
S 1.404766 0.025790 1.305593

Mo 3.158707 -1.225345 0.003994
S 4.421415 0.742865 0.683948
S 5.386473 -0.662447 -0.484346
S 2.177739 -1.539658 -1.854762
S 3.134835 -3.015756 1.161179
S -0.953600 2.473838 1.838124
S -2.866775 -2.752014 -0.866492
S -4.731254 0.069653 -1.846197
H 0.453985 -0.926071 1.361477

E= -5382.786732
S 1.500674 -0.871035 -0.785005
Mo 3.772889 -0.810115 0.061439
S 3.633159 1.625228 -0.250299
S 5.409356 0.909209 0.424804
Mo 0.105380 0.950221 -0.463417
S -1.005063 1.905101 1.452085
S 0.971468 1.427556 1.691593
S -1.875451 -0.262741 -1.399570
Mo -3.883217 -0.754150 0.030433
S -4.076472 1.665653 -0.131578
S -5.533401 0.650706 0.927555
S -2.994450 -1.811052 1.648670
S -4.824119 -2.116942 -1.315374
S 0.591664 2.425465 -1.896996
S 4.734685 -2.153094 -1.286127
S 3.565377 -1.688458 1.987531
H -1.350976 -1.499676 -1.471757

[Mo3S13H]- XIII
E= -5382.799106
S 1.264585 -0.503828 0.575664
Mo 3.695716 -0.782169 0.159682
S 3.717114 1.596889 -0.317513
S 5.392749 0.515307 -0.836666
Mo -0.118419 1.059933 -0.219135
S -1.759333 3.182444 0.420682
S -0.581628 2.165046 1.799791
S -1.656144 0.048283 -1.542554
Mo -3.332298 -1.021380 -0.058765
S -4.570573 1.023109 -0.515120
S -5.469549 -0.367229 0.729074
S -2.173470 -1.402412 1.690070
S -3.625852 -2.813076 -1.171115
S 1.126852 2.208194 -1.478823
S 3.559642 -2.445230 -1.173392
S 4.314561 -1.408232 2.099767
H -2.912678 2.443683 0.487322

E= -5382.781350
S 1.729487 -1.019183 -0.773484
Mo 3.910528 -0.617418 -0.012170
S 3.745011 1.666029 -0.980179
S 5.542898 1.200398 -0.251663
Mo 0.048090 0.548832 -0.177251
S -1.185717 1.430596 1.825630
S 0.672997 0.537935 2.129985
S -1.673516 -0.685813 -0.999428
Mo -3.978649 -0.609046 -0.131911
S -3.763988 1.751349 -0.537116
S -5.611907 1.091857 0.118985
S -3.697519 -1.439439 1.832829
S -4.843344 -2.030234 -1.470530
S 0.394989 2.315197 -1.327423
S 5.014167 -2.178401 -0.952836
S 3.856229 -0.885523 2.099900
H -2.035244 0.384245 2.061225

[Mo3S13H]- XIV
E= -5382.784116
S 1.950812 0.571759 -1.364596
Mo 3.570388 -0.858450 -0.135063
S 4.607524 1.305103 0.184352
S 5.551071 -0.332894 1.024828
Mo 0.110488 1.214732 -0.292878
S -0.710246 1.080037 1.902009
S 1.079842 2.114743 1.599980
S -1.506543 -0.177232 -1.004575
Mo -3.599604 -0.868232 0.071232
S -4.318415 1.300532 -0.717952
S -5.718195 0.150076 0.283354
S -2.885262 -1.272233 2.049113

S -3.893328 -2.682878 -1.011173
S -0.744666 3.044105 -1.436044
S 4.083959 -2.159310 -1.745658
S 2.274995 -1.841807 1.241577
H 0.241828 3.901913 -1.101618

E= -5382.783726
S 1.291990 -0.715255 -1.087460
Mo 3.500381 -0.898847 0.049526
S 3.757256 1.425198 -0.587336
S 5.334601 0.546606 0.414458
Mo 0.122871 1.025393 -0.354867
S -0.569946 0.495704 1.932724
S 0.639191 2.111401 1.698608
S -1.923844 0.806709 -1.282713
Mo -3.655120 -0.612187 -0.282914
S -3.551383 1.028590 1.534602
S -4.894837 -0.490144 1.758462
S -2.724613 -2.519213 -0.223124
S -5.105249 -0.515870 -1.839438
S 0.614395 2.978387 -1.605694
S 4.250112 -2.541565 -1.085763
S 2.861404 -1.551878 1.974657
H 1.673222 3.458187 -0.925016

[Mo3S13H]- XV
E= -5382.773360
S -0.053269 -0.837631 1.419872
Mo 0.169890 1.374603 0.152461
S 0.587786 3.855396 -0.257177
S 0.396402 2.552459 -1.800421
Mo 1.836438 -0.979671 -0.327043
S 1.698821 -3.345197 -0.244768
S 3.038721 -2.473672 1.068766
Mo -2.037994 -0.395884 0.248592
S -3.311037 -1.937380 -1.349758
S -3.413960 0.090903 -1.585056
S 2.547246 1.143321 0.782524
S 1.344272 1.703538 2.347837
S -0.261510 -0.504661 -1.454805
S 3.048038 -0.430712 -2.000278
S -3.254430 -1.502315 1.944119
S -2.028407 1.823700 0.865485
H -4.088808 -2.164041 1.110153

E= -5382.769824
S 0.126990 -0.862355 1.434552
Mo 0.093257 1.355560 0.261069
S 0.183150 3.897535 -0.064905
S -0.088933 2.663494 -1.640880
Mo 1.869675 -0.859830 -0.446622
S 1.956107 -3.232728 -0.421529
S 3.292197 -2.259989 0.825002
Mo -1.945471 -0.637280 0.267799
S -3.642359 -1.605919 -1.252764
S -3.578247 0.370187 -1.408386
S 2.538245 1.313255 0.610836
S 1.480986 1.777445 2.304130
S -0.311366 -0.482858 -1.461055
S 2.882424 -0.153952 -2.202628
S -2.617619 -2.374325 1.761482
S -2.031412 1.495472 1.225028
H -3.775974 -2.779091 1.203567

[Mo3S13H]- XVI
E= -5382.780646
S -0.307196 -0.914789 -1.494465
Mo -0.100190 1.317715 -0.270048
S -0.085714 3.857424 0.077202
S 0.213933 2.556863 1.604937
Mo -1.883419 -0.799697 0.505458
S -2.060714 -3.173915 0.478580
S -3.457211 -2.142622 -0.642956
Mo 1.903106 -0.726480 -0.683992
S 3.645471 -1.273738 0.907674
S 3.517517 -0.128609 2.643364
S -2.518374 1.379926 -0.551115
S -1.517564 1.770827 -2.302119
S 0.426861 -0.574455 1.293605
S -2.716957 -0.056340 2.335640
S 2.781275 -2.103974 -2.074767
S 2.102026 1.417072 -1.314816

H 3.007463 -1.063339 3.468225

E= -5382.769952
S -0.297135 -0.897388 -1.530020
Mo -0.185138 1.315925 -0.346315
S -0.246558 3.732313 0.025552
S 0.354486 2.731296 1.627987
Mo -1.855739 -0.823300 0.538255
S -1.915882 -3.202481 0.546631
S -3.401569 -2.256849 -0.536426
Mo 1.934026 -0.705528 -0.702093
S 3.652668 -1.210456 0.936472
S 3.536140 0.009871 2.623170
S -2.634365 1.303605 -0.515081
S -1.695318 1.715700 -2.305596
S 0.456988 -0.527026 1.251868
S -2.664115 -0.075762 2.380509
S 2.823448 -2.122540 -2.043580
S 2.126908 1.412365 -1.339334
H 2.956552 -0.860408 3.471981

[Mo3S13H]- XVII
E= -5382.774379
S -0.218148 -0.698863 -1.475146
Mo -0.071699 1.355668 -0.151249
S 0.365906 3.846699 0.294153
S 0.812239 2.404515 1.651911
Mo -2.000627 -0.685008 0.397431
S -2.279960 -3.028200 0.162667
S -3.561017 -1.844687 -0.952744
Mo 1.940595 -0.980060 -0.258157
S 3.195035 -0.969985 1.781746
S 4.264011 -0.296865 0.160793
S -2.444217 1.645387 -0.399409
S -1.438760 2.158603 -2.106957
S 0.223728 -0.688136 1.408142
S -2.893823 -0.032382 2.236623
S 2.167108 -2.924304 -1.068319
S 1.972319 1.124762 -1.603153
H 2.901974 1.850107 -0.941912

E= -5382.764100
S -0.214416 -0.667240 -1.511913
Mo -0.077189 1.376099 -0.209168
S 0.179452 3.746216 0.249266
S 0.880411 2.583292 1.714692
Mo -1.990322 -0.714338 0.422487
S -2.179059 -3.061782 0.167583
S -3.507966 -1.918225 -0.935882
Mo 1.961008 -0.940682 -0.259113
S 3.194107 -0.976145 1.790045
S 4.304560 -0.322377 0.189891
S -2.521554 1.582939 -0.360621
S -1.572625 2.113016 -2.100238
S 0.237738 -0.621069 1.388030
S -2.911713 -0.126660 2.266775
S 2.161848 -2.877687 -1.099365
S 2.041159 1.163326 -1.581384
H 3.002073 1.833015 -0.906704

[Mo3S13H]- XVIII
E= -5382.770306
S 0.070119 -0.827173 1.470524
Mo 0.124900 1.341420 0.232166
S 0.333197 3.877476 -0.340800
S 0.290327 2.479257 -1.853875
Mo 1.838399 -0.966768 -0.320903
S 1.695202 -3.325147 -0.406563
S 3.097268 -2.560408 0.909985
Mo -2.079207 -0.605126 0.297985
S -3.397207 -1.782741 -1.431575
S -3.527567 0.260271 -1.392347
S 2.557294 1.232987 0.712043
S 1.381144 1.818727 2.305754
S -0.269781 -0.531170 -1.418141
S 3.033947 -0.235607 -1.959071
S -3.051813 -1.715621 1.850083
S -2.010376 1.665174 1.014095
H 1.668756 3.986064 -0.150200

E= -5382.755208
S -0.021637 -0.841896 -1.473933

Mo -0.191498 1.315366 -0.227014
S -0.311653 3.841455 0.249970
S -0.094303 2.584814 1.858132
Mo -1.852505 -0.938730 0.374147
S -1.751103 -3.320677 0.254328
S -3.132996 -2.400079 -0.978038
Mo 2.073793 -0.540222 -0.375950
S 3.319116 -1.890182 1.348863
S 3.500535 0.062937 1.635984
S -2.611322 1.222826 -0.640310
S -1.499214 1.749189 -2.303549
S 0.305753 -0.539775 1.400246
S -2.956468 -0.367974 2.121349
S 3.168436 -1.591216 -1.910016
S 2.110275 1.670985 -0.975368
H -1.657866 3.984097 0.207771

[Mo3S13H]- XIX
E= -5382.780817
S -0.294157 -1.129710 0.862099
Mo 0.082764 1.264960 0.005520
S 0.479742 3.787293 -0.004196
S 0.767910 2.695225 -1.679479
Mo 2.095605 -0.828956 -0.188627
S 2.262815 -3.217555 -0.264663
S 3.010990 -2.279813 1.418727
Mo -2.429747 -0.529623 0.275157
S -2.944486 -2.297294 -1.221411
S -3.821717 -0.461788 -1.664340
S 2.249095 1.188154 1.205189
S 0.640754 1.419983 2.450477
S 0.345176 -0.398303 -1.920429
S 3.654066 -0.046700 -1.413580
S -3.571608 -0.812620 2.034439
S -2.183821 1.781375 0.134322
H 1.041700 0.280060 -2.860563

E= -5382.769508
S -0.277699 -1.125255 0.862211
Mo 0.004249 1.152954 -0.011121
S 0.196883 3.658171 0.018543
S 0.860523 2.826743 -1.641167
Mo 2.180961 -0.760751 -0.154342
S 2.407135 -3.123134 -0.342998
S 3.070810 -2.264504 1.419975
Mo -2.420525 -0.481329 0.243107
S -2.930677 -2.587597 -0.756757
S -3.922291 -0.950708 -1.556154
S 2.146816 1.248037 1.308866
S 0.438993 1.450371 2.429898
S 0.477754 -0.483283 -1.959438
S 3.751556 0.169957 -1.253518
S -3.470666 -0.258893 2.068756
S -2.205346 1.659627 -0.623011
H 1.182576 0.230800 -2.864293

[Mo3S13H]- XX
E= -5382.771066
S 0.121713 -0.664014 1.489563
Mo 0.019688 1.492772 0.152568
S 0.204787 3.978394 -0.098110
S 0.066736 2.775008 -1.769671
Mo 1.754977 -0.955030 -0.327081
S 1.363832 -3.157675 -1.003693
S 2.748763 -2.973935 0.521062
Mo -2.068916 -0.617806 0.386151
S -3.355595 -1.904850 -1.247443
S -3.595754 0.131456 -1.272559
S 3.154370 0.264424 1.525508
S 2.061979 2.088407 1.184543
S -0.282369 -0.351967 -1.449432
S 3.116934 0.010102 -1.677142
S -2.922972 -1.652436 2.052988
S -2.065923 1.677495 1.024721
H 2.494533 -0.163859 2.625870

E= -5382.754497
S 0.104745 -0.455951 1.509956
Mo -0.105465 1.540936 0.089663
S 0.119019 4.000482 -0.106643
S 0.524204 2.849697 -1.760479
Mo 1.804996 -1.042787 -0.314546

S 1.169596 -3.274106 -0.666717
S 2.563097 -2.999317 0.842772
Mo -2.072051 -0.540502 0.381215
S -2.926429 -2.243459 -1.096343
S -3.650210 -0.416080 -1.516558
S 3.126925 0.437686 1.437427
S 1.960647 2.222363 1.241203
S -0.201212 -0.258615 -1.482090
S 3.234662 -0.361431 -1.750726
S -2.913206 -1.215916 2.222896
S -2.297897 1.829332 0.553025
H 2.622827 -0.056149 2.590510

[Mo3S13H]- XXI
E= -5382.771608
S -0.793396 -0.511665 -1.698512
Mo 0.173574 1.268632 -0.167476
S 0.661598 3.677549 0.489148
S 0.597759 2.212950 1.892363
Mo -2.049506 -0.674174 0.101881
S -2.758540 -2.901296 0.597748
S -3.883246 -1.789509 -0.771922
Mo 2.094238 -0.907693 -0.224006
S 3.247115 -1.802556 1.644976
S 4.373198 -0.615768 0.363251
S -2.278535 1.834034 -0.390101
S -1.145067 2.369871 -2.017287
S 0.162144 -0.807950 1.219474
S -2.735842 0.368539 2.201708
S 1.948661 -2.380746 -1.739817
S 2.237534 1.217969 -1.193508
H -3.302961 -0.786917 2.602883

E= -5382.759802
S -0.149572 -0.829484 -1.480074
Mo 0.088656 1.347776 -0.208439
S 0.208676 3.861214 0.316617
S 0.232075 2.503134 1.800601
Mo -1.930451 -0.742449 0.173112
S -2.377460 -3.103003 0.455201
S -3.437070 -2.065587 -1.000835
Mo 1.980567 -0.806570 -0.330436
S 3.145043 -2.123657 1.389261
S 3.479323 -0.163426 1.571635
S -2.376733 1.539545 -0.642260
S -1.175845 2.042069 -2.247055
S 0.173917 -0.607637 1.377534
S -3.007152 0.084634 2.151923
S 2.826493 -1.980449 -1.920600
S 2.263930 1.429503 -0.997975
H -2.718451 -0.937505 2.978488

[Mo3S13H]- XXII
E= -5382.769147
S -0.170090 -0.896164 1.135944
Mo -0.050508 1.408875 0.006729
S 0.172762 3.903412 -0.045501
S 0.528834 2.856952 -1.746250
Mo 1.934218 -0.702424 -0.309192
S 1.867862 -3.120542 -0.440760
S 2.813417 -2.686094 1.351174
Mo -2.295717 -0.641067 0.290031
S -2.466354 -2.541738 -1.109279
S -3.523971 -0.864048 -1.743597
S 2.274406 1.313902 1.107935
S 0.719228 1.678544 2.377210
S 0.521985 -0.135654 -1.917864
S 3.946125 -0.288467 -0.979094
S -3.532406 -0.917253 1.989089
S -2.326227 1.689562 -0.004119
H 4.095162 -2.624692 0.923936

E= -5382.740684
S -0.149960 -0.848394 -1.462041
Mo 0.159415 1.346901 -0.217056
S 0.350835 3.870798 0.221435
S 0.368192 2.552658 1.748972
Mo -1.899043 -0.638562 0.349664
S -2.435603 -2.993741 0.117290
S -3.906853 -1.859498 -0.789354
Mo 1.967714 -0.871033 -0.343283
S 3.088591 -2.204442 1.407584

S 3.508653 -0.265647 1.568946
S -2.278380 1.603328 -0.597210
S -1.126014 1.973855 -2.266344
S 0.210492 -0.558067 1.437366
S -3.094631 0.044247 2.066547
S 2.831384 -2.118237 -1.873809
S 2.333813 1.338036 -1.040901
H -4.787891 -1.725245 0.232676

[Mo3S13H]- XXIII
E= -5382.800692
S 2.795598 -0.439396 2.195641
Mo 3.486490 -0.273520 0.185014
S 3.797738 -2.144447 -1.321570
S 5.346995 -1.701505 -0.021231
S 1.332769 -0.245282 -1.091647
Mo -0.297152 0.993691 -0.256667
S -0.036551 3.281004 -0.892235
S 0.248364 2.802240 1.105045
Mo -2.663653 -0.454449 0.038806
S -5.234629 -0.089553 -0.608294
S -4.440996 0.719506 1.134873
S -2.026861 0.771249 -1.784127
S -1.081143 -0.188871 1.617690
S -2.473738 -2.556755 -0.877866
S -3.476089 -2.665634 0.930103
S 4.186937 1.700595 -0.211053
H -5.093026 0.979677 -1.425693

E= -5382.783066
S 2.974001 0.398451 2.052522
Mo 3.279126 -0.360709 0.088857
S 2.325765 -2.411310 -0.769181
S 4.067422 -2.573631 0.334991
S 1.362974 0.577568 -1.218269
Mo -0.399830 1.454320 -0.200695
S -0.569170 3.747396 -0.784078
S 0.245629 3.332255 1.004420
Mo -2.419793 -0.542218 0.070958
S -4.976080 -0.955656 -0.543939
S -4.432592 -0.196797 1.320479
S -2.144933 0.943806 -1.666747
S -0.970413 0.290316 1.689943
S -1.301291 -2.403130 -1.035942
S -2.289207 -2.934674 0.622604
S 4.826448 0.725699 -0.903538
H -5.195978 0.196769 -1.215305

[Mo3S13H]- XXIV
E= -5382.796361
S -3.541776 -1.897523 -1.727744
Mo -3.320083 -0.460509 -0.157770
S -2.048342 -0.764418 1.861815
S -3.957169 -1.581097 1.803513
S -1.276501 0.638184 -1.115553
Mo 0.535767 1.470305 -0.184883
S 0.024554 3.438344 1.000514
S 0.812171 3.727222 -0.902516
Mo 2.391051 -0.648681 0.112784
S 4.108713 -0.223817 1.565002
S 4.836059 -1.057430 -0.188671
S 0.992310 0.315898 1.740361
S 2.251336 0.821932 -1.629664
S 1.128426 -2.610779 0.248038
S 2.164529 -2.716012 -1.547236
S -4.667336 1.171229 -0.432985
H 3.285512 -3.354527 -1.143490

E= -5382.770667
S 1.743285 0.173569 1.378793
Mo 0.657589 2.136765 0.428147
S 0.654311 3.616706 -1.472393
S 2.476643 2.856295 -0.869910
S -1.830535 1.840149 0.039517
Mo -2.408499 -0.288953 0.126859
S -3.676233 -1.398975 -1.591260
S -4.720263 -0.396665 -0.113513
Mo 1.575137 -1.529810 -0.128357
S 0.748460 -3.531668 0.726584
S 2.676719 -3.128715 1.372459
S -0.583850 -1.255512 -1.332589
S -1.934821 -1.177831 1.981136

S 0.817204 0.229547 -1.722542
S 3.328557 -1.721471 -1.692020
S 0.509214 3.226595 2.241524
H 4.043381 -2.668476 -1.051877

[Mo3S13H]- XXV
E= -5382.766072
S -1.768333 0.825622 1.453678
Mo -1.438735 -1.263908 0.345907
S -2.813547 -2.679370 -1.029207
S -3.782658 -1.256458 0.108608
S 0.384045 -2.206025 -0.996696
Mo 1.858983 -0.720074 -0.189178
S 3.699554 -1.939533 -1.017410
S 3.820515 -1.387623 0.983086
Mo -0.235918 1.611119 -0.043723
S 1.140585 3.562555 0.030118
S -0.562453 3.763427 1.133979
S 1.929290 1.046103 -1.460069
S 1.387772 0.621781 1.802690
S -1.248931 0.482846 -1.920612
S -1.857545 2.419643 -1.599502
S -0.969321 -2.359275 2.107196
H 2.514565 1.361152 1.719985

E= -5382.764176
S 1.302636 1.187724 -1.415012
Mo 2.402059 -0.498092 -0.467283
S 2.960412 -1.097641 1.806974
S 4.027698 0.448134 0.946277
S 0.676849 -2.210129 -0.161415
Mo -1.433879 -1.524395 0.150653
S -2.622605 -3.228812 1.263067
S -3.179648 -2.854090 -0.708867
Mo -0.760144 1.422532 -0.024142
S -2.769333 2.750686 -0.236975
S -1.329100 3.275807 -1.570652
S -2.072143 0.110477 1.522188
S -1.613143 -0.117513 -1.833901
S 0.729244 1.489480 2.002419
S 0.023705 3.250910 1.405600
S 3.502948 -1.438052 -2.013623
H -2.937817 0.126457 -1.784883

[Mo3S13H]- XXVI
E= -5382.759003
S 1.096709 -0.955492 1.635627
Mo 2.385843 0.383297 0.419360
S 3.243980 0.795016 -1.820074
S 4.176474 -0.672569 -0.718730
S 0.739817 2.192623 -0.172519
Mo -1.356539 1.382248 -0.245074
S -3.164277 2.700733 -0.970281
S -2.425459 3.657710 0.731327
Mo -0.984549 -1.448429 0.022449
S -3.007706 -2.545065 -0.161618
S -2.017363 -3.209303 1.509449
S -1.729247 -0.133171 -1.857066
S -1.774423 0.212482 1.609697
S 0.973017 -1.450676 -1.552250
S 0.437094 -3.204799 -0.658599
S 3.433521 1.495513 1.898926
H -1.593888 4.553104 0.154878

E= -5382.795962
S -2.504257 -2.659096 -1.305262
Mo -2.842105 -0.828420 -0.287900
S -4.502520 -0.668943 1.444276
S -5.159694 -0.423260 -0.502043
S -1.274327 -0.847129 1.519778
Mo -0.137603 0.584011 0.210750
S -0.252426 2.936966 0.638610
S -1.852482 4.029870 -0.174434
Mo 2.781305 -0.317468 0.019102
S 4.246725 1.444651 -0.075355
S 4.501655 0.244454 -1.742843
S 1.628824 0.956632 1.702478
S 1.131193 -0.323124 -1.534066
S 2.631783 -2.064587 1.611430
S 3.962464 -2.327365 0.060374
S -1.947958 0.917910 -1.400403
H -1.410793 4.127177 -1.442640

[Mo3S13H]- XXVII
E= -5382.764285
S -1.671295 0.992590 1.491517
Mo -1.790935 -1.027370 0.342074
S -3.309078 -2.228193 -1.121116
S -4.097981 -0.739356 0.068073
S 0.173604 -2.119254 -0.899082
Mo 2.079519 -0.766047 -0.076489
S 3.228346 -2.876524 -0.157501
S 4.391288 -1.155144 -0.054925
Mo -0.041931 1.610020 -0.032178
S 1.599261 3.322523 0.135431
S -0.083540 3.724277 1.225492
S 1.801230 0.761076 -1.608790
S 1.615464 0.230571 1.772220
S -1.315786 0.530804 -1.892980
S -1.521995 2.557018 -1.572429
S -1.474662 -2.314945 2.014330
H 0.282884 -3.264441 -0.206951

E= -5382.786473
S -2.228149 -2.373765 -1.046564
Mo -3.230980 -0.613118 -0.389871
S -4.616413 -0.473453 1.592058
S -5.518185 -1.098018 -0.165653
S -1.460482 0.068520 1.280399
Mo 0.424191 1.410973 0.323035
S -0.757090 3.448321 0.615484
S 0.612011 3.341857 -0.959539
Mo 2.738490 -0.658346 0.044929
S 4.637600 0.617785 -0.277401
S 4.479894 -0.883106 -1.700667
S 2.124641 1.154182 1.686959
S 1.062457 -0.158756 -1.356787
S 2.012929 -2.047050 1.822045
S 3.008342 -2.975995 0.274789
S -3.044316 0.948053 -1.826718
H -2.143203 1.043420 1.905613

[Mo3S13H]- XXVIII
E= -5382.774687
S -1.670415 1.443915 1.363518
Mo -1.936813 -0.726327 0.283814
S -3.502186 -1.822223 -1.127372
S -4.192021 -0.178858 -0.089613
S -0.292701 -2.195718 -0.836782
Mo 1.630613 -1.202746 -0.149317
S 3.189854 -2.795691 -0.889102
S 3.174993 -2.455260 1.173701
Mo 0.577887 1.513281 -0.082008
S 2.269124 3.073743 -0.086841
S 0.888724 3.587923 1.321764
S 2.199495 0.412783 -1.584594
S 1.289762 0.123108 1.706485
S -1.030447 0.738803 -1.781276
S -1.040235 2.768095 -1.484402
S -1.853808 -1.749252 2.147603
H -2.293075 2.241403 0.466032

E= -5382.773263
S 0.917704 -1.735952 1.040322
Mo 2.585836 -0.028384 0.321075
S 4.251970 0.043613 -1.345774
S 4.084374 -1.751117 -0.289900
S 1.196376 1.467960 -1.027856
Mo -0.894407 1.705675 -0.219030
S -1.700605 3.784142 -1.027126
S -1.229658 3.709213 1.009083
Mo -1.493394 -1.072505 0.035140
S -3.704135 -1.603224 0.474216
S -2.508063 -2.560879 1.802118
S -2.405882 0.555314 -1.482322
S -1.104698 0.509895 1.721092
S -0.274053 -1.641589 -2.061744
S -1.263868 -3.178182 -1.271865
S 3.137838 0.985584 2.083082
H 1.325732 -2.757456 0.265044

[Mo3S13H]- XXIX
E= -5382.788468
S 2.430955 -0.980986 2.010314

Mo 3.088915 0.048636 0.257480
S 2.524602 -0.919948 -1.847088
S 3.901238 -2.178310 -0.932391
S 1.736739 1.874918 -0.022573
Mo -0.675965 1.484788 -0.083947
S -0.742314 3.885288 -0.082126
S -2.545023 2.852070 -0.102640
Mo -2.094016 -0.956033 -0.061906
S -4.153008 -0.518947 -1.008666
S -4.294974 -0.557372 1.051695
S -0.967801 0.167401 -1.861513
S -1.000211 0.162782 1.691836
S -0.883675 -2.832170 -0.651683
S -2.091432 -3.142018 1.012582
S 5.057077 0.862015 0.470347
H 3.049995 -3.046009 -0.337856

E= -5382.756432
S 1.303342 -1.404319 0.980905
Mo 2.419793 0.428848 0.328165
S 3.826079 0.209973 -1.609726
S 4.574147 -0.970868 -0.078348
S 0.865676 1.803118 -0.910779
Mo -1.288188 1.546897 -0.207078
S -2.459561 3.421699 -1.101974
S -2.182656 3.388883 0.974669
Mo -1.192519 -1.283647 0.065459
S -3.207753 -2.331166 0.535997
S -1.788543 -2.954818 1.847950
S -2.470666 0.078538 -1.472439
S -1.249417 0.356137 1.734017
S 0.102022 -1.599154 -2.055950
S -0.520039 -3.304689 -1.256276
S 3.118186 1.624573 1.945294
H 3.985318 -2.154645 -0.367748

[Mo3S13H]- XXX
E= -5382.781435
S 2.455231 -1.645042 1.698337
Mo 2.609207 -0.105633 0.234890
S 3.415324 0.532006 -2.023601
S 4.372756 -0.938437 -0.942692
S 0.972835 1.841633 -0.171681
Mo -1.240782 1.579403 -0.046827
S -2.121704 3.644846 -0.793498
S -2.442302 3.180781 1.218224
Mo -1.624838 -1.245779 -0.128745
S -3.722714 -2.017763 -0.648222
S -3.004863 -2.933985 1.017800
S -2.077435 0.424135 -1.801513
S -1.603949 0.058388 1.702878
S 0.739777 -1.308038 -1.077294
S -0.067580 -2.973488 -0.150233
S 3.553475 1.463477 1.747002
H 3.267719 2.608187 1.100568

E= -5382.759775
S -1.241543 1.273148 1.497723
Mo -2.240866 -0.348188 0.337921
S -3.260154 -1.054095 -1.760810
S -4.323918 0.278686 -0.592296
S -0.592383 -2.156444 0.077713
Mo 1.530857 -1.420896 -0.106395
S 2.641486 -3.272174 -1.116329
S 3.322178 -2.682052 0.766704
Mo 0.860482 1.350797 0.009374
S 2.708830 2.862283 -0.155146
S 1.549210 3.316390 1.407772
S 1.969724 0.089327 -1.717891
S 1.726552 -0.004982 1.709855
S -1.000395 1.145208 -1.688052
S -0.418208 3.022981 -1.241054
S -3.200438 -1.652991 2.046156
H -4.414935 -1.076437 2.132663

[Mo3S13H]- XXXI
E= -5382.800712
S 1.147060 -0.183920 -1.863642
Mo 2.848811 -0.412803 -0.168212
S 4.584164 1.356277 0.677577
S 3.509938 1.733983 -1.044369
S 1.102572 -1.876891 0.469564

S 2.460350 -1.553435 1.975647
Mo -0.391888 0.283430 -0.084626
S 1.329829 1.198141 1.542642
S 0.132161 2.479050 0.429289
Mo -3.187044 -0.302645 -0.139963
S -4.906796 0.342013 1.397142
S -4.988684 1.216987 -0.496271
S -3.582496 -2.224232 -0.952489
S -1.705523 -0.557681 1.623764
S -1.891228 0.804520 -1.733554
S 4.368408 -1.652030 -1.003029
H 5.709026 0.820216 0.141285

E= -5382.802736
S -0.972988 0.845278 -1.314898
Mo -2.894567 0.809708 0.043699
S -5.932637 -1.012926 -0.593963
S -4.126217 -0.458212 -1.516314
S -1.309474 0.290803 1.826230
S -3.166222 -0.662211 1.897920
Mo 0.340586 -0.582691 -0.006919
S -0.735333 -2.596711 0.532104
S 0.768501 -2.729630 -0.859589
Mo 3.349575 0.546937 -0.152787
S 4.700123 -0.948028 1.176957
S 5.476093 -0.331794 -0.640754
S 3.631325 2.651099 -0.117412
S 1.751761 0.198642 1.593816
S 2.025959 -0.014636 -1.852950
S -3.792454 2.723946 0.208647
H -6.509959 0.204003 -0.564408

[Mo3S13H]- XXXII
E= -5382.804366
S -0.956830 0.957253 -1.594568
Mo -2.725110 0.230749 -0.092328
S -4.720526 -1.250052 -0.172409
S -3.363624 -1.291232 -1.712860
S -1.305115 1.454826 1.514972
S -2.931086 0.507107 2.324929
Mo 0.109555 -0.162266 0.053726
S -1.394265 -1.673892 1.156626
S -0.013716 -2.472487 -0.177817
Mo 3.315445 0.313687 -0.235394
S 4.326577 -1.035759 1.490327
S 5.252152 -1.013519 -0.361691
S 3.995967 2.270611 -0.711342
S 1.701029 0.719900 1.471812
S 1.910965 -0.403768 -1.794624
S -4.012146 2.123069 -0.694534
H -5.225515 1.675953 -0.313271

E= -5382.805247
S 1.251915 -0.180418 -1.401930
Mo 3.009788 -0.442233 0.094634
S 5.138280 -0.064279 -0.771862
S 4.292057 -1.820596 -1.473346
S 1.460406 0.803555 1.660207
S 3.225153 1.696221 1.086295
Mo -0.378614 0.979254 -0.145916
S 0.132671 3.231934 0.193684
S -1.370659 2.852024 -1.160121
Mo -3.017740 -0.862164 -0.068820
S -4.674497 0.379246 1.167824
S -5.298147 -0.563686 -0.566070
S -2.790478 -2.958118 0.166211
S -1.519017 0.033685 1.571943
S -1.885442 -0.170348 -1.861043
S 2.829204 -2.191268 1.641317
H 3.572653 -3.111213 0.994537

[Mo3S13H]- XXXIII
E= -5382.801774
S 1.127618 -0.674023 -1.376547
Mo 3.130006 -0.564828 0.043299
S 5.012161 0.909728 -0.169742
S 3.964905 0.490233 -1.906633
S 1.258001 -0.695159 1.571548
S 2.912208 0.306996 2.271699
Mo -0.395618 0.538513 -0.099073
S 0.533334 2.506194 0.968560
S -0.452281 2.740909 -0.837164

Mo -3.063199 -0.402696 -0.149543
S -5.261081 -0.231705 1.142331
S -4.769306 1.081078 -0.399665
S -3.427513 -2.689978 -0.583598
S -1.820382 0.017182 1.683329
S -1.830944 0.060444 -1.949008
S 3.901545 -2.521042 0.115543
H -4.562200 -2.795237 0.132905

E= -5382.801752
S -1.032310 -0.727421 1.243816
Mo -3.133699 -0.598288 -0.019046
S -5.141006 0.575428 0.597166
S -3.902486 -0.023529 2.144862
S -1.419157 -0.281332 -1.758828
S -3.205580 0.723122 -2.006070
Mo 0.253411 0.680496 -0.048132
S -0.848082 2.681672 -0.595577
S 0.643666 2.841785 0.811623
Mo 3.265486 -0.467522 0.125292
S 4.801998 1.100665 -0.727011
S 5.584616 -0.317367 0.595578
S 3.272356 -2.802977 -0.230870
S 1.695146 -0.107439 -1.636067
S 1.979023 0.123255 1.806925
S -3.714588 -2.577898 -0.424046
H 4.404190 -3.144238 0.415225

[Mo3S13H]- XXXIV
E= -5382.812339
S 1.062266 -0.447191 -1.533998
Mo 3.066816 -0.576583 -0.113549
S 4.928329 0.939432 0.032248
S 3.862190 0.939845 -1.743556
S 1.193291 -1.088355 1.306431
S 2.834277 -0.315519 2.279689
Mo -0.387459 0.589302 -0.020847
S 0.935811 2.264766 1.145187
S -0.283189 2.860718 -0.418103
Mo -3.017952 -0.473944 0.006816
S -4.938867 0.586211 0.939449
S -5.405374 0.049797 -1.017205
S -3.092203 -2.600085 -0.141021
S -1.740634 0.096888 1.823608
S -1.980100 0.470881 -1.774703
S 3.887312 -2.474713 -0.512935
H -5.988750 -1.151300 -0.803107

E= -5382.787470
S 1.252998 -0.286098 -1.693061
Mo 3.139809 -0.538215 -0.138024
S 4.971189 0.983316 0.256070
S 4.024208 1.118616 -1.580871
S 1.204589 -1.245163 1.160196
S 2.768392 -0.409942 2.233225
Mo -0.225700 0.491563 -0.073739
S 0.812145 2.288442 1.070478
S -0.683894 2.860875 -0.187457
Mo -3.063739 -0.492299 0.082117
S -4.889598 0.874242 0.699160
S -5.486877 0.155070 -1.169204
S -3.498249 -2.584459 0.174722
S -1.781814 0.047163 1.819739
S -1.941144 0.057892 -1.775121
S 4.026945 -2.386661 -0.619256
H -6.177843 -0.935829 -0.772804

[Mo3S13H]- XXXV
E= -5382.803948
S 1.116028 -0.107837 -1.719758
Mo 2.980759 -0.532985 -0.152315
S 4.784862 0.886747 0.536689
S 3.918949 1.317552 -1.292830
S 0.999874 -1.442138 0.882973
S 2.503404 -0.916824 2.194632
Mo -0.390131 0.583121 -0.117301
S 1.072605 1.990186 1.309581
S -0.214620 2.856383 -0.044335
Mo -3.059296 -0.446410 -0.110341
S -4.988469 0.208015 1.111239
S -5.162364 0.311658 -0.959264
S -2.807454 -2.532766 -0.363311

S -1.740344 -0.058402 1.904112
S -1.999275 0.729774 -1.787073
S 3.885319 -2.274076 -0.916839
H -2.212176 1.151167 2.265183

E= -5382.788170
S 1.380088 0.077109 -1.884234
Mo 3.013334 -0.483909 -0.159287
S 4.611283 0.961617 0.996762
S 3.756113 1.695098 -0.718621
S 1.024175 -1.663450 0.545682
S 2.371254 -1.209565 2.048961
Mo -0.370842 0.313124 -0.242105
S 1.035909 2.067984 1.013252
S -0.457639 2.718043 -0.160289
Mo -3.098844 -0.446204 0.005080
S -4.845363 0.798925 1.025162
S -4.974065 0.582970 -1.041255
S -3.292571 -2.548646 0.184781
S -1.648821 0.032041 1.894285
S -1.858064 -0.032083 -1.922986
S 4.221194 -1.941593 -1.077926
H -2.009096 1.298265 2.187946

[Mo3S13H]- XXXVI
E= -5382.810314
S -1.140566 -0.840000 1.085230
Mo -3.174308 -0.429830 -0.171193
S -5.223277 0.367251 0.785585
S -4.084709 -0.888092 1.980731
S -1.418380 0.537275 -1.657784
S -3.127694 1.646960 -1.285465
Mo 0.445711 0.601490 0.118858
S -0.067057 2.894920 -0.055488
S 1.630312 2.508585 1.043268
Mo 3.018159 -0.694647 -0.078743
S 4.862543 0.328756 -1.153481
S 5.010179 0.132983 0.913485
S 3.007131 -2.799602 -0.279732
S 1.573186 0.036069 -1.757131
S 1.738157 -0.533088 1.986734
S -3.664729 -2.051333 -1.424634
H 2.316869 0.514445 2.604219

E= -5382.802556
S 1.241165 -0.693800 -1.343941
Mo 3.262955 -0.537743 0.053161
S 5.277617 0.707716 -0.393302
S 4.122722 0.181409 -2.028783
S 1.458822 -0.362368 1.737328
S 3.188054 0.721589 2.064108
Mo -0.187075 0.532769 -0.040612
S 0.660732 2.612225 0.678519
S -0.761728 2.691763 -0.806477
Mo -3.546956 -0.643720 0.002820
S -5.081544 0.575082 1.303039
S -4.923135 1.148389 -0.702194
S -4.151898 -2.642629 -0.362708
S -1.630979 -0.570746 1.397656
S -1.962820 -0.070534 -1.858404
S 3.893802 -2.512894 0.404694
H -1.507737 -1.318061 -2.078094

[Mo3S13H]- XXXVII
E= -5382.823566
S -1.348707 1.076294 -1.244165
Mo -3.337800 0.098359 0.068631
S -4.999457 -1.305765 -0.698907
S -3.717352 -0.632846 -2.172027
S -0.305651 2.161697 0.170669
S -4.177187 -0.310110 2.305456
Mo 0.699165 0.045581 -0.047969
S -1.385673 -1.096388 1.156531
S -0.319724 -2.044360 -0.356986
Mo 3.499190 0.190214 0.030984
S 5.001537 -1.325952 1.091936
S 5.020637 -1.327425 -0.990602
S 4.215182 2.184918 0.068624
S 1.989947 -0.065551 1.804194
S 2.068474 0.062112 -1.833585
S -4.067362 2.057323 0.413675
H -3.737969 -1.777637 2.393894

E= -5382.773976
S 1.519037 0.494017 -1.486892
Mo 3.018574 -0.634861 -0.093585
S 5.108882 0.446675 0.421636
S 4.538913 0.594806 -1.531238
S 0.888202 -0.954741 1.138937
S 2.516365 -0.289670 2.188727
Mo -0.597627 0.907728 -0.120044
S 0.845128 2.630725 1.244058
S -0.935149 2.972490 -0.792570
Mo -2.981490 -0.651133 0.042426
S -5.153014 0.237078 0.568924
S -4.857779 -0.224841 -1.407715
S -2.794975 -2.685532 0.608526
S -1.993059 0.624571 1.703482
S -1.555469 -0.369560 -1.768214
S 3.349319 -2.666920 -0.573897
H -0.079603 2.941630 2.170281

[Mo3S13H]- XXXVIII
E= -5382.825190
S 0.886406 -1.356317 -0.733006
Mo 3.058728 -0.549748 0.129149
S 4.763540 0.743459 -1.010771
S 3.411134 -0.287796 -2.194165
S 1.496147 -0.030326 1.885504
S 3.155090 1.198786 1.778833
Mo -0.474327 0.359028 0.032295
S -0.257448 2.667747 0.652754
S 0.910965 2.379298 -1.032608
Mo -3.158428 -0.492817 -0.111283
S -5.016703 0.248326 1.184154
S -5.082250 0.711047 -0.846732
S -3.296128 -2.548912 -0.597157
S -1.765610 -0.336395 1.762836
S -1.875050 0.542662 -1.757800
S 4.044339 -2.279788 0.802571
H 2.118215 2.279923 -0.417401

E= -5382.803844
S 1.092671 -0.677698 -1.292160
Mo 3.150396 -0.587783 0.031428
S 5.214828 0.516768 -0.567359
S 3.969886 -0.042517 -2.125166
S 1.479763 -0.270625 1.877900
S 3.201278 0.889186 1.855522
Mo -0.357533 0.333643 0.168839
S 0.118104 2.564198 0.720326
S -0.515886 3.968204 -0.708164
Mo -3.219134 -0.616550 -0.238840
S -4.728768 0.085116 1.494641
S -5.442466 0.198658 -0.431377
S -3.355529 -2.516610 -1.172485
S -1.666532 -0.930159 1.541603
S -2.010289 0.815237 -1.505130
S 3.728061 -2.555218 0.508992
H 0.541417 3.856367 -1.534164

[Mo3S13H]- XXXIX
E= -5382.820395
S -1.326502 0.702589 -1.651605
Mo -3.147377 0.313657 -0.006609
S -4.766067 -1.350926 0.344215
S -3.859074 -1.394549 -1.504017
S -0.901819 1.716850 0.084452
S -3.227725 0.590257 2.437326
Mo 0.605290 -0.213842 -0.129636
S -1.273187 -1.447804 1.036451
S -0.080768 -2.405065 -0.376714
Mo 3.351968 0.337971 0.039513
S 4.958040 -1.017886 1.167060
S 5.078499 -0.995621 -0.910553
S 3.829842 2.403763 0.111133
S 1.824357 -0.083403 1.765103
S 2.019678 0.073082 -1.873248
S -4.172479 2.098837 -0.550418
H -3.659746 -0.628935 2.795789

E= -5382.784689
S -1.045441 1.155169 -1.108370
Mo -3.170975 0.462122 -0.006181

S -4.712332 -1.225509 -0.702194
S -3.419543 -0.541284 -2.150284
S -1.229069 0.974793 1.425929
S -3.725981 -0.427282 2.218620
Mo 0.360112 -0.346776 0.094817
S -0.960320 -2.172854 0.770758
S 0.489027 -2.577368 -0.636062
Mo 3.360902 0.465645 -0.097695
S 4.749289 -1.127805 1.052696
S 5.342796 -0.569245 -0.852745
S 3.826804 2.531133 -0.003413
S 1.858285 0.135513 1.722310
S 1.885359 0.096740 -1.771784
S -4.201673 2.296067 -0.063685
H -4.816856 -1.170683 1.952058

[Mo3S13H]- XXXX
E= -5382.819720
S 1.466874 -0.266428 1.990655
Mo 3.027414 0.410857 0.153873
S 4.761277 -0.693787 -1.054291
S 4.323105 -1.471007 0.804872
S 0.899855 1.593720 -0.476229
S 2.272353 1.280580 -1.965653
Mo -0.536271 -0.421134 0.057485
S 1.303784 -1.573204 -1.212276
S 0.040461 -2.667533 0.005970
Mo -3.224721 0.405427 0.014638
S -4.992425 -0.854029 -0.976909
S -5.016832 -0.731926 1.099174
S -3.503125 2.505929 -0.108806
S -1.834893 -0.196455 -1.768832
S -1.828920 0.048115 1.855489
S 3.923148 2.086889 1.083379
H 1.775663 -1.570118 2.083487

E= -5382.801266
S -1.428748 -0.047668 -1.937496
Mo -3.109052 0.444016 -0.146787
S -4.828943 -0.829185 0.913144
S -4.253470 -1.470996 -0.960767
S -1.047319 1.595912 0.633318
S -2.478002 1.174644 2.058760
Mo 0.393066 -0.380337 0.021088
S -1.290176 -1.673875 1.165294
S -0.087195 -2.681668 -0.170651
Mo 3.373194 0.382737 -0.108697
S 4.913752 -0.909007 1.183270
S 5.421157 -0.592501 -0.805964
S 3.681856 2.475884 -0.254208
S 1.867722 0.105806 1.705588
S 1.980304 -0.349351 -1.765381
S -4.068761 2.113442 -1.011287
H -1.717540 -1.332486 -2.213277

[Mo3S13H]- XXXXI
E= -5382.794625
S 1.497340 -0.273129 -1.530399
Mo 3.382460 -0.405361 -0.386050
S 4.129688 0.831042 1.490790
S 4.515506 1.656031 -0.362284
S 0.560385 -1.115032 1.708532
S 2.464409 -1.901941 1.341662
Mo -0.551677 0.464581 -0.089043
S 0.713498 2.485099 0.903046
S -0.451677 2.623833 -0.761706
Mo -3.202817 -0.494031 -0.001079
S -5.121887 0.776517 0.618477
S -4.973402 0.281934 -1.396127
S -3.369847 -2.546817 0.502835
S -1.993407 0.554552 1.700503
S -1.722776 -0.412209 -1.812860
S 4.674932 -1.809226 -1.314632
H 0.861267 -0.148410 2.593796

E= -5382.787488
S 1.224784 -0.547225 -0.892852
Mo 3.469034 -0.651324 -0.006387
S 5.542852 0.442267 -0.418966
S 4.516387 -0.297196 -2.088088
S 1.027126 0.538915 2.095126
S 3.038640 1.001336 1.659719

Mo -0.457263 0.766862 -0.003359
S 0.245007 3.014898 0.201722
S -1.047581 2.594189 -1.335583
Mo -3.284802 -0.755373 -0.085681
S -4.967712 0.783685 0.703663
S -5.429783 -0.352381 -0.963667
S -3.318697 -2.817204 0.416259
S -1.967300 0.217792 1.643919
S -1.855007 -0.410814 -1.764152
S 3.663306 -2.591926 0.818705
H 0.714959 1.651719 2.795061

[Mo3S11H]- I
E= -4586.285908
S -0.349664 -1.211556 0.902348
Mo 0.870573 0.500454 -0.095742
S 2.457618 0.516439 1.776557
Mo 3.520109 -0.327297 0.037029
S 2.287919 -0.202846 -1.848597
Mo -2.517507 -0.647760 -0.128457
S -3.241768 -2.450139 -0.940900
S -4.489522 0.325990 0.943269
S -3.014143 -0.472247 2.160762
S -0.957875 0.137706 -1.856474
S -2.713431 1.223269 -1.583355
S 0.968432 2.955509 -0.488455
S -0.333452 2.441589 1.036530
S 4.562814 -2.169703 0.368262
H -1.504225 2.429144 0.342005

E= -4586.288791
S -0.346902 -1.234636 0.909742
Mo 0.893479 0.471215 -0.098301
S 2.415055 0.767804 1.660504
Mo 3.615092 -0.264634 0.050150
S 2.272092 -0.331254 -1.787570
Mo -2.539410 -0.682536 -0.066475
S -3.376330 -2.531470 -0.623977
S -4.404411 0.525972 0.941066
S -2.955529 -0.238392 2.211869
S -0.986491 -0.176849 -1.854739
S -2.721904 0.958372 -1.795143
S 0.579342 2.763198 -0.806961
S -0.525012 2.456450 0.918826
S 4.989716 -1.851646 0.505998
H -1.738450 2.268648 0.340442

[Mo3S11H]- II
E= -4586.322309
S -1.428196 -0.552049 1.876664
Mo -0.164257 0.612684 0.118140
S 1.575031 0.792324 1.690523
Mo 2.415992 -0.576795 0.031294
S 0.759484 -0.538376 -1.617887
Mo -2.767438 -0.859625 0.127368
S -3.437527 -2.841328 -0.282408
S -2.170518 0.567996 -1.597306
S -3.967934 1.059593 -0.621206
S 0.096982 2.917891 -0.666876
S -1.026587 2.951367 1.061762
S 4.085290 -0.243265 -1.650102
S 4.557758 0.459700 0.251302
S 2.452430 -2.554238 0.794904
H -2.279864 2.858656 0.544338

E= -4586.319783
S 1.358019 -0.643729 -1.797224
Mo 0.138545 0.626733 -0.104340
S -1.606868 0.780265 -1.688568
Mo -2.404783 -0.615272 -0.032979
S -0.746950 -0.564139 1.617758
Mo 2.798446 -0.842410 -0.099315
S 3.709866 -2.746294 0.227597
S 2.112218 0.611604 1.603473
S 3.885645 1.153500 0.593340
S -0.206149 2.978988 0.572878
S 0.991992 2.896078 -1.103125
S -4.061499 -0.277202 1.662484
S -4.558341 0.404625 -0.234215
S -2.414117 -2.592034 -0.799556
H 2.226165 2.873235 -0.538823

[Mo3S11H]- III
E= -4586.275163
S 0.551696 -0.307869 -1.683326
Mo 2.411428 -0.681706 -0.113041
S 4.302918 0.747523 0.395691
S 3.351503 1.044740 -1.422805
S 0.385555 -1.273112 1.064696
S 1.952447 -0.626192 2.256011
Mo -0.906684 0.648242 -0.151173
S 0.551890 2.403464 1.076702
S -0.838498 3.013823 -0.325341
Mo -3.265039 -0.415828 -0.013456
S -3.838520 -2.487295 -0.050576
S -2.406464 0.456349 1.849042
S -2.618517 0.590076 -1.904484
S 3.238481 -2.536736 -0.664751
H -0.187451 2.473951 2.208368

E= -4586.274262
S 0.719371 -0.254306 -1.725589
Mo 2.555360 -0.685641 -0.146260
S 4.362600 0.759648 0.573582
S 3.447164 1.209683 -1.232608
S 0.520455 -1.423728 0.866308
S 2.014639 -0.944620 2.211478
Mo -0.871412 0.552989 -0.172051
S 0.717358 2.232856 1.193632
S -0.631958 2.886628 -0.233881
Mo -3.606926 -0.216420 0.009706
S -4.918478 -1.918125 -0.022913
S -2.200664 0.187028 1.757040
S -2.455371 0.473978 -1.850833
S 3.477031 -2.435567 -0.869532
H -0.069295 2.285422 2.294460

E= -4586.269544
S 1.399045 0.702245 -1.382149
Mo 2.775541 -0.546650 -0.108945
S 5.025129 0.097798 0.591423
S 4.763247 -0.683357 -1.308852
S 0.252089 0.265816 1.999541
S 2.325816 0.390874 2.003187
Mo -0.745170 0.686033 -0.141691
S -0.617260 3.296578 0.023173
S -1.600048 2.469511 -1.596539
Mo -3.461928 -0.884395 0.064150
S -5.351265 -1.894196 -0.089687
S -2.824060 0.820119 1.382334
S -1.583154 -1.186313 -1.249674
S 2.071864 -2.539492 0.062011
H -1.657084 3.457183 0.876078

[Mo3S11H]- IV
E= -4586.359057
S -1.176973 0.770629 -0.500194
Mo -3.553911 0.061686 -0.007568
S -3.345400 -1.015151 1.814480
S -3.701787 -1.266704 -1.671258
Mo 0.806756 -0.812863 0.023236
S 0.220977 -1.437356 1.947169
S 3.117136 -1.647004 -0.120957
Mo 3.787640 0.507935 -0.032997
S 1.756007 1.492460 -0.162504
S 4.774055 0.969525 1.806468
S 0.001280 -2.142141 -1.425762
S 5.029013 1.016621 -1.697229
S -3.814349 2.467161 -0.102050
S -5.528740 1.324427 0.128891
H -0.999901 1.696669 0.454939

E= -4586.268973
S -1.007831 -0.001706 1.141452
Mo -3.117264 -0.343754 -0.219621
S -2.493816 -1.926150 -1.515450
S -3.064490 1.550808 -1.193005
Mo 1.128143 0.766333 -0.067215
S 0.706513 -0.999561 -1.555097
S 2.584791 -0.083310 -1.836990
Mo 3.542537 -0.649647 0.271870
S 2.287596 0.372456 1.888547
S 4.438638 -2.580647 0.545924
S 0.277802 2.948226 0.834812

S 1.546268 2.900309 -0.786160
S -3.980097 -0.696683 2.002908
S -5.327823 -0.806063 0.430313
H -0.724263 -1.305980 1.312490

E= -4586.283131
S 0.929376 -0.204237 -1.882780
Mo 2.467830 -0.655042 -0.019613
S 2.558770 -2.777306 -0.066155
S 1.413570 -0.021524 1.858552
Mo -0.297136 0.552765 0.145995
S -1.351776 -1.750182 0.442907
S -1.916634 -0.329267 1.863253
Mo -3.313073 -0.383964 -0.140149
S -2.247013 1.133732 -1.438361
S -5.382114 -0.809652 -0.560689
S 0.740848 2.681639 -0.446597
S -0.407535 2.727192 1.185912
S 4.055019 0.499736 -1.392489
S 4.581977 0.215610 0.598841
H 0.388089 -1.429718 -2.020074

[Mo3S11H]- V
E= -4586.354215
S 1.617633 -0.454629 1.535629
Mo 0.791251 0.719971 -0.203194
S 2.329911 0.388157 -1.810713
Mo 3.400429 -0.536028 0.042086
S 5.040493 0.673996 0.697845
S 3.900605 -2.581150 -0.367593
S -0.930497 2.419352 -0.199535
S 0.987796 2.932471 0.388439
S -0.946540 -0.831455 -0.968051
Mo -3.004741 -0.663743 -0.070820
S -4.024583 -2.374153 -0.777326
S -3.955692 1.177665 -1.141052
S -4.391968 1.084301 0.878197
S -2.619327 -1.036801 2.242663
H -1.976742 -2.212490 2.084951

E= -4586.291156
S -1.898738 -0.158516 -0.821697
Mo -0.374488 1.415987 0.130553
S -1.241027 2.445985 1.751548
Mo -3.957228 -0.774774 -0.105013
S -5.000756 -2.247666 -1.242413
S -4.932266 -0.073428 1.656906
S 1.512935 2.439020 -0.829895
S -0.312290 2.794528 -1.780800
S 0.974056 -0.260378 1.243064
Mo 2.889961 -0.984259 0.302613
S 3.557319 -2.533342 1.575001
S 4.334056 0.839446 0.583720
S 4.561775 -0.150033 -1.222018
S 2.151067 -2.017401 -1.704504
H 1.255648 -2.843489 -1.125032

E= -4586.326112
S -2.413915 0.398124 -1.760490
Mo -0.601259 0.597563 -0.200641
S -1.803123 -0.108857 1.646575
Mo -3.470828 -0.462159 0.066595
S -5.234590 0.651697 0.540126
S -3.906623 -2.543220 -0.147943
S 1.000797 2.248288 0.779578
S -0.216148 2.881521 -0.721631
S 0.854892 -0.960531 -0.981838
Mo 3.044295 -0.675068 -0.136914
S 4.105784 -2.463179 -0.516812
S 2.509856 -0.544869 2.222590
S 3.812172 0.872263 1.548024
S 3.787138 0.959557 -1.720865
H 3.227431 0.413233 -2.816725

[Mo3S11H]- VI
E= -4586.354023
S 1.602435 -0.344924 1.560738
Mo 0.894270 0.959928 -0.116920
S 2.402438 0.573915 -1.738488
Mo 3.295945 -0.691750 -0.000353
S 5.162744 0.108400 0.677107
S 3.340047 -2.758779 -0.567061

S -0.845775 2.658829 -0.045834
S -1.091464 3.142698 0.525961
S -0.954435 -0.409887 -1.132840
Mo -3.096169 -0.726219 0.153474
S -3.569439 -2.677127 -0.566902
S -3.631677 1.283614 -1.110118
S -5.057430 0.562687 0.201320
S -2.389183 -0.837144 2.156694
H -0.368916 -1.598776 -0.889668

E= -4586.341777
S 2.056241 -0.388261 1.665384
Mo 0.804957 0.787306 -0.009125
S 2.271389 0.541916 -1.708368
Mo 3.516823 -0.602340 -0.072142
S 5.369873 0.385142 0.323987
S 3.805152 -2.639634 -0.649681
S -0.712408 2.571633 -0.389524
S 0.828730 2.869198 0.985971
S -0.903851 -0.998995 -0.178525
Mo -3.345745 -0.582741 0.216746
S -3.947390 -2.622426 0.384256
S -3.060144 0.534548 -1.925233
S -4.937038 0.571627 -1.060079
S -3.295725 0.329006 2.140384
H -0.590701 -1.751346 0.892389

E= -4586.305798
S -1.171926 1.798296 -0.890222
Mo 0.793921 2.111517 0.242134
S 0.522147 3.650400 1.674340
Mo -2.580945 -0.004709 -0.284119
S -4.260815 -0.007561 -1.607072
S -3.047270 -0.003696 1.816479
S 3.098561 1.548067 -0.398500
S 2.107494 2.852582 -1.611095
S 0.779025 0.001123 1.593270
Mo 0.801763 -2.108844 0.242246
S 0.538432 -3.649230 1.674406
S 3.104239 -1.536491 -0.399070
S 2.116942 -2.843138 -1.612440
S -1.167024 -1.804566 -0.887708
H -0.535916 -0.000722 1.950861

[Mo3S11H]- VII
E= -4586.367374
S 1.570360 -0.760502 1.524702
Mo 0.593128 0.555965 -0.080015
S 2.263811 1.006506 -1.539605
Mo 3.246694 -0.479215 -0.041731
S 4.940046 0.459705 0.876593
S 3.716143 -2.330110 -1.004948
S -0.440611 2.927635 -0.620259
S 0.190900 2.423206 1.292476
S -0.865262 -0.651841 -1.312107
Mo -2.862156 -0.711458 0.136220
S -3.429934 -2.738510 -0.180976
S -3.593136 1.105811 -1.307198
S -4.872218 0.536001 0.219023
S -1.936571 -0.471658 2.049137
H -1.758400 2.557876 -0.557301

E= -4586.363036
S -1.359116 -1.195570 -1.372474
Mo -0.195984 0.439845 -0.128877
S -2.146953 1.022674 1.184505
Mo -3.079709 -0.702241 0.058223
S -3.528438 -2.352116 1.342378
S -4.818003 -0.079931 -1.023366
S -1.070730 4.133670 0.314868
S 0.135801 2.730360 -0.676030
S 1.022022 -0.280527 1.614172
Mo 2.680263 -0.639469 -0.078643
S 2.755865 -2.745297 -0.285587
S 4.143858 0.504984 1.444564
S 4.899934 0.085752 -0.429586
S 1.558040 0.288201 -1.816403
H -0.468436 4.083187 1.517840

E= -4586.334465
S -1.661549 -1.037615 -1.576559
Mo -0.253539 0.163899 -0.175560

S -1.919852 0.293239 1.663538
Mo -3.224550 -0.617484 0.083366
S -4.684830 0.797890 -0.609246
S -4.149055 -2.428804 0.750509
S -1.633956 3.627857 0.327647
S -0.168233 2.445249 -0.613367
S 1.193997 -0.811303 1.397163
Mo 3.020030 -0.596920 -0.043389
S 3.861542 -2.502279 -0.440853
S 4.298182 0.814228 1.561981
S 4.589691 1.296057 -0.349056
S 1.646641 0.080729 -1.753582
H -2.722768 2.917251 -0.036302

[Mo3S11H]- VIII
E= -4586.285276
Mo -2.712802 -0.935779 0.112386
S -4.013168 -0.006243 -1.313364
S -2.170516 -2.991969 -0.155250
S -2.210526 0.153080 1.994317
Mo -0.685357 0.869488 0.140682
S 1.038456 0.957057 1.700979
S 0.267261 -0.438656 -1.575478
Mo 1.884402 -0.238800 -0.039252
S 3.419641 1.167400 -1.243672
S 4.341587 0.660234 0.548089
H 3.994428 1.741501 1.284586
S -0.950947 2.576892 -1.388580
S -1.204716 3.204970 0.576063
S 2.082941 -2.289913 1.002436
S 3.123948 -2.300833 -0.787094

E= -4586.280434
Mo 3.870556 -0.616556 0.012070
S 5.154221 -2.065870 -0.898863
S 4.542427 0.366303 1.786809
S 1.757942 -0.314968 -0.970109
Mo 0.068574 0.981951 -0.270080
S -1.669585 0.760001 -1.763387
S -0.703509 -0.162377 1.643337
Mo -2.305626 -0.443714 0.090315
S -4.071570 0.748772 1.182824
S -4.876805 -0.070854 -0.549747
H -4.733462 0.989493 -1.378058
S 0.594342 2.851535 0.976759
S 0.526464 3.234130 -1.066390
S -2.127289 -2.555527 -0.815104
S -3.118748 -2.647403 1.000197

E= -4586.262927
Mo 3.496397 -0.765597 0.029487
S 4.908521 -1.951729 -1.059928
S 3.841059 -0.404493 2.110578
S 1.739975 0.178131 -1.239488
Mo 0.075725 1.297228 -0.236822
S -1.751509 0.978085 -1.643512
S -0.607264 0.190533 1.653317
Mo -2.202166 -0.503016 0.092421
S -4.116361 0.089203 1.414855
S -4.792619 -0.549665 -0.449632
H -4.882236 0.637305 -1.091227
S 1.059434 3.069991 0.979576
S 0.240351 3.591200 -0.860073
S -1.428981 -2.432833 -1.129645
S -2.383602 -2.873369 0.593804

[Mo3S11H]- IX
E= -4586.379493
Mo -0.015575 0.584337 -0.034905
S 1.463539 -0.064450 -1.868676
Mo 2.773404 -0.505626 -0.132420
S 1.550024 -0.086701 1.690092
S 3.346486 -2.561847 -0.238259
S -1.488127 -0.047610 1.768998
S -4.414094 -1.537518 1.170242
Mo -2.980957 0.017192 0.043342
S -4.428321 -1.633001 -0.916495
S -3.913230 1.921810 -0.013892
S -1.551526 -0.165879 -1.732963
S 0.044388 2.686750 -0.080276
S 4.518027 0.984228 -0.695414
S 5.091543 0.298694 1.190909

H 5.872007 -0.739537 0.819029

E= -4586.354980
Mo -0.195516 0.574032 -0.030732
S -1.141645 -0.893088 1.452200
Mo -2.796421 -0.415462 -0.101914
S -2.028750 1.448512 -1.184117
S -3.038585 -2.099693 -1.382978
S 1.170914 -0.392217 -1.558448
S 3.812069 -2.341432 -0.109318
Mo 3.135148 -0.086080 -0.228110
S 3.922160 -1.279605 1.686398
S 4.509899 1.187603 -1.221857
S 1.879911 1.227412 1.430380
S 0.683004 2.676349 0.499729
S -4.460541 -0.179980 1.575718
S -5.314116 0.495738 -0.202314
H -5.924006 -0.638166 -0.614527

E= -4586.284244
Mo -0.330814 0.810894 -0.026492
S 0.965304 0.011497 -1.820122
Mo 2.434213 -0.749086 -0.243716
S 1.279925 -0.304199 1.613665
S 3.014360 -2.783112 -0.573748
S -1.913477 0.197316 1.923885
S -2.058126 -0.059492 -1.704255
Mo -3.077619 -0.761701 0.318142
S -3.964684 0.738251 -1.263045
S -4.089103 -2.602129 0.713972
S -1.241196 3.011728 -0.332487
S 0.335740 2.848281 0.950807
S 4.250333 0.669143 -0.603743
S 5.594966 0.167599 0.946437
H 6.132545 -0.922539 0.364969

[Mo3S11H]- X
E= -4586.311711
Mo 2.592584 0.372649 -0.126923
S 1.440099 -0.911413 -1.844394
H 1.968457 -2.136478 -1.622476
S 1.087508 0.526429 1.655463
S 2.815298 2.278029 -1.029810
Mo -0.077921 -0.479057 0.008726
S -2.076714 -1.049968 -1.668696
S -1.162486 1.721836 -0.659107
S -5.072038 0.226786 -0.204262
Mo -2.929431 0.211980 -0.069130
S 4.482202 -1.052223 -0.353990
S 4.298886 -0.088258 1.480847
S -0.784213 -2.735088 0.562504
S -1.862924 -1.257642 1.550637
S -2.199880 2.197915 1.103947

E= -4586.350193
Mo -2.892423 -0.413678 -0.153171
S -1.915865 1.362807 -1.522751
H -2.353603 2.470567 -0.887622
S -1.229080 -0.978243 1.390017
S -3.070640 -1.967460 -1.578402
Mo -0.227296 0.468850 -0.034084
S 1.171900 -0.481680 -1.551551
S 4.032655 -2.199825 -0.238186
S 4.313189 1.448006 -1.087120
Mo 3.093881 -0.041269 -0.200515
S -4.852080 0.889365 0.151440
S -4.510848 -0.577508 1.589238
S 0.536320 2.540907 0.723393
S 1.738327 1.037866 1.568996
S 4.001049 -1.265142 1.628298

E= -4586.287014
Mo -2.349105 -0.731313 0.087787
S -0.861141 -0.534716 -1.855549
H -0.148455 -1.673894 -1.744576
S -1.583611 0.698371 1.699714
S -2.002409 -2.732470 0.715984
Mo 0.103952 0.766767 0.013715
S 2.255468 1.036000 -1.565761
S 1.373582 -0.916611 1.405797
S 4.403505 -1.965203 -0.995022
Mo 3.050910 -0.499228 -0.222473

S -4.123847 -0.398886 -1.446350
S -4.604370 -0.055161 0.546555
S -0.650331 3.009594 -0.851991
S 0.573053 3.083012 0.718494
S 3.114269 0.098095 2.054712

[Mo3S11H]- XI
E= -4586.279865
S -3.694040 1.710280 1.565508
Mo -2.809184 0.203357 -0.171572
S -3.403342 1.649673 -1.605010
S -0.718228 -0.339060 -1.562321
Mo 1.140870 -0.133466 0.168600
S 2.629940 -1.666003 -0.797167
Mo 3.912316 -0.147241 0.247709
S 2.569263 1.247988 1.399008
S 0.339978 1.426691 -1.451568
S -4.573987 -1.173264 0.386474
S -3.227675 -2.025294 -0.929932
S -0.981141 0.199576 1.609726
S -0.066579 -1.662053 1.515217
S 5.443946 0.769471 -0.939607
H -3.338266 1.040633 2.675797

E= -4586.284780
S -3.750873 -2.138320 -0.873131
Mo -2.831833 -0.123564 0.221111
S -3.416753 -0.973508 2.072954
S -0.749491 0.900498 1.337263
Mo 1.150927 0.070981 -0.170810
S 2.594687 1.830889 0.203530
Mo 3.942178 0.053850 -0.268275
S 2.548873 -1.632600 -0.803785
S 0.344698 -0.761371 1.892421
S -4.593032 0.964691 -0.797939
S -3.255281 2.226696 0.144510
S -0.998859 -0.828567 -1.387852
S -0.061564 0.916371 -2.012023
S 5.614264 -0.389202 1.005065
H -3.400138 -1.902482 -2.149320

E= -4586.263030
S 3.652028 -1.763346 1.557765
Mo 2.889687 -0.219300 -0.174896
S 3.500595 -1.635681 -1.634054
S 0.794202 0.283888 -1.548160
Mo -0.990250 0.124115 0.247709
S -2.648979 1.518999 -0.919356
Mo -4.075360 -0.019279 -0.019018
S -2.572889 -1.207115 1.326148
S -0.188524 -1.507617 -1.332073
S 4.659059 1.143531 0.390000
S 3.288492 2.034445 -0.873676
S 1.084894 0.027592 1.671609
S 0.101301 1.853954 1.426986
S -6.164804 -0.380067 -0.373171
H 3.302778 -1.089823 2.668318

[Mo3S11H]- XII
E= -4586.285908
S -0.349664 -1.211556 0.902348
Mo 0.870573 0.500454 -0.095742
S 2.457618 0.516439 1.776557
Mo 3.520109 -0.327297 0.037029
S 2.287919 -0.202846 -1.848597
Mo -2.517507 -0.647760 -0.128457
S -3.241768 -2.450139 -0.940900
S -4.489522 0.325996 0.943269
S -3.014143 -0.472247 2.160762
S -0.957875 0.137706 -1.856474
S -2.713431 1.223269 -1.583358
S 0.968432 2.955509 -0.488455
S -0.333452 2.441581 1.036530
S 4.562814 -2.169703 0.368262
H -1.504225 2.429144 0.342005

E= -4586.288790
S 0.347433 -1.235672 -0.909140
Mo -0.893555 0.470275 0.097952
S -2.415004 0.767451 -1.660653
Mo -3.615565 -0.264256 -0.050093
S -2.272229 -0.331138 1.787499

Mo 2.539943 -0.682259 0.066450
S 3.377646 -2.530903 0.623725
S 4.404296 0.527041 -0.941281
S 2.955591 -0.237897 -2.211927
S 0.986940 -0.177036 1.854420
S 2.722024 0.958645 1.795398
S -0.580127 2.761997 0.807330
S 0.524894 2.456446 -0.918368
S -4.991000 -1.850599 -0.505856
H 1.738035 2.268742 -0.339352

E= -4586.271205
S 0.603255 -1.001703 -1.243772
Mo -0.731126 0.293162 0.184976
S -2.440549 0.630789 -1.681961
Mo -3.763006 -0.420704 -0.204532
S -2.244650 -0.903075 1.493243
Mo 2.698264 -0.609750 -0.018289
S 3.544732 -2.510524 0.307041
S 4.625219 0.743739 -0.689386
S 3.239644 0.224629 -2.142955
S 1.061515 -0.454718 1.827143
S 2.714870 0.804079 1.889259
S -0.952121 2.563511 1.122716
S 0.325094 2.579638 -0.507176
S -5.857794 -0.894876 -0.282867
H 1.519070 2.462430 0.128892

[Mo3S11H]- XIII
E= -4586.281524
S 2.623261 -1.351286 2.161952
Mo 2.586724 -0.465212 -0.126756
S 3.463253 -2.086978 -1.195251
S 0.681550 -0.288105 -1.736238
Mo -1.034704 0.442317 0.020711
S -2.686013 0.910116 -1.623748
Mo -3.771090 0.046076 0.130535
S -2.339777 -0.194729 1.855740
S 0.271024 -1.644635 -0.254468
S 4.355079 0.919390 0.591295
S 3.443760 1.509067 -1.157938
S 0.909586 1.259892 1.327526
S -0.114376 2.592827 0.101085
S -4.999334 -1.655565 -0.306053
H 3.472738 -0.493494 2.748970

E= -4586.284287
S 2.668545 -1.222677 2.240064
Mo 2.618139 -0.453030 -0.096387
S 3.507495 -2.145647 -1.037732
S 0.748077 -0.367702 -1.744573
Mo -1.040312 0.405297 -0.038947
S -2.626095 0.647424 -1.741138
Mo -3.805347 0.072549 0.098507
S -2.357895 -0.008078 1.830458
S 0.295234 -1.660171 -0.215147
S 4.370712 0.979083 0.556443
S 3.461248 1.468031 -1.225082
S 0.905073 1.260474 1.285517
S -0.147271 2.558450 0.045763
S -5.185064 -1.561837 -0.073659
H 3.322926 -0.199900 2.812109

E= -4586.267338
S 2.812428 -1.507411 2.006792
Mo 2.737831 -0.404788 -0.178800
S 3.729508 -1.822822 -1.411808
S 0.798121 -0.175832 -1.727986
Mo -0.889570 0.304092 0.135356
S -2.620584 0.850150 -1.564470
Mo -3.975608 -0.177479 -0.048388
S -2.402628 -0.698162 1.602544
S 0.501720 -1.685528 -0.368305
S 4.402078 1.017803 0.697022
S 3.455645 1.722586 -0.989277
S 0.948511 1.129477 1.482411
S -0.187171 2.524316 0.422023
S -6.089178 -0.574424 -0.071734
H 3.773392 -0.799125 2.621576

[Mo3S11H]- XIV
E= -4586.282986

S 0.912940 0.427378 -1.921161
Mo -0.946356 0.445022 -0.014523
S -2.539622 0.796014 -1.726435
Mo -3.686722 0.029148 0.044590
S -2.335657 -0.136740 1.816824
Mo 2.525049 -0.484875 -0.222336
S 3.391752 -2.008615 -1.412089
S 4.298386 0.426534 1.090118
S 3.821407 1.467713 -0.625889
S 0.390939 -1.683270 0.251957
S 1.796717 -1.655329 1.760381
S 0.860523 1.326420 1.426479
S -0.258401 2.665165 0.316572
S -4.883921 -1.705167 -0.352336
H 1.256196 1.727981 -1.915398

E= -4586.285627
S -0.934330 0.381684 1.939677
Mo 0.949505 0.479244 0.038182
S 2.506005 0.653559 1.792007
Mo 3.683372 0.015372 -0.020544
S 2.343949 0.055862 -1.813824
Mo -2.515495 -0.503670 0.200112
S -3.351979 -2.091504 1.326212
S -4.302032 0.417860 -1.086415
S -3.857331 1.402538 0.670957
S -0.356761 -1.650811 -0.310936
S -1.755705 -1.584487 -1.821743
S -0.882749 1.388803 -1.373152
S 0.240092 2.697928 -0.232175
S 4.873641 -1.752480 0.215489
H -1.294875 1.677036 1.956933

E= -4586.272764
S -1.054634 0.635940 1.890606
Mo 0.791228 0.265534 0.101852
S 2.449445 0.387680 1.768896
Mo 3.870639 -0.212481 0.035739
S 2.394492 -0.600548 -1.630020
Mo -2.679928 -0.363347 0.234390
S -3.692416 -1.657152 1.569543
S -4.344633 0.529870 -1.222826
S -3.802670 1.727331 0.365148
S -0.655498 -1.792681 -0.074011
S -2.034091 -1.793020 -1.599917
S -0.804407 1.086876 -1.574008
S 0.401203 2.471148 -0.629862
S 6.020140 -0.302713 0.054424
H -1.272379 1.948697 1.689215

[Mo3S11H]- XV
E= -4586.343329
S 0.150293 -0.175115 1.737313
Mo -0.015466 1.509266 0.088880
S 1.826674 1.191615 -1.492624
Mo 1.506761 -0.828714 -0.110007
S 0.149599 -2.123192 -1.380603
Mo -1.279761 -0.879205 -0.022827
S -1.677082 0.935523 -1.643944
S -2.492430 1.321136 0.211546
S -2.535091 -2.222601 1.371225
S -3.355685 -2.207029 -0.531765
S 2.926623 -2.099400 1.249032
S 3.824622 -1.388220 -0.483707
S 0.575380 3.195160 1.513902
S -0.018958 4.035716 -0.270637
H 1.132446 0.926732 -2.616746

E= -4586.328739
S 0.088845 -0.185845 1.719957
Mo 0.367883 1.456204 0.044311
S 1.990437 0.595838 -1.591727
Mo 1.207997 -1.194002 -0.108629
S -0.445049 -2.048650 -1.394891
Mo -1.509055 -0.481358 -0.013405
S -1.426151 1.379005 -1.618344
S -2.100586 1.964640 0.251145
S -3.064417 -1.471555 1.401246
S -3.859873 -1.186608 -0.481079
S 2.256822 -2.776948 1.259037
S 3.268139 -2.411204 -0.527819
S 1.807838 2.851719 1.447129

S 1.107093 3.813465 -0.192492
H 3.223762 0.822844 -1.090211

[Mo3S11H]- XVI
E= -4586.340753
S -0.205912 0.074203 1.728696
Mo 0.815401 -1.207719 0.039218
S -0.881928 -2.005100 -1.280544
Mo -1.715131 -0.244238 -0.088382
S -1.465666 1.706093 -1.315288
Mo 0.380704 1.549742 -0.011988
S 1.853530 0.294637 -1.568140
S 3.313932 -0.001443 -0.081504
S 0.610428 3.366083 1.424760
S 1.603219 3.623808 -0.388723
S -3.516082 -0.642401 1.294728
S -4.132031 -0.572355 -0.703815
S 1.650609 -2.818835 1.506517
S 2.313441 -3.196157 -0.432596
H 3.502412 -1.363512 -0.377111

E= -4586.327357
S -0.477360 -0.041050 1.724549
Mo 0.733490 -1.283160 0.094367
S -1.022017 -1.952631 -1.275063
Mo -1.912839 -0.163863 -0.182934
S -1.287553 1.720134 -1.370118
Mo 0.455657 1.391285 0.057237
S 1.863207 0.138274 -1.475891
S 3.918263 0.258085 -0.861945
S 0.764149 3.114546 1.632046
S 1.920785 3.287524 -0.083359
S -3.831411 -0.355614 1.147726
S -4.219297 -0.198407 -0.893607
S 1.603683 -2.716880 1.732242
S 2.419994 -3.041070 -0.159728
H 3.956002 -1.065659 -0.553746

[Mo3S11H]- XVII
E= -4586.319182
S 0.280100 -0.006294 1.783445
Mo -0.184638 1.541590 0.077637
S 1.543968 1.386191 -1.439818
Mo 1.640881 -0.490732 -0.089944
S 0.564417 -2.251867 -1.061883
Mo -1.058334 -1.051326 0.120789
S -1.928351 -0.152464 -2.288196
S -2.485147 0.878596 -0.542015
S -2.117730 -2.211452 1.771868
S -2.945204 -2.782400 -0.034032
S 3.477520 -0.903079 1.251013
S 3.964415 -1.152434 -0.769443
S -0.619118 3.242032 1.545268
S -0.594730 4.018953 -0.359075
H -2.954553 -1.032895 -2.270359

E= -4586.329465
S 0.487783 -0.017971 1.841270
Mo -0.704880 1.350580 0.295530
S 0.912337 1.832467 -1.258955
Mo 1.751182 -0.003541 -0.173955
S 0.920297 -1.829243 -1.273531
Mo -0.708101 -1.361299 0.278089
S -1.914878 0.084477 -3.257950
S -2.151206 0.095110 -1.000069
S -1.134899 -3.004461 1.907462
S -2.246455 -3.217980 0.162296
S 3.791298 -0.016579 0.981089
S 3.988615 0.012550 -1.093993
S -1.102707 2.984490 1.942944
S -2.236521 3.212231 0.214643
H -3.227333 -0.148270 -3.429161

[Mo3S11H]- XVIII
E= -4586.321669
S -0.148893 0.000159 1.702507
Mo 0.714654 -1.395515 0.041481
S -1.156225 -1.841397 -1.268479
Mo -1.724845 0.000893 -0.033463
S -1.154256 1.842447 -1.268630
Mo 0.716158 1.394800 0.041429
S 1.750833 -0.000922 -1.679596

S 2.856527 -0.001490 0.057501
S 1.311869 3.191809 1.380601
S 1.889383 3.509222 -0.582978
S -3.633639 0.002296 1.285368
S -4.127910 0.001795 -0.745004
S 1.308262 -3.193217 1.380648
S 1.885652 -3.511162 -0.582862
H -0.156285 -0.000103 3.058047

E= -4586.300660
S -0.461468 -0.102682 1.955349
Mo 1.715958 -0.539570 -0.043840
S 0.493669 -2.346160 -0.916351
Mo -1.267083 -1.178884 -0.099553
S -1.840058 0.465944 -1.591316
Mo -0.486993 1.401565 0.027086
S 1.438683 1.386795 -1.519485
S 1.904607 1.963932 0.405793
S -1.601739 2.996825 1.278441
S -1.163166 3.735362 -0.605984
S -2.768702 -2.398915 1.223305
S -3.200474 -2.470468 -0.813831
S 3.421654 -1.278952 1.366072
S 3.979997 -1.126399 -0.638596
H -1.647071 0.104824 2.590582

[Mo3S11H]- XIX
E= -4586.371098
S -0.109327 -0.017013 1.767406
Mo 0.834484 -1.302476 0.010172
S -0.992907 -1.957970 -1.300233
Mo -1.620131 -0.147983 -0.057222
S -1.317935 1.743665 -1.301428
Mo 0.595785 1.416349 0.012291
S 1.784407 0.152282 -1.731574
S 2.829412 0.244643 0.042020
S 1.001947 3.182852 1.447222
S 1.589783 3.671167 -0.479944
S -3.524493 -0.288870 1.352875
S -4.226899 -0.375680 -0.610016
S 1.539777 -2.975484 1.441289
S 2.207614 -3.347940 -0.485803
H -4.527875 0.926211 -0.809160

E= -4586.341222
S -0.109645 -0.037912 1.750837
Mo 0.778880 -1.352289 -0.010124
S -1.225292 -1.864304 -1.298598
Mo -1.613492 -0.003466 -0.079116
S -1.127138 1.862469 -1.308390
Mo 0.733281 1.374784 0.026141
S 1.864258 0.040188 -1.700705
S 2.891575 0.058798 0.097935
S 1.229272 3.099122 1.484925
S 1.899176 3.569498 -0.416917
S -3.514773 0.046758 1.342005
S -4.233757 0.078453 -0.617939
S 1.012637 -3.474821 1.349420
S 1.853529 -3.516333 -0.467621
H -4.381580 1.410199 -0.789025

[Mo3S11H]- XX
E= -4586.352516
S -0.145932 -0.034726 1.762335
Mo 0.998561 -1.191874 0.036192
S -0.695934 -2.043728 -1.332785
Mo -1.587248 -0.355893 -0.096900
S -1.471501 1.524116 -1.357213
Mo 0.425013 1.468247 0.014306
S 1.811791 0.361999 -1.690256
S 2.792948 0.589560 0.107532
S 0.547689 3.293549 1.429389
S 1.092659 3.839963 -0.496267
S -3.719878 -0.626513 1.296062
S -3.979440 -0.877742 -0.732767
S 1.852622 -2.783586 1.479584
S 2.591937 -3.077770 -0.436249
H -3.957050 0.697919 1.479052

E= -4586.335606
S -0.268527 0.104246 1.685884
Mo 0.702542 -1.360235 0.047808

S -1.025824 -2.013043 -1.325022
Mo -1.733173 -0.128622 -0.149665
S -1.087843 1.713352 -1.402881
Mo 0.795226 1.404789 -0.050111
S 1.921927 -0.075737 -1.651869
S 2.841868 -0.013912 0.196161
S 1.258209 3.189853 1.388058
S 2.034087 3.433942 -0.523407
S -3.893718 1.022288 0.893437
S -4.063758 -0.738187 -0.214671
S 1.192857 -3.004584 1.602548
S 1.968510 -3.518795 -0.245411
H -4.157587 1.940066 -0.062630

[Mo3S11H]- XXI
E= -4586.354243
S 0.120344 -0.030865 1.756116
Mo -0.091192 1.540639 0.012420
S 1.823762 1.272567 -1.276587
Mo 1.572612 -0.643011 -0.048697
S 0.375479 -2.163401 -1.309242
Mo -1.106962 -0.973897 -0.027416
S -1.635684 0.675159 -1.687218
S -2.625458 1.104547 0.071901
S -2.594643 -2.458513 1.418487
S -3.053804 -2.510443 -0.584425
S 3.260317 -1.319906 1.374845
S 3.832877 -1.622810 -0.613301
S 0.097536 3.371413 1.412994
S -0.370724 3.975068 -0.514582
H -3.407300 -1.481718 1.891305

E= -4586.341621
S 0.054890 -0.258861 1.693408
Mo 0.616612 1.383809 0.041548
S 2.090113 0.390602 -1.419078
Mo 1.146957 -1.310789 -0.163874
S -0.656160 -2.139523 -1.213904
Mo -1.606389 -0.216825 -0.014103
S -1.180570 1.559196 -1.617050
S -1.754060 2.286450 0.239359
S -3.399698 -1.572860 1.230897
S -3.986477 -0.648258 -0.527226
S 2.274373 -2.766410 1.296320
S 3.040626 -2.729463 -0.640716
S 1.701952 2.751359 1.558282
S 1.595250 3.681034 -0.291092
H -3.085355 -2.812447 0.782800

[Mo3S11H]- XXII
E= -4586.367924
S 0.121002 -0.062432 1.755172
Mo 0.454713 1.486564 0.006525
S 2.153372 0.558349 -1.275428
Mo 1.221829 -1.148821 -0.068434
S -0.450034 -2.128589 -1.319542
Mo -1.403751 -0.488221 0.007232
S -1.276766 1.228349 -1.713013
S -2.073934 1.973066 0.046251
S -3.049393 -1.388951 1.496072
S -3.846050 -1.375239 -0.426021
S 2.575279 -2.370826 1.347183
S 2.993353 -2.852995 -0.643219
S 1.277881 3.115181 1.425063
S 1.080843 3.863500 -0.497262
H -3.546068 -2.630542 -0.827649

E= -4586.342157
S 0.012706 0.258844 1.690876
Mo -1.636851 0.263589 -0.027026
S -0.644611 2.130331 -1.279528
Mo 1.095432 1.346999 -0.143029
S 2.105979 -0.350815 -1.390468
Mo 0.594319 -1.338676 0.020172
S -1.162038 -1.509709 -1.659048
S -1.752206 -2.296342 0.168367
S 1.651716 -2.788329 1.602374
S 1.695121 -3.720325 -0.258662
S 2.090776 2.887207 1.321438
S 2.963145 2.838859 -0.573998
S -3.351241 1.355027 1.337933
S -3.930295 0.689656 -0.522362

H 2.913368 -3.330755 -0.695584

[Mo3S11H]- XXIII
E= -4586.355849
S 0.079390 0.422706 1.708196
Mo -1.269310 -0.599113 0.034679
S -2.821699 -1.454431 1.654780
S -3.274840 -1.962133 -0.307154
Mo 0.012996 1.785091 -0.211597
S -2.519445 1.627315 -0.077695
S -1.623681 0.986454 -1.819652
Mo 1.481582 -0.458519 -0.010295
S 3.676437 -1.600393 -0.440615
S 3.279931 -0.749275 1.405127
S 1.785493 1.272804 -1.567631
S 0.423084 3.684109 1.175540
S 0.217909 -2.600505 0.321027
S 0.141780 -1.816664 -1.568294
H 0.708997 4.487048 0.124863

E= -4586.334051
S 0.114972 0.262252 1.785251
Mo -1.352186 -0.441265 0.014187
S -3.227800 -1.310954 1.434467
S -3.546281 -1.468630 -0.526610
Mo 0.277758 1.794380 0.008740
S -2.325851 1.923249 0.168330
S -1.440170 1.369810 -0.610167
Mo 1.393032 -0.670327 0.001615
S 3.413974 -2.099205 -0.512096
S 3.076843 -1.414677 1.408486
S 2.132159 1.102148 -1.276987
S 1.119209 3.960049 0.595574
S -0.206037 -2.681377 0.127738
S -0.094647 -1.680588 -1.662519
H 2.356698 3.928377 0.065753

E= -4586.296642
S 0.141849 0.302480 1.812466
Mo -0.831773 -1.020328 0.000942
S -1.865623 -2.814566 1.413785
S -2.196363 -3.082909 -0.521857
Mo -0.818379 1.730247 0.139856
S -2.934477 0.294132 0.330197
S -2.084088 0.412958 -1.553631
Mo 1.691573 0.144294 -0.032190
S 4.052442 -0.145259 -0.608822
S 3.545472 0.158190 1.387174
S 1.277350 2.220260 -0.878183
S -1.957627 3.874695 0.271141
S 1.274814 -2.392384 -0.093481
S 0.794921 -1.316027 -1.784343
H -2.518389 3.937918 -0.952664

[Mo3S11H]- XXIV
E= -4586.334827
S -0.060529 0.352925 -1.755087
Mo 1.294739 -0.585685 -0.015068
S 2.893812 -1.464163 -1.569500
S 3.357675 -1.388951 0.413919
Mo -0.018530 1.879079 0.032671
S 2.433493 1.657314 -0.023705
S 1.580737 1.129968 1.766717
Mo -1.442596 -0.542605 -0.046363
S -3.664823 -1.709419 0.439151
S -3.278993 -0.804557 -1.371811
S -1.909399 1.316977 1.476592
S -0.573707 3.763831 -0.869789
S -0.142771 -2.637115 -0.226447
S -0.111348 -1.768052 1.630104
H -1.398030 0.886351 2.645628

E= -4586.279684
S 0.025705 0.089029 -1.890359
Mo 1.380959 -0.427304 0.005384
S 2.987603 -1.607549 -1.334206
S 3.472742 -1.574334 0.682796
Mo -0.008297 1.839340 -0.267450
S 2.467934 1.804283 -0.599470
S 1.842883 1.642118 1.351371
Mo -1.379841 -0.315403 0.016536
S -3.610319 -1.352016 0.724178

S -3.191922 -1.482026 -1.209872
S -1.479741 1.556195 1.722685
S -2.357500 1.792622 -0.924633
S -0.057181 -2.482551 0.134268
S -0.042214 -1.337964 1.817702
H -0.626316 1.176451 2.720924

E= -4586.236382
S 0.044759 0.115862 -1.856631
Mo 1.496438 -0.440318 0.002841
S 3.204717 -1.506077 -1.317665
S 3.604122 -1.363453 0.718954
Mo -0.221479 1.944859 -0.280368
S 2.328214 1.932411 -0.596923
S 1.639261 1.784641 1.337986
Mo -1.350635 -0.376377 0.021151
S -3.514760 -1.567778 0.705260
S -3.060940 -1.688178 -1.219953
S -1.627150 1.466450 1.725501
S -2.527744 1.619973 -0.932239
S 0.087378 -2.492281 0.129275
S 0.066407 -1.336261 1.809864
H -0.729823 1.172181 2.712912

[Mo3S11H]- XXV
E= -4586.287637
S 0.049501 0.145790 -1.894739
Mo 1.380479 -0.437356 -0.009497
S 3.037044 -1.598019 -1.318799
S 3.442316 -1.584828 0.716076
Mo -0.017474 1.837396 -0.234900
S 2.490306 1.800191 -0.535107
S 1.765008 1.597181 1.386758
Mo -1.378755 -0.312196 -0.021972
S -3.652539 -1.293948 0.763506
S -3.234925 -1.418787 -1.248969
S -1.209404 1.303820 1.844691
S -2.224214 2.021244 -0.825163
S -0.055021 -2.501382 0.031173
S -0.098355 -1.320364 1.728298
H -4.293936 -0.103812 0.823865

E= -4586.274151
S 0.031902 0.089645 -1.898457
Mo 1.408554 -0.432964 -0.001015
S 3.016391 -1.640884 -1.298944
S 3.504546 -1.544131 0.717787
Mo 0.084791 1.871660 -0.294255
S 2.564877 1.793525 -0.507035
S 1.801603 1.591594 1.394930
Mo -1.369665 -0.370882 -0.007783
S -3.665341 -1.421492 0.699684
S -3.121096 -1.533055 -1.291278
S -1.683234 1.677921 1.358199
S -2.437924 1.898560 -0.558317
S -0.035824 -2.498863 0.277041
S -0.024975 -1.197738 1.858261
H -4.409354 -0.289483 0.698326

E= -4586.228037
S 0.055978 0.150632 -1.825134
Mo 1.581701 -0.422570 0.009800
S 3.311426 -1.417884 -1.304342
S 3.697134 -1.327561 0.742707
Mo -0.220192 2.027237 -0.296941
S 2.314341 2.051328 -0.513834
S 1.555461 1.704947 1.372473
Mo -1.338032 -0.483726 0.016863
S -3.522026 -1.702162 0.627596
S -2.917008 -1.791772 -1.345142
S -1.916251 1.520579 1.392621
S -2.685350 1.647504 -0.529567
S 0.195183 -2.497396 0.220043
S 0.123669 -1.239703 1.835584
H -4.386806 -0.655732 0.583602

[Mo3S11H]- XXVI
E= -4586.356511
S -0.055706 0.377352 1.734798
Mo 1.237765 -0.662214 0.026797
S 2.765347 -1.643825 1.600268
S 3.195689 -2.072467 -0.386118

Mo -1.509359 -0.417469 0.011228
S -0.327655 -2.618691 0.242549
S -0.230223 -1.759413 -1.613205
Mo 0.041615 1.764949 -0.154956
S -1.770858 1.386808 -1.480815
S -0.188777 3.912487 0.883855
S -3.765240 -1.443631 -0.443522
S -3.309596 -0.680257 1.425395
S 2.581195 1.502964 0.001788
S 1.654398 0.991579 -1.763949
H 0.881908 3.972319 1.694426

E= -4586.264623
S -0.028106 0.110179 1.894602
Mo 1.383011 -0.431248 -0.034474
S -0.024667 -1.237845 -1.859981
S -0.039347 -2.460796 -0.234255
Mo -1.398087 -0.374465 -0.009135
S -1.709281 1.683855 -1.407276
S -2.441073 1.912048 0.511386
Mo 0.031378 1.850091 0.295383
S 2.507414 1.759144 0.605367
S 1.822624 1.648111 -1.332312
S -3.041921 -1.512951 1.305723
S -3.488531 -1.483906 -0.720887
S 3.291971 -1.434348 -1.130340
S 2.952861 -1.549871 1.613477
H 2.484231 -2.801828 1.497444

E= -4586.237984
S -0.024891 0.019287 1.836170
Mo -1.424673 -0.399531 -0.049601
S -3.033957 -1.635000 1.242486
S -3.528189 -1.391182 -0.763204
Mo -0.047079 1.873563 0.383105
S -2.516879 1.827915 0.556598
S -1.753342 1.690864 -1.351332
Mo 1.597481 -0.550945 -0.051349
S 3.399674 -1.068731 -1.309888
S 2.775918 -1.800767 1.691992
S 1.736668 1.842441 -1.209212
S 2.484484 1.767392 0.709889
S 0.001443 -2.481154 -0.410923
S 0.006557 -1.090428 -1.905245
H 1.959621 -1.659844 2.752197

[Mo3S11H]- XXVII
E= -4586.312365
S 0.131093 0.201533 -1.832515
Mo 1.438919 -0.581426 -0.036071
S 3.294611 -0.979307 -1.312579
S 3.637080 -1.641940 0.623501
Mo 0.048751 1.837262 -0.127420
S 1.259226 3.557172 -0.657536
S 1.301338 0.974369 1.791312
Mo -1.295355 -0.540659 -0.010798
S -3.315193 -1.759178 0.705748
S -2.922257 -1.727731 -1.323297
S -1.879282 1.506997 1.340867
S -2.368714 1.666096 -0.627796
S 0.136929 -2.683181 -0.251514
S 0.216736 -0.820090 2.100787
H 0.057704 -2.753268 -1.591496

E= -4586.278242
S -0.000536 0.074255 -1.897826
Mo 1.341299 -0.404372 0.059365
S 3.180820 -1.597390 -1.120615
S 3.371236 -1.568589 0.895923
Mo -0.000483 1.847372 -0.336891
S 2.459676 1.833164 -0.670374
S 1.814244 1.730210 1.287048
Mo -1.341435 -0.404951 0.059565
S -3.372275 -1.568126 0.894555
S -3.178915 -1.597401 -1.122312
S -1.812816 1.727638 1.289125
S -2.460846 1.833257 -0.667271
S 0.000413 -2.557967 -0.230579
S 0.000613 -0.862356 2.013022
H 0.000212 -2.745218 -1.576782

E= -4586.250977

S 0.000437 0.085200 -1.901679
Mo 1.341860 -0.409129 0.040405
S 3.289097 -1.606112 -1.034285
S 3.455859 -1.501447 0.936532
Mo -0.000574 1.869869 -0.331451
S 2.505154 1.808953 -0.661907
S 1.817535 1.720347 1.274603
Mo -1.340957 -0.410086 0.040658
S -3.454630 -1.501387 0.937732
S -3.288723 -1.608017 -1.033246
S -1.820733 1.721494 1.272477
S -2.505791 1.805906 -0.664952
S 0.000709 -2.611752 -0.330711
S 0.000188 -0.899486 1.967784
H 0.000585 -2.746641 -1.681257

[Mo3S11H]- XXVIII
E= -4586.282974
S 0.001142 -0.091813 -2.021242
Mo 1.332140 -0.683746 0.020678
S 3.366587 -1.728304 -0.848584
S 3.236804 -1.425229 1.178520
Mo 0.002263 1.647695 -0.438113
S 2.401318 1.608567 -0.707778
S 1.683797 2.704769 0.888728
Mo -1.334380 -0.678474 0.020392
S -3.237400 -1.421130 1.179130
S -3.370077 -1.724964 -0.847368
S -1.681566 2.703015 0.887694
S -2.397139 1.608912 -0.711233
S -0.002717 -2.590600 -0.215540
S -0.000610 -0.294697 2.100307
H -0.003185 -1.566413 2.553667

E= -4586.270836
S 0.000224 0.112803 -1.914594
Mo 1.334507 -0.430109 0.025592
S 3.042155 -1.674214 -1.193385
S 3.326545 -1.691833 0.819931
Mo 0.001115 1.852907 -0.312148
S 2.450314 1.846382 -0.698342
S 1.867243 1.730722 1.270397
Mo -1.334916 -0.428525 0.025306
S -3.325888 -1.692657 0.820806
S -3.045432 -1.671429 -1.192288
S -1.866193 1.731821 1.269606
S -2.448059 1.849762 -0.699362
S -0.001928 -2.430058 -0.154925
S -0.000707 -0.600390 2.209571
H -0.002029 -1.933999 2.373852

E= -4586.238067
S -0.000042 0.112129 -1.909471
Mo 1.337751 -0.423422 0.016586
S 3.143866 -1.681256 -1.128768
S 3.457737 -1.620176 0.830018
Mo -0.000156 1.872014 -0.310583
S 2.494359 1.796661 -0.695045
S 1.878392 1.705488 1.256175
Mo -1.337912 -0.422058 0.016668
S -3.457967 -1.619916 0.829582
S -3.142505 -1.682197 -1.129019
S -1.878564 1.705033 1.256407
S -2.494630 1.796127 -0.694761
S 0.000167 -2.465091 -0.202814
S 0.000236 -0.616172 2.171777
H -0.000952 -1.954104 2.298305

[Mo3S11H]- XXIX
E= -4586.238195
S 0.000004 0.143957 1.877277
Mo -1.390819 -0.409825 0.008089
S -3.054906 -1.585308 1.281061
S -3.466628 -1.518427 -0.751613
Mo 0.000003 1.892051 0.283723
S -2.485752 1.899276 0.484759
S -1.733336 1.592929 -1.403590
Mo 1.390816 -0.409824 0.008083
S 3.466633 -1.518425 -0.751603
S 3.054893 -1.585315 1.281067
S 1.733337 1.592930 -1.403599
S 2.485762 1.899248 0.484750

S -0.000008 -2.481936 -0.238098
S -0.000004 -1.223147 -1.841270
H 0.000025 -0.493367 3.098170

E= -4586.243192
S -0.355331 0.376331 2.163123
Mo -1.358083 -0.422087 0.007802
S -3.060150 -1.556695 1.276455
S -3.380377 -1.619527 -0.765389
Mo -0.033647 1.846700 0.227850
S -2.525940 1.882814 0.248628
S -1.635243 1.494336 -1.560892
Mo 1.456578 -0.410888 -0.087846
S 3.549583 -1.551670 -0.666620
S 3.032839 -1.519770 1.351631
S 1.816073 1.790679 -1.343573
S 2.413834 1.832350 0.634329
S 0.058597 -2.450297 -0.077655
S 0.008718 -1.392087 -1.820991
H -1.485293 0.840134 2.767439

E= -4586.226717
S -0.934832 0.599160 2.208710
Mo -1.433694 -0.479513 0.005439
S -3.368020 -1.497878 1.043169
S -3.314717 -1.687106 -1.017580
Mo -0.257198 1.837820 0.199618
S -2.675030 1.780221 -0.416804
S -1.330311 1.139499 -1.838509
Mo 1.723488 -0.438226 -0.054219
S 3.987425 -0.643909 -0.872471
S 3.475211 -1.879515 0.709044
S 1.852154 1.964702 -0.955614
S 2.066738 1.846126 1.109771
S 0.120488 -2.197797 0.754841
S 0.170642 -1.905850 -1.276177
H -2.164994 1.074201 2.490716

[Mo3S11]- I
E= -4585.700310
S 0.535563 -0.552589 -1.434159
Mo 2.571974 -0.641891 -0.058633
S 4.496767 0.794523 -0.161072
S 3.393341 0.596043 -1.903308
S 0.722257 -0.864623 1.474412
S 2.422873 -0.011323 2.260025
Mo -0.897162 0.616227 -0.029727
S 0.188183 2.442765 1.169426
S -0.852147 2.861755 -0.566296
Mo -3.548004 -0.301757 -0.049866
S -4.478291 -2.223717 -0.194678
S -2.335204 0.071859 1.794084
S -2.460710 0.361596 -1.863133
S 3.284495 -2.616810 -0.212458

E= -4585.697920
S 0.612628 -0.595169 -1.369192
Mo 2.699244 -0.600860 -0.065643
S 4.678246 0.718923 -0.443374
S 3.452956 0.384338 -2.079264
S 0.960097 -0.646014 1.678032
S 2.713843 0.353805 2.119727
Mo -0.723761 0.536076 0.116149
S 0.316159 2.463291 0.987890
S -1.183887 2.781853 -0.386658
Mo -3.712806 -0.472653 -0.128497
S -5.750317 -1.158784 -0.085662
S -2.156372 -0.524908 1.616265
S -2.428943 0.235213 -1.821371
S 3.346064 -2.601777 -0.011664

E= -4585.668185
S 1.222942 0.674303 -1.455029
Mo 2.669949 -0.544884 -0.041166
S 4.886148 0.155107 0.517916
S 4.348216 0.409798 -1.468057
S 0.502327 -0.876375 1.445918
S 2.249636 -0.049689 2.206096
Mo -0.734162 0.650191 -0.055488
S -0.311561 3.039053 0.586090
S -1.516430 2.900904 -0.990645
Mo -3.454080 -0.832169 0.041697

S -5.509175 -1.287606 -0.369040
S -2.802352 0.628396 1.545818
S -1.827660 -1.058705 -1.449372
S 2.743426 -2.627175 -0.425432

[Mo3S11]- II
E= -4585.748296
S 1.145559 0.954572 -0.000383
Mo 3.317397 0.058612 -0.000006
S 3.455759 -1.157844 -1.739752
S 3.455412 -1.156977 1.740356
Mo -0.678587 -0.768594 -0.000011
S -0.015944 -1.817060 -1.721092
S -3.018906 -1.646526 -0.000174
Mo -3.727743 0.485514 -0.000045
S -1.721602 1.517202 -0.000044
S -4.857201 0.958206 -1.759389
S -0.016141 -1.816278 1.721595
S -4.857008 0.958081 1.759454
S 3.864025 2.513986 -0.000308
S 5.424497 1.281867 -0.000101

E= -4585.686559
S 1.234257 1.364300 -0.164668
Mo 2.802562 -0.541021 0.136354
S 1.658941 -2.182747 -0.642553
S 2.887466 -0.599577 2.269999
Mo -1.044278 1.223641 0.044511
S -0.700849 -1.056655 1.168035
S -2.331886 0.075702 1.832959
Mo -2.708372 -1.337689 -0.179337
S -2.132442 0.277028 -1.764294
S -3.990828 -2.950591 -0.776735
S -1.059076 3.463045 -0.870056
S -2.153409 3.121071 0.834871
S 4.081742 0.988064 -1.227232
S 5.000065 -0.780083 -0.664335

E= -4585.685819
S 0.873054 -0.432831 -1.715484
Mo 2.492074 -0.718068 -0.087368
S 2.932864 -2.801245 -0.086277
S 1.436655 -0.076310 1.779355
Mo -0.328934 0.531701 0.143516
S -1.436576 -1.763432 0.566685
S -2.007445 -0.236456 1.877121
Mo -3.331856 -0.416797 -0.177666
S -2.237954 1.186344 -1.375797
S -5.394873 -0.819223 -0.442239
S 0.746858 2.662636 -0.447419
S -0.354196 2.761935 1.208561
S 3.836622 0.858122 -1.300768
S 4.672871 0.243764 0.455247

[Mo3S11]- III
E= -4585.767116
S 1.589446 -0.769600 1.549288
Mo 0.463036 0.449714 -0.075148
S 2.078752 0.885001 -1.605883
Mo 3.209338 -0.404367 -0.040983
S 4.814984 0.756595 0.776929
S 3.854096 -2.256028 -0.899336
S -0.689635 2.601574 -0.617653
S 0.202751 2.501524 1.177368
S -0.881756 -0.888594 -1.350960
Mo -2.761425 -0.671846 0.152339
S -3.448678 -2.685108 0.214938
S -3.494168 1.010868 -1.433166
S -4.745560 0.645016 0.156355
S -1.671472 -0.156690 1.937075

E= -4585.747520
S 2.402304 -0.044752 -1.780653
Mo 0.697466 -0.552203 -0.191998
S 2.063288 -0.279152 1.686724
Mo 3.593306 0.454920 0.109131
S 5.405131 -0.676394 0.212696
S 3.975541 2.547876 0.294163
S -0.678034 -2.413364 0.711396
S -0.072283 -2.539927 -1.229411
S -0.867114 1.033592 -0.420297
Mo -3.277182 0.573226 -0.174528

S -4.018001 2.562176 -0.356525
S -2.608405 -0.429503 1.945765
S -4.602494 -0.441109 1.539509
S -3.660609 -0.568793 -1.927704

[Mo3S11]- II
E= -4585.718010
S -1.713408 -0.995859 -1.554263
Mo -0.308794 0.255418 -0.214576
S -2.038901 0.686805 1.500283
Mo -3.285743 -0.542197 0.094244
S -4.923354 0.580165 -0.706331
S -3.971265 -2.355028 1.002106
S -0.733099 3.909491 0.486432
S 0.014165 2.578393 -0.776929
S 1.056631 -0.707231 1.405678
Mo 2.916930 -0.723790 -0.023787
S 3.623850 -2.705914 -0.278669
S 4.260060 0.710278 1.505384
S 4.615140 1.029408 -0.428818
S 1.588900 -0.077764 -1.776560

[Mo3S11]- IV
E= -4585.762211
Mo -3.189242 -0.389405 0.069312
S -3.805114 -1.772515 1.571470
S -4.783679 0.307693 -1.172360
S -1.460767 -1.288112 -1.201116
Mo -0.339938 0.408759 -0.180629
S 0.856939 -0.320639 1.610745
S 1.212513 0.886957 -1.802207
Mo 2.467818 -0.073078 -0.052429
S 3.568588 1.942802 0.165306
S 4.235996 0.518400 1.523120
S -1.418224 2.512689 -0.280817
S -2.154974 1.367284 1.301632
S 3.130583 -2.437787 0.281419
S 3.404215 -1.575746 -1.567362

E= -4585.680724
Mo 3.824765 -0.665229 0.022302
S 5.071134 -2.156912 -0.871828
S 4.472696 0.249745 1.841778
S 1.740632 -0.280139 -1.002416
Mo 0.078342 1.036371 -0.283682
S -1.690502 0.832280 -1.750631
S -0.696683 -0.089160 1.635922
Mo -2.302704 -0.386681 0.081810
S -4.084410 0.778472 1.108117
S -4.811887 -0.322703 -0.440235
S 0.659134 2.905829 0.941672
S 0.501953 3.286705 -1.095285
S -2.126074 -2.583660 -0.799501
S -3.237051 -2.579667 0.903776

E= -4585.706211
Mo 1.886283 -1.485155 0.213362
S 1.094974 -3.267272 -0.658098
S 3.450727 -1.906215 1.609298
S 2.583608 -0.009593 -1.370234
Mo 0.938655 1.387431 -0.330574
S -1.057733 1.473339 -1.564412
S 0.238268 -0.142947 1.300346
Mo -1.901065 0.002823 -0.016993
S -2.957037 0.988865 1.910572
S -4.216944 0.475892 0.376647
S 2.625477 3.018612 0.042061
S 0.702296 3.724692 0.198066
S -2.316514 -1.754591 -1.693463
S -2.572288 -2.351089 0.201505

[Mo3S11]- V
E= -4585.783415
Mo -2.843667 -0.402401 -0.098632
S -1.785406 1.107365 -1.544396
S -1.175996 -0.731332 1.517397
S -3.100025 -2.219477 -1.155729
Mo -0.139545 0.413057 -0.137895
S 1.138733 -0.923050 -1.455715
S 3.947367 -2.157327 0.057168
S 4.054989 1.278563 -1.373804
Mo 2.914184 -0.039219 -0.176313
S -4.807371 0.949526 -0.116960

S -4.477683 -0.144359 1.623337
S 0.594960 2.585066 0.341257
S 1.717148 1.229270 1.480381
S 4.074481 -0.899266 1.710769

E= -4585.755424
Mo -2.824416 -0.399179 -0.203927
S -2.049283 1.588726 -1.089198
S -1.204736 -0.930399 1.389757
S -2.901919 -1.910885 -1.678757
Mo -0.228053 0.604641 -0.008384
S 1.144634 -0.300995 -1.568274
S 3.722227 -2.368089 -0.165995
S 4.518352 1.185639 -1.119269
Mo 3.093708 -0.092651 -0.205051
S -5.061636 0.642715 0.077974
S -4.589305 -0.671246 1.502738
S 0.687242 2.684630 0.587774
S 1.835475 1.179557 1.482092
S 3.790696 -1.395780 1.676735

E= -4585.681883
Mo -2.868616 -0.792371 0.149748
S -1.611554 -0.388962 -1.703782
S -1.023434 -0.265357 1.519160
S -3.357495 -2.850436 0.329151
Mo 0.234240 0.612449 -0.250116
S 1.612185 -0.725327 -1.539032
S 2.020981 0.231854 1.642903
S 4.892589 -2.176203 -0.283846
Mo 3.496803 -0.562326 -0.142411
S -4.740515 0.592471 -0.623909
S -4.319334 0.872095 1.309590
S -0.570124 2.543271 -1.311395
S 1.006169 2.844711 -0.012403
S 3.826662 1.270283 1.310852

[Mo3S11]- VI
E= -4585.702873
S -3.069325 1.431179 -1.403310
Mo -3.227461 -0.333075 -0.225942
S -3.868231 -1.985903 -1.421272
S -0.873909 -1.076842 0.121309
Mo 1.165557 0.541511 -0.206774
S 2.064837 -0.215963 1.824226
Mo 3.755003 -0.304443 0.349424
S 3.120182 0.505123 -1.620719
S 0.205926 -0.972378 -1.648786
S -4.858886 0.019201 1.428207
S -2.973215 -0.354483 2.198763
S 1.090169 2.806710 -0.565958
S -0.118912 2.243732 1.012761
S 4.836982 -2.148358 0.293417

E= -4585.670031
S 3.556822 1.885522 -0.749070
Mo 2.853172 -0.032635 0.221604
S 3.179295 -0.293085 2.297456
S 0.845695 -1.461463 -0.465856
Mo -1.186050 0.168762 -0.040471
S -2.489488 -0.559755 -1.803577
Mo -3.976240 0.150667 -0.227052
S -2.715756 1.081549 1.421528
S -0.375174 -1.653465 1.199807
S 5.112045 -0.387382 -0.656834
S 3.734473 -1.794528 -1.106597
S 0.861684 1.556362 0.744374
S -0.028776 1.959541 -1.069238
S -5.649383 -1.086130 0.308546

E= -4585.665591
S -2.833696 -1.074836 -1.712363
Mo -3.180801 0.300939 0.174978
S -4.318132 -0.635066 1.700255
S -0.904614 0.641022 1.139598
Mo 1.172840 -0.481163 0.207511
S 2.083419 1.479163 -0.753831
Mo 4.079434 0.469619 -0.195936
S 3.242222 -1.391129 0.896564
S -0.097420 -1.015705 2.129090
S -4.471230 1.727155 -1.211985
S -3.097080 2.667256 0.047137

S -1.528244 -2.583134 -1.120378
S 0.436480 -1.887652 -1.430417
S 6.050675 1.313265 -0.173372

[Mo3S11]- VII
E= -4585.702433
S -0.223818 -1.583764 0.328360
Mo 0.872192 0.384884 0.034803
S 2.367664 0.271514 1.890095
Mo 3.592149 -0.083046 0.058181
S 2.423928 0.452641 -1.776594
Mo -2.441583 -0.523029 -0.201163
S -3.374093 -2.141179 -1.194616
S -4.180457 0.402003 1.181460
S -2.842584 -0.853803 2.128006
S -0.980575 0.299276 -1.937674
S -2.675707 1.413157 -1.619714
S 0.316370 2.668641 -0.007332
S -0.816495 1.576473 1.334260
S 4.676028 -1.924330 -0.042281

E= -4585.694871
S -0.576331 -1.224398 0.981476
Mo 0.758829 0.401107 0.019873
S 2.427485 0.047048 1.832958
Mo 3.626646 -0.303900 0.026622
S 2.309711 -0.254691 -1.766315
Mo -2.671083 -0.557515 -0.149763
S -3.398978 -2.321234 -1.042378
S -4.653489 0.455644 0.832753
S -3.305816 -0.455316 2.114551
S -1.008624 0.190392 -1.813679
S -2.742072 1.315503 -1.586460
S 1.312043 2.811402 -0.397190
S -0.093371 2.363164 0.998684
S 5.229161 -1.719208 0.116677

E= -4585.673286
S -0.627422 -1.060944 1.165018
Mo 0.705214 0.383379 -0.050176
S 2.490762 0.454173 1.753184
Mo 3.705713 -0.549796 0.145502
S 2.156041 -0.721206 -1.558201
Mo -2.686743 -0.583068 -0.077131
S -3.353949 -2.415690 -0.874493
S -4.737483 0.443746 0.740781
S -3.419548 -0.326208 2.142565
S -1.031363 0.035789 -1.879301
S -2.723684 1.207481 -1.596651
S 1.140768 2.811484 -0.731638
S -0.211704 2.602662 0.711787
S 5.791600 -1.063887 0.079186

[Mo3S11]- VIII
E= -4585.702874
S -3.069504 1.434201 -1.399523
Mo -3.227589 -0.332686 -0.226141
S -3.867452 -1.983167 -1.425245
S -0.874118 -1.076804 0.120538
Mo 1.165699 0.541633 -0.206401
S 2.065202 -0.216785 1.824178
Mo 3.755144 -0.304838 0.349113
S 3.120111 0.505609 -1.620608
S 0.205558 -0.970700 -1.649638
S -4.859768 0.015965 1.428042
S -2.974154 -0.358178 2.198579
S 1.090419 2.806983 -0.564268
S -0.118140 2.243357 1.014603
S 4.837054 -2.148767 0.292342

E= -4585.690429
S -3.136166 1.817749 -0.752627
Mo -3.320205 -0.247676 -0.244572
S -4.021128 -1.383456 -1.912002
S -0.975714 -1.066468 -0.185433
Mo 1.149328 0.439028 -0.072060
S 2.153782 -1.119597 1.416649
Mo 3.919599 -0.330262 0.262086
S 3.087794 1.169201 -1.188449
S 0.079674 -0.534650 -1.902847
S -4.932488 -0.432197 1.455735
S -3.049887 -1.067108 2.036732

S 0.018583 2.547123 -0.182700
S 0.637706 2.033869 1.671950
S 5.547449 -1.599830 -0.313827

E= -4585.644814
S 2.891645 -0.570211 2.258950
Mo 2.736846 -0.510022 -0.021032
S 3.685330 -2.222924 -0.848115
S 0.794258 -0.621425 -1.613698
Mo -0.888487 0.354936 0.041016
S -2.628742 0.328045 -1.745083
Mo -3.970404 -0.185418 0.019991
S -2.394493 -0.145321 1.749659
S 0.444634 -1.733875 0.082784
S 4.586677 0.952291 0.420345
S 3.519757 1.422475 -1.250012
S 0.950368 1.555542 1.071887
S -0.207804 2.564915 -0.350931
S -6.071260 -0.635688 0.119280

[Mo3S11]- IX
E= -4585.700310
S 0.535671 -0.551815 -1.434579
Mo -0.897174 0.616405 -0.029817
S -2.460994 0.361806 -1.863139
Mo -3.547901 -0.301853 -0.049762
S -2.335165 0.072035 1.794167
Mo 2.571909 -0.641905 -0.058794
S 3.284257 -2.616765 -0.214131
S 4.497134 0.794144 -0.159878
S 3.393457 0.597593 -1.902214
S 0.721867 -0.865450 1.473720
S 2.422337 -0.012665 2.260226
S 0.188630 2.442514 1.169405
S -0.852711 2.862075 -0.565638
S -4.477426 -2.224159 -0.194710

E= -4585.697918
S 0.613050 -0.596174 -1.368430
Mo -0.723870 0.536328 0.115507
S -2.428816 0.232492 -1.821901
Mo -3.712714 -0.473176 -0.128147
S -2.156216 -0.523527 1.616618
Mo 2.699523 -0.600730 -0.064879
S 3.346004 -2.601651 -0.007094
S 4.678379 0.718417 -0.444552
S 3.454196 0.380006 -2.080497
S 0.960233 -0.643216 1.678991
S 2.713889 0.357609 2.118840
S 0.314757 2.465083 0.985431
S -1.185464 2.781309 -0.389487
S -5.750233 -1.159207 -0.084432

E= -4585.668184
S 1.223155 0.674944 -1.454983
Mo -0.734274 0.650385 -0.056047
S -1.827636 -1.058723 -1.449677
Mo -3.453871 -0.831965 0.041645
S -2.802175 0.629267 1.545098
Mo 2.669833 -0.544975 -0.041085
S 2.745495 -2.626604 -0.428323
S 4.884947 0.156186 0.520079
S 4.348590 0.412213 -1.466168
S 0.501561 -0.879654 1.442809
S 2.247456 -0.015961 2.206791
S -0.311128 3.038621 0.587711
S -1.515625 2.902185 -0.989514
S -5.509071 -1.287716 -0.368168

[Mo3S11]- X
E= -4585.715092
S -0.000002 0.110771 -1.898935
Mo -0.000002 1.851663 -0.279049
S -1.772679 1.651484 1.383392
S -2.466075 1.871749 -0.550293
Mo -1.379747 -0.401403 0.007776
S -0.000001 -2.452182 0.284790
S 0.000006 -1.199233 1.894694
Mo 1.379749 -0.401399 0.007775
S 1.772680 1.651493 1.383390
S 2.466076 1.871745 -0.550294
S -2.978297 -1.584704 -1.322721

S -3.459932 -1.544837 0.695190
S 3.459929 -1.544843 0.695189
S 2.978296 -1.584703 -1.322721

E= -4585.680027
S 0.000018 0.117520 -1.921976
Mo 0.000034 1.877534 -0.288206
S -1.733715 1.619789 1.385252
S -2.501289 1.849692 -0.516100
Mo -1.383108 -0.393771 -0.016029
S -0.000048 -2.492410 0.162710
S -0.000038 -1.277309 1.803567
Mo 1.383100 -0.393819 -0.016013
S 1.733716 1.619714 1.385314
S 2.501349 1.849633 -0.516010
S -3.119049 -1.611706 -1.224864
S -3.536052 -1.462145 0.753855
S 3.536046 -1.462173 0.753817
S 3.118995 -1.611707 -1.224912

[Mo3S11]- XI
E= -4585.702162
S -0.025700 0.042242 1.863538
Mo -0.954990 -1.263924 0.059851
S -2.865979 -2.072579 1.168306
S -2.804889 -2.374486 -0.899739
Mo -0.777571 1.401469 0.093708
S -3.039072 1.503370 -0.427105
S -2.206134 3.326292 0.186519
Mo 1.507475 -0.071320 0.017922
S 3.897076 -0.265495 -0.596158
S 3.431076 -0.231501 1.427196
S 0.843214 1.615830 -1.635226
S 1.533775 2.458170 0.113862
S 1.135645 -2.551890 0.066582
S 0.691840 -1.623793 -1.717910

E= -4585.680773
S -0.305022 -0.056620 1.692689
Mo -0.961549 -1.527036 -0.029230
S -2.330936 -3.355116 0.610148
S -3.255515 -1.789630 -0.462555
Mo -0.776372 1.606368 0.084898
S -3.071607 2.068577 -0.027946
S -1.819954 3.750981 0.197804
Mo 1.432478 -0.084718 0.003989
S 3.864875 -0.191319 -0.450353
S 3.268373 -0.212790 1.539398
S 0.875207 1.643211 -1.655599
S 1.567922 2.420705 0.115466
S 1.284817 -2.599558 0.017357
S 0.723627 -1.664304 -1.733007

[Mo3S11]- XII
E= -4585.660019
Mo 0.843423 -1.275289 0.096207
Mo -1.374535 0.000141 0.139230
Mo 0.843388 1.275369 0.096569
S 2.033414 2.131057 -1.653975
S 2.213428 3.478582 -0.077306
S -1.331398 2.470187 -0.110592
S -0.955728 1.759273 1.782204
S -2.782217 0.000597 -1.896624
S -4.094081 -0.000778 -0.406416
S -1.331668 -2.469909 -0.110487
S -0.955056 -1.758773 1.782138
S 2.212490 -3.478911 -0.076726
S 2.033657 -2.131840 -1.653795
S 2.137434 -0.000067 1.550062

E= -4585.639669
Mo -1.440204 -0.896561 0.090979
Mo 0.004962 1.318329 0.137135
Mo 1.433131 -0.905409 0.091317
S 2.524394 -1.837446 -1.712125
S 3.643173 -2.067437 0.034940
S 2.459860 1.360954 -0.065208
S 1.745496 0.898776 1.813614
S 0.010588 2.793871 -1.850814
S 0.015488 4.055727 -0.317592
S -2.449451 1.377576 -0.067341
S -1.739933 0.910710 1.812173

S -3.657650 -2.043404 0.036598
S -2.538381 -1.822752 -1.711411
S -0.008045 -2.357017 1.188662

[Mo3S11]- XIII
E= -4585.648254
Mo -1.295288 -0.537990 0.043627
Mo 1.295196 -0.538152 0.043636
Mo 0.000129 1.765023 0.030179
S 2.467623 1.581184 -0.225562
S 1.747432 1.345644 1.681490
S 2.654894 -1.398588 -1.744316
S 3.417173 -1.876986 0.123869
S -0.000169 -2.609265 -0.075774
S -0.000139 -1.733047 1.763310
S -3.417330 -1.876708 0.123928
S -2.655125 -1.398360 -1.744282
S -2.467404 1.581499 -0.225646
S -1.747288 1.345901 1.681432
S 0.000237 3.230413 -1.666733

E= -4585.627826
Mo 1.159053 0.726814 0.064550
Mo -1.394160 0.437311 0.105581
Mo 0.286709 -1.915607 0.019693
S -2.157877 -1.807885 -0.464655
S -1.657370 -1.615843 1.528464
S -2.742940 1.227828 -1.771293
S -3.667920 1.536503 0.029638
S -0.358955 2.664036 0.114030
S -0.199988 1.655034 1.893654
S 3.146908 2.375410 -0.003733
S 2.330386 1.856310 -1.777761
S 2.608217 -1.200499 -0.369383
S 2.006916 -1.033746 1.595970
S 0.557168 -3.684506 -1.273216

[Mo3S11]- XIV
E= -4585.726809
S -0.195817 0.000067 -1.785606
Mo -1.011062 -1.472491 -0.069409
S 0.701027 -1.688179 1.634920
S 1.289438 -2.520824 -0.137156
Mo 1.401900 -0.000315 -0.006161
S 1.290749 2.520231 -0.136961
S 0.701909 1.687785 1.635061
Mo -1.010225 1.472915 -0.069321
S -2.187219 0.000502 1.500927
S -3.058152 0.000794 -0.354411
S 3.318156 -0.000742 -1.451810
S 3.791407 -0.000808 0.572896
S -2.011889 3.362932 -0.548896
S -2.013717 -3.362045 -0.548625

E= -4585.705874
S -0.162525 -0.000070 -1.796964
Mo -1.070349 -1.431387 -0.071038
S 0.668154 -1.711263 1.589241
S 1.283229 -2.491995 -0.202299
Mo 1.455474 -0.081283 -0.004924
S 1.285316 2.489784 -0.203917
S 0.671808 1.710937 1.588795
Mo -1.068257 1.432675 -0.070699
S -1.958545 0.001198 1.695925
S -2.978628 0.001601 -0.642712
S 3.455322 -0.002248 -1.426034
S 3.767770 -0.000309 0.610815
S -2.117336 3.313467 -0.413836
S -2.121345 -3.311115 -0.414029

[Mo3S11]- XV
E= -4585.773930
S 0.174571 -0.128489 1.725464
Mo -0.265440 1.470144 0.017896
S 1.642187 1.463550 -1.302770
Mo 1.668498 -0.495005 -0.102738
S 0.564261 -2.080212 -1.321523
Mo -1.118397 -1.108541 -0.012797
S -1.728006 0.542715 -1.727496
S -2.710633 0.837474 0.062435
S -2.146788 -2.605377 1.447993
S -2.911095 -2.724987 -0.468807

S 3.413050 -1.129076 1.343124
S 4.002318 -0.956657 -0.636693
S -0.261773 3.238515 1.512269
S -0.785328 3.892724 -0.377695

E= -4585.739451
S -0.319837 -0.001909 1.614368
Mo 0.768375 -1.422833 -0.037599
S -1.023866 -1.820830 -1.379586
Mo -1.887804 -0.007378 -0.110183
S -1.038542 1.811328 -1.380474
Mo 0.756635 1.428167 -0.037203
S 1.998881 0.008029 -1.603484
S 2.820078 0.011565 0.295444
S 1.165577 3.148640 1.507871
S 2.043228 3.441959 -0.349479
S -3.985576 1.028097 0.311215
S -3.977591 -1.059400 0.310544
S 1.195038 -3.138173 1.508384
S 2.074945 -3.423938 -0.349215

[Mo3S11]- XVI
E= -4585.761912
S -0.094604 0.350871 1.744232
Mo -0.153989 1.875552 -0.038887
S 1.505778 1.208797 -1.716831
S 2.381600 1.764885 0.059177
Mo 1.316120 -0.541606 0.006057
S -0.030371 -2.654504 0.270643
S -0.058046 -1.773277 -1.583126
Mo -1.454914 -0.541413 0.006732
S -1.858900 1.166333 -1.477694
S 3.118983 -1.420219 1.510873
S 3.383303 -1.725790 -0.459341
S -3.591583 -1.791373 -0.483291
S -3.247608 -0.980199 1.393944
S -0.739996 3.774074 0.809924

E= -4585.730489
S 0.045898 0.455985 -1.707753
Mo -0.825121 1.888754 -0.021339
S -1.877617 0.518538 1.664236
S -2.990056 0.437595 -0.070081
Mo -0.902649 -0.000665 0.000976
S 1.144703 -2.437915 -0.154819
S 0.793426 -1.544607 1.668347
Mo 1.711724 0.031044 0.026045
S 1.259908 2.090024 1.029782
S -2.102523 -2.586113 -1.513444
S -2.257443 -2.980207 0.448125
S 4.058484 -0.328903 0.574606
S 3.549450 0.129407 -1.404055
S -1.582110 3.833470 -0.549859

[Mo3S11]- XVII
E= -4585.748536
Mo -1.465371 -0.596479 0.015267
S -0.017786 0.065518 -1.782694
Mo 0.199494 1.754236 -0.106959
Mo 1.258450 -0.838625 0.016914
S -0.194826 -1.881766 1.471049
S 2.389010 -2.341894 -1.322015
S 3.228954 -2.308614 0.570314
S 2.683949 1.250772 -0.253228
S -2.339841 1.741603 -0.642712
S -1.496526 1.364924 1.584487
S 1.773558 1.001857 1.573458
S -2.884181 -1.829748 -1.334774
S -3.561981 -1.755914 0.631939
S 0.439290 3.855270 -0.688227

E= -4585.709208
Mo -1.420250 -0.733996 0.045065
S -0.000012 -0.144208 -1.801678
Mo 0.000005 1.713643 -0.234575
Mo 1.420252 -0.733983 0.045049
S 0.000012 -1.729815 1.589679
S 2.721417 -2.202629 -1.232466
S 3.465360 -1.894973 0.677594
S 2.482824 1.467456 -0.429272
S -2.482821 1.467449 -0.429208
S -1.680956 1.272619 1.493120

S 1.681014 1.272643 1.493075
S -2.721453 -2.202557 -1.232497
S -3.465388 -1.894955 0.677577
S -0.000015 3.944098 -0.426715

[Mo3S11]- XVIII
E= -4585.769613
Mo 0.557180 -0.629722 0.000047
S 1.887538 -0.198621 1.808507
Mo 3.155406 0.533346 -0.000021
S 1.887499 -0.198744 -1.808472
S 3.167325 2.645147 -0.000096
S -1.207840 0.770666 0.000020
S -3.896990 2.333356 0.000194
Mo -3.542562 -0.070605 -0.000042
S -5.578365 1.150240 0.000092
S -3.607751 -1.274796 -1.755071
S -3.607715 -1.275135 1.754757
S 0.130480 -2.706982 0.000124
S 5.189767 -0.403358 1.003070
S 5.189740 -0.403448 -1.003083

E= -4585.755424
Mo -0.228205 0.603526 -0.008272
S -1.205380 -0.930745 1.390467
Mo -2.824774 -0.399775 -0.203576
S -2.049302 1.587779 -1.089066
S -2.902967 -1.912422 -1.677433
S 1.144845 -0.302492 -1.567674
S 3.724008 -2.367187 -0.164993
Mo 3.094150 -0.092167 -0.205212
S 3.792767 -1.393823 1.677202
S 4.517454 1.186294 -1.121272
S 1.835710 1.179746 1.481825
S 0.686787 2.683914 0.586717
S -4.589793 -0.667082 1.503611
S -5.062201 0.643110 0.075398

[Mo3S11]- XIX
E= -4585.782714
Mo 2.852478 -0.530052 -0.000038
S 1.527172 -0.074604 1.777438
S 1.527200 -0.074231 -1.777444
S 3.273895 -2.607113 -0.000259
Mo 0.002655 0.570702 0.000052
S -1.490769 -0.118815 1.761624
S -4.404767 -1.589961 1.016990
S -3.859053 1.945633 0.000158
Mo -2.912470 0.052536 -0.000011
S 4.716632 0.654294 1.021300
S 4.716611 0.654567 -1.021081
S 0.039049 2.673892 0.000264
S -1.490744 -0.118477 -1.761667
S -4.404717 -1.589799 -1.017330

E= -4585.755424
Mo -2.824768 -0.399770 -0.203580
S -2.049296 1.587774 -1.089097
S -1.205382 -0.930718 1.390479
S -2.902964 -1.912422 -1.677429
Mo -0.228206 0.603544 -0.008268
S 1.144831 -0.302497 -1.567668
S 3.724000 -2.367197 -0.164987
S 4.517458 1.186276 -1.121269
Mo 3.094143 -0.092178 -0.205214
S -5.062190 0.643108 0.075417
S -4.589794 -0.667127 1.503596
S 0.686787 2.683931 0.586721
S 1.835711 1.179761 1.481819
S 3.792753 -1.393824 1.677202

[Mo3S10H]- I
E= -4188.122863
S -1.933779 0.868760 -1.670157
Mo -0.414659 0.373266 -0.059007
S 0.254932 2.461822 0.601874
S 1.557783 0.946989 1.575448
Mo 2.626845 -0.301596 0.035177
S 4.743846 -0.367792 -1.099803
S 3.657170 1.417049 -1.143648
Mo -3.197530 -0.250896 -0.074378
S -4.730405 1.038872 0.683559

S -3.923192 -2.100613 -0.869990
S -1.604996 -0.639516 1.576400
S 0.907871 -1.209473 -1.160052
S 3.387185 -1.790053 1.700519
H 4.321818 -2.489210 1.018336

E= -4188.123418
S -1.965197 0.605773 -1.793099
Mo -0.356782 0.348777 -0.154163
S 0.422948 2.555795 -0.255793
S 1.372350 1.489975 1.278431
Mo 2.556225 -0.274884 0.111044
S 4.447728 -1.013331 -1.210862
S 4.267087 1.021546 -0.744864
Mo -3.162071 -0.254474 -0.010053
S -4.690987 1.122559 0.596367
S -3.922311 -2.196440 -0.503121
S -1.548362 -0.366047 1.657250
S 0.911296 -1.293869 -1.145115
S 2.990247 -1.311987 2.152164
H 3.873556 -2.239179 1.731508

[Mo3S10H]- II
E= -4188.140679
S 1.770765 0.515480 -1.765554
Mo 0.430796 -0.285107 -0.102394
S -1.194552 -1.383581 -1.616716
S -1.135027 -2.189856 0.270889
Mo -2.387348 -0.160971 0.314268
S -5.036490 1.852534 -0.576222
S -3.877646 0.317796 -1.438741
Mo 3.252457 0.292754 0.011457
S 4.866112 -0.979771 -0.619621
S 3.878221 2.184911 0.799212
S 1.925093 -0.885244 1.513994
S -0.807973 1.454625 0.685492
S -3.426869 -0.551826 2.148201
H -5.814180 1.078060 0.205116

E= -4188.122138
S -1.932995 0.351727 -1.879690
Mo -0.416138 0.305973 -0.144379
S 0.427513 2.474086 -0.444941
S 1.266949 1.597450 1.275796
Mo 2.478810 -0.219194 0.429437
S 5.041433 -0.822887 -1.681384
S 4.189964 0.858445 -0.741469
Mo -3.231422 -0.263173 -0.064026
S -4.776839 1.186623 0.273676
S -3.980571 -2.252254 -0.334981
S -1.707738 -0.159830 1.683961
S 0.928004 -1.419052 -0.812139
S 3.243161 -1.278969 2.124892
H 5.905425 -1.156878 -0.702870

[Mo3S10H]- III
E= -4188.156322
S -1.771828 -0.015497 1.773390
Mo -3.087109 0.207788 0.002172
S -1.774939 0.005194 -1.769622
Mo -0.228887 -0.619450 -0.000677
S 1.276279 0.012847 1.769518
Mo 2.647226 0.474785 0.003902
S 3.028604 2.562251 0.024490
S -0.249657 -2.725850 -0.017854
S 1.268309 0.047357 -1.764875
S -4.653618 -1.226216 0.001033
S -3.982063 2.396545 -0.011234
S 4.473766 -0.685357 1.030357
S 4.469566 -0.662342 -1.056218
H -5.262359 2.005195 0.109561

E= -4188.125148
S -1.798138 -0.285993 1.628096
Mo 0.012458 -0.841349 0.000001
S 0.191582 -2.946093 0.000017
Mo -3.254855 0.266488 -0.000001
S -4.974254 -1.010876 -0.000026
S -3.763043 2.577178 0.000029
S -1.798118 -0.285957 -1.628096
S 1.320348 -0.117115 -1.813213
Mo 2.523955 0.576520 -0.000008

S 4.589529 -0.332467 0.999415
S 4.589529 -0.332524 -0.999371
S 1.320334 -0.117072 1.813205
S 2.526724 2.696918 -0.000037
H -5.097322 2.394320 0.000039

[Mo3S10H]- IV
E= -4188.145898
S -1.900103 -0.417820 1.869795
Mo -0.175840 -0.546383 -0.041262
S -0.254288 -2.656430 -0.082891
Mo -3.172106 0.266445 -0.019159
S -4.660362 -1.204517 -0.418150
S -4.008605 2.195376 0.348331
S -1.686362 0.399111 -1.700611
S 1.305366 0.035001 -1.817305
Mo 2.655931 0.462173 -0.025230
S 4.348357 -0.743761 1.168144
S 4.450417 -0.835065 -0.912028
S 1.192358 0.173169 1.736208
S 3.132930 2.526596 -0.115960
H -1.650710 0.799539 2.388803

E= -4188.116913
S -1.893773 -0.336635 1.896287
Mo -0.351090 -0.440572 -0.070736
S -0.245993 -2.552850 -0.127935
Mo -3.226350 0.228271 -0.011269
S -4.701491 -1.288985 -0.297783
S -4.029892 2.187167 0.311815
S -1.776316 0.329715 -1.766596
S 1.322952 0.289498 -1.706020
Mo 2.861696 0.547855 -0.019305
S 4.099494 -1.229779 1.192773
S 4.247578 -1.350208 -0.795218
S 1.155393 0.566179 1.549566
S 3.805428 2.448920 -0.140131
H -1.672861 0.898095 2.386911

[Mo3S10H]- V
E= -4188.152895
S 2.054534 0.598115 1.723260
Mo 0.026190 0.584741 -0.118972
S 0.136876 2.918321 0.183874
Mo 3.168748 -0.307899 0.047504
S 4.728940 0.961073 -0.687760
S 3.947750 -2.231375 0.564260
S 1.488316 -0.507562 -1.556120
S -1.582578 0.945920 -1.652277
Mo -2.575278 -0.482648 -0.099075
S -4.252275 -0.100707 1.547905
S -4.597180 0.772600 -0.304696
S -0.928564 -0.599616 1.549587
S -2.698715 -2.403115 -0.981610
H 1.220600 2.985410 0.980018

E= -4188.142245
S 2.060569 0.727567 1.681389
Mo 0.120834 0.661730 0.018725
S 0.207835 3.025507 0.068878
Mo 3.081182 -0.360875 0.019238
S 4.727406 0.751670 -0.787023
S 3.719435 -2.312423 0.634819
S 1.377878 -0.501024 -1.545699
S -1.612202 1.107311 -1.546140
Mo -2.459522 -0.465885 -0.126012
S -4.369070 -0.203582 1.433628
S -4.734513 0.466401 -0.406476
S -0.999958 -0.449064 1.677817
S -2.405915 -2.374256 -1.034829
H 1.271855 3.201545 0.876265

[Mo3S10H]- VI
E= -4188.152235
S -1.732832 0.156711 1.710745
Mo -0.164349 -0.542168 -0.008732
S -0.025996 -2.638477 -0.070995
Mo -3.200130 0.238828 -0.022895
S -4.603925 -1.375509 0.083133
S -4.207230 2.127666 -0.100660
S -1.795505 0.023683 -1.770755
S 1.196414 0.301487 -1.759116

Mo 2.619708 0.468150 0.001454
S 4.367591 -0.958645 0.739968
S 4.439257 -0.393185 -1.260361
S 1.373799 -0.267287 1.945914
S 2.881826 2.532706 0.410049
H 0.986018 0.931599 2.420514

E= -4188.133505
S 1.585254 0.135832 -1.649141
Mo 0.410241 -1.015480 0.104480
S 0.734030 -3.096472 0.044792
Mo 3.114627 0.532468 -0.002592
S 4.879647 -0.643525 -0.277379
S 3.594707 2.609823 0.136624
S 1.903637 -0.155099 1.790220
S -1.351756 -0.500323 1.589007
Mo -2.753655 0.512303 0.009091
S -4.794904 -0.349619 -0.833510
S -4.819499 0.381957 1.129943
S -1.453766 -0.832361 -1.684702
S -2.172316 2.497079 -0.451022
H -2.071441 -1.986853 -1.378471

[Mo3S10H]- VII
E= -4188.158854
S -1.803011 0.128260 1.753166
Mo -0.218559 -0.475348 0.000021
S -0.130138 -2.574853 -0.000525
Mo -3.232495 0.252689 -0.000005
S -4.621724 -1.378685 -0.000292
S -4.258225 2.134977 0.000311
S -1.802998 0.128866 -1.753138
S 1.266317 0.298962 -1.746453
Mo 2.624817 0.301144 0.000148
S 4.980585 -0.207396 -0.000317
S 3.635015 -1.783383 -0.000224
S 1.266470 0.297611 1.746919
S 3.343896 2.592804 0.000073
H 4.682975 2.508982 0.000756

E= -4188.134408
S 1.776405 0.185757 -1.719096
Mo 3.278115 0.298909 -0.027496
S 1.902848 -0.003359 1.744803
Mo 0.253470 -0.587605 0.044223
S -1.315173 0.051138 -1.754554
Mo -2.726518 0.349964 -0.074209
S -3.126334 2.626461 0.364898
S 0.280959 -2.688828 0.012771
S -1.240572 0.100477 1.714871
S 4.741255 -1.258022 -0.171983
S 4.218753 2.220985 0.049724
S -5.009401 -0.099025 -0.643311
S -4.077222 -1.474562 0.575631
H -4.237088 2.850348 -0.365812

[Mo3S10H]- VIII
E= -4188.159890
S -1.838505 0.098588 1.725533
Mo -0.213543 -0.605084 0.025031
S -0.212956 -2.709378 0.032117
Mo -3.218544 0.288027 -0.054703
S -4.699666 -1.263350 -0.066945
S -4.137083 2.226249 -0.101174
S -1.760768 0.056528 -1.764376
S 1.307935 0.013892 -1.710952
Mo 2.530830 0.447121 0.123405
S 4.298439 -0.999979 0.741728
S 4.824630 -0.307291 -1.154133
S 1.209821 -0.027040 1.867480
S 3.024962 2.523185 0.234967
H 5.583875 0.754839 -0.804726

E= -4188.130812
S 2.008197 0.262871 -1.702633
Mo 0.374829 -0.489655 -0.084777
S 0.166981 -2.579569 -0.282986
Mo 3.416308 0.232923 0.081015
S 4.800782 -1.395588 -0.026638
S 4.449285 2.096377 0.287203
S 1.897808 -0.053443 1.745649
S -1.307711 0.201781 1.546443

Mo -2.869188 0.526915 -0.093885
S -4.220332 -1.289362 -0.791892
S -4.851830 -0.921204 1.166851
S -1.189655 0.528433 -1.644172
S -3.806510 2.445033 -0.099041
H -5.874092 -0.072992 0.920644

[Mo3S10H]- IX
E= -4188.132300
S 1.035716 0.002249 -1.757660
Mo 2.442845 -0.000212 0.099378
S 3.880523 1.729016 -0.999976
S 3.229949 1.981332 0.955537
Mo -0.383121 -0.000027 -0.019715
S -1.832287 -1.788518 -0.127013
Mo -3.245561 -0.000029 0.020882
S -4.232190 -0.002561 1.897315
S 0.807589 -0.002549 1.851027
S -1.832183 1.788815 -0.122052
S 3.230419 -1.983542 0.951275
S 3.881828 -1.725927 -1.003345
S -4.693611 0.002282 -1.841278
H -5.806923 0.001715 -1.084173

E= -4188.119477
S 1.059988 -0.317541 1.670750
Mo 2.574038 0.038990 -0.011987
S 4.191300 -1.641124 0.856518
S 3.349821 -1.869270 -1.027301
Mo -0.484921 -0.070109 -0.038687
S -1.849513 1.720396 0.254951
Mo -3.305708 -0.033212 -0.022198
S -4.461560 0.125987 -1.810007
S 0.823511 0.066431 -1.830744
S -1.900444 -1.851969 -0.073886
S 2.741668 2.311387 -0.598494
S 4.189508 1.603499 0.692102
S -4.614539 0.083723 1.950203
H -5.379050 -1.002408 1.715138

[Mo3S10H]- X
E= -4188.110586
S 0.996593 0.013196 1.725174
Mo 2.444710 0.000196 -0.108501
S 3.886525 -1.665262 1.078704
S 3.323689 -1.966231 -0.895574
Mo -0.384275 -0.060333 -0.026730
S -1.835850 1.882231 0.079011
Mo -3.327256 -0.028149 0.054960
S -4.464834 -0.059206 -1.757513
S 0.830714 -0.131300 -1.873149
S -1.843211 -1.808315 0.094168
S 3.206821 1.973659 -1.014615
S 3.783319 1.800908 0.975643
S -4.444449 0.053132 1.875372
H -1.822580 2.222967 -1.224143

E= -4188.100095
S 1.001136 -0.327056 1.621478
Mo 2.557812 0.043948 -0.010039
S 4.205954 -1.588725 0.872753
S 3.391105 -1.849977 -1.018814
Mo -0.502362 -0.217193 -0.147372
S -1.739978 1.783923 0.352320
Mo -3.350530 -0.007791 0.078905
S -4.548453 0.481835 -1.624310
S 0.857615 0.039770 -1.892889
S -2.027957 -1.883370 -0.326183
S 2.658416 2.339287 -0.558210
S 4.105629 1.651335 0.745303
S -4.397046 -0.291269 1.928566
H -1.709366 1.911493 1.697041

[Mo3S10H]- XI
E= -4188.139384
S -1.668594 0.051514 -1.779084
Mo -0.050820 0.689448 -0.044382
S -0.721328 2.823163 -0.780564
S 0.669545 2.791350 0.769099
Mo -2.773887 -0.503829 0.043914
S -4.567978 0.612894 0.285475
S -3.255336 -2.803240 -0.136032

S -1.349242 -0.117623 1.740135
S 1.663987 0.025474 1.774048
Mo 2.871128 -0.571487 -0.005488
S 4.617999 0.642391 -0.262312
S 1.365652 -0.195571 -1.700687
S 3.399859 -2.646596 0.072417
H -4.422727 -2.733622 0.530267

E= -4188.124670
S -1.875090 0.540710 -1.602317
Mo 0.111925 0.885926 0.007889
S -0.348702 3.069943 -0.711781
S 1.207283 2.852075 0.627009
Mo -2.954843 -0.516083 0.025156
S -4.855718 0.343636 0.459726
S -3.025154 -2.847520 -0.332492
S -1.418624 0.035560 1.611410
S 1.726627 0.020776 1.806330
Mo 2.794845 -0.738874 -0.010053
S 4.613311 0.320649 -0.407682
S 1.207755 -0.343904 -1.642969
S 3.167192 -2.840235 0.145182
H -4.362976 -2.932532 -0.204355

[Mo3S10H]- XII
E= -4188.128437
S 0.895065 -0.967528 1.297141
Mo 2.458726 0.035479 0.018028
S 4.439179 -0.384067 1.429963
S 4.185370 -1.460423 -0.318769
Mo -0.319474 0.041140 -0.370633
S -1.655511 1.619853 0.588589
Mo -3.161052 -0.105622 0.218495
S -4.782949 0.669535 -0.957990
S 1.386394 -1.004585 -2.033176
S -1.860588 -1.478299 -1.121758
S 1.295778 1.850275 -1.028091
S 2.447758 2.314928 0.653589
S -3.769551 -1.081754 2.025640
H 1.620545 -0.028859 -2.929594

E= -4188.109376
S 1.149470 -0.616222 1.585984
Mo 2.555757 0.013168 -0.027394
S 4.657488 -0.408594 1.204469
S 4.163062 -1.613506 -0.410417
Mo -0.253108 0.061155 -0.167659
S -1.922463 1.724010 -0.105585
Mo -3.319114 -0.087962 0.134217
S -4.693508 -0.177919 -1.508472
S 1.195607 -1.211041 -1.783894
S -1.804687 -1.778574 0.081644
S 1.357703 1.860426 -1.064068
S 2.843095 2.313699 0.326881
S -4.356181 -0.035428 2.008492
H 1.258175 -0.336810 -2.805426

[Mo3S10H]- XIII
E= -4188.133001
S 0.899545 1.012600 1.494191
Mo 2.323653 0.015989 -0.009277
S 3.389873 -1.526047 1.466598
S 4.222731 -1.702256 -0.426630
Mo -0.520684 -0.003603 0.002876
S -1.893822 1.503419 -0.943979
Mo -3.406484 -0.009139 0.004966
S -4.549925 -0.999314 -1.516900
S 0.885619 -1.034475 -1.484615
S -1.884080 -1.511916 0.957147
S 3.153935 1.625721 -1.408987
S 4.220136 1.700555 0.358832
S -4.559672 0.970443 1.526021
H 5.193432 -0.756017 -0.286496

E= -4188.123956
S 0.830764 0.485018 1.752331
Mo 2.419138 0.032570 0.059590
S 3.651753 -1.724676 1.136729
S 4.296849 -1.590367 -0.833755
Mo -0.548616 -0.047994 0.038107
S -1.894103 1.665720 -0.573947
Mo -3.418315 -0.014869 -0.016711

S -4.554689 -0.590705 -1.741761
S 0.856997 -0.658156 -1.618844
S -1.953150 -1.726693 0.605920
S 3.016350 2.003903 -1.138427
S 4.090790 1.679416 0.579609
S -4.612567 0.582918 1.661156
H 5.343377 -0.749744 -0.665527

[Mo3S10H]- XIV
E= -4188.159784
S -1.251857 -0.142349 1.748210
Mo 0.246366 0.563497 0.000234
S 1.782796 -0.085322 -1.777452
Mo 3.092254 -0.304725 -0.003156
Mo -2.720693 -0.013341 0.001187
S -4.143906 -1.640766 1.032444
S -4.153008 -1.616176 -1.056168
S -3.667813 1.883656 0.023948
S -1.260789 -0.107804 -1.754353
S 1.787646 -0.102169 1.772664
S 0.306433 2.664872 0.016156
S 3.987706 -2.492363 0.009542
H 5.269114 -2.102547 -0.102946

E= -4188.132068
S -1.274356 0.023209 -1.788638
Mo -2.696246 0.032813 -0.000017
S -3.938255 -1.680790 -0.000135
Mo 0.030858 -0.785842 0.000003
S 1.822998 -0.197148 -1.634775
Mo 3.267393 0.367167 0.000008
S 3.732523 2.689468 -0.000123
S -0.060590 -2.890390 -0.000031
S -1.274453 0.023052 1.788667
S 1.822888 -0.196946 1.634779
S -3.870252 1.979660 0.995968
S -3.870144 1.979805 -0.995840
S 5.012494 -0.875488 0.000151
H 5.070172 2.535266 -0.000072

[Mo3S10H]- XV
E= -4188.158818
S -1.269473 -0.107289 1.766884
Mo 0.216594 0.566973 0.019164
S 1.810328 -0.078089 -1.766259
Mo 3.069912 -0.439663 -0.003206
S 4.821340 1.144754 -0.031953
Mo -2.714779 0.007160 -0.005682
S -4.163165 -1.592732 1.032979
S -4.125721 -1.618132 -1.055234
S -3.650980 1.909692 -0.031432
S -1.232578 -0.123562 -1.750468
S 1.775145 -0.174025 1.770196
S 0.294967 2.669476 0.029759
S 3.880098 -2.403883 -0.023152
H 5.748112 0.332930 0.507282

E= -4188.134013
S -1.348864 -0.141944 1.788407
Mo -2.752845 0.097617 0.000012
S -3.670685 2.004071 0.000123
Mo 0.071432 0.430894 0.000011
S 1.752228 -0.425935 1.635105
Mo 3.294102 -0.392623 0.000011
S 4.473286 -2.177540 0.000063
S 0.344791 2.527802 0.000021
S -1.348913 -0.141774 -1.788427
S 1.752065 -0.426255 -1.634959
S -4.251123 -1.613503 -0.995985
S -4.251058 -1.613659 0.995828
S 4.579413 1.592081 -0.000267
H 5.768816 0.959200 0.000015

[Mo3S10H]- XVI
E= -4188.150313
S -1.182557 -0.213678 1.728387
Mo -2.711563 0.002703 0.009892
S -3.644657 1.897100 0.189413
Mo 0.193013 0.544905 -0.027285
S 1.926372 0.278337 1.877186
Mo 3.165692 -0.388633 -0.038547

S 3.962019 -2.343820 0.269665
S 0.355893 2.645676 -0.030666
S -1.304371 -0.016961 -1.793408
S 1.669542 -0.439976 -1.711332
S -4.199455 -1.506351 -1.098610
S -4.070447 -1.714162 0.974718
S 4.687508 1.055488 -0.405729
H 1.622454 -0.943396 2.355483

E= -4188.123195
S -1.345631 -0.229489 1.770860
Mo -2.797547 0.053871 0.004986
S -3.801035 1.908361 0.158227
Mo -0.014801 0.503010 0.006989
S 1.909208 -0.009098 1.783338
Mo 3.507572 -0.353885 -0.043846
S 4.663143 -2.140007 0.216894
S 0.264701 2.601073 0.024321
S -1.407781 0.024092 -1.813087
S 1.573372 -0.727509 -1.313603
S -4.211414 -1.641999 -1.118461
S -4.193553 -1.803463 0.866064
S 4.582002 1.408339 -0.626181
H 2.272406 1.227781 2.164619

[Mo3S10H]- XVII
E= -4188.152734
S -0.953161 -0.426237 1.640741
Mo 0.057197 0.588210 -0.112258
S 1.409341 -0.677139 -1.537215
Mo 3.124514 -0.418161 0.010204
S 4.672277 0.802785 -0.826217
Mo -2.680393 -0.046201 0.121447
S -3.532444 -2.236799 0.513111
S -3.858162 -1.472421 -1.386598
S -3.888532 1.490975 0.935752
S -1.522744 0.827010 -1.704293
S 2.056948 0.572141 1.679068
S 0.309892 2.924352 -0.022311
S 3.905252 -2.317804 0.606585
H 1.365976 3.008624 0.807567

E= -4188.141070
S 0.955261 -0.459629 -1.660455
Mo 2.614922 -0.011682 -0.097669
S 3.790918 1.596735 -0.816029
Mo -0.151839 0.594565 0.032283
S -2.118860 0.813434 -1.566989
Mo -3.113696 -0.425235 0.005450
S -3.695699 -2.342387 -0.758602
S -0.251761 2.934915 -0.025226
S 1.485037 0.615849 1.772839
S -1.433571 -0.640405 1.571971
S 4.050416 -1.508564 1.268630
S 3.668774 -2.203554 -0.558443
S -4.793117 0.577513 0.882438
H 0.807380 3.236323 0.755207

[Mo3S10H]- XVIII
E= -4188.156374
S -1.367467 0.426462 1.899878
Mo -2.703678 -0.017365 -0.051298
S -3.755644 1.801577 -0.289166
Mo 0.204574 0.596878 -0.029362
S 1.697146 -0.191536 1.725338
Mo 3.172957 -0.393573 0.008151
S 4.056106 -2.344271 -0.031127
S 0.243664 2.692495 -0.147388
S -1.186666 -0.311883 -1.717997
S 1.806781 -0.115063 -1.763215
S -4.007469 -1.823364 -0.907684
S -3.864073 -1.698856 1.164731
S 4.678557 1.126670 0.108236
H -1.116840 -0.805212 2.381309

E= -4188.132658
S -1.345977 -0.035338 1.749204
Mo -3.093899 -0.008643 -0.079074
S -3.768316 2.001124 -0.171816
Mo 0.444069 0.555699 -0.038290
S 1.897494 -0.251998 1.692333
Mo 3.409360 -0.395859 -0.010263

S 4.283212 -2.344137 -0.106468
S 0.308061 2.657030 -0.032248
S -1.203548 -0.423683 -1.417297
S 2.011756 -0.026143 -1.764653
S -4.637897 -1.532830 -0.985219
S -4.359190 -1.627644 1.087929
S 4.916389 1.112619 0.140709
H -1.532027 1.185735 2.280725

[Mo3S10H]- XIX
E= -4188.157567
S 1.285666 0.014652 -1.746200
Mo 2.620574 -0.187750 0.000224
S 3.710820 1.947570 0.000486
Mo -0.265536 0.625244 -0.000217
S -1.782340 -0.103433 -1.756962
Mo -3.186400 -0.384225 0.000061
S -3.993813 -2.370778 -0.000039
S -0.314973 2.725990 -0.000305
S 1.285426 0.014358 1.746323
S -1.782138 -0.103650 1.756884
S 4.880565 -1.044466 0.000061
S 3.326970 -2.407434 -0.000388
S -4.747721 1.083507 0.000236
H 5.021804 1.661652 -0.001239

E= -4188.135935
S -1.211655 -0.251631 1.781163
Mo 0.244515 0.495807 0.015636
S 1.807905 -0.171742 -1.753102
Mo 3.249553 -0.355125 -0.019551
S 4.695234 1.228984 -0.027813
Mo -2.590274 -0.071263 0.012472
S -4.211555 -1.724258 0.910207
S -4.537269 -1.327889 -1.011787
S -3.811386 1.915479 0.074095
S -1.252642 -0.162726 -1.770114
S 1.847386 -0.191237 1.745526
S 0.260298 2.602604 0.047581
S 4.215184 -2.271472 -0.040052
H -2.783344 2.746627 0.349351

[Mo3S10H]- XX
E= -4188.164656
S 1.299583 -0.146404 -1.713885
Mo 2.624569 0.049716 0.097241
S 3.818483 1.815664 0.079804
Mo -0.209826 0.587575 -0.020366
S -1.760139 -0.283480 -1.736703
Mo -3.213943 -0.399595 -0.014201
S -4.075397 -2.360105 0.125611
S -0.295933 2.680175 -0.188565
S 1.193799 0.107852 1.842751
S -1.847810 0.003072 1.736402
S 3.722346 -1.887003 0.922769
S 4.442726 -1.591762 -1.009905
S -4.746675 1.092142 -0.176561
H 5.550666 -0.865629 -0.739765

E= -4188.131368
S 1.392133 -0.373338 1.580657
Mo 2.873272 -0.048295 -0.131741
S 4.571033 -1.347395 -0.147936
Mo -0.434541 -0.958524 0.074733
S -1.737151 0.273281 1.717024
Mo -3.159056 0.588881 -0.024981
S -3.665356 2.657156 -0.247238
S -0.842088 -3.006019 0.329751
S 1.318158 -0.826958 -1.610411
S -1.830650 -0.120010 -1.725141
S 3.227710 -1.633520 -0.904489
S 4.047073 2.170088 1.018608
S -4.922990 -0.609541 0.159404
H 5.327697 1.860859 0.719889

[Mo3S10H]- XXI
E= -4188.165123
S 1.307004 -0.167994 -1.708839
Mo -0.200815 0.592039 -0.025627
S -1.843545 0.038492 1.737372
Mo -3.205545 -0.399290 -0.007644
S -4.742626 1.084480 -0.198685

Mo 2.636325 0.057929 0.100137
S 4.444200 -1.572568 -0.975030
S 3.728935 -1.873674 0.959435
S 3.806108 1.834468 0.060421
S 1.196628 0.134748 1.843697
S -1.750387 -0.309439 -1.730273
S -0.288488 2.681553 -0.226119
S -4.061707 -2.359655 0.166523
H 3.603534 -2.375071 -1.664434

E= -4188.132175
S 1.402463 -0.367825 1.584394
Mo -0.414029 -0.976739 0.075266
S -1.812320 -0.148049 -1.727089
Mo -3.136970 0.579669 -0.032393
S -4.909972 -0.604633 0.156690
Mo 2.887800 -0.035694 -0.130018
S 3.946369 2.203376 0.993673
S 3.170681 2.177331 -0.946177
S 4.593522 -1.316930 -0.128688
S 1.341654 -0.862970 -1.600588
S -1.720806 0.264887 1.713259
S -0.820499 -3.022474 0.345917
S -3.628193 2.650787 -0.267178
H 2.847942 2.600096 1.672671

[Mo3S10H]- XXII
E= -4188.129373
S 1.287332 -0.730058 1.661399
Mo 0.071803 0.438209 0.059814
S 0.691504 2.654855 0.770468
S -0.738268 2.730158 -0.618538
Mo 2.835317 -0.533701 -0.014860
S 4.469592 0.678719 0.642183
S 3.402207 -2.482691 -0.668334
S 1.737441 0.535279 -1.863683
S -1.207647 -0.764056 -1.543783
Mo -2.876101 -0.496814 0.014233
S -4.313038 0.930214 -0.696500
S -1.732415 0.254664 1.794825
S -3.818765 -2.362832 0.471873
H 2.250160 1.768853 -1.684421

E= -4188.132036
S -1.292796 -0.728447 -1.639493
Mo -0.003240 0.464384 -0.034620
S -0.761176 2.659623 -0.801288
S 0.629495 2.703710 0.653186
Mo -2.845056 -0.540564 0.006703
S -4.497049 0.643927 -0.645788
S -3.425326 -2.490741 0.637465
S -1.761489 0.500812 1.867469
S 1.260768 -0.692725 1.590369
Mo 2.892253 -0.491952 -0.019528
S 4.392030 0.901941 0.619346
S 1.727943 0.283638 -1.787389
S 3.753262 -2.398997 -0.473202
H -2.256800 1.737707 1.661905

[Mo3S10H]- XXIII
E= -4188.140788
S -1.477696 -0.507828 -1.740481
Mo 0.032571 0.370382 0.021163
S -1.080642 2.425535 -0.678569
S 0.473865 2.524488 0.689780
Mo -2.818573 -0.509758 0.023559
S -4.482583 1.162453 -0.056003
S -3.801604 -2.390039 0.121207
S -1.448686 -0.350694 1.775295
S 1.608678 -0.344728 1.744956
Mo 3.010911 -0.377751 -0.030323
S 4.444499 1.214142 0.021471
S 1.541976 -0.110726 -1.758692
S 3.977365 -2.284928 -0.157334
H -5.528980 0.316519 0.009167

E= -4188.136562
S 1.332568 -0.652129 1.659206
Mo 0.008254 0.455523 0.005767
S 0.695740 2.687127 0.779642
S -0.584546 2.666544 -0.759575
Mo 2.791833 -0.558608 -0.047881

S 4.623494 0.836664 0.466549
S 3.470834 -2.520602 -0.504111
S 1.763529 0.344870 -1.763079
S -1.304470 -0.707571 -1.578290
Mo -2.930184 -0.473145 0.034637
S -4.450759 0.882570 -0.640545
S -1.775088 0.366745 1.765136
S -3.765741 -2.383386 0.530742
H 5.375098 -0.131631 1.023240

[Mo3S10H]- XXIV
E= -4188.142465
S 1.283872 -0.730938 1.611796
Mo 0.195139 0.468699 0.001454
S 0.395984 2.648110 0.947625
S -0.764214 2.813122 -0.755084
Mo 2.893810 -0.524389 -0.032907
S 4.550094 0.634395 0.674866
S 3.449196 -2.465707 -0.739245
S 1.762833 0.626875 -1.679468
S -1.180991 -0.791815 -1.474276
Mo -2.906441 -0.034412
S -4.357406 0.853180 -0.714270
S -1.815082 0.232077 1.790999
S -3.816323 -2.440082 0.432712
H 0.207246 3.103360 -1.654757

E= -4188.134801
S -1.256796 -0.718676 -1.568976
Mo -0.008131 0.540749 -0.083068
S -0.613001 2.794735 -0.846125
S 0.643104 2.904416 0.784941
Mo -2.910216 -0.565906 0.054349
S -4.601377 0.508092 -0.695125
S -3.480406 -2.518832 0.707801
S -1.832746 0.572523 1.660168
S 1.227400 -0.696399 1.533191
Mo 2.906643 -0.580328 -0.019175
S 4.618222 0.442541 0.764240
S 1.914065 0.653077 -1.627541
S 3.429507 -2.539242 -0.697904
H -0.275940 2.994607 1.776820

[Mo3S10H]- XXV
E= -4188.150247
S -1.988432 0.686206 -1.764400
Mo -0.226958 0.412701 -0.180934
S 0.734773 2.549842 -0.480850
S 1.410282 1.549085 1.225707
Mo 2.468665 -0.402927 0.218767
S 4.141241 -0.831877 -1.423183
S 4.482071 0.786044 -0.155828
Mo -3.009058 -0.138801 0.040675
S -4.454363 1.255471 0.755793
S -4.000246 -2.176584 -0.623204
S -1.406091 -0.425224 1.630824
S 0.840984 -1.220151 -1.279543
S 2.564556 -1.700538 1.889002
H -4.967659 -2.137219 0.313522

E= -4188.122614
S -1.957056 0.597577 -1.807656
Mo -0.454367 0.278305 -0.057693
S 0.486044 2.378558 0.171969
S 1.459952 1.091652 1.517288
Mo 2.867948 -0.430395 0.135388
S 4.346393 -0.328130 -1.709687
S 4.308131 1.348134 -0.463931
Mo -3.218303 -0.097608 -0.066010
S -4.610639 1.422588 0.475790
S -4.271451 -2.185384 -0.445874
S -1.768641 -0.510457 1.645724
S 0.954660 -1.275651 -0.998306
S 3.501247 -1.779949 1.646434
H -5.379912 -1.655705 -0.998760

[Mo3S10H]- XXVI
E= -4188.130148
S -2.002397 1.148276 -1.548605
Mo -0.241894 0.441727 -0.164048
S 0.808575 2.565068 -0.164807
S 1.340340 1.346490 1.442768

Mo 2.463894 -0.418361 0.172160
S 4.117532 -0.545204 -1.527002
S 4.481030 0.815591 0.004642
Mo -3.083938 -0.188652 -0.042573
S -4.528467 0.988139 1.018375
S -3.854781 -1.947859 -0.982435
S -1.381551 -0.942036 1.508453
S 0.820519 -1.023694 -1.432560
S 2.558358 -1.966828 1.614329
H -1.545098 -0.064616 2.516837

E= -4188.104374
S -2.063058 1.350100 -1.403906
Mo -0.380798 0.533087 -0.083651
S 0.828094 2.618292 -0.105198
S 1.430016 1.309120 1.399266
Mo 2.548443 -0.467681 0.114054
S 4.301321 -0.668788 -1.452778
S 4.400074 0.986720 -0.190101
Mo -3.116857 -0.219612 -0.065828
S -4.534366 0.777767 1.199587
S -3.885108 -1.810347 -1.215024
S -1.416759 -1.164041 1.374655
S 0.780220 -1.070819 -1.281551
S 2.756189 -1.895002 1.668664
H -1.679074 -0.451408 2.489198

[Mo3S10H]- XXVII
E= -4188.126442
S -1.922770 1.160862 -1.481765
Mo -0.267988 0.275572 -0.116264
S 1.145532 2.622723 -0.289664
S 1.255042 1.319434 1.394309
Mo 2.480420 -0.452234 0.201231
S 4.139935 -0.677447 -1.500453
S 4.309872 0.977798 -0.251302
Mo -3.142397 -0.164690 -0.040357
S -4.590246 1.033397 0.999933
S -3.987297 -1.859607 -1.040057
S -1.490599 -0.810823 1.463321
S 0.853147 -1.298700 -1.255801
S 2.723069 -1.780399 1.835238
H 0.087576 3.340964 0.146232

E= -4188.142245
S 2.060744 0.728017 1.681186
Mo 0.120766 0.661761 0.018630
S 0.207820 3.020596 0.068750
S -1.612436 1.107441 -1.546037
Mo -2.459511 -0.465958 -0.126053
S -4.369045 -0.203904 1.433718
S -4.734540 0.466610 -0.406150
Mo 3.081225 -0.360874 0.019298
S 4.727590 0.751473 -0.787099
S 3.719292 -2.312404 0.635134
S 1.377823 -0.501205 -1.545552
S -0.999911 -0.449100 1.677735
S -2.405848 -2.374219 -1.035098
H 1.272012 3.201725 0.875899

[Mo3S10H]- XXVIII
E= -4188.108779
S -2.054018 0.492773 -1.875826
Mo -0.310074 0.395139 -0.382407
S 0.393849 2.660692 -0.418091
S 1.829048 1.930689 0.983354
Mo 2.446010 -0.386928 0.244091
S 4.142980 -1.157911 -1.243305
S 4.513681 0.645622 -0.279403
Mo -3.068990 -0.246881 0.069255
S -4.593165 1.312813 0.629889
S -3.782897 -2.254669 -0.144377
S -1.286416 -0.223861 1.572953
S 0.859262 -1.296507 -1.256082
S 2.361932 -1.432208 2.083111
H 1.040172 1.729197 2.064994

E= -4188.126898
S 2.172113 -0.432032 -1.709764
Mo 0.718777 -0.480797 0.077731
S 0.038023 -2.436094 0.472908
S -3.388303 0.207357 2.338906

Mo -3.337074 0.461243 -0.023398
S -3.283132 -1.283431 -1.617529
S -4.866773 -1.320798 -0.258508
Mo 3.676577 0.258429 -0.063606
S 5.239003 -1.163569 0.231762
S 4.440634 2.209989 -0.461766
S 2.166689 0.261229 1.713775
S -0.956939 0.953411 -0.222798
S -4.184958 2.306281 -0.630573
H -2.469445 1.129779 2.686831

[Mo3S10H]- XXIX
E= -4188.126582
S 1.914825 -1.193670 -1.488304
Mo 0.352958 -0.322377 -0.077386
S -1.376378 -2.028845 -0.627718
S -1.250469 -1.427938 1.358280
Mo -2.478075 0.302092 0.203369
S -4.142076 0.497980 -1.476069
S -4.580982 -0.832871 0.053434
Mo 3.171259 0.108927 -0.021857
S 4.586801 -1.166838 0.965906
S 4.010810 1.828531 -0.988002
S 1.528976 0.766498 1.510722
S -0.799310 1.484443 -1.157437
S -2.580465 1.783953 1.723667
H -0.925665 0.897161 -2.364941

E= -4188.114795
S 1.961923 -0.940691 -1.579797
Mo 0.249170 -0.337749 -0.057900
S -1.499541 -1.963368 -0.765088
S -1.356812 -1.555003 1.274960
Mo -2.529438 0.297362 0.213594
S -4.232698 0.624610 -1.402325
S -4.676964 -0.757007 0.079174
Mo 3.284188 0.096876 -0.007423
S 4.760327 -1.246878 0.765020
S 4.185201 1.874273 -0.789356
S 1.677267 0.590147 1.570697
S -0.864438 1.452433 -1.192038
S -2.519567 1.716222 1.799651
H -1.119810 0.911667 -2.401691

[Mo3S10H]- XXX
E= -4188.128415
S 1.876506 -0.020756 -1.623058
Mo 0.828563 1.334254 -0.067693
S -1.118005 2.008854 -1.069772
Mo -1.620387 0.030888 0.001833
S 0.084998 -0.149768 1.615578
Mo 0.656014 -1.394910 -0.263571
S 1.265965 -3.726981 0.087099
S 2.657123 -2.512922 1.062519
S -1.296836 -1.731162 -1.443671
S 2.191440 3.389434 -0.522919
S 1.854613 2.755133 1.443455
S -4.105053 0.217352 -0.300529
S -3.280931 0.002603 1.608396
H 3.626898 -2.458271 0.122564

E= -4188.110303
S 1.145194 1.662477 -1.380943
Mo -0.754387 1.452160 -0.129587
S -2.258005 0.117357 -1.246888
Mo -0.936070 -1.286267 -0.006265
S 0.131501 0.094498 1.638247
Mo 1.635461 -0.264891 -0.117270
S 3.929145 -1.015717 -0.228907
S 3.838408 0.701391 0.952846
S 0.768523 -2.111448 -1.268408
S -2.041439 3.460637 -0.536944
S -1.319171 3.160498 1.387367
S -2.482131 -3.244236 -0.277353
S -1.827363 -2.668448 1.622983
H 4.155274 1.645790 0.039130

[Mo3S10H]- XXXI
E= -4188.145356
S -0.734239 -2.020282 -1.306446
Mo 1.035527 -1.218045 -0.055183
S 2.137764 0.377305 -1.284920

Mo 0.550697 1.489215 -0.054740
S 0.046265 0.001692 1.711675
Mo -1.507367 -0.275646 -0.033264
S -4.088839 -0.734497 -0.496675
S -3.337468 -0.573267 1.445213
S -1.387378 1.626467 -1.310306
S 2.603482 -3.109662 -0.578454
S 2.241688 -2.543751 1.404061
S 1.367109 3.808821 -0.572623
S 1.226779 3.145624 1.407571
H -4.514590 0.532764 -0.691656

E= -4188.111011
S -1.862880 1.321192 -1.201081
Mo -1.525059 -0.705257 -0.102118
S -0.263233 -2.011255 -1.408960
Mo 1.416254 -0.939743 -0.074169
S -0.011719 -0.182179 1.686777
Mo 0.086219 1.478956 -0.019589
S 0.325233 4.105928 -0.346117
S 0.370039 3.237950 1.550305
S 1.809133 0.994396 -1.400196
S -3.821899 -1.405704 -0.464848
S -2.974318 -1.773055 1.406863
S 3.441682 -2.084387 -0.647983
S 2.944172 -2.027402 1.377524
H 1.649228 4.166085 -0.609748

[Mo3S10H]- XXXII
E= -4188.118717
S -1.073979 1.899088 -1.262030
Mo -1.598875 -0.002589 -0.087145
S -1.067212 -1.901842 -1.263074
Mo 0.780880 -1.406444 -0.024787
S -0.004161 -0.000133 1.686977
Mo 0.776168 1.408820 -0.024843
S 2.436512 3.140862 -0.327666
S 1.384426 3.098626 1.471872
S 1.857083 0.002968 -1.721247
S -4.058434 -0.005647 -0.636846
S -3.398102 -0.004022 1.348130
S 2.445763 -3.134041 -0.327171
S 1.391966 -3.095651 1.471443
H 3.134960 0.005616 -1.301620

E= -4188.102248
S 0.939757 -1.912692 -1.252502
Mo 1.746176 -0.143812 -0.092105
S 1.223057 1.810450 -1.241827
Mo -0.671961 1.395602 -0.052042
S 0.159637 -0.034549 1.688895
Mo -0.960532 -1.256678 -0.032372
S -2.715163 -2.877968 -0.384926
S -1.954045 -2.672340 1.553644
S -1.741116 0.140744 -1.887261
S 4.111736 -0.135267 -0.588749
S 3.525963 -0.411182 1.396829
S -2.331315 3.098436 -0.269638
S -1.326650 2.990228 1.547298
H -3.044443 0.278627 -1.574363

[Mo3S10H]- XXXIII
E= -4188.098597
S -1.998815 0.733752 -1.272925
Mo -1.245786 -1.038474 -0.018679
S 0.363214 -2.099868 -1.270706
Mo 1.522215 -0.559754 -0.018116
S -0.000482 0.001334 1.641177
Mo -0.276228 1.598046 -0.020218
S -0.685303 3.978920 -0.654188
S -0.597112 3.432455 1.362880
S 1.637867 1.362796 -1.271600
S -3.098342 -2.588926 -0.652043
S -2.680996 -2.224844 1.365051
S 3.787518 -1.398960 -0.651203
S 3.272002 -1.196392 1.365814
H -0.001262 0.003316 2.998447

E= -4188.075807
S -1.922599 -0.001951 -1.585675
Mo -0.840439 -1.345133 -0.075290
S 1.135724 -2.048987 -0.939320

Mo 1.882269 0.001884 -0.127986
S -0.220618 0.000270 1.873461
Mo -0.843340 1.343665 -0.075403
S -2.321353 3.216173 -0.643270
S -1.900684 2.841439 1.364483
S 1.131030 2.050556 -0.941074
S -2.315600 -3.220384 -0.643290
S -1.898511 -2.842064 1.364688
S 4.244268 0.002152 -0.641729
S 3.633197 0.001754 1.360716
H -1.374223 -0.000806 2.600673

[Mo3S10H]- XXXIV
E= -4188.128415
S 1.876107 -0.020886 -1.622938
Mo 0.828647 1.334159 -0.067613
S -1.117890 2.009081 -1.069688
Mo -1.620501 0.031271 0.002040
S 0.084942 -0.149625 1.615797
Mo 0.655570 -1.394993 -0.263302
S 1.266136 -3.727056 0.086206
S 2.657245 -2.513269 1.062135
S -1.297153 -1.730836 -1.443524
S 2.191378 3.389381 -0.523318
S 1.856655 2.754081 1.443142
S -4.105167 0.217303 -0.300591
S -3.281185 0.003043 1.608449
H 3.626823 -2.457982 0.122021

E= -4188.110303
S -1.141302 -1.663550 -1.382817
Mo 0.756193 -1.450672 -0.128673
S 2.259132 -0.115741 -1.245933
Mo 0.934966 1.286980 -0.006287
S -0.133479 -0.093441 1.637988
Mo -1.636454 0.261870 -0.118516
S -3.929447 1.015482 -0.225964
S -3.839694 -0.705362 0.950249
S -0.769809 2.108826 -1.269942
S 2.044927 -3.458585 -0.534859
S 1.321672 -3.158344 1.388997
S 2.483292 3.242457 -0.277073
S 1.821046 2.673449 1.622609
H -4.159008 -1.646521 0.033911

[Mo3S9H]- I
E= -3789.801812
S 0.644733 -0.612365 -1.893425
Mo 2.201777 -0.987177 -0.297644
S 3.596740 0.832897 0.345415
S 1.856527 0.466238 1.502453
Mo -0.119513 0.607450 -0.024448
S 0.690644 2.837709 -0.919478
S -0.417475 2.980651 0.811938
S -2.186549 0.936604 -1.401649
Mo -2.765871 -0.362966 0.267571
S -4.061270 -2.026298 -0.136062
S -1.115430 -0.595829 1.773738
S 2.664070 -3.044088 0.087301
H 1.959620 2.794403 -0.433788

E= -3789.800775
S -0.665457 -0.607332 1.894704
Mo -2.224855 -0.977712 0.292531
S -3.598424 0.849973 -0.365170
S -1.847819 0.472267 -1.506300
Mo 0.115498 0.598891 0.032831
S -0.689497 2.836179 0.903152
S 0.448708 2.969775 -0.808884
S 2.179513 0.908238 1.414678
Mo 2.781450 -0.362097 -0.265948
S 4.114223 -2.000061 0.118302
S 1.115855 -0.625042 -1.749711
S -2.699372 -3.034370 -0.081653
H -1.951562 2.804531 0.398761

[Mo3S9H]- II
E= -3789.836591
Mo 0.329045 0.614682 0.152660
Mo 2.613111 -0.629863 -0.051183
S 2.148274 0.166558 1.952513
S 2.254118 0.756316 -1.709488

S 3.013756 -2.707399 -0.391171
S -0.881803 -0.385156 -1.688702
S -3.961722 0.822326 -0.110937
Mo -2.384051 -0.632196 -0.011539
S -1.018544 -0.297115 1.802270
S 0.642335 2.860717 0.838835
S -0.556931 2.935319 -0.839592
H 0.395240 3.038582 -1.795981
S -3.129211 -2.642116 0.022434

E= -3789.781491
Mo -0.235958 0.656399 -0.230513
Mo -2.739078 -0.562670 -0.123349
S -1.131044 -0.870831 -1.698608
S -2.149681 1.058726 1.250729
S -3.566442 -2.343128 0.747552
S 0.806464 -0.358024 1.776017
S 2.806972 0.266570 1.977793
Mo 2.294548 -0.774627 -0.077206
S 1.819007 0.603771 -1.737874
S -0.546962 2.943609 -1.120596
S 0.742542 2.997546 0.478509
H -0.120626 3.305375 1.476027
S 3.012963 -2.717467 -0.634218

E= -3789.775201
Mo -0.369345 0.784875 -0.125451
Mo -2.713391 -0.800953 -0.222980
S -1.203873 -0.633288 -1.864264
S -2.281699 0.708747 1.367023
S -3.294737 -2.765280 0.418957
S 0.690341 -1.011767 1.338712
S 2.397685 -0.085138 2.187878
Mo 2.532490 -0.594178 -0.106858
S 1.908746 1.018449 -1.455865
S -0.940819 3.055308 -0.908472
S 0.250261 3.144359 0.787376
H -0.697100 3.280966 1.744578
S 3.962061 -2.034530 -0.785247

[Mo3S9H]- III
E= -3789.905969
S -0.001769 3.744861 1.043708
Mo -0.000779 1.756487 -0.264530
S 1.831345 1.188834 -1.508372
Mo 1.380915 -0.552652 -0.045320
S -0.000008 0.384470 1.624817
Mo -1.379931 -0.554073 -0.045315
S -1.832600 1.186660 -1.508000
S -2.878926 -1.344618 1.526571
S 0.001483 -2.050920 -1.104889
S 2.877017 -1.346624 1.527584
S 3.497649 -1.836053 -0.406644
S -3.494594 -1.840722 -0.407629
H -0.002170 3.335800 2.322614

E= -3789.876818
S -0.024000 4.103162 0.629212
Mo -0.009280 1.845856 -0.158639
S 1.877165 1.248574 -1.321219
Mo 1.351854 -0.615900 -0.053633
S -0.000885 0.383878 1.651266
Mo -1.344254 -0.628459 -0.053423
S -1.889530 1.229723 -1.321288
S -2.936405 -1.347567 1.511641
S 0.010254 -1.997434 -1.306120
S 2.949787 -1.322148 1.512040
S 3.335573 -2.044301 -0.390151
S -3.316186 -2.074459 -0.390229
H -0.021817 3.866311 1.956706

E= -3789.843336
S 1.744426 3.721059 0.566374
Mo 0.527187 1.731110 0.069309
S 2.309165 0.787727 -1.076380
Mo 1.175696 -0.963291 -0.107068
S -0.025765 0.119926 1.686963
Mo -1.714738 -0.237425 -0.076824
S -1.337215 1.925911 -1.152616
S -3.464192 -0.793909 1.408074
S -0.464432 -1.702556 -1.461530
S 2.210916 -2.459738 1.396894

S 2.970381 -2.517276 -0.531038
S -3.967210 -0.736080 -0.628823
H 0.880709 4.202455 1.485782

[Mo3S9H]- IV
E= -3789.833964
S 0.730924 -0.356334 -1.779903
Mo 2.368758 -0.429021 -0.037341
S 2.866410 -2.458429 0.401400
S 4.039930 0.770288 -0.607241
Mo -0.316970 0.745829 0.192605
S 1.304343 0.484849 1.788497
S -1.942333 0.117993 2.024851
Mo -2.413197 -0.882213 0.086230
S -3.334779 0.303340 -1.447990
S -1.806714 -2.906674 -0.329454
S -0.191627 2.584211 -1.264291
S -0.732086 3.045243 0.682735
H 0.234113 -1.604789 -1.640406

E= -3789.809226
S -1.338349 0.007642 2.033016
Mo -2.548048 0.350658 -0.031911
S -4.463752 -0.641423 0.112271
S -2.775419 2.468670 -0.176792
Mo 0.247811 -0.443255 0.213110
S 1.540318 -2.118373 1.259382
S 2.173175 -1.677409 -0.712886
Mo 2.847808 0.575711 -0.371997
S 1.059123 1.743140 0.428717
S 4.869977 0.941905 0.274599
S -0.990763 -0.028420 -1.844882
S -1.395457 -1.888474 -1.016517
H -1.859639 -1.206894 2.305321

E= -3789.791523
S 1.325039 -0.090823 -1.596786
Mo 3.235128 0.347043 -0.075849
S 5.065931 -0.325037 -0.966497
S 3.199427 2.385318 0.565159
Mo -0.674331 -0.529484 -0.125782
S -1.951684 -1.964298 -1.473501
S -2.791123 -1.670082 0.454869
Mo -3.203608 0.663419 0.350151
S -1.208944 1.726187 -0.011761
S -5.069053 1.358392 -0.458048
S 2.569195 -1.127720 1.597157
S 0.443625 -1.468903 1.613677
H 1.679483 -1.371285 -1.826143

[Mo3S9H]- V
E= -3789.862307
S 3.110616 -1.624344 -1.275785
Mo 1.496391 -0.581127 0.147709
S 1.080509 1.337536 1.620160
Mo -0.459124 1.505954 -0.208459
S 0.012596 -0.233149 -1.642692
Mo -1.181131 -1.339903 0.054630
S 0.427161 -2.146400 1.450330
S -2.502721 -2.793456 -0.837010
S -2.132297 0.371014 1.386509
S 0.055004 3.280249 -1.319417
H 2.405786 -1.815139 -2.406274
S 2.991836 1.178152 0.768233
S -2.815424 1.833418 0.016129

E= -3789.853342
S -0.492311 3.301441 -1.361201
Mo -0.337279 1.476816 0.150643
S -1.650870 0.096737 1.719802
Mo -1.243234 -1.180453 -0.239403
S 0.272776 -0.034581 -1.621339
Mo 1.944117 -0.208278 0.056773
S 1.555571 1.602126 1.423296
S 3.886062 -0.109808 -0.857623
S 1.286334 -2.167542 1.141225
S -3.088373 -1.669782 -1.203317
H 0.005806 2.768859 -2.493507
S -2.550972 1.837292 0.932800
S -0.173041 -3.260161 0.066165

E= -3789.826278

S 0.331323 3.322361 1.335909
Mo 0.406347 1.452935 -0.124511
S 2.056559 0.085138 -1.652229
Mo 1.520056 -1.152941 0.286208
S -0.353703 -0.261335 1.400775
Mo -2.171497 -0.221569 -0.066145
S -1.533852 1.458142 -1.484163
S -4.058982 -0.023170 0.928154
S -1.790229 -2.334331 -0.833306
S 3.143572 -1.781619 1.527644
H -0.913052 3.173398 1.833058
S 2.561835 2.012518 -0.941371
S 0.343915 -2.881906 -0.646802

[Mo3S9H]- VI
E= -3789.855252
S 2.554330 2.454366 -1.252015
Mo 0.809810 1.267177 -0.094898
S -0.918908 1.424564 1.669416
Mo -1.792449 -0.046257 -0.026390
S -0.260272 0.166552 -1.763849
Mo 0.565620 -1.535020 -0.097903
S 2.496558 -0.194231 0.705614
S 0.938077 -3.003201 -1.615967
S -1.456740 -1.964689 1.083073
S -3.767063 0.343238 -0.801543
H 3.595328 1.597665 -1.285402
S -0.413415 3.182567 0.648366
S 1.697400 -1.684507 1.982619

E= -3789.848893
S 2.885813 -2.389598 -1.093134
Mo 1.501266 -0.733511 -0.007909
S 1.596242 1.128943 1.585724
Mo -0.130979 1.697448 0.009680
S 0.054059 0.059855 -1.673955
Mo -1.668628 -0.598109 -0.103870
S -0.291269 -2.564943 0.269416
S -3.394415 -0.682239 -1.353560
S -1.905389 1.272662 1.319959
S -0.023873 3.633424 -0.927055
H 2.014194 -3.367712 -1.405435
S 3.304128 0.805335 0.398481
S -1.568039 -2.013255 1.829976

E= -3789.826777
S 1.970117 -2.863779 -1.548696
Mo 1.112345 -1.142471 -0.066591
S 1.647039 0.411393 1.768715
Mo 0.762960 1.608148 -0.093454
S -0.168912 0.089838 -1.680620
Mo -2.016046 -0.003407 -0.078466
S -1.062323 -2.228687 0.435773
S -3.911867 0.120145 -1.024155
S -1.372939 2.107058 0.729187
S 1.957250 3.225656 -0.835556
H 1.005273 -2.877319 -2.486692
S 3.227346 -0.732083 0.937707
S -1.979096 -1.163169 1.999157

[Mo3S9H]- VII
E= -3789.938162
S -1.532182 0.110307 1.750373
Mo 0.022377 -0.570045 0.000138
S -1.531993 0.110252 -1.750336
Mo -2.955919 0.295300 -0.000059
S -4.412051 -1.278403 -0.000096
S -3.898014 2.222497 -0.000111
S 1.538309 0.064550 -1.777951
S 0.030783 -2.673594 0.000204
S 1.538187 0.065142 1.777999
Mo 2.828764 0.367896 -0.000041
S 3.593355 2.350492 -0.000162
S 4.599679 -1.198102 -0.000195
H 5.583482 -0.282602 0.002835

E= -3789.898149
S -1.764938 0.853265 -1.669466
Mo -0.123024 0.318088 -0.140414
S -1.288302 -0.597415 1.600935
Mo -2.942913 -0.201356 0.021626
S -4.399551 1.133720 0.858919

S -3.789882 -2.032080 -0.702411
S 1.720615 1.154682 1.416615
S 0.783528 2.470530 0.068483
S 1.100126 -1.183569 -1.363225
Mo 2.782548 -0.402509 0.018594
S 3.643577 -1.951245 1.207884
S 4.432828 0.903334 -1.035533
H 4.894355 -0.016930 -1.907081

E= -3789.867055
S -1.776054 0.432176 -1.725203
Mo -0.142578 0.225684 0.013461
S -1.616493 -0.439074 1.664577
Mo -3.179147 -0.165067 -0.031497
S -4.572897 1.384300 0.447208
S -4.190623 -2.000709 -0.455718
S 1.838066 0.991006 1.476754
S 0.809985 2.340390 0.187299
S 1.208685 -1.353175 -1.020507
Mo 3.075583 -0.387848 -0.045799
S 4.352403 -1.746732 1.010074
S 4.269349 1.225757 -1.300861
H 5.179257 0.400659 -1.856838

[Mo3S9H]- VIII
E= -3789.940529
S -1.541276 0.108939 1.746617
Mo 0.042499 -0.557459 0.000010
S -1.541186 0.109515 -1.746577
Mo -2.961964 0.317201 0.000006
S -4.441101 -1.234535 -0.000288
S -3.883211 2.254333 0.000313
S 1.524355 0.082402 -1.781405
S 0.064104 -2.659130 -0.000338
S 3.808159 2.401325 0.000003
Mo 2.850136 0.238909 0.000053
S 4.350428 -1.263361 -0.000148
S 1.524397 0.081773 1.781550
H 5.077117 1.956512 0.001459

E= -3789.897098
S 1.656147 -0.295010 1.686133
Mo 0.152423 0.445278 -0.030168
S 1.758342 0.058168 -1.764415
Mo 3.176911 -0.270282 -0.015242
S 4.569427 1.337922 0.192162
S 4.189612 -2.145757 -0.176799
S -1.423089 -0.645904 -1.392198
S -0.174668 2.526369 0.039465
S -1.615543 -0.299596 1.748987
Mo -3.316756 -0.269049 -0.035303
S -4.608627 -1.968237 0.055459
S -4.267155 1.625540 -0.326137
H -1.879369 0.854296 2.387444

E= -3789.849751
S -2.010402 -0.855633 1.596896
Mo -0.231706 -0.449595 0.085869
S -1.538915 0.633877 -1.536288
Mo -3.228169 0.235947 -0.019633
S -4.743976 -1.025113 -0.852295
S -4.055117 2.071463 0.706685
S 1.839805 -0.993820 -1.403909
S 1.042125 -2.474997 -0.152735
S 1.486485 0.417937 1.738461
Mo 3.242596 0.393151 -0.011550
S 3.337350 2.351569 -0.853366
S 5.096169 -0.550017 0.468801
H 1.869353 -0.743356 2.307222

[Mo3S9H]- IX
E= -3789.849929
S -0.809658 -0.849771 -1.427232
Mo 0.118377 0.526112 0.104805
S -1.649688 1.123776 1.485720
Mo -2.608107 -0.301707 -0.054406
S -4.115568 0.748588 -1.160761
S -3.322645 -2.089698 0.886274
S 1.259002 2.887226 0.544743
S 0.613048 2.287428 -1.339144
S 1.190657 -0.641845 1.938474
Mo 2.572152 -0.875401 0.161185

S76

S 2.451057 -2.553764 -1.145162
S 4.008475 0.644592 -0.365824
H 2.543430 2.437321 0.440058

E= -3789.773969
S 1.560831 -0.234248 0.526793
Mo -0.068476 1.236012 -0.313478
Mo 3.685155 -0.840272 0.148157
S 4.682023 -2.005446 1.641218
S 4.850894 -0.123082 -1.493891
S -1.954474 2.710898 0.588805
S -0.200761 2.479237 1.684432
S -1.467380 -0.499628 -1.055534
Mo -3.338484 -1.198433 -0.033767
S -4.702067 -2.368399 -1.188507
S -4.061102 -0.193891 1.733652
H -2.754269 1.738758 1.137675

E= -3789.850284
S 1.616105 -1.257350 1.274265
Mo 0.104691 -0.100972 -0.034333
S 1.663051 1.073517 -1.279535
Mo 3.181748 -0.106634 0.008245
S 4.387053 1.190727 1.204367
S 4.389150 -1.421048 -1.167043
S -1.563277 3.636787 0.032815
S -1.586294 0.996336 1.184331
S -1.307958 -1.465662 -1.263823
Mo -2.955273 -0.455606 0.006409
S -3.945099 -1.844516 1.292553
S -4.359797 0.637112 -1.185167
H -2.595937 3.120487 -0.657720

[Mo3S9H]- X
E= -3789.816294
Mo -3.582307 -0.067138 -0.256469
S -5.013167 0.489305 1.239384
S -2.177729 1.563878 -0.946324
S -2.250062 -1.824242 0.239213
Mo -0.755898 -0.107160 -0.202355
S 0.459225 0.540156 1.593427
S 0.808789 -0.681578 -1.763536
Mo 2.075108 -0.030288 0.025524
S 3.060650 1.988102 -0.848075
S 3.828636 1.647965 1.050525
H 2.999825 2.434452 1.776519
S 2.945494 -1.908775 1.061042
S 4.091303 -1.429925 -0.599277

E= -3789.785472
Mo 3.129340 0.195423 0.076517
S 3.270989 1.894872 -1.222311
S 3.324157 0.512537 2.186534
S 2.769505 -1.934913 -0.766707
Mo 0.746217 -0.783792 -0.272609
S -0.558707 0.269262 -1.810931
S -0.598479 -1.046327 1.558247
Mo -1.942510 -0.000377 0.027128
S -2.263025 2.109108 1.119806
S -3.395145 2.104981 -0.621022
H -2.528364 2.722560 -1.456945
S -3.385623 -1.555953 -0.886710
S -4.079896 -0.978270 0.977685

E= -3789.767476
Mo 3.672258 0.098301 0.019355
S 4.890712 1.314988 -1.258367
S 4.381743 -0.344398 1.990640
S 2.214151 -1.414902 -1.014625
Mo 0.525695 -0.233363 0.005528
S -0.719447 1.264121 -1.174017
S -0.963145 -1.304366 1.378113
Mo -2.259340 0.019674 0.027031
S -3.220046 1.440128 1.718650
S -4.054701 1.940901 -0.114728
H -3.252007 2.976769 -0.453860
S -3.157779 -1.242693 -1.683241
S -4.257097 -1.536932 0.049669

[Mo3S9H]- XI
E= -3789.920428

Mo -0.297418 0.001506 -0.090915
S 1.071259 -1.717512 -0.693209
Mo 2.546146 -0.159245 0.221003
S 1.156451 1.695282 0.400564
S 3.180909 -0.866798 2.118908
S -1.710131 0.557028 -1.762374
S -1.634042 -0.511247 1.642109
Mo -3.182044 0.052487 -0.021432
S -4.380002 -1.653418 -0.536019
S -4.287830 1.799450 0.558134
S 4.102831 -0.400579 -1.548462
S 4.605752 1.323201 -0.488142
H 5.516110 0.814033 0.372329

E= -3789.845240
Mo -0.362738 -0.194996 0.296459
S 1.112779 0.887780 1.678869
Mo 2.431096 0.239205 -0.116290
S 0.993069 -1.164999 -1.271656
S 2.939624 1.974488 -1.252266
S -1.870452 -1.598982 1.345509
S -1.668529 1.453720 -0.771246
Mo -3.163939 -0.223623 0.044830
S -3.226905 2.061740 0.590724
S -4.448160 -1.216219 -1.364122
S 4.168638 -0.633048 1.237839
S 4.539980 -1.275120 -0.713841
H 5.373701 -0.294362 -1.126908

E= -3789.817156
Mo -0.246705 0.178704 0.113423
S 1.219535 0.558073 1.838235
Mo 2.605984 0.298060 0.002834
S 1.141206 -0.521427 -1.582881
S 3.410094 2.204129 -0.522966
S -1.871868 1.763551 -0.256785
S -1.800494 -1.403928 1.097477
Mo -3.475233 0.030285 -0.116196
S -2.729787 -2.160387 -0.659675
S -5.530461 0.666744 -0.029638
S 4.089958 -1.191972 1.093219
S 4.650254 -1.228131 -0.920609
H 5.615060 -0.282486 -0.904618

[Mo3S9H]- XII
E= -3789.851007
Mo -2.834291 -0.558429 0.073763
S -4.527084 0.802576 -0.809416
H -4.910862 -0.118590 -1.714397
S -1.988305 -0.275565 2.046292
S -2.691514 -2.545445 -0.616795
Mo -0.398947 0.668960 0.127255
S 0.662510 -0.226266 -1.667883
S 3.538857 -1.855272 -0.949791
S 3.417925 1.857980 -0.671065
Mo 2.401862 0.077367 -0.132610
S -0.957414 2.673554 -0.274410
S 1.183226 0.482185 1.807370
S 3.851089 -1.399576 1.063275

E= -3789.831288
Mo -3.122227 -0.270318 0.185278
S -2.333929 1.483527 -1.255816
H -2.698674 2.627918 -0.634177
S -1.485086 -0.642757 1.746508
S -4.406290 -1.821437 -0.562323
Mo -0.431465 0.633563 0.119119
S 0.328783 -0.578956 -1.629537
S 2.806165 -2.496296 -0.395131
S 3.503863 1.065628 -1.419758
Mo 2.218973 -0.197315 -0.298285
S 0.493039 2.746574 0.606523
S 1.450118 1.144545 1.573898
S 3.315640 -1.500637 1.359228

E= -3789.802729
Mo -3.375519 -0.307425 0.161292
S -2.551841 1.533871 -1.142737
H -2.852387 2.686311 -0.497683
S -1.692165 -0.892385 1.600829
S -4.677328 -1.750833 -0.749297
Mo -0.686767 0.542631 0.090625

S 0.558992 -0.369060 -1.573941
S 3.361154 -2.335091 -0.518019
S 3.848133 1.327921 -1.228757
Mo 2.586912 -0.117965 -0.324939
S 0.225335 2.533606 0.880077
S 1.435794 0.959302 1.574991
S 3.543059 -1.482984 1.379641

[Mo3S9H]- XIII
E= -3789.812187
S 4.131946 1.075326 1.018656
Mo 2.319832 -0.232702 0.130016
S 3.420702 -2.033479 -0.282042
S 0.529180 -1.287281 1.325963
Mo -0.425473 0.230652 -0.318510
S -1.864169 -1.517377 -1.260305
Mo -3.114330 -0.024030 -0.162601
S -2.120003 1.978240 -0.114754
S 0.661386 0.674074 1.896520
S 1.347826 1.771957 -1.176679
S 1.260467 -0.088546 -2.030520
S -4.384729 -0.644039 1.462638
H 3.517096 2.233369 1.314368

E= -3789.843074
S -3.948040 -2.128392 -0.219885
Mo -2.577603 -0.190223 -0.062618
S -4.089666 1.319043 -0.066082
S -1.314884 -0.067138 -1.880026
Mo 0.210164 0.554487 -0.094800
S 1.739745 -0.538708 -1.677318
Mo 3.291145 -0.266904 -0.032087
S 2.012243 0.441383 1.678289
S 0.149690 2.656556 -0.394177
S -1.312458 0.475207 1.832911
S -0.863825 -1.483418 1.327201
S 5.391823 -0.737184 -0.102825
H -3.029667 -3.086683 -0.010161

E= -3789.798742
S -4.188511 -1.672562 -0.929168
Mo -2.868554 0.089095 0.013430
S -4.290713 1.655193 0.357558
S -1.207846 0.692015 -1.622632
Mo 0.589989 -0.010573 0.106370
S 1.861555 -1.085104 -1.492311
Mo 3.370355 -0.334233 0.056424
S 2.114525 0.482211 1.774737
S -0.026869 2.127619 -0.636372
S -1.344332 -0.175355 1.892255
S -0.742145 -1.870534 0.832445
S 5.158350 0.678008 -0.568966
H -3.199380 -2.563996 -1.122151

[Mo3S9H]- XIV
E= -3789.801812
S 0.644733 -0.612365 -1.893425
Mo -0.119513 0.607450 -0.024448
S -2.186549 0.936604 -1.401649
Mo -2.765871 -0.362966 0.267571
S -1.115430 -0.595829 1.773738
Mo 2.201777 -0.987177 -0.297644
S 2.664070 -3.044088 0.087301
S 1.856527 0.466238 1.502453
S 3.596740 0.832897 0.345415
S -0.417475 2.980051 0.811938
S 0.690644 2.837709 -0.919478
S -4.061270 -2.026298 -0.136062
H 1.959620 2.794403 -0.433788

E= -3789.800774
S -0.665675 -0.607462 1.894982
Mo 0.115368 0.598818 0.032948
S 2.178974 0.907711 1.415259
Mo 2.781697 -0.361603 -0.265862
S 1.116250 -0.624191 -1.749872
Mo -2.224835 -0.977762 0.292704
S -2.698263 -3.034480 -0.082407
S -1.848024 0.471881 -1.506387
S -3.598713 0.849683 -0.365388
S 0.448862 2.969370 -0.808650
S -0.690400 2.835887 0.902704

S 4.114374 -1.999714 0.117961
H -1.952184 2.804024 0.397608

E= -3789.778920
S 0.720663 -1.063753 -1.362121
Mo -0.412202 0.549810 -0.060165
S -2.255795 0.556039 -1.604332
Mo -3.030118 -0.451219 0.217885
S -1.471778 -0.350923 1.842872
Mo 2.729585 -0.819718 -0.192854
S 4.018602 -2.531247 -0.160888
S 1.632309 0.450378 1.550625
S 3.344937 1.331717 0.660887
S -0.553704 2.979937 0.473230
S 0.515890 2.603385 -1.256359
S -4.191489 -2.240640 -0.005310
H 1.780696 2.529075 -0.741994

[Mo3S9H]- XV
E= -3789.846611
S 3.388523 2.319773 -0.381042
Mo 2.320060 0.203693 -0.208695
S 3.907193 -1.126801 -0.734759
S 1.502363 -0.908839 1.749322
Mo -0.285501 -0.846414 0.126819
S -2.205641 -0.658246 1.832215
Mo -2.667795 0.503250 -0.020039
S -3.721382 -0.413711 -1.642274
S 0.860231 1.054633 1.690216
S 0.675876 0.151376 -1.749174
S -0.491186 -2.879394 -0.431438
S -2.406922 2.632454 -0.075390
H 2.451065 3.117919 0.157612

E= -3789.843074
S -3.946860 -2.129573 -0.217593
Mo -2.577577 -0.190487 -0.062399
S -4.090511 1.317905 -0.067689
S -1.312691 0.477650 1.832374
Mo 0.210104 0.555039 -0.095242
S 2.012235 0.443797 1.677675
Mo 3.290979 -0.267137 -0.031818
S 1.739217 -0.541021 -1.676340
S -0.863059 -1.481238 1.328623
S -1.314758 -0.069236 -1.879898
S 0.149906 2.656836 -0.396969
S 5.391562 -0.737896 -0.102424
H -3.027867 -3.087046 -0.006832

E= -3789.799606
S -3.762581 2.150845 0.787261
Mo -2.873144 0.098797 -0.042910
S -4.494466 -1.147288 -0.679247
S -1.196516 0.538592 -1.737130
Mo 0.587377 -0.253166 -0.007377
S 2.096140 -0.807052 -1.662789
Mo 3.380724 -0.148238 0.110326
S 1.931254 0.189421 1.825707
S -0.331430 1.908939 -0.414704
S -1.414349 -0.998050 1.525903
S -0.390395 -2.377991 0.314959
S 4.996182 1.232848 -0.195136
H -4.929596 1.654072 1.241183

[Mo3S9H]- XVI
E= -3789.820822
S 1.111817 -1.600195 -0.793329
Mo -0.718458 -0.041583 0.225385
S -2.095535 -1.889571 -0.307051
Mo -3.426878 -0.053023 -0.481151
S -1.975782 1.711461 -0.659696
Mo 2.968522 -0.100514 -0.103902
S 4.503597 -0.330870 -1.552940
S 2.774937 2.121703 0.605770
S 1.205968 1.565030 -0.647000
S -0.547498 0.103767 2.326542
S 3.418436 -1.210599 1.660185
S -5.362737 0.111547 0.438755
H 0.894912 -1.121352 -2.033711

E= -3789.805607
S 0.911363 -0.379788 -1.961132

Mo -0.598054 -0.445153 -0.081162
S -2.465130 -1.729030 -0.634793
Mo -3.245683 0.376935 -0.343691
S -1.467706 1.722399 -0.014412
Mo 2.355874 -0.038284 -0.001782
S 4.036571 -1.352428 -0.192146
S 3.001924 1.916251 1.173455
S 2.954887 2.088436 -0.893525
S 0.904070 -2.231707 0.890618
S 0.833768 -0.387504 1.835738
S -4.850574 0.577944 1.066655
H 0.743524 0.879903 -2.408675

E= -3789.771626
S -0.966601 -1.015756 -1.803020
Mo 0.757477 0.132764 -0.311022
S 2.042161 -1.850356 -0.106623
Mo 3.423651 -0.170850 0.479248
S 2.231763 1.731817 0.629143
Mo -2.490348 0.022469 -0.110092
S -4.211873 0.326747 -1.305757
S -3.295060 -0.701960 2.047522
S -2.510689 -2.157070 0.807411
S -1.028419 1.878867 -0.817760
S -1.943586 2.023917 1.045004
S 5.300848 -0.050546 -0.557625
H -0.909496 -2.314667 -1.454314

[Mo3S9H]- XVII
E= -3789.907444
S 0.001850 3.657966 1.171388
Mo 0.000772 1.756449 -0.246194
S -1.829938 1.202777 -1.498738
Mo -1.381541 -0.550802 -0.045648
S -3.502223 -1.824343 -0.423421
S -2.873998 -1.368757 1.516930
S 1.831443 1.200663 -1.498265
Mo 1.380556 -0.552246 -0.045881
S 3.499599 -1.828661 -0.423988
S 2.875023 -1.367514 1.516154
S 0.000183 0.368796 1.633993
S -0.001503 -2.039887 -1.116543
H 0.001979 4.540485 0.144198

E= -3789.877742
S -1.672257 3.723530 0.655799
Mo -0.529999 1.711407 0.047661
S -2.187698 0.752751 -1.247210
Mo -1.139318 -0.921128 -0.073525
S -2.929698 -2.571228 -0.538863
S -2.203120 -2.360466 1.407519
S 1.431811 1.842991 -1.140428
Mo 1.608954 -0.217772 -0.074954
S 3.904382 -0.554592 -0.616228
S 3.373130 -0.703523 1.392273
S 0.048605 0.155346 1.698995
S 0.555715 -1.828242 -1.327556
H -2.598653 3.849059 -0.314428

[Mo3S9H]- XVIII
E= -3789.880456
S -0.065278 3.677228 1.057054
Mo -0.054315 1.779401 0.026625
S -1.884591 1.321979 -1.272325
Mo -1.402215 -0.572384 -0.071113
S -3.527556 -1.809339 -0.580130
S -2.991906 -1.372504 1.396108
S 1.759562 1.367642 -1.520883
Mo 1.446344 -0.625262 -0.064833
S 3.753560 -1.161345 -0.346953
S 2.823411 -1.368661 1.371289
S 0.064069 0.152211 1.666535
S 0.030597 -1.890031 -1.320200
H 1.037938 1.050681 -2.616454

E= -3789.864007
S 1.582122 3.502124 0.883978
Mo 0.626212 1.741227 0.079486
S -1.436834 1.837813 -1.088761
Mo -1.627442 -0.196858 -0.087288
S -3.862472 -0.965662 -0.568966
S -3.366034 -0.594865 1.423388

S 1.856484 0.743107 -1.731220
Mo 1.129783 -0.951205 -0.070647
S 3.212096 -2.060196 -0.351022
S 2.210151 -2.401458 1.438923
S -0.042991 0.179721 1.694025
S -0.547418 -1.834899 -1.325719
H 0.919086 0.596163 -2.699160

[Mo3S9H]- XIX
E= -3789.883291
S 0.000201 3.823651 0.744957
Mo 0.000006 1.861583 -0.152563
S -1.873780 1.248774 -1.347512
Mo -1.421495 -0.556163 -0.025686
S -3.114327 -2.264874 -0.216491
S -3.090882 -1.108412 1.520330
S 1.873810 1.249051 -1.347700
Mo 1.421651 -0.555950 -0.025953
S 3.113839 -2.265510 -0.216148
S 3.090389 -1.108885 1.520533
S 0.000222 0.330912 1.623453
S 0.000079 -1.687339 -1.669123
H 0.000372 -2.955635 -1.220275

E= -3789.863409
S 3.609541 1.767491 0.715161
Mo 1.783675 0.934982 -0.065855
S 0.355897 2.269250 -1.214833
Mo -1.177362 0.879160 -0.020688
S -3.445054 1.640106 -0.327418
S -2.657720 1.687666 1.611132
S 2.029705 -1.022322 -1.273432
Mo 0.115484 -1.441141 -0.072331
S -0.806567 -3.626086 -0.283631
S 0.093970 -3.162677 1.530271
S 0.410936 0.212224 1.673068
S -1.330276 -0.663222 -1.911161
H -2.482382 -1.304943 -1.633767

[Mo3S9H]- XX
E= -3789.859650
S 0.002715 3.829620 0.787944
Mo 0.001080 1.863244 -0.119319
S -1.838089 1.233892 -1.368351
Mo -1.419777 -0.581585 -0.010065
S -3.512908 -1.836195 -0.561010
S -3.027373 -1.423168 1.431378
S 1.838714 1.231975 -1.369430
Mo 1.418941 -0.583126 -0.010766
S 3.512370 -1.838007 -0.560164
S 3.024498 -1.426453 1.431935
S 0.000569 0.330065 1.573575
S -0.001273 -1.965895 -1.180680
H 0.002114 0.488316 2.923136

E= -3789.836563
S 0.000267 3.790655 1.029525
Mo -0.000202 2.117751 -0.303137
S -2.081986 1.356942 -1.025902
Mo -1.353595 -0.568603 -0.057848
S -3.240351 -2.038448 -0.609851
S -2.875682 -1.589583 1.390497
S 2.081958 1.357923 -1.025713
Mo 1.353905 -0.567946 -0.057765
S 3.241620 -2.037502 -0.609165
S 2.873186 -1.592002 1.391226
S -0.000031 -0.030564 1.909925
S 0.000737 -1.715710 -1.509898
H -0.000027 -1.237831 2.537207

[Mo3S9H]- XXI
E= -3789.891321
S 0.451710 3.622171 1.250355
Mo 0.214916 1.838148 0.047761
S -1.824104 1.627323 -1.023838
Mo -1.417143 -0.423885 -0.067542
S -3.675436 -1.456804 -0.428658
S -2.861957 -1.333154 1.496574
S 1.836426 1.325748 -1.505760
Mo 1.320912 -0.626019 -0.361279
S 3.551469 -1.380790 0.275201
S 2.149176 -2.786343 0.911248

S 0.217601 0.085186 1.564118
S -0.279577 -1.622552 -1.676096
H 1.970318 -2.398852 2.194230

E= -3789.871109
S -0.702743 3.687048 0.837903
Mo -0.268250 1.809222 -0.134497
S -2.017089 1.064339 -1.401509
Mo -1.376393 -0.685010 -0.030890
S -3.501380 -1.920920 -0.314215
S -2.669315 -1.728534 1.594872
S 1.686362 1.499253 -1.293534
Mo 1.475131 -0.550950 -0.079148
S 3.414062 -1.995053 -0.237107
S 3.839079 -0.380163 1.012182
S 0.080727 0.279436 1.620838
S 0.037880 -2.038959 -1.186124
H 4.438165 0.459857 0.137558

[Mo3S9H]- XXII
E= -3789.907605
S -0.222288 3.796565 0.803137
Mo -0.096808 1.832506 -0.101816
S -1.912355 1.173771 -1.364604
Mo -1.371825 -0.632524 -0.045957
S -3.424028 -2.013719 -0.496681
S -2.913430 -1.469146 1.459122
S 1.778097 1.332049 -1.368048
Mo 1.355031 -0.495202 -0.030709
S 3.682255 -1.719154 -0.436455
S 3.000144 -1.268601 1.487384
S -0.055753 0.330851 1.668319
S 0.085799 -1.972036 -1.242119
H 4.476217 -0.650061 -0.664609

E= -3789.872831
S 0.544073 3.803898 0.817678
Mo 0.212599 1.861735 -0.070420
S -1.592405 1.546112 -1.373521
Mo -1.547693 -0.486006 -0.052758
S -3.601466 -1.581855 -0.584245
S -3.275876 -1.178131 1.432013
S 2.069838 1.124994 -1.236160
Mo 1.248271 -0.657927 -0.036757
S 3.372549 -2.213097 -0.413360
S 2.658522 -1.780896 1.502383
S -0.097506 0.327174 1.683238
S -0.120529 -1.853172 -1.375224
H 4.331370 -1.268121 -0.527044

[Mo3S9H]- XXIII
E= -3789.876022
S -2.118958 3.092364 1.037470
Mo -0.929089 1.795409 -0.165082
S -2.298165 0.412497 -1.335111
Mo -0.974371 -0.989077 -0.060654
S -2.496215 -2.952230 -0.328739
S -1.793768 -2.406602 1.568587
S 1.396464 1.859402 -1.265840
Mo 1.651315 -0.004317 -0.118592
S 3.821054 -0.950473 -0.348118
S 3.404410 0.023654 1.452048
S 0.080089 0.408024 1.561346
S 0.713151 -1.771491 -1.345316
H -0.738899 2.873042 -1.479425

E= -3789.860336
S -0.000134 3.594753 1.109098
Mo -0.000150 1.891930 -0.245994
S -1.912386 1.207331 -1.371394
Mo -1.390679 -0.573663 -0.049445
S -3.391068 -1.961986 -0.396322
S -3.044797 -1.223771 1.500258
S 1.912059 1.207638 -1.371701
Mo 1.390863 -0.573349 -0.049587
S 3.391173 -1.962016 -0.396113
S 3.044784 -1.223471 1.500300
S 0.000102 0.206273 1.664996
S 0.000202 -1.988887 -1.237436
H -0.000406 3.019611 -1.535905

[Mo3S8H]- I

E= -3391.561593
Mo 1.483148 -0.127759 -0.054783
S 3.882915 -0.611722 -0.662875
S 3.575050 -0.590177 1.377296
H 3.836324 0.696958 1.718957
S 0.539584 -1.715792 -1.383221
S -0.027594 0.142852 1.807588
Mo -1.146323 -0.814008 -0.084343
S -2.902832 -1.934436 1.087045
S -3.225061 -1.517105 -0.937786
S -2.516084 2.681418 0.072497
Mo -0.645976 1.592339 0.064266
S 1.245771 1.793651 -1.271471

E= -3391.561593
Mo 1.483148 -0.127759 -0.054783
S 3.882915 -0.611722 -0.662875
S 3.575050 -0.590177 1.377296
H 3.836324 0.696958 1.718957
S 0.539584 -1.715792 -1.383221
S -0.027594 0.142852 1.807588
Mo -1.146323 -0.814008 -0.084343
S -2.902832 -1.934436 1.087045
S -3.225061 -1.517105 -0.937786
S -2.516084 2.681418 0.072497
Mo -0.645976 1.592339 0.064266
S 1.245771 1.793651 -1.271471

[Mo3S8H]- II
E= -3391.582510
S 0.646171 2.176961 2.269531
Mo 0.431693 1.606827 0.005196
S -1.474569 1.960842 -1.242706
Mo -1.412267 -0.136966 -0.351861
S -3.239787 -1.632512 0.248728
S -2.508644 -0.283749 1.672837
S 2.256843 1.180585 -1.283517
Mo 1.113995 -0.728818 -0.398241
S 3.079869 -1.763845 0.583808
S 1.226322 -2.065963 1.498491
S -0.359055 -1.577459 -1.920339
H 0.361890 0.958399 2.776718

E= -3391.571920
S 1.690834 1.992467 1.988776
Mo 0.732664 1.468327 -0.070108
S -1.427844 2.128228 -0.564715
Mo -1.781852 -0.115438 -0.142043
S -4.160800 -0.540566 -0.192057
S -3.118328 -0.721059 1.627536
S 2.133844 0.940845 -1.765759
Mo 1.157312 -0.784792 -0.397498
S 3.327906 -1.721921 0.129102
S 1.837542 -1.842285 1.581405
S -0.685250 -1.772381 -1.356191
H 1.892315 0.726679 2.435735

[Mo3S8H]- III
E= -3391.541956
S -0.686170 -1.195329 -1.979555
Mo 0.722947 -1.069217 0.048902
S 2.804706 -0.775905 1.295442
S 2.941429 -1.857423 -0.520313
Mo -1.621263 0.149958 -0.071214
S -3.761572 -0.566705 -0.846583
S -3.575850 -0.160465 1.179992
S -0.880659 2.256180 -0.276978
S -0.341071 -0.124955 1.963872
Mo 1.215289 1.108262 0.217376
S 2.670271 1.943361 -1.160203
H -0.050230 -0.238278 -2.683452

E= -3391.547697
S -0.692746 -1.296981 -1.852174
Mo 0.800517 -0.957075 0.047570
S 2.642488 -1.897793 1.252596
S 2.573505 -2.367534 -0.733300
Mo -1.616939 0.135891 -0.062429
S -3.696926 -0.893746 -0.448601
S -3.447547 -0.045502 1.430977
S -0.988670 2.095274 -1.017440
S -0.099391 0.361068 1.822494

Mo 1.083703 1.447991 -0.017667
S 3.018754 2.424872 -0.198961
H -0.177268 -0.400412 -2.723357

[Mo3S8H]- IV
E= -3391.558692
S 1.885545 2.140890 1.491416
Mo 1.164119 0.777923 -0.287638
S 3.117693 -0.725434 -0.090329
S 1.660792 -1.327283 -1.472226
Mo -0.073760 -1.394841 0.248655
S -2.493067 -1.296902 0.325141
S -1.803092 -1.312903 -1.636123
Mo -1.342706 0.826308 -0.171811
S -1.959966 2.109653 1.452472
S -0.095726 1.922087 -1.851998
S 0.309318 -2.204106 2.207908
H 0.654590 2.309589 2.033181

E= -3391.527109
S 2.598317 1.609715 1.465825
Mo 1.413591 0.523036 -0.271829
S 3.028387 -1.301562 -0.285200
S 1.298944 -1.661904 -1.413457
Mo -0.482561 -1.382754 0.230820
S -2.846800 -0.725760 0.252355
S -2.129936 -0.651800 -1.708922
Mo -1.202983 1.105571 -0.161332
S -1.401539 2.270346 1.640734
S 0.332490 1.980218 -1.699678
S -0.257322 -2.297742 2.155928
H 1.461417 2.129994 1.976928

[Mo3S8H]- V
E= -3391.641965
S -0.109235 0.081812 1.582698
Mo -1.204186 -1.196131 -0.073930
S -2.264971 0.301549 -1.450077
Mo -0.737996 1.481437 -0.208571
S -1.492729 3.317102 0.642695
S 1.182233 1.628696 -1.471601
Mo 1.672117 0.020155 0.104486
S 3.261214 0.761842 1.324588
S 2.353604 -2.155625 -0.511762
S 0.377705 -2.225655 -1.336410
S -2.452682 -2.405525 1.520824
H -2.339480 -1.696485 2.661324

E= -3391.621579
Mo 1.693082 0.739949 -0.108903
Mo -1.752154 0.456453 0.098149
Mo 0.179463 -1.586204 -0.203517
S 0.079402 0.066497 1.510401
S 2.076515 -1.087777 -1.433150
S 0.223057 -3.493303 0.796104
S -1.649900 -1.198754 -1.521695
S -3.610201 0.310974 1.152458
S -1.364882 2.764244 -0.352654
S 0.469963 2.307635 -1.281090
S 3.282982 1.308818 1.526332
H 2.832633 0.718359 2.652125

[Mo3S8H]- VI
E= -3391.628261
S 1.421566 -1.796183 -0.168091
Mo 2.790704 -0.007778 0.005014
S 4.899041 0.131913 -1.015354
Mo -0.106345 -0.062387 -0.021702
Mo -2.962995 0.097576 -0.020049
S -4.412347 -1.780612 0.046818
S 1.331136 1.724963 0.158701
S -1.547851 -0.259835 1.733583
S -1.521374 0.085062 -1.804307
S 4.883611 -0.062666 1.065074
S -3.988587 1.963940 0.128712
H -5.340380 -1.256584 -0.779210

E= -3391.631342
S -1.406362 -1.802595 0.117408
Mo -2.792357 -0.008872 -0.003841
S -4.902934 0.112167 1.029548
Mo 0.098824 -0.072979 0.016600

Mo 2.959121 0.093540 0.012208
S 4.453618 -1.749048 -0.017782
S -1.311676 1.720488 -0.114194
S 1.552458 -0.229775 -1.750407
S 1.530294 0.033544 1.801358
S -4.895527 -0.030460 -1.062199
S 3.940467 1.980762 -0.100972
H 5.479867 -1.052274 0.507226

[Mo3S8H]- VII
E= -3391.690448
S -1.354114 1.743835 0.002621
Mo -2.917113 0.000246 -0.000034
S -4.065937 0.030067 -1.812503
Mo -0.030159 -0.070199 -0.000301
S 1.412767 -0.112327 -1.789205
Mo 2.829528 0.083194 0.000152
S 3.732609 2.000082 0.003188
S -1.443873 -1.817431 -0.003345
S 1.412478 -0.117700 1.788695
S -4.063897 0.023294 1.813765
S 4.339973 -1.726504 -0.002690
H 5.425160 -0.929234 -0.000753

E= -3391.673388
S -1.439789 1.454007 -0.922124
Mo -3.015094 -0.015920 -0.002148
S -4.196030 -0.961050 -1.514190
Mo 0.057065 -0.003592 0.021759
S 1.481768 -0.990157 -1.457097
Mo 2.887189 0.084354 -0.019018
S 3.976059 1.652551 -0.971870
S -1.471385 -1.475797 0.946354
S 1.459905 0.918584 1.565466
S -4.229382 0.937869 1.477575
S 4.282385 -1.653062 0.785408
H 5.158756 -0.850480 1.422796

[Mo3S8H]- VIII
E= -3391.515765
S 2.045946 -0.271347 2.111576
Mo 2.767793 -0.665082 -0.129980
S 2.523406 -2.660142 -0.900813
Mo 0.641659 0.403676 0.442987
S -1.149840 -1.101360 0.043837
Mo -3.277019 -0.389191 -0.151681
S -3.818481 1.687709 -0.261338
S -0.143262 2.310682 -1.190796
S 0.848914 2.744610 0.582172
S 4.278224 0.645044 -0.933499
S -4.842808 -1.798154 0.173820
H -1.435806 2.412354 -0.775072

E= -3391.520538
S 1.984433 -0.324153 2.081457
Mo 2.816016 -0.624015 -0.120700
S 2.681155 -2.589266 -0.981972
Mo 0.614042 0.353351 0.368674
S -1.100084 -1.125697 -0.016603
Mo -3.287252 -0.393345 -0.096794
S -3.799382 1.680790 -0.405900
S -0.154761 2.341050 -1.156900
S 0.646355 2.662433 0.735586
S 4.300713 0.784600 -0.790992
S -4.840320 -1.831347 0.191507
H -1.487614 2.313844 -0.848519

[Mo3S8H]- IX
E= -3391.478668
Mo -1.109549 0.014058 0.021846
S 0.255307 -0.406534 -1.741839
Mo 1.744679 -0.054021 -0.029562
S 0.314774 0.357741 1.752066
S 2.635958 -2.091688 0.667912
S 3.607233 -1.427346 -1.044162
S 2.737651 2.044065 -0.738811
S 3.679441 1.397934 0.994021
H 2.983022 2.107882 1.912945
S -2.549038 -1.767014 0.502316
Mo -3.825291 0.011949 -0.046696
S -2.493592 1.834636 -0.368230

E= -3391.496346
Mo -1.093184 -0.011283 -0.001908
S 0.292238 -0.462829 -1.752414
Mo 1.751837 -0.056609 -0.035388
S 0.306005 0.405274 1.725246
S 2.665064 -2.061893 0.744282
S 3.624254 -1.440009 -0.994331
S 2.734998 2.045705 -0.758405
S 3.679289 1.438421 0.986826
H 2.967893 2.149960 1.892833
S -2.541815 -1.773389 0.426122
Mo -3.881251 0.036940 0.014145
S -2.486205 1.795595 -0.434858

[Mo3S8H]- X
E= -3391.600124
Mo -3.374743 -0.066423 -0.333896
S -4.959816 0.052358 1.111643
S -1.959612 1.701599 -0.477398
S -2.022844 -1.874875 -0.235416
Mo -0.557926 -0.086395 -0.134125
S 0.649962 0.047275 1.788487
Mo 2.279043 0.264275 0.142289
S 2.977405 2.283156 0.134243
S 1.072994 -0.273727 -1.747109
S 3.751452 -1.322830 1.109833
S 4.495092 -0.909716 -0.798403
H 5.378176 0.066948 -0.493368

E= -3391.606721
Mo -3.382935 -0.058127 -0.302809
S -5.045828 0.067473 1.059714
S -1.911460 1.694287 -0.302809
S -1.992612 -1.876227 -0.254899
Mo -0.548995 -0.102181 -0.148317
S 0.654467 -0.019019 1.782403
Mo 2.287437 0.266696 0.143404
S 2.943587 2.293633 0.183524
S 1.085762 -0.240681 -1.764097
S 3.763374 -1.320919 1.105798
S 4.484179 -0.883788 -0.804231
H 5.365141 0.095570 -0.500754

[Mo3S8H]- XI
E= -3391.628260
S 4.413052 -1.779896 -0.045651
Mo 2.962955 0.097704 0.020306
Mo 0.106257 -0.062597 0.021370
S -1.421340 1.796610 0.167627
Mo -2.790669 -0.008305 -0.005688
S -4.884780 -0.061782 -1.063814
S -4.897749 0.132544 1.016672
S 1.520873 0.086099 1.804207
S 3.988105 1.964218 -0.129335
S -1.331395 1.724590 -0.159486
S 1.548241 -0.261060 -1.733433
H 5.341048 -1.254977 0.779857

E= -3391.631341
S 4.453595 -1.749055 -0.017672
Mo 2.959121 0.093553 0.012251
Mo 0.098825 -0.072984 0.016506
S -1.406344 -1.802615 0.117288
Mo -2.792357 -0.008901 -0.003966
S -4.895762 -0.030436 -1.061923
S -4.902700 0.112226 1.029824
S 1.530210 0.033528 1.801331
S 3.940480 1.980774 -0.100854
S -1.311689 1.720466 -0.114346
S 1.552549 -0.229746 -1.750436
H 5.479828 -1.052304 0.507399

[Mo3S8H]- XII
E= -3391.471416
S -3.895217 -1.376301 -0.000613
Mo -2.052668 0.161637 -0.000154
S -0.661253 -1.299109 -1.658745
S -0.558047 0.730008 -1.817629
Mo 0.843693 -0.109814 0.000610
S -0.662276 -1.297838 1.660532
S -0.559001 0.731589 1.817844
S -3.142237 2.017789 -0.001266

S 2.016760 2.066681 -0.000213
Mo 3.192610 0.157496 -0.000473
S 2.459263 -1.961536 0.000176
H -3.280534 -2.571903 -0.000703

E= -3391.473716
S -4.003234 -1.259834 -0.000016
Mo -2.040432 0.141326 0.000014
S -0.621745 -1.330268 -1.676003
S -0.569598 0.718759 -1.801465
Mo 0.806504 -0.119135 -0.000026
S -0.621764 -1.330220 1.675987
S -0.569505 0.718801 1.801449
S -3.311586 1.931693 0.000059
S 2.032418 2.043266 -0.000085
Mo 3.271599 0.194162 0.000011
S 2.529387 -1.905625 0.000076
H -3.412111 -2.472009 0.000007

[Mo3S8H]- XIII
E= -3391.541441
S 0.701000 -1.251947 -1.334126
Mo 2.352373 -1.100964 0.177383
S 4.349978 -1.037551 -0.618824
S 1.871763 0.442277 1.679672
Mo -0.015453 0.484796 0.109695
S 1.178290 2.428352 -1.096871
S -0.122464 2.994256 0.395634
S -1.845622 0.778201 -1.624032
Mo -2.724734 -0.256012 0.090525
S -3.892307 -2.023893 -0.270168
S -1.369534 -0.190499 1.903580
H 2.350521 2.404447 -0.417196

E= -3391.541240
S 0.692504 -1.268254 -1.322932
Mo 2.347340 -1.103633 0.182178
S 4.336515 -1.023501 -0.631923
S 1.872804 0.442660 1.681368
Mo -0.016610 0.483890 0.110190
S 1.183688 2.417818 -1.099000
S -0.119755 2.994523 0.386983
S -1.842867 0.780287 -1.626825
Mo -2.722361 -0.250054 0.090604
S -3.872496 -2.028545 -0.273455
S -1.369528 -0.181539 1.906540
H 2.354635 2.396297 -0.416908

[Mo3S8H]- XIV
E= -3391.639395
S -3.370628 2.323020 0.310890
Mo -2.427070 0.207953 -0.116417
S -1.520074 -0.630989 1.765429
S 0.442274 -2.763530 -0.461680
Mo 0.227488 -0.767953 0.184961
S 2.389558 2.551343 -0.524254
S -0.703651 0.472233 -1.550368
S -3.931732 -1.069075 -0.900844
S 3.904920 -0.737403 -1.111312
Mo 2.642870 0.511488 0.080544
S 1.765767 -0.199883 2.033386
H -2.241043 2.906074 0.758330

E= -3391.668033
S -1.930030 2.818938 0.602749
Mo -2.035081 0.580427 -0.118182
S -1.904796 -0.968436 1.580822
S -0.149442 -3.388440 -0.604431
Mo -0.042004 -1.478966 0.329770
S 2.145761 2.489742 0.837352
S 0.017694 0.269617 -1.274150
S -3.741565 0.295665 -1.356584
S 3.684679 0.251100 -1.481905
Mo 2.066999 0.579147 -0.127595
S 1.941544 -1.117262 1.446836
H -0.597874 2.999730 0.461253

[Mo3S8H]- XV
E= -3391.616396
S 1.615858 0.392410 1.894032
Mo 2.515323 -0.474627 -0.151619
S 4.210487 0.711146 -0.683431

Mo -0.178587 0.684801 0.133307
S 0.062328 2.819501 0.339502
S -1.541656 -0.506479 1.725589
Mo -3.011802 -0.158506 0.078446
S -4.405298 -1.695441 -0.443788
S -2.079802 0.982195 -1.525309
S 0.875132 -0.236803 -1.727094
S 2.952574 -2.552603 0.108746
H 1.318834 -0.792875 2.462419

E= -3391.621444
S 1.489161 -0.091957 1.924340
Mo 2.674891 -0.371052 -0.129786
S 4.295918 1.015088 -0.187221
Mo -0.153827 0.565946 0.110254
S 0.038339 2.611579 0.625646
S -1.624704 -0.682198 1.581221
Mo -3.150543 -0.269402 -0.061318
S -5.232954 -0.810792 -0.124301
S -1.854509 0.590280 -1.686091
S 1.174364 0.063211 -1.778044
S 3.292941 -2.413283 -0.278253
H 1.181232 -1.381514 2.158971

[Mo3S8H]- XVI
E= -3391.669271
S -0.333912 -0.080003 1.610509
Mo 1.353547 0.014174 -0.043878
Mo -0.973128 -1.365510 -0.241246
Mo -1.088631 1.354220 -0.050662
S -2.303314 0.020334 -1.508095
S -1.864170 -2.973816 1.251950
H -2.258523 -3.819654 0.269872
S 0.914491 -1.774466 -1.462686
S 0.834165 1.941634 -1.185847
S -2.108923 2.954542 0.987069
S 3.836291 0.086568 -0.376910
S 3.025586 0.056365 1.548581

E= -3391.640100
S -0.125231 0.108487 1.669543
Mo 1.490639 -0.250925 -0.068935
Mo -1.310791 -1.145651 0.084397
Mo -0.714019 1.516956 -0.115386
S -2.346724 0.420611 -1.293731
S -3.253700 -2.444803 0.589574
H -4.141111 -2.068689 -0.350835
S 0.452947 -2.087034 -1.051130
S 1.201000 1.616759 -1.394478
S -1.349712 3.342797 0.855999
S 3.825125 -0.644801 -0.543273
S 3.257314 -0.498720 1.451725

[Mo3S8H]- XVII
E= -3391.643164
S -0.191600 0.110654 1.619665
Mo 1.443353 0.165825 -0.070781
Mo -0.929262 -1.426058 0.056782
Mo -1.218934 1.284683 -0.131809
S -2.365483 -0.307259 -1.343847
S -1.704205 -3.102032 1.177822
S 0.922543 -1.839351 -1.444149
S 0.639773 1.852844 -1.391744
S -2.420672 2.815053 0.810140
S 3.771967 -0.297347 -0.280100
S 3.172767 0.785444 1.395827
H 0.402014 -1.315020 -2.573890

E= -3391.618983
S -0.237961 0.066809 1.656623
Mo 1.445654 0.197448 -0.027144
Mo -0.825410 -1.470563 -0.007716
Mo -1.313176 1.256518 -0.062243
S -2.353372 -0.398493 -1.316444
S -1.416909 -3.272567 1.029186
S 1.062601 -1.703255 -1.510848
S 0.436436 1.933124 -1.344701
S -2.721634 2.630017 0.828683
S 3.824690 0.380990 -0.448709
S 3.193042 0.483250 1.526729
H 0.512850 -1.220928 -2.649996

[Mo3S8H]- XVIII
E= -3391.638961
S -0.308949 0.000194 1.635278
Mo 1.359861 -0.000352 -0.057966
Mo -1.015568 -1.428059 -0.040398
Mo -1.014913 1.428421 -0.040696
S -2.489601 0.000333 -1.361547
S -1.953139 -3.101689 0.948353
S 0.822801 -1.874620 -1.312924
S 0.823812 1.873974 -1.313089
S -1.951559 3.102669 0.947901
S 3.849156 -0.001248 -0.483585
S 3.087101 0.000359 1.465666
H -1.907914 0.000026 -2.576567

E= -3391.622250
S -0.209564 0.086539 1.670061
Mo 1.447872 0.266090 -0.089523
Mo -0.678954 -1.521425 0.016566
Mo -1.416537 1.196889 0.015813
S -2.254578 -0.488441 -1.506802
S -1.406739 -3.290492 1.020233
S 1.166139 -1.702879 -1.299892
S 0.435671 1.941209 -1.260490
S -2.930880 2.564332 0.723831
S 3.825036 0.359125 -0.483825
S 3.169801 0.711673 1.452096
H -1.518195 -0.442340 -2.643344

[Mo3S8H]- XIX
E= -3391.620550
S -0.321743 0.000127 1.516951
Mo 1.404486 0.000068 -0.011932
Mo -1.073795 -1.423257 -0.091561
Mo -1.073833 1.423260 -0.091713
S -2.316100 -0.000091 -1.434491
S -2.075964 -3.059209 0.914461
S 0.864985 -1.851533 -1.282780
S 0.864955 1.851513 -1.282952
S -2.075902 3.059137 0.914560
S 3.865769 -0.000227 -0.493489
S 3.172774 0.000120 1.480560
H -0.448395 0.000075 2.873596

E= -3391.599491
S -0.037961 0.360356 1.809185
Mo 1.454956 -0.081782 -0.063411
Mo -1.238957 -1.438456 -0.185912
Mo -1.016177 1.348849 -0.137121
S -2.484218 0.098637 -1.377913
S -2.316711 -2.641609 1.229936
S 0.825980 -2.092880 -1.005353
S 0.888158 1.720102 -1.395560
S -1.905161 3.079039 0.810233
S 3.808838 -0.159509 -0.607393
S 3.283388 -0.002542 1.401763
H 0.610417 1.412786 2.392279

[Mo3S8H]- XX
E= -3391.642699
S 0.402368 -0.089840 1.602253
Mo -1.205499 0.431791 -0.079013
Mo 1.556490 1.027914 -0.020065
Mo 0.414864 -1.838146 -0.129776
S 2.463355 -0.258347 -1.160209
S 2.785710 2.550142 0.868089
S -0.090439 1.993516 -1.327693
S -1.460203 -1.455684 -1.367049
S 0.126692 -3.561749 1.089634
S -3.527732 1.288796 -0.481838
S -2.781212 1.092064 1.468011
H 1.137448 -2.649497 -1.447319

E= -3391.626481
S 0.198836 0.142580 1.652605
Mo -1.407485 0.188659 -0.079055
Mo 1.294304 1.235749 -0.048090
Mo 0.863822 -1.566326 -0.181839
S 2.437271 -0.257052 -1.327168
S 2.535839 2.730519 0.877272
S -0.523252 1.970623 -1.280027
S -1.155717 -1.738290 -1.294204

S 1.417419 -3.080456 1.268258
S -3.796511 0.367488 -0.477880
S -3.167704 0.401729 1.481568
H 1.334133 -2.633705 -1.429433

[Mo3S8H]- XXI
E= -3391.650794
S -0.286848 -0.075922 1.623774
Mo 1.306898 0.225534 -0.083229
Mo -0.882430 -1.487013 -0.125363
Mo -1.260114 1.278264 0.015485
S -2.393827 -0.222067 -1.338699
S -1.562939 -3.327933 0.798909
S 1.010300 -1.550276 -1.468645
S 0.508903 2.043520 -1.258843
S -2.428173 2.731525 1.122409
S 3.704111 0.728192 -0.414864
S 3.419293 -0.273137 1.380026
H 3.563993 -1.567459 1.005425

E= -3391.632405
S -0.187243 -0.115276 1.596045
Mo 1.453331 0.163809 -0.086275
Mo -1.095103 -1.408245 -0.150026
Mo -1.134663 1.349225 0.007617
S -2.397475 0.025805 -1.392016
S -2.244334 -2.972708 0.790980
S 0.848332 -1.840918 -1.278305
S 0.670009 2.099292 -1.178139
S -2.239320 2.805832 1.167720
S 3.787748 0.751046 -0.183822
S 3.561998 -0.908840 1.065828
H 3.814817 -1.908832 0.192031

[Mo3S8H]- XXII
E= -3391.668664
S -0.353460 -0.001766 1.636863
Mo 1.314225 0.042980 -0.036820
Mo -1.028756 -1.420127 -0.074906
Mo -1.105599 1.376119 -0.076112
S -2.334710 -0.057692 -1.413592
S -1.997797 -3.091895 0.906755
S 0.892284 -1.832310 -1.307531
S 0.790119 1.892825 -1.305696
S -2.163274 2.994947 0.902754
S 3.957329 0.109716 -0.399612
S 3.099607 0.064270 1.509258
H 4.203873 -1.206327 -0.578005

E= -3391.634161
S 0.490397 0.016316 1.605783
Mo -1.267176 -0.086973 -0.036707
Mo 0.956067 1.622957 -0.066606
Mo 1.151658 -1.509394 -0.076953
S 2.494948 0.145202 -1.033398
S 1.672686 3.496272 0.727666
S -0.983970 1.763114 -1.353762
S -0.762504 -1.898616 -1.344864
S 2.085310 -3.272628 0.741342
S -3.917542 -0.231306 -0.365257
S -3.023865 -0.155568 1.529717
H -4.193494 1.078680 -0.544494

[Mo3S7H]- I
E= -2993.374353
Mo -0.282294 -0.054261 -0.180616
S -1.682841 1.764425 -0.365873
Mo -3.106154 0.001466 -0.289414
S -1.770921 -1.819196 -0.352821
S -4.618499 0.039078 1.232988
S 1.347151 -0.134039 -1.804701
S 4.124769 -1.679440 0.325047
H 3.234084 -2.686798 0.235758
S 0.964809 -0.049955 1.735044
Mo 2.569866 0.086697 0.105612
S 3.582179 1.958061 0.172179

E= -2993.307649
Mo -0.075526 0.659489 -0.142665
S -1.346758 0.201453 1.820321
Mo -2.822195 -0.201048 0.176070
S -1.905927 0.172629 -1.772158

S81

S -4.096260 -1.915947 0.345376
S 0.056876 2.730799 -0.727217
S 1.830752 1.064154 1.569958
H 1.548112 0.199806 2.569255
S 1.110903 -0.900197 -1.525354
Mo 2.739859 -0.446872 -0.037020
S 4.668044 -1.395749 0.137982

E= -2993.315280
Mo 0.004954 0.042737 0.422693
S 1.469076 1.639099 -0.618497
Mo 2.972912 -0.052791 -0.286580
S 1.610298 -1.785386 0.215452
S 5.123012 -0.014172 -0.451815
S -0.184892 0.350210 2.510263
S -1.676721 1.931463 -0.117803
H -1.329714 2.312408 -1.366234
S -1.419959 -1.760624 -0.388557
Mo -2.901589 -0.082965 -0.436893
S -5.037934 -0.260938 -0.274107

[Mo3S7H]- II
E= -2993.319941
S -1.588364 -1.084012 1.809758
Mo -2.435031 0.388021 0.035524
S -3.717375 -0.468799 -1.446511
S -2.538006 2.472406 0.511300
Mo 0.188198 -0.759785 0.056014
S 0.224192 -2.477369 -1.176962
S 0.761203 1.106652 -1.223087
Mo 2.519735 0.729315 0.121460
S 1.871003 -0.713848 1.717547
S 4.405324 0.362695 -0.830266
H -2.149494 -2.180737 1.265603

E= -2993.308992
S 1.652245 1.933684 -0.138023
Mo 2.880029 -0.071518 -0.502390
S 1.383588 -1.741079 -0.463574
S 5.000521 -0.277845 -0.223996
Mo 0.028688 0.047043 0.444667
S 0.271551 0.238638 2.530827
S -1.511698 1.685260 -0.481975
Mo -2.966136 -0.036370 -0.241996
S -1.634686 -1.774332 0.223596
S -5.088801 -0.050595 -0.574961
H 1.248073 2.335778 -1.362119

E= -2993.297068
S -1.431124 0.786137 1.090742
Mo -3.447217 -0.294979 0.073948
S -3.550439 -2.421470 -0.181705
S -5.149083 0.959184 -0.292816
Mo 0.754592 0.776036 -0.090021
S 0.929886 2.492808 -1.327022
S 2.235394 0.809749 1.677034
Mo 2.989762 -0.803548 0.256700
S 1.279738 -1.156362 -1.213884
S 4.978642 -0.619840 -0.515556
H -1.168011 -0.058638 2.104949

[Mo3S7H]- III
E= -2993.316042
S -0.918434 -0.421169 -1.918501
Mo 0.038819 0.790800 -0.048727
S 0.024018 2.913186 -0.091471
Mo -2.342510 -0.411090 -0.143366
S -3.817856 1.123443 0.063856
S -2.535765 -2.188012 1.040958
S 0.865385 -0.212493 1.917972
Mo 2.256384 -0.312477 0.121162
S 3.723550 1.206391 0.026070
S 2.696839 -2.427148 -0.797838
H 1.383083 -2.731009 -0.877675

E= -2993.353934
S -1.343244 -0.069451 -1.806304
Mo 0.207729 -0.003187 -0.178941
S -0.950818 0.039898 1.728697
Mo -2.669242 -0.007404 0.122549
S -3.805478 1.810940 0.220253
S -3.804857 -1.818932 0.285134

S 1.640406 -1.798521 -0.388265
Mo 3.114388 -0.048017 -0.253414
S 4.743337 -0.056007 1.141498
S 1.713401 1.900357 -0.271721
H 1.495321 2.329014 -1.536838

E= -2993.343410
S -1.252905 0.459639 -1.688536
Mo 0.258410 -0.066945 -0.000086
S -1.133833 -0.245676 1.803679
Mo -2.699556 -0.011224 0.070701
S -3.994662 1.660422 0.433264
S -3.788855 -1.826360 -0.244197
S 1.692168 -1.818971 -0.425888
Mo 3.121008 -0.016738 -0.231368
S 4.955325 -0.032694 0.888573
S 1.646414 1.905584 -0.250086
H 1.467365 2.354956 -1.517280

[Mo3S7H]- IV
E= -2993.299638
S -1.357287 -0.406559 2.068697
Mo -0.113593 -0.858227 0.001294
S -0.506329 -2.721083 -0.909171
Mo -2.282882 0.671026 0.305007
S -3.666868 -0.295198 -1.011830
S -1.728355 2.708633 -0.108470
S 0.917666 0.398815 -1.851446
Mo 2.631751 0.060223 -0.226125
S 3.909946 1.707460 0.259416
S 1.783743 -1.162038 1.442201
H 0.478129 1.652570 -1.597735

E= -2993.292513
S 1.106795 -0.102168 2.005958
Mo -0.092807 0.717718 0.279655
S -0.009931 2.782691 -0.143173
Mo 0.497433 -0.309696 0.061989
S 4.066153 1.081756 -0.237318
S 2.626051 -2.226765 -0.959638
S -0.728024 -0.411452 -1.821424
Mo -2.522022 -0.392356 -0.175925
S -4.112910 1.020390 -0.394549
S -2.630478 -2.005679 1.217999
H -0.151879 -1.618340 -1.645876

E= -2993.295252
S -1.313868 -0.833180 -0.381731
Mo 0.665729 0.387888 -0.437918
S 0.625803 2.483902 -0.771718
Mo -3.466867 -0.167520 0.036768
S -4.008825 1.782555 0.723823
S -4.985713 -1.676636 0.008615
S 1.428135 -0.016783 1.842444
Mo 3.156997 -0.644796 0.274384
S 5.111379 0.188558 0.564565
S 2.160241 -0.743332 -1.793385
H 0.779481 -1.135378 2.242405

[Mo3S7H]- V
E= -2993.284666
Mo -1.591363 -0.305527 0.052907
S -2.954232 -1.913626 -0.297845
S -2.547645 1.695011 0.881312
S -2.911355 1.633155 -1.167521
H -4.130087 1.044803 -1.184325
S 0.065613 -0.469511 -1.706457
S -0.515123 -0.685508 2.063595
Mo 1.056829 -1.071850 0.353759
S 3.361007 -1.144666 -0.372888
Mo 1.944219 0.737513 -0.460222
S 2.059443 2.499488 0.814410

E= -2993.265438
Mo 1.918476 -0.158036 -0.189184
S 3.099627 -1.718842 -1.038895
S 2.833147 2.027645 -0.223499
S 3.754085 1.005578 1.349775
H 4.855606 0.549466 0.713310
S 0.683070 -0.895600 1.635648
S 0.216137 0.371671 -1.709380
Mo -0.884840 -0.717676 -0.042563

S -2.960293 -1.844816 -0.094751
Mo -2.845311 0.432802 0.512709
S -3.173602 2.182661 -0.701008

E= -2993.246666
Mo -2.013751 -0.177029 0.126396
S -3.284036 -1.898356 0.300590
S -3.050821 1.882359 0.653120
S -3.772419 1.388191 -1.247981
H -4.906148 0.742381 -0.896891
S -0.582873 -0.320247 -1.684924
S -0.540705 -0.190058 1.909351
Mo 0.799053 -0.659947 0.108479
S 2.851256 -1.851754 -0.023794
Mo 3.249062 0.379116 -0.462158
S 3.346026 2.145349 0.746311

[Mo3S7H]- VI
E= -2993.288981
Mo -2.085850 0.508775 -0.234035
S -2.463163 -0.914260 1.768103
H -1.959751 -0.149998 2.756200
S -2.122201 -1.318402 -1.589549
S -1.668436 2.581005 -0.722836
Mo -0.391546 -0.885020 0.181563
S 1.043958 -0.481601 2.180194
S 1.255353 -0.713511 -1.685799
S 2.141814 2.398021 0.184103
Mo 2.003939 0.279770 0.324241
S 3.177983 -1.288629 -1.019871

E= -2993.284963
Mo -2.772729 0.030325 -0.301804
S -2.066271 -1.508213 1.461817
H -2.020103 -0.643649 2.494765
S -1.148901 0.032064 -1.912625
S -4.059037 1.707014 0.112273
Mo -0.131505 -0.719083 0.048442
S 0.617717 0.642456 1.783648
S 1.812017 -1.117236 -1.390814
S 3.201953 2.388328 -0.297805
Mo 2.322894 0.510846 0.272044
S 3.294798 -1.637165 0.038543

E= -2993.281700
Mo 2.903765 -0.009575 0.194005
S 1.298497 -0.997026 1.696383
H 1.370249 -0.292351 2.853569
S 1.811831 1.673455 -0.925901
S 4.391793 -1.257598 -0.739790
Mo 0.136164 0.439441 0.095432
S -0.757947 -1.382591 -1.110889
S -1.880383 2.051993 -0.465782
S -4.347929 -1.470270 0.127699
Mo -2.573674 -0.326352 -0.346430
S -1.825424 1.128586 1.389541

[Mo3S7H]- VII
E= -2993.406509
S 0.711972 -2.236056 1.084378
Mo 1.673050 -0.533814 -0.004194
S 3.611995 -0.730173 -0.909998
S 1.562327 1.326442 1.380879
Mo -0.342816 1.497437 0.092619
S -2.012020 0.643422 1.428148
Mo -1.385465 -1.124539 0.110069
S 0.088933 -0.055898 -1.583497
S -0.731143 3.389058 -0.873123
S -2.979373 -1.781384 -1.138249
H -1.723340 -2.128143 1.446624

E= -2993.312412
S -2.190049 -2.668609 0.009259
Mo -2.346540 -0.333015 0.008146
S -3.052807 0.537345 1.807132
S -2.996817 0.658664 -1.750098
Mo 0.192634 0.757752 0.003242
S 1.206395 -0.299557 -1.774308
Mo 2.545319 -0.703603 0.031969
S 1.283211 -0.095948 1.839410
S 0.241135 2.885062 -0.111677
S 4.608077 -0.113326 -0.050663

H -2.025673 -2.745737 -1.325896

E= -2993.271926
S -2.070846 -2.487563 -1.121072
Mo -2.290020 -0.421123 0.001379
S -3.080041 -0.477707 1.988701
S -2.168440 1.648717 -1.131185
Mo 0.069596 0.636707 0.038641
S 1.187163 -0.265309 -1.742551
Mo 2.612508 -0.570429 0.070612
S 1.208808 -0.048816 1.876552
S -0.600620 2.809534 -0.170906
S 4.705119 -0.068729 0.074250
H -3.365792 -2.858550 -1.027190

[Mo3S7H]- VIII
E= -2993.327764
Mo -2.612792 -0.401245 0.348605
S -0.772901 -0.817636 1.659939
Mo 0.058011 0.558074 0.040159
Mo 2.743785 -0.109211 -0.297238
S 4.013960 -1.742147 0.275396
S 1.995507 1.263291 1.285884
S 1.056997 -0.580956 -1.727074
S -1.043621 2.649585 -0.048533
S -1.919637 1.176438 -1.269918
S -3.586132 -2.107817 -0.483038
H -3.844944 0.547877 1.073400

E= -2993.331212
Mo 2.584278 -0.315462 -0.390432
S 0.749373 -1.386724 -1.127801
Mo -0.118583 0.387672 0.070359
Mo -2.910834 0.011452 0.186415
S -4.438714 -1.363320 -0.469982
S -1.717206 1.431503 -1.209743
S -1.338173 -0.439745 1.832023
S 1.808544 1.079587 1.404270
S 1.833204 2.060147 -0.407374
S 4.067945 -1.613902 0.446473
H 3.256277 0.205491 -1.872223

E= -2993.312185
Mo 2.883738 -0.112483 -0.460708
S 1.403423 -1.782790 -0.286991
Mo -0.017094 0.054124 0.443124
Mo -2.965741 -0.054460 -0.292133
S -5.107229 -0.028089 -0.552309
S -1.459640 1.621955 -0.647271
S -1.629001 -1.762987 0.325437
S 0.197990 0.436713 2.521496
S 1.697195 1.950516 -0.249870
S 5.025038 -0.281393 -0.359342
H 2.117681 2.275562 0.989737

[Mo3S7H]- IX
E= -2993.326723
S 1.489660 -1.144750 1.650383
Mo 2.654866 -0.013518 0.022141
S 3.861634 -1.256550 -1.222243
S 2.328317 2.335789 -0.093321
Mo -0.174363 -0.139677 0.433364
S -1.866788 1.026541 1.538979
Mo -2.964648 -0.299983 0.075761
S -1.391675 -1.622604 -0.863675
S 0.936761 1.184252 -1.183865
S -4.321116 0.636473 -1.297307
H 3.745427 0.487077 1.223636

E= -2993.334012
S 1.728691 1.894524 -0.714295
Mo 2.640886 -0.126386 0.190640
S 4.735347 -0.122044 0.709765
S 1.644440 -1.487026 -1.254710
Mo -0.176632 0.026412 -0.263461
S -1.576356 -1.829836 -0.472691
Mo -2.986507 -0.051873 -0.157131
S -1.662648 1.776438 -0.631607
S 0.934778 0.063831 1.788474
S -4.560083 -0.004721 1.304773
H 2.027883 1.718917 -2.017382

E= -2993.335907
S 1.639401 1.816075 -0.862217
Mo 2.703590 -0.147987 0.013432
S 4.862914 -0.039808 0.039447
S 1.463585 -1.552426 -1.200862
Mo -0.128197 0.031616 -0.017220
S -1.609994 -1.786246 0.189191
Mo -3.008799 -0.010015 0.274689
S -1.677740 1.808859 0.051574
S 1.296662 0.065383 1.865954
S -4.944036 -0.076684 -0.657857
H 1.710406 1.545781 -2.181500

[Mo3S7H]- X
E= -2993.355831
S -1.348626 -0.013805 -1.901607
Mo 0.283901 -0.062466 -0.125167
S 1.774479 -1.824761 -0.325282
S 1.653912 1.766868 -0.463905
Mo 3.085572 0.018567 -0.299433
S 4.547007 0.105412 1.263948
S -0.948644 0.025280 1.767002
S -3.772222 -1.788087 0.307803
H -1.483318 -1.317412 -2.225937
Mo -2.636099 0.025322 0.154402
S -3.738307 1.860196 0.200433

E= -2993.281643
S -1.311070 -0.940612 1.830239
Mo 0.126326 0.215097 0.277129
S 1.897404 1.535816 1.024171
S 1.259753 -1.619831 -0.586110
Mo 2.959461 -0.252063 0.065455
S 4.893742 -0.186438 -0.888246
S -1.160186 0.931912 -1.520319
S -2.414148 2.192191 -0.307216
H -1.579476 -0.065766 2.835680
Mo -2.667472 -0.123833 0.024348
S -4.164855 -1.486828 -0.692944

E= -2993.325747
S -1.586555 -1.168852 -1.529965
Mo 0.418474 -0.042951 -0.290189
S 1.906409 -1.773830 -0.565484
S 1.771729 1.827805 -0.360829
Mo 3.205005 0.063463 -0.196997
S 4.635996 0.005250 1.402621
S -0.956163 -0.071062 1.563852
S -4.571856 -0.964195 0.952008
H -1.511457 -2.340795 -0.873597
Mo -2.857692 0.074618 0.188855
S -3.115284 2.041466 -0.624484

[Mo3S7H]- XI
E= -2993.263747
S 0.289166 -0.885331 -1.661012
Mo -1.079433 -0.990889 0.403783
S -3.243871 0.501092 0.728647
S -3.083863 -0.447083 -1.134889
Mo -0.979078 0.884433 -0.500662
S 2.391089 2.041855 -0.293417
S 0.644964 2.018255 0.905267
Mo 1.551644 -0.167714 0.153854
S 0.627942 -1.117315 2.064353
S 3.433091 -1.334075 -0.767066
H 4.352136 -0.923231 0.132988

E= -2993.321862
S -0.129973 0.229646 1.706025
Mo -0.975921 1.232635 -0.303472
S -3.326098 -1.810829 0.543228
S -2.730082 2.456938 -0.292225
Mo -1.320025 -1.145913 0.179768
S 3.366415 -1.467993 -0.495676
S 0.179453 -2.211385 -0.995461
Mo 1.769097 -0.129295 0.021184
S 0.856843 1.347066 -1.629926
S 2.916371 1.464367 1.394279
H 4.000799 1.663141 0.621941

E= -2993.284251
S -0.003395 -0.126639 1.751930
S -0.877081 0.987585 1.878299

Mo 1.131020 -1.294713 -0.018473
S 2.986691 2.265759 0.106446
S 3.109244 -2.125080 0.025223
Mo 1.143618 1.146490 0.051677
S -2.220063 2.239526 0.063207
S -0.728242 1.682977 -1.341730
Mo -1.697435 -0.129474 0.020380
S -0.615916 -1.976811 -1.269607
S -3.766109 -1.216187 0.455894
H -4.437875 -0.233411 1.087674

[Mo3S7H]- XII
E= -2993.312622
S 0.151787 0.254897 -1.786550
Mo 1.634480 0.300823 0.061909
S 1.812943 -2.013985 0.653493
S 3.506364 1.175707 -0.607811
Mo -0.197791 -1.618369 -0.382282
S -2.700745 -0.977302 -0.662041
S -1.933332 -1.204699 1.264318
Mo -1.137892 0.835193 0.101603
S 0.456018 1.283553 1.922751
S -2.088922 2.730255 -0.384986
H 0.184719 0.283986 2.801575

E= -2993.293795
S 0.097867 -0.233557 -1.770320
Mo -1.307346 -1.120831 0.004476
S -2.738603 2.197973 -0.196046
S -3.338283 -1.858933 -0.003665
Mo -0.799917 1.271474 -0.067385
S 1.621571 2.152327 0.026042
S 0.831866 1.246885 1.726737
Mo 1.769597 -0.266546 -0.039403
S 0.634986 -2.245627 1.015918
S 3.740942 -0.838344 -0.674443
H 0.576437 -1.863618 2.309545

E= -2993.264942
S 0.091581 -0.115727 -1.751885
Mo -1.085414 -1.256374 0.034926
S -3.096517 2.155333 -0.199521
S -2.979844 -2.286226 -0.008470
Mo -1.188522 1.147362 -0.126655
S 2.441174 2.065518 0.114086
S 0.630959 1.868082 1.227503
Mo 1.773988 -0.180392 -0.064282
S 0.700264 -1.642594 1.651403
S 3.501642 -1.240051 -0.784750
H 0.369641 -0.714356 2.578585

[Mo3S7H]- XIII
E= -2993.262237
S -0.877081 0.987585 1.878299
Mo -1.827030 -0.288860 0.012455
S -0.879221 -2.215196 -0.957676
S -3.805464 -0.658557 0.784019
Mo 1.130884 -1.167953 -0.416534
S 2.829721 -0.736034 1.337547
S 3.326753 0.055730 -0.534016
Mo 1.072822 0.877998 0.365142
S 0.209772 2.525979 -1.101606
S -1.714320 1.419715 -1.400878
H -1.262944 2.242676 1.544341

E= -2993.229556
S -0.251473 -0.706782 -1.901422
Mo -1.603608 0.044509 -0.037095
S -1.336491 2.328495 0.505792
S -3.549817 -0.303499 -0.944191
Mo 0.780307 1.566674 -0.150920
S 3.137324 -1.110987 -0.931338
S 3.076599 0.533572 0.419749
Mo 1.004127 -0.736165 0.192507
S -0.543559 -0.652908 2.108781
S -0.960973 -2.262162 0.863408
H -0.740484 -1.962426 -2.121096

E= -2993.168371
S 0.164188 0.803966 2.175390
Mo -1.390392 0.725082 0.222687
S -2.426563 -1.190290 -0.958048

S -2.241861 -1.485455 1.095744
Mo -0.028805 -1.551117 -0.175113
S 3.241841 -0.376878 0.731945
S 2.393073 -1.433262 -0.912652
Mo 1.143109 0.517579 -0.101874
S -0.333530 1.507381 -1.856078
S -0.090907 2.851714 -0.288267
H 0.295817 2.120333 2.472085

[Mo3S7H]- XIV
E= -2993.287450
S -0.202117 -0.182765 -1.847838
Mo 0.830588 1.222175 -0.288948
S 1.808962 0.210949 1.624907
S 2.840482 -0.076257 -1.050083
Mo 0.971203 -1.358408 -0.218902
S -3.421024 -0.732860 -0.531616
S -0.555096 -1.977275 1.367547
Mo -1.459786 -0.097984 0.126593
S -0.071804 1.244663 1.896794
S -1.361442 2.294412 -0.373085
H 1.028389 -2.656164 -1.373228

E= -2993.273257
S -0.030285 0.112117 -1.740616
Mo -1.711785 -0.036256 -0.090884
S -1.316509 2.137881 0.817947
S -3.673640 -0.209491 -0.975276
Mo 0.803645 1.612398 -0.008781
S 3.094456 -1.344515 -0.920259
S 3.131974 0.416005 0.264828
Mo 1.036332 -0.742193 0.227913
S -0.716268 -1.101161 1.906853
S -0.939960 -2.382603 0.271172
H 1.819621 2.922389 0.619176

E= -2993.328299
S 0.000215 -0.256838 1.398997
Mo 1.920671 -0.388017 0.053152
S 1.962339 1.684860 -1.017749
S 3.672678 -0.878971 1.188582
Mo -0.001091 1.786962 0.146264
S -3.671752 -0.878886 1.189315
S -1.963607 1.682667 -1.019059
Mo -1.919937 -0.389210 0.053137
S -1.103049 -2.110160 -1.222157
S 1.104288 -2.108279 -1.222794
H -0.002792 3.440827 0.670602

[Mo3S7H]- XV
E= -2993.361694
S -3.707602 -0.651223 0.479201
Mo -1.701375 -0.209609 -0.194447
S -0.387270 -0.152465 1.757396
S -1.315527 1.918910 -1.079528
Mo 1.070733 -0.968134 -0.176901
S 2.651395 -0.458387 -1.500804
S 2.163333 2.691088 0.227217
Mo 0.328089 1.581622 0.452579
S -0.633273 -1.691818 -1.572578
S 1.851932 -2.520594 1.436706
H 2.739417 -3.131081 0.626512

E= -2993.335819
S -3.333853 1.383235 -0.657204
Mo -1.600214 0.344789 0.136695
S -0.114788 0.411166 -1.703298
S -1.941067 -1.944496 0.530863
Mo 1.098623 0.750653 0.277306
S 1.678453 -1.442628 1.275662
S 2.654805 -1.139021 -0.530835
Mo 0.109410 -1.603631 -0.528194
S -0.458149 1.268492 1.931073
S 2.448718 2.586116 -0.480250
H 1.525711 3.378129 -1.060063

E= -2993.271881
S -4.087985 -0.535413 -0.003343
Mo -2.024675 0.152306 0.004354
S -0.564862 -0.743536 -1.605024
S -0.557244 -0.736775 1.611599
Mo 0.717761 0.780860 -0.001737

S 2.684138 -0.440672 1.031724
S 2.676130 -0.441090 -1.042416
Mo 0.918645 -1.848326 0.001415
S -1.252002 2.274336 -0.008377
S 2.049445 2.789050 0.005107
H 1.145363 3.782298 0.002321

[Mo3S7H]- XVI
E= -2993.301095
S -3.158872 -1.443449 -0.784164
Mo -1.320278 -0.541046 -0.007672
S -2.196800 1.669174 0.783589
S 0.103018 -0.112862 -1.840177
Mo 1.484025 -0.321320 0.082833
S 3.390879 -0.928850 -0.768285
S 1.610637 1.891874 0.996669
Mo -0.127326 1.746860 -0.458884
S 0.250388 -2.472607 0.508720
S 0.013533 -1.031853 1.982291
H -1.734219 1.708436 2.058101

E= -2993.169897
S 3.751233 -1.462534 -0.102238
Mo 1.945408 -0.255430 -0.004436
S 0.177358 -1.109000 1.402250
S 0.054543 -0.924299 -1.483972
Mo -0.532968 0.876740 0.024868
S -2.865277 0.753466 -1.041886
S -2.827888 0.666687 1.042924
Mo -1.889683 -1.311123 -0.029675
S 1.470861 1.962672 -1.018038
S 1.485135 1.968156 1.056485
H 0.108783 -0.710636 2.699814

E= -2993.184201
S 3.767423 -1.438288 -0.051865
Mo 1.941761 -0.259583 0.010554
S 0.194628 -0.256838 1.468252
S 0.074395 -0.996283 -1.472532
Mo -0.528725 0.873679 0.006195
S -2.845832 0.710069 -1.028460
S -2.857594 0.757410 1.069400
Mo -1.908940 -1.321963 -0.037614
S 1.458515 1.917483 -1.086504
S 1.503982 1.995271 0.985534
H 0.099733 -0.571009 2.735169

[Mo3S7H]- XVII
E= -2993.232598
S 3.518429 -1.687765 -0.000457
Mo 1.838823 -0.308450 0.008966
S 0.052277 -0.780308 1.562827
S 0.036065 -0.801084 -1.541851
Mo -0.516535 0.988397 -0.009925
S -2.821487 0.630454 -1.035577
S -2.790391 0.694180 1.040003
Mo -1.728104 -1.352212 0.009554
S 1.583258 1.937912 -1.052019
S 1.572729 1.963266 1.014049
H -1.369791 -3.071343 -0.152589

E= -2993.250051
S 3.511689 -1.030154 -0.446561
Mo 1.634562 -0.000264 -0.089032
S 0.356113 -0.383781 1.753615
S -0.047801 -0.359765 -1.752981
Mo -0.849736 0.810085 0.243679
S -2.984565 1.377683 -0.648738
S -2.855569 -0.567915 0.311936
Mo -0.738584 -1.829352 -0.061897
S 0.932488 2.341566 -0.750638
S 1.068692 2.005777 1.268278
H -1.638920 -3.314295 0.345899

E= -2993.273618
S -3.645374 -1.183918 -0.001173
Mo -1.731809 -0.179401 0.000312
S -0.044926 -0.864199 -1.586090
S -0.044938 -0.864944 1.586328
Mo 0.835203 0.934850 0.000198
S 2.069986 2.777288 -0.001385
S 2.942637 -0.438508 0.000606

Mo 1.281230 -1.964906 -0.000244
S -1.192233 1.990424 1.027539
S -1.192398 1.990586 -1.026408
H 1.561743 -3.710495 -0.001865

[Mo3S7H]- XVIII
E= -2993.229121
S 3.305828 -1.718255 -0.000253
Mo 1.642951 -0.318686 0.000113
S 0.063913 -0.609421 1.742893
S 0.063913 -0.609302 -1.742684
Mo -0.631919 1.077983 -0.000131
S -2.842776 0.260193 -1.036023
S -2.842771 0.260670 1.035903
Mo -1.279516 -1.393495 0.000082
S 1.517967 1.955268 -1.028079
S 1.517687 1.955560 1.028198
H -1.263887 2.720917 -0.001956

E= -2993.243467
S 3.503603 -1.648826 -0.000337
Mo 1.799207 -0.299736 -0.000116
S 0.101711 -0.758756 1.626749
S 0.101091 -0.756540 -1.626986
Mo -0.584302 1.003238 -0.000009
S -2.855655 0.471833 -1.042809
S -2.854023 0.472761 1.043186
Mo -1.587186 -1.401724 -0.000210
S 1.527258 1.943919 -1.031038
S 1.524884 1.942756 1.032127
H -1.146152 2.650952 -0.000190

E= -2993.241556
S 3.597265 -1.581293 -0.001026
Mo 1.853110 -0.286241 0.000069
S 0.116045 -0.849380 1.572465
S 0.115614 -0.849086 -1.571854
Mo -0.574415 0.973353 0.000302
S -2.857936 0.544674 -1.045087
S -2.858261 0.544605 1.043981
Mo -1.686246 -1.393446 0.000217
S 1.512854 1.940326 -1.033053
S 1.514028 1.940469 1.033039
H -1.116605 2.620984 -0.000098

[Mo3S7H]- XIX
E= -2993.429715
S 3.059926 -1.657105 1.059582
Mo 1.412082 -0.779045 -0.031926
S 0.022143 -2.201655 -1.216232
Mo -1.395845 -0.806590 -0.032377
S -0.001272 0.113793 1.582655
Mo -0.015258 1.558792 -0.264038
S -1.867802 0.945742 -1.482198
S -0.037485 3.422418 1.188744
S -3.025250 -1.718854 1.058404
S 1.849275 0.981587 -1.482180
H -0.033685 2.952585 2.449957

E= -2993.397813
S 3.075091 -1.939810 -0.864951
Mo 1.368497 -1.041442 0.092973
S 1.899735 0.666085 1.541700
Mo 0.320153 1.524075 0.098821
S 0.138212 -0.015636 -1.651765
Mo -1.547062 -0.607980 -0.133588
S -1.724419 1.339926 1.139628
S -3.882308 -0.868365 -0.544160
S 0.790850 3.430776 -0.810017
S -0.389181 -2.276494 1.011422
H -4.474370 -0.119134 0.405656

E= -2993.379117
S 2.256990 -2.844449 -0.875470
Mo 0.992738 -1.383177 0.059299
S 2.037490 0.000568 1.558940
Mo 0.991923 1.383644 0.059288
S -0.106309 -0.000128 -1.529854
Mo -1.894812 -0.000602 0.050205
S -1.120396 1.990446 0.970754
S -4.142824 -0.000256 -0.694493
S 2.255485 2.845551 -0.875349

S -1.119084 -1.991410 0.970589
H -4.755302 0.000513 0.508897

[Mo3S7H]- XX
E= -2993.399589
S 3.103258 -1.648554 -1.039126
Mo 1.446468 -0.771013 0.032086
S 1.850604 1.035834 1.375983
Mo -0.006608 1.614623 0.100501
S 0.000316 0.010109 -1.595086
Mo -1.439555 -0.783027 0.032021
S -1.859936 1.020408 1.375115
S -3.090105 -1.672642 -1.038769
S -0.014920 3.511235 -0.947920
S 0.009590 -2.304568 1.280313
H 0.006312 -1.773628 2.518287

E= -2993.378082
S -0.184034 3.493744 -0.945832
Mo -0.124525 1.557216 0.001465
S -1.786402 0.945292 1.450478
Mo -1.472608 -0.888055 0.069429
S -0.047562 -0.087913 -1.642175
Mo 1.546640 -0.762862 -0.051280
S 0.068305 -2.204935 1.154372
S 3.443318 -1.438859 -0.828795
S -3.260789 -1.661937 -0.845091
S 1.728707 1.090201 1.546215
H 2.735991 1.765959 0.949460

E= -2993.366251
S 2.826921 -2.432928 -0.771339
Mo 1.227843 -1.260415 0.043447
S 1.844298 0.252942 1.660086
Mo 0.727506 1.474029 0.070115
S -0.083947 -0.074355 -1.550231
Mo -1.986543 -0.175782 -0.020011
S -1.367344 1.931914 0.913309
S -4.067513 -0.355278 -0.535614
S 1.878551 3.042979 -0.831995
S -0.873901 -2.275905 0.882428
H -1.202837 -3.017226 -0.195464

[Mo3S7H]- XXI
E= -2993.382300
S -0.801424 3.434090 1.017373
Mo -0.376931 1.614579 -0.079582
S 1.556868 1.459178 -1.356789
Mo 1.587234 -0.481124 -0.079192
S 0.000557 -0.000356 1.466916
Mo -1.210273 -1.133673 -0.079397
S 0.484709 -2.079155 -1.355980
S -2.575501 -2.409330 1.017662
S 3.376304 -1.022720 1.016470
S -2.041651 0.618873 -1.357726
H 0.000949 -0.000102 2.836349

E= -2993.348830
S -2.167838 -2.797904 0.892745
Mo -0.911535 -1.374223 -0.145774
S -2.009527 0.002197 -1.631741
Mo -0.907611 1.375834 -0.145964
S -0.089589 -0.000227 1.539446
Mo 1.884838 -0.001910 0.155580
S 1.131128 2.006751 -0.939845
S 4.032846 -0.003987 0.367092
S -2.159333 2.802992 0.893123
S 1.126345 -2.009170 -0.939465
H -0.583558 0.002104 2.816967

E= -2993.335833
S 1.844786 3.053018 0.796540
Mo 0.703677 1.452493 -0.078959
S 1.806689 0.269669 -1.697110
Mo 1.195965 -1.254341 -0.093746
S 0.280459 -0.040679 1.804258
Mo -2.075143 -0.226776 -0.133389
S -0.900015 -2.160009 -0.722892
S -4.001635 -0.427906 0.764502
S 2.780550 -2.531088 0.607213
S -1.437099 1.897632 -0.907440
H 1.391287 0.232026 2.534792

[Mo3S7H]- XXII
E= -2993.396282
S -1.285729 3.251046 -1.051749
Mo -0.544417 1.533782 0.034606
S -2.114732 0.320899 1.492407
Mo -0.975996 -1.302671 0.034115
S 0.009963 -0.001559 -1.598203
Mo 1.609595 -0.244419 0.087545
S 0.756089 -1.998760 1.360082
S 3.478431 -0.528082 -0.970428
S -2.192827 -2.724269 -1.051048
S 1.318248 1.684712 1.358915
H -3.256732 0.495099 0.797206

E= -2993.378081
S 3.443518 -1.437499 -0.830026
Mo 1.546854 -0.763158 -0.050952
S 1.728412 1.089087 1.547676
Mo -0.123678 1.556959 0.001475
S -0.047447 -0.088367 -1.641936
Mo -1.473022 -0.887055 0.069365
S -1.785690 0.945479 1.450838
S -3.261627 -1.660444 -0.845085
S -0.184628 3.492987 -0.946602
S 0.067228 -2.205468 1.153399
H 2.737267 1.763751 0.952467

E= -2993.366250
S -2.825752 -2.434846 -0.770431
Mo -1.227148 -1.260951 0.043356
S 0.875171 -2.275656 0.881504
Mo 1.986756 -0.174772 -0.020390
S 0.083452 -0.073763 -1.550290
Mo -0.728480 1.473943 0.070106
S 1.366271 1.932654 0.912801
S -1.880031 3.042685 -0.831554
S 4.068134 -0.354727 -0.534174
S -1.844217 0.251841 1.660136
H 1.204183 -3.016261 -0.196923

[Mo3S7H]- XXIII
E= -2993.388384
S -2.548837 2.871865 -0.138437
Mo -0.997810 1.397786 -0.004696
S -1.195201 0.000325 1.797231
Mo -0.998188 -1.397698 -0.004510
S -0.934466 -0.000136 -1.818065
Mo 2.176224 0.000059 0.142852
S 1.191563 -2.095751 0.113157
S 4.212665 -0.000737 -0.390874
S -2.549254 -2.871765 -0.138063
S 1.192019 2.095892 0.113515
H 2.534701 -0.001231 1.771445

E= -2993.392174
S -2.448281 2.649548 -0.767196
Mo -0.943060 1.386461 0.086409
S -1.712350 0.000721 1.762725
Mo -0.944249 -1.386052 0.086335
S 0.017578 -0.000209 -1.556645
Mo 1.982445 -0.000908 0.073494
S 1.094541 -2.233056 0.546359
S 4.022922 -0.000211 -0.520863
S -2.451513 -2.646687 -0.767257
S 1.096356 2.231271 0.546913
H 2.096252 -0.001114 1.753441

E= -2993.369831
S 2.053799 3.202857 0.756656
Mo 0.979598 1.524971 -0.029341
S 2.061018 0.004891 -1.433943
Mo 0.986871 -1.520862 -0.029702
S 0.027951 0.000064 1.520915
Mo -1.965707 -0.004634 -0.143597
S -1.083364 -2.107099 -0.856168
S -3.883673 -0.006460 0.754365
S 2.068137 -3.193776 0.757322
S -1.093246 2.101326 -0.856891
H -2.441964 -0.006817 -1.765223

[Mo3S7H]- XXIV

E= -2993.393856
S -3.838686 -0.001760 -0.602749
Mo -1.740337 -0.000812 -0.108175
S -1.117724 -1.851109 1.178954
Mo 0.843142 -1.437219 0.051686
S 0.320986 0.000023 -1.630975
Mo 0.841567 1.438015 0.051656
S 1.969905 0.001023 1.475204
S 2.018778 3.061482 -0.737079
S 2.022233 -3.059281 -0.737123
S -1.119775 1.849672 1.179175
H -1.755117 -0.000106 -1.803540

E= -2993.393856
S 4.007060 -0.000421 0.426311
Mo 1.994121 -0.000271 -0.278467
S 1.164887 2.233456 0.221770
Mo -0.915361 1.390563 0.089428
S -0.476544 0.000094 -1.715722
Mo -0.915752 -1.390523 0.089234
S -1.343187 -0.000043 1.874951
S -2.548500 -2.714490 -0.324132
S -2.547107 2.715675 -0.323907
S 1.164396 -2.233777 0.221964
H 2.417574 0.001813 -1.907949

E= -2993.367038
S -4.083097 -0.000522 -0.103745
Mo -1.976123 -0.000376 0.224654
S -1.172728 2.049485 -0.646493
Mo 0.988260 1.504628 -0.069646
S 0.374625 0.000294 1.627556
Mo 0.988900 -1.504307 -0.069536
S 1.862652 0.000417 -1.612474
S 2.165621 -3.194914 0.519259
S 2.164410 3.195555 0.519708
S -1.171963 -2.050194 -0.645800
H -2.275905 0.000385 1.882011

[Mo3S7H]- XXV
E= -2993.408591
S -1.702690 1.788080 -0.322771
Mo -3.084047 0.000033 -0.305700
S -4.425995 0.001085 1.343476
Mo -0.227620 -0.000568 -0.179631
Mo 2.646736 0.000191 0.117364
S 3.783659 1.816223 0.229244
S -1.703489 -1.788717 -0.321897
S 1.308905 -0.000246 -1.807992
S 0.945524 -0.000525 1.730207
S 3.784926 -1.815078 0.229269
H -3.926297 0.001351 -1.817960

E= -2993.398519
S -1.719235 1.792879 -0.302390
Mo -3.125495 0.000279 -0.285066
S -4.638857 0.001534 1.219944
Mo -0.309063 -0.000972 -0.142528
Mo 2.726670 0.000263 0.100086
S 3.915158 1.774310 0.203533
S -1.720990 -1.793687 -0.301141
S 1.327558 -0.001391 -1.770359
S 1.022145 0.000191 1.718127
S 3.916642 -1.772681 0.205376
H -3.907435 -0.000394 -1.814114

[Mo3S13H3]+ I
E= -5383.560805
S 0.211180 -0.321443 -1.257971
Mo 2.391557 -0.054671 -0.167998
Mo -1.446917 -1.313925 0.260750
Mo -1.058776 1.431730 -0.075771
S -2.099255 0.478388 1.653113
S -2.479226 0.279526 -1.793287
S 1.156545 2.036776 0.347134
S 3.920975 1.244779 -1.275424
S -0.092139 -2.341259 1.498467
S 2.876211 -1.661683 -1.899077
S 3.571268 -1.517964 1.200555
S 2.844078 0.165176 2.071914
S -2.462128 -3.184742 -0.984593
S -3.622542 -2.420374 0.420164

S -2.393066 3.318246 -0.732684
S -1.395985 3.708631 0.919343
H 4.080609 -2.157800 -1.558873
H 3.834858 2.377049 -0.541685
H -3.696449 0.584229 -1.295080

E= -5383.574067
S 1.097595 -1.434683 1.304435
Mo -2.685148 -0.248438 0.017310
Mo 2.738890 -0.333272 -0.071902
Mo 0.093510 0.603549 0.176968
S 1.756414 0.914392 -1.578887
S 2.077737 1.294180 1.684364
S -1.047140 -1.089694 -1.201306
S -1.597505 0.675298 1.999878
S 1.944325 -2.528643 -0.237456
S -3.214567 -1.759578 1.779000
S -4.374652 0.650714 -1.381481
S -4.618922 -1.295471 -1.032664
S 5.020981 0.346613 0.186701
S 4.756125 -0.919406 -1.327756
S -0.434973 3.018672 0.256277
S -1.537707 1.963736 -1.032974
H -3.950470 -2.711498 1.168915
H -1.941619 1.986574 1.930953
H 2.464122 2.429606 1.070239

[Mo3S13H3]+ II
E= -5383.551576
S 1.679432 -0.027929   0.000000
Mo -0.247656   2.649246   0.000000
Mo 0.143563 -0.852695   1.827322
Mo 0.143563 -0.852695 -1.827322
S -1.380762 -1.302086   0.000000
S   1.600257 -2.029145   0.000000
S -0.711299   1.503284 -1.878639
S   1.903461 -0.842903 -3.044272
S -0.711299   1.503284   1.878639
S   1.903461 -0.842903   3.044272
S   1.839535   3.647596   0.000000
S -1.491622   4.314991   0.000000
S -0.817384 -2.944252   2.887083
S -1.633670 -1.140083   3.399254
S -0.817384 -2.944252 -2.887083
S -1.633670 -1.140083 -3.399254
H   2.600996   2.532987   0.000000
H   0.038183 -3.131605   3.925292
H   0.038183 -3.131605 -3.925292

E= -5383.581463
S -1.879630 0.003053 1.688249
Mo -1.475747 -1.354024 -0.076883
S -3.309113 -2.769750 -0.390231
S -2.382092 -3.295541 1.371612
S -0.418832 0.070267 -1.766131
S -2.441794 -0.166864 -1.967671
Mo -1.301200 1.445296 -0.001502
S -2.619420 3.210748 -0.768230
S -2.390543 3.465368 1.273624
S 0.764541 2.222798 0.630878
S 2.290629 1.924788 -0.781226
Mo 3.198824 -0.070793 -0.025327
S 5.149935 -0.032525 -0.800526
S 2.234667 -1.964707 -0.918890
S 0.510455 -2.518104 0.144443
S 3.314118 -0.128182 2.274030
H 4.073848 -1.229068 2.462915
H -1.354940 4.339277 1.288380
H -1.604465 -4.311929 0.925724

[Mo3S13H3]+ III
E= -5383.656700
S 0.004700 0.004005 1.826825
Mo -1.140582 1.073105 0.010050
S 0.446470 1.905547 -1.631420
S 0.657892 2.814514 0.174310
Mo 1.501389 0.457623 0.010560
S 2.108940 -1.971344 0.170466
S 1.430434 -1.331027 -1.632796
Mo -0.352988 -1.521874 0.008153
S -1.875817 -0.566499 -1.628484
S -2.759283 -0.834972 0.177282

S 3.558891 0.959408 1.371508
S 3.799715 1.160026 -0.649228
S -0.892916 -3.861513 -0.658175
S -0.941622 -3.559654 1.363759
S -2.892941 2.715088 -0.655112
S -2.766117 2.435286 1.366617
H -1.974769 3.466757 1.753044
H 3.301401 2.232533 1.761667
H 0.291484 -3.973001 1.748452

E= -5383.610039
S -0.019822 -0.000042 1.823385
Mo -0.850104 1.359554 0.019467
S 0.907892 1.769501 -1.616780
S 1.374908 2.485898 0.244734
Mo 1.492093 0.000274 -0.021306
S 1.375776 -2.485405 0.244292
S 0.908257 -1.768871 -1.617043
Mo -0.849653 -1.359816 0.019429
S -2.003508 -0.000327 -1.634214
S -2.948460 -0.000458 0.163418
S 4.936680 -0.000391 1.096021
S 3.917559 0.001423 -0.647166
S -2.076996 -3.435403 -0.599694
S -2.007716 -3.105702 1.417987
S -2.078212 3.434776 -0.599505
S -2.008809 3.104878 1.418072
H -0.951415 3.864172 1.797597
H 6.182491 0.001989 0.570182
H -0.950047 -3.864703 1.797338

E= -5383.563995
S 0.004117 0.032828 1.818592
Mo -1.374123 -0.653093 -0.012138
S -1.677288 1.186161 -1.606602
S -2.435575 1.597162 0.255169
Mo 0.052345 1.663787 0.044386
S 2.532819 1.428720 0.234904
S 1.734785 1.074733 -1.619180
Mo 1.321675 -0.743711 -0.023445
S -0.074487 -1.995533 -1.614849
S -0.096161 -2.774740 0.297304
S 0.238554 3.717439 1.493268
S 0.121827 4.081573 -0.516877
S 3.390548 -2.012583 -0.618237
S 4.164046 -2.657120 1.134566
S -3.527277 -1.773906 -0.608639
S -4.297732 -2.453592 1.131812
H -5.427935 -2.992559 0.621632
H -1.050037 3.871282 1.886383
H 5.231463 -3.310227 0.622620

[Mo3S13H3]+ IV
E= -5383.668573
S 0.003636 -0.002201 1.785755
Mo -1.113302 -1.100899 -0.009209
S -1.855152 0.511644 -1.678922
S -2.799438 0.775307 0.113687
Mo -0.390009 1.513257 -0.008554
S 2.077776 2.031129 0.105363
S 1.374459 1.346523 -1.684835
Mo 1.511842 -0.420393 -0.011460
S 0.485731 -1.869743 -1.684823
S 0.727983 -2.812330 0.108088
S -0.868801 3.348976 1.502459
S -0.983587 3.982009 -0.451011
S 3.945625 -1.141775 -0.454270
S 3.344385 -0.920293 1.499622
S -2.891388 -2.911201 -0.455000
S -2.472699 -2.429889 1.499862
H -3.971380 -2.127433 -0.691161
H 4.510148 0.067037 -0.692477
H -2.313499 3.867392 -0.684576

E= -5383.618033
S 0.470547 0.004887 1.892204
Mo -1.435132 -0.006254 0.458111
S -1.262505 1.753812 -1.226320
S -1.284231 2.480641 0.695670
Mo 0.843551 1.361780 -0.036534
S 2.925029 0.005790 -0.490118
S 1.500122 0.002260 -1.956108

Mo 0.856616 -1.355112 -0.033149
S -1.250260 -1.771415 -1.218178
S -1.266479 -2.485534 0.706948
S 2.140857 2.980960 1.223283
S 2.028972 3.537866 -0.753426
S 1.992912 -3.563578 -0.729439
S 2.184092 -2.952884 1.224079
S -4.850437 -0.047922 -1.007576
S -3.899695 -0.024638 0.776980
H -6.114589 -0.054710 -0.529747
H 3.139560 -3.082293 -1.268696
H 0.980773 4.395630 -0.723491

E= -5383.573275
S -0.041715 0.006024 1.624387
Mo -0.938958 -1.443270 -0.008766
S -1.979320 -0.064166 -1.739074
S -3.050451 -0.100198 0.009502
Mo -1.031721 1.388051 -0.016120
S 1.327931 2.522522 0.352587
S 0.956567 1.694548 -1.477048
Mo 1.970627 0.068730 0.134252
S 1.057203 -1.626212 -1.474714
S 1.515247 -2.417988 0.354226
S -2.100270 2.987502 1.426927
S -2.190485 3.642802 -0.528195
S 4.402537 0.125468 -0.820612
S 4.070436 0.158376 1.224001
S -1.950494 -3.772611 -0.508803
S -1.891578 -3.103583 1.443194
H -3.209173 -3.421071 -0.865813
H 4.623247 -1.195793 -1.018694
H -3.421622 3.209638 -0.890905

[Mo3S13H3]+ V
E= -5383.575826
S 0.043652 -0.034111 1.752771
Mo -1.567540 -0.194729 0.005189
S -1.134835 1.655058 -1.515189
S -2.357769 2.356886 0.030633
Mo 0.807621 1.349629 -0.030780
S 3.335447 0.880408 0.562990
S 2.511788 0.090058 -1.210366
Mo 0.898795 -1.371377 -0.016156
S -0.781734 -1.675727 -1.782716
S -1.207054 -2.657966 -0.024319
S 0.678286 3.405202 1.107881
S 1.588656 3.682634 -0.653112
S 2.318154 -3.388843 -0.545974
S 2.349771 -2.629923 1.299276
S -4.084865 -0.646294 -0.389052
S -3.390969 -0.610864 1.551863
H -3.557702 2.224946 -0.591602
H -4.049160 -1.972158 -0.663041
H 3.877618 2.014968 0.053042

E= -5383.584380
S 0.019831 0.022290 1.813323
Mo -1.375330 -0.683516 0.002886
S -1.939454 1.426899 -1.173099
S -3.005703 1.251279 0.585277
Mo 0.254902 1.593159 0.027565
S 2.724532 1.273999 0.517096
S 1.204222 0.549814 -2.011850
Mo 1.356068 -0.830539 0.006128
S 0.009256 -1.177837 -2.003958
S -0.081975 -2.867627 0.372058
S 0.002771 3.571772 1.251129
S 0.541174 3.980980 -0.622975
S 3.385604 -2.138656 -0.694198
S 3.130195 -2.039915 1.252704
S -3.372633 -1.994766 -0.783945
S -3.139921 -2.008485 1.173915
H -4.162576 0.754769 0.075296
H -0.085085 -2.868629 1.719247
H 2.704370 1.195583 1.861490

E= -5383.574370
S 0.020985 0.069623 1.791975
Mo -1.137049 -1.024033 0.010157
S -2.163874 0.803269 -1.268391
S -3.227746 0.457089 0.475899

Mo -0.154656 1.607768 -0.017502
S 2.298233 1.965835 0.479153
S 1.059403 0.805302 -2.025839
Mo 1.544772 -0.448760 0.013817
S 0.354751 -1.180933 -1.981513
S 0.684776 -2.781994 0.435745
S -1.207762 3.460933 1.280669
S -0.605724 3.994874 -0.534199
S 3.852497 -1.187714 -0.653609
S 3.567124 -1.125449 1.290639
S -2.704268 -2.846512 -0.744545
S -2.513380 -2.718493 1.214174
H -4.219293 -0.311667 -0.042702
H 0.673265 -2.746200 1.782394
H 2.276953 1.930984 1.825949

[Mo3S13H3]+ VI
E= -5383.526931
S 0.167661 0.017741 1.977314
Mo 1.392613 -0.843723 0.127497
S -1.254044 -2.359177 -1.568456
S -0.224028 -2.753797 0.223006
Mo -1.454659 -0.634973 0.373806
S -1.713225 1.397205 -0.863712
S -1.828202 1.368960 -2.972653
Mo 0.333118 1.610761 0.235138
S 1.291290 -0.621594 -2.492743
S 2.065488 0.993410 -1.294503
S -2.968562 -0.694981 2.036614
S -3.915712 -1.232332 0.313328
S 1.095193 3.902901 -0.022127
S 0.169609 3.443693 1.712006
S 3.572553 -2.149073 -0.169161
S 2.979796 -1.552095 1.633660
H -2.508399 2.529063 -3.052019
H -2.361273 -3.075874 -1.263266
H 2.479560 -1.173692 -2.816426

E= -5383.543708
S -0.178182 0.584306 1.703986
Mo 1.757910 0.358162 0.135888
S 1.849517 -3.514313 -0.425278
S 1.201758 -1.916689 0.776828
Mo -1.085228 -1.170235 0.347486
S -2.189558 -0.136071 -1.531732
S -0.771381 -1.581607 -2.193902
Mo -0.946423 1.544311 -0.292601
S 2.626656 -0.787392 -1.855308
S 0.915613 1.900763 -1.453839
S -2.482182 -1.744314 2.046126
S -2.610721 -3.075116 0.500708
S -2.787151 2.864826 -0.879370
S -1.834270 3.358883 0.870323
S 3.993070 1.033658 0.325462
S 2.826776 1.513891 1.906969
H -1.678494 -2.568884 -2.381600
H 1.307076 -4.415672 0.418635
H 2.909441 0.216937 -2.705065

E= -5383.546876
S -0.223672 -0.242921 -1.382164
Mo -2.097989 -0.658747 0.054602
S 1.668332 -2.992568 -0.653917
S 2.607268 -1.770479 -1.948914
Mo 1.703354 -0.570730 0.095385
S 1.413616 1.348351 1.587360
S 1.542748 -1.542959 2.255902
Mo -0.290727 1.519507 0.207227
S -1.740845 -2.579687 1.265862
S -2.286725 1.243884 1.288514
S 3.342648 1.094405 -0.981096
S 4.107502 -0.072243 0.402859
S -0.511183 3.986838 0.377471
S -0.120640 3.264507 -1.437372
S -4.527811 -1.087042 -0.112591
S -3.560050 -0.827968 -1.830706
H 1.686553 -2.871256 2.082751
H 2.714779 -3.476220 0.059621
H -2.995143 -2.987680 1.555316

[Mo3S13H3]+ VII
E= -5383.482598

S 0.068609 -0.179998 1.875765
Mo 1.582094 -0.196738 -0.004968
S 0.653369 -1.568248 -1.768625
S 1.116352 -2.660336 -0.115493
Mo -0.990893 -1.254329 0.012148
S -2.906806 0.375441 0.183099
S -2.469878 -0.105340 -1.791782
Mo -0.682038 1.553392 0.308952
S 1.863291 1.717062 -1.607070
S 1.763816 2.312903 0.372015
S -1.985198 -2.814544 1.505674
S -2.386320 -3.206514 -0.457740
S -1.434159 3.460844 -0.862044
S -1.671890 3.669496 1.099820
S 4.004918 -0.682617 -0.569393
S 3.612973 -0.577339 1.349255
H -3.372540 -1.110064 -1.953006
H 3.214483 1.767754 -1.788848
H 0.307981 -0.808334 3.048607

E= -5383.482522
S -0.064375 -0.184631 1.878657
Mo 1.011842 -1.238675 0.013466
S -0.627545 -1.573574 -1.770183
S -1.073422 -2.674543 -0.117705
Mo -1.575495 -0.219225 -0.003619
S -1.798058 2.284292 0.386040
S -1.903353 1.697616 -1.595436
Mo 0.658630 1.560211 0.311890
S 2.473027 -0.065281 -1.791531
S 2.902365 0.420868 0.183664
S -3.609032 -0.629509 1.340656
S -3.991377 -0.209140 -0.577584
S 1.371715 3.473660 -0.871351
S 1.615385 3.699218 1.088105
S 2.436564 -3.168441 -0.460397
S 2.028666 -2.784728 1.504127
H -3.256300 1.728110 -1.765526
H 3.390119 -1.056696 -1.953538
H -0.291782 -0.814765 3.053116

E= -5383.515874
S 0.001812 0.002244 1.836946
Mo -1.588747 -0.162688 0.063303
S -1.240975 1.687499 -1.489634
S -1.662289 2.343190 0.376227
Mo 0.705420 1.408436 0.001304
S 2.850662 0.384436 0.543408
S 1.215005 -0.013552 -2.029246
Mo 1.178129 -1.213998 0.127237
S -1.528087 -1.922604 -1.741491
S -1.114379 -2.633454 0.145500
S 1.590998 3.483496 1.084078
S 1.777717 3.479977 -0.870090
S 2.599564 -3.040470 -0.741393
S 2.401445 -3.047497 1.229280
S -4.090338 -0.201390 -0.326105
S -3.546153 -0.490446 1.531423
H 2.539162 0.204184 -2.140390
H -2.835328 -2.290764 -1.844132
H -0.165233 0.250180 3.157590

[Mo3S13H3]+ VIII
E= -5383.535832
S -0.006254 -0.047280 1.781505
Mo 1.516270 0.417347 0.002126
S 1.394605 -1.670359 -1.367811
S 2.674852 -1.957384 0.250588
Mo -0.605133 -1.586867 0.101178
S -2.911502 -0.687406 0.239863
S -2.001406 -0.488403 -1.576310
Mo -1.121208 1.123810 0.022072
S 0.403161 1.456813 -1.814298
S 0.725416 2.786144 0.639801
S -0.603983 -3.510354 1.298022
S -1.350970 -3.868227 -0.549491
S -2.681842 2.888213 -0.789739
S -2.683874 2.686230 1.165804
S 3.661502 1.248410 -0.936990
S 3.649229 1.209590 1.033182
H -0.050516 0.053003 3.131678
H 0.730149 2.798143 1.999042

H 3.840428 -1.667072 -0.382553

E= -5383.535852
S -0.005439 -0.046667 1.780640
Mo 1.517439 0.414265 0.000994
S 1.391049 -1.673027 -1.368331
S 2.671080 -1.963031 0.249681
Mo -0.608670 -1.585653 0.101131
S -2.912999 -0.681102 0.242088
S -2.004471 -0.484657 -1.575094
Mo -1.119010 1.126061 0.021495
S 0.404685 1.453571 -1.816201
S 0.731864 2.785079 0.636534
S -0.610738 -3.508982 1.298169
S -1.359422 -3.865705 -0.548781
S -2.674044 2.894670 -0.788169
S -2.678307 2.691913 1.167377
S 3.663310 1.242873 -0.934518
S 3.652398 1.200442 1.035689
H -0.047853 0.054894 3.130747
H 0.737418 2.798497 1.995780
H 3.837101 -1.675689 -0.383934

E= -5383.530886
S -0.338176 0.365078 2.047317
Mo 1.253547 -1.135693 -0.011090
S -0.604756 -2.240545 -1.179702
S -1.523126 -2.833803 0.599671
Mo -1.552027 -0.310065 0.037390
S -1.861321 2.166165 -0.190936
S -1.095193 1.197595 -1.803291
Mo 0.542977 1.452864 -0.007645
S 1.809309 0.253370 -1.734375
S 2.751969 0.640750 1.000426
S -3.778705 -0.319604 1.164518
S -3.891886 -0.684503 -0.770547
S 1.448698 3.618296 -0.831695
S 1.083260 3.632433 1.097616
S 2.848890 -2.862049 -0.858760
S 2.599391 -2.868533 1.099586
H -1.188090 1.291785 2.559579
H 2.474959 0.574798 2.321140
H -2.729428 -3.199473 0.098554

[Mo3S13H3]+ IX
E= -5383.600283
S 0.000073 0.014512 1.767205
Mo 1.388931 -0.791864 0.021820
S -0.002882 -1.926225 -1.615615
S -0.003997 -2.922584 0.159351
Mo -1.391241 -0.788217 0.022096
S -2.528585 1.464416 0.111616
S -1.652027 0.962080 -1.652109
Mo 0.002288 1.635184 0.033690
S 1.654466 0.957635 -1.652415
S 2.532749 1.457316 0.111160
S -3.139086 -1.759721 1.409590
S -3.552272 -1.999671 -0.583073
S 0.006049 3.951737 -0.599893
S 0.005305 3.560505 1.420494
S 3.546575 -2.009845 -0.582753
S 3.133806 -1.767941 1.409830
H 0.000942 -0.136422 3.111962
H 4.364994 -0.952986 -0.812766
H -4.367753 -0.940392 -0.812840

E= -5383.598396
S -0.272854 0.168361 2.017783
Mo 1.381491 -0.865052 -0.109120
S -0.119318 -1.961515 -1.690888
S -0.109817 -2.874105 0.136280
Mo -1.377428 -0.715529 0.008955
S -2.457617 1.579316 0.038183
S -1.559788 1.009724 -1.694552
Mo 0.062001 1.560939 0.017676
S 1.787845 1.006709 -1.627639
S 2.545695 1.325087 0.238212
S -3.138707 -1.644047 1.419154
S -3.600832 -1.883316 -0.562639
S 0.196887 3.993880 -0.624095
S 0.140352 3.678763 1.313303
S 3.539165 -2.282075 -0.365927

S 2.875945 -1.838095 1.537966
H -1.300879 0.801920 2.649032
H 4.444120 -1.293922 -0.563873
H -3.149210 -3.142054 -0.782929

E= -5383.569320
S -0.703222 0.091251 2.051349
Mo 1.927638 -0.182024 -0.052531
S 0.756423 -1.964262 -1.329132
S 0.986218 -2.399533 0.668646
Mo -1.160492 -1.236042 0.035355
S -2.966367 0.496564 -0.316626
S -1.630406 0.240987 -1.832659
Mo -0.619343 1.450155 0.008108
S 1.403153 1.832004 -1.346140
S 1.661863 2.157859 0.658979
S -2.566686 -2.754976 1.288673
S -2.615636 -3.208326 -0.714372
S -1.437114 3.692385 -0.779441
S -1.523631 3.450733 1.165695
S 4.256768 -0.954642 -0.756590
S 3.960810 -0.380002 1.199551
H -1.951225 0.353237 2.499471
H 4.123918 -2.301058 -0.665869
H -1.695174 -4.200609 -0.779665

[Mo3S13H3]+ X
E= -5383.591901
S -0.000957 0.058356 1.805004
Mo 1.360238 -0.829302 0.045292
S -0.072731 -1.954532 -1.546591
S -0.104875 -2.891899 0.250631
Mo -1.419520 -0.729663 0.045311
S -2.481527 1.546919 0.114089
S -1.623691 1.000664 -1.638828
Mo 0.057890 1.641688 0.039724
S 1.696095 0.884106 -1.635000
S 2.580519 1.366969 0.120843
S -3.334765 -1.803702 1.276894
S -3.495202 -1.814719 -0.758605
S 0.138339 3.951690 -0.634982
S 0.127522 3.588096 1.391094
S 3.358917 -2.049279 -0.760306
S 3.297600 -1.864810 1.272403
H 0.000905 -0.000780 3.156173
H -4.062829 -0.709249 1.612739
H 2.756459 -3.050092 1.651016

E= -5383.590433
S -0.352638 0.135827 2.046853
Mo 1.550787 -0.551362 -0.066784
S 0.339586 -2.046920 -1.559635
S 0.511663 -2.784247 0.329255
Mo -1.199406 -0.993946 0.025535
S -2.746441 0.993551 -0.022075
S -1.692103 0.611873 -1.712499
Mo -0.280974 1.543005 0.027064
S 1.579608 1.371253 -1.564534
S 2.185794 1.834087 0.321721
S -2.978761 -2.303520 1.257026
S -2.973788 -2.554866 -0.767357
S -0.663640 3.935680 -0.662929
S -0.696317 3.649359 1.279773
S 3.816643 -1.366648 -0.651665
S 3.520341 -1.142592 1.363919
H -1.506576 0.549927 2.640097
H -2.261368 -3.372503 1.682784
H 3.211697 -2.406025 1.747207

E= -5383.551305
S -1.062140 0.021225 1.928317
Mo 1.889120 -0.515906 0.047838
S 0.700587 -2.273278 -1.352487
S 0.606719 -2.534238 0.695498
Mo -1.120887 -1.045179 -0.285966
S -2.641710 0.885144 -0.821807
S -1.087549 0.538384 -2.095889
Mo -0.360009 1.476726 0.034487
S 1.867070 1.748473 -0.912252
S 1.867062 1.707492 1.140922
S -4.292701 -2.135593 1.130071
S -2.907391 -2.549034 -0.363913

S -0.785206 3.853933 -0.666722
S -1.192936 3.497699 1.219501
S 4.088490 -0.977778 -0.820085
S 3.969500 -1.410221 1.184546
H -2.333469 0.433269 2.119480
H -5.374510 -2.562689 0.449806
H 4.485862 -0.282818 1.732444

[Mo3S13H3]+ XI
E= -5383.565277
S -0.153501 -0.764800 -1.474424
Mo -0.209398 1.367163 -0.220748
S -0.619053 3.854184 0.346598
S -0.223452 2.503828 1.840510
Mo -1.733573 -1.079579 0.252330
S -1.753505 -3.365545 0.523894
S -3.170941 -2.559037 -0.752799
Mo 2.008861 -0.469586 -0.244458
S 3.631433 -1.543336 1.415472
S 3.926923 0.337592 0.903274
S -2.599388 1.145189 -0.753955
S -1.460266 1.827702 -2.301048
S 0.371299 -0.525920 1.436093
S -2.767627 -0.030711 2.110243
S 2.709657 -2.163388 -1.671859
S 1.876711 1.705721 -1.141019
H 3.936996 -2.398393 -1.153570
H -3.617205 -1.075994 2.230112
H 0.620164 4.374822 0.168527

E= -5383.565485
S -0.110147 -0.866038 -1.433577
Mo -0.131658 1.348598 -0.288541
S -0.391593 3.882869 0.153798
S -0.083696 2.584994 1.714005
Mo -1.794841 -0.931644 0.313480
S -1.891880 -3.286824 0.483926
S -3.264052 -2.431745 -0.713807
Mo 2.000337 -0.599823 -0.231362
S 3.707137 -1.568505 1.233256
S 3.616728 0.382690 1.431509
S -2.550086 1.213937 -0.745147
S -1.409038 1.737684 -2.361452
S 0.305659 -0.491192 1.453206
S -2.825673 -0.103788 2.256057
S 2.675907 -2.244894 -1.761005
S 1.978686 1.542122 -1.195058
H 3.868414 -2.648166 -1.279681
H -3.973360 0.389948 1.746228
H 0.876493 4.317777 -0.048184

[Mo3S13H3]+ XII
E= -5383.572847
S 0.116211 -0.748666 1.496517
Mo 0.190122 1.403897 0.230705
S 0.556403 3.911481 -0.286678
S 0.216535 2.586313 -1.813922
Mo 1.731060 -0.953115 -0.419044
S 1.528415 -3.327582 -0.476694
S 3.037922 -2.744762 0.796985
Mo -1.968973 -0.503291 0.256775
S -3.555711 -1.582465 -1.421361
S -3.814708 0.330532 -1.036720
S 2.593612 1.203163 0.671879
S 1.504039 1.810591 2.280147
S -0.341597 -0.432567 -1.486310
S 3.086190 -0.390225 -1.945779
S -2.762376 -2.128242 1.718657
S -1.898753 1.698035 1.136483
H -3.941398 -2.421679 1.124615
H -0.695839 4.402224 -0.115538
H 2.385553 -2.741692 1.985335

E= -5383.572304
S 0.113061 -0.806874 1.457580
Mo 0.153583 1.387558 0.257185
S 0.453382 3.915887 -0.198324
S 0.132307 2.618505 -1.755084
Mo 1.772860 -0.890602 -0.443590
S 1.649587 -3.271922 -0.544298
S 3.137714 -2.659580 0.740141
Mo -1.972109 -0.579263 0.244985

S -3.609459 -1.603964 -1.265264
S -3.728841 0.354064 -1.317934
S 2.554323 1.245672 0.715784
S 1.430895 1.767221 2.333948
S -0.323830 -0.437933 -1.490282
S 3.089581 -0.253844 -1.973667
S -2.689669 -2.188865 1.787109
S -1.953214 1.597539 1.157365
H -3.851121 -2.632962 1.265889
H -0.808833 4.372119 -0.007222
H 2.484542 -2.696764 1.927732

[Mo3S13H3]+ XIII
E= -5383.557620
S 1.196217 1.039307 -1.476595
Mo 2.001410 -0.506279 -0.044607
S 4.451739 -0.718490 -0.705469
S 3.055239 -1.945039 -1.571635
S 0.947372 1.531993 1.761007
S 2.903943 1.272228 1.295242
Mo -1.825559 -1.023196 -0.108586
S -3.281462 -2.980493 0.877308
S -3.843576 -1.932949 -0.828947
Mo -0.690475 1.560002 0.004513
S -2.005687 3.346435 0.479464
S -0.742508 3.711015 -1.079123
S 1.961847 -1.716406 2.043974
S 0.126709 -2.111353 -0.346939
S -1.966495 0.302864 1.667214
S -1.747361 0.423069 -1.817346
H 4.516880 0.276390 -1.623801
H 2.876432 -1.065037 2.788801
H -2.674779 -4.048340 0.309092

E= -5383.559764
S 1.842472 0.990208 -1.423847
Mo 1.927991 -0.699002 -0.035188
S 4.137196 -1.482712 -0.981889
S 2.532803 -2.757504 -1.053021
S 1.123907 0.590422 1.894100
S 3.150676 0.219374 1.713468
Mo -2.119455 -0.434766 -0.193781
S -4.081074 -2.009270 0.322353
S -4.237531 -0.588541 -1.185583
Mo -0.014479 1.684829 -0.017118
S -0.753135 3.734178 0.772471
S 0.806480 3.829851 -0.549064
S -0.526812 -3.180565 1.627164
S -0.320027 -2.010817 -0.102772
S -1.833537 0.814669 1.557569
S -1.308270 0.930486 -1.844953
H 4.098918 -0.961747 -2.233241
H -0.225699 -4.353174 1.033904
H -3.753981 -3.106112 -0.400969

[Mo3S13H3]+ XIV
E= -5383.564115
S 0.113744 -0.428146 -1.595302
Mo -1.708592 -0.618623 0.070326
S -3.700950 -1.546080 -1.187294
S -3.968151 -0.840191 0.656872
Mo 1.886572 -0.810095 -0.055515
S 4.001951 -1.355394 -0.797386
S 2.990686 -2.819011 0.206721
Mo 0.015862 1.567911 -0.058706
S -0.318676 3.800755 -0.436712
S 1.008416 3.575347 1.064883
S 0.041298 -1.932777 1.324683
S -1.132720 -3.171324 0.104291
S 2.325687 1.380369 -1.273082
S 1.720082 0.496228 1.690068
S -2.122423 1.417611 -1.373843
S -1.358992 1.019070 1.725221
H -1.957585 -3.591126 1.089158
H -2.912713 2.167050 -0.581428
H 3.129738 2.034633 -0.410022

E= -5383.538387
S -0.019533 0.021849 1.678527
Mo -1.763614 0.120270 0.023051
S -3.477456 -1.290564 0.902993
S -3.960100 -0.617902 -0.910822

Mo 0.654583 1.428905 -0.163126
S 0.755034 3.472822 1.152146
S 1.348381 3.780196 -0.714025
Mo 0.961200 -1.362581 0.012783
S 2.658265 -2.257847 1.391902
S 2.679093 -3.125513 -0.409137
S -0.988588 1.543606 -1.688728
S -2.702801 2.076446 1.013157
S 3.392453 1.006911 0.311652
S 2.340617 0.196613 -1.325545
S -0.787525 -3.273674 0.245348
S -0.878905 -1.985241 -1.403708
H -3.330465 1.577665 2.095593
H -0.077104 -4.277590 -0.322892
H 3.873540 2.099703 -0.326605

[Mo3S13H3]+ XV
E= -5383.577655
S -0.044420 -0.144045 -1.766908
Mo 1.128355 -1.319254 -0.075634
S 2.388988 -2.374881 -1.717563
S 3.196674 -2.349560 0.185026
Mo 0.480082 1.373851 -0.048618
S 2.772793 1.925685 -1.085498
S 1.226149 3.288356 -1.177188
Mo -1.895251 -0.241808 -0.089025
S -4.197010 0.194581 0.790837
S -3.220300 -1.436583 1.432492
S 1.514691 0.146546 1.843149
S 3.560099 0.526381 2.094079
S -1.798552 2.212604 -0.266740
S -1.266971 1.565311 1.601213
S -2.938753 -0.817716 -2.111102
S -0.601631 -2.409017 0.637768
H 3.384416 1.196765 3.250734
H -4.219850 -0.900967 -1.690336
H 3.413504 2.319579 0.044197

E= -5383.580049
S 0.100019 -0.390784 1.766632
Mo -1.058801 -1.399535 -0.044504
S -2.042288 -2.891407 1.433259
S -3.034367 -2.598391 -0.348404
Mo -0.578069 1.257106 0.212269
S -2.524948 2.103779 1.595712
S -1.743950 3.386263 0.184920
Mo 1.911337 -0.192702 0.071542
S 4.225259 0.555890 -0.628700
S 3.578818 -1.027731 -1.554479
S -1.816409 0.280836 -1.634700
S -3.918550 0.463045 -1.507528
S 1.663138 2.204669 0.604019
S 1.192880 1.780489 -1.363780
S 3.047194 -1.010250 1.932091
S 0.753940 -2.095705 -1.104836
H -3.974860 1.477324 -2.393821
H 4.312143 -1.148428 1.472176
H -3.556634 1.575358 0.883406

[Mo3S13H3]+ XVI
E= -5383.558518
S -0.694237 -0.407484 1.692964
Mo 1.245027 -1.119599 0.136467
S 3.697461 -1.650742 -0.187580
S 2.426589 -2.439639 -1.557386
Mo -2.134582 -0.311543 -0.124831
S -4.331026 -0.664513 0.417235
S -3.384904 -2.251403 -0.467409
Mo 0.052875 1.371608 0.306011
S 0.775314 3.619868 0.388366
S 2.524294 2.920376 -0.457634
S -0.455273 -1.442222 -1.463254
S 1.193283 -2.888684 1.629225
S -2.322926 2.161727 0.278715
S -1.569248 1.538319 -1.524550
S 2.100198 0.710245 1.663144
S 1.752046 1.205391 -1.434985
H 2.031541 -3.766142 1.030780
H 1.614637 0.208376 2.816075
H 4.109290 -0.521660 -0.817637

E= -5383.579534

S -0.011222 0.391384 1.743732
Mo 1.062558 1.323497 -0.106852
S 1.497977 3.701875 0.943135
S 2.987633 2.629357 -0.039949
Mo 0.623717 -1.281155 0.192514
S 2.099036 -2.409620 1.629301
S 1.796640 -3.509737 0.005219
Mo -1.879028 0.154901 0.050200
S -4.208506 -0.627797 -0.487313
S -3.677338 0.970352 -1.462396
S 2.143517 -0.319343 -1.426420
S 4.204049 -0.510663 -0.922952
S -1.601870 -2.237176 0.593307
S -1.160606 -1.813305 -1.384237
S -2.938150 1.135035 1.905485
S -0.718162 1.756599 -1.404649
H 4.609732 -0.584772 -2.204951
H -4.213787 1.277010 1.483056
H 1.091744 4.512857 -0.060536

[Mo3S13H3]+ XVII
E= -5383.610445
S 1.469061 0.632996 -1.618961
Mo 2.951683 -0.667272 -0.201437
S 5.009035 0.026615 1.143800
S 4.152286 1.369556 -0.167385
S 0.736203 -1.460781 0.156239
S 2.009083 -1.580726 1.774657
Mo -0.369470 0.830141 -0.125501
S 0.018402 2.580952 1.338638
S 0.114983 3.397893 -0.569833
Mo -2.889805 -0.550330 -0.019511
S -4.776431 -0.247694 1.352138
S -5.374030 -0.127854 -0.628344
S -2.650646 -2.520441 -0.716763
S -1.505847 -0.158427 1.750500
S -2.129121 1.008106 -1.550469
S 3.889330 -2.087298 -1.407347
H -1.128395 3.928308 -0.620237
H 4.425547 0.408401 2.304827
H -5.775227 -1.403294 -0.843670

E= -5383.598451
S 1.096253 -0.617520 -1.492660
Mo 3.120438 -0.594968 -0.110443
S 5.147191 0.938014 -0.266706
S 3.633243 1.110874 -1.655949
S 1.466519 -1.196073 1.563697
S 3.122590 -0.150000 2.204966
Mo -0.307319 0.127020 0.163474
S 0.363694 2.096326 1.084146
S 0.008247 3.699449 -0.212166
Mo -3.242855 -0.504769 -0.193800
S -4.837416 0.119282 1.427286
S -5.401379 0.907604 -0.401791
S -3.819452 -2.135537 -1.383583
S -1.747877 -1.230763 1.397347
S -1.961714 0.965881 -1.337885
S 4.122991 -2.359402 -0.585646
H 0.442682 4.625899 0.664742
H 4.787417 1.903676 0.612418
H -6.267392 -0.045616 -0.821775

[Mo3S13H3]+ XVIII
E= -5383.608575
S 0.662538 -1.368658 -1.009659
Mo 2.773070 -0.753442 0.101958
S 4.768665 0.493594 -0.812050
S 3.236701 0.024971 -2.090597
S 1.189297 -0.491862 1.888131
S 2.907347 0.634885 2.019346
Mo -0.643542 0.194128 0.029859
S 4.630704 2.490468 -0.203889
S 0.082326 2.391947 0.229615
Mo -3.401855 -0.155396 -0.129838
S -5.090241 0.616259 1.270663
S -5.015636 1.453966 -0.594284
S -3.936540 -2.141583 -1.123682
S -2.006587 -0.613016 1.661758
S -1.979730 0.816275 -1.684947
S 3.728215 -2.574364 0.430354
H 1.037638 2.257618 1.176211

H 5.669983 2.868159 -0.976748
H -4.102915 -2.833457 0.025244

E= -5383.572983
S 0.914248 0.501079 -1.265350
Mo 3.006549 -0.547836 -0.212253
S 4.790273 0.465507 0.958789
S 3.667598 1.707307 -0.225305
S 1.473987 -2.507530 0.425312
S 3.142576 -2.111444 1.553099
Mo -0.758967 1.240658 -0.087962
S 0.307379 2.643862 1.695915
S -0.768204 3.720958 -0.514261
Mo -2.783813 -0.693922 -0.133285
S -4.539267 -1.357974 1.443740
S -5.226515 -0.639371 -0.270921
S -2.065471 -2.344747 -1.199688
S -1.341700 -0.161622 1.627432
S -2.627339 1.233157 -1.409955
S 3.812922 -1.444838 -1.914318
H -1.991448 3.986602 -0.017161
H -0.664754 2.607411 2.629136
H 0.530131 -1.817312 1.123236

[Mo3S13H3]+ XIX
E= -5383.576945
S -0.995269 0.768368 1.069340
Mo -3.082956 -0.432684 0.165138
S -4.800122 0.334135 -1.271271
S -3.630105 1.772296 -0.401928
S -1.551358 -2.474211 0.012687
S -3.203851 -2.353989 -1.201559
Mo 0.885453 1.295759 0.125560
S 0.777523 2.979074 -1.458173
S 0.911125 3.891528 0.403441
Mo 2.688625 -0.885480 0.084827
S 4.094256 -1.676993 -1.634597
S 5.021922 -0.810604 -0.016774
S 1.874251 -2.433430 1.265107
S 1.150295 -0.240729 -1.542567
S 2.789338 1.014613 1.638187
S -3.956642 -0.887013 2.006420
H 2.241355 4.130123 0.453137
H -0.599649 -1.944979 -0.804494
H 2.029362 0.627140 2.686288

E= -5383.574813
S 0.789561 0.040937 -1.304163
Mo 2.991622 -0.566920 -0.226532
S 4.666547 0.840023 0.677865
S 3.466559 1.680692 -0.765035
S 1.695089 -2.563093 0.799789
S 3.239376 -1.686252 1.835548
Mo -0.660547 1.034608 0.036664
S 0.372958 2.365191 1.701920
S 0.153956 3.456538 -0.051497
Mo -2.952986 -0.567944 -0.180785
S -4.803601 -1.050377 1.329335
S -5.295911 0.132762 -0.181721
S -2.517264 -2.307616 -1.245317
S -1.477657 -0.410304 1.611112
S -2.405585 1.311851 -1.650853
S 3.894988 -1.728059 -1.708103
H -0.990121 4.130940 0.216275
H 0.632471 -1.901822 1.329808
H -1.986437 0.664958 -2.760751

[Mo3S13H3]+ XX
E= -5383.571552
S 0.876162 -1.181152 -1.018967
Mo 2.980240 -0.335949 -0.059071
S 5.323808 0.118570 -0.166988
S 3.199828 0.778129 -2.123685
S 1.432307 -0.328810 1.783993
S 3.143752 0.768205 2.009233
Mo -0.263147 0.499448 0.030860
S 0.780446 2.578393 0.473411
S -0.603544 2.600423 -0.980335
Mo -3.150533 -0.565481 -0.018759
S -4.866243 0.878312 1.046566
S -5.263094 0.323577 -0.812599
S -3.508978 -2.618983 0.132135

S89

S -1.705865 0.031845 1.733166
S -1.901270 -0.158019 -1.803883
S 3.445626 -2.614924 -0.044849
H 2.097596 0.387047 -2.791326
H 5.669174 0.296071 1.123296
H 4.790766 -2.608935 0.005576

E= -5383.571413
S -0.873896 1.185470 -1.015183
Mo -2.978242 0.335360 -0.061007
S -5.320683 -0.123363 -0.174761
S -3.188622 -0.783933 -2.123609
S -1.434213 0.329923 1.784444
S -3.145555 -0.768347 2.006805
Mo 0.264751 -0.497134 0.033747
S -0.771596 -2.580733 0.482993
S 0.609835 -2.600382 -0.972513
Mo 3.142844 0.565542 -0.015265
S 4.879255 -0.856488 1.041885
S 5.242940 -0.337705 -0.834488
S 3.504128 2.618059 0.136105
S 1.707042 -0.036412 1.739289
S 1.896374 0.160729 -1.804409
S -3.447833 2.613694 -0.050171
H -2.085099 -0.391856 -2.788489
H -5.669517 -0.299766 1.114728
H -4.793041 2.605162 -0.002397

[Mo3S13H3]+ XXI
E= -5383.561439
S -1.895496 0.705853 1.491429
Mo -1.464478 -1.280411 0.358012
S -2.903494 -3.001953 -0.867781
S -3.801336 -1.438092 0.134034
S -1.197870 0.020110 -1.901931
S -2.279382 1.753221 -1.812491
Mo -0.679795 1.740311 -0.100763
S 0.350066 3.439301 1.188409
S -1.428735 3.923131 0.303796
Mo 2.329438 -0.432527 0.011235
S 4.134145 -1.694587 -0.842827
S 4.753448 0.203661 -0.316479
S 0.761122 -2.075909 -0.822997
S 1.544464 1.344077 -1.062130
S 2.186217 -0.378377 2.102418
S -0.889150 -2.570070 1.935118
H 1.062933 -3.161618 -0.089319
H -2.888919 -2.508755 -2.128956
H 4.705046 0.834878 -1.515158

E= -5383.551357
S -1.095043 0.747523 1.673815
Mo -2.274151 -0.686719 0.424803
S -4.105134 -1.085482 -1.432474
S -4.181678 0.561252 -0.177247
S -1.043266 0.772665 -1.703093
S -1.062564 2.719367 -1.101418
Mo 0.665161 1.539586 -0.052974
S 2.445647 3.163247 0.016848
S 1.028143 3.489864 1.361498
Mo 1.884457 -1.151840 -0.205020
S 2.700613 -3.388819 -0.214865
S 4.208204 -2.039475 0.208528
S -0.386865 -2.099920 -0.579591
S 2.126068 0.436657 -1.701319
S 1.525889 0.014352 1.651585
S -2.934860 -2.153705 1.772577
H -0.418029 -3.241901 0.128477
H -3.508048 -0.525319 -2.510304
H 4.754039 -1.878259 -1.021734

[Mo3S13H3]+ XXII
E= -5383.536912
S 1.224496 -1.727963 -0.365052
Mo 2.672813 -0.113182 0.218238
S 4.166292 0.965563 -1.288139
S 4.863799 -0.627610 -0.219640
S -0.991063 -1.149429 -2.710635
S -1.663875 -2.895641 -1.854858
Mo -1.271148 -1.492039 -0.057702
S -2.633133 -2.227480 1.656037
S -0.661251 -2.719871 1.798497

Mo -1.259687 1.589911 0.129528
S -0.872523 3.872559 -0.315135
S -2.821386 3.248758 -0.401442
S 1.031803 1.445294 -0.831732
S -3.102695 0.081471 -0.470525
S -1.155810 1.240970 2.186794
S 2.524703 0.400934 2.248052
H 1.557518 2.669810 -0.643165
H -3.883879 0.081608 0.627147
H -2.186477 -0.629294 -3.082245

E= -5383.552660
S -3.367591 -0.258723 -2.341988
Mo -3.610879 -0.217032 -0.251860
S -4.201068 -2.202073 1.145707
S -5.693878 -1.341598 0.172684
S 1.846273 -2.848060 0.456056
S 3.635366 -2.676433 -0.601146
Mo 2.961492 -0.552547 0.011399
S 4.742177 0.656079 0.703542
S 5.054649 0.032149 -1.230147
Mo 0.545627 1.101326 0.103476
S -1.089901 2.782027 -0.163962
S 0.794426 3.357449 0.462496
S -1.260395 -0.668970 0.434612
S 1.759723 0.177912 2.027066
S 1.788220 0.522915 -1.630841
S -3.943563 1.753257 0.426209
H -1.403835 -0.667299 1.773404
H 2.422111 1.237030 2.538444
H 2.308653 -3.077990 1.707142

[Mo3S13H3]+ XXIII
E= -5383.554023
S 0.933800 1.987028 -0.704428
Mo 2.008784 0.261982 0.214029
S 4.235124 0.915124 -0.090976
S 3.589947 0.332713 -1.851733
S -0.119651 -0.079916 1.556856
S 2.576813 0.728233 2.483402
Mo -1.132689 -1.372337 -0.206285
S -1.388296 -3.463755 0.930828
S -2.464214 -3.189880 -0.762423
Mo -1.406526 1.365500 0.029746
S -3.172655 2.798770 0.407803
S -1.637077 3.670565 -0.556184
S 2.352761 -2.390768 0.290981
S 1.052171 -1.725538 -1.237038
S -2.999157 -0.286222 1.147602
S -1.772681 0.133210 -1.852312
H 3.445390 -2.462554 -0.504651
H -4.022602 -0.253253 0.271089
H 3.865112 1.126694 2.460930

E= -5383.562824
S 1.537528 1.427742 -0.747272
Mo 2.437012 -0.505460 0.209308
S 4.735200 0.463610 0.125407
S 4.224636 -0.546598 -1.467190
S 0.067421 0.002864 1.501733
S 3.053600 -0.479311 2.463849
Mo -1.920922 -1.037353 -0.273905
S -3.226891 -2.564731 1.146046
S -4.325601 -1.534871 -0.131976
Mo -0.739825 1.468192 -0.026888
S -1.413445 3.665311 0.688341
S -0.541037 3.752095 -1.069551
S 1.961414 -2.649074 -0.571439
S -1.128725 -2.329891 -1.715549
S -2.246814 0.840248 1.866544
S -2.204668 0.900970 -1.594564
H 2.946637 -2.971722 -1.432507
H -3.345429 1.565495 1.560315
H 1.913722 -0.941861 3.018425

[Mo3S13H3]+ XXIV
E= -5383.580304
S 1.403298 -0.880002 -0.484704
Mo 3.834121 -0.586195 -0.015004
S 5.593100 0.503368 -1.018257
S 3.796497 0.736400 -1.985833
S -0.065775 0.147250 2.263250

S 3.573939 0.139690 1.926846
Mo -3.594586 -0.710183 -0.163195
S -5.524731 0.563038 -0.718176
S -5.342383 -1.304138 -1.512801
Mo -0.467789 0.847042 0.315357
S -0.590758 3.180844 0.202233
S 1.155948 2.332801 -0.410564
S 4.425090 -2.786206 0.298330
S -3.492389 -2.078112 1.424670
S -2.901899 1.295915 1.097321
S -1.601065 -0.575574 -1.276442
H 4.642035 -3.028066 -1.015329
H -3.263686 2.213182 0.179345
H 1.346371 -0.717416 -1.818690

E= -5383.522979
S -0.638291 -2.315768 -0.443124
Mo -2.089355 -0.455056 0.157477
S -4.071708 -1.487594 0.732805
S -3.870289 -1.152570 -1.261999
S 0.331343 0.074813 1.758542
S -1.558022 -0.543500 2.430592
Mo 0.888175 1.568531 -0.105169
S 1.932343 3.564767 0.375690
S 0.102607 3.827379 -0.469760
Mo 1.661406 -1.228104 -0.002601
S 3.710212 -2.247532 0.089474
S 2.285231 -3.407789 -0.755952
S -2.759401 1.980982 -0.190488
S -1.278476 1.169758 -1.474460
S 2.978550 0.673330 1.045747
S 1.667211 0.144812 -1.798332
H -3.826439 1.745169 -0.991967
H 3.884730 0.880913 0.071758
H -0.688716 -2.309057 -1.787254

[Mo3S13H3]+ XXV
E= -5383.546168
S -0.606424 -1.911463 -0.933039
Mo -2.059177 -0.468481 -0.026914
S -4.063710 -1.533928 0.570676
S -4.001702 -0.510529 -1.207111
S 0.377716 -0.427529 1.875323
S -1.484665 -1.206135 2.214914
Mo 0.593788 1.457283 0.100015
S 1.606165 3.426809 0.516129
S 0.303400 3.762470 -0.958124
Mo 1.653322 -1.140922 -0.122789
S 3.647134 -2.257475 0.109836
S 2.242921 -3.245221 -0.987709
S -1.808401 1.799972 1.018407
S -1.252973 1.059090 -1.794614
S 2.744638 0.671435 1.311855
S 1.811496 0.476066 -1.680046
H -1.780300 1.456990 2.322631
H 3.671033 1.135193 0.449680
H -2.033455 2.139874 -1.589335

E= -5383.527581
S 1.317907 1.449906 -0.188580
Mo 2.861195 -0.439599 -0.040924
S 3.481987 -0.548099 2.213145
S 4.816759 0.239875 0.888527
S -0.417805 -1.078466 -0.603144
S 0.931778 -1.708847 0.844548
Mo -2.764068 -0.795830 -0.037000
S -3.418721 -2.958308 -0.488524
S -4.796306 -1.779065 0.504109
Mo -0.959531 1.329100 -0.100098
S -1.299126 3.440600 1.094875
S -1.126261 3.651886 -0.852073
S 3.166357 -2.489576 -1.085728
S 3.730948 0.441874 -2.105839
S -1.795040 0.230254 1.955621
S -2.666374 0.825792 -1.635238
H 4.282193 -2.224384 -1.803260
H -2.759157 1.061092 2.410581
H 3.880390 1.743889 -1.797612

[Mo3S13H3]+ XXVI
E= -5383.588290
S -1.048694 -0.555410 -0.494724

Mo -3.468115 -0.599960 -0.459186
S -3.403128 -1.218364 1.861573
S -5.333098 -1.117483 1.148368
Mo 0.066895 1.131665 0.546263
S 1.282824 2.663907 -0.744073
S -0.698016 2.801286 -1.341703
S 1.841015 0.194089 1.574804
Mo 3.385289 -0.917347 0.051390
S 4.688577 1.114427 0.117514
S 5.558457 -0.335961 -1.057442
S 2.259467 -1.504087 -1.641926
S 3.967146 -2.576540 1.209653
S -1.001084 2.040247 2.097881
S -3.874417 -2.071089 -1.910801
S -4.093852 1.326237 -1.096928
H 5.115116 0.014811 -2.289443
H -5.685132 0.139386 1.513618
H -1.084012 3.862622 -0.594898

E= -5383.561667
S 0.779109 -0.569761 -0.711838
Mo 3.043188 -0.696526 0.280513
S 3.675043 0.082611 -1.932629
S 5.284598 -0.283138 -0.710494
Mo -0.504892 1.540208 -0.307353
S -2.061635 2.558578 1.159151
S -0.194896 2.445250 2.039081
S -2.271878 0.629393 -1.752622
Mo -2.771001 -1.222092 -0.167414
S -4.164928 0.551839 -0.885408
S -3.709709 -1.254327 1.991478
S -0.595713 -0.928282 0.876935
S -3.022440 -3.089620 -1.064453
S 0.493242 2.909916 -1.541926
S 3.165015 -2.732208 0.791775
S 3.066393 0.532745 2.001783
H -3.139232 -2.379833 2.467427
H 5.537053 0.955558 -0.218598
H 0.300583 3.669582 1.736515

[Mo3S13H3]+ XXVII
E= -5383.568544
S -1.292745 0.592904 0.288125
Mo -3.709581 0.387025 0.237224
S -3.174528 -1.255205 -1.519455
S -5.635964 0.354848 -1.136454
Mo 0.338346 -0.833063 -0.278818
S 2.123964 -2.545235 0.534827
S 1.100294 -1.431646 1.882530
S 1.702460 0.111799 -1.812248
Mo 3.320618 1.002869 -0.210905
S 4.100865 -1.472703 0.086248
S 4.485628 -0.144955 1.537397
S 2.122465 2.346618 0.898060
S 4.678544 2.083905 -1.382479
S -0.953819 -2.227988 -1.269101
S -4.108949 2.663303 0.533660
S -4.147353 -0.633744 1.999817
H -6.459361 1.117313 -0.384554
H -3.835923 -2.326176 -1.043460
H -3.592608 2.751547 1.778118

E= -5383.560858
S 1.266430 -0.708808 0.364035
Mo 3.551601 -0.449031 0.209698
S 2.807427 0.752024 -1.910828
S 5.169478 -0.979405 -1.459765
Mo -0.393218 0.865233 -0.164831
S -1.342523 2.931037 0.630095
S -0.253603 1.984608 2.004791
S -1.865045 0.111835 -1.730081
Mo -3.237388 -0.911842 -0.069585
S -4.997870 0.735224 -0.715221
S -5.449049 -0.447562 0.804023
S -1.963041 -0.765460 1.654440
S -3.395556 -2.904911 -0.700128
S 0.981892 1.944733 -1.524852
S 4.288339 -2.406032 1.244913
S 4.103512 1.164174 1.413355
H 6.147420 -1.505130 -0.695301
H 3.646976 1.804322 -1.963687
H 3.917568 -2.065628 2.497749

[Mo3S13H3]+ XXVIII
E= -5383.588410
S -1.179678 -0.104492 0.863800
Mo -3.055702 -0.549438 -0.683006
S -4.272462 -1.174909 1.543003
S -5.176452 -1.519781 -0.256798
Mo 0.344239 1.324158 0.062670
S 0.774838 1.049451 -1.971494
S -4.891858 0.653556 2.364014
S 2.164801 1.104638 1.330701
Mo 3.553077 -0.735010 0.445359
S 4.814407 1.100824 -0.959485
S 5.018167 -0.899061 -1.404802
S 2.158880 -2.271310 0.049848
S 4.649039 -1.251540 2.155552
S -0.514455 3.433979 0.399154
S -2.189506 -1.865292 -2.078554
S -3.439979 1.293403 -1.622088
H 3.786456 1.432525 -1.777946
H -5.746952 0.081875 3.235417
H -0.039186 4.026338 -0.714078

E= -5383.550963
S -1.941626 0.603609 -1.359370
Mo -3.814706 -0.436179 -0.134291
S -2.352946 -2.423183 0.289641
S -4.191637 -2.535522 1.001350
Mo -0.140091 1.169006 -0.189070
S 1.154315 2.707688 -1.366003
S -0.902646 3.128289 0.914977
S 1.277913 -0.541589 -0.599890
Mo 3.685099 -0.763673 -0.259606
S 3.495357 0.458870 1.905016
S 5.329633 -0.023581 1.342107
S 4.349726 0.114305 -2.064987
S 3.940730 -2.850098 -0.315381
S 0.145943 0.462673 2.067973
S -5.271841 -0.444672 -1.648444
S -4.304074 0.992610 1.334609
H 1.813997 1.882145 -2.207585
H -1.632155 3.622180 -0.106868
H -0.516100 1.400826 2.773531

[Mo3S13H3]+ XXIX
E= -5383.564266
S -0.955191 -0.863967 -1.235840
Mo -3.201448 -0.946460 -0.157317
S -1.767219 -0.149719 1.710913
S -3.779876 0.216208 1.827233
Mo -0.452094 1.392913 0.045835
S 1.268712 1.778392 -1.539453
S -1.923477 2.309715 -1.101062
S 1.485305 0.005941 1.554822
Mo 3.288249 -0.886694 0.142282
S 3.167738 1.580351 -0.613746
S 4.316396 0.275742 -1.660443
S 2.466774 -2.635627 -0.709561
S 4.796216 -1.435965 1.489075
S -0.073075 2.855938 1.821722
S -3.828335 -2.942130 -0.084097
S -4.209237 0.091260 -1.723340
H -0.747091 3.929686 1.364859
H -0.254923 -1.691780 -0.438060
H 0.908646 -1.125997 1.999998

E= -5383.540766
S 1.652997 -0.919481 -0.579573
Mo 4.080087 -0.579132 -0.138560
S 3.995341 1.456494 -1.562281
S 5.748839 1.045158 -0.731659
Mo 0.041511 0.669419 0.276451
S -1.080637 0.513883 2.268243
S 0.983779 0.573297 2.400905
S -1.718608 -0.364436 -1.036544
Mo -4.057549 -0.627094 -0.248991
S -4.207537 1.814786 -0.801144
S -5.871533 0.952415 -0.175373
S -3.826606 -1.286170 1.739764
S -4.738712 -2.193700 -1.477603
S -0.003386 2.724417 -0.718386
S 4.895610 -2.403949 -0.791796

S 3.919965 -0.532311 1.972984
H 1.203977 3.136904 -0.265420
H 1.511410 -1.026260 -1.914665
H -1.397624 -1.651183 -1.274370

[Mo3S13H3]+ XXX
E= -5383.567046
S 2.864394 -2.066989 -1.336539
Mo -0.994545 1.367227 -0.144945
S -1.892693 3.357570 1.097465
S -2.743219 2.725740 -0.649281
Mo 3.257871 -0.414291 -0.109800
S 3.952022 -1.114088 1.960134
S 2.201981 -0.031143 1.963294
Mo -2.163235 -1.219560 -0.015679
S -4.252354 -1.863631 -0.774343
S -4.006745 -1.789627 1.258740
S 1.379758 0.925040 -1.085906
S 0.945183 2.605021 0.038644
S -1.692415 0.012303 -2.073076
S 4.974021 0.715204 -1.147000
S -0.582958 -2.865303 -0.004070
S -1.492062 0.171301 1.701471
H -0.906329 -3.353942 -1.223073
H -2.907981 0.440528 -2.468057
H 5.131905 1.609264 -0.143548

E= -5383.541355
S 0.012995 -0.693774 -1.488360
Mo -0.295491 1.382285 -0.410353
S -0.736996 3.784542 0.338519
S -0.834495 2.414636 1.743682
Mo -1.628376 -1.037056 0.308221
S -1.736743 -3.404661 -0.035371
S -3.104603 -2.265973 -0.958506
Mo 2.012189 -0.334162 -0.109347
S 3.658526 -1.003348 1.573183
S 4.458748 0.079417 0.151423
S -2.762774 1.038674 -0.530097
S -1.880362 1.677120 -2.245710
S 0.503552 -1.271424 1.649967
S -2.549025 -0.509304 2.399787
S 2.722080 -1.565932 -1.961480
S 1.941383 1.948136 -0.197896
H 4.065437 -1.619330 -1.799310
H 0.858639 -2.574513 1.611056
H -3.710191 0.079320 2.044115

[Mo3S13H3]+ XXXI
E= -5383.636313
S 0.031250 -0.048426 1.806676
Mo -0.915393 -1.273456 -0.005670
S -2.087823 -2.956988 1.369158
S -2.373609 -3.257192 -0.555758
Mo -0.640034 1.424292 0.024192
S -1.512901 3.010721 1.767402
S -1.710611 3.543574 -0.913621
Mo 1.559054 -0.168495 -0.007081
S 4.078491 -0.465488 -0.488666
S 3.466626 -0.379210 1.473208
S 1.118459 1.576821 -1.647736
S 1.680902 2.355699 0.153483
S -1.976387 0.207033 -1.607913
S -2.871883 0.296516 0.218471
S 1.175511 -2.657097 0.072991
S 0.764286 -1.743184 -1.701348
H -0.662082 4.380580 -0.809098
H 4.433260 0.823423 -0.708485
H -0.440562 3.813213 1.895504

E= -5383.636272
S 0.030961 -0.048663 1.806734
Mo -0.914526 -1.274048 -0.005955
S -2.085068 -2.958539 1.369153
S -2.371127 -3.259995 -0.555449
Mo -0.641136 1.423797 0.024297
S -1.516544 3.009330 1.767100
S -1.710985 3.544101 -0.913469
Mo 1.559009 -0.167453 -0.006960
S 4.078631 -0.462840 -0.488389
S 3.466618 -0.377074 1.473459
S 1.117510 1.577863 -1.647264

S 1.679155 2.356814 0.154217
S -1.976282 0.205832 -1.608271
S -2.872249 0.294401 0.217937
S 1.177393 -2.656190 0.072559
S 0.765436 -1.742439 -1.701707
H -0.661797 4.380227 -0.805894
H 4.432622 0.826307 -0.708090
H -0.446624 3.815388 1.892831

[Mo3S13H3]+ XXXII
E= -5383.619321
S -0.000698 -0.121262 1.807136
Mo -1.372478 -0.766594 -0.026003
S -3.135965 -1.853777 1.319706
S -3.494255 -1.981677 -0.612567
Mo -0.009843 1.597758 0.122096
S 0.020704 2.841180 2.099764
S 0.102747 4.066873 -0.876225
Mo 1.351483 -0.763944 -0.030722
S 3.519589 -2.050973 -0.557777
S 3.016431 -1.770736 1.415834
S 1.634902 1.023644 -1.645014
S 2.532121 1.452993 0.142094
S -1.705533 1.037269 -1.597730
S -2.542095 1.445591 0.218900
S -0.023590 -2.887879 0.029029
S -0.023037 -1.858047 -1.727731
H -0.591909 4.028788 -2.030683
H 4.361101 -1.008199 -0.761519
H -0.895119 4.664990 -0.200075

E= -5383.619348
S -0.000437 -0.122079 1.807957
Mo -1.372520 -0.766289 -0.025233
S -3.134752 -1.851521 1.319045
S -3.495942 -1.983832 -0.612569
Mo -0.009508 1.597854 0.122498
S 0.021437 2.843612 2.097884
S 0.104227 4.066373 -0.878570
Mo 1.351170 -0.764444 -0.030503
S 3.518553 -2.051950 -0.558518
S 3.016441 -1.771985 1.415410
S 1.634641 1.023251 -1.644811
S 2.532706 1.451903 0.142037
S -1.707024 1.036725 -1.596951
S -2.540488 1.448126 0.220468
S -0.023913 -2.887478 0.028754
S -0.024235 -1.857640 -1.728008
H -0.590697 4.028134 -2.032845
H 4.360226 -1.009348 -0.762468
H -0.892938 4.666076 -0.202755

[Mo3S13H3]+ XXXIII
E= -5383.580465
S 0.051428 3.994843 0.299925
Mo 0.018715 1.886444 -0.102405
Mo 1.403360 -0.658717 -0.128619
S 3.568561 -1.840514 -0.773339
S 3.124319 -1.696986 1.225213
S -0.008201 0.201251 1.537854
S -0.277488 -0.001589 3.612492
Mo -1.400299 -0.610135 -0.172765
S -3.184417 -1.590155 1.148880
S -3.596163 -1.731209 -0.857824
S -1.592542 1.241634 -1.771447
S -2.520554 1.683064 -0.017686
S -0.045720 -2.756080 -0.036516
S 0.010697 -1.733698 -1.803249
S 1.686005 1.206683 -1.699299
S 2.598038 1.591637 0.077763
H 0.813466 0.723071 3.933817
H -3.151393 -2.983991 -1.122787
H 4.399948 -0.780056 -0.936093

E= -5383.575860
S 0.942256 3.747983 1.222187
Mo 0.593484 1.821571 0.272560
Mo 1.307172 -0.871800 -0.025861
S 3.148422 -2.655448 -0.283388
S 2.191318 -2.504799 1.532287
S -0.246840 -0.001642 1.566583
S -3.359001 -1.290363 3.519237

Mo -1.225385 -0.130735 -0.613429
S -3.375906 -0.890245 0.218336
S -3.421369 -0.615449 -1.842427
S -0.686078 1.972081 -1.785826
S -1.853623 2.248849 -0.133045
S -0.447235 -2.517692 -0.800579
S 0.268005 -1.216828 -2.202500
S 2.463847 1.036753 -1.061361
S 2.829379 0.868339 0.942870
H -4.684376 -1.529807 3.463852
H -3.178972 -1.874193 -2.279209
H 4.251175 -1.900159 -0.059948

[Mo3S13H3]+ XXXIV
E= -5383.610511
S -1.406676 -2.894788 1.709559
Mo -0.284287 -1.612381 0.440646
S -3.856025 -0.543848 -0.119386
S -1.876650 -0.488219 -0.993984
Mo -0.579923 1.149644 0.273423
S 0.706995 1.539062 -1.783609
S 1.421473 2.543492 -0.139639
Mo 1.851038 0.047498 -0.222473
S 2.000273 -2.442877 0.063384
S 1.056510 -1.819729 -1.640922
S 0.699542 -0.027845 1.872483
S -2.375978 3.022175 0.089228
S -1.799438 2.221568 1.922835
S 4.004458 0.338968 0.851284
S 4.216112 0.238990 -1.193641
H 4.239443 1.554796 -1.515887
H -3.471601 2.255054 -0.136195
S -5.093426 -0.861237 -1.697993
H -5.369296 0.418814 -2.028540

E= -5383.592967
S -1.688394 -2.711642 1.672821
Mo -0.392955 -1.555154 0.478742
S -4.010003 -0.350222 -0.182083
S -1.959229 -0.383081 -0.947957
Mo -0.555199 1.135252 0.249678
S 0.812276 1.538552 -1.745876
S 1.569759 2.464769 -0.067837
Mo 1.986528 0.022491 -0.217111
S 1.875708 -2.472414 0.212117
S 1.021859 -1.859975 -1.561862
S 0.728923 -0.019307 1.873069
S -2.236526 3.059492 0.017725
S -1.902399 2.229909 1.881228
S 4.145355 0.230294 0.786078
S 4.339526 0.019902 -1.260635
H 4.449373 1.314423 -1.644892
H -3.342548 2.363510 -0.350480
S -5.154682 -0.948659 -1.749251
H -5.393298 0.251467 -2.320216

[Mo3S13H3]+ XXXV
E= -5383.612386
S -1.354701 -2.973102 1.624146
Mo -0.232636 -1.648416 0.394919
S 0.688054 -0.064943 1.869787
Mo 1.849365 0.092065 -0.215528
S 4.212368 0.389989 -1.164966
S 3.983157 0.443149 0.879578
S -1.847534 -2.552834 -1.032906
Mo -0.622167 1.100961 0.287018
S -1.834922 2.147216 1.957351
S -2.477801 2.918513 0.135012
S 2.084352 -2.397300 0.034368
S 1.138356 -1.779231 -1.670426
S -3.799670 -0.755491 -0.123898
S -5.107614 -0.446697 -1.648411
S 0.658346 1.567055 -1.759984
S 1.330161 2.566353 -0.095802
H 4.188936 1.711628 -1.462589
H -3.556043 2.120489 -0.061496
H -5.165303 -1.708591 -2.126651

E= -5383.594156
S -1.639894 -2.774503 1.635959
Mo -0.362263 -1.579258 0.457987
S 0.735661 -0.043973 1.873083

Mo 1.987390 0.051065 -0.218766
S 4.337795 0.108790 -1.267166
S 4.143863 0.286214 0.782742
S -1.952165 -0.417883 -0.948242
Mo -0.573742 1.108726 0.268568
S -1.930404 2.159439 1.918489
S -2.304862 2.988675 0.063102
S 1.923014 -2.451173 0.177609
S 1.055973 -1.830149 -1.586982
S -3.999147 -0.438861 -0.168044
S -5.171044 -0.637372 -1.814343
S 0.780394 1.564232 -1.725489
S 1.523858 2.482117 -0.036827
H 4.421835 1.410544 -1.633143
H -3.393848 2.260648 -0.297454
H -5.234795 -1.985609 -1.858786

[Mo3S12H2]+ I
E= -4984.776360
S -1.710621 0.137872 1.786672
Mo -0.060972 0.823817 0.173419
S 1.346177 -0.174917 1.708377
Mo 2.741312 -0.755621 -0.067408
S 1.563973 -0.016906 -1.761168
Mo -2.703390 -0.223262 -0.153822
S 2.863942 -2.845849 -0.101254
S -4.423259 -1.980614 0.848439
S -3.048061 -2.469165 -0.626924
S -1.349848 0.361644 -1.803319
S -4.385125 1.298410 -0.616167
S 4.951954 -0.023896 -0.767539
S 4.596655 0.374714 1.138415
S 0.711415 2.912996 -0.739434
S -0.488640 2.930765 0.924696
H -3.747464 -2.406463 1.940926
H -5.342352 0.838331 0.214416

E= -4984.725942
S 1.732702 1.788274 -0.564652
Mo -0.642659 1.612724 0.017833
S -1.159207 0.212641 -1.676345
Mo -1.687891 -1.231310 0.112715
S -2.159273 0.368165 1.576928
Mo 2.078551 -0.374009 0.233525
S 0.348193 -2.134835 0.508935
S 4.024764 -0.518382 -1.418491
S 2.472068 -1.849041 -1.578938
S 0.792383 0.990393 1.823810
S 3.565944 -0.683373 1.959468
S -3.166594 -2.926247 0.572540
S -3.286621 -2.255369 -1.343122
S -2.305384 3.240206 0.189469
S -0.721168 3.780543 -0.941887
H 3.660442 0.425235 -2.321156
H 4.718595 -0.943862 1.306675

[Mo3S12H2]+ II
E= -4984.794906
S 1.053183 -0.552918 -1.469111
Mo -0.292531 0.700331 -0.049562
S -1.940472 1.088365 -1.549011
Mo -2.779749 -0.572707 -0.152433
S -1.241411 -0.570267 1.581658
Mo 2.771153 -0.670768 0.110220
S 3.022386 -2.713786 0.544914
S 5.222952 0.001210 0.361357
S 4.288867 0.283254 -1.460917
S 1.996453 0.455973 1.782115
S -0.267333 2.740839 1.168694
S 0.732328 3.057415 -0.610537
S -4.678018 -0.601221 1.383697
S -5.046269 0.341570 -0.319554
S -2.652025 -2.402504 -1.143712
H -0.284507 3.533166 -1.368160
H 5.081583 1.232003 0.909182

E= -4984.778473
S -1.759771 0.968832 1.458220
Mo 0.079439 0.607621 -0.040251
S 1.233393 -0.572762 1.547183
Mo 2.817068 -0.530185 -0.140602
S 1.959393 1.100369 -1.469108

Mo -2.584888 -0.749960 0.225184
S -2.480702 -2.513710 1.345112
S -4.535058 -1.284835 -1.377197
S -4.769960 0.126717 0.122188
S -1.013092 -0.777922 -1.486703
S 0.067474 2.979209 -0.300255
S -1.748963 3.826142 0.183166
S 5.074040 0.416400 -0.316858
S 4.684491 -0.415050 1.439204
S 2.814356 -2.375708 -1.117049
H -1.275772 5.089663 0.116237
H -4.221828 -0.486610 -2.424573

[Mo3S12H2]+ III
E= -4984.751316
S 0.761563 -1.217803 -1.164091
Mo -0.496630 0.178224 0.098312
S -2.057276 0.975239 -1.420528
Mo -3.292131 -0.365679 -0.077461
S -1.889299 -0.905645 1.615839
Mo 2.875833 -0.641558 -0.026399
S 3.880483 -2.463738 0.086846
S 4.851702 0.718622 -0.845904
S 3.261160 0.403169 -2.112984
S 1.342743 -0.595650 1.837025
S 3.032885 0.574299 1.986948
S 0.353782 2.244454 0.571352
S -0.880400 3.828162 0.022522
S -4.980569 -1.745656 -0.800059
S -5.556961 -0.057694 0.220704
H -0.105045 4.759937 0.611477
H 4.531028 1.934456 -0.341187

E= -4984.737367
S 0.842491 -0.503524 -1.410215
Mo -0.518974 0.550335 0.169723
S -2.362926 1.172253 -1.336353
Mo -3.448744 -0.313144 -0.107682
S -1.895033 -0.998174 1.357406
Mo 2.855113 -0.718743 -0.078365
S 3.461824 -2.713759 -0.175535
S 5.176633 0.264767 -0.486706
S 3.688225 0.527155 -1.895047
S 1.168068 -0.701477 1.690687
S 2.973395 0.226223 2.068613
S -0.029809 2.504086 1.391403
S 0.415349 2.991556 -0.561934
S -5.106795 -1.662587 -0.930469
S -5.681504 -0.155705 0.377404
H -0.744726 3.580260 -0.935223
H 5.075450 1.431884 0.192772

[Mo3S12H2]+ IV
E= -4984.704593
S -0.042202 -1.502096 -0.324234
Mo 2.339705 -0.640504 -0.086688
S 3.995562 -1.948678 -1.038937
S 4.527332 -0.791220 0.584187
Mo -0.123725 1.340604 -0.071157
S -0.841032 3.438257 -0.072786
S 0.271985 3.596948 0.705473
Mo -2.334531 -0.770214 -0.101659
S -3.475663 -2.747347 -0.456638
S -4.502368 -1.274198 0.554604
S 1.836253 1.113085 -1.448040
S 1.473767 0.779287 1.831184
S -1.837668 0.575101 -1.787914
S -2.184458 1.085857 1.490521
S 1.050333 -2.284521 1.215032
H -1.659747 0.450222 2.558615
H 2.289437 1.846958 1.741456

E= -4984.746188
S 1.455820 0.025957 -1.849810
Mo 0.986771 -1.268419 0.118347
S 2.379944 -3.203496 -0.624716
S 2.335050 -2.917780 1.324038
Mo 0.551698 1.337272 -0.020300
S 1.180142 3.518860 -1.039050
S 1.543732 3.423124 0.889826
Mo -1.900386 -0.278166 -0.046160
S -3.868626 -1.508255 -0.624068

S -4.057759 -0.140419 0.850289
S -2.879883 0.393085 -0.434588
S 0.823555 0.088603 2.116331
S -1.364368 1.204275 -1.615120
S -1.559235 1.868374 1.219553
S -0.850615 -2.310154 -0.655053
H -1.299273 1.508794 2.495839
H 2.139420 0.207606 2.402825

[Mo3S12H2]+ V
E= -4984.738402
S 1.810471 0.946178 -1.192385
Mo -0.316723 0.907445 0.027832
S -1.756669 0.807764 -1.710910
Mo -2.636409 -0.740345 -0.214657
S -1.713121 -0.042983 1.747041
Mo 3.058066 -0.464932 0.086822
S 5.553647 0.037349 -0.567159
S 4.666613 -1.833714 -0.841470
S 0.913336 -1.242587 0.842577
S 2.292854 -0.546327 2.267126
S -0.563145 2.790933 1.325547
S -0.001513 3.512724 -0.534912
S -4.828712 -0.941576 0.853115
S -4.912913 -0.314388 -1.026746
S -1.995945 -2.668454 -0.724807
H -1.225740 3.868632 -0.989882
H 5.380070 0.561611 -1.802292

E= -4984.738420
S 1.809668 0.945310 -1.193363
Mo -0.316867 0.908180 0.027435
S -1.757979 0.809046 -1.710461
Mo -2.636065 -0.739988 -0.214393
S -1.713698 -0.041457 1.747170
Mo 3.056849 -0.466676 0.085416
S 5.553440 0.037116 -0.563976
S 4.667320 -1.833892 -0.841760
S 0.912369 -1.241299 0.844845
S 2.294041 -0.544059 2.266796
S -0.563090 2.792030 1.324513
S -0.000750 3.513151 -0.535970
S -4.827803 -0.942616 0.854162
S -4.913396 -0.319467 -1.026985
S -1.992715 -2.667317 -0.724042
H -1.224748 3.869385 -0.991314
H 5.381712 0.562662 -1.798817

[Mo3S12H2]+ VI
E= -4984.772062
S 1.043975 0.873385 -1.061974
Mo -0.864885 1.287866 -0.053132
S -2.543954 1.283064 -1.539962
Mo -2.905997 -0.603553 -0.200567
S -1.431678 -0.146363 1.571673
Mo 3.041470 -0.242429 0.032659
S 5.388162 -0.264513 -0.430311
S 4.224963 0.632013 -1.812151
S 1.754051 -2.195518 0.212223
S 3.592996 -2.335910 1.042883
S 2.821357 1.205301 1.777331
S -0.767108 3.395994 0.873775
S -4.728912 -1.181534 1.322020
S -5.332619 -0.406071 -0.399181
S -2.221325 -2.288926 -1.224449
H -2.008961 3.472629 1.395898
H 3.845782 0.833489 2.577769

E= -4984.772063
S 1.043697 0.873193 -1.060629
Mo -0.865269 1.287213 -0.051860
S -2.543983 1.284061 -1.539125
Mo -2.906599 -0.603724 -0.201519
S -1.432846 -0.148131 1.571700
Mo 3.042433 -0.241756 0.032472
S 5.387367 -0.263951 -0.439306
S 4.220692 0.618340 -1.822439
S 1.751445 -2.190690 0.229794
S 3.593407 -2.329928 1.053904
S 2.831488 1.217329 1.768757
S -0.767221 3.394541 0.876820
S -4.730122 -1.182297 1.320255

S -5.333081 -0.406261 -0.400950
S -2.221654 -2.288100 -1.226810
H -2.009073 3.470902 1.398993
H 3.858349 0.848720 2.567571

[Mo3S12H2]+ VII
E= -4984.786073
S 1.075094 -0.396985 -1.193624
Mo -0.464657 0.781757 -0.075123
S -2.183510 1.282412 -1.445088
Mo -2.915695 -0.544665 -0.179907
S -1.371807 -0.542579 1.552682
Mo 3.184353 -0.739254 0.039948
S 3.716432 -2.546192 -0.858241
S 5.109566 0.486343 0.312599
S 3.751452 1.332008 -0.972902
S 2.429776 -1.150249 2.189756
S 0.040962 2.431629 1.469950
S 0.567108 3.183961 -0.395375
S -4.779981 -0.800077 1.380260
S -5.237418 0.231891 -0.248755
S -2.701159 -2.283540 -1.311548
H -0.556317 3.886316 -0.672779
H 2.123999 -2.453459 2.030827

E= -4984.776838
S 1.047543 -0.978960 -1.073458
Mo -0.308476 0.532653 0.090697
S -1.761591 0.903558 -1.622541
Mo -2.883170 -0.524730 -0.180909
S -1.536804 -0.480394 1.711172
Mo 3.070157 -0.742760 0.074774
S 3.839077 -2.622948 0.532506
S 4.619983 1.163958 0.140732
S 4.346273 0.388630 -1.665713
S 1.801463 0.109313 1.964336
S -0.248632 2.674561 1.115565
S 0.912892 2.777501 -0.587486
S -4.919023 -0.223412 1.139483
S -5.031830 0.534778 -0.687630
S -2.831903 -2.451006 -0.979233
H 0.000093 3.220420 -1.485182
H 1.303296 -1.086491 2.329855

[Mo3S12H2]+ VIII
E= -4984.744119
S -1.009107 0.152264 1.432514
Mo 0.470807 0.914061 -0.017701
S 2.327725 1.653616 1.039871
Mo 2.873768 -0.481851 0.263357
S 1.197353 -0.839018 -1.308964
Mo -3.070411 -0.509967 0.164997
S -5.273993 0.332888 -0.056394
S -3.943244 1.599287 0.743582
S -1.865183 -2.660086 -0.599673
S -3.920117 -2.621428 -0.494853
S -0.211972 2.082542 -1.915665
S -0.466045 3.342807 -0.281103
S 4.596920 -1.236145 -1.301284
S 5.224432 0.142238 -0.022984
S 2.685619 -1.846816 1.829246
H 0.684237 4.050319 -0.356878
H -1.677355 -2.418884 -1.919239

E= -4984.744909
S -0.983797 0.182679 1.658231
Mo 0.361734 0.897143 0.057120
S 2.266666 1.765790 0.913286
Mo 2.833508 -0.389696 0.209874
S 1.053756 -0.893565 -1.195292
Mo -2.922138 -0.575564 0.245089
S -4.986490 0.323828 -0.492528
S -3.989685 1.423678 0.859201
S -1.839256 -2.910410 0.137063
S -3.254306 -2.381175 -1.261819
S -0.552432 1.914103 -1.829381
S -0.694950 3.273736 -0.260069
S 4.450182 -1.173825 -1.451250
S 5.125300 0.299885 -0.310940
S 2.825306 -1.672603 1.856228
H 0.414572 4.009228 -0.498954
H -2.609681 -3.582278 1.027813

[Mo3S12H2]+ IX
E= -4984.719562
S 0.827498 -0.287842 -1.601495
Mo -0.451005 0.342116 0.187508
S -2.166320 0.783577 -1.598602
Mo -3.446626 -0.214693 -0.112098
S -1.985595 -0.926256 1.466258
Mo 2.863714 -0.516460 -0.241904
S 3.896807 -2.108924 -1.070950
S 4.855578 0.881680 0.409472
S 3.512251 1.268016 -1.881058
S 1.124189 -1.502465 1.103375
S 2.755278 -0.804749 2.126063
S 0.901497 1.710992 1.551031
S -0.494794 2.659245 0.388340
S -5.337688 -1.345767 -0.727468
S -5.607747 0.437062 0.291508
H 2.751641 2.243809 -1.347146
H 4.177641 1.862643 1.036328

E= -4984.719723
S 0.825799 -0.221942 -1.620742
Mo -0.445349 0.323844 0.199916
S -2.166323 0.865083 -1.552499
Mo -3.448362 -0.202820 -0.116612
S -1.987330 -0.992619 1.422742
Mo 2.858320 -0.502533 -0.264547
S 3.905766 -2.032613 -1.188534
S 4.844671 0.870033 0.456404
S 3.471017 1.385544 -1.793581
S 1.122780 -1.574146 1.015990
S 2.749700 -0.936863 2.082821
S 0.928430 1.611547 1.617553
S -0.455562 2.632909 0.500480
S -5.343542 -1.297783 -0.783069
S -5.606746 0.434667 0.321142
H 2.701639 2.313814 -1.191579
H 4.166245 1.808450 1.144493

[Mo3S12H2]+ X
E= -4984.769232
S 2.420934 -0.680194 2.210784
Mo -1.966776 -1.177558 0.071612
S -1.411726 0.358054 1.742094
Mo -1.045967 1.551440 -0.110804
S -1.581391 0.174855 -1.799559
Mo 3.027505 -0.194796 0.257906
S 4.798996 0.923852 0.373169
S 2.346356 -1.256433 -2.034601
S 3.604552 -2.255990 -0.752898
S -0.519730 -2.698325 0.102894
S 1.474347 1.650520 -0.451511
S -4.100949 -1.999354 -0.783647
S -4.004999 -1.892460 1.194677
S -0.669466 3.923981 -0.238874
S -2.580231 3.233547 -0.064572
H 1.804971 2.539736 0.499737
H 1.147916 -1.774198 -1.653016

E= -4984.728489
S 1.499133 0.822906 -1.719337
Mo -0.161340 1.620509 0.016084
S -1.559430 0.546605 -1.625511
Mo -2.170652 -0.736655 0.134025
S -2.088465 0.786747 1.641230
Mo 2.022303 -0.818153 -0.325133
S 2.347988 -2.515278 -1.546441
S 3.717838 -1.619952 1.551004
S 4.177271 -0.070665 0.256724
S 1.136181 0.757253 1.589295
S -0.116796 -2.060429 0.594062
S -0.989502 3.692707 0.621949
S 0.493046 3.704101 -0.778180
S -3.563248 -2.755961 0.308580
S -4.429440 -1.209448 -0.582805
H -0.268243 -3.113675 -0.230830
H 3.281949 -0.903151 2.612736

[Mo3S12H2]+ XI
E= -4984.735767
S -1.542682 0.498257 1.699241

Mo 0.009380 1.467929 0.003285
S 1.630851 0.357030 1.684594
Mo 2.055242 -0.876383 -0.056385
S 1.580733 0.454049 -1.730410
Mo -1.892149 -0.850851 0.034847
S -3.625856 -2.546720 0.953368
S -4.113407 -1.203574 -0.560179
S -1.503727 0.700683 -1.723409
S -1.878487 2.609184 -1.096825
S 0.007293 -2.353840 -0.300351
S 1.526915 3.341471 -0.142048
S 0.236413 3.541170 1.335566
S 3.139667 -2.996089 -0.096595
S 4.298060 -1.296409 -0.037786
H 0.020221 -3.144679 0.790501
H -3.356452 -3.647850 0.213421

E= -4984.732523
S 1.554977 0.557742 -1.681223
Mo -0.079185 1.444415 -0.030714
S -1.636683 0.322994 -1.684469
Mo -2.032167 -0.934795 0.056388
S -1.568692 0.390477 1.737380
Mo 1.945135 -0.795140 -0.031636
S 3.693264 -2.500259 -0.906137
S 4.183816 -1.082651 0.537608
S 1.491215 0.764728 1.700759
S 1.818619 2.657816 1.030668
S 0.068534 -2.337639 0.294782
S -1.663200 3.388295 0.210688
S -0.409918 3.506113 -1.302676
S -3.053771 -3.082058 0.107443
S -4.262797 -1.418063 0.208380
H 0.085400 -3.115559 -0.805105
H 3.449869 -3.571995 -0.115723

[Mo3S12H2]+ XII
E= -4984.740170
S -1.142166 -1.784013 -1.321793
Mo 1.060904 -1.474907 -0.007803
S 1.878926 -0.052181 -1.615781
Mo 1.159031 1.375748 0.006234
S 2.615153 -0.095762 1.466818
Mo -2.063977 -0.215646 -0.101115
S -1.100523 1.667199 -1.341278
S -2.297738 2.498156 0.186407
S -3.455766 -0.867786 1.685610
S -4.367676 -0.475023 -0.109864
S -0.211234 0.002199 1.479912
S 2.700056 2.958688 0.617681
S 1.220990 3.658690 -0.571815
S 2.594932 -3.095333 0.503748
S 1.133386 -3.748469 -0.719088
H -3.385464 2.711533 -0.583294
H 3.741827 -0.151605 0.727081

E= -4984.726671
S 1.289553 1.739241 -1.296919
Mo -0.975390 1.579802 -0.032721
S -1.771945 0.203132 -1.626072
Mo -1.266336 -1.348949 0.025695
S -2.614240 0.267769 1.409956
Mo 2.124915 0.081685 -0.126199
S 0.962892 -1.811327 -1.226523
S 2.093487 -2.628084 0.383524
S 3.590556 0.662034 1.616653
S 4.437284 0.096578 -0.167465
S 0.223421 0.050830 1.428468
S -2.938812 -2.841217 0.686641
S -1.673524 -3.545068 -0.742062
S -2.375715 3.311117 0.574021
S -0.879714 3.840802 -0.680955
H 3.130751 -3.046875 -0.396295
H -3.716566 0.387352 0.642691

[Mo3S12H2]+ XIII
E= -4984.707163
S -0.396114 -2.147069 -0.483718
Mo 1.630846 -0.999888 0.039457
S 1.651352 0.461122 -1.733886
Mo 0.820574 1.833213 -0.097705
S 2.740983 0.970666 1.309517

Mo -1.897140 -0.498258 0.076839
S -1.354991 1.562934 -1.240596
S -2.824866 2.102355 0.180923
S -3.890455 -1.673449 0.359312
S -3.565153 -0.989003 -1.527683
S 0.114559 0.208165 1.801951
S -1.688236 -0.565968 2.415731
S 1.432967 3.814904 -0.396956
S 3.773030 -1.889496 0.249229
S 2.560255 -2.938001 -0.967375
H -3.863446 2.012281 -0.678492
H 3.730408 1.240305 0.434472

E= -4984.706641
S -0.322501 -2.229601 -0.257419
Mo 1.666630 -0.985055 0.024887
S 1.657151 0.456107 -1.755432
Mo 0.764205 1.873053 -0.112176
S 2.795876 1.072515 1.163705
Mo -1.868577 -0.542874 0.108692
S -1.315210 1.371070 -1.400273
S -2.883467 1.998196 -0.134251
S -3.831860 -1.714955 0.510734
S -3.508056 -1.269374 -1.447202
S 0.152792 0.355606 1.772401
S -1.679209 -0.292570 2.440993
S 1.062632 3.941959 -0.262993
S 3.802501 -1.842439 0.284031
S 2.602801 -2.944353 -0.920975
H -3.873740 1.733864 -1.015416
H 3.723728 1.336355 0.223382

[Mo3S12H2]+ XIV
E= -4984.760992
S -1.322159 0.929382 -0.335806
Mo -0.155315 -1.090889 -0.464267
S -1.255380 -2.311433 -1.736745
Mo -3.608728 0.719041 0.139729
S -4.315603 2.671686 0.438931
S -3.923478 -0.473112 1.859870
S -4.771574 -0.312070 -1.571579
S 0.803638 -2.628101 1.170390
S -0.725903 -1.571423 1.861655
S 1.726076 -0.569760 -1.581149
Mo 3.127739 0.784013 -0.112146
S 3.501288 2.455009 -1.335211
S 4.624460 -1.107018 -0.125927
S 5.380750 0.483368 0.940083
S 1.942872 1.292657 1.570372
H 5.012546 0.157089 2.203507
H -4.927575 0.784984 -2.340920

E= -4984.764352
S -1.387634 -0.450828 -1.668370
Mo -0.033319 0.736772 -0.053205
S -1.805204 0.670633 1.749947
Mo -3.024399 -0.637928 -0.128810
S -4.775266 -1.149984 -1.159239
S -3.454130 1.455897 0.746235
S -2.660870 -2.445583 1.291985
S 0.414457 3.052614 0.565702
S -0.804740 2.915763 -0.987859
S 1.124637 -0.418378 1.615416
Mo 2.691650 -0.649686 -0.055444
S 2.777807 -2.674427 -0.594404
S 4.454935 0.049459 1.356884
S 5.131184 -0.053068 -0.597073
S 1.836438 0.630784 -1.670678
H 4.985978 1.238557 -0.976022
H -3.236932 -3.429331 0.572539

[Mo3S12H2]+ XV
E= -4984.755257
S 0.185477 0.326574 -1.563164
Mo -1.852872 -0.679721 -0.482361
S -3.124105 -0.401054 1.458838
S -2.448989 -2.286674 1.129246
Mo 1.635180 -0.810927 0.073080
S 3.305866 -0.235817 -1.571843
S 3.866718 -1.354359 0.015910
Mo 0.345507 1.940842 0.107149
S 1.490514 3.562618 -0.534816

S94

S -3.108420 -0.877954 -2.137262
S -0.048403 -2.523979 -0.809369
S 1.408203 0.727691 1.763761
S 1.535968 -2.322741 1.940315
S -2.047874 1.946623 -0.349515
S -1.445737 2.621841 1.503186
H 1.404660 -3.501474 1.302034
H 0.116665 -2.330957 -2.137096

E= -4984.725528
S 1.437304 2.159274 -0.200545
Mo -1.340572 -1.469322 0.006058
S -3.221762 -2.449451 -1.019590
S -1.809452 -3.711906 -0.233860
Mo 1.871803 -0.346292 0.083148
S 3.868978 0.208782 -0.962461
S 3.701233 -1.723883 -0.313967
Mo -1.012571 2.164308 -0.066851
S -1.803154 3.951983 0.633673
S 0.129371 -0.674416 -1.497977
S 0.777801 -2.383180 1.113678
S 0.339467 2.655661 -1.900224
S 1.896712 0.381079 2.313961
S -2.835931 0.559846 0.148468
S -1.405705 0.366241 1.661434
H 1.984178 -0.774167 3.005292
H 1.034292 -3.311472 0.174377

[Mo3S12H2]+ XVI
E= -4984.750506
S 1.339283 -1.076292 -0.621810
Mo -0.440206 0.089092 0.053100
S 0.414644 2.153275 0.506863
Mo 3.681461 -0.304625 -0.125341
S 4.104791 -1.312327 1.664481
S 2.552464 2.087026 0.078566
S 5.303121 1.485836 -0.250628
S 4.445848 -1.379962 -1.762242
S -2.175474 0.466443 1.857173
S -0.853702 -1.117100 2.024022
S -1.701194 -0.045653 -1.837254
Mo -3.264538 -0.302708 -0.143956
S -5.028997 1.308109 0.418808
S -4.943966 0.811896 -1.493095
S -3.882311 -2.289355 -0.004370
H 5.260011 1.910267 1.026205
H 2.525730 2.385482 -1.234158

E= -4984.698490
S 0.975667 -0.428369 0.780959
Mo -0.514516 1.013637 -0.031694
S 0.921382 2.084024 -1.410227
Mo 3.371642 -0.793967 0.222772
S 4.177697 -0.545609 2.145802
S 2.939175 1.227239 -1.365778
S 5.273428 -0.305297 -1.209934
S 3.172623 -2.835096 -0.239851
S -1.720456 3.308739 0.100147
S -0.917759 2.584023 1.750108
S -1.833784 -0.012391 -1.706801
Mo -3.273411 -0.757389 -0.110240
S -5.559595 -0.845643 -0.314023
S -4.544059 -2.650141 -0.310313
S -2.330193 -0.252857 1.759320
H 5.771334 0.739236 -0.522335
H 2.846637 0.586993 -2.543374

[Mo3S12H2]+ XVII
E= -4984.719567
S -0.924622 -0.665142 -0.323608
Mo 0.059255 1.262241 0.407460
S -0.852965 2.093752 2.101801
Mo -3.355213 -0.795491 -0.332573
S -4.022691 0.963400 -1.303355
S -3.230306 -1.033001 2.149027
S -5.047145 -1.120438 1.376605
S -3.649401 -2.467346 -1.574306
S 1.073908 2.781246 -1.094485
S -0.962041 2.672271 -1.458888
S 2.123085 0.414583 1.198402
Mo 3.618917 -0.637799 -0.100291
S 2.932976 -1.370923 -1.933284

S 6.084895 -0.132991 0.117720
S 5.307497 -1.885139 0.926726
H 6.494181 -0.564504 -1.100696
H -1.389510 3.744185 -0.750030

E= -4984.719668
S -0.923149 -0.672157 -0.310380
Mo 0.057304 1.265119 0.402796
S -0.846406 2.107253 2.096405
Mo -3.351304 -0.802295 -0.329140
S -4.010603 0.941748 -1.332455
S -3.252613 -0.997679 2.158700
S -5.062135 -1.088339 1.370134
S -3.644937 -2.494415 -1.542917
S 1.071640 2.773708 -1.109986
S -0.964090 2.657630 -1.473833
S 2.123786 0.420749 1.193462
Mo 3.621055 -0.635987 -0.098333
S 2.940320 -1.370189 -1.932829
S 6.087225 -0.135997 0.128274
S 5.303332 -1.885519 0.936542
H 6.500322 -0.569758 -1.088056
H -1.394543 3.733931 -0.773437

[Mo3S12H2]+ XVIII
E= -4984.761464
S -0.455349 -1.713075 1.716560
H -0.354034 -0.803015 2.709376
Mo 1.343755 -1.099818 0.008322
S 3.279240 -2.099912 1.117581
S 2.950484 -2.783199 -0.715111
Mo -1.726942 -0.607556 -0.087698
S -3.973012 -0.917503 0.506560
S -3.395304 -2.003423 -0.843991
S -1.592631 1.379251 1.507192
H -2.540708 2.134153 0.920575
Mo 0.358942 1.777513 -0.054518
S -1.294059 1.022042 -1.616209
S 0.110132 4.003372 0.482391
S 1.506473 3.575188 -0.953920
S 1.828853 0.421146 -1.539654
S 1.558608 0.771172 1.583948
S -0.278867 -2.240147 -1.139249

E= -4984.743805
S -0.654144 -1.909382 1.499959
H -0.507200 -1.177882 2.625039
Mo 1.288715 -1.213978 -0.049327
S 2.549156 -3.109747 0.813553
S 3.379552 -2.175486 -0.727772
Mo -1.816034 -0.419499 -0.084913
S -4.012744 -0.387481 0.661790
S -3.595351 -1.662435 -0.883342
S -1.401421 1.383609 1.671991
H -2.280768 2.295497 1.219630
Mo 0.545463 1.598187 -0.041895
S -1.415004 1.310013 -1.453457
S 1.576428 3.586082 0.881817
S 0.627509 3.963271 -0.809293
S 1.779677 0.602504 -1.637560
S 1.662402 0.297090 1.633853
S -0.369439 -1.874736 -1.429478

[Mo3S12H2]+ XIX
E= -4984.769232
S -1.030407 0.176595 1.096194
Mo 0.897597 1.030368 0.324740
S 1.207947 3.385961 0.801751
S -0.086235 3.103179 -0.676047
S 1.037854 -0.537645 -1.524103
S 2.447032 0.959093 -1.604768
Mo -2.987562 -0.393102 -0.245236
S -4.135939 -0.310437 1.878377
S -5.372302 -0.851945 0.328546
S -3.219872 1.171000 -1.641876
S -2.470680 -2.214512 -1.189347
S 2.434250 0.357949 1.887850
Mo 2.787987 -1.005438 0.081080
S 2.311839 -2.967858 0.653366
S 5.046951 -1.169835 -0.400058
H 5.298966 0.043160 -0.926561
H -5.342870 -2.204639 0.423881

E= -4984.752666
S -0.460747 -2.003915 0.898449
Mo -2.277777 -0.643556 0.344728
S -1.175395 3.011210 -0.090753
Mo 0.815734 1.654011 0.028366
S 1.820817 3.696770 -0.508637
Mo 1.446060 -1.077298 -0.031988
S 0.493619 0.302111 -1.719655
S 2.720576 -2.555708 -1.464261
S 2.870123 -3.088220 0.441457
S 1.835012 0.427538 1.840274
S 3.154976 0.717884 0.305120
S -2.824300 -1.477464 -1.787826
S -3.383955 0.507923 -1.629714
S -3.760272 -1.106206 1.729147
S -1.299053 1.463317 1.270693
H 3.105490 3.356992 -0.719708
H -2.296579 1.126569 -2.155447

[Mo3S12H2]+ XX
E= -4984.746851
S 0.934754 1.355095 -1.592216
Mo -0.831846 1.541389 -0.283309
S -2.437831 3.271349 -0.290346
S -0.718275 3.658028 0.725037
S -0.392426 0.105067 1.420807
Mo 2.007647 -0.089202 0.208959
S 3.576491 -0.048221 -1.556140
S 4.474818 -0.876591 0.083831
S 2.582738 1.267350 1.718819
S 1.597986 -2.305069 0.926091
S -2.505675 0.282478 -1.408465
Mo -1.880425 -1.378821 -0.049034
S -2.593539 -3.146912 -0.949764
S 0.462549 -2.064550 -0.758331
S -3.230132 -1.518056 1.850047
H -2.710329 -0.568702 2.652472
H 4.281264 -2.192222 -0.180204

E= -4984.731851
S 0.879665 1.457290 -1.390065
Mo -1.008237 1.542097 -0.198444
S -1.580320 3.939808 -0.739138
S -1.363874 3.477384 1.182217
S -0.318480 0.106943 1.456699
Mo 2.027085 -0.077015 0.224680
S 3.462127 0.006436 -1.645982
S 4.478667 -0.892641 -0.115034
S 2.730447 1.211854 1.733041
S 1.635574 -2.328076 0.852249
S -2.670297 0.384425 -1.222286
Mo -1.849874 -1.461644 -0.075249
S -2.671465 -3.017567 -1.231023
S 0.423548 -2.148596 -0.793192
S -2.943268 -1.996639 1.894116
H -2.333316 -1.159419 2.756358
H 4.239248 -2.194943 -0.403439

[Mo3S12H2]+ XXI
E= -4984.742982
S 0.126274 -0.843123 1.410119
Mo -2.098000 -1.003033 -0.096669
S -2.530128 1.025938 0.909107
Mo -0.334165 1.265162 0.212963
S -0.263556 -0.617261 -1.529330
Mo 1.806161 -0.707605 -0.185751
S 2.640288 0.700618 -1.915512
S -0.568458 3.703122 -0.123008
S -0.400634 2.646342 -1.777649
S 2.008391 1.626392 0.932893
S 0.633633 1.935148 2.404688
S 2.428179 -2.879414 -0.610802
S 3.540159 -1.846880 0.799815
S -3.613689 -1.227016 -1.526642
S -2.361155 -2.842087 1.287914
H -3.588252 -3.235488 0.889515
H 3.651576 -0.163023 -2.157811

E= -4984.734067
S -0.095965 -0.913446 -1.394193
Mo 2.053154 -1.077194 0.133860

S 2.635244 0.920386 -0.883410
Mo 0.446557 1.247967 -0.255568
S 0.233856 -0.503332 1.566612
Mo -1.794388 -0.556069 0.244195
S -2.794973 0.480348 2.108128
S 0.820466 3.695223 -0.033083
S 0.462006 2.748776 1.654037
S -1.933325 1.664181 -0.878544
S -0.607723 1.824978 -2.417532
S -2.480872 -2.841269 0.066310
S -3.873754 -1.589051 -0.603886
S 3.503368 -1.348718 1.627987
S 2.314066 -2.961372 -1.193165
H 3.496474 -3.394897 -0.710139
H -4.038368 0.750091 1.657493

[Mo3S12H2]+ XXII
E= -4984.739784
S -0.132861 -0.827695 -1.510664
Mo 1.903617 -0.664013 -0.181615
S 1.971700 1.380792 -1.423314
Mo -0.126425 1.389719 -0.485452
S 0.198824 -0.206905 1.405536
Mo -1.946452 -0.634348 0.225811
S -3.051190 0.259309 2.072697
S -0.275763 3.847855 -0.514440
S -0.034308 3.056966 1.279473
S -2.351297 1.266181 -1.098204
S -2.261876 -2.971096 0.390869
S -3.439866 -2.028606 -0.937120
S 3.443274 -1.433571 1.719379
S 3.838007 0.277310 0.831172
S 2.464740 -2.653085 -1.215211
H 3.603499 -2.941769 -0.543228
H -2.404686 -0.374544 3.073249

E= -4984.742764
S -0.136883 -0.871780 -1.447748
Mo 1.903210 -0.670212 -0.082480
S 2.076556 1.263431 -1.295827
Mo -0.139769 1.362703 -0.469439
S 0.104801 -0.163898 1.456758
Mo -1.996115 -0.614007 0.220050
S -3.131003 0.423659 1.976025
S -0.142455 3.812534 -0.692645
S 0.111298 3.186020 1.160655
S -2.322698 1.292914 -1.154257
S -2.364479 -2.920427 0.454269
S -3.483572 -2.007365 -0.951399
S 3.286286 -0.615574 1.944066
S 4.347761 -0.618658 0.291591
S 2.212955 -2.776908 -1.019418
H 3.470768 -3.066264 -0.620651
H -2.635527 -0.293867 3.006042

[Mo3S12H2]+ XXIII
E= -4984.737906
S 1.450927 1.939589 0.271933
Mo -0.913789 1.400280 0.160513
S -1.270788 0.450161 -1.860164
Mo -1.289327 -1.218225 -0.195893
S -2.646387 0.211809 1.226189
Mo 2.080184 -0.287614 0.245005
S 0.738464 -2.231315 -0.500693
S 3.203669 -0.991121 2.111012
S 4.314572 0.486867 -0.851742
S 3.075101 -0.817858 -1.833883
S 0.045030 -0.298363 1.635275
S -2.555316 -3.169387 0.592452
S -3.197004 -2.374265 -1.118958
S -2.322462 3.302290 0.595072
S -1.037849 3.709521 -0.842069
H 3.911136 1.669457 -1.374915
H 4.484738 -0.722789 1.779896

E= -4984.736298
S 1.412032 1.944920 -0.104195
Mo -1.005344 1.564975 0.037372
S -1.362497 0.193864 -1.746307
Mo -1.371822 -1.312583 0.005251
S -2.719699 0.235131 1.199955
Mo 2.134478 -0.209647 0.270606

S 0.831672 -2.165647 -0.254653
S 3.193774 -0.597013 2.274702
S 4.412293 0.463123 -0.816195
S 3.251161 -1.015097 -1.643469
S 0.011219 -0.063923 1.546119
S -3.291782 -2.635252 0.266193
S -1.966174 -3.517167 -0.935445
S -2.666487 3.161673 0.160963
S -0.997563 3.799281 -0.799611
H 4.011069 1.532450 -1.544891
H 4.454652 -0.190069 2.020363

[Mo3S12H2]+ XXIV
E= -4984.736729
S -0.671259 -1.674783 -1.334468
Mo 1.159406 -1.267053 -0.171969
S 2.013685 0.292751 -1.757632
Mo 1.668598 1.768214 -0.077421
S 2.157144 0.471720 1.628150
Mo -1.958471 0.190484 0.173820
S -0.532074 2.250417 -0.008143
S -3.296487 1.360720 1.656809
S -4.034425 -0.473490 -1.135582
S -2.700391 0.861025 -1.958839
S -0.416666 -0.917918 1.774021
S -2.212116 -1.821300 1.477401
S 2.823968 3.516326 -0.170236
S 3.018104 -2.417557 0.766258
S 1.961237 -3.322849 -0.738181
H -3.587634 -1.623179 -1.697893
H -2.704257 2.573091 1.678920

E= -4984.714030
S -0.777678 -1.375541 -1.474690
Mo 1.141777 -1.237988 -0.065210
S 2.008053 0.257683 -1.781900
Mo 1.724469 1.699545 -0.103113
S 2.165705 0.422121 1.640100
Mo -1.876266 -0.025282 -0.003897
S -0.545821 2.129665 -0.154230
S -2.270593 1.823646 1.836749
S -4.265342 -0.325078 -0.731067
S -3.199982 1.158520 -1.643766
S -0.403628 -1.122554 1.819972
S -2.330343 -1.725716 1.558563
S 2.864798 3.461391 -0.198810
S 2.895914 -2.585451 0.545320
S 1.710102 -3.345884 -0.936420
H -4.111468 -1.347974 -1.609400
H -3.086639 2.659525 1.165529

[Mo3S12H2]+ XXV
E= -4984.792639
Mo -2.828981 -0.630942 0.304948
S -1.816805 0.323481 1.952692
S -1.113386 -0.719283 -1.293127
Mo 0.248353 0.675603 -0.069104
S 1.371834 -0.457712 1.593891
S 1.832202 1.102182 -1.612931
Mo 2.782088 -0.510416 -0.224656
S 2.710940 -2.354486 -1.216552
S 4.851938 0.617174 -0.332547
S 4.886972 -0.757485 1.214479
S -0.730860 2.923977 -0.639826
S 0.097465 2.995955 1.145103
S -3.361622 -2.579550 0.866047
S -4.614242 -0.307239 -1.697707
H -3.954836 0.615231 -2.432553
S -4.737759 0.710449 0.106043
H 5.466699 -1.812897 0.593589

E= -4984.773170
Mo 2.718662 -0.587006 -0.240394
S 1.819883 0.933147 -1.631117
S 1.278188 -0.454612 1.541524
Mo 0.006716 0.784153 0.005556
S -1.246958 -0.489172 -1.514233
S -1.801294 0.917303 1.652659
Mo -2.709379 -0.577260 0.245647
S -2.712069 -2.482889 1.126555
S -4.823896 0.447300 0.256945
S -4.763234 -0.856429 -1.350664

S 0.583349 3.097399 0.769416
S -0.608406 3.073413 -0.802661
S 2.620546 -2.487509 -1.117047
S 4.780626 -0.917339 1.295314
H 4.499331 -0.024011 2.272274
S 4.883866 0.340490 -0.347338
H -5.340875 -1.948874 -0.795846

[Mo3S12H2]+ XXVI
E= -4984.794905
Mo -0.292758 0.701022 -0.049724
Mo 2.771223 -0.670457 0.110681
S 1.053140 -0.552574 -1.468645
S 1.997625 0.457934 1.781896
S -1.241275 -0.569511 1.581820
S -1.940728 1.088205 -1.549212
Mo -2.779474 -0.573040 -0.152414
S -2.651321 -2.403012 -1.143336
S -4.678037 -0.602258 1.383229
S -5.046166 0.340705 -0.319968
S -0.268109 2.741235 1.168883
S 0.731630 3.057975 -0.610389
S 4.289009 0.280854 -1.462173
S 5.223491 -0.000066 0.359972
H 5.083219 1.231352 0.906675
S 3.021006 -2.713333 0.546824
H -0.285059 3.534139 -1.367942

E= -4984.750654
Mo -0.247061 0.510261 -0.101935
Mo 3.121780 -0.725915 -0.058448
S 1.383279 -0.537943 -1.657822
S 1.056787 -1.255761 0.937863
S -1.561122 0.104144 1.818404
S -1.806673 0.426974 -1.779753
Mo -2.881237 -0.509325 0.049832
S -2.864433 -2.588912 -0.145747
S -4.908486 0.134392 1.258388
S -5.039893 0.382388 -0.704355
S 0.061152 2.620184 0.765984
S 0.717852 2.716597 -1.200425
S 4.202284 1.379666 -0.215300
S 4.322371 0.638637 1.720207
H 3.280952 1.270820 2.312987
S 4.274383 -2.396612 -0.540600
H -0.407236 3.198237 -1.779406

[Mo3S12H2]+ XXVII
E= -4984.719270
Mo 1.293657 -0.733162 0.025347
Mo -1.294653 -0.731484 0.025310
Mo 0.000945 1.497097 0.073332
S -1.758152 0.981338 1.698024
S -2.452803 1.428899 -0.156342
S -2.970031 -1.510622 -1.666104
S -3.503401 -2.020148 0.239845
H -2.386080 -2.645394 -2.127202
S -0.001372 -2.042870 1.623346
S -0.001825 -2.800745 -0.261525
S 2.968059 -1.514452 -1.666037
S 3.500723 -2.024723 0.239918
H 2.382664 -2.648455 -2.127188
S 2.454626 1.425717 -0.156251
S 1.759356 0.979083 1.698088
S 0.002512 3.209917 -1.697177
S 0.002655 4.134285 0.044642

E= -4984.699784
Mo 0.908757 -1.185913 0.062886
Mo -1.822986 -0.055493 -0.034306
Mo 0.800952 1.253999 0.071901
S -1.185873 1.930761 1.352697
S -1.336158 2.244275 -0.680485
S -3.997051 -0.037869 -1.307921
S -4.115530 -0.106391 0.743315
H -4.146230 -1.345366 -1.632716
S -1.044621 -2.031516 1.290971
S -1.139835 -2.280166 -0.755266
S 2.276801 -2.435366 -1.622551
S 2.280351 -3.314155 0.232569
H 1.327071 -3.141133 -2.283807
S 2.944451 0.121435 0.341849

S 1.745247 0.056688 1.989899
S 1.882961 2.607980 -1.674512
S 2.162805 3.491669 0.070452

[Mo3S12H2]+ XXVIII
E= -4984.802018
S -0.000124 -0.125116 1.799746
Mo -1.345850 -0.886952 -0.014636
S -1.687301 0.857793 -1.626201
S -2.523267 1.360758 0.165443
Mo 0.000539 1.461276 0.019144
S 2.524255 1.359004 0.165391
S 1.687876 0.856487 -1.626247
Mo 1.345196 -0.887822 -0.014551
S -0.000706 -2.140583 -1.388738
S 0.000450 3.512183 1.393911
S 0.002120 3.909609 -0.536240
S 3.130450 -1.998036 1.381525
S 3.353771 -2.190968 -0.649057
S -3.355203 -2.188820 -0.649313
S -3.131881 -1.996090 1.381280
H 2.489541 -3.147088 1.719004
H -2.491721 -3.145554 1.718783

E= -4984.784455
S 0.031912 -0.248203 1.744203
Mo -1.252369 -1.096406 -0.093944
S -1.770248 0.650723 -1.659684
S -2.702341 1.013060 0.126321
Mo -0.221109 1.433019 0.038354
S 2.247287 1.835782 0.234257
S 1.554870 1.252310 -1.609484
Mo 1.633695 -0.586442 -0.016675
S 0.301102 -2.243811 -1.199047
S -0.560930 3.376218 1.532723
S -0.634127 3.879167 -0.369993
S 3.234196 -2.140993 1.213629
S 3.838943 -1.346981 -0.595397
S -3.197801 -2.443580 -0.693433
S -2.810162 -2.492069 1.324089
H 2.798101 -3.362910 0.821764
H -2.050424 -3.610263 1.442394

[Mo3S12H2]+ XXIX
E= -4984.798668
S -0.000051 0.225626 -1.814745
Mo 1.352905 -0.604101 -0.001685
S 1.687122 1.235360 1.577813
S 2.501106 1.599839 -0.251961
Mo 0.000662 1.857876 -0.069517
S -2.499876 1.601643 -0.251655
S -1.685967 1.236288 1.577991
Mo -1.353544 -0.603419 -0.001692
S -0.000800 -2.707709 -0.114689
S -0.000574 -1.728478 1.668369
S 0.002167 3.970530 -0.578107
S -3.236412 -1.581653 -1.364615
S -3.408075 -1.813034 0.662338
S 3.406505 -1.815493 0.662384
S 3.234952 -1.584056 -1.364533
H -2.694683 -2.767419 -1.737993
H 2.692167 -2.769350 -1.737891

E= -4984.758978
S -0.000070 0.206007 -1.749715
Mo 1.539547 -0.621533 0.013876
S 1.720290 1.278256 1.576766
S 2.519682 1.627872 -0.272009
Mo 0.000155 1.881845 -0.061008
S -2.519615 1.628030 -0.271708
S -1.719882 1.278220 1.576873
Mo -1.539642 -0.621474 0.013870
S -0.000006 -2.611104 -0.178385
S -0.000080 -1.659602 1.620480
S 0.000015 3.939343 -0.666657
S -3.400148 -1.622786 -1.353358
S -3.487869 -1.884055 0.688784
S 3.487802 -1.884067 0.688776
S 3.399759 -1.623337 -1.353428
H -2.855888 -2.797523 -1.753024
H 2.855319 -2.798128 -1.752675

[Mo3S12H2]+ XXX
E= -4984.824951
S 0.016406 0.230492 -1.796735
Mo -1.376474 -0.544063 -0.005035
S -0.069091 -1.789531 1.617066
S -0.106835 -2.694267 -0.202013
Mo 1.342814 -0.650799 -0.012864
S 2.570674 1.547672 -0.149280
S 1.734597 1.088513 1.652505
Mo 0.075646 1.742853 0.013524
S -2.417866 1.737001 -0.162962
S -1.636670 1.223327 1.648910
S 3.082098 -1.717453 -1.404339
S 3.415806 -1.982501 0.518082
S 0.301123 3.939741 -0.768487
S -3.505861 -1.656245 0.623791
S -3.189756 -1.923704 -1.396627
H -0.980444 4.324780 -0.922636
H -3.897018 -0.509143 -1.772214

E= -4984.781309
S 0.000560 0.028177 -1.870375
Mo -1.431620 -0.470851 0.013359
S -0.190198 -1.550843 1.795448
S -0.325468 -2.711618 0.128112
Mo 1.263904 -0.766518 0.005774
S 2.666799 1.245953 -0.496028
S 1.928427 1.115087 1.412335
Mo 0.243088 1.776745 -0.235679
S -2.254907 1.827641 -0.489221
S -1.567708 1.525762 1.419141
S 2.862901 -2.137829 -1.289543
S 3.230773 -2.205840 0.642978
S 0.558969 4.140280 -0.136251
S -3.591899 -1.378301 0.755519
S -3.314180 -1.558421 -1.268641
H 0.740954 4.376549 1.179137
H -3.971692 -0.470791 -1.739737

[Mo3S12H2]+ XXXI
E= -4984.809608
Mo -0.983372 -1.309392 -0.002644
Mo -0.511635 1.364379 0.014513
Mo 1.548857 -0.389656 -0.030984
S 0.039233 -0.128437 1.792845
S 3.902437 -0.838047 -0.652030
S 3.534372 -1.135787 1.342222
H 3.869784 0.054497 1.902432
S 1.881101 2.132091 0.179794
S 1.274810 1.393328 -1.623493
S -1.344147 3.284707 1.423422
S -1.317306 3.621133 -0.596418
H -0.170147 3.837196 1.817615
S -2.837442 0.403053 0.170056
S -1.893252 0.250645 -1.634964
S -2.423684 -3.280976 -0.534658
S -1.903301 -3.071997 1.369983
S 0.714594 -1.995336 -1.419088

E= -4984.787026
Mo -0.984982 -1.336827 -0.068892
Mo -0.526362 1.341937 0.026881
Mo 1.712131 -0.259455 -0.024312
S 0.093406 -0.237764 1.751902
S 4.026924 -0.544381 -0.593158
S 3.549346 -1.582758 1.129712
H 3.961733 -0.708294 2.078268
S 1.794092 2.236901 0.263610
S 1.260073 1.549759 -1.595266
S -1.436464 3.167510 1.513185
S -1.417638 3.596229 -0.488723
H -0.284052 3.743196 1.936301
S -2.857110 0.399794 0.079157
S -1.835238 0.252774 -1.687005
S -2.616397 -3.180600 -0.561178
S -2.052510 -3.017581 1.326902
S 0.734796 -2.161907 -1.215952

[Mo3S12H2]+ XXXII
E= -4984.838258
S 0.098721 -0.000010 1.787330
Mo 0.856695 -1.344696 -0.013911
S -0.922759 -1.664127 -1.661196
S -1.371518 -2.517962 0.147229
Mo -1.493510 0.000066 0.011628
S -1.371306 2.518089 0.147115
S -0.922536 1.664146 -1.661257
Mo 0.856819 1.344604 -0.013903
S 2.111716 -0.000106 -1.411506
S -3.501695 0.000318 1.452563
S -3.955438 0.000111 -0.464698
S 2.174456 2.662665 1.408216
S 2.242375 3.484675 -0.495189
S 2.241952 -3.484937 -0.495127
S 2.174289 -2.662764 1.408216
H 3.394065 2.943320 -0.953566
H 3.393651 -2.943788 -0.953713

E= -4984.792622
S 0.026433 -0.262045 1.745169
Mo -1.304828 -1.031793 -0.065179
S -1.676292 0.700755 -1.746637
S -2.673106 1.101959 0.002648
Mo -0.177830 1.431580 0.014040
S 2.313356 1.719968 0.213198
S 1.582302 1.203894 -1.640121
Mo 1.586348 -0.651473 -0.021385
S 0.174334 -2.318969 -1.131475
S -0.462061 3.360266 1.543307
S -0.491873 3.895236 -0.351579
S 3.050277 -2.027112 1.298986
S 3.915477 -1.602558 -0.529135
S -3.439723 -2.423604 -0.492392
S -2.635516 -2.294342 1.413076
H 3.581663 -2.703573 -1.244660
H -2.874401 -3.580772 -0.910011

[Mo3S12H2]+ XXXIII
E= -4984.804903
S -0.000055 0.209122 -1.793608
Mo 1.350980 -0.598002 0.006299
S 1.682822 1.267090 1.584064
S 2.497456 1.615217 -0.256190
Mo -0.000103 1.859015 -0.063200
S -2.497700 1.614892 -0.256002
S -1.682837 1.266901 1.584188
Mo -1.350921 -0.598130 0.006347
S 0.000195 -2.731177 0.029713
S 0.000108 -1.628971 1.750501
S -0.000390 3.970917 -0.587996
S -2.961592 -1.626963 -1.482750
S -3.557551 -1.843074 0.474191
S 3.557743 -1.842610 0.474301
S 2.961892 -1.626666 -1.482685
H -3.078505 -3.078174 0.759758
H 3.078867 -3.077775 0.759881

E= -4984.760558
S 0.000041 0.187641 -1.731029
Mo 1.553391 -0.603543 0.003231
S 1.725728 1.304921 1.587263
S 2.513487 1.646425 -0.277396
Mo -0.000104 1.866594 -0.044860
S -2.513638 1.646115 -0.277468
S -1.725902 1.304681 1.587211
Mo -1.553254 -0.603750 0.003189
S 0.000163 -2.601943 -0.121750
S 0.000107 -1.590991 1.658404
S -0.000181 3.927690 -0.665417
S -3.163120 -1.645325 -1.429615
S -3.668737 -1.934379 0.551349
S 3.668683 -1.934514 0.551334
S 3.163302 -1.644971 -1.429616
H -3.155104 -3.168072 0.781234
H 3.154826 -3.168174 0.780906

[Mo3S12H]+ I
E= -4984.163602
S -1.663538 0.707824 1.654474
Mo -1.672883 -0.731902 0.008419
S 0.009896 -2.279998 -1.067231
Mo 0.035905 1.717010 0.019124
S -0.728005 3.772276 0.722712
S 0.640827 3.814910 -0.797121

S 1.447858 0.875249 1.637412
Mo 1.762833 -0.774234 -0.023147
S 3.919135 -1.023527 0.810523
S 3.339530 -2.337728 -0.653806
S 1.727322 0.810679 -1.574589
S -1.425829 0.840134 -1.631284
S 0.027273 -2.258630 1.005192
S -4.111372 -1.016180 -0.663464
S -3.222156 -2.445394 0.528312
H -4.660949 -0.210549 0.277285

E= -4984.149351
S -1.515292 1.956644 -0.217586
Mo -2.159535 -0.328352 -0.349281
S -3.441297 -0.795829 -1.927281
Mo 0.856384 1.522040 -0.094802
S 0.849937 3.840231 0.781182
S 2.441975 3.307330 -0.262812
S 1.109910 0.304492 1.726977
Mo 1.425590 -1.343698 -0.067877
S 2.876242 -2.398570 1.491885
S 2.791838 -3.134925 -0.419788
S 2.624804 0.322615 -1.225063
S -0.070786 -0.045387 -1.639450
S -0.712585 -2.277156 -0.002028
S -4.119191 0.422383 1.221746
S -2.940149 -1.195516 1.697647
H -3.468891 1.399470 1.895413

[Mo3S12H]+ II
E= -4984.196693
S -1.267194 0.194120 1.609635
Mo -2.514407 -0.825446 -0.085517
S -2.275221 0.739575 -1.792418
Mo -0.640945 1.215076 -0.296219
S 0.344717 3.255006 1.070291
S -1.142608 3.475939 -0.364770
S 2.971284 0.639506 1.970774
Mo 2.874752 -0.552882 0.230845
S 1.995993 -2.414943 0.670244
S 1.294079 0.592988 -1.261549
S 4.428610 -0.264747 -1.718558
S 5.182324 -1.151500 -0.125100
S -1.569049 -2.601804 -0.642417
S -4.926083 -0.992135 -0.463850
S -4.389462 -1.265118 1.424250
H 1.426953 3.546369 0.312886

E= -4984.199122
S 2.246460 0.987446 -1.613971
Mo 2.841662 -0.688076 -0.089504
S 1.281169 -0.332456 1.598405
Mo 0.505678 0.820731 -0.204106
S -0.314045 3.210104 -0.924097
S 0.174207 2.749670 1.039190
S -1.123374 -0.373665 -1.215876
Mo -3.109320 -0.260096 0.201873
S -2.362441 -0.479276 2.160667
S -3.883743 1.688723 -0.075848
S -5.095947 -1.628522 0.205458
S -3.837530 -2.201127 -1.203025
S 2.510088 -2.550436 -0.966894
S 4.673841 -0.841184 1.520253
S 5.210052 -0.083654 -0.230403
H -1.656594 3.022521 -0.860640

[Mo3S12H]+ III
E= -4984.146742
S 0.017111 0.240923 -1.636766
Mo -0.845535 -1.615195 -0.179420
S 1.523043 -1.917260 -0.422367
Mo 2.138329 0.412845 -0.346349
S 0.835534 2.530458 0.169935
Mo -1.436344 1.284983 -0.015075
S -0.978795 -0.031895 1.704954
S 3.505851 -0.838517 1.200961
S 2.952670 0.986697 1.833131
S 3.458159 0.978459 -1.845062
S -3.586420 2.125137 0.024438
S -2.138473 3.418892 0.639713
S -2.674839 -0.628707 -1.078785
S -1.410955 -3.854763 -0.522789

S -1.175822 -3.416182 1.419701
H 0.796020 3.037530 -1.077567

E= -4984.150421
S 0.205221 -0.130158 -1.630630
Mo 1.571618 -0.742668 0.160633
S 1.668138 1.125981 1.549082
Mo -0.012705 1.547273 0.076581
S -1.580859 0.882540 1.921497
Mo -1.775055 -0.561963 -0.164611
S -0.115480 -1.807281 1.450293
S 0.574545 3.402834 -1.335224
S -0.103838 3.986793 0.438830
S -2.368957 1.390527 -1.033626
S -2.482295 -2.480396 -1.259357
S -3.533494 -1.932070 0.430264
S 1.168672 -3.070799 0.412735
S 3.297984 -1.303196 -1.508035
S 4.002186 -0.807855 0.265469
H -2.631204 1.698331 1.729934

[Mo3S12H]+ IV
E= -4984.169955
S 1.110766 -1.033001 -1.273937
Mo 3.057720 -0.365164 0.044078
S 2.804617 0.937483 1.996465
S 1.322766 -0.479368 1.746095
Mo -0.495416 0.046622 0.005533
S -1.876459 1.895004 -0.644463
S -0.375795 2.237742 0.752774
S -2.040092 -0.888037 -1.848950
Mo -3.179108 -0.210753 -0.088006
S -5.214545 0.937177 0.002841
S -5.267375 -1.124847 0.086260
S -1.839141 -0.991371 1.593802
S 4.192970 -2.085703 0.338334
S 4.966757 1.178185 -0.612780
S 3.554825 0.657809 -2.022947
H 4.477074 2.373212 -0.203265

E= -4984.152695
S 1.270827 -0.491509 -1.733603
Mo 3.074386 -0.310043 -0.082468
S 2.632679 -0.152503 2.235027
S 1.339092 -1.408293 1.216792
Mo -0.355275 -0.133694 -0.157500
S -1.767224 1.838638 -0.321392
S -0.290427 1.866747 1.112078
S -2.100163 -1.024241 -1.754701
Mo -3.259816 -0.213986 -0.051985
S -5.082025 1.267775 -0.020342
S -5.479197 -0.749309 0.006275
S -2.072651 -0.901433 1.644546
S 4.424739 -1.826018 -0.542572
S 4.783595 1.542249 0.232258
S 3.502169 1.619232 -1.377389
H 4.126966 2.338377 1.110365

[Mo3S12H]+ V
E= -4984.171761
S -1.197928 -0.704438 1.680207
Mo -2.773012 -0.139844 0.025525
S -3.028444 -0.648302 -2.261914
S -1.337096 -1.410184 -1.359959
Mo 0.181952 0.109311 -0.000221
S -0.395329 2.338929 -0.150201
S -2.439699 2.112064 -0.164525
S 1.771809 0.418002 1.762743
Mo 3.145148 -0.339690 0.132075
S 3.884830 -2.217069 0.675005
S 1.705471 -0.604194 -1.642583
S 4.715216 0.887675 -1.314928
S 4.918176 1.261801 0.621495
S -5.334831 0.318468 0.147415
S -4.381172 -0.874092 1.542478
H -5.367748 1.490834 0.826534

E= -4984.193986
S 0.974768 -0.071111 1.733674
Mo 2.761705 0.245427 0.047455
S 3.606328 2.080093 -1.198724
S 1.974749 2.430144 -0.047871

Mo -0.435541 -0.661881 0.113971
S 0.347856 -2.419282 -1.124159
S 1.982655 -1.158755 -1.583434
S -2.152263 -1.653389 1.140409
Mo -3.049431 0.302203 0.201616
S -3.277943 1.691735 1.741279
S -1.301501 1.005264 -1.160055
S -4.743029 0.698193 -1.508468
S -5.156575 -0.830547 -0.318606
S 5.150997 -0.654046 -0.207614
S 4.183205 -0.697618 1.619035
H 4.949302 -1.932359 -0.615156

[Mo3S12H]+ VI
E= -4984.149823
S -2.891286 0.374134 2.103164
Mo -3.000856 -0.361428 0.147515
S -2.860553 1.317733 -1.434379
S -1.051188 0.263376 -1.270296
Mo 0.731259 1.412087 0.018434
S 1.251849 3.800044 0.525015
S -0.654777 3.353098 -0.124660
S 1.128315 0.000496 1.723998
Mo 2.262614 -0.964932 -0.088719
S 1.110987 -2.466466 -0.999519
S 2.427356 0.932306 -1.435130
S 4.635259 -1.423543 -0.394463
S 3.960658 -1.851861 1.424801
S -2.646786 -2.640675 -0.434718
S -4.507029 -2.146527 0.152487
H 1.848397 4.205657 -0.624451

E= -4984.147947
S 1.472156 1.101415 -1.569385
Mo 2.783555 -0.219620 -0.132546
S 2.089572 -2.337301 0.984491
S 1.048221 -1.695518 -0.653163
Mo -0.191984 0.479639 0.025601
S 0.847368 2.504989 1.190600
S 1.693083 0.629810 1.775306
S -1.817971 1.629923 -1.078951
Mo -2.895325 -0.257447 -0.250447
S -3.048563 -1.688499 -1.764292
S -1.402439 -0.983901 1.361801
S -4.766104 -0.480246 1.313984
S -5.012544 0.954766 -0.031762
S 5.025742 -0.700105 0.244457
S 4.663933 0.896057 -0.978898
H 0.078454 2.589721 2.303481

[Mo3S12H]+ VII
E= -4984.175129
S -1.603885 -0.449503 1.929984
Mo -2.939247 -0.564567 0.195859
S -1.140777 -1.136340 -1.349193
Mo 0.246239 0.374191 0.237683
S 0.003019 2.487821 1.092579
S -1.432814 2.235949 -0.300043
S 1.618736 -0.610871 1.736104
Mo 2.917119 -0.426178 -0.190044
S 3.098575 -2.348475 -0.991019
S 1.570093 0.831652 -1.580283
S 4.866883 0.928997 -0.779749
S 4.926158 0.189277 1.058067
S -4.121955 -2.261456 0.472305
S -3.790943 0.694231 -1.824512
S -4.537309 1.198682 -0.056773
H -0.705163 -2.264156 -0.746371

E= -4984.175187
S -1.604049 -0.445320 1.928727
Mo -2.939870 -0.566455 0.195692
S -1.141393 -1.133402 -1.351191
Mo 0.246533 0.376666 0.235111
S 0.006682 2.491311 1.090912
S -1.427232 2.242733 -0.303313
S 1.615712 -0.611056 1.735023
Mo 2.916252 -0.427997 -0.189755
S 3.095905 -2.350556 -0.990620
S 1.572549 0.832610 -1.581076
S 4.867536 0.924538 -0.777088
S 4.922619 0.187532 1.062154

S -4.118300 -2.265826 0.474685
S -3.793165 0.694517 -1.821779
S -4.538045 1.195929 -0.052314
H -0.703512 -2.261177 -0.749921

[Mo3S12H]+ VIII
E= -4984.158046
S -1.072730 0.373077 1.885123
Mo -0.063817 1.496391 -0.055639
S -2.498434 1.321337 -0.776066
S -1.134095 0.301612 -1.910019
Mo -1.718889 -0.870232 0.137625
S -3.579101 -1.826410 1.108744
S -3.438550 -2.668176 -0.799952
S 0.193854 -2.156652 0.106263
Mo 2.069149 -0.805966 -0.092520
S 1.830410 0.743281 -1.624840
S 4.143794 -1.072079 0.947918
S 3.737449 -2.286840 -0.664741
S 1.424896 0.637251 1.613833
S -0.561880 3.625320 1.005642
S 0.472969 3.597668 -0.774021
H -4.327950 -1.878364 -1.443705

E= -4984.147866
S 1.197294 1.019092 -1.727170
Mo 2.032766 -0.419966 -0.298288
S 0.657641 -2.238012 -0.428890
Mo -1.477826 -1.399059 0.052479
S -3.472459 -2.348530 -0.741962
S -2.483061 -3.364350 0.744687
Mo -0.576269 1.402832 0.117510
S -1.355596 3.472515 -0.998180
S -2.394680 2.955979 0.594592
S -1.665382 0.214033 -1.586869
S -1.643759 -0.017915 1.782226
S 1.429729 0.904080 1.544863
S 1.153549 2.860789 0.981222
S 4.093150 -1.707097 0.918244
S 4.256913 -0.610376 -0.857555
H 4.522387 -0.763240 1.785247

[Mo3S12H]+ IX
E= -4984.154684
S 1.526249 0.887829 -1.689706
Mo 2.119027 -0.321372 0.026733
S 1.378894 0.940957 1.710863
Mo -1.923737 -0.755072 0.037347
S -4.038839 -1.200179 -0.861586
S -3.365832 -2.448559 0.629619
Mo -0.183676 1.699510 0.029859
S 0.365452 3.804185 -0.769356
S -1.008105 3.723331 0.751396
S -1.549375 0.765286 -1.631344
S -1.779112 0.701647 1.667556
S 0.209765 -1.853616 0.056834
S 0.401833 -3.903340 -0.160769
S 4.388147 -0.499190 0.006695
S 3.405735 -2.309809 0.137047
H 0.555207 -3.905448 -1.501404

E= -4984.123803
S -1.491424 1.555178 1.373399
Mo -2.129596 -0.183898 0.203971
S -0.346257 0.138907 -1.435990
Mo 1.609516 -1.113801 -0.137525
S 2.989251 -2.590523 1.108830
S 2.442321 -3.148946 -0.770467
Mo 0.733786 1.673870 -0.001013
S 0.331926 3.936947 0.431053
S 1.947707 3.490374 -0.708311
S 1.664271 0.512649 1.665656
S 2.562030 0.443298 -1.385552
S -0.601321 -1.944542 1.063414
S -1.708598 -2.836532 -0.488615
S -3.779802 0.211936 -1.421979
S -4.407730 -0.540942 0.377566
H -2.613609 -3.444051 0.307774

[Mo3S12H]+ X
E= -4984.130502
S 0.716968 0.837261 1.906459

Mo 0.441231 2.055193 -0.168071
S -2.524205 -0.333497 2.177184
Mo -2.109389 -0.441131 0.101688
S -1.851826 2.001707 0.002613
Mo 1.680708 -0.916208 -0.025520
S 2.469048 -0.240254 2.050176
S -4.020934 -0.126513 -1.151037
S -3.425876 -2.079700 -0.910966
S -0.147972 0.006381 -1.418953
S -0.430699 -2.317743 0.616161
S 3.518015 -1.587098 -1.192872
S 2.395462 -3.096826 -0.387177
S 2.478003 1.208186 -0.893618
S 0.822605 4.083935 -0.523091
H -0.504544 -3.003310 -0.538128

E= -4984.152093
S 0.295787 -0.954862 -1.580486
Mo -1.419242 1.927590 0.044212
S -2.058720 0.556495 1.731197
Mo -1.527549 -1.119613 0.152598
S -2.143536 0.608992 -1.601030
Mo 2.174801 0.058632 -0.320939
S 0.820720 2.174850 0.084321
S -3.258248 -2.409154 -0.715980
S -2.103366 -3.287812 0.708020
S 1.904999 -2.157575 -1.206263
S 0.409114 -1.335384 1.699955
S 3.937204 -0.878648 1.104340
S 3.250221 0.843711 1.745464
S 3.328815 0.948511 -1.805923
S -2.411274 3.775412 0.077142
H 0.876127 -2.550146 1.361319

[Mo3S12H]+ XI
E= -4984.191061
S 1.692232 0.085470 1.846267
Mo 2.837661 -0.655063 0.106783
S 4.613425 0.482515 -1.207597
S 5.049566 0.154220 0.695664
Mo 0.034664 0.726578 -0.014393
S -1.656833 0.247956 -1.892585
Mo -2.813296 -0.586860 -0.204868
S -1.316470 -0.358201 1.538177
S 1.365073 -0.192591 -1.644344
S -0.686850 2.876837 -0.615083
S 0.799205 2.817919 0.736858
S 3.034562 -2.734169 0.211958
S -3.187079 -2.613532 -0.586160
S -4.788055 0.656244 -0.422366
S -4.805849 -0.127193 1.498079
H -4.286082 0.916746 2.182140

E= -4984.135987
S -1.231128 1.298160 -0.330925
Mo -3.438616 0.912518 0.063546
S -4.631892 -0.886014 -0.902077
S -4.274145 -1.025067 1.093927
Mo -0.193720 -0.885045 -0.464155
S 1.701473 -0.506448 -1.606935
Mo 3.193937 0.664982 -0.072823
S 2.021440 1.235322 1.599658
S -1.426081 -1.929967 -1.783540
S 0.464488 -2.517511 1.134105
S -0.876472 -1.191866 1.838788
S -4.536045 2.652186 0.408519
S 3.754576 2.327539 -1.233887
S 4.499058 -1.362813 -0.131175
S 5.376564 0.103500 1.015335
H 4.943428 -0.232734 2.255470

[Mo3S12H]+ XII
E= -4984.172144
S 1.438108 -0.670349 0.816856
Mo 3.729649 -0.509464 -0.042497
S 3.625828 -1.048268 -2.078040
Mo -0.328258 0.317595 -0.143003
S -1.678407 -1.508898 -0.671696
Mo -3.535374 -0.423942 0.182140
S -3.890983 -0.978968 2.171157
S 0.298810 1.391172 -1.820205
S -2.474493 1.753256 0.368855

S -0.883952 1.633588 1.684502
S 4.707309 -1.997049 1.088173
S 3.682187 1.801132 0.658519
S 5.508508 1.240534 -0.102854
S -4.993027 0.970746 -1.150481
S -5.375059 -1.029471 -1.020462
H 6.189975 0.945234 1.031962

E= -4984.129044
S -0.844893 -0.537071 -0.456357
Mo -3.275533 -0.707896 -0.409192
S -3.595550 -2.364534 -1.667820
Mo 0.249614 1.223426 0.455142
S 2.079256 0.335261 1.558878
Mo 3.479999 -0.639293 -0.057024
S 2.846650 -0.327764 -2.043998
S -0.911049 2.056423 1.961812
S 1.593918 3.026618 -0.558108
S -0.102837 2.643187 -1.498588
S -3.987887 1.086192 -1.283400
S -3.171095 -1.031501 1.973334
S -5.102028 -1.105054 1.262929
S 5.741836 -0.874496 0.297980
S 4.606196 -2.593067 0.390698
H -5.511629 0.170930 1.467302

[Mo3S12H]+ XIII
E= -4984.147273
S 1.489932 -0.516112 -1.966349
Mo 1.380925 -1.827728 0.100803
S 2.438089 -3.603726 -0.139684
Mo 0.994713 1.617930 -0.395128
S -1.131299 1.100273 -1.584960
Mo -2.329392 -0.330156 -0.299046
S -2.358661 -0.664165 2.051411
S -3.531026 0.835679 1.300639
S 2.176718 2.793808 -1.645555
S -0.454358 3.140491 0.662181
S 1.172856 2.591913 1.757299
S -0.770479 -2.262278 -0.178858
S 2.728039 0.103766 0.764057
S 1.696245 -0.901153 2.237716
S -3.754011 -1.180634 -1.573688
H 2.824948 -0.327705 -2.025763

E= -4984.131169
S 1.036321 -0.539638 -1.052905
Mo 3.339630 -0.864876 -0.115199
S 4.135760 -2.166532 -1.559180
Mo -0.422870 1.323985 -0.206638
S -2.172186 0.810846 -1.616703
Mo -3.630864 -0.570042 -0.444775
S -2.934559 -1.827359 1.376581
S -4.005933 -0.142830 1.828835
S 0.444915 3.067061 -0.977494
S -1.334693 1.802184 1.853516
S 0.120576 0.379061 1.938316
S 2.820809 -1.915420 1.636668
S 3.704809 1.594316 -0.200540
S 5.206914 0.521273 0.508894
S -5.230488 -1.289532 -1.581745
H 1.316453 -0.035667 -2.270194

[Mo3S12H]+ XIV
E= -4984.161510
S -0.838717 1.124840 1.759496
Mo 0.711146 1.610508 -0.136638
S -1.355272 1.357236 -1.451812
Mo -1.918588 -0.249756 0.003696
S -0.555291 -0.977793 1.826652
Mo 1.145982 -1.388715 0.004339
S -0.918157 -2.169609 -0.934440
S -4.024461 0.224749 0.861940
S -3.932420 -1.195629 -0.637158
S 2.114292 3.375692 0.342912
S 0.622829 3.755111 -1.003756
S 2.224315 0.374788 1.490318
S 1.654157 0.138889 -1.630002
S 3.057292 -2.542810 0.550821
S 1.900819 -3.423198 -0.889400
H 3.390263 0.498161 0.832216

E= -4984.154418
S 0.613944 -1.315875 1.699379
Mo -0.934400 -1.549318 -0.067750
S 1.208627 -1.815018 -1.265238
Mo 1.775960 -0.025380 -0.000776
S 0.641367 1.370716 1.663831
Mo -0.894371 1.571763 -0.090498
S 1.233598 1.665017 -1.362007
S 3.876839 0.150884 1.245384
S 4.107571 -0.215643 -0.691413
S -2.629924 -3.004822 0.513669
S -1.233096 -3.722273 -0.794785
S -2.230475 0.046177 1.429819
S -1.597409 0.000907 -1.667923
S -2.531431 3.100261 0.458903
S -1.108800 3.744197 -0.859166
H -3.394953 0.050756 0.751733

[Mo3S12H]+ XV
E= -4984.188946
S 0.934042 -0.758087 -1.247168
Mo 3.029519 -0.801176 0.015486
S 4.312399 -1.898697 -1.223148
Mo -0.617831 0.636101 -0.390867
S -2.285492 0.472818 -1.905851
Mo -3.096898 -0.566725 -0.010763
S -5.080560 0.393476 0.695469
S -0.093296 2.916697 -0.812416
S 1.166453 2.252828 0.648758
S -1.232723 -0.776985 1.493117
S -1.970043 1.137213 1.638235
S 3.069673 1.762632 -0.425936
S 4.282249 0.990061 0.986217
S 2.523300 -1.977022 1.693508
S -3.458054 -2.566769 -0.528722
H -5.908399 -0.435019 0.025044

E= -4984.176284
S 1.284326 1.312302 -0.363378
Mo 2.891225 -0.461542 0.197782
S 2.038991 -2.266987 -0.494682
Mo -0.977597 1.226405 0.030081
S -2.174362 0.500194 -1.761011
Mo -2.432109 -1.181985 -0.232144
S -4.662467 -1.674216 0.143762
S -0.935276 3.509731 -1.021136
S -1.825574 3.352736 0.732020
S -0.654667 -0.856108 1.321189
S -2.214795 0.322352 1.927649
S 4.391129 0.962891 -1.215290
S 5.207903 -0.662684 -0.449242
S 2.977119 -0.429265 2.302442
S -1.759559 -2.931481 -1.175310
H -4.988081 -0.712334 1.027556

[Mo3S12H]+ XVI
E= -4984.154379
S 0.969967 1.226174 -1.585586
Mo 2.009676 -0.169835 0.159198
S 1.284273 -2.153786 1.245337
Mo -0.635778 1.803688 -0.126600
S -2.470251 0.561165 -1.010138
Mo -2.128117 -1.504951 -0.032534
S -2.761656 -1.658243 1.978080
S -2.237814 3.525311 -0.228117
S -0.322755 4.037807 0.308599
S -0.105275 0.630907 1.619035
S 3.206915 -0.676172 -1.799071
S 4.222746 -1.539246 -0.244891
S 3.162491 1.099184 1.364571
S -3.268916 -2.797563 -1.228576
S 0.068681 -2.419545 -0.401142
H 3.702699 -2.789835 -0.292260

E= -4984.143758
S 1.057871 1.333549 -1.488932
Mo 2.028914 -0.189948 0.185386
S 1.178485 -2.183959 1.242522
Mo -0.661445 1.700817 -0.091850
S -2.605333 0.757538 -0.798181
Mo -2.175875 -1.450496 -0.049410
S -2.877419 -1.785654 1.904653

S -1.183213 4.023545 -0.956881
S -0.916198 3.820624 0.997117
S 0.051913 0.606895 1.698852
S 3.077616 -0.764920 -1.847143
S 4.090148 -1.726898 -0.352263
S 3.347180 0.978701 1.315682
S -3.288275 -2.620772 -1.388766
S -0.027118 -2.414164 -0.419287
H 3.462553 -2.927394 -0.371259

[Mo3S12H]+ XVII
E= -4984.145377
S -0.461790 -0.526608 -1.863843
Mo -1.841675 -0.558264 0.356800
S -3.684151 -1.698732 -0.615097
S -2.196700 -2.821850 0.204135
Mo 2.298067 -1.049705 0.124612
S 2.165275 -2.681701 -1.216311
Mo 0.403965 1.220487 -0.273256
S -0.986851 1.438591 -2.306219
S -2.164715 1.706761 -0.583044
S 2.548769 0.957204 -1.034547
S 0.336123 -0.670367 1.375005
S 3.921101 -1.258163 1.448187
S 0.715172 3.628153 -0.017592
S 0.638156 2.604222 1.677664
S -2.964974 0.309971 2.191297
H -1.981606 0.474560 3.103940

E= -4984.144707
S -0.477509 -0.524862 -1.826080
Mo -1.858969 -0.556027 0.331228
S -3.827672 -1.583559 -0.524540
S -2.359825 -2.797841 0.217571
Mo 2.278360 -1.094609 0.111611
S 2.100024 -2.730299 -1.220613
Mo 0.436115 1.217200 -0.284202
S -0.969096 1.447691 -2.311917
S -2.125559 1.731839 -0.576334
S 2.564998 0.911676 -1.047985
S 0.340225 -0.673634 1.374844
S 3.908326 -1.327956 1.423116
S 0.773730 3.625479 -0.019898
S 0.700280 2.613259 1.674730
S -2.762263 0.424837 2.223655
H -1.781788 0.338196 3.152432

[Mo3S12H]+ XVIII
E= -4984.149854
S -0.207813 -0.890746 -1.448249
Mo -2.034545 -0.501966 0.205453
S -3.641383 -1.788551 -0.920288
S -2.571391 -2.744705 0.507357
Mo 1.891030 -0.972647 -0.150355
S 2.223032 -2.968314 -0.705503
Mo -0.037615 1.338370 -0.487679
S -2.217895 1.419705 -1.180992
S 2.022140 1.031475 -1.499740
S 0.128633 -0.301991 1.392960
S 3.237337 -0.677706 1.903628
S 4.209770 -0.226420 0.264319
S 0.121418 3.795024 -0.562175
S 0.335936 3.010082 1.237744
S -2.998060 0.707183 1.960619
H -2.660101 -0.118377 2.973525

E= -4984.150115
S -0.206517 -0.886674 -1.449887
Mo -2.038327 -0.487441 0.204526
S -3.649094 -1.768444 -0.931334
S -2.585421 -2.742348 0.482582
Mo 1.887879 -0.979607 -0.147076
S 2.211217 -2.978438 -0.696369
Mo -0.026491 1.341429 -0.492139
S -2.209232 1.429877 -1.178706
S 2.036070 1.022063 -1.498962
S 0.123580 -0.300944 1.390991
S 3.226133 -0.682865 1.909495
S 4.209608 -0.243689 0.273208
S 0.180068 3.791444 -0.565516
S 0.303183 3.009318 1.245573
S -3.011254 0.687520 1.973248

H -2.622259 -0.113124 2.987721

[Mo3S12H]+ XIX
E= -4984.181903
S 1.209796 1.742568 -0.694570
Mo 2.638978 0.083990 -0.104201
S -0.390274 -0.055290 1.770755
Mo -1.333166 -1.350905 -0.034707
S -1.441532 -3.534967 -0.890925
S -3.046365 -2.869289 0.179394
Mo -1.132133 1.496045 0.033710
S -1.177884 3.701696 -0.876284
S -2.753196 3.088650 0.251195
S -1.808037 0.130709 -1.670644
S -2.420952 0.114932 1.646574
S 1.086451 -1.695288 -0.848036
S 2.313290 -2.090453 0.763596
S 3.491546 0.591706 2.011669
S 4.213063 0.173458 -1.467008
H 4.291032 1.601591 1.606842

E= -4984.161760
S -1.327629 -0.807568 -1.816255
Mo -1.838313 0.742130 -0.062029
S -1.706701 -0.746337 1.605614
Mo 2.215976 0.531666 0.001315
S 4.433434 1.016327 0.232370
S 3.281969 2.638098 -0.273434
Mo -0.077641 -1.449343 0.009946
S -0.356647 -3.743962 -0.701707
S 0.493049 -3.612426 1.076877
S 1.960237 -1.102920 -1.443965
S 1.408451 -0.358134 1.819292
S 0.243898 1.871504 -0.854569
S -0.923854 2.812920 0.550372
S -4.061381 1.702091 0.839415
S -3.951298 0.748999 -1.001207
H -4.497390 0.675572 1.607437

[Mo3S12H]+ XX
E= -4984.148695
S 1.116923 1.237619 -1.584999
Mo 1.929022 -0.127172 -0.062547
S 2.424654 1.527298 1.611915
S 0.595609 0.636312 1.784090
Mo -1.934684 -1.372316 -0.215600
S -3.505638 -2.744712 -0.475781
Mo -0.784509 1.475843 -0.053913
S -0.678085 3.731238 -0.629731
S -2.178231 3.203269 0.631854
S -1.818516 0.140504 -1.805696
S -2.227463 -0.030760 1.490033
S 0.327616 -2.231968 -0.232735
S 0.474132 -3.257345 1.581123
S 4.266457 -0.134641 -0.438840
S 3.226438 -1.737300 -1.123847
H 0.804860 -4.442024 1.028323

E= -4984.153995
S 0.961977 0.774163 -1.872577
Mo 1.910644 -0.243588 -0.145875
S 1.841168 1.999309 0.974383
S 0.893168 0.462206 1.905880
Mo -2.063855 -1.203236 -0.183645
S -3.707734 -2.506260 -0.354055
Mo -0.424231 1.378490 0.035652
S -0.840992 3.611045 -0.882100
S -1.548099 3.388787 0.947005
S -2.023810 0.341515 -1.712791
S -2.118970 0.126579 1.555242
S 0.166029 -2.196882 -0.340100
S 0.251674 -3.426529 1.349369
S 4.217302 -0.154803 -0.156138
S 3.393970 -1.954421 -0.684319
H 0.481604 -4.565292 0.665670

[Mo3S12H]+ XXI
E= -4984.193593
S -2.029988 0.215909 1.921534
Mo 0.260061 0.746804 -0.100008
S -0.014017 2.714882 1.328588
S -0.669845 3.033042 -0.507398

Mo -2.872681 -0.705161 0.185425
S -5.169200 0.073080 0.197987
S -4.277990 0.443120 -1.526513
S -1.078797 -0.539972 -1.396590
S -3.083737 -2.770539 0.476585
S 1.291429 -0.512544 1.544183
Mo 2.767709 -0.493274 -0.217711
S 4.798515 -0.915964 1.284440
S 4.872235 0.573307 -0.151225
S 1.925843 1.252417 -1.519730
S 2.692391 -2.260084 -1.342642
H 5.376814 -1.937943 0.608862

E= -4984.193488
S -2.026432 0.245988 1.913634
Mo 0.258945 0.758057 -0.102915
S -0.000521 2.731129 1.325043
S -0.639872 3.052177 -0.516389
Mo -2.867428 -0.700923 0.189436
S -5.166219 0.067884 0.205285
S -4.301869 0.384540 -1.543513
S -1.082597 -0.526766 -1.400023
S -3.058009 -2.763684 0.507103
S 1.285776 -0.500529 1.546233
Mo 2.759124 -0.500182 -0.217356
S 4.788770 -0.929985 1.284880
S 4.870855 0.552372 -0.157529
S 1.928501 1.244627 -1.526486
S 2.671206 -2.272333 -1.333123
H 5.359681 -1.958678 0.613248

[Mo3S12H]+ XXII
E= -4984.199031
S 2.386053 -0.513662 2.167117
Mo 3.122092 -0.259372 0.206817
S 3.869847 1.695510 -0.044975
S 1.120004 -0.366064 -1.204330
Mo -0.508287 0.825080 -0.206123
S 0.384716 3.197179 -0.895386
S -0.182442 2.747479 1.051346
S -1.283992 -0.334089 1.597140
Mo -2.839899 -0.695298 -0.090368
S -5.212056 -0.102562 -0.223213
S -4.668415 -0.868997 1.521392
S -2.253648 0.984261 -1.614858
S 5.117751 -1.612950 0.177377
S 3.863427 -2.166226 -1.242623
S -2.500370 -2.555152 -0.969677
H -0.758094 3.767186 -1.342681

E= -4984.198193
S 2.138581 0.487693 1.867661
Mo 3.010497 -0.210277 0.051264
S 4.237047 1.268680 -0.799852
S 1.117717 -0.397518 -1.415469
Mo -0.353102 0.759341 -0.114195
S 0.530323 3.166213 -0.707983
S -0.271620 2.749789 1.151906
S -1.182332 -0.536175 1.576924
Mo -2.754177 -0.668630 -0.115622
S -5.082155 0.089245 -0.204403
S -4.598867 -0.844690 1.474938
S -2.071762 1.053587 -1.536586
S 4.604966 -1.860518 0.818002
S 3.397838 -2.603637 -0.995834
S -2.529777 -2.485417 -1.115409
H -0.574518 3.625741 -1.341931

[Mo3S12H]+ XXIII
E= -4984.129283
S -1.994049 0.212835 1.739553
S -2.840269 0.309320 -0.107344
Mo -0.616142 1.356369 0.070008
S -1.666092 3.769917 0.021858
S -1.332673 2.897386 -1.714458
Mo 1.466132 -0.164228 0.030398
S 1.219459 1.625361 1.667845
S 1.654226 2.275469 -0.204865
Mo -0.896028 -1.195042 0.065339
S 1.124978 -2.583591 -0.203872
S 0.828795 -1.854580 1.669943
S 3.291282 -0.240068 -1.683124

S 4.005924 -0.442169 0.221302
S -1.929018 -2.540578 -1.721898
S -2.442408 -3.326354 0.011908
H 3.211097 -1.525339 -2.110879

E= -4984.129303
S -1.994136 0.213333 1.739222
S -2.840094 0.310022 -0.107767
Mo -0.615814 1.356604 0.069794
S -1.664781 3.770172 0.022553
S -1.332294 2.898100 -1.714203
Mo 1.466128 -0.164591 0.030475
S 1.219743 1.625155 1.667771
S 1.654873 2.275003 -0.204956
Mo -0.896348 -1.194888 0.065099
S 1.124436 -2.583820 -0.203997
S 0.828193 -1.854862 1.669841
S 3.291256 -0.240871 -1.683031
S 4.005877 -0.443192 0.221379
S -1.930105 -2.540424 -1.721624
S -2.442800 -3.325686 0.012647
H 3.210761 -1.526111 -2.110823

[Mo3S12H]+ XXIV
E= -4984.214795
S -0.002842 -0.126121 1.794780
Mo 1.391448 -0.766699 -0.031594
S 3.519566 -1.857341 -0.669010
S 3.243276 -1.767746 1.362047
Mo -1.292763 -0.996427 -0.004084
S -2.641004 -2.448805 1.380129
S -3.193510 -2.535036 -0.524479
Mo -0.146521 1.457398 0.020189
S -0.346168 3.906829 -0.498594
S -0.333037 3.479938 1.424827
S -1.770012 0.736579 -1.639027
S -2.648221 1.129656 0.167804
S 0.167196 -2.118413 -1.407071
S 2.373063 1.574056 0.172899
S 1.589062 1.015055 -1.626048
H 2.691212 -2.977815 1.638449

E= -4984.214827
S -0.003708 -0.125717 1.794458
Mo 1.388412 -0.771880 -0.031541
S 3.512273 -1.871084 -0.668525
S 3.236286 -1.779618 1.362484
Mo -1.296866 -0.991580 -0.004134
S -2.650568 -2.437962 1.381167
S -3.202682 -2.523079 -0.523752
Mo -0.141005 1.458061 0.019582
S -0.329779 3.907116 -0.497880
S -0.319646 3.481436 1.425793
S -1.766700 0.742491 -1.639936
S -2.644111 1.140168 0.166283
S 0.158984 -2.119263 -1.406779
S 2.378818 1.565133 0.172753
S 1.593193 1.008764 -1.626281
H 2.679507 -2.987417 1.639363

[Mo3S12H]+ XXV
E= -4984.204540
S 0.020986 0.220899 -1.811054
Mo -1.365740 -0.565402 0.003079
S -3.456321 -1.701055 0.662425
S -3.275775 -1.483928 -1.366408
Mo 1.338966 -0.650059 -0.006269
S 3.070341 -1.755862 -1.381359
S 3.397677 -1.973751 0.549120
Mo 0.080300 1.853089 -0.067341
S 0.162743 3.961731 -0.579515
S 1.739069 1.180052 1.578221
S 2.572108 1.516549 -0.252284
S -0.091405 -2.714243 -0.104451
S -0.050145 -1.727469 1.675525
S -2.426652 1.677037 -0.255483
S -1.629791 1.294338 1.578677
H -2.773455 -2.689113 -1.732336

E= -4984.204188
S 0.019542 0.216728 -1.811629
Mo -1.371424 -0.560123 0.003076

S -3.464143 -1.687484 0.664859
S -3.285900 -1.471736 -1.364669
Mo 1.334253 -0.655159 -0.006496
S 3.060330 -1.764580 -1.382236
S 3.408195 -1.973156 0.545170
Mo 0.090796 1.849413 -0.067676
S 0.176506 3.960191 -0.577717
S 1.747979 1.166849 1.578364
S 2.577627 1.506023 -0.253156
S -0.103991 -2.715538 -0.100915
S -0.059987 -1.724526 1.676829
S -2.418282 1.687497 -0.257552
S -1.624365 1.302576 1.577416
H -2.788407 -2.678974 -1.730210

[Mo3S12H]+ XXVI
E= -4984.230684
S -0.000027 0.221803 -1.795493
Mo 0.024919 1.734978 0.016938
S 0.201639 3.936677 -0.763621
Mo -1.372139 -0.583140 -0.011047
S -3.163531 -1.553403 -1.407693
S -3.527365 -1.780716 0.513822
Mo 1.345840 -0.625699 -0.009886
S 3.456625 -1.899339 0.515614
S 3.106060 -1.651958 -1.405875
S -0.032607 -1.797546 1.620655
S -0.047013 -2.707594 -0.200942
S -2.467101 1.681260 -0.163074
S -1.675267 1.180767 1.649634
S 2.520654 1.598287 -0.150011
S 1.699612 1.122213 1.654812
H -1.088863 4.294964 -0.907785

E= -4984.230724
S -0.000033 0.221334 -1.795148
Mo 0.024928 1.734941 0.016907
S 0.201655 3.936443 -0.764132
Mo -1.372334 -0.583267 -0.010740
S -3.163138 -1.553705 -1.408537
S -3.527058 -1.780031 0.513170
Mo 1.346019 -0.625841 -0.009573
S 3.456291 -1.898720 0.514978
S 3.105666 -1.652238 -1.406706
S -0.032612 -1.796653 1.620900
S -0.047033 -2.708026 -0.199432
S -2.467051 1.681197 -0.163342
S -1.675474 1.181019 1.649542
S 2.520625 1.598195 -0.150293
S 1.699854 1.122453 1.654717
H -1.088828 4.294765 -0.908402

[Mo3S12H]+ XXVII
E= -4984.214942
S 0.009355 -0.125733 1.790840
Mo 1.426962 -0.696214 -0.038453
S 0.267255 -2.085991 -1.426890
Mo -1.243606 -1.055560 -0.006051
S -2.505627 -2.584250 1.373635
S -3.060511 -2.687842 -0.530047
Mo -0.213737 1.452177 0.022589
S -1.806562 0.659550 -1.634268
S -2.696409 1.002583 0.177040
S 2.295762 1.689266 0.175054
S 1.538081 1.101230 -1.628778
S -0.496436 3.457537 1.436170
S -0.535370 3.891124 -0.485470
S 3.621690 -1.650287 -0.653930
S 3.211281 -1.834786 1.346219
H 3.795865 -0.735334 1.887251

E= -4984.214973
S 0.008078 -0.125353 1.790534
Mo 1.422540 -0.704843 -0.038333
S 0.254294 -2.087871 -1.426505
Mo -1.250413 -1.048000 -0.006079
S -2.521820 -2.568016 1.374741
S -3.076453 -2.669324 -0.529282
Mo -0.204867 1.453560 0.021925
S -1.801908 0.669699 -1.635266
S -2.690465 1.019560 0.175374
S 2.305857 1.675245 0.174946

S 1.545219 1.091448 -1.628992
S -0.475257 3.460750 1.437111
S -0.509784 3.893383 -0.484791
S 3.611248 -1.672895 -0.653538
S 3.199967 -1.853664 1.346753
H 3.791468 -0.757558 1.887048

[Mo3S12H]+ XXVIII
E= -4984.232704
S -0.086207 0.071883 1.790367
Mo -1.449681 -0.673939 -0.002297
S -3.768859 -1.738138 -0.483456
S -3.267215 -1.079067 1.418938
Mo -0.017223 1.603885 -0.028129
S -0.347977 3.569047 1.348173
S -0.061628 4.049260 -0.553872
Mo 1.254954 -0.784039 0.014999
S 3.343465 -2.088997 -0.470377
S 2.950215 -1.869582 1.447488
S 1.668781 0.944413 -1.639955
S 2.504281 1.402977 0.171640
S -1.792892 1.130427 -1.409679
S -0.192010 -2.850565 0.142541
S -0.115103 -1.883050 -1.662606
H -4.455728 -0.665786 -0.939342

E= -4984.232734
S -0.085778 0.072040 1.790023
Mo -1.450049 -0.672896 -0.002303
S -3.770131 -1.735329 -0.482958
S -3.267583 -1.076658 1.419337
Mo -0.015953 1.604199 -0.028221
S -0.345064 3.569083 1.348939
S -0.058474 4.049221 -0.553196
Mo 1.254449 -0.784973 0.014481
S 3.340286 -2.092369 -0.469548
S 2.948969 -1.871580 1.448520
S 1.668710 0.943225 -1.640751
S 2.505712 1.401092 0.170332
S -1.792147 1.131958 -1.409462
S -0.193903 -2.850357 0.142385
S -0.116754 -1.883034 -1.662839
H -4.456279 -0.662455 -0.938699

[Mo3S12H]+ XXIX
E= -4984.207350
S -0.000607 0.213180 -1.800850
Mo -1.365028 -0.560049 0.004367
S -3.608005 -1.737148 0.480264
S -3.027997 -1.511213 -1.480241
Mo 1.335360 -0.648473 0.000153
S 3.045319 -1.777424 -1.386148
S 3.405258 -1.953045 0.542672
Mo 0.066911 1.851341 -0.062979
S 0.138410 3.960813 -0.589656
S 1.755617 1.201020 1.559465
S 2.555372 1.513000 -0.290910
S -0.077433 -2.726249 -0.033692
S -0.036800 -1.678880 1.716455
S -2.439425 1.695365 -0.217021
S -1.609232 1.300263 1.606790
H -3.171815 -2.993296 0.741210

E= -4984.206958
S -0.002687 0.210494 -1.803053
Mo -1.368133 -0.557049 0.003421
S -3.612733 -1.729380 0.485356
S -3.035046 -1.507380 -1.476385
Mo 1.332066 -0.650543 -0.002091
S 3.037449 -1.780981 -1.383473
S 3.422675 -1.947156 0.540971
Mo 0.072763 1.847919 -0.063169
S 0.140975 3.961333 -0.583602
S 1.763176 1.190070 1.558477
S 2.555924 1.509340 -0.293713
S -0.084225 -2.727529 -0.032023
S -0.041809 -1.676845 1.716096
S -2.434682 1.700355 -0.218823
S -1.606758 1.303421 1.605776
H -3.177445 -2.985601 0.747578

[Mo3S11H3]+ I

E= -4587.092542
S -0.798887 -0.931021 1.624262
Mo 0.502770 0.101998 -0.063607
S 0.396828 2.375960 -0.430123
Mo -2.424726 -1.036671 0.030200
S -1.462683 -0.168814 -1.739748
S -3.623446 1.727033 0.997313
S -4.003906 2.925977 -0.629910
S -4.472597 -0.156476 0.592616
S -2.930655 -3.034685 -0.335399
S 2.062089 0.419480 1.724306
Mo 3.085388 -0.438575 -0.006624
S 5.613421 0.017948 0.696193
S 4.566288 1.090694 -0.765417
S 1.631794 -1.078069 -1.647608
H 5.417840 0.832454 1.757486
H -5.230373 3.347150 -0.259018
H -0.703517 2.488383 -1.200970

E= -4587.121804
S 1.560695 0.508859 -2.179517
Mo -0.132620 1.287142 -0.848646
S 0.554915 3.456651 -0.557150
Mo 1.790546 -0.923686 -0.419439
S 0.010866 -0.159610 0.993275
S 3.558664 0.772356 0.981796
S 3.051162 0.674632 2.985929
S 3.972016 -1.164987 0.313171
S 1.404774 -2.873573 -1.079483
S -2.293033 1.162282 -1.503110
Mo -2.261635 -0.458122 0.180740
S -4.616353 0.047438 0.913492
S -3.150187 -0.195198 2.351378
S -2.429593 -2.358213 -0.659236
H -4.654480 1.396391 0.787964
H 4.302104 0.846350 3.458631
H -0.274697 3.803036 0.453126

[Mo3S11H3]+ II
E= -4587.124331
S 1.096851 -0.590174 -1.891543
Mo 0.054052 0.618681 -0.180681
S -1.767674 1.304736 -1.390071
Mo -2.528767 -0.410177 -0.037325
S -0.762206 -0.706940 1.454969
Mo 2.647688 -0.891548 -0.270716
S 5.091243 -0.162236 0.014458
S 3.519313 0.864227 0.939234
S 2.209205 -2.494798 0.984781
S 0.678653 2.336718 1.275634
S 1.210002 2.947576 -0.638860
S -4.076992 -0.152016 1.717798
S -4.925998 0.517979 -0.047403
S -2.724529 -2.200484 -1.111289
H 0.117976 3.687034 -0.940740
H 5.445899 -1.039359 0.982361
H -5.594646 -0.593248 -0.438630

E= -4587.112956
S 1.295495 -0.696375 -1.499235
Mo -0.005506 0.687125 0.059874
S -1.693719 0.683009 -1.632542
Mo -2.491170 -0.683139 -0.008339
S -1.085253 -0.301995 1.799782
Mo 2.806458 -0.462057 0.064150
S 4.832414 -1.989640 0.331228
S 5.026818 -0.123209 -0.562229
S 2.007838 0.789988 1.622521
S -0.400512 2.985463 0.631858
S 0.842799 2.957214 -1.005463
S -4.375027 -0.149248 1.311378
S -4.930825 -0.234191 -0.681009
S -2.314962 -2.710654 -0.548702
H -0.063897 3.079990 -2.004149
H 5.163003 -1.700647 1.614114
H -5.390987 -1.506136 -0.750132

[Mo3S11H3]+ III
E= -4587.101731
S 1.215864 -0.108090 -1.774716
Mo -0.102029 0.616474 0.124887
S -1.792989 0.458620 -1.663304

Mo -2.951863 -0.435617 -0.026012
S -1.693234 -0.305612 1.769558
Mo 2.699755 -0.281651 -0.087680
S 4.288971 -2.074286 0.924196
S 3.705183 -2.175789 -1.060047
S 1.300936 -0.392442 1.703536
S 3.956348 1.405980 -0.030522
S -0.437376 2.688068 1.088606
S 0.473697 2.980719 -0.735204
S -5.142855 -0.063809 0.184682
S -4.939562 -2.091545 -0.439082
H -0.613529 3.239362 -1.504939
H 5.470689 -1.424301 0.799514
H -4.943142 -2.730723 0.751954

E= -4587.072330
S -1.281354 0.073163 1.923701
Mo 0.090312 0.813278 0.046297
S 1.891904 0.893005 1.592742
Mo 2.590167 -0.492601 0.034683
S 0.953470 -0.741296 -1.461816
Mo -2.551613 -0.532096 0.242848
S -2.259895 -2.924559 -0.663438
S -3.845020 -2.439975 0.620806
S -1.851238 0.742481 -1.618441
S -3.596758 1.325870 -0.589321
S 0.668926 2.935188 -1.002829
S -0.522940 3.255083 0.634656
S 4.799744 -0.349714 -0.691148
S 4.586095 -2.071076 0.453989
H 0.400141 3.508079 1.594527
H -2.865131 -2.801536 -1.867721
H 4.365729 -2.997708 -0.509986

[Mo3S11H3]+ IV
E= -4587.111921
S 1.345583 -1.991999 -0.459116
Mo 0.318232 0.265090 -0.237796
S -1.452990 -0.771943 -1.495299
Mo -3.012388 -0.329499 0.108541
S -1.575853 1.504972 0.968062
Mo 3.068532 -0.234161 0.133514
S 4.154786 1.060957 1.704467
S 4.506318 -1.421536 -0.854709
S -4.691288 1.344350 -0.076961
S -5.154522 -0.549465 -0.663310
S -2.763961 -1.617723 1.749765
S 1.215119 -0.161699 1.775814
S 1.003245 2.403144 -0.862742
S 2.119933 0.909340 -1.756972
H 5.375698 1.012324 1.130134
H -1.900404 2.399629 0.014110
H 1.498989 -2.206392 -1.787112

E= -4587.110038
S -1.821151 -0.090488 2.015874
Mo -0.449845 1.062850 0.171044
S 1.242157 0.253412 1.674818
Mo 2.639807 -0.516119 0.051923
S 1.592514 1.131570 -1.446467
Mo -2.615440 -0.924109 -0.078015
S -2.410395 -3.208785 -0.143338
S -4.593381 -0.310553 -0.354014
S 4.708637 0.522001 -0.508844
S 4.734946 -0.927484 0.922818
S 1.923042 -2.286851 -0.831645
S -1.322493 -0.116240 -1.688145
S -0.637338 3.257711 -0.735776
S -2.029536 2.802425 0.616616
H -3.673315 -3.514001 0.222990
H 2.217853 2.219607 -0.956621
H -2.866535 0.716798 2.295257

[Mo3S11H3]+ V
E= -4587.127449
S -1.637372 0.085895 -1.867282
Mo -0.013429 0.597202 -0.064382
S 1.425821 -0.419674 -1.608958
Mo 3.024829 -0.071378 0.024913
S 1.624111 0.486976 1.904195
Mo -2.996265 -0.153886 0.119288
S -3.732097 2.021536 0.075828

S -4.644646 -1.514861 0.947527
S -3.934877 -2.033045 -0.913802
S -1.419531 -0.406142 1.639974
S 4.486468 -1.527410 1.101631
S 4.048689 -2.025677 -0.847718
S 4.055676 1.687519 -0.436344
S -0.009226 2.677540 -0.183046
H -4.912593 1.758934 -0.531493
H 1.381829 -0.733664 2.423778
H -1.313159 -1.169131 -2.236769

E= -4587.116168
S -1.614007 0.271330 -1.768791
Mo 0.208057 0.423928 0.032582
S 1.610021 0.193206 -1.788384
Mo 3.038049 0.059665 0.001618
S 1.609187 -0.285715 1.923696
Mo -3.385377 -0.216412 -0.040488
S -4.957473 -1.220928 -1.394158
S -3.479344 -1.054028 2.030628
S -1.379297 -1.233775 0.894978
S -3.950107 1.795664 0.093503
S 4.408719 -1.898230 0.544889
S 4.582716 -1.274628 -1.325707
S 3.948916 1.897245 0.352696
S -0.128471 2.425864 0.527711
H -4.664716 -2.473064 -0.977409
H 1.438922 -1.624002 1.964747
H -1.338598 -0.980669 -2.180204

[Mo3S11H3]+ VI
E= -4587.145814
S -0.343696 -0.114055 -0.769689
Mo 1.128137 1.390871 0.362040
S 0.259104 2.164827 2.099019
Mo -2.724187 -0.113283 -0.310388
S -3.488326 1.623578 -1.212113
S 0.299964 -2.359428 2.042492
S -3.392750 -0.254414 1.885921
S -3.500521 -1.818313 -1.246483
S 2.724011 2.803487 -0.603785
S 0.861385 3.280875 -1.373411
S 2.786836 -0.047361 1.128475
Mo 1.207866 -1.490897 0.373001
S 2.209555 -3.206974 -0.792236
S 2.542322 -1.754537 -2.251224
H 3.828529 -1.477700 -1.945261
H -3.353317 1.069424 2.143687
H 0.502399 4.291014 -0.545289

E= -4587.106139
S 1.499426 -1.538916 1.193745
Mo 0.014957 -0.477097 -0.357903
S -0.066745 -1.786278 -1.987390
Mo 2.828458 0.124679 0.446851
S 1.433514 1.335425 -0.889134
S 4.529586 -1.297275 -0.338831
S 4.875988 0.603359 -1.093369
S 3.410698 1.239994 2.126646
S -1.749816 1.112795 -1.343641
S -1.586528 2.948064 -0.306363
S -1.508455 -1.259885 1.404576
Mo -2.960842 -0.061003 0.268961
S -5.109920 0.475626 1.041077
S -5.196508 -0.868898 -0.547856
H -5.258490 -2.058132 0.100928
H 4.293134 0.491660 -2.309195
H -2.602549 3.529979 -0.975287

[Mo3S11H3]+ VII
E= -4587.093078
S -0.801936 -0.954091 1.626220
Mo 0.503624 0.071349 -0.059070
S 0.160933 2.304662 -0.509818
Mo -2.437843 -1.030852 0.035547
S -1.449725 -0.209905 -1.743547
S -3.556428 1.757490 0.983774
S -3.884430 2.974352 -0.640936
S -4.465427 -0.096672 0.575496
S -2.988539 -3.018539 -0.317515
S 1.652803 -1.114885 -1.639429
S 2.050347 0.397975 1.738787

Mo 3.082945 -0.427736 -0.005939
S 5.626435 0.031407 0.663626
S 4.544041 1.126857 -0.757391
H 5.441063 0.821957 1.744273
H -5.115705 3.399052 -0.289445
H 1.218966 2.864607 0.114325

E= -4587.114305
S -0.860648 -0.838118 1.702209
Mo 0.349100 0.273736 0.030384
S -0.198086 2.490092 -0.258172
Mo -2.364087 -1.128177 0.009704
S -1.378966 -0.185997 -1.733686
S -3.876355 1.457495 0.874966
S -4.238346 2.642076 -0.767753
S -4.534051 -0.486254 0.408893
S -2.601150 -3.173678 -0.371578
S 1.799087 -0.616770 -1.588577
S 1.985265 0.714687 1.715132
Mo 3.181985 -0.074367 0.059294
S 5.617419 -0.911211 0.149861
S 5.160989 1.011984 -0.491004
H 5.880987 -0.687575 1.460440
H -5.528058 2.924804 -0.491114
H 0.630662 3.103783 0.611984

[Mo3S11H3]+ VIII
E= -4587.206766
S 0.099054 -0.002566 1.757527
Mo -0.680151 1.360542 -0.001427
Mo 1.638950 -0.027639 -0.056499
Mo -0.723676 -1.337185 -0.004209
S 1.120830 -1.817671 -1.305823
S -1.205715 3.097000 1.486525
S -1.824482 3.637147 -0.418982
H -0.770659 4.386872 -0.815457
S -1.303710 -3.059598 1.480144
S -1.934011 -3.578428 -0.427195
H -0.901526 -4.357906 -0.822769
S 3.482829 -0.075029 1.367096
S 4.184873 -0.123273 -0.588476
H 4.469040 1.187137 -0.766185
S -1.756154 0.030249 -1.745939
S -2.836585 0.047534 0.014353
S 1.181070 1.829870 -1.305850

E= -4587.160464
S -0.067132 -0.193651 1.728616
Mo 1.530187 -0.741245 -0.000033
Mo -1.546024 -0.892527 -0.032001
Mo -0.160509 1.434687 -0.018709
S -1.903639 0.890737 -1.419649
S 3.131317 -1.697928 1.409341
S 3.739810 -1.940289 -0.566022
H 3.289585 -3.194472 -0.805783
S -0.709512 3.144714 1.486810
S -0.455725 3.972851 -0.399252
H -1.741683 4.018927 -0.816901
S -3.300627 -1.652369 1.287489
S -3.738848 -2.116295 -0.696428
H -3.331727 -3.406417 -0.722675
S 1.510728 0.969018 -1.739941
S 2.342539 1.652766 0.031851
S 0.025486 -2.345603 -0.843027

[Mo3S11H3]+ IX
E= -4587.153304
S -0.222571 -0.278003 1.639517
Mo 1.480751 -0.284890 0.005635
Mo -0.934036 -1.420104 -0.292338
Mo -0.743835 1.296520 -0.048753
S 1.159359 1.569685 -1.477717
S 1.582194 2.263170 0.400278
S 0.990577 -1.946881 -1.468318
S 3.909821 -0.406482 -0.408361
S 3.426056 -0.679120 1.565973
H 3.344625 -2.032046 1.659751
S -3.061380 -2.364434 0.859753
S -1.576247 -3.659666 0.203389
H -2.735472 -2.265292 2.169698
S -1.832151 3.041970 1.421358
S -1.740334 3.486279 -0.580887

H -3.069792 2.495418 1.539801
S -1.964096 0.158346 -1.609989

E= -4587.140731
S -0.227080 -0.238791 1.657819
Mo 1.473041 -0.701895 0.000816
Mo -1.471213 -0.907958 -0.227914
Mo -0.206879 1.493958 0.008160
S 1.616625 1.194400 -1.516290
S 2.313787 1.621601 0.373956
S -0.044853 -2.130675 -1.362205
S 3.574561 -1.709840 -0.575832
S 2.840476 -2.485644 1.194691
H 2.259367 -3.626140 0.750236
S -2.847128 -2.668582 1.095819
S -3.773795 -1.391837 -0.251786
H -2.670852 -3.758586 0.312224
S -0.527168 3.415405 1.613180
S -0.383984 3.924843 -0.370714
H -1.870168 3.328449 1.797348
S -1.860581 1.026864 -1.462663

[Mo3S11H3]+ X
E= -4587.162598
S -0.948959 -1.047360 -1.218602
Mo 0.078713 0.547105 -0.008917
S 1.726016 1.388678 -1.339403
Mo 2.728249 -0.357080 -0.175379
S 4.772181 -0.653197 1.361558
S 4.748857 0.845867 -0.067562
Mo -2.749017 -0.086671 -0.133197
S -3.854940 -1.186180 1.640747
S -3.922871 -2.341657 -0.075379
S -3.917263 1.092474 -1.417133
S -1.723675 1.399340 1.509936
S -0.947824 2.899035 0.244855
S 1.221213 -0.558151 1.597923
S 2.801496 -2.074426 -1.373989
H -5.132378 -1.968030 -0.557253
H 5.423119 -1.629945 0.685477
H -1.992094 3.026327 -0.600725

E= -4587.134955
S 1.224489 0.044146 1.617049
Mo -0.234485 0.765756 -0.022431
S -2.002936 1.811224 0.894905
Mo -2.780622 -0.302155 0.239874
S -4.625294 -1.244918 -1.280181
S -4.834869 0.632919 -0.433573
Mo 2.988956 -0.150315 0.109574
S 3.167053 -1.883576 -1.512969
S 3.353644 -2.643301 0.403253
S 4.734710 0.838696 0.707212
S 1.824329 1.253981 -1.517444
S 1.090398 2.956010 -0.500065
S -1.071720 -0.959632 -1.217116
S -2.876888 -1.525317 1.937511
H 4.702325 -2.646795 0.533417
H -5.293912 -1.999765 -0.375981
H 1.963306 3.004804 0.530549

[Mo3S11H3]+ XI
E= -4587.160214
S -1.885093 0.942115 -1.752365
Mo 0.065800 1.240858 -0.191689
S 0.610577 3.236447 -0.337155
Mo -2.843698 -0.631993 -0.082635
S -4.853921 -0.957563 -0.589784
S -1.664261 -2.346282 -0.483762
S -2.546987 -0.284068 2.254231
S -2.108917 1.398282 1.146594
S 1.231532 0.025852 -1.803009
Mo 2.519549 -0.194646 0.064979
S 3.560974 -2.304566 -0.887403
S 2.900732 -2.299778 1.070033
S 1.095116 0.494454 1.890985
S 4.105780 1.162380 0.122072
H 0.326293 -0.588711 2.157348
H -1.476917 0.137033 -2.752850
H 4.872765 -2.021893 -0.698944

E= -4587.128394

S -2.086436 0.999298 -1.685501
Mo -0.215316 1.655455 -0.160261
S -0.072499 3.724149 -0.260222
Mo -2.639961 -0.836256 -0.085321
S -4.655365 -1.337967 -0.363436
S -1.391534 -2.371477 -0.836245
S -2.074263 -0.713366 2.220434
S -2.143482 1.168045 1.369539
S 1.362816 0.696501 -1.613635
Mo 2.709145 -0.275187 0.021145
S 2.886308 -2.595896 -0.963503
S 2.374002 -2.392315 1.033138
S 1.356471 0.981983 1.669728
S 4.618259 0.563542 0.100296
H 0.627618 0.011719 2.267213
H -1.504278 0.350302 -2.712064
H 4.225760 -2.770442 -0.858261

[Mo3S11H3]+ XII
E= -4587.159361
S -1.758096 -0.128401 -1.868237
Mo -0.114999 0.681874 -0.053305
S -0.084767 2.713314 -0.532974
Mo -3.012462 -0.496994 -0.114332
S -4.495697 1.293908 0.174092
S -4.238447 -2.168988 -0.448646
S -1.293468 -1.323882 1.376182
S -1.849527 0.644127 1.761276
S 1.208582 -0.579974 -1.594049
Mo 2.740317 0.035626 -0.064248
S 4.221687 -1.910342 -0.736663
S 3.861575 -1.570567 1.268469
S 1.498257 0.810180 1.841344
S 3.864999 1.683912 -0.686756
H -5.380290 0.923714 -0.773690
H 1.272976 -0.330761 2.525785
H 5.405793 -1.266827 -0.877555

E= -4587.132111
S 1.791672 -0.208850 -1.811320
Mo 0.289430 -1.184558 -0.140057
S 0.567593 -3.226022 -0.382202
Mo 2.962934 0.664654 -0.127986
S 4.669597 -0.761025 0.554403
S 3.956909 2.352308 -0.868845
S 1.439472 1.508785 1.422720
S 1.663912 -0.542517 1.787240
S -1.435082 -0.413713 -1.608115
Mo -3.066371 0.084742 -0.040887
S -3.634573 2.419266 -0.794889
S -3.161536 2.111406 1.198864
S -1.657940 -1.188264 1.521660
S -4.807420 -1.045857 -0.265118
H 5.657876 -0.343684 -0.261623
H -1.308495 -0.292181 2.463591
H -2.442752 2.824454 -1.297102

[Mo3S11H2]+ I
E= -4586.510710
S -1.389269 -0.993481 1.907734
Mo -2.281959 -0.999459 -0.172631
S -2.562980 -2.968180 -0.818136
Mo 0.342162 0.206312 0.829928
S 2.087317 -0.958595 1.918711
Mo 3.035800 -0.419669 -0.046367
S 2.628319 -1.786448 -1.567827
S 0.247243 2.215990 1.390916
S -0.574472 -0.066899 -1.335468
S -3.700651 1.738758 0.356260
S -4.370390 -0.096295 -0.446202
S -3.268325 2.976799 -1.223559
S 4.963704 1.048381 -0.929868
S 3.003364 1.764569 -0.783263
H 5.461100 1.490162 0.250189
H -4.514999 3.454530 -1.417982

E= -4586.511563
S -1.099210 -1.027381 1.670528
Mo -2.475551 -1.147444 -0.086801
S -2.833961 -3.144225 -0.596434
Mo 0.267894 0.383621 0.196013
S 2.005207 -0.321581 1.732520

Mo 3.363318 -0.080961 -0.030117
S 1.863464 0.471412 -1.611621
S -0.200557 2.345073 0.709804
S -1.265660 -0.145713 -1.666436
S -3.954223 1.559393 0.770552
S -4.614770 -0.362589 0.207907
S -4.056890 2.753376 -0.896918
S 5.673791 0.923880 -0.023595
S 5.423853 -1.114720 -0.373647
H 5.764258 1.398174 -1.291256
H -5.358721 3.091965 -0.793283

[Mo3S11H2]+ II
E= -4586.526175
S -0.911000 -0.904173 1.715962
Mo -2.343840 -1.108050 -0.024992
S -2.492960 -3.140697 -0.490362
Mo 0.287482 0.269287 0.059521
S 1.969430 0.099033 1.777051
Mo 3.287200 0.030766 -0.018573
S 1.863880 -0.059104 -1.730148
S -0.241491 2.495711 0.170746
S -1.192554 -0.148591 -1.727442
S -3.879351 1.412931 0.841149
S -4.532407 -0.520072 0.299149
S -4.184401 2.637636 -0.781422
S 5.375652 0.968778 -0.159726
S 5.302758 -1.080850 -0.000706
H -5.471652 2.948709 -0.523720
H 0.535453 2.817548 1.225548

E= -4586.521130
S -1.341872 -0.788702 1.868874
Mo -2.386284 -1.068005 -0.077214
S -2.432480 -3.101268 -0.563683
Mo 0.310933 0.326162 0.422740
S 1.977553 1.606739 -0.883290
Mo 3.313997 0.012030 -0.142552
S 1.933966 -1.235752 1.137376
S -0.161050 2.193201 1.691673
S -0.940879 -0.016953 -1.511480
S -4.021194 1.422889 0.344913
S -4.616445 -0.547230 -0.113973
S -3.967561 2.488249 -1.413452
S 5.065015 -0.833238 -1.351335
S 5.536891 0.356430 0.274400
H -5.265584 2.855414 -1.421823
H 0.731346 3.086873 1.216544

[Mo3S11H2]+ III
E= -4586.546684
S 1.079533 -0.677758 -1.420470
Mo 2.593869 -0.052269 0.117198
S 1.682432 1.461107 1.416809
Mo -0.092863 0.772379 -0.040582
S -0.343637 3.035267 -0.568039
S -1.927413 0.684511 -1.652513
Mo -2.617087 -0.523329 0.029077
S -2.393416 -2.707601 -0.647475
S -1.188100 -0.127109 1.774795
S -4.493114 0.272374 1.311992
S -5.010433 -0.172200 -0.558140
S 4.678721 -1.354458 -0.550879
S 4.600901 0.725498 -0.724166
S 3.736753 -1.685172 1.288067
H 0.547670 3.661945 0.228068
H -2.427907 -3.198051 0.613125

E= -4586.471144
S 1.128474 -0.249984 -1.548741
Mo 2.789875 0.297475 -0.055598
S 1.700082 1.075139 1.635862
Mo -0.448393 0.731249 -0.156199
S -0.628598 3.019119 0.210447
S -2.097627 0.830260 -1.675563
Mo -2.884636 -0.595495 -0.025949
S -2.836467 -2.624038 -1.073341
S -1.189725 -0.587907 1.539066
S -4.541121 -0.468038 1.609711
S -5.010979 0.368583 -0.188067
S 4.798341 -1.324227 -0.518447
S 4.957466 0.783529 -0.713821

S 5.283876 -1.953950 1.281375
H 0.422294 3.276548 1.013880
H -2.629367 -3.367952 0.035778

[Mo3S11H2]+ IV
E= -4586.519799
S -1.274946 -0.972806 -1.699286
Mo -2.633417 -0.178821 -0.198785
S -1.491561 0.206218 1.610888
Mo 0.266775 -0.777105 0.199356
S 0.459340 -2.728719 0.908568
S 1.762815 -0.617407 -1.658114
Mo 2.925625 0.526885 -0.082622
S 2.866682 2.567573 -1.134467
S 1.556985 0.593953 1.705588
S 4.886333 0.418711 1.158936
S 4.908050 -0.605241 -0.629210
S -4.888848 0.801934 -0.779813
S -4.750691 -1.111785 0.020825
S -5.291250 2.223564 0.690564
H -6.604612 2.309015 0.394638
H 3.241588 3.294762 -0.060183

E= -4586.516146
S 1.318070 -0.921514 1.735752
Mo 2.661581 -0.158925 0.195182
S 1.493979 0.219809 -1.610991
Mo -0.189893 -0.783451 -0.157245
S -0.352664 -2.758039 -0.811715
S -1.715472 -0.509563 1.663264
Mo -2.942825 0.528456 0.057520
S -3.067849 2.614600 1.039713
S -1.585097 0.555304 -1.680355
S -5.307074 0.648746 -0.642382
S -4.730412 -1.101732 0.096100
S 4.928014 0.837751 0.744693
S 4.783818 -1.085837 -0.027435
S 5.311282 2.239760 -0.750666
H 6.628940 2.328300 -0.476357
H -4.066703 3.227762 0.371499

[Mo3S11H2]+ V
E= -4586.540782
S 1.296852 -0.709201 -1.425060
Mo 2.994648 -0.443662 0.051204
S 2.154184 0.704426 1.666748
Mo -0.097470 0.684770 -0.066156
S 0.842126 2.976521 -0.962924
S -0.209530 2.868776 0.811005
S -1.726563 0.754502 -1.653490
Mo -2.546260 -0.665947 -0.017918
S -2.387218 -2.661987 -0.627109
S -1.020593 -0.371813 1.707449
S -4.367401 -0.234964 1.407096
S -4.989428 -0.081132 -0.560387
S 4.630584 -2.004709 0.409919
S 5.208485 -0.247936 -0.526074
H -0.168099 3.292891 -1.807928
H -5.474397 -1.329392 -0.766306

E= -4586.518855
S -2.007112 0.937730 1.351783
Mo -3.041896 -0.528282 0.055440
S -1.470365 -1.045409 -1.455383
Mo -0.118663 0.442008 -0.143782
S -1.124777 3.948796 0.282922
S 0.107474 2.625295 -0.753347
S 1.199539 -0.254717 1.614948
Mo 2.722953 -0.657733 -0.076195
S 3.076833 -2.711069 -0.312267
S 1.605983 0.109022 -1.863002
S 4.649294 0.626717 -0.431709
S 4.724434 -0.070488 1.516751
S -4.623433 -2.009627 0.799807
S -5.289268 -0.443015 -0.376338
H -0.686759 5.012036 -0.420299
H 5.488600 -1.175515 1.344207

[Mo3S11H2]+ VI
E= -4586.578605
S -1.129919 -1.063898 -1.253247
Mo -2.878554 0.012305 -0.136525

S -3.985114 1.269446 -1.382783
Mo 0.132904 0.426017 -0.091065
S -1.714382 1.309091 1.506941
S -0.654895 2.594077 0.258461
S 1.284989 -0.546630 1.598940
Mo 2.811821 -0.372696 -0.149074
S 3.045088 -2.193594 -1.158559
S 1.706271 1.096297 -1.579860
S 4.727867 0.994660 -0.125141
S 4.829695 -0.351463 1.444615
S -4.208540 -2.153536 -0.003347
S -4.087060 -0.936222 1.661289
H -5.375018 -1.714854 -0.535572
H 5.571849 -1.333081 0.878545

E= -4586.513275
S -1.867721 0.545428 1.746141
Mo -2.900864 -0.435397 0.110230
S -1.530286 -0.601953 -1.600800
Mo -0.135796 0.572840 -0.007401
S 0.508833 2.833414 0.572782
S -0.827781 2.778509 -0.888120
S 1.210458 -0.434007 1.625030
Mo 2.621166 -0.626919 -0.172708
S 2.923029 -2.637319 -0.716507
S 1.526679 0.390608 -1.830509
S 4.569397 0.655881 -0.365756
S 4.720554 -0.367277 1.432240
S -5.048987 -1.769958 0.499312
S -5.118688 0.139627 -0.315928
H -5.046765 -2.534961 -0.620379
H 5.449695 -1.434266 1.029110

[Mo3S11H2]+ VII
E= -4586.483963
S -1.085999 -0.346838 1.886226
Mo -2.502793 -0.532085 0.125904
S -3.561793 1.399267 -0.124234
S -1.829568 0.922686 -1.620846
Mo -0.021474 0.706631 0.092798
S -0.632089 3.083011 0.789134
S 0.792825 2.930713 -0.679017
S 1.926726 0.782835 1.597857
Mo 2.551582 -0.517775 -0.021510
S 4.659682 -1.937190 0.348612
S 4.724216 -0.202641 -0.792456
S 0.945976 -0.722285 -1.540759
S -2.997861 -2.437412 -1.048554
S -3.301910 -2.592693 0.967271
H 0.137113 3.220032 1.896138
H 4.472377 -2.875670 -0.611845

E= -4586.510649
S -0.854228 -0.206877 -1.702914
Mo -2.630521 0.308121 -0.029528
S -3.747507 2.338410 0.540595
S -2.129665 2.555584 -0.629710
Mo 0.393569 -0.692008 0.075321
S 0.286521 -2.898522 0.856337
S -1.499947 -0.316221 1.707781
S 2.263449 -1.514802 -1.130176
Mo 3.031342 0.275014 -0.113036
S 5.307077 1.304767 -0.775811
S 5.120953 0.073345 0.886290
S 1.418423 1.123882 1.161278
S -4.835864 -0.595117 0.247203
S -3.693338 -1.556979 -1.081571
H -0.712388 -2.874749 1.762650
H 5.174047 2.527882 -0.207286

[Mo3S11H2]+ VIII
E= -4586.515814
S -0.757634 -0.186595 -1.902235
Mo -2.353510 0.270520 -0.239528
S -2.826761 2.215317 1.199803
S -2.505108 2.456327 -0.820323
Mo 0.288483 -0.556833 0.046349
S -0.584001 -2.351980 1.259591
S -1.342532 -0.489707 1.833185
S 2.169574 -1.706946 -0.877559
Mo 3.009006 0.177057 -0.125129
S 5.413867 0.787880 -0.828678

S 5.007968 -0.012214 1.044826
S 1.377196 1.362543 0.818349
S -4.738159 -0.581215 0.380939
S -3.750058 -1.238490 -1.314678
H -4.474044 -1.604284 1.227572
H 5.397262 2.114349 -0.550150

E= -4586.501206
S -0.753332 -0.260877 -1.855311
Mo -2.507655 0.237063 -0.215962
S -3.572206 2.220208 0.628500
S -1.966165 2.569139 -0.508184
Mo 0.321575 -0.425316 0.069550
S -0.613835 -2.052247 1.487727
S -1.303205 -0.123118 1.845727
S 2.119323 -1.778993 -0.661481
Mo 3.066504 0.141718 -0.145787
S 5.519307 0.470008 -0.895223
S 5.042085 -0.015901 1.067526
S 1.502861 1.516629 0.645413
S -4.620055 -1.049302 0.420318
S -3.758605 -1.355816 -1.486659
H -4.116083 -2.101448 1.110637
H 5.599522 1.820264 -0.811955

[Mo3S11H2]+ IX
E= -4586.559683
S -1.870252 0.987073 -1.731025
Mo -2.807618 -0.625315 -0.086482
S -1.582556 -2.308048 -0.495587
Mo 0.082384 1.247200 -0.166749
S -2.542660 -0.302502 2.257201
S -2.099180 1.391779 1.171192
S 1.239998 0.091668 -1.826521
Mo 2.520932 -0.225734 0.033900
S 4.090511 1.139026 0.099806
S 1.107211 0.425413 1.887237
S 0.639033 3.243347 -0.247234
S 3.023100 -2.407168 1.027779
S 3.407094 -2.285659 -0.909752
S -4.804822 -0.986747 -0.618889
H 0.323650 -0.651686 2.132935
H -1.462571 0.202387 -2.748352

E= -4586.528525
S -2.056940 1.026944 -1.679305
Mo -2.622158 -0.824361 -0.099333
S -1.326277 -2.336736 -0.819351
Mo -0.193042 1.650479 -0.134046
S -2.126475 -0.712753 2.225099
S -2.151689 1.165468 1.368054
S 1.399456 0.746785 -1.609276
Mo 2.709516 -0.308562 -0.004043
S 4.597981 0.560892 0.079594
S 1.330688 0.875905 1.687166
S -0.036369 3.720081 -0.169532
S 2.483654 -2.543351 0.981220
S 2.840516 -2.528199 -0.970340
S -4.620947 -1.351438 -0.440712
H 0.572157 -0.100102 2.238287
H -1.471017 0.385184 -2.708473

[Mo3S11H2]+ X
E= -4586.558588
S -1.752073 -0.049296 -1.863285
Mo -2.995700 -0.489880 -0.117654
S -4.219251 -2.150417 -0.511890
Mo -0.096696 0.685031 -0.028475
S -1.270775 -1.371028 1.334244
S -1.821319 0.583362 1.791541
S 1.200701 -0.520392 -1.636446
Mo 2.760604 0.015027 -0.103008
S 3.836648 1.693409 -0.705497
S 1.540560 0.730017 1.845405
S -0.061330 2.733874 -0.426131
S 4.033275 -1.621707 1.212406
S 4.120223 -1.895345 -0.745882
S -4.482228 1.283451 0.247489
H -5.372613 0.946166 -0.707108
H 1.316979 -0.428481 2.499579

E= -4586.548187

S -2.009604 0.471380 1.724074
Mo -3.008325 -0.475067 0.019432
S -4.689577 0.595951 -0.622718
Mo -0.115106 0.648776 0.023224
S -0.788132 2.937018 -0.541492
S 0.499257 2.855499 0.966410
S 1.055476 -0.505604 1.665355
Mo 2.458668 -0.635789 -0.133082
S 2.287821 -2.531637 -0.977746
S 1.536808 0.791022 -1.850195
S -1.425485 -0.497438 -1.601213
S 4.664301 0.420176 -0.340249
S 4.420861 -0.667788 1.297235
S -3.639693 -2.612009 0.619226
H -4.813279 -2.666004 -0.040100
H 2.140794 1.968225 -1.580988

[Mo3S11H2]+ XI
E= -4586.549337
S 1.683376 0.554879 1.814220
Mo 3.379145 -0.190613 0.137039
S 4.016726 1.752745 -0.407358
Mo -0.126277 0.364581 -0.018684
S 0.252696 2.245765 -0.817277
S -1.567091 0.461424 1.761696
Mo -2.963085 0.100127 -0.032792
S -3.806308 1.889101 -0.673177
S -1.496163 -0.578963 -1.834015
S -4.405873 -1.855347 -0.321922
S -4.571845 -0.975527 1.443234
S 4.912068 -1.201932 1.149704
S 2.816812 -1.233281 -1.920774
S 1.402188 -1.619416 -0.465228
H -1.392484 -1.914415 -1.669429
H 1.436172 -0.628735 2.410196

E= -4586.517811
S -1.545741 -0.767111 1.325915
Mo -3.511642 0.106633 0.043763
S -3.429482 -1.207449 -1.600115
Mo 0.661661 -1.163136 0.233951
S 0.623290 -3.097086 -0.566031
S 2.321518 -0.878018 1.753166
Mo 3.058185 0.233951 -0.154184
S 4.260345 -1.004296 -1.318874
S 1.019141 0.491210 -1.491732
S 3.577079 2.631411 -0.241435
S 4.484315 1.648442 1.220163
S -5.111176 -0.394751 1.306716
S -4.181120 2.214764 -0.915951
S -2.516610 2.403796 0.133581
H 0.492229 1.655222 -1.050744
H -1.261786 0.237351 2.176020

[Mo3S11H2]+ XII
E= -4586.547948
S -1.441732 -0.976050 -1.317029
Mo -3.303708 -0.250709 -0.114862
S -4.095583 1.249085 -1.341171
Mo 0.150019 0.327892 -0.049721
S -0.200137 2.344341 -0.443960
S 1.541807 -0.526926 -1.698791
Mo 2.998656 0.074611 -0.048298
S 3.799332 1.961751 -0.415091
S 1.617233 0.375509 1.919218
S 4.486788 -1.501485 1.099647
S 4.600164 -1.563272 -0.875568
S -4.923557 -1.858455 -0.200396
S -3.197401 0.818938 1.943665
S -1.610104 -0.497828 1.700764
H -4.215814 -2.714557 0.574269
H 1.498225 -0.870542 2.426130

E= -4586.536190
S 1.202300 0.875655 -0.587098
Mo 3.378567 0.089812 0.115454
S 3.308565 -0.686226 2.054959
Mo -0.496993 -0.539435 -0.130076
S -0.059664 -2.567747 0.119206
S -1.981476 -0.278483 -1.833460
Mo -3.273147 0.043899 0.056083
S -4.297130 -1.715204 0.487984

S -1.642287 0.154347 1.882105
S -4.389723 2.125299 0.704051
S -4.769770 1.528195 -1.147501
S 3.515716 -1.606198 -1.474652
S 5.627021 0.910037 -0.290087
S 4.296840 2.361023 -0.059672
H 4.786830 -2.032889 -1.329048
H -1.307048 1.462104 1.894301

[Mo3S11H2]+ XIII
E= -4586.514179
S 0.146015 0.007029 -0.515206
Mo 2.604992 -0.119109 -0.358545
S 3.197684 1.564789 -1.476474
Mo -1.712043 -1.230136 0.269807
S -3.320137 0.471457 0.222437
Mo -1.438819 1.641340 -0.107201
S -1.579136 3.704738 -1.129422
S -1.212737 3.684068 0.898649
S -1.507120 -1.758515 2.284003
S -3.099347 -2.654989 -0.969613
S -1.163035 -3.389241 -1.019624
S 3.063594 -1.924170 -1.354066
S 2.362721 -0.013561 2.033437
S 4.333321 -0.101995 1.442780
H 4.582281 -1.430387 1.551754
H -1.204898 -4.271388 0.007257

E= -4586.510021
S -0.161273 -0.474430 -1.205909
Mo 2.016877 -1.166404 -0.218917
S 3.186670 -0.728469 -1.919409
Mo -2.054346 -0.446714 0.244528
S -2.047719 1.773180 1.005551
Mo -0.015502 1.540813 0.114034
S 0.739394 3.047608 -1.589371
S 0.961616 3.820084 0.236492
S -1.917996 -1.659630 1.939150
S -4.234804 -0.179950 -0.556160
S -3.435090 -1.904375 -1.378226
S 1.858217 -3.242404 0.057190
S 1.385884 0.439046 1.603262
S 3.829560 -0.451060 1.321659
H 3.497771 -1.167670 2.413881
H -3.904307 -2.829141 -0.506671

[Mo3S11H2]+ XIV
E= -4586.505852
S 0.919392 -0.605151 -0.867851
Mo 3.241590 -0.776650 -0.042865
S 3.778150 -2.610275 -0.919293
Mo -0.804495 0.175491 0.321383
S -2.115757 1.570170 -1.003934
Mo -3.507939 -0.066098 -0.388263
S -5.501336 0.519041 0.625086
S -5.922967 -0.947420 -0.789930
S -0.442693 1.158615 2.135021
S -2.310833 -1.576117 0.708418
S 3.095983 -1.062522 2.032277
S 3.583153 1.535348 -1.219784
S 5.167371 0.584824 -0.353227
S 2.740771 2.946777 0.085985
H -6.275114 -0.178008 -1.848113
H 3.390833 3.990172 -0.466893

E= -4586.511279
S 1.114658 -1.058763 -1.661371
Mo 2.513590 -1.137143 0.079520
S 2.931062 -3.121146 0.594245
Mo -0.278123 0.321259 -0.176776
S -2.022017 -0.484085 -1.637164
Mo -3.373991 0.058164 0.079159
S -5.508324 0.990528 -0.041566
S -5.618895 -1.048692 0.368675
S 0.122378 2.287461 -0.718331
S -1.831452 0.362107 1.680686
S 1.300848 -0.158234 1.669990
S 3.908651 1.605516 -0.807679
S 4.626589 -0.296173 -0.245035
S 3.998760 2.808653 0.853747
H -5.827491 -1.555948 -0.872171
H 5.289402 3.182529 0.732907

[Mo3S11H2]+ XV
E= -4586.600428
S -0.000020 0.132725 1.757334
Mo -1.345803 -0.693197 0.005433
Mo -0.000184 1.661831 -0.073412
Mo 1.345953 -0.692900 0.005439
S 1.832479 1.146544 -1.323120
S -3.080499 -1.225609 1.490479
S -3.613521 -1.859189 -0.412545
H -4.374532 -0.815225 -0.813849
S 3.080770 -1.224925 1.490494
S 3.613932 -1.858394 -0.412528
H 4.374756 -0.814290 -0.813816
S -0.000431 3.624425 1.315214
S -0.000450 4.086909 -0.621509
S 0.000194 -1.763851 -1.732495
S 0.000309 -2.826718 0.037676
S -1.832690 1.146127 -1.323105

E= -4586.557752
S 0.064103 -0.267104 1.705264
Mo 0.498214 1.386385 0.012537
Mo 1.197727 -1.225402 -0.159838
Mo -1.604510 -0.355670 0.006868
S -0.448768 -2.278312 -1.136416
S 1.429989 2.868059 1.571560
S 1.348787 3.811191 -0.275976
H 2.610989 3.592729 -0.710997
S -3.195538 -1.589838 1.332897
S -4.046884 -0.958442 -0.440694
H -3.904430 -2.059049 -1.217733
S 2.610853 -2.548052 1.288961
S 3.201519 -2.609220 -0.604568
S -1.261393 1.404980 -1.684561
S -1.911487 2.087066 0.162002
S 2.049651 0.494869 -1.429287

[Mo3S11H2]+ XVI
E= -4586.566566
S -0.224583 -0.179737 1.666357
Mo 1.422486 -0.514786 0.005981
Mo -1.186943 -1.192832 -0.231124
Mo -0.468638 1.467202 -0.028400
S 1.429895 1.312456 -1.543589
S 1.974322 1.983454 0.319653
S 0.624226 -2.115848 -1.380866
S 3.782031 -1.104786 -0.403845
S 3.276083 -1.187313 1.582041
H 2.946711 -2.495280 1.743864
S -3.378535 -1.834593 0.938574
S -2.282937 -3.295042 -0.053248
H -2.966337 -2.029626 2.212714
S -1.504780 3.118084 1.371682
S -1.197217 3.764795 -0.489499
S -1.885405 0.465556 -1.588996

E= -4586.551776
S -0.147331 -0.278662 1.661925
Mo 1.606737 -0.295375 -0.001819
Mo -1.196345 -1.215099 -0.233348
Mo -0.561423 1.415939 0.030716
S 1.283345 1.562102 -1.532333
S 1.835834 2.162474 0.366004
S 0.486299 -2.055985 -1.363433
S 3.889251 -0.768574 -0.570806
S 3.368714 -1.674339 1.213727
H 3.084920 -2.928621 0.787025
S -2.100006 -3.267195 1.079325
S -3.297480 -2.266395 -0.287015
H -1.638650 -4.276932 0.303672
S -1.546934 2.983561 1.597469
S -1.422206 3.746783 -0.228162
S -2.043420 0.554731 -1.468188

[Mo3S11H2]+ XVII
E= -4586.558503
Mo 0.000009 1.875633 -0.267020
Mo -1.362818 -0.364880 0.019663
Mo 1.362809 -0.364898 0.019664
S 0.000000 0.136893 -1.885752
S 1.776950 1.643347 1.385548

S 2.454173 1.856525 -0.544858
S -1.776943 1.643372 1.385545
S -2.454165 1.856504 -0.544867
S -3.585345 -1.520577 0.611966
S -2.971382 -1.555233 -1.348486
S -0.000010 -1.190776 1.873348
S 0.000003 -2.462414 0.270224
S 3.585337 -1.520592 0.611967
S 2.971381 -1.555226 -1.348488
H 3.126317 -2.717564 1.052381
H -3.126320 -2.717541 1.052396

E= -4586.506773
Mo -0.267103 2.008082 -0.282032
Mo -1.324568 -0.442107 0.033035
Mo 1.482830 -0.398452 -0.003121
S 0.000392 0.187845 -1.839210
S 1.565072 1.741733 1.364027
S 2.223262 2.008972 -0.569934
S -1.919346 1.493279 1.429815
S -2.688586 1.646678 -0.472524
S -3.456710 -1.779727 0.595867
S -2.840695 -1.723663 -1.364456
S 0.119112 -1.254120 1.831909
S 0.153578 -2.485271 0.190093
S 3.882911 -1.131781 0.642966
S 3.200933 -1.437789 -1.284488
H 3.642614 -2.346145 1.192442
H -2.910066 -2.948316 1.011487

[Mo3S10H2]+ I
E= -4188.297927
S -0.827060 -0.555124 -1.921986
Mo 0.488676 -0.068641 -0.201855
S -0.816783 0.199097 1.579202
Mo -2.325888 0.128808 -0.232968
S -3.850962 -1.591101 -0.791566
S -4.202516 -0.912599 1.119176
S -5.772305 0.473203 1.144082
S -2.946947 2.061833 -0.728113
S 2.114816 -1.736929 0.058762
Mo 3.309367 0.123559 -0.159475
S 4.809654 0.427435 1.561101
S 5.851042 -0.479587 0.003499
S 1.832507 1.768311 -0.590122
H 5.772012 -1.774199 0.390704
H -6.665678 -0.414947 1.625268

E= -4188.286227
S -0.802507 0.309178 -1.939367
Mo 0.574711 0.059909 -0.149033
S -0.918927 -0.242026 1.521772
Mo -2.430633 0.255418 -0.237879
S -3.868340 -1.276247 -1.292134
S -4.207633 -1.278457 0.747178
S -5.874069 -0.115849 1.226367
S -3.255885 2.165982 -0.059761
S 1.988522 -1.690962 -0.414233
Mo 3.381039 0.070025 0.012009
S 5.147322 0.194560 1.487853
S 5.893722 -0.355654 -0.447614
S 1.943718 1.847358 0.105211
H 5.891000 -1.700686 -0.607929
H -6.680698 -1.184303 1.389443

[Mo3S10H2]+ II
E= -4188.339089
S -0.360012 -2.317682 -1.398222
Mo 1.260268 -1.587689 0.042042
S 2.046658 -2.913146 1.763500
Mo -1.184313 -0.491103 -0.295518
S -3.471024 -0.927380 -0.903420
S -3.346160 -0.132389 0.977545
S -3.692763 1.943982 0.959998
S -0.672381 1.259685 -1.626809
S 2.627016 -0.198966 -1.176221
Mo 1.073509 1.100464 -0.136285
S 2.093318 3.289861 -0.624233
S 1.708644 2.917632 1.297633
S 0.188617 -0.234514 1.601621
H -4.905950 1.836146 1.537793
H 2.677872 -3.739705 0.889851

E= -4188.243764
S 0.109266 -1.889967 -1.325527
Mo -1.710750 -0.815587 -0.603165
S -3.670137 -1.128568 -1.768924
Mo 1.536992 -0.859382 0.324142
S 3.552645 -0.562077 -0.800703
S 2.424541 0.879909 -1.773517
S 2.873072 2.736937 -0.963339
S 2.184873 -2.429959 1.539586
S -1.864333 -1.079693 1.667744
Mo -1.002749 0.979457 1.261598
S -2.411173 2.600123 0.407553
S -1.306153 1.499008 -1.034158
S 1.181306 1.021067 1.754535
H 3.875905 3.014464 -1.820491
H -3.645145 -0.151472 -2.699668

[Mo3S10H2]+ III
E= -4188.291232
S 1.485385 -0.739222 -1.489840
Mo -0.039579 0.559725 -0.199600
S -1.030158 -0.198460 1.701018
Mo -2.606703 -0.475516 0.047818
S -4.636434 0.599266 -0.520441
S -4.331521 0.295016 1.455511
Mo 3.046497 -0.172781 0.048965
S 5.246878 0.223287 -0.446291
S 4.824689 -1.478977 0.657400
S 1.952071 1.002180 1.514534
S -0.110971 2.858290 -0.446773
S -1.616102 0.371139 -1.832642
S -2.721093 -2.707951 -0.403475
H 0.844358 3.258984 0.415470
H -2.657263 -3.132063 0.878853

E= -4188.288183
S 1.423610 -0.807143 -1.431902
Mo 0.037581 0.616718 -0.116323
S -1.107945 0.079345 1.794600
Mo -2.547079 -0.478296 0.102217
S -4.886180 -0.050618 -0.602195
S -4.329327 0.770821 1.123279
Mo 3.019081 -0.180572 0.031724
S 5.215375 0.104678 -0.550099
S 4.776491 -1.490326 0.699381
S 1.969901 1.140195 1.435010
S -0.119000 2.837293 -0.716805
S -1.657171 0.264968 -1.765798
S -2.504899 -2.763831 -0.112304
H 0.816062 3.390760 0.082448
H -2.712230 -2.986507 1.206945

[Mo3S10H2]+ IV
E= -4188.281584
S -1.034683 -2.150386 -0.443184
Mo 0.219465 -0.233799 -0.178153
S 1.648570 0.127523 -1.854091
Mo 3.017627 0.015722 0.043608
S 4.085643 1.656302 1.304974
S 4.312419 1.789817 -0.717619
Mo -2.594929 -0.534133 -0.232200
S -4.196850 -0.753160 1.408385
S -5.098894 0.078635 -0.282041
S -5.291895 2.133623 -0.060621
S -1.458546 1.382270 -0.168948
S 1.390256 -0.300231 1.710826
S 4.085954 -2.000035 0.120782
H -6.603350 2.090346 0.251676
H 4.560926 -1.927735 -1.143845

E= -4188.276602
S -1.119127 -1.823340 -0.689044
Mo 0.301546 -0.164261 -0.052383
S 1.577698 0.615224 -1.727800
Mo 3.096200 -0.010886 -0.068875
S 4.444899 1.143017 1.439428
S 4.461581 1.826232 -0.485844
Mo -2.739562 -0.357224 0.095123
S -4.692909 -0.894779 1.230946
S -5.129254 -0.071632 -0.626942
S -5.551209 1.966562 -0.474028

S -1.262835 1.358668 0.601919
S 1.658614 -0.733976 1.631673
S 4.044085 -1.999493 -0.674467
H -6.886975 1.807631 -0.574087
H 4.338565 -1.631809 -1.941671

[Mo3S10H2]+ V
E= -4188.311677
S -1.699717 0.065072 1.778300
Mo -0.148641 0.636069 -0.027401
S 1.326574 -0.025205 -1.833501
Mo 2.665990 -0.512137 -0.094076
S 4.809133 0.344258 1.154208
S 4.404500 0.904304 -0.799092
Mo -2.958262 -0.266938 0.035702
S -5.110457 0.609821 0.043598
S -5.220364 -1.461774 0.180887
S -1.754139 0.003688 -1.757882
S -0.152333 2.718740 -0.037600
S 1.371640 -0.073749 1.701843
S 3.166501 -2.553172 -0.193668
H -5.378109 -1.800128 -1.122488
H 5.635069 -0.705329 0.931592

E= -4188.283906
S 1.714604 -0.265435 1.738232
Mo 0.138663 -0.621245 -0.083969
S -1.357163 0.305256 -1.775136
Mo -2.779488 0.548684 -0.064070
S -4.889709 -0.550068 1.113862
S -4.454928 -0.866600 -0.887120
Mo 3.183748 0.101517 0.088313
S 5.437100 -0.500389 -0.015999
S 5.228688 1.560049 0.239465
S 1.767510 0.283930 -1.648389
S 0.047815 -2.675300 -0.388166
S -1.469492 -0.123036 1.651576
S -3.422929 2.543013 0.099535
H 5.354273 1.978555 -1.044828
H -5.780976 0.462516 0.995643

[Mo3S10H2]+ VI
E= -4188.301187
S -1.755567 1.201979 -1.610577
Mo 0.248192 1.254389 -0.119517
S 0.877338 3.228174 -0.140981
Mo -2.722713 -0.535617 -0.096919
S -4.802959 -0.506129 -0.341152
S -1.915779 -2.287335 -0.953766
S -2.101460 -0.692707 2.193012
S -1.696671 1.194587 1.461932
S 1.421046 0.033014 -1.739084
Mo 2.786871 -0.671570 -0.021501
S 2.942160 -2.765807 0.065237
S 1.569373 0.259678 1.823381
S 4.683172 0.227389 -0.095732
H 0.729936 -0.768800 2.094285
H -1.379081 0.500798 -2.697275

E= -4188.273041
S -1.638819 1.153149 -1.677930
Mo 0.235353 1.760178 -0.136409
S 0.498650 3.815320 -0.250387
Mo -2.213450 -0.636154 -0.042252
S -4.187663 -1.257023 -0.268512
S -0.884656 -2.296676 -1.030361
S -1.451796 -0.665663 2.196954
S -1.674409 1.261745 1.436712
S 1.753687 0.654670 -1.588445
Mo 2.217676 -0.914524 0.020651
S 0.909126 -2.791325 -0.062918
S 1.797765 0.897151 1.605738
S 4.251366 -1.371401 0.065613
H 0.996224 0.289074 2.509771
H -1.030566 0.512820 -2.696732

[Mo3S10H2]+ VII
E= -4188.339001
S -3.687888 -1.981562 0.950369
Mo -0.160355 0.373706 0.112931
S -1.126889 -1.064045 -1.304217
Mo -2.888578 -0.298908 -0.002752

S -4.515083 0.781038 -1.234994
S -1.864225 0.826527 1.802840
S -1.700131 2.226175 0.302090
S 1.178363 -0.713385 1.600079
Mo 2.580598 -0.278843 -0.200827
S 4.498693 -0.265918 1.298314
S 4.569099 1.148927 -0.084557
S 1.354891 1.374596 -1.497825
S 2.746704 -1.937218 -1.445672
H -5.297327 -0.297953 -1.449796
H 1.710845 2.545648 -0.925837

E= -4188.310093
S -3.890620 -1.923370 1.088968
Mo -0.073334 0.343457 -0.057112
S -1.355650 -1.109458 -1.239931
Mo -3.096126 -0.292270 0.044008
S -4.844191 0.682081 -1.081712
S -2.020611 1.133954 1.572035
S -1.021612 2.447845 0.277534
S 1.149003 -0.585373 1.607269
Mo 2.650256 -0.339683 -0.143455
S 4.501392 -0.147064 1.424019
S 4.650182 1.072898 -0.128495
S 1.496004 1.100019 -1.729495
S 2.840129 -2.140824 -1.168426
H -4.091728 1.276209 -2.034848
H 1.833851 2.349326 -1.337983

[Mo3S10H2]+ VIII
E= -4188.293530
S 1.949538 -1.673679 -1.371701
Mo 0.125109 -0.160498 -0.316342
S -1.062649 1.663217 0.796545
Mo -2.639003 -0.114746 0.288788
S -4.651166 -0.366350 -1.057417
S -4.378231 1.474706 -0.381701
Mo 3.040159 -0.033506 0.140387
S 1.813884 1.441587 -1.378736
S 2.878042 2.299741 0.185582
S 1.462820 -0.754437 1.570814
S 4.973663 -0.771057 0.505743
S -1.478829 -1.547970 -1.117678
S -2.942334 -1.046499 2.124935
H -1.284173 2.570112 -0.179566
H 2.145211 -1.110735 -2.581660

E= -4188.293517
S 1.949038 -1.670556 -1.375385
Mo 0.125283 -0.160960 -0.312802
S -1.062347 1.658486 0.808180
Mo -2.639144 -0.116271 0.287431
S -4.654159 -0.362570 -1.051054
S -4.370859 1.481421 -0.386920
Mo 3.039807 -0.033194 0.138935
S 1.808589 1.444326 -1.374917
S 2.873858 2.299706 0.190211
S 1.466324 -0.760308 1.570536
S 4.975120 -0.768451 0.499301
S -1.477830 -1.541994 -1.125637
S -2.942244 -1.056706 2.119452
H -1.279539 2.568862 -0.165530
H 2.141946 -1.104675 -2.584404

[Mo3S10H2]+ IX
E= -4188.320319
S -1.410848 -1.351264 1.270273
Mo -0.089304 0.190651 0.158614
S 1.744663 1.992788 -0.276759
Mo 2.707861 -0.252134 0.027045
S 4.729115 -1.322183 0.039119
S 4.821174 0.698763 -0.277976
Mo -2.898092 -0.268368 -0.072911
S -1.685204 2.048063 0.284205
S -1.630153 1.101516 -1.551755
S -3.723154 -1.652401 -1.411875
S -4.773740 0.377406 1.112819
S 1.231994 -0.833782 -1.564548
S 1.577700 -0.439393 1.909665
H -4.285560 1.444347 1.773943
H 1.921239 2.497223 0.959946

E= -4188.280213
S -1.447420 -1.561902 -0.272070
Mo 0.114908 0.266493 0.037843
S 2.032318 1.910001 0.663696
Mo 2.977686 -0.286039 -0.061593
S 4.996981 -1.300496 -0.396118
S 5.094876 0.614416 0.336825
Mo -3.288241 -0.311156 -0.032437
S -1.427724 2.042387 -0.129586
S -3.134684 1.595038 -1.268926
S -4.895879 -1.391931 -0.783263
S -3.918419 0.062068 2.156749
S 1.609757 0.019013 -1.812539
S 1.645734 -1.275684 1.370585
H -2.794145 0.718584 2.513928
H 2.122688 1.764320 2.000458

[Mo3S10H2]+ X
E= -4188.283382
S 0.288015 0.081840 1.514429
Mo -0.612438 -1.389346 -0.176628
S -1.358196 -3.110710 1.312809
S -1.575209 -3.617420 -0.606863
Mo -1.350626 1.291859 0.252294
S -1.640320 3.267068 -1.325208
S 0.066128 3.147660 -0.156666
S -2.843744 1.546566 1.693988
S 1.139656 -1.727915 -1.594501
Mo 1.943922 -0.193642 -0.118163
S 4.102340 -0.415364 0.720582
S 3.882807 1.505108 -0.041359
S -2.161064 -0.221145 -1.317934
H 3.597508 2.195751 1.089092
H -1.200116 2.740635 -2.492618

E= -4188.299449
S -1.318309 0.070719 -1.850037
Mo 0.035757 0.139681 -0.021509
S 1.593058 1.797974 -0.876536
S 1.747761 1.576803 1.183513
Mo -2.814073 0.174413 -0.067786
S -4.594453 -1.235392 1.090977
S -4.124997 -1.605641 -0.891611
S -3.752697 2.040365 -0.188732
S 1.162045 -1.790813 -0.059526
Mo 2.925925 -0.157868 -0.031849
S 4.742368 -1.645333 0.014237
S 5.431670 0.317289 -0.058043
S -1.389805 0.164887 1.768181
H 5.677791 0.542330 1.254718
H -3.823630 -2.157505 1.714560

[Mo3S10H2]+ XI
E= -4188.291355
S -1.114266 -0.108240 1.753837
Mo 0.020391 0.632411 -0.078785
S 1.352887 -0.799647 -1.456827
Mo -2.561604 -0.539140 -0.007781
S -4.764311 0.382256 -0.533116
S -4.492822 0.014786 1.395062
S -2.516514 -2.583638 -0.443658
S -1.619925 0.602816 -1.764414
S 1.906688 1.056320 1.490944
Mo 2.856189 -0.262220 0.067115
S 5.065713 -1.470246 0.529133
S 5.018115 0.270388 -0.603632
S -0.051139 2.927401 -0.451722
H 5.347982 -0.971934 1.757584
H 0.872193 3.404118 0.409654

E= -4188.291031
S -1.058064 -0.149640 1.724901
Mo 0.026618 0.707401 -0.090641
S 1.409315 -0.563148 -1.572407
Mo -2.523378 -0.562705 -0.022558
S -4.781107 0.267402 -0.477009
S -4.446492 -0.116844 1.437104
S -2.437591 -2.595715 -0.503732
S -1.622113 0.613882 -1.773080
S 1.888648 1.097155 1.509712
Mo 2.888808 -0.072035 -0.010273
S 5.432679 -0.198406 -0.256579

S 4.375152 -1.724980 0.676317
S -0.177791 3.003534 -0.378898
H 5.517219 -0.674101 -1.523637
H 0.694566 3.490553 0.528185

[Mo3S10H2]+ XII
E= -4188.273319
Mo 3.283366 -0.632170 -0.036618
S 3.717972 1.230413 -1.305007
S 3.312531 2.904913 -0.159386
H 3.914294 3.757998 -1.014010
S 3.833916 -0.261811 1.958971
S 4.505827 -2.108029 -0.894532
S 1.038196 -1.507897 -0.147183
Mo -0.541875 0.063542 0.156239
S 0.049311 2.028915 0.585838
S -1.988373 -0.616754 1.844821
S -1.991954 0.080842 -1.683694
Mo -3.302145 -0.343719 0.056681
S -5.114689 1.071525 0.246892
S -5.780875 -0.646445 -0.720450
H -5.676598 -0.250122 -2.010955

E= -4188.262382
Mo 3.326808 -0.719737 -0.007396
S 3.957670 1.081320 -1.280029
S 3.664227 2.787318 -0.140574
H 4.251828 3.607951 -1.035761
S 3.807919 -0.332131 2.004183
S 4.472435 -2.309349 -0.762616
S 1.036157 -1.414843 -0.238419
Mo -0.493270 0.201237 0.107411
S 0.329517 2.071380 0.573831
S -2.015865 -0.455941 1.686508
S -1.945566 0.347805 -1.660372
Mo -3.509733 -0.113294 -0.032300
S -5.606912 0.863733 0.163034
S -5.817998 -1.140826 -0.352449
H -5.956981 -1.048060 -1.698080

[Mo3S10H2]+ XIII
E= -4188.378073
S -0.000054 0.036710 1.719087
Mo 0.073576 1.584626 -0.064283
Mo 1.310721 -0.833257 -0.035241
Mo -1.382498 -0.707289 -0.038918
S -3.002456 -1.513410 1.424418
S -3.677714 -1.827029 -0.518087
S 0.183678 4.010846 -0.555937
S 0.148346 3.510891 1.372946
H -3.311721 -3.118292 -0.686754
S 2.832834 -1.805010 1.432882
S 3.440348 -2.242534 -0.507875
H 4.369885 -1.275832 -0.685858
S 1.886521 0.979161 -1.317552
S -0.098985 -2.142772 -1.280425
S -1.783373 1.152070 -1.320259

E= -4188.328080
S -0.041589 0.115657 1.673050
Mo -1.578943 0.758114 -0.049557
Mo 1.505566 0.795404 -0.028501
Mo 0.030271 -1.502073 -0.076840
S 0.041126 -3.271957 1.435708
S 0.018668 -4.065888 -0.485427
S -3.573520 2.125710 -0.592038
S -3.492715 1.404764 1.261910
H 1.338265 -4.314698 -0.648828
S 3.132938 1.622228 1.417114
S 3.720383 2.011349 -0.542797
H 3.306655 3.294965 -0.655657
S -0.034310 2.173282 -1.040389
S 1.893794 -1.071316 -1.312281
S -1.841931 -1.115139 -1.326714

[Mo3S10H2]+ XIV
E= -4188.342114
S -0.061528 0.080427 1.615904
Mo 1.438213 -0.722278 -0.025478
S 1.706036 1.089128 -1.426701
Mo -0.123834 1.567621 -0.197860
S -1.826221 0.707962 -1.536468

Mo -1.299053 -0.920198 -0.093299
S -2.889923 -2.694952 -0.080295
S -3.456814 -1.204367 1.248823
S 0.250000 -2.220777 -1.233467
S 0.504873 3.649591 1.181867
S -0.973983 3.779281 -0.269479
S 3.121073 -1.440997 1.525531
S 3.674903 -1.698719 -0.375720
H -2.990940 -1.699332 2.419706
H 1.572606 4.097992 0.479125

E= -4188.318571
S 0.098685 -0.166920 1.623183
Mo 1.683323 0.165322 -0.100869
Mo -0.866429 -1.379463 -0.183122
Mo -0.847109 1.343902 0.018653
S -1.757578 2.837711 1.671578
S -2.178509 3.429637 -0.182314
S 0.891396 2.079544 -1.203925
S -2.253241 0.115926 -1.269555
S 3.851835 -0.939180 0.784395
S 3.919534 0.863203 -0.251905
H 3.908231 -0.487726 2.058581
S -1.065697 -3.633570 1.049469
S -2.504098 -3.063169 -0.335189
H -1.669754 -3.265205 2.203290
S 0.937084 -1.629246 -1.455592

[Mo3S10H]+ I
E= -4187.732029
S 1.906614 1.184977 -1.619067
Mo 1.941765 -0.552120 -0.084273
S 1.819866 -2.351227 -1.125062
Mo -0.000148 1.458051 -0.451626
S -1.906488 1.184200 -1.619564
Mo -1.941555 -0.552465 -0.084267
S -1.819970 -2.351958 -1.124468
S -0.000447 3.325389 0.903332
S 4.289619 -0.230316 0.395206
S 3.241137 -0.759572 1.987608
S 0.000008 -0.117135 1.312471
S -3.241261 -0.759996 1.987447
S -4.289217 -0.229405 0.395175
H -0.000393 2.835126 2.157710

E= -4187.634936
S 1.591977 0.699246 -1.960669
Mo 2.206600 -0.699066 -0.187821
S 2.630082 -2.649430 -0.807801
Mo -0.145773 1.185578 -0.628421
S -1.951831 0.694951 -1.918700
Mo -2.311378 -0.717206 -0.152181
S -1.487340 -2.632718 -0.384037
S -0.183611 3.450939 -0.312891
S 3.767232 -0.228612 1.501677
S 2.408606 1.300865 1.797647
S 0.599166 0.123432 1.416668
S -4.153969 -0.664364 1.258085
S -2.475645 0.289299 1.934207
H -1.391394 3.551412 0.286803

[Mo3S10H]+ II
E= -4187.675749
S 0.243182 -0.476427 -1.430395
Mo 1.793628 0.125501 0.097485
S 0.773631 1.248561 1.712998
S 2.854591 -1.487630 1.392048
Mo -0.944346 0.741115 0.133878
S -2.813316 0.750811 -1.494335
Mo -3.341212 -0.692637 0.060023
S -3.087230 -2.634485 -0.674211
S -2.039852 -0.351094 1.870729
S -1.177010 3.037229 -0.190260
S 3.513972 1.446501 -0.704770
S 3.767754 -0.518597 -1.413249
S 4.522515 -1.694439 0.125430
H -0.270722 3.565976 0.658067

E= -4187.656623
S 0.440398 0.021158 -1.605901
Mo 2.400609 -0.209870 -0.398937
S 0.995101 1.426173 1.505627

S 2.723535 1.884842 0.472634
Mo -0.958193 0.896059 0.052999
S -2.886000 0.735318 -1.407461
Mo -3.126328 -0.790768 0.160366
S -2.673413 -2.666489 -0.646040
S -1.737025 -0.324653 1.880484
S -1.381682 3.166098 -0.137113
S 3.885909 -0.437049 -1.838157
S 3.177874 -1.351236 1.649833
S 1.901513 -2.410160 0.573032
H -0.415030 3.688293 0.643038

[Mo3S10H]+ III
E= -4187.710231
S 1.414626 -0.703611 -1.458848
Mo 3.045457 -0.217634 0.058049
S 2.014763 0.910509 1.585477
Mo -0.068404 0.629621 -0.206263
S -1.677142 0.708407 -1.768090
Mo -2.602241 -0.526929 -0.018528
S -2.577946 -2.534086 -0.580430
S -1.016748 -0.236177 1.653636
S 0.002101 2.950811 -0.246676
S -4.798881 0.491420 -0.370418
S -4.476946 -0.113391 1.487105
S 5.238135 0.186842 -0.466379
S 4.826451 -1.558168 0.569695
H 1.083268 3.186678 0.522021

E= -4187.710204
S 1.413960 -0.705835 -1.457479
Mo 3.045779 -0.216902 0.057495
S 2.015357 0.911565 1.584835
Mo -0.068218 0.629685 -0.206269
S -1.677066 0.709172 -1.767983
Mo -2.602376 -0.526335 -0.018626
S -2.578448 -2.533488 -0.580510
S -1.017102 -0.235340 1.653696
S 0.003535 2.950890 -0.247457
S -4.800116 0.489647 -0.370303
S -4.476925 -0.113416 1.487562
S 5.239339 0.184516 -0.466729
S 4.824776 -1.558811 0.571263
H 1.085257 3.186743 0.520447

[Mo3S10H]+ IV
E= -4187.724268
S -1.355680 1.865211 0.162758
Mo -2.716089 0.083395 0.007334
S -1.338418 -1.695007 -0.133742
Mo 0.122649 0.090164 0.018049
S 1.427703 0.237161 -1.775621
Mo 2.940871 0.124201 0.020702
S 3.821525 2.229646 -0.004323
S 1.432796 -0.062379 1.812027
S 4.259498 -1.413700 -1.116493
S 4.309328 -1.520019 0.920431
S -4.349102 0.043765 1.631644
S -5.043174 -0.923136 -0.086396
S -4.336222 0.317348 -1.612920
H 4.155832 2.231842 1.306597

E= -4187.710671
S 1.416129 1.626014 -0.212936
Mo 2.852719 -0.179607 0.023927
S 1.154326 -1.790798 0.229459
Mo -0.182167 0.014623 -0.006859
S -1.499373 0.300206 1.781174
Mo -2.970121 0.175909 -0.033880
S -3.688673 2.341850 -0.116710
S -1.500331 -0.177003 -1.813473
S -4.464928 -1.163545 1.151214
S -4.521888 -1.339194 -0.880701
S 4.485295 -0.153485 1.651768
S 5.169658 0.761723 -0.101900
S 4.486335 -0.580554 -1.554277
H -4.002882 2.337722 -1.431763

[Mo3S10H]+ V
E= -4187.771686
S 1.003699 -1.875898 -1.298371
Mo -0.834019 -1.339383 -0.056014

S -2.109793 0.062900 -1.333218
Mo 1.543518 -0.044590 -0.029521
S 1.109779 1.815878 -1.297963
Mo -0.756093 1.385643 -0.053176
S -1.684094 3.070808 1.387618
S -1.919626 3.521409 -0.539087
S -0.035191 0.000226 1.719280
S 4.098211 -0.173325 -0.501032
S 3.346918 -0.113059 1.437880
S -2.115111 -3.405333 -0.548527
S -1.847840 -2.978784 1.379590
H 4.405731 1.132701 -0.672860

E= -4187.771745
S 0.941039 -1.909073 -1.298265
Mo -0.878429 -1.311969 -0.056472
S -2.105461 0.132611 -1.334309
Mo 1.540732 -0.096436 -0.029553
S 1.169834 1.776768 -1.298804
Mo -0.709713 1.410514 -0.053862
S -1.582318 3.124185 1.387846
S -1.796633 3.584158 -0.539478
S -0.036060 0.001065 1.718678
S 4.090956 -0.308504 -0.498521
S 3.339765 -0.220596 1.439467
S -1.949235 -2.913513 1.380519
S -2.224907 -3.334317 -0.547892
H 4.439551 0.986867 -0.672609

[Mo3S10H]+ VI
E= -4187.687305
S -2.153506 2.451137 -0.319360
Mo -2.761536 0.558037 0.309657
S -1.657317 -0.197214 2.115533
Mo -0.186199 -0.868282 0.391100
S 0.643886 0.402725 -1.347166
Mo 2.548460 0.426550 -0.009134
S 2.881441 2.374553 0.658847
S 1.725932 -0.892898 1.700379
S -0.585690 -2.814729 -0.263974
S 4.042010 -0.098096 -1.870639
S 4.689252 -0.747665 -0.111264
S -3.211789 -0.856333 -1.452280
S -4.981128 0.123251 -0.920052
H -5.519917 -0.800512 -0.088568

E= -4187.710466
S 1.697369 0.053618 -1.767580
Mo 2.930708 0.283795 -0.003679
S 1.704142 0.054687 1.764835
Mo 0.105505 0.645792 0.001005
S -1.369382 -0.032754 -1.772343
Mo -2.683405 -0.542997 -0.000217
S -3.056979 -2.601224 -0.005221
S -1.367383 -0.041205 1.773021
S 0.104120 2.730772 0.004594
S -4.622478 0.598612 -0.987567
S -4.621299 0.594707 0.994103
S 5.087651 0.612412 0.005712
S 5.185653 -1.462638 -0.079128
H 5.319432 -1.770194 1.234583

[Mo3S10H]+ VII
E= -4187.691927
S 1.918832 0.468042 -1.698908
Mo 2.817116 -0.691696 0.034878
S 4.712812 0.085334 0.545348
Mo 0.056854 0.896375 0.010785
S -1.960893 0.443805 1.866077
Mo -2.853818 -0.650530 -0.038467
S -3.035678 -2.715087 0.279120
S 1.107949 -0.316227 1.620742
S 0.954308 2.931889 -0.610919
S -0.714807 3.054567 0.493270
S -1.141392 -0.281018 -1.573127
S 2.945351 -2.760556 -0.343410
S -4.670527 0.161511 -0.706641
H -2.701629 1.566383 1.752930

E= -4187.692069
S 1.808118 0.208666 -1.770857
Mo 2.795691 -0.583536 0.030377

S 4.654246 0.407193 0.484728
Mo 0.003234 0.776182 0.013008
S -1.825560 0.269803 1.903929
Mo -2.861077 -0.629946 -0.038466
S -3.149247 -2.699018 0.184396
S 1.203890 -0.364593 1.661389
S 0.810467 2.851070 -0.709089
S -0.743036 2.953617 0.559284
S -1.213763 -0.279096 -1.629862
S 3.428948 -2.620128 -0.248188
S -4.653202 0.331427 -0.569738
H -2.523379 1.423543 1.937520

[Mo3S10H]+ VIII
E= -4187.744408
S -4.191078 -1.644536 0.968263
Mo -3.024228 -0.211300 -0.002996
S -4.350838 1.023729 -1.421922
Mo -0.084439 0.195222 0.033529
S 1.321921 1.058741 -1.509805
Mo 2.666393 -0.287406 -0.148491
S 2.989164 -2.113979 -1.098567
S -1.317160 -1.376723 -1.050368
S -1.940540 0.870244 1.772870
S -1.428173 2.133234 0.211484
S 1.255017 -0.598648 1.683607
S 4.571094 0.233798 1.290678
S 4.586773 1.201706 -0.437961
H -5.363405 0.145307 -1.578267

E= -4187.744511
S 4.190987 1.642603 0.970825
Mo 3.023683 0.211128 -0.002755
S 4.350499 -1.021484 -1.423846
Mo 0.085305 -0.195585 0.032502
S -1.320950 -1.059604 -1.511216
Mo -2.665688 0.284612 -0.148362
S -2.983710 2.114361 -1.093904
S 1.316993 1.379148 -1.047948
S 1.937751 -0.870247 1.772024
S 1.431593 -2.133026 0.208848
S -1.254336 0.592806 1.684667
S -4.565538 -0.243492 1.297993
S -4.602024 -1.180163 -0.447270
H 5.361134 -0.140964 -1.580938

[Mo3S10H]+ IX
E= -4187.717014
S 1.889124 -1.417492 -1.629136
Mo 3.005914 -0.096797 0.146791
S 4.845835 -1.074095 0.422028
Mo 0.087776 -0.082840 -0.289162
S -1.381773 -1.712041 -0.789993
Mo -2.639952 -0.063371 0.296174
S -2.897691 -0.589468 2.296040
S -1.162491 1.742763 0.136489
S -4.632041 -0.624790 -1.007105
S -4.523271 1.283522 -0.487292
S 1.989882 1.649225 -1.169228
S 3.174357 2.189923 0.432882
S 1.377020 -0.769569 1.561163
H 2.079750 -0.641340 -2.713267

E= -4187.706845
S -1.950179 -1.630326 1.348145
Mo -3.057214 0.081093 -0.038820
S -5.117572 -0.319724 -0.033816
Mo -0.105532 -0.327324 0.021303
S 1.319837 -0.736669 1.713106
Mo 2.687054 -0.233151 -0.119037
S 3.556377 -2.023337 -0.738389
S 1.120656 0.316264 -1.756602
S 4.210323 1.084890 1.270199
S 4.148743 1.652228 -0.625227
S -1.335616 1.541631 1.057166
S -2.593559 2.357454 -0.369314
S -1.993469 -0.917809 -1.667286
H -1.869646 -1.059568 2.567516

[Mo3S10H]+ X
E= -4187.701826
S -1.522757 -0.877096 -1.414659

Mo -3.210643 -0.243408 -0.063898
S -3.329990 -1.364190 1.943728
Mo 0.282123 0.252667 -0.252148
S 1.288668 -1.840950 0.061074
Mo 2.839012 -0.145071 0.097732
S 4.835575 -0.817204 0.970935
S 4.958924 0.045435 -0.893146
S 1.744093 1.192276 1.507370
S 1.643100 0.985176 -1.804165
S -1.151362 1.787516 0.920758
S -3.096102 1.997567 0.140240
S -4.999535 -0.698205 -1.010504
H -2.170463 -0.861140 2.423077

E= -4187.681542
S 1.079899 -0.819007 -0.132742
Mo 3.531657 -0.442228 0.033887
S 4.145539 -2.369761 -1.067343
Mo -0.640613 0.555001 0.125629
S -2.146646 -0.192141 1.724682
Mo -3.584177 -0.203206 -0.051406
S -5.349796 -1.640363 -0.350975
S -5.821203 0.319997 0.033264
S -2.115957 0.486694 -1.662464
S -0.020878 2.512106 0.516111
S 3.034965 1.704268 -0.824566
S 5.000605 1.256988 -0.432930
S 3.761856 -0.906934 2.057067
H 4.017445 -1.831340 -2.302301

[Mo3S10H]+ XI
E= -4187.689038
-0.065778 -0.104041 -1.643493
0.364126 1.788662 -0.244189
1.281299 3.152521 -1.535895
1.377210 -0.792421 0.179273
1.972261 1.076718 1.268391
3.082485 -1.580039 -1.189220
2.872327 -2.559814 0.606236
-0.205196 -1.705307 1.685641
-1.455546 -0.850798 0.060554
-3.800451 -0.803665 -0.385380
-2.770778 -2.521222 -0.772659
-0.992689 2.849865 1.604475
-2.073009 1.689983 0.209793
-0.810711 1.971414 2.616985

E= -4187.714743
S 1.087111 -0.268594 1.768724
Mo 2.751450 0.138252 0.166442
S 3.586539 1.984579 0.680656
Mo -0.078201 0.137490 -0.097142
S 1.456319 0.362086 -1.753272
S -1.595615 1.779422 0.728802
S -1.889970 1.737904 -1.319904
S -1.371079 -1.742575 -0.459513
Mo -2.904677 -0.108469 -0.222706
S -4.563550 -0.279021 1.438354
S -5.032790 -1.117157 -0.359092
S 4.655118 -1.045276 -1.247193
S 4.027104 -1.733721 0.821329
H 3.972972 -1.867773 -1.859245

[Mo3S10]+ XII
E= -4187.710037
S 1.293810 -0.169461 -1.747881
Mo 2.624483 -0.517394 0.040683
S 2.627820 -2.565095 0.438883
Mo -0.058479 0.670887 -0.003765
S 0.073053 2.741140 -0.169164
S 1.450499 0.317084 1.976973
S -1.688859 0.030320 1.717130
S -1.741121 0.079470 -1.762206
Mo -3.062027 -0.184809 -0.019349
S -5.263059 0.453126 0.018423
S -4.878023 -1.580398 -0.052591
S 4.661575 0.729543 0.612546
S 4.646947 -0.052175 -1.208425
H 1.910671 1.578421 2.083114

E= -4187.686733
S 0.255526 -0.146555 1.506559

Mo -1.784189 -0.653145 0.303581
S -3.230974 -0.537504 1.792662
Mo 1.977937 -0.138946 -0.180050
S 1.753062 -1.627241 -1.639072
S 3.724756 -1.102766 1.474549
S 4.203274 0.454910 0.196509
S 1.560844 1.910878 -1.221698
Mo -0.278559 1.617374 0.044195
S -2.297587 1.269982 -1.141097
S -2.247488 2.877895 0.195444
S -1.314522 -2.994114 -0.134795
S -2.443958 -2.136855 -1.515909
H 4.155116 -2.159953 0.745055

[Mo3S10H]+ XIII
E= -4187.704193
S 1.350931 1.897853 -0.599589
Mo 2.238031 -0.438118 -0.257438
S 0.379524 -1.672986 -0.756744
Mo -0.766396 1.736623 -0.072382
S -1.763912 3.746620 0.303831
S -1.042892 0.419369 1.774898
S -2.000485 0.654694 -1.667267
Mo -1.746808 -0.852274 0.015527
S -3.725718 -1.877918 0.454026
S -2.225723 -3.199528 0.063490
S 3.442397 -1.389358 1.460523
S 3.054249 0.595819 1.719354
S 3.444329 -0.558087 -1.961460
H -3.045894 3.394680 0.543341

E= -4187.695016
S -1.104847 -0.055758 1.696424
Mo -2.601083 -0.552177 -0.017696
S -1.660688 0.608180 -1.711570
Mo 0.099621 0.758483 -0.067688
S 0.131351 3.059082 -0.347852
S 1.373670 -0.717985 -1.443525
S 2.056545 1.219533 1.382587
Mo 2.996830 -0.221742 0.017259
S 4.634825 -1.717484 0.674099
S 5.255454 -0.140531 -0.471620
S -4.873034 0.185715 -0.537568
S -4.524153 -0.000410 1.403570
S -2.531540 -2.603821 -0.393374
H -0.926811 3.264012 -1.157481

[Mo3S10H]+ XIV
E= -4187.753869
S 0.081034 0.114033 1.653423
Mo 0.668648 1.425379 -0.186004
Mo 0.851398 -1.334297 -0.062938
Mo -1.582782 -0.083126 -0.001258
S -3.411981 -0.099347 1.560256
S -4.033420 -0.355218 -0.313810
S -1.297709 1.683915 -1.386397
S -1.027620 -1.967838 -1.184264
S 2.494777 2.768005 1.022791
S 1.107573 3.753578 -0.170803
H 1.947151 2.940795 2.248431
S 2.028156 -2.836827 1.387695
S 2.183058 -3.350962 -0.536602
S 1.919116 0.085977 -1.516041

E= -4187.753929
S 0.079355 0.113602 1.652779
Mo 0.658633 1.429614 -0.186078
Mo 0.860983 -1.328653 -0.063364
Mo -1.583156 -0.094023 -0.002015
S -3.410366 -0.127541 1.561140
S -4.030305 -0.380832 -0.314146
S -1.309214 1.675299 -1.386629
S -1.013306 -1.974518 -1.185070
S 2.473514 2.785241 1.025133
S 1.080269 3.761259 -0.169282
H 1.923106 2.953189 2.250249
S 2.045973 -2.823439 1.388241
S 2.211544 -3.331883 -0.536922
S 1.919135 0.100025 -1.515809

[Mo3S10]+ I
E= -4187.110930

S 1.446579 -0.772232 1.639848
Mo 2.920609 -0.279543 -0.031632
S 3.993731 -2.027661 -0.702264
Mo 0.125444 0.252386 0.043332
S -1.129772 -1.259224 -1.382553
Mo -2.793089 -0.574277 -0.015209
S -1.745779 -0.461479 1.867268
S 1.639753 0.647270 -1.671023
S -1.295318 2.205788 -0.812366
S -0.274473 2.389100 0.951559
S 4.513318 1.026261 0.600232
S -4.485922 -1.805255 0.098719
S -3.326149 1.636195 -0.580208

E= -4187.078498
S 1.189972 -0.644208 1.497118
Mo 2.973292 -0.584130 0.006576
S 3.380015 -2.504110 -0.758574
Mo 0.164938 0.651890 -0.110143
S -1.185310 -0.637797 -1.537726
Mo -2.861769 -0.598678 0.026449
S -1.956164 0.443993 1.705617
S 1.931195 0.869229 -1.509634
S -0.637559 2.952934 -0.850673
S 0.090307 2.817785 0.976480
S 4.708935 0.323131 0.782429
S -3.561202 -2.566403 0.543228
S -4.685900 0.339104 -0.645831

[Mo3S10]+ II
E= -4187.128387
S -1.896300 0.527315 -1.592757
Mo -2.044797 -1.116259 0.097069
S -1.984474 -3.079197 -0.670071
Mo -0.283461 1.369696 -0.274831
S -0.135720 -0.439130 1.351532
Mo 1.794674 -0.547411 -0.097249
S 1.780818 1.484204 -1.216153
S -0.478898 3.781102 -0.363663
S -1.046184 2.927311 1.350730
S -3.771022 -0.835456 1.258025
S 1.564101 -2.031460 -1.532191
S 3.189697 -1.238167 1.794060
S 4.178641 -0.324841 0.342395

E= -4187.125321
S -2.001804 0.541110 -1.528873
Mo -2.018633 -1.156272 0.114950
S -1.933939 -3.095233 -0.712273
Mo -0.331917 1.338565 -0.252886
S -0.092307 -0.464880 1.348761
Mo 1.822184 -0.519644 -0.109095
S 1.692968 1.499157 -1.245396
S -0.812555 3.743298 -0.451791
S -0.850359 2.995840 1.395506
S -3.716861 -0.953460 1.332880
S 1.623517 -2.018629 -1.531565
S 3.278614 -1.174969 1.744358
S 4.199688 -0.186685 0.296849

[Mo3S10]+ III
E= -4187.065957
S 1.804422 -0.492614 1.728014
Mo 3.292627 -0.502243 0.077457
S 3.554686 -2.440184 -0.660562
Mo 0.771577 0.691201 -0.064847
S -0.459429 -0.725011 -1.306442
Mo -2.373739 -0.647382 0.144507
S -1.600423 0.379274 1.852965
S 2.553198 0.936577 -1.512569
S 0.069867 2.906325 -0.591459
S 0.543861 2.662770 1.339984
S -2.705930 -2.668479 0.593669
S -3.574897 0.440056 -1.757372
S -4.622827 0.204649 -0.098659

E= -4187.082208
S -2.368707 0.427578 -1.613758
Mo -3.316634 -0.492696 0.098781
S -4.548067 -2.122866 -0.356601
Mo -0.269203 0.546509 0.157891
S 0.704496 -0.528462 -1.608020

Mo 2.443246 -0.167032 -0.128876
S 1.309342 0.504469 1.785728
S -1.636530 -0.903785 1.538875
S -1.212899 2.710791 1.006401
S -0.160413 2.804357 -0.668688
S 3.597532 1.435673 -0.801500
S 3.516526 -2.272035 -0.754872
S 3.798020 -1.758521 1.136969

[Mo3S10]+ IV
E= -4187.065957
S 1.804118 -0.492932 1.727457
Mo 3.293111 -0.502687 0.077709
S 3.555152 -2.440545 -0.660462
Mo 0.772073 0.691586 -0.065498
S -0.459662 -0.724521 -1.306070
Mo -2.374529 -0.647170 0.144749
S -1.602151 0.379919 1.853170
S 2.554095 0.936487 -1.512375
S 0.070611 2.906773 -0.590785
S 0.544452 2.662423 1.340682
S -2.705890 -2.668458 0.593836
S -3.574807 0.440374 -1.757635
S -4.623889 0.203621 -0.099835

E= -4187.082153
S 1.536767 -0.850671 1.451476
Mo 3.297015 -0.431394 0.089198
S 4.520941 -2.069749 -0.355497
Mo 0.216549 0.617528 0.127255
S -0.739385 -0.438822 -1.650550
Mo -2.301118 -0.609288 0.052660
S -1.448384 0.890970 1.620526
S 2.411390 0.507406 -1.633676
S 0.307866 2.878970 -0.783391
S 1.176040 2.824211 0.982461
S -2.214165 -2.531237 0.852987
S -4.192712 -0.455371 -1.482258
S -4.541030 0.355075 0.291499

[Mo3S10]+ V
E= -4187.123074
S -1.896362 0.187464 -1.786531
Mo -3.203840 -0.238602 0.109620
S -4.237649 -2.033336 -0.301093
Mo -0.279925 0.195031 -0.191236
S 1.040070 -1.411527 -1.162064
Mo 2.608758 -0.028873 -0.191738
S -1.464416 -0.355220 1.699874
S 1.405372 1.459018 1.247162
S 0.334171 2.440268 -0.220342
S -4.511322 1.299336 0.718510
S 3.647915 1.022644 -1.658760
S 4.037025 -1.892501 0.388190
S 3.942086 -0.525979 1.812609

E= -4187.073749
S 1.234189 -0.599845 1.536104
Mo 3.019272 -0.687594 0.050376
S 3.345016 -2.663614 -0.603908
Mo 0.260679 0.653794 -0.134081
S -1.149919 -0.651527 -1.503060
Mo -2.809060 -0.433273 0.039118
S 2.036518 0.716589 -1.544546
S -0.417158 2.950307 -1.026844
S 0.263162 2.876463 0.820644
S 4.791804 0.190273 0.775949
S -1.869072 0.637966 1.665774
S -4.422539 -2.008830 0.411940
S -5.048088 -0.221716 -0.415014

[Mo3S10]+ VI
E= -4187.102926
S -1.570519 0.335815 1.591197
Mo -3.251249 0.324814 -0.022576
S -3.440505 2.198886 -0.960420
Mo -0.357792 -0.834023 -0.046991
S 0.898190 0.358285 -1.524980
Mo 2.646853 0.594307 0.094996
S 1.539977 0.148630 1.897314
S -2.187187 -1.320429 -1.313103
S 0.483464 -2.704489 0.402884

S -5.120748 -0.362127 0.659217
S -3.175595 2.614420 0.053247
S 3.971548 -0.984400 -1.306181
S 4.775926 -0.507974 0.434075

E= -4187.112472
S -1.853872 -0.063037 1.734704
Mo -3.205810 0.287228 0.000126
S -4.128399 2.238805 0.001181
Mo -0.198400 -0.696132 -0.000200
S 1.302713 0.013543 -1.732652
Mo 2.676772 0.527841 -0.000202
S 1.302322 0.013686 1.732187
S -1.853344 -0.060934 -1.734562
S -0.172532 -2.773186 -0.000511
S 3.095624 2.571191 -0.000400
S 4.591129 -0.643655 -0.989975
S 4.590599 -0.643210 0.991570

[Mo3S10]+ VII
E= -4187.120127
Mo -0.417350 -0.005065 -0.074238
Mo 2.580979 -0.003843 -0.022179
S 1.066677 0.023317 1.680955
S 0.883547 -0.036712 -1.859966
S 2.980789 2.166251 -0.809112
S 4.143954 1.668162 0.745393
S 2.993867 -2.191918 -0.742678
S 4.187522 -1.612123 0.763286
S -1.817542 -1.739780 -0.002009
Mo -3.447672 0.001002 0.083747
S -4.519776 0.032205 1.895174
S -4.734794 -0.023109 -1.581250
S -1.813631 1.734457 -0.056533

E= -4187.120317
Mo -0.441057 -0.000219 -0.043553
Mo 2.555975 0.000043 -0.016723
S 1.049614 -0.000235 1.700675
S 0.874190 -0.000324 -1.827345
S 3.140765 2.111990 -0.844011
S 4.185833 1.588190 0.788493
S 3.141871 -2.111659 -0.844003
S 4.186298 -1.587584 0.788781
S -1.841968 -1.734171 -0.001958
Mo -3.478342 0.000013 0.067902
S -4.595408 0.000169 1.852919
S -4.720509 0.000105 -1.631560
S -1.841702 1.733944 -0.002007

[Mo3S10]+ VIII
E= -4187.151323
S 4.349319 1.379621 1.324251
Mo 3.177702 0.236307 0.008024
S 2.103505 -1.336576 1.380383
S 0.973605 -2.326215 -0.046748
Mo 0.052780 -0.218344 -0.145769
Mo -2.665625 0.347731 -0.047812
S -3.013908 2.343064 -0.530756
S 4.366818 -0.659137 -1.477697
S 1.391980 1.477265 -0.881747
S -1.131946 0.270744 1.708824
S -1.414835 -0.599786 -1.793164
S -4.626600 -1.019824 -0.549255
S -4.480688 -0.489101 1.352998

E= -4187.124701
S -4.025134 -1.749692 1.292737
Mo -3.171413 -0.322645 0.004787
S -2.093342 1.245603 1.423203
S -1.232392 2.464997 -0.025595
Mo -0.190214 0.383210 -0.075811
Mo 2.733492 -0.342091 -0.114528
S 3.017543 -2.239004 -0.919948
S -4.617264 0.562404 -1.243555
S -1.353755 -1.207305 -1.186485
S 1.133080 -0.426970 1.598747
S 1.494954 0.970892 -1.559493
S 4.795422 0.937062 -0.352997
S 4.529745 0.181017 1.460460

[Mo3S10]+ IX
E= -4187.078314
S 0.762832 -0.141082 -1.659127
Mo -0.424774 0.703364 0.089864
S -2.286466 0.387669 -1.680677
Mo -3.381869 -0.320089 0.070021
S -1.829874 -0.443732 1.682311
Mo 2.313646 -0.737656 -0.008660
S 2.515201 -2.815337 -0.081723
S 4.539119 0.044719 0.557701
S 4.032718 0.507171 -1.299536
S 1.217553 -0.166208 1.829629
S 0.507127 2.690112 0.896954
S -1.022664 2.916983 -0.398985
S -4.516432 -2.050044 -0.243513

E= -4187.078719
S -0.768624 -0.144684 1.658533
Mo 0.419114 0.687867 -0.093414
S 2.301161 0.376161 1.680305
Mo 3.388688 -0.312788 -0.079047
S 1.789690 -0.534080 -1.641718
Mo -2.330915 -0.727388 0.012450
S -2.537523 -2.804877 0.076044
S -4.555888 0.064115 -0.546258
S -4.042981 0.515333 1.312046
S -1.248842 -0.145149 -1.831418
S -0.487448 2.692698 -0.900002
S 1.066538 2.888647 0.370118
S 4.607078 -1.983353 0.242379

[Mo3S10]+ X
E= -4187.104875
S 4.007286 -1.392776 1.609681
Mo 3.094604 -0.085858 0.238281
S 1.854060 -1.489772 -1.208482
S 0.905829 -0.035605 -2.361781
Mo 0.062355 0.136341 -0.219627
Mo -2.661512 -0.005704 0.311078
S -1.545581 1.890699 -0.682527
S -2.323467 2.053985 1.268483
S 4.520302 1.070619 -0.790182
S 1.424430 1.240316 1.224167
S -1.120288 -1.629128 0.683105
S -4.479021 -0.351033 -1.136121
S -4.544100 -1.474852 0.528107

E= -4187.053657
S -4.622182 0.761492 -1.052164
Mo -3.007201 0.250948 0.193526
S -2.284873 -1.849046 -0.595317
S -0.625510 -2.175788 0.633959
Mo -0.032949 -0.313762 -0.584673
Mo 2.370707 0.161115 -0.055822
S 2.695256 2.077690 1.360544
S 2.833317 2.388355 -0.612545
S -3.587819 0.189163 2.216830
S -1.139483 1.643125 -0.154839
S 1.513469 -0.345661 -2.233125
S 3.276728 -1.168986 1.734259
S 3.698384 -1.778385 -0.124308

[Mo3S10]+ XI
E= -4187.151441
Mo 0.085772 -0.034369 -0.000095
Mo -2.945883 0.271456 -0.041857
S -1.336459 0.044526 -1.764011
S -1.383120 -0.117242 1.710293
S -4.601798 -1.275944 0.854980
S -4.610428 -1.135268 -1.123924
S -3.624073 2.234531 0.044530
S 1.401741 -1.836263 -0.158826
S 1.417523 1.763449 0.015458
Mo 2.880328 -0.057293 0.241872
S 3.467466 -0.157458 2.239608
S 4.600711 -0.985393 -1.223748
S 4.615366 0.993104 -1.119151

E= -4187.151314
Mo 0.084103 -0.042923 0.005423
Mo -2.943009 0.268197 -0.059253
S -1.336626 -0.112474 -1.759374

S -1.386190 0.003390 1.717700
S -4.628707 -1.175048 0.942844
S -4.598221 -1.221779 -1.040594
S -3.598605 2.239071 -0.132784
S 1.406663 -1.846727 -0.011469
S 1.408705 1.755591 -0.123071
Mo 2.878904 -0.035990 0.245113
S 3.468652 0.026072 2.243616
S 4.604749 -1.072680 -1.138721
S 4.607087 0.907714 -1.200264

[Mo3S10]+ XII
E= -4187.112606
S -1.307881 -0.185032 -1.797434
Mo -2.730062 0.338622 -0.025945
S -4.710392 -0.807082 0.842635
S -4.636594 -0.717855 -1.135573
Mo 0.008536 -0.195388 0.057013
S 1.781269 -1.612345 1.273147
S 1.487631 -1.934862 -0.762423
Mo 2.972993 0.000441 -0.017838
S -1.442252 -0.366233 1.791429
S 1.220373 1.674592 0.087419
S -3.006328 2.402874 0.066134
S 4.779939 1.495576 0.209756
S 5.174132 -0.326781 -0.609818

E= -4187.112643
S -1.305025 -0.173001 -1.798504
Mo -2.730151 0.336617 -0.025796
S -4.704912 -0.826629 0.835345
S -4.643358 -0.700117 -1.141254
Mo 0.010134 -0.190607 0.057521
S 1.780325 -1.612480 1.271019
S 1.484075 -1.931660 -0.764320
Mo 2.971773 0.001950 -0.017124
S -1.442590 -0.376813 1.788736
S 1.223841 1.678777 0.097849
S -3.007622 2.399894 0.081359
S 4.785995 1.487257 0.210508
S 5.168412 -0.333624 -0.619067

[Mo3S10]+ XIII
E= -4187.065957
Mo -0.772046 0.691558 -0.065464
S -1.804107 -0.492961 1.727463
Mo -3.293091 -0.502658 0.077701
S -2.554054 0.936520 -1.512362
S -0.070602 2.906760 -0.590795
S -0.544413 2.662244 1.340672
S 0.459659 -0.724527 -1.306109
Mo 2.374491 -0.647182 0.144722
S 3.574824 0.440399 -1.757607
S 4.623840 0.203660 -0.099762
S 2.705895 -2.668465 0.593800
S 1.602073 0.379861 1.853163
S -3.555167 -2.440508 -0.660478

E= -4187.082153
Mo -0.216748 0.617701 0.127744
S -1.537540 -0.849049 1.452562
Mo -3.297307 -0.431137 0.089160
S -2.411484 0.507359 -1.633700
S -0.307745 2.878463 -0.784636
S -1.175407 2.825131 0.981463
S 0.738674 -0.439413 -1.649998
Mo 2.300957 -0.609267 0.052679
S 4.192337 -0.456033 -1.482474
S 4.541103 0.354884 0.291014
S 2.213556 -2.531019 0.853467
S 1.448562 0.891280 1.620535
S -4.517671 -2.072008 -0.355887

[Mo3S10]+ XIV
E= -4187.076467
S -3.068226 -1.719538 -1.104049
Mo -3.097962 -0.092767 0.230159
S -2.891115 2.307660 -0.502411
S -4.652412 1.452520 -0.758090
S -3.993732 -0.650396 2.049340
S -0.760477 0.341587 1.002786
S 0.182626 -1.442865 1.462449

Mo 1.195332 -0.456817 -0.407406
S 0.455799 -1.099550 -2.251241
S 2.053870 1.717544 -0.676863
Mo 3.835477 0.466490 -0.161808
S 4.423050 0.981813 1.772765
S 3.176894 -1.670652 -0.104664

E= -4187.067674
S 3.201049 -1.451992 1.400251
Mo 3.220016 -0.043862 -0.162632
S 2.838099 2.423442 0.172659
S 4.622888 1.730239 0.652197
S 4.247711 -0.810675 -1.828119
S 0.908348 0.114720 -1.115045
S 0.062871 -1.771414 -1.320697
Mo -1.059379 -0.526853 0.306281
S -0.460341 -0.919165 2.261018
S -2.076330 1.661610 0.054547
Mo -3.941273 0.442607 0.187297
S -5.489668 0.997491 -1.103729
S -3.180459 -1.637971 -0.041815

[Mo3S10]+ XV
E= -4187.081866
S 0.691885 -0.834028 -1.193314
Mo -0.809254 0.723714 -0.273215
S -2.471656 -0.308989 -1.797980
Mo -3.745468 -0.172962 -0.009089
S -2.374204 0.551791 1.588564
Mo 2.544786 -0.430768 0.250838
S 2.953537 -1.999326 1.558375
S 4.693061 0.251427 -0.663241
S 3.768086 -1.065984 -1.797737
S 0.799579 0.692370 1.688970
S 2.572962 1.668837 1.279093
S -0.562163 2.652467 -1.023300
S -4.795008 -1.923522 0.443167

E= -4187.080289
S 0.731844 -1.074700 -1.021551
Mo -0.774354 0.601894 -0.377481
S -2.457061 -0.740684 -1.654358
Mo -3.766259 -0.125206 0.002051
S -2.351511 0.740012 1.492092
Mo 2.573888 -0.369626 0.319793
S 3.038123 -1.684961 1.865243
S 4.696338 0.218978 -0.713386
S 3.814382 -1.301433 -1.601284
S 0.803102 0.929193 1.572722
S 2.547249 1.869628 0.992821
S -0.574959 2.353794 -1.488921
S -5.084853 -1.590864 0.702671

[Mo3S10]+ XVI
E= -4187.114229
S 1.279292 -0.093764 1.721678
Mo -0.212446 0.642896 0.000042
S 1.279080 -0.094811 -1.721322
Mo 2.765098 -0.011389 0.000085
S 4.203818 -1.728707 -0.990832
S 4.204256 -1.728285 0.990923
S 3.778569 1.812795 -0.000482
S -0.156947 2.719325 -0.000464
S -1.877355 0.016521 -1.731404
Mo -3.217642 -0.383679 0.000029
S -4.063807 -2.370792 0.000337
S -1.877496 0.017155 1.731449
S -5.023811 0.800017 -0.000291

E= -4187.113949
S -1.281495 -0.096732 -1.720636
Mo 0.212554 0.632562 -0.000092
S -1.281785 -0.095382 1.720899
Mo -2.768626 -0.008113 0.000024
S -4.214094 -1.719481 0.991245
S -4.213452 -1.720465 -0.990520
S -3.775358 1.819732 -0.000786
S 0.170711 2.709141 -0.000699
S 1.874515 -0.005361 1.733079
Mo 3.218572 -0.383438 0.000106
S 4.105332 -2.352373 0.000416
S 1.874650 -0.005872 -1.733054

S 5.001911 0.834139 -0.000045

[Mo3S10]+ XVII
E= -4187.101865
S -0.915846 0.133514 -1.559128
Mo 0.449042 -1.028804 -0.161402
S -0.120023 -3.027950 0.125274
Mo -2.717872 0.081516 0.018344
S -4.106542 1.837654 0.929638
S -3.001556 2.488440 -0.571790
S -1.769650 -0.722735 1.781005
S -4.123856 -1.270587 -0.739929
S 1.410931 0.152617 1.612468
Mo 3.111571 0.543831 0.060053
S 5.057750 0.136875 0.750146
S 2.367277 -1.158966 -1.378004
S 2.989320 2.490210 -0.731791

E= -4187.113949
S 1.281391 -0.096850 -1.720529
Mo -0.212546 0.632560 0.000106
S -0.170693 2.709139 -0.000566
Mo 2.768630 -0.008107 0.000026
S 4.214178 -1.719483 0.991087
S 4.213318 -1.720497 -0.990677
S 1.281886 -0.095258 1.721005
S 3.775384 1.819725 -0.000941
S -1.874618 -0.005287 1.733106
Mo -3.218574 -0.383435 0.000050
S -5.001912 0.834147 -0.000266
S -1.874555 -0.005940 -1.733026
S -4.105340 -2.352367 0.000332

[Mo3S10]+ XVIII
E= -4187.088947
S 0.005206 -0.024118 -1.066622
Mo -1.779018 -1.355654 -0.032413
S -1.402329 -3.246503 0.803759
Mo 2.244131 -0.482841 -0.022939
S 4.344738 0.684841 -0.150549
S 2.948660 1.631607 -1.173953
S 2.679687 -2.370342 -0.834117
S 1.884256 -0.635953 2.045256
S -3.315609 -1.476082 -1.452586
S -2.220918 0.186790 1.647251
Mo -1.254634 1.672646 0.144259
S -2.631572 2.486534 -1.210411
S -0.219626 3.198579 1.158591

E= -4187.036227
S 1.189190 1.049000 1.112956
Mo -1.096179 1.328144 0.296446
S -0.419710 2.709419 -1.183000
Mo 2.781773 -0.155181 -0.249154
S 3.988212 -2.206609 0.205420
S 2.667883 -1.849948 1.624033
S 4.304106 1.295785 -0.377260
S 1.919818 -0.469740 -2.142135
S -1.897829 2.403664 1.898612
S -3.195265 0.846806 -1.009481
Mo -2.837161 -1.257508 -0.480827
S -1.047621 -1.206044 0.802463
S -4.485921 -2.350405 0.206423

[Mo3S10]+ XIX
E= -4187.165199
S 0.000935 0.001718 1.720570
Mo -0.569993 1.462250 -0.046621
Mo 1.551814 -0.237922 -0.046550
Mo -0.980621 -1.224543 -0.044905
S -2.185225 -2.723078 1.395263
S -2.504372 -3.123017 -0.530850
S -1.458742 3.726717 -0.534431
S -1.262824 3.256328 1.392386
S 3.453294 -0.521247 1.393394
S 3.955893 -0.611260 -0.533151
S 1.320686 1.646896 -1.315756
S 0.766868 -1.970370 -1.312570
S -2.089664 0.317879 -1.312402

E= -4187.165344
S 0.000593 -0.000020 1.718843

Mo 1.506955 0.441239 -0.047179
Mo -0.371470 -1.525078 -0.047427
Mo -1.135458 1.084090 -0.047138
S -2.522588 2.410787 1.396757
S -2.895390 2.763151 -0.529509
S 3.840598 1.125160 -0.531686
S 3.350979 0.978339 1.395014
S -0.821908 -3.391137 1.395886
S -0.949453 -3.887771 -0.530324
S 1.527551 -1.458768 -1.315364
S -2.029760 -0.593854 -1.313334
S 0.499308 2.053454 -1.314204

[Mo3S9H3]+ I
E= -3790.644155
S -0.036147 3.559111 1.302377
Mo -0.041331 1.793591 -0.166398
S -1.861878 1.227843 -1.400034
Mo -1.433183 -0.579346 -0.076291
S -3.071719 -2.231717 -0.388895
S -3.193218 -1.082579 1.318358
S 1.920232 1.368527 -1.490760
Mo 1.438482 -0.509805 0.029472
S 3.665870 -1.436372 -0.046255
S 2.485117 -2.048051 1.464331
S -0.049361 0.300415 1.644208
S 0.145537 -1.670710 -1.620268
H 1.392163 1.090071 -2.704474
H 0.174261 -2.946988 -1.183228
H -0.123975 4.486968 0.313809

E= -3790.636355
S 0.015319 3.610550 1.088792
Mo -0.041416 1.730022 -0.245852
S -1.860949 1.179577 -1.490319
Mo -1.395987 -0.478554 0.017380
S -3.595001 -1.587781 -0.219937
S -2.852217 -1.503499 1.627993
S 1.713501 0.949323 -1.754948
Mo 1.389717 -0.645220 0.023513
S 3.186651 -2.175891 -0.118988
S 3.404990 -0.685811 1.260264
S 0.081497 0.378973 1.666950
S -0.119206 -2.041429 -1.283246
H 2.788025 1.647585 -1.317558
H -0.314011 -1.562911 -2.538961
H -0.064566 4.468708 0.039820

[Mo3S9H3]+ II
E= -3790.652809
S -2.166957 -3.165290 0.843313
Mo -0.851275 -1.756485 -0.023986
S 1.132573 -2.135814 -1.087504
Mo 1.575648 -0.047875 -0.106917
S 3.639859 0.941620 -0.435518
S 3.358249 0.024697 1.373051
S -2.110461 -0.421067 -1.579387
Mo -0.878020 0.942934 0.050380
S -2.205680 3.191720 -0.231568
S -1.516980 2.533879 1.616005
S 0.035349 -0.437464 1.701220
S 0.653460 1.534549 -1.738283
H -3.354241 -0.495422 -1.060756
H 0.191925 0.813817 -2.790599
H -3.495089 2.792218 -0.147954

E= -3790.645083
S -0.006142 3.760785 0.858783
Mo -0.088711 1.844522 -0.038313
S -1.941277 1.283014 -1.251384
Mo -1.392746 -0.578565 -0.046867
S -3.490924 -1.842164 -0.457290
S -2.979492 -1.566490 1.450535
S 1.812844 1.362965 -1.432955
Mo 1.372892 -0.541656 0.007312
S 3.616874 -1.824339 -0.374002
S 2.908246 -1.377140 1.532080
S -0.016475 0.281224 1.691948
S 0.031328 -1.915166 -1.445758
H 1.260736 1.165953 -2.652735
H -0.149017 -1.385498 -2.682156
H 4.488356 -0.804114 -0.545937

[Mo3S9H3]+ III
E= -3790.668539
S 1.331086 0.284076 -1.686601
Mo 2.943834 0.319520 -0.039827
S 3.794537 2.230019 0.262409
Mo -0.010729 -0.495741 0.069647
Mo -2.769260 0.312797 -0.021510
S -4.516226 -1.140764 0.255629
S 1.571393 -0.139041 1.743508
S -1.452314 0.435655 1.735829
S 0.112604 -2.783738 0.198404
S -1.668663 -0.494669 -1.721900
S 4.419230 -1.152092 -0.396185
S -3.405416 2.487315 -0.348516
H -4.123167 2.232488 -1.468246
H -5.073365 -0.455754 1.282630
H -0.664673 -3.141097 -0.844634

E= -3790.655891
S 1.891905 0.884511 1.600235
Mo 3.015250 -0.410506 -0.018147
S 3.576679 -2.315811 0.679074
Mo 0.175710 0.701077 0.163953
Mo -2.904465 -0.361607 -0.019665
S -4.766097 0.712374 0.731281
S 1.184904 -0.513426 -1.475060
S -1.947789 0.795625 -1.577934
S -0.187243 2.949675 -0.288321
S -1.253807 -0.529562 1.533871
S 4.659917 0.627801 -0.824739
S -3.373869 -2.484756 -0.711237
H -4.373364 -2.209087 -1.581219
H -5.230850 -0.270886 1.537114
H 1.017781 3.440636 0.071433

[Mo3S9H3]+ IV
E= -3790.677563
S 0.301210 3.750647 0.773146
Mo 0.156832 1.839533 -0.126095
S -1.684834 1.336877 -1.456945
Mo -1.482556 -0.477844 -0.150974
S -3.122935 -2.185138 -0.125268
S -3.588814 -0.739379 1.279925
S 1.991069 1.115929 -1.297893
Mo 1.317518 -0.617092 0.017095
S 3.546601 -1.982274 -0.179358
S 2.771075 -1.373288 1.650220
S -0.143506 0.274250 1.604464
S -0.052975 -2.004383 -1.412255
H 0.070979 -1.407027 -2.618607
H 4.441040 -0.991009 -0.398297
H -4.437524 0.033067 0.559244

E= -3790.665783
S 0.054968 3.368262 0.190090
Mo 0.206388 1.404469 -0.532054
S -1.575353 0.722806 -1.843308
Mo -1.830014 -0.656700 -0.063228
S -3.977127 -0.160382 0.764595
S -3.303905 0.884937 1.451837
S 2.260956 0.945753 -1.469509
Mo 2.256948 -0.486987 0.302616
S 2.870254 -2.593089 -0.360849
S 3.619912 0.167637 1.731216
S 0.104889 -0.167294 1.246551
S -1.538242 -2.785105 -0.900204
H -1.007940 -3.363208 0.201371
H 1.995580 -2.671440 -1.388510
H -3.848785 1.692707 0.512405

[Mo3S9H3]+ V
E= -3790.685931
S 0.081170 3.637255 1.019849
Mo 0.061113 1.759716 -0.315053
S -1.772848 1.133343 -1.534901
Mo -1.488697 -0.567762 -0.044994
S -3.200788 -2.146192 -0.180504
S -3.299845 -0.806497 1.376078
S 1.935076 1.096256 -1.453405
Mo 1.332903 -0.522450 0.026485
S 3.545494 -1.897428 -0.147962

S 2.772819 -1.266786 1.677786
S -0.129305 0.423581 1.610469
S 0.024831 -2.057194 -1.306505
H 0.200762 -1.525660 -2.537169
H 4.445423 -0.911280 -0.364695
H 0.024753 4.456407 -0.062996

E= -3790.641271
S 0.009776 3.648777 0.911349
Mo 0.058031 1.724140 -0.354217
S -1.709188 1.021820 -1.671417
Mo -1.407858 -0.529601 -0.067899
S -3.557513 -1.715700 -0.371891
S -3.221573 -0.920340 1.426584
S 2.018490 1.119087 -1.326135
Mo 1.438225 -0.591584 0.102226
S 3.392424 -1.922457 -0.648391
S 2.626767 -1.042427 1.926252
S -0.099081 0.480803 1.603761
S 0.021506 -2.331001 -0.824504
H 0.116171 -2.190319 -2.163769
H 4.341590 -0.971302 -0.608992
H 0.123765 4.420542 -0.201605

[Mo3S9H3]+ VI
E= -3790.659473
S -0.135147 3.714124 0.969129
Mo -0.049938 1.798044 -0.317973
S -1.849364 1.015382 -1.494215
Mo -1.448417 -0.643911 0.019403
S -3.167125 -2.228255 -0.409266
S -3.306435 -1.073015 1.299410
S 1.827395 1.180745 -1.476282
Mo 1.398697 -0.498631 0.023103
S 3.573553 -1.808763 -0.355863
S 2.992790 -1.260746 1.557356
S -0.061662 0.461240 1.571394
S 0.115084 -2.007457 -1.070690
H 4.435825 -0.803497 -0.635370
H -0.180445 4.534593 -0.110347
H 0.104829 0.845758 2.864336

E= -3790.648190
S -0.040603 3.671637 1.010193
Mo -0.034306 1.756034 -0.291038
S -1.892684 1.163219 -1.471333
Mo -1.448818 -0.599453 -0.079349
S -3.544684 -1.847566 -0.349413
S -3.029371 -1.369954 1.523157
S 1.804653 1.144257 -1.523363
Mo 1.361508 -0.527945 -0.019747
S 3.479126 -1.933605 -0.446582
S 3.010318 -1.269752 1.461007
S 0.187221 0.556022 1.771350
S 0.005247 -2.061860 -1.048642
H 4.357984 -0.974364 -0.818767
H -0.058291 4.474009 -0.083864
H 1.140654 1.259230 2.466283

[Mo3S9H3]+ VII
E= -3790.670064
S -1.708385 -0.849682 1.594906
Mo -3.067335 0.093164 -0.140687
S -4.336117 1.794372 0.736477
Mo -0.183982 0.023982 -0.051821
S 1.114581 1.593993 0.808984
Mo 2.628497 -0.129493 0.233228
S 3.162047 -1.140913 1.974426
S 1.141064 -1.479825 -1.004729
S -1.591259 0.916212 -1.635320
S 4.387210 -0.274657 -1.452484
S 4.358485 1.443994 -0.467709
S -4.171075 -1.815671 -0.732491
H -5.073566 1.047250 1.588876
H -4.839443 -1.352886 -1.815189
H -1.633359 -2.180954 1.363111

E= -3790.669039
S 1.694089 -1.019416 1.508948
Mo 3.051958 0.112529 -0.119096
S 4.021002 -1.793478 -0.895579
Mo 0.193063 0.045939 -0.037529

S -1.123199 -1.331449 -1.176248
Mo -2.621012 -0.152475 0.214647
S -3.155844 -1.377127 1.812594
S -1.117407 1.490041 1.010620
S 1.589619 1.138350 -1.503313
S -4.359905 1.486154 -0.286809
S -4.370793 -0.090641 -1.485982
S 4.568176 1.548425 0.849391
H 4.579890 -1.294292 -2.023828
H 3.694560 2.551321 1.090623
H 1.585397 -2.322469 1.158339

[Mo3S9H3]+ VIII
E= -3790.674889
S -1.589563 -0.279877 1.698198
Mo -3.043165 -0.027917 -0.027982
S -4.191047 1.938382 0.065228
Mo -0.244407 -0.006941 -0.104261
S 1.141769 1.916226 0.267361
Mo 2.615418 -0.036226 0.262085
S 3.074083 -0.280140 2.277728
S 1.167979 -1.729461 -0.424501
S -1.706160 0.251732 -1.830364
S 4.441369 -0.931276 -1.058129
S 4.309577 1.045739 -1.133221
S -4.450970 -1.832884 -0.216833
H -4.654777 1.787887 1.329227
H -3.530368 -2.818013 -0.137485
H 1.262980 2.440581 -0.972550

E= -3790.675051
S -1.558138 0.401804 1.633747
Mo -3.041106 -0.045594 -0.031789
S -4.184283 1.916059 -0.232340
Mo -0.242435 -0.037845 -0.146117
S 1.156825 1.882269 -0.486288
Mo 2.608309 0.062438 0.265763
S 3.022337 0.574472 2.240124
S 1.157067 -1.762277 0.209557
S -1.733363 -0.473578 -1.823967
S 4.453311 -1.258532 -0.585617
S 4.338987 0.548206 -1.395051
S -4.437087 -1.816438 0.401243
H -4.824742 1.615378 -1.387496
H -3.574060 -2.822889 0.144630
H 1.308040 1.897762 -1.829635

[Mo3S9H3]+ IX
E= -3790.684336
S -1.709009 -0.898454 1.548744
Mo -3.017103 0.034842 -0.033427
S -4.051603 1.947727 0.641091
Mo -0.199336 -0.067791 0.017044
S 1.074930 1.564723 0.818702
Mo 2.614472 -0.080249 0.143349
S 3.413281 -0.824659 2.146785
S 1.139816 -1.690905 -0.718954
S -1.621082 0.764492 -1.621842
S 4.071185 -0.324755 -1.644555
S 3.990028 1.533222 -0.802747
S -4.437155 -1.564725 -0.840016
H -4.798241 1.294600 1.567455
H -3.573299 -2.584062 -1.037718
H 3.727892 -2.062844 1.702398

E= -3790.676730
S 1.733084 1.064467 -1.432579
Mo 3.057975 -0.042159 0.015548
S 4.131092 1.315759 1.496963
Mo 0.247346 -0.010591 -0.048592
S -1.036542 1.386833 1.132567
Mo -2.583094 0.139210 -0.067225
S -3.422640 1.844032 -1.354262
S -1.212056 -1.302509 -1.199837
S 1.659401 -1.211749 1.323536
S -4.625085 -1.242259 -0.049496
S -3.850307 -0.754573 1.729063
S 4.475637 -1.405277 -1.160206
H 4.805687 1.989725 0.532156
H 3.610875 -1.941952 -2.047724
H -4.391431 1.205317 -2.045123

[Mo3S9H3]+ X
E= -3790.703243
S -1.659421 -0.736025 1.589876
Mo -3.041558 0.049370 -0.015451
S -4.072782 2.004008 0.531731
Mo -0.229232 -0.033624 -0.072991
S 1.082634 1.669882 0.498015
Mo 2.580623 -0.130995 0.222237
S 3.131482 -0.913952 2.078154
S 1.088919 -1.699188 -0.719457
S -1.726769 0.650768 -1.721731
S 4.166056 -0.427741 -1.495255
S 4.543632 1.322532 -0.456312
S -4.464474 -1.630705 -0.624317
H -4.795060 1.417399 1.520107
H -3.591874 -2.650394 -0.777798
H 3.945511 2.240245 -1.253008

E= -3790.688173
S -1.672497 -0.282178 1.651787
Mo -3.192493 0.030396 -0.051394
S -4.411038 1.919860 0.291829
Mo -0.142181 -0.018255 -0.022655
S 1.203796 1.759755 0.153568
Mo 2.657234 -0.081772 0.234543
S 3.234536 -0.452258 2.207900
S 1.155531 -1.802641 -0.331180
S -1.655536 0.282064 -1.730477
S 4.222161 -0.756212 -1.394541
S 4.640712 1.163689 -0.741132
S -4.616883 -1.748215 -0.281553
H -5.154791 1.928132 -0.839061
H -4.052444 -2.248000 -1.403609
H 4.047222 1.907002 -1.705273

[Mo3S9H3]+ XI
E= -3790.663835
S 1.303121 -0.329288 1.688290
Mo 2.938254 -0.340549 0.041305
S 3.806981 -2.231475 -0.330514
Mo 0.036582 0.465798 -0.073107
Mo -2.843124 -0.275742 -0.010691
S -4.231743 1.106576 -0.705106
S 1.590818 0.144979 -1.759536
S -1.342765 -0.699162 -1.611692
S 0.046993 2.759628 -0.270946
S -1.703292 0.742921 1.802583
S 4.393701 1.131492 0.466016
S -3.763652 -2.289182 0.573228
H -5.046711 -1.879111 0.668707
H -0.575456 3.135943 0.866033
H -1.512371 -0.319964 2.612773

E= -3790.648731
S 1.874587 0.863776 1.565680
Mo 2.925194 -0.430492 -0.016935
S 3.394943 -2.373646 0.664982
Mo 0.058465 0.709351 0.044194
Mo -2.853633 -0.347431 0.001849
S -4.506052 0.682413 0.744148
S 1.135980 -0.507782 -1.538803
S -1.894289 0.848685 -1.551233
S 0.007467 2.994036 -0.229775
S -1.286610 -0.449522 1.827008
S 4.632330 0.543171 -0.782661
S -3.436632 -2.367656 -0.896619
H -4.542665 -2.589988 -0.154004
H 1.070577 3.397270 0.496718
H -0.736576 -1.662832 1.590812

[Mo3S9H3]+ XII
E= -3790.662327
S -1.531837 -0.066484 -1.840208
Mo -3.080629 0.070246 0.025930
S -4.620217 -1.638949 -0.015909
Mo -0.243153 -0.013348 0.208026
S 1.110873 -1.904621 -0.399046
Mo 2.590667 0.043715 -0.257991
S 3.008419 0.458540 -2.255638
S 1.169117 1.688946 0.592346
S -1.776632 -0.311890 1.864755
S 4.443398 0.802269 1.109429

S 4.312462 -1.172038 0.983705
S -3.822823 2.015098 0.137922
H -5.666670 -0.864612 -0.376965
H -1.512305 1.220836 -2.245815
H 1.285670 -2.515911 0.794520

E= -3790.661253
S -1.526959 -0.209375 1.827319
Mo -3.081225 -0.069177 -0.035645
S -4.638864 1.595816 0.271741
Mo -0.246145 0.059589 -0.206117
S 1.130900 1.858462 0.575196
Mo 2.597720 -0.092876 0.240273
S 2.993082 -0.869272 2.134208
S 1.157440 -1.560573 -0.863541
S -1.781668 0.616800 -1.787476
S 4.488586 -0.593440 -1.177935
S 4.275639 1.343524 -0.800706
S -3.798739 -1.981218 -0.453570
H -5.677074 0.762598 0.501626
H -1.495516 -1.542642 2.035301
H 1.027225 1.871995 1.921827

[Mo3S9H3]+ XIII
E= -3790.693769
S 1.728693 -1.140931 -1.528242
Mo 3.117282 0.006187 0.087973
S 4.694499 1.336263 -0.919726
Mo 0.223200 0.068532 -0.081913
S -1.187017 1.346249 -1.230278
Mo -2.599089 -0.197669 -0.141930
S -3.207564 -1.701787 -1.457264
S -0.984470 -1.176286 1.286770
S 1.635416 1.388016 1.137297
S -4.059035 0.229902 1.655066
S -4.594111 1.356758 0.002121
S 3.813532 -1.360068 1.496741
H 5.761413 0.585900 -0.567693
H 1.663066 -2.413968 -1.089354
H -4.002090 2.542111 0.283823

E= -3790.669483
S -1.664065 1.172128 -1.451950
Mo -3.167676 -0.005536 0.035562
S -4.630840 -1.353248 -1.114461
Mo -0.343811 -0.102597 0.094048
S 1.180762 -1.215802 -1.184359
Mo 2.685753 0.242420 -0.116132
S 3.411135 1.712605 -1.414380
S 1.074510 1.229136 1.274011
S -1.808581 -1.399409 1.244318
S 4.246773 -0.355350 1.538117
S 4.581524 -1.469177 -0.177985
S -4.002421 1.375616 1.356771
H -5.728978 -0.606948 -0.865207
H -1.711662 2.423507 -0.944559
H 3.900688 -2.600617 0.122355

[Mo3S9H3]+ XIV
E= -3790.674225
S -1.778479 1.815885 -0.699923
Mo -3.081474 -0.057607 0.094688
S -4.660164 -0.723261 -1.433898
Mo -0.190579 0.080250 -0.140470
S 1.182322 -0.320657 -1.843287
Mo 2.627240 0.137410 -0.045308
S 3.501345 2.230984 -0.290189
S 1.030623 0.491349 1.659532
S -1.532477 -1.727805 0.232862
S 3.898818 -1.204036 1.354778
S 4.043022 -1.596766 -0.639296
S -3.766636 0.337309 2.021376
H -5.730898 -0.308617 -0.722137
H -1.734054 2.669119 0.342967
H 3.853123 2.069224 -1.586302

E= -3790.666225
S -1.800700 1.672381 -1.000020
Mo -3.116557 -0.044374 0.079443
S -4.695653 -0.931230 -1.333042
Mo -0.239284 0.035457 -0.155524
S 1.256800 -0.602631 -1.720000

S114

Mo 2.592750 0.136139 -0.006989
S 3.494626 2.220111 -0.332121
S 0.963212 0.754358 1.561896
S -1.579825 -1.694261 0.466697
S 3.743860 -1.487840 1.278601
S 4.610424 -1.173867 -0.499371
S -3.797092 0.644752 1.923388
H -5.765104 -0.414928 -0.689248
H -1.768584 2.685350 -0.110926
H 4.453036 1.957856 -1.247371

[Mo3S9H3]+ XV
E= -3790.658641
S 1.935557 -0.434167 1.798123
Mo 3.084453 0.103008 -0.136318
S 4.597286 -1.539827 -0.675208
Mo 0.284793 -0.167553 0.309576
S -1.251335 -1.991297 0.060045
Mo -2.666646 -0.025811 0.144624
S -3.576877 -0.314502 2.008274
S -1.099845 1.734436 0.731858
S 1.284101 0.132830 -1.638315
S -3.852219 1.343325 -1.321656
S -3.953768 -0.692708 -1.682088
S 3.837792 2.036996 0.033883
H 5.657917 -0.718724 -0.831348
H -1.045316 -2.396296 -1.211553
H -0.852868 2.508602 -0.346762

E= -3790.652536
S 2.225078 -1.911623 0.298202
Mo 2.904941 0.257513 0.042618
S 4.433795 0.380076 -1.686195
Mo 0.270314 -0.772298 -0.006323
S -1.235858 -0.917456 -1.861264
Mo -2.545178 -0.127670 0.036441
S -3.741742 -1.777882 0.425013
S -1.002157 -0.210590 1.927202
S 0.979838 1.359580 -0.540259
S -3.514249 2.000517 0.710831
S -3.673233 1.616586 -1.225865
S 3.642877 1.010069 1.849354
H 5.430070 0.935865 -0.968059
H -1.026203 0.178542 -2.623778
H -0.696661 1.080310 2.184571

[Mo3S9H3]+ XVI
E= -3790.691224
S 1.525255 -0.150236 1.675148
Mo 3.115121 0.087052 -0.013676
S 4.692378 -1.586413 0.088467
Mo 0.301061 -0.167801 -0.188986
S -1.287497 -1.984140 -0.276810
Mo -2.560686 0.043703 0.246742
S -2.886921 0.221191 2.295125
S -0.969713 1.679530 -0.266201
S 1.778165 -0.134445 -1.887073
S -4.167205 1.126323 -1.069050
S -4.788977 -0.811247 -0.669983
S 3.845140 2.039269 0.037332
H 5.761059 -0.772262 0.218095
H -1.143053 -2.623749 0.900429
H -4.398807 -1.445368 -1.801187

E= -3790.676908
S -1.745753 -0.063401 1.695685
Mo -3.220586 -0.045966 -0.069445
S -4.617231 1.791219 -0.002234
Mo -0.193806 -0.069210 0.003633
S 1.150096 1.906760 -0.058017
Mo 2.639327 -0.011987 0.229194
S 3.145952 0.018517 2.249920
S 1.197986 -1.824809 -0.089977
S -1.697444 0.127917 -1.757183
S 4.248888 -1.058915 -1.126490
S 4.683331 0.958997 -0.946140
S -4.306511 -1.821988 -0.180948
H -5.796096 1.141293 0.054808
H 1.243170 2.210187 -1.373506
H 4.156639 1.440613 -2.097194

[Mo3S9H3]+ XVII

E= -3790.701183
S -1.646722 1.521717 -0.875204
Mo -3.116645 -0.030084 0.034487
S -4.575574 -0.813242 -1.568125
Mo -0.289486 -0.043162 -0.024287
S 1.252101 -0.775220 -1.566192
Mo 2.531585 0.239246 0.012230
S 3.344095 2.198409 -0.866983
S 1.011897 0.759244 1.660468
S -1.643390 -1.694912 0.681498
S 3.749251 -1.143612 1.370020
S 4.618678 -1.247956 -0.518326
S -3.984501 0.794373 1.743709
H -5.702466 -0.467278 -0.910909
H 4.024427 -2.370804 -0.985427
H 4.395614 2.285278 -0.019554

E= -3790.690394
S -1.772747 1.081132 -1.333715
Mo -3.239140 -0.033889 0.036438
S -4.577630 -1.495293 -1.132359
Mo -0.205273 0.042988 -0.004200
S 1.214941 -1.296060 -1.146851
Mo 2.575116 0.170986 -0.032459
S 3.664781 1.696315 -1.375266
S 1.098030 1.468671 1.149979
S -1.680362 -1.125953 1.321256
S 3.877729 -0.743219 1.641547
S 4.737709 -1.302831 -0.166992
S -4.362115 1.294855 1.183427
H -5.776933 -1.042550 -0.715342
H 4.208719 -2.540377 -0.305248
H 2.873317 2.777478 -1.225825

[Mo3S9H3]+ XVIII
E= -3790.668565
S -1.668217 1.724685 -0.557100
Mo -3.198165 -0.024760 0.052838
S -4.603085 -0.206343 -1.503129
Mo -0.196752 -0.145844 -0.175063
S 1.269704 -0.383392 -1.814366
Mo 2.604527 0.270118 0.019146
S 3.102791 2.291394 -0.113762
S 0.927988 0.103945 1.693157
S -1.799599 -1.971483 0.004778
S 4.101490 -1.053297 1.267894
S 4.695217 -0.940638 -0.710394
S -4.019922 0.298370 1.965010
H 4.191494 -2.095019 -1.210546
H -1.466025 2.475275 0.545183
H -1.630937 -2.371711 1.281244

E= -3790.643371
S -1.819794 1.785482 -0.657509
Mo -3.243837 -0.066387 -0.013111
S -4.318562 -0.794059 -1.674119
Mo -0.339057 -0.004263 0.029541
S 1.159514 -0.613102 -1.553985
Mo 2.713375 0.271936 -0.007006
S 3.452142 2.130117 -0.602441
S 1.092630 0.597690 1.672621
S -1.760324 -1.853331 0.678400
S 4.255184 -0.947034 1.285235
S 4.597046 -1.289845 -0.730918
S -4.399605 0.612641 1.613412
H 3.908185 -2.442247 -0.909258
H -1.762494 1.626367 -1.997709
H -1.758067 -1.695045 2.020040

[Mo3S9H3]+ XIX
E= -3790.649311
S -1.760965 1.843075 -0.302834
Mo -3.179071 -0.062329 0.049480
S -4.538880 -0.151685 -1.553868
Mo -0.171108 0.023750 -0.138497
S 1.211727 0.025646 -1.859009
Mo 2.652067 0.169109 0.002306
S 3.445027 2.298465 0.165696
S 1.015663 0.119996 1.712312
S -1.651562 -1.898828 -0.188323
S 3.984023 -1.347551 1.134792
S 4.139704 -1.357839 -0.897494

S -4.053160 -0.027347 1.965882
H -1.625568 2.435191 0.901620
H -1.474999 -2.400388 1.051366
H 3.756030 2.420053 -1.145601

E= -3790.640306
S -1.770513 1.723200 -0.710355
Mo -3.211557 -0.039215 0.054886
S -4.619927 -0.408989 -1.464742
Mo -0.217244 -0.055330 -0.206481
S 1.324055 -0.364113 -1.804184
Mo 2.616843 0.158457 0.028553
S 3.387452 2.313457 0.065989
S 0.900300 0.407995 1.628215
S -1.721388 -1.920788 0.130409
S 3.859953 -1.561741 1.079069
S 4.721252 -0.910048 -0.608187
S -4.029080 0.390084 1.948344
H -1.605001 2.570513 0.325658
H -1.531799 -2.225244 1.430297
H 4.405337 2.265538 -0.821141

[Mo3S9H3]+ XX
E= -3790.681920
S 1.317955 -0.387824 1.611467
Mo 2.974267 -0.366829 -0.030374
S 3.410201 -2.342771 -0.591771
Mo -0.204322 0.634577 0.186951
Mo -2.832617 -0.355983 -0.047812
S -4.298911 1.038899 -0.545427
S 1.910152 0.726466 -1.812077
S -1.176339 -0.278662 -1.644128
S -0.210936 2.929007 -0.044996
S -1.729590 0.268186 1.848493
S 4.691176 0.604604 0.691008
S -3.603136 -2.506856 0.224502
H -4.897898 -2.246510 -0.053762
H 0.235467 3.159889 1.210922
H 2.325508 1.975724 -1.518431

E= -3790.664451
S -1.886301 1.008460 -1.447750
Mo -3.008294 -0.380249 -0.027160
S -3.386500 -2.259865 -0.893465
Mo 0.005021 0.691437 -0.033482
Mo 2.895117 -0.355304 -0.022588
S 4.558686 0.770083 -0.584639
S -1.318403 -0.696216 1.658480
S 1.843275 0.568783 1.679152
S 0.308011 2.952146 0.183564
S 1.283969 -0.281983 -1.666490
S -4.777425 0.491648 0.703917
S 3.505727 -2.515225 0.473911
H 4.721038 -2.519016 -0.109541
H -0.671622 3.446194 -0.603465
H -1.603469 0.320444 2.501745

[Mo3S9H3]+ XXI
E= -3790.645360
S 1.171342 0.078675 1.430508
Mo 3.120554 0.032662 0.086333
S 4.238427 -1.698531 0.563318
Mo 0.321983 -0.035671 -0.602119
S -1.128783 -1.919840 -0.482157
Mo -2.471250 -0.024248 0.281772
S -2.406713 -0.047429 2.358251
S -1.183190 1.803974 -0.686688
S 2.083434 -0.088220 -1.999775
S -4.721290 1.027822 -0.347450
S -4.359080 -0.976771 -0.717745
S 4.195823 1.829731 0.384844
H -0.793481 -2.618367 0.623488
H -0.892583 2.673517 0.304938
H -5.347487 0.939062 0.850471

E= -3790.638191
S -2.048844 -1.410724 -1.174215
Mo -3.252133 0.157598 0.106693
S -4.424478 -0.734535 1.613982
Mo -0.247439 -0.371208 -0.303176
S 1.141716 -1.466895 1.298552
Mo 2.659632 -0.160016 -0.100023

S 3.583987 -1.654343 -1.205895
S 1.170689 0.972860 -1.669650
S -1.313597 1.190774 0.970383
S 4.231837 1.823399 0.165334
S 3.801259 0.618706 1.792547
S -4.404477 1.470967 -1.072231
H 1.016050 -0.757808 2.442575
H 1.077971 2.242042 -1.211680
H 5.374023 1.244720 -0.278578

[Mo3S9H3]+ XXII
E= -3790.651350
S 1.714099 1.099079 -1.323824
Mo 3.318553 -0.069281 0.034269
S 4.580293 1.240128 1.095554
Mo 0.281990 0.037597 -0.013406
S -1.071785 1.467759 1.088595
Mo -2.582535 0.138413 -0.058132
S -3.366388 1.711579 -1.509978
S -1.176892 -1.408684 -1.289784
S 1.597272 -1.011722 1.424955
S -4.745109 -1.339294 0.093876
S -3.904978 -0.389634 1.747426
S 4.397875 -1.525270 -1.041502
H -1.156168 -2.550309 -0.568171
H -5.721409 -0.448677 -0.195871
H -4.269010 1.013316 -2.235743

E= -3790.651521
S -1.705597 -1.089385 -1.335023
Mo -3.311509 0.066055 0.032633
S -4.561637 -1.250864 1.096569
Mo -0.283003 -0.027586 -0.014032
S 1.061300 -1.463253 1.092484
Mo 2.576366 -0.142841 -0.057140
S 3.354283 -1.710916 -1.517824
S 1.181943 1.419601 -1.283394
S -1.598459 1.014744 1.430055
S 4.742194 1.332619 0.094426
S 3.903609 0.378756 1.747372
S -4.401763 1.518326 -1.035871
H 1.177320 2.559617 -0.558699
H 5.715775 0.440361 -0.199737
H 4.255118 -1.010439 -2.243621

[Mo3S9H3]+ XXIII
E= -3790.662031
S -1.644211 1.449060 0.865248
Mo -3.275659 -0.079427 0.084551
S -4.728971 0.931828 -1.049491
Mo -0.211351 0.103888 -0.213737
S 1.223201 1.293922 -1.463696
Mo 2.557395 0.170185 0.035156
S 3.338891 2.012266 1.162417
S 1.054982 -1.114093 1.200625
S -1.776858 -1.391249 -1.351168
S 4.588609 -1.403646 0.539277
S 3.996171 -0.935900 -1.399657
S -4.121625 -1.252727 1.611585
H 5.603315 -0.517827 0.670360
H 4.152121 1.429839 2.069534
H -1.594590 -2.518502 -0.632854

E= -3790.664282
S 1.672340 1.394106 -0.958525
Mo 3.306680 -0.042319 -0.045775
S 4.464840 0.922737 1.417613
Mo 0.200525 0.016061 0.052551
S -1.119324 1.049960 1.552226
Mo -2.572863 0.181793 0.008800
S -3.352701 2.172458 -0.837915
S -1.206558 -0.991466 -1.403077
S 1.769493 -1.603282 1.049580
S -4.701243 -1.249425 -0.570766
S -3.960384 -1.077322 1.366271
S 4.495667 -0.953889 -1.522296
H -5.682902 -0.320943 -0.502208
H -4.250953 1.728765 -1.742723
H 1.697406 -2.562295 0.100930

[Mo3S9H3]+ XXIV
E= -3790.699540

S 1.674329 1.422653 -1.042398
Mo 3.121431 -0.117063 -0.069457
S 4.676493 0.946171 1.255328
Mo 0.301647 0.059184 0.077287
S -1.121692 1.286922 1.427433
Mo -2.513191 0.225294 0.008622
S -3.399980 2.042064 -1.103882
S -1.153741 -1.070546 -1.281457
S 1.627465 -1.344388 1.215895
S -4.571609 -1.388340 -0.365966
S -3.717119 -1.054717 1.499943
S 3.867667 -1.364248 -1.566004
H -5.615932 -0.533686 -0.268897
H -4.469465 1.452583 -1.675160
H 5.761103 0.440555 0.630792

E= -3790.689122
S 1.767781 1.286430 -1.220698
Mo 3.179059 -0.117203 -0.046024
S 4.694508 1.097762 1.192521
Mo 0.374546 0.045769 0.044365
S -0.996807 1.319094 1.275832
Mo -2.646452 0.182370 -0.012913
S -3.472487 2.001382 -1.128842
S -1.124445 -1.151233 -1.179032
S 1.701528 -1.238982 1.334615
S -4.681003 -1.422663 -0.309605
S -4.026416 -0.786959 1.563522
S 4.022888 -1.484492 -1.378022
H -5.691687 -0.543732 -0.505263
H -4.376845 1.429168 -1.953141
H 5.799351 0.529925 0.665811

[Mo3S9H3]+ XXV
E= -3790.698122
S -1.916172 0.927002 -1.626103
Mo -2.795187 -0.447414 0.001376
S -3.020010 -2.366061 -0.784586
Mo -0.236860 0.665716 -0.141518
Mo 2.876102 -0.289812 0.002531
S 4.464660 0.777918 -0.837839
S -1.157347 -0.483415 1.599648
S 1.938172 0.781737 1.621727
S 0.145525 2.919658 0.230231
S 1.165748 -0.552828 -1.523442
S -4.721161 0.469631 0.865178
S 3.627441 -2.316069 0.788329
H 4.727607 -2.427178 0.016899
H -1.059515 3.444517 -0.075145
H -5.548093 -0.535097 0.507626

E= -3790.692794
S 1.879618 0.735719 1.618196
Mo 2.889735 -0.425353 0.028356
S 3.465625 -2.322899 0.679172
Mo 0.010356 0.641961 0.011455
Mo -2.919431 -0.306847 0.012170
S -4.580507 0.783277 0.647607
S 1.260046 -0.586375 -1.547276
S -1.858530 0.726379 -1.626032
S -0.061494 2.939213 -0.127694
S -1.323455 -0.385120 1.635174
S 4.721289 0.727245 -0.754896
S -3.562211 -2.417499 -0.644159
H -4.810364 -2.421886 -0.136473
H 0.967298 3.298129 0.668444
H 5.609260 -0.285228 -0.796628

[Mo3S9H3]+ XXVI
E= -3790.706003
S -1.524754 0.134870 1.738830
Mo -2.913184 0.357000 -0.001945
S -3.847645 2.225770 0.009131
Mo 0.046106 -0.530887 0.004938
Mo 2.895300 0.243513 -0.019465
S 4.242711 -1.314135 -0.321124
S -1.562997 0.167150 -1.746782
S 1.456401 0.366893 -1.709589
S 0.107778 -2.601723 -0.139795
S 1.629350 -0.300750 1.925975
S -4.499477 -1.319633 -0.014480
S 3.868759 2.316669 0.118237

H 5.115212 1.892810 0.418646
H -5.606720 -0.566674 0.126683
H 1.384176 0.947780 2.380011

E= -3790.657547
S -1.734314 0.410862 -1.797116
Mo -2.930430 -0.221307 0.034797
S -3.705515 -2.135148 -0.296442
Mo -0.157894 0.261089 -0.093996
Mo 2.892206 -0.248005 -0.073956
S 4.293064 0.753048 -1.260163
S -1.380378 -0.306218 1.733442
S 1.803078 1.298907 1.285730
S 0.702868 2.377217 -0.133458
S 1.141162 -1.512852 -1.170819
S -4.563262 1.331451 0.529284
S 3.926987 -1.499691 1.531958
H 4.921238 -2.059006 0.806026
H -5.608836 0.480737 0.501961
H 1.185523 -1.157638 -2.474166

[Mo3S9H3]+ XXVII
E= -3790.650675
S -1.689854 1.196284 -1.591465
Mo -2.719967 -0.307114 -0.040909
S -2.881573 -2.171625 -0.934653
Mo -0.044488 0.585277 0.088751
Mo 2.669473 -0.413042 -0.036520
S 4.191005 0.277407 -1.322262
S -1.293462 -0.432662 1.901629
S 1.930110 1.339828 1.413718
S 1.086443 2.580508 -0.049214
S 0.755172 -1.021462 -1.258457
S -4.649946 0.710194 0.656847
S 3.288848 -2.024125 1.179967
H -5.482822 -0.297104 0.313198
H -0.822584 -1.696826 1.936082
H -1.493253 0.389340 -2.662558

E= -3790.635228
S -1.729830 0.963161 -1.793752
Mo -2.859896 -0.272740 -0.073610
S -3.461245 -2.186563 -0.675344
Mo -0.059284 0.423971 -0.059365
Mo 2.844027 -0.365959 -0.012979
S 4.291823 0.438794 -1.308351
S -1.412705 -0.295204 1.855127
S 1.891669 1.283264 1.402700
S 1.006720 2.451006 -0.079325
S 0.971250 -1.236427 -1.162059
S -4.546796 0.951502 0.901234
S 3.681254 -1.778174 1.302198
H -5.377724 1.103265 -0.154137
H -1.016190 -1.583028 1.959335
H -1.523897 0.036553 -2.754011

[Mo3S9H3]+ XXVIII
E= -3790.662852
S -1.759035 1.101497 -1.638969
Mo -2.835040 -0.281091 -0.002478
S -3.558924 -2.016122 -0.943451
Mo 0.008260 0.506341 -0.004835
Mo 2.667715 -0.360564 -0.063813
S 4.118300 0.660373 -1.153050
S -1.146647 -0.948265 1.586376
S 1.801701 1.214891 1.522152
S 0.881879 2.608125 0.243292
S 0.936181 -0.853417 -1.521352
S -4.309399 0.859229 0.981026
S 3.377811 -2.274305 0.975834
H -1.331057 -0.130965 2.644065
H -2.154644 2.316358 -1.207232
H 4.696595 -2.134328 0.720731

E= -3790.640210
S -1.776755 0.931899 -1.729160
Mo -2.958349 -0.240848 0.002292
S -3.677781 -2.090846 -0.692700
Mo -0.090009 0.400896 -0.025658
Mo 2.810425 -0.298253 -0.138226
S 4.302094 0.658815 -1.258014
S -1.403705 -0.526998 1.826238

S 1.888031 1.129608 1.466895
S 0.853152 2.467047 0.222415
S 0.991947 -1.120626 -1.329417
S -4.458105 1.046927 0.715100
S 3.773255 -1.870568 1.235840
H -1.026917 -1.819502 1.727206
H -1.581447 -0.006907 -2.678918
H 4.727453 -2.373107 0.423440

[Mo3S9H3]+ XXIX
E= -3790.657807
S -1.691773 0.660223 -1.771905
Mo -2.846356 -0.171628 -0.061954
S -3.847752 -2.133869 -0.690427
Mo -0.071810 0.319765 -0.133637
Mo 2.878652 -0.334714 0.034423
S 4.325453 0.379085 -1.317396
S -1.330723 -0.545550 1.751075
S 1.810525 1.414639 1.237513
S 0.927539 2.376301 -0.388056
S 1.067295 -1.363271 -1.078543
S -4.192659 1.326049 1.012467
S 3.716531 -1.613442 1.479626
H -1.437719 0.533897 2.561546
H -4.980580 1.709934 -0.018878
H -4.473122 -2.410232 0.476695

E= -3790.653448
S 1.733523 -0.992073 -1.645156
Mo 2.868474 0.135742 -0.075655
S 3.598250 2.221192 -0.648064
Mo 0.093079 -0.330935 -0.142345
Mo -2.902426 0.311633 -0.012180
S -4.378096 -0.697890 -1.122908
S 1.328301 0.810243 1.627210
S -1.737544 -1.122593 1.481870
S -0.891876 -2.409016 0.085980
S -1.137726 1.092749 -1.365375
S 4.401117 -1.264322 0.906129
S -3.721794 1.829429 1.193853
H 1.044501 2.107049 1.356197
H 4.939550 -0.363600 1.759287
H 4.426140 1.882585 -1.664518

[Mo3S9H3]+ XXX
E= -3790.697403
S 0.079562 3.531228 1.359085
Mo 0.011134 1.803424 -0.170167
S -0.004507 0.270468 1.585790
Mo 1.353233 -0.587359 -0.134710
S -0.158965 -1.800521 -1.412117
Mo -1.429657 -0.474290 -0.107776
S -2.664413 -2.137805 1.448366
S -3.694936 -1.158870 -0.060966
S -1.834571 1.368548 -1.429789
S 1.814986 1.150783 -1.477332
S 3.092130 -2.194146 -0.374056
S 3.421077 -1.044079 1.316761
H 4.246758 -0.085752 0.827428
H -2.378424 -3.310655 0.832206
H 0.068037 4.472178 0.379935

E= -3790.675500
S 0.180758 3.328824 1.685804
Mo 0.098546 1.787651 -0.037751
S 0.004681 0.058898 1.578599
Mo 1.458291 -0.545569 -0.206687
S -0.016929 -1.654902 -1.451709
Mo -1.556713 -0.410905 -0.135517
S -2.887674 -2.368716 0.939996
S -3.846173 -0.880615 -0.153008
S -1.764493 1.624048 -1.290332
S 1.938624 1.417163 -1.320213
S 3.685878 -1.268028 -0.302815
S 2.678853 -2.395827 1.119508
H 3.026000 -1.734762 2.248468
H -2.785916 -3.326658 -0.009843
H 0.178352 4.378475 0.826174

[Mo3S9H3]+ XXXI
E= -3790.732561
S -0.005656 3.629534 1.114108

Mo -0.006138 1.776922 -0.265497
S 0.000457 0.417141 1.634549
Mo 1.363168 -0.526353 -0.040000
S 0.008851 -2.020510 -1.131322
Mo -1.357165 -0.538254 -0.036647
S -2.905432 -1.291079 1.529651
S -3.521135 -1.918092 -0.354627
S -1.850674 1.162996 -1.486303
S 1.838322 1.181240 -1.489239
S 3.583602 -1.805304 -0.375224
S 2.930679 -1.252993 1.519663
H -0.002017 4.466648 0.043941
H -4.411855 -0.942280 -0.645690
H 3.155325 -3.088510 -0.408288

E= -3790.690358
S -1.225646 4.044339 0.364756
Mo -0.494094 1.862430 0.103062
S -0.024425 0.266752 1.730513
Mo 1.472846 -0.267616 -0.065250
S 0.479989 -1.829663 -1.405424
Mo -1.111005 -0.899374 -0.058297
S -2.307737 -2.266634 1.392879
S -2.886288 -2.724648 -0.550811
S -2.175287 0.827541 -1.099543
S 1.529128 1.798748 -1.038287
S 3.900991 -1.011194 -0.567943
S 3.170276 -0.936423 1.376766
H -1.527979 4.397237 -0.903823
H -4.014914 -1.982785 -0.640227
H 3.721538 -2.324036 -0.842069

[Mo3S9H3]+ XXXII
E= -3790.633409
Mo 0.386944 1.400467 -0.215229
Mo -1.406856 -0.365392 -0.215436
Mo 1.019220 -1.035614 -0.215624
S -0.591308 -2.117917 -1.455884
S 2.129665 0.546829 -1.455498
S -1.538387 1.570141 -1.456031
S -2.570747 -0.698572 1.758135
S -4.000409 -0.958086 0.248775
S 1.168744 3.943348 0.248101
S 0.681965 2.575163 1.758034
S 2.832740 -2.981974 0.248554
H 2.027119 -4.066790 0.235935
H 2.510811 3.785810 0.235881
H -4.533891 0.283377 0.238036
S 1.889302 -1.877668 1.757954

E= -3790.612191
Mo -0.777505 -1.212760 -0.252248
Mo 1.833235 0.034883 -0.149582
Mo -0.811626 1.164945 -0.256291
S 1.158337 2.087727 -0.953456
S -2.079124 -0.030365 -1.748516
S 1.220399 -2.041498 -0.964458
S 3.230839 0.046761 1.668845
S 4.454734 0.016887 -0.024011
S -2.511681 -3.315835 0.194544
S -1.719380 -2.004945 1.693007
S -2.523713 3.252066 0.189117
H -1.634944 4.254060 0.367999
H -3.677723 -2.588318 -0.018925
H 4.692874 -1.311986 -0.110102
S -1.832448 1.921037 1.657561

[Mo3S9H2]+ I
E= -3790.089670
S -0.268056 3.769927 0.903989
Mo -0.147912 1.876992 -0.030977
S -1.930396 1.220255 -1.286176
Mo -1.291771 -0.626544 -0.063013
S -3.397555 -2.089391 -0.504800
S -2.812192 -1.560511 1.420235
S 1.879990 1.531689 -1.294350
Mo 1.424835 -0.517061 -0.050046
S 3.611847 -1.632634 -0.438625
S 2.936757 -1.598354 1.438159
S 0.031622 0.316869 1.663141
S 0.164639 -1.889431 -1.317856
H 1.500820 1.251808 -2.559196

H -4.343660 -1.148758 -0.730750

E= -3790.055450
S -1.372514 3.617932 -0.027802
Mo -0.369568 1.775269 -0.106988
S 1.866052 1.839260 -0.271188
Mo 2.077647 -0.525581 -0.122598
S 2.902419 -0.858822 2.012928
S 3.570028 -1.081798 -1.468169
S -0.891014 0.623589 1.941512
Mo -1.317725 -0.821100 -0.010711
S -3.463300 -1.383833 0.932947
S -3.124808 -2.224382 -0.842687
S -1.200045 0.530927 -1.843024
S 0.428468 -2.209118 -0.082515
H 0.326669 0.222291 2.384447
H 3.833866 0.116933 2.075973

[Mo3S9H2]+ II
E= -3790.126437
S 0.069363 3.615873 1.137053
Mo 0.030118 1.771320 -0.251384
S -1.831618 1.204369 -1.465674
Mo -1.355703 -0.513969 -0.030963
S -3.537697 -1.869630 -0.347944
S -2.906885 -1.256866 1.535789
S 1.849114 1.135625 -1.499185
Mo 1.376122 -0.565816 -0.055896
S 3.452424 -1.858504 -0.404290
S 3.021753 -1.404147 1.486295
S 0.038392 0.396346 1.635813
S -0.017697 -2.002027 -1.154964
H -4.416524 -0.881081 -0.632732
H 0.099569 4.459943 0.072660

E= -3790.069348
S 0.023150 3.719344 0.864527
Mo -0.127011 1.738323 -0.305737
S -2.076385 1.130641 -1.226678
Mo -1.502727 -0.705807 0.151926
S -3.233259 -2.005449 -0.859371
S -2.455008 -1.094051 2.061517
S 1.588865 1.106622 -1.688261
Mo 1.374577 -0.526802 -0.096798
S 3.583747 -1.560270 -0.501368
S 3.170394 -1.122360 1.392905
S 0.183748 0.519028 1.623837
S 0.084709 -2.177100 -0.857301
H -2.913396 -1.912074 -2.167354
H -0.289226 4.409571 -0.263963

[Mo3S9H2]+ III
E= -3790.113830
S -1.085534 3.618844 0.816654
Mo -0.384256 1.853462 -0.105867
S -2.010191 0.894384 -1.410401
Mo -1.212750 -0.754531 -0.056301
S -3.153515 -2.423252 -0.454417
S -2.643755 -1.782299 1.457961
S 1.665579 1.668101 -1.201622
Mo 1.516445 -0.321768 -0.051820
S 3.869556 -1.334360 -0.458344
S 3.143495 -0.992049 1.461440
S 0.018223 0.351252 1.651300
S 0.381196 -1.928677 -1.216576
H -4.179964 -1.582597 -0.720651
H 4.602696 -0.209350 -0.627742

E= -3790.065989
S -0.640307 3.834862 0.432232
Mo -0.415951 1.826597 -0.125897
S -2.272203 0.998437 -1.067403
Mo -1.645834 -0.951317 0.170379
S -2.776736 -2.359178 -1.350597
S -2.860987 -1.361753 1.815787
S 1.404841 1.459323 -1.475038
Mo 1.676201 -0.376193 -0.045323
S 4.017095 -1.280500 -0.616945
S 3.515352 -0.718348 1.325059
S 0.085443 0.428109 1.607687
S 0.380107 -2.172746 -0.449802
H -2.075977 -2.065568 -2.464865

H 4.628849 -0.147393 -1.035553

[Mo3S9H2]+ IV
E= -3790.063411
S -1.662088 0.276597 -1.823507
Mo -3.016921 -0.166731 0.041853
S -4.058050 -1.959471 -0.367181
Mo -0.135686 0.181780 -0.175637
Mo 2.785420 -0.254539 -0.011621
S 4.305468 0.668181 -1.441439
S -1.334885 -0.342175 1.669451
S 1.694377 1.282761 1.336523
S 0.659545 2.367199 -0.096897
S 1.236209 -1.479235 -1.079581
S -4.309798 1.402464 0.608293
S 3.827955 -1.517405 1.561817
H 4.540852 -2.342887 0.758702
H 5.141286 1.218833 -0.531381

E= -3790.057895
S -1.743139 0.993143 -1.503754
Mo -3.107749 -0.200403 0.001062
S -3.880287 -1.985869 -0.803744
Mo -0.108736 0.335399 -0.080541
Mo 2.839837 -0.322875 -0.079707
S 4.402787 0.866664 -1.239033
S -1.366292 -0.600755 1.546088
S 1.819991 1.035797 1.509627
S 0.928433 2.408227 0.216794
S 1.109345 -1.183176 -1.293368
S -4.639159 1.019081 0.777250
S 3.764063 -1.972474 1.199259
H 4.515923 -1.235742 2.049036
H 4.971398 -0.163538 -1.909075

[Mo3S9H2]+ V
E= -3790.071909
S -0.010389 3.858379 0.681268
Mo -0.008529 1.879428 -0.079677
S -1.811082 1.219573 -1.354399
Mo -1.428607 -0.598136 -0.014549
S -3.470876 -1.820648 -0.588892
S -3.199441 -1.460060 1.355374
S 1.821430 1.237629 -1.320426
Mo 1.381090 -0.574248 0.015809
S 3.553610 -1.848413 -0.535708
S 3.033841 -1.419714 1.426958
S -0.041170 0.333316 1.617515
S -0.001985 -1.929279 -1.212672
H 4.409583 -0.829429 -0.783985
H -0.038698 0.401059 2.973202

E= -3790.057864
S -1.420989 3.577618 -0.298973
Mo -0.359146 1.770201 -0.134299
S -1.005873 0.383305 -1.843524
Mo -1.358089 -0.786221 0.086548
S -2.947769 -2.390289 -0.882657
S -3.579196 -1.430351 0.745079
S 1.887569 1.879348 -0.132450
Mo 2.108848 -0.478540 0.102449
S 3.056454 -1.277524 -1.821607
S 3.439408 -0.783961 1.680567
S -1.024933 0.774328 1.955813
S 0.436122 -2.089825 0.421917
H 4.328642 -0.864424 -1.633481
H -2.229099 1.353551 2.149538

[Mo3S9H2]+ VI
E= -3790.103747
S -1.665712 -0.813317 1.528340
Mo -3.027212 0.030156 -0.042411
S -4.184098 1.890264 0.610313
Mo -0.201944 -0.004503 -0.071470
S 1.093283 1.662695 0.615122
Mo 2.603510 -0.109101 0.238704
S 3.142927 -0.921829 2.079389
S 1.127824 -1.626031 -0.802724
S -1.695613 0.835394 -1.648080
S 4.373644 -0.413663 -1.411309
S 4.318969 1.402805 -0.624445
S -4.238067 -1.804417 -0.674336

H -5.001471 1.183593 1.429867
H -5.091925 -1.069209 -1.428758

E= -3790.090476
S 1.664802 -0.076350 1.679429
Mo 3.172373 0.000785 -0.058644
S 4.452610 -1.877014 -0.220494
Mo 0.124560 -0.003363 -0.008542
S -1.196958 -1.799534 -0.114963
Mo -2.672463 -0.006827 0.245061
S -3.242710 -0.049349 2.249373
S -1.197086 1.796288 -0.050594
S 1.625515 0.078114 -1.746816
S -4.412079 1.020142 -1.128965
S -4.417052 -0.960568 -1.173018
S 4.440210 1.890512 0.052140
H 5.184765 -1.741405 0.909536
H 5.111449 1.780567 -1.117752

[Mo3S9H2]+ VII
E= -3790.093991
S -1.712166 1.502711 -1.170482
Mo -3.099323 -0.022040 0.099147
S -4.676654 -1.052172 -1.212881
Mo -0.203772 -0.038069 -0.086148
S 1.165772 -0.987365 -1.549480
Mo -2.618177 0.207643 -0.125723
S 3.225017 1.943453 -1.104990
S 1.048328 0.795589 1.539665
S -1.617003 -1.623164 0.761738
S 4.277549 -0.531477 1.505397
S 4.344874 -1.514449 -0.213164
S -3.796122 0.942138 1.808402
H -5.743572 -0.413802 -0.684525
H -1.643328 2.613154 -0.408781

E= -3790.069074
S -1.624715 1.505571 -1.080524
Mo -3.144143 0.012756 0.068615
S -4.667051 -0.931610 -1.369106
Mo -0.325514 -0.178214 0.027298
S 1.182118 -0.935950 -1.505580
Mo 2.700668 0.221126 -0.135042
S 3.332381 1.957936 -1.099772
S 1.114555 0.767716 1.516918
S -1.814354 -1.692486 0.826308
S 4.417248 -0.499506 1.442877
S 4.454302 -1.469164 -0.288287
S -3.915994 1.006047 1.732240
H -5.736538 -0.252368 -0.900428
H -1.621764 2.577406 -0.257317

[Mo3S9H2]+ VIII
E= -3790.093318
S 1.568497 -0.121718 1.705711
Mo 3.095768 0.111764 -0.039103
S 4.676538 -1.559660 -0.008778
Mo 0.273804 -0.155443 -0.109537
S -1.266992 -2.018639 -0.211531
Mo -2.599163 -0.001724 0.262465
S -3.007944 0.009256 2.303363
S -1.044057 1.671601 -0.166843
S 1.677960 -0.105259 -1.858825
S -4.396479 1.163623 -0.857524
S -4.345602 -0.778742 -1.260575
S 3.824281 2.064430 -0.010941
H 5.750608 -0.744773 0.058268
H -1.087045 -2.546599 1.016130

E= -3790.080141
S -1.717468 -0.020623 1.698036
Mo -3.193199 -0.072782 -0.068063
S -4.604496 1.753247 -0.063946
Mo -0.165508 -0.065800 0.010312
S 1.152078 1.926365 -0.120161
Mo 2.658682 0.037608 0.247011
S 3.161472 0.237354 2.257370
S 1.262041 -1.804981 -0.028913
S -1.666910 0.058375 -1.757216
S 4.480060 -1.076185 -0.911504
S 4.318132 0.846910 -1.360209
S -4.263554 -1.860607 -0.120945

H -5.778131 1.096083 0.015568
H 1.237517 2.187163 -1.444653

[Mo3S9H2]+ IX
E= -3790.093931
S -1.693108 1.795063 -0.064491
Mo -3.093100 -0.053271 0.027647
S -4.558763 -0.064453 -1.748193
Mo -0.276664 0.054157 -0.039389
S 1.252088 0.111159 -1.755236
Mo 2.606481 0.183022 0.062239
S 3.521899 2.289481 0.122076
S 1.038838 0.064522 1.795165
S -1.566932 -1.784787 -0.168738
S 3.514691 -1.893242 0.634923
S 4.521260 -0.984035 -0.853076
S -3.963604 -0.131919 1.921812
H -5.684300 -0.113941 -1.005046
H 4.680297 1.961201 0.736342

E= -3790.082221
S 1.717616 1.381589 -1.084150
Mo 3.166596 -0.096035 -0.053730
S 4.664838 1.026028 1.288214
Mo 0.358208 0.006643 0.071747
S -1.012298 1.128545 1.432376
Mo -2.663065 0.163642 -0.024995
S -3.411505 2.015647 -1.106434
S -1.149358 -1.098039 -1.247821
S 1.719598 -1.374417 1.218879
S -4.687360 -1.265174 -0.390029
S -4.214426 -0.828024 1.492003
S 4.028335 -1.311788 -1.514434
H 5.778083 0.537780 0.702613
H -4.458140 1.553860 -1.827214

[Mo3S9H2]+ X
E= -3790.111180
S 1.712143 -0.186559 1.690767
Mo 3.203806 0.083041 -0.051227
S 4.612159 -1.714466 -0.283503
Mo 0.176817 -0.018536 -0.003318
S -1.106069 -1.815195 -0.274746
Mo -2.619158 -0.083766 0.228972
S -3.229113 -0.399106 2.203227
S -1.168212 1.759885 0.123381
S 1.655468 0.193790 -1.752939
S -4.571642 1.144522 -0.878496
S -4.147514 -0.811823 -1.404231
S 4.227035 1.886126 0.127632
H 5.785953 -1.053552 -0.216877
H -5.515564 0.947715 0.073485

E= -3790.085566
S 1.833843 -0.831722 1.471018
Mo 3.297343 0.115486 0.003961
S 4.751839 -1.442443 -0.880059
Mo 0.272100 -0.045618 -0.040805
S -1.189162 -1.617580 -0.823193
Mo -2.599214 -0.219506 0.163381
S -3.601705 -1.191395 1.815230
S -1.240449 1.457487 0.755626
S 1.790250 0.842137 -1.541389
S -4.609414 1.519562 -0.335011
S -4.243733 -0.045062 -1.642441
S 4.363635 1.692988 0.857484
H 5.915471 -0.854653 -0.541666
H -5.626720 0.995911 0.390886

[Mo3S9H2]+ XI
E= -3790.083772
S 1.839177 1.539822 -1.069411
Mo 3.279089 -0.111180 0.042166
S 4.505181 0.737894 1.524251
Mo 0.175484 0.059645 -0.023690
S -1.104915 0.966663 1.542737
Mo -2.635679 0.218420 -0.087337
S -3.321463 1.921788 -1.083259
S -1.152084 -0.992595 -1.459686
S 1.552499 -1.445396 0.943143
S -4.528291 -1.494640 -0.296260
S -4.098870 -0.635486 1.538059

S 4.390652 -1.150938 -1.405146
H -5.515374 -0.673470 -0.728661
H 1.811696 2.510519 -0.130056

E= -3790.062910
S 1.758172 1.393534 -1.117629
Mo 3.357881 -0.090056 -0.018330
S 4.749550 0.965435 1.153731
Mo 0.278780 -0.033957 0.199459
S -1.219639 1.264991 1.335777
Mo -2.740151 0.251862 -0.110671
S -3.514666 1.703916 -1.403384
S -1.169140 -1.142440 -1.158070
S 1.821942 -1.293912 1.283235
S -4.560273 -1.565393 -0.244335
S -4.293831 -0.466400 1.490502
S 4.304795 -1.296033 -1.453745
H -5.554731 -0.856759 -0.832477
H 1.870730 2.467913 -0.304079

[Mo3S9H2]+ XII
E= -3790.065556
S 1.842571 1.888387 -0.142253
Mo 3.237803 -0.119902 0.027859
S 4.276167 -0.089970 1.853080
Mo 0.138136 0.105877 -0.080136
S -1.111808 0.263370 1.752504
Mo -2.650295 0.149229 -0.015399
S -3.514263 2.256475 0.052933
S -1.212052 -0.028262 -1.854163
S 1.487774 -1.701644 0.031430
S -4.102860 -1.468407 -0.874989
S -3.976158 -1.393911 1.142832
S 4.532002 -0.353933 -1.613329
H 1.875397 2.063801 -1.481676
H -3.894402 2.303923 -1.244645

E= -3790.058291
S 1.857331 1.717908 -0.774055
Mo 3.284669 -0.117834 -0.001803
S 4.566025 0.443402 1.568276
Mo 0.178516 0.096615 0.016221
S -1.151045 0.833213 1.652504
Mo -2.628241 0.145225 -0.002681
S -3.569844 2.190934 -0.432113
S -1.205365 -0.585004 -1.635531
S 1.553209 -1.552825 0.710577
S -4.577276 -1.243259 -0.629128
S -3.846185 -1.491519 1.213254
S 4.339802 -0.912590 -1.635028
H 1.896439 2.509679 0.319980
H -4.430478 1.877885 -1.425453

[Mo3S9H2]+ XIII
E= -3790.060409
S -1.672225 1.140685 -1.376036
Mo -3.010224 -0.221314 -0.005386
S -3.636105 -1.998475 -0.945037
Mo -0.022128 0.350625 -0.004235
Mo 2.741582 -0.380533 -0.070097
S 3.951946 0.646023 -1.423828
S -1.292688 -0.597385 1.589295
S 1.798817 1.259368 1.445220
S 1.225304 2.625977 -0.060073
S 0.974017 -1.336544 -1.445834
S -4.635408 0.837843 0.818488
S 3.717365 -2.020017 1.208348
H 4.995446 -1.695311 0.911124
H 0.320539 3.326183 0.668328

E= -3790.068751
S 1.893295 0.801512 1.593251
Mo 2.899159 -0.372914 0.005567
S 3.662630 -2.272850 0.685272
Mo 0.004469 0.649633 -0.019421
Mo -2.910935 -0.326683 0.030305
S -4.574341 0.766947 0.654899
S 1.278884 -0.565735 -1.579365
S -1.867738 0.674537 -1.640753
S 0.113905 2.946333 -0.066618
S -1.301627 -0.358079 1.639601
S 4.715590 0.545603 -0.704146

S -3.544819 -2.457169 -0.567922
H -4.785762 -2.459019 -0.042708
H -0.919782 3.259912 -0.875777

[Mo3S9H2]+ XIV
E= -3790.068846
S 1.651980 1.802617 0.159992
Mo 3.179765 -0.049403 0.056765
S 3.996604 -0.484082 1.948907
Mo 0.178360 -0.068240 -0.215177
S -0.980456 -0.554542 1.590717
Mo -2.622780 0.254628 0.084533
S -3.124761 2.196786 0.638183
S -1.259498 0.347455 -1.838356
S 1.782937 -1.827379 -0.739932
S -4.483168 -0.821118 -1.062587
S -4.293686 -1.359222 0.833087
S 4.589144 0.378444 -1.445706
H 1.442032 2.065824 1.466296
H 1.607935 -2.682534 0.287723

E= -3790.045628
S -1.711316 -1.424488 1.197986
Mo -3.236460 0.100723 0.027265
S -4.276513 1.380723 1.327991
Mo -0.141032 -0.250437 -0.267090
S 0.977984 1.426246 0.809116
Mo 2.608833 -0.133970 0.198110
S 3.041141 -1.362514 1.828678
S 1.433019 -1.369893 -1.408131
S -1.662974 1.302158 -1.386042
S 4.586127 0.110264 -1.210412
S 4.313345 1.619721 0.044953
S -4.493173 -1.045737 -1.196485
H -1.510612 -0.734610 2.341881
H -1.527956 2.465643 -0.712317

[Mo3S9H2]+ XV
E= -3790.051459
S 1.477149 0.458206 1.625235
Mo 3.213928 -0.014700 -0.028762
S 4.483458 -1.556774 0.629247
Mo 0.202064 -0.169641 -0.287556
S -1.201622 -1.809334 0.237256
Mo -2.609185 0.067548 0.271606
S -2.941457 0.560550 2.266041
S -1.129366 1.779667 -0.675990
S 1.810415 -0.712374 -1.768854
S -4.352280 0.673505 -1.328722
S -4.542186 -1.136279 -0.539095
S 4.249350 1.770480 -0.457018
H 1.413786 1.803689 1.734827
H -0.955051 2.660951 0.333482

E= -3790.053651
S -1.827625 -1.058458 1.538130
Mo -3.252697 0.053249 -0.111185
S -4.378842 1.552712 0.835808
Mo -0.172294 0.103867 0.124976
S 1.285743 1.659572 0.830738
Mo 2.663611 -0.105635 0.201529
S 3.323114 -1.000947 1.963180
S 1.091275 -1.717190 -0.792109
S -1.537643 0.959783 -1.451575
S 4.131624 -0.270491 -1.744071
S 4.419437 1.342762 -0.629685
S -4.463947 -1.289452 -1.189059
H -1.842402 -2.312579 1.037021
H 1.130173 -2.696431 0.137831

[Mo3S9H2]+ XVI
E= -3790.046523
S 1.736075 0.000227 1.771118
Mo 3.248026 -0.000029 -0.112491
S 4.412099 -1.746876 -0.242143
Mo 0.235062 0.000094 0.164600
S -1.190923 -1.937314 0.248449
Mo -2.673460 -0.000006 0.161787
S -3.331127 0.000143 2.150248
S -1.191059 1.937416 0.248145
S 1.400842 -0.000103 -1.688552
S -4.120743 1.034641 -1.339955

S -4.120726 -1.034969 -1.339753
S 4.412266 1.746684 -0.242482
H -1.055904 2.403303 -1.012606
H -1.055743 -2.403371 -1.012235

E= -3790.037947
S -2.025648 1.836721 0.002543
Mo -3.226394 -0.189740 -0.000259
S -4.388685 -0.454018 -1.738237
Mo -0.221983 0.483579 0.000579
S 1.179476 0.317854 -1.924187
Mo 2.672818 0.178579 0.000300
S 3.593073 2.034227 0.003234
S 1.179225 0.311963 1.925021
S -1.284612 -1.534093 -0.002331
S 4.019057 -1.588987 0.987982
S 4.019308 -1.585835 -0.992619
S -4.388379 -0.458956 1.737167
H 1.064012 -0.955468 2.381254
H 1.064402 -0.948137 -2.384445

[Mo3S9H2]+ XVII
E= -3790.060735
S -1.675922 -1.027645 1.406384
Mo -3.243627 0.066910 -0.053631
S -4.450492 1.458599 0.962833
Mo -0.215525 -0.061399 0.056624
S 1.160283 1.326989 1.202856
Mo 2.638415 -0.068994 0.112475
S 3.358130 -1.476371 1.755531
S 1.181117 -1.660069 -1.079194
S -1.482899 1.124329 -1.311809
S 4.054096 0.228462 -1.678701
S 4.080908 1.705981 -0.262289
S -4.375367 -1.281676 -1.209735
H 1.093557 -1.244818 -2.359753
H 3.779748 -2.466492 0.936069

E= -3790.044340
S 1.682296 -1.539967 -0.777816
Mo 3.296304 0.044900 0.046915
S 4.530713 0.810778 -1.475234
Mo 0.268886 -0.020539 -0.017339
S -1.079058 0.772476 -1.644876
Mo -2.613146 -0.096972 -0.133567
S -3.425287 -1.944966 -1.175674
S -1.221927 -0.931414 1.653708
S 1.587536 1.609377 0.694695
S -4.665032 0.405616 1.174959
S -3.963571 1.856274 0.000785
S 4.403486 -0.694951 1.679342
H -1.228565 0.017764 2.615694
H -4.343800 -2.459632 -0.326365

[Mo3S9H2]+ XVIII
E= -3790.082779
S -1.643108 -0.430303 1.655293
Mo -3.276362 0.057589 -0.051252
S -4.470924 1.724645 0.419388
Mo -0.247074 -0.009529 0.001207
S 1.167964 1.693330 0.451783
Mo 2.610348 -0.112509 0.218802
S 3.185980 -0.831392 2.090199
S 1.139367 -1.906440 -0.542112
S -1.577018 0.592035 -1.664988
S 4.117644 -0.389598 -1.572873
S 4.487739 1.392341 -0.586583
S -4.423325 -1.624298 -0.591147
H 1.131823 -1.812278 -1.889705
H 5.468790 0.994031 0.258503

E= -3790.054531
S -1.756169 -0.302061 1.679913
Mo -3.218733 0.035678 -0.052212
S -4.578579 1.680589 0.226389
Mo -0.190174 0.102048 0.030025
S 1.278556 1.778695 0.341861
Mo 2.635907 -0.110691 0.227018
S 3.166348 -0.792296 2.127753
S 1.088284 -1.838322 -0.529832
S -1.715852 0.330151 -1.732015
S 4.137547 -0.535181 -1.545082

S 4.594995 1.261160 -0.625932
S -4.605850 -1.593906 -0.378352
H 1.168237 -1.804150 -1.879973
H 5.549281 0.847397 0.241819

[Mo3S9H2]+ XIX
E= -3790.086809
S -1.646058 1.618959 -0.548977
Mo -3.282645 -0.066039 -0.037081
S -4.401366 -0.642565 -1.725905
Mo -0.249316 0.007013 0.040043
S 1.248541 -0.565897 -1.616314
Mo 2.556563 0.226860 0.046057
S 3.375217 2.259626 -0.639544
S 1.108638 0.559885 1.789030
S -1.607973 -1.671718 0.562308
S 3.822608 -1.294461 1.209785
S 4.556339 -1.293440 -0.739372
S -4.508124 0.467664 1.590118
H 5.600760 -0.447850 -0.583417
H 4.200785 2.389942 0.426586

E= -3790.074366
S -1.764399 1.248555 -1.175553
Mo -3.371785 -0.074464 -0.013244
S -4.497614 -1.297534 -1.304129
Mo -0.338241 0.030792 0.032479
S 1.166691 -1.109976 -1.233096
Mo 2.687181 0.164402 -0.009081
S 3.677349 1.893182 -1.136911
S 1.050759 1.245547 1.315645
S -1.710673 -1.284765 1.196925
S 4.079345 -0.858572 1.519474
S 4.746251 -1.380455 -0.382515
S -4.607863 1.070979 1.247428
H 5.720501 -0.453156 -0.544061
H 3.001438 2.951126 -0.638698

[Mo3S9H2]+ XX
E= -3790.078097
S 1.770445 0.827150 1.757998
Mo 2.967591 -0.252072 -0.033559
S 3.764403 -2.107928 0.547544
Mo -0.044672 0.423093 0.034636
Mo -2.758831 -0.341408 0.037338
S -4.201655 0.618266 1.190913
S 1.262138 -0.466085 -1.615520
S -1.802003 1.272696 -1.449604
S -0.861056 2.577447 -0.103390
S -1.094683 -1.047640 1.437064
S 4.464331 1.018915 -0.779275
S -3.529537 -2.115457 -1.185343
H -4.849434 -1.875864 -1.027684
H 1.599636 -0.205697 2.608045

E= -3790.053308
S 1.831999 0.685998 1.779474
Mo 3.137464 -0.223046 -0.040100
S 4.068419 -2.037627 0.461790
Mo 0.069661 0.293247 0.029688
Mo -2.980780 -0.298923 0.113914
S -4.398424 0.753789 1.239246
S 1.428148 -0.489634 -1.614711
S -1.916237 1.186965 -1.347320
S -0.743866 2.449924 -0.150385
S -1.179704 -1.218602 1.241719
S 4.540410 1.196940 -0.687693
S -4.007913 -1.775339 -1.313195
H -5.143891 -2.009057 -0.622110
H 1.672034 -0.423292 2.532261

[Mo3S9H2]+ XXI
E= -3790.098762
S -1.759722 0.864789 -1.649489
Mo -2.866028 -0.280295 0.007371
S -3.408374 -2.166421 -0.701744
Mo -0.139955 0.356585 -0.126562
Mo 2.829137 -0.272778 -0.043323
S 4.165243 0.712156 -1.300502
S -1.275997 -0.488777 1.653621
S 1.790403 1.279194 1.384098
S 0.706102 2.496720 0.073119

S 1.099519 -1.219364 -1.234096
S -4.623524 0.981419 0.801829
S 3.802551 -1.845049 1.310848
H 5.081683 -1.673048 0.914877
H -5.593360 0.090827 0.507760

E= -3790.071790
S -1.857020 0.716200 -1.638161
Mo -3.037954 -0.252721 0.006571
S -3.862947 -2.068636 -0.600408
Mo -0.068350 0.333020 -0.128382
Mo 2.961875 -0.285709 -0.082194
S 4.475336 0.715597 -1.134174
S -1.394560 -0.558019 1.555342
S 1.872867 1.191072 1.350205
S 0.783463 2.463915 0.074830
S 1.210598 -1.145723 -1.327167
S -4.688779 1.143737 0.793391
S 3.886684 -1.802986 1.373519
H 4.992462 -2.154779 0.683416
H -5.736729 0.299472 0.726704

[Mo3S9H2]+ XXII
E= -3790.077277
S -1.821107 1.250668 -1.408915
Mo -2.834461 -0.274067 -0.024243
S -3.256803 -2.039995 -1.050132
Mo -0.137772 0.430110 -0.085680
Mo 2.802458 -0.429011 -0.003329
S 4.344883 0.394597 -1.175739
S -1.234179 -0.638636 1.594010
S 1.730436 1.216836 1.406869
S 1.228027 0.613959 -0.101383
S 0.960651 -1.076079 -1.329658
S -4.665214 0.719033 0.968568
S 3.480090 -1.922203 1.315402
H -5.559065 -0.219031 0.593287
H 0.421077 3.392787 0.658923

E= -3790.046445
S -1.937684 1.548315 -0.938389
Mo -3.033624 -0.228069 -0.038259
S -3.993561 -1.370764 -1.496180
Mo -0.070330 0.434396 -0.071873
Mo 2.931601 -0.467205 -0.006511
S 4.713664 0.290743 -0.837024
S -1.310274 -1.342485 0.874274
S 1.769682 1.115894 1.421089
S 1.523504 2.645846 -0.026386
S 1.279225 -0.714713 -1.590106
S -4.551030 0.437843 1.563228
S 3.265898 -2.143516 1.227917
H -5.686751 0.027582 0.966336
H 0.774809 3.454716 0.757884

[Mo3S9H2]+ XXIII
E= -3790.048843
S 1.801316 0.954770 1.753075
Mo 2.914470 -0.241174 -0.028632
S 3.536503 -2.150276 0.586470
Mo -0.008525 0.510322 0.063702
Mo -2.711772 -0.485973 0.015396
S -4.313805 0.134104 1.242044
S 1.217642 -0.329427 -1.644251
S -1.869309 1.252630 -1.411569
S -1.343774 2.684885 0.060799
S -0.897194 -1.091754 1.354360
S 4.514471 0.879403 -0.807355
S -3.221986 -1.979244 -1.387641
H -0.532593 3.438660 -0.723231
H 1.595529 -0.013499 2.668746

E= -3790.027230
S 1.693715 0.293147 1.854347
Mo 3.147726 -0.164708 -0.036933
S 4.281829 -1.911264 0.248967
Mo 0.043571 0.127153 -0.007960
Mo -3.013529 -0.332563 0.036675
S -4.209685 0.735028 1.405671
S 1.492177 -0.447795 -1.662443
S -1.794780 1.213743 -1.379853
S -0.961768 2.450333 0.127361

S -1.268941 -1.487273 1.012180
S 4.357235 1.512789 -0.419834
S -4.153860 -1.524547 -1.275197
H -0.079253 3.133463 -0.646351
H 1.638266 -0.935117 2.412297

[Mo3S9H2]+ XXIV
E= -3790.083226
S 0.036473 3.452055 1.425576
Mo -0.022455 1.730711 -0.101163
S -1.833301 1.296054 -1.408485
Mo -1.403223 -0.526405 -0.097793
S -3.564528 -1.616759 -0.502654
S -3.019885 -1.456077 1.410279
S 1.811488 1.301201 -1.598893
Mo 1.455789 -0.608920 -0.058849
S 3.655607 -1.322321 -0.328720
S 2.728546 -1.846947 1.425970
S 0.048388 0.192727 1.651049
S -0.011121 -1.902242 -1.254837
H 1.134823 1.028350 -2.737890
H -0.026157 4.402374 0.457090

E= -3790.068173
S 1.128711 3.858598 0.645773
Mo 0.292084 1.769512 0.054648
S -1.559340 1.580808 -1.273369
Mo -1.477648 -0.350129 -0.049556
S -3.705375 -1.244933 -0.581450
S -3.314236 -0.991900 1.360232
S 2.078852 1.020803 -1.348692
Mo 1.185452 -0.804696 -0.012398
S 3.067186 -2.366710 -0.499991
S 2.530732 -2.194208 1.408270
S 0.003026 0.223124 1.750161
S -0.326341 -1.819878 -1.366180
H 1.495104 0.840219 -2.558770
H 0.058140 4.291651 1.349542

[Mo3S9H2]+ XXV
E= -3790.085237
S 0.393671 3.676323 0.822690
Mo 0.124159 1.843251 -0.201014
S -0.026110 0.273603 1.577835
Mo 1.348412 -0.653700 -0.073011
S -0.123419 -1.976605 -1.246134
Mo -1.467661 -0.501152 -0.087658
S -3.586525 -0.602516 1.351002
S -3.276490 -2.019073 -0.135254
S -1.780212 1.262623 -1.439963
S 1.882384 1.015667 -1.472001
S 3.044444 -2.309273 -0.159551
S 3.390975 -1.039012 1.442720
H 4.247431 -0.148126 0.884362
H -3.153155 -1.272399 2.444849

E= -3790.060561
S -0.252180 3.923778 0.610537
Mo -0.100072 1.954946 -0.112916
S -0.036681 0.282224 1.568854
Mo 1.419441 -0.660559 -0.060310
S 0.040576 -1.898171 -1.474027
Mo -1.369321 -0.701994 -0.160972
S -3.520826 -0.958508 1.303754
S -2.881106 -2.461063 0.011336
S -1.920866 1.151118 -1.344816
S 1.809839 1.424246 -1.173043
S 3.145056 -2.236176 -0.056007
S 3.656672 -0.696602 1.248990
H 4.452669 0.040459 0.440071
H -3.002441 -1.414471 2.466983

[Mo3S9H2]+ XXVI
E= -3790.124058
S 0.075676 3.715738 0.987374
Mo 0.030438 1.770745 -0.259984
S 0.039577 0.405873 1.632279
Mo 1.375114 -0.570372 -0.054044
S -0.020403 -2.009799 -1.146887
Mo -1.355246 -0.515110 -0.028624
S -2.906561 -1.253858 1.541202
S -3.535106 -1.874866 -0.340688

S -1.833505 1.196568 -1.466843
S 1.846852 1.122999 -1.503324
S 3.449601 -1.865407 -0.398026
S 3.027041 -1.393589 1.490284
H 0.011282 3.409032 2.295126
H -4.414909 -0.888589 -0.629674

E= -3790.084450
S -0.161488 4.226805 0.371349
Mo -0.065435 1.926546 0.119934
S 0.045006 0.256767 1.732473
Mo 1.382015 -0.570843 -0.090730
S 0.067816 -1.864990 -1.432347
Mo -1.277729 -0.656490 -0.046945
S -2.699223 -1.804630 1.389143
S -3.386654 -2.084936 -0.553499
S -1.973728 1.286804 -1.024674
S 1.854969 1.411466 -1.085084
S 3.442501 -1.850595 -0.592410
S 2.994351 -1.631572 1.336120
H -0.221821 4.642976 -0.912833
H -4.346707 -1.131852 -0.599239

[Mo3S9H2]+ XXVII
E= -3790.025879
Mo 1.296280 -0.597106 -0.170375
Mo -0.051075 1.496842 -0.504549
Mo -1.240233 -0.684052 -0.168579
S -1.940374 0.827076 -1.720509
S 0.082531 -2.292423 -1.139457
S 1.866311 0.957435 -1.731434
S -1.105304 2.950878 1.148358
S 0.894036 2.987476 1.175680
S 3.590310 -1.822074 0.363828
S 2.468473 -0.829779 1.823453
S -3.449950 -2.055399 0.402313
H -4.385184 -1.118709 0.127753
H 3.157061 -3.085538 0.572946
S -2.342328 -1.026596 1.848169

E= -3790.002190
Mo -0.821764 -1.203877 -0.250409
Mo 1.851150 -0.036850 -0.046789
Mo -0.768250 1.163173 -0.249865
S 1.270132 2.020932 -0.867109
S -2.027620 0.035040 -1.791184
S 1.186573 -2.069171 -0.897660
S 3.580932 -0.067566 1.583872
S 4.364905 -0.092375 -0.822742
S -2.700218 -3.095321 0.161897
S -1.816950 -1.962097 1.684013
S -2.368213 3.367109 0.162123
H -1.428642 4.300617 0.428034
H -3.810717 -2.353520 -0.040964
S -1.846295 1.945334 1.618117

[Mo3S9]+ I
E= -3788.882661
S 1.248679 -0.066711 1.797308
Mo -0.067017 -0.001974 0.000126
S 1.248473 -0.066944 -1.797195
Mo 2.733040 0.243794 -0.000049
S 4.452872 -1.178594 -0.990432
S 3.319734 2.243049 -0.000201
S 4.452992 -1.178594 0.990268
S -1.571404 -1.750374 0.000290
Mo -3.116708 -0.051211 0.000111
S -5.179391 -0.099138 -1.022283
S -5.179849 -0.099012 1.021686
S -1.609059 1.695866 0.000068

E= -3788.882627
S 1.247701 -0.068741 1.797174
Mo -0.067528 0.000201 -0.000232
S 1.247961 -0.068649 -1.797449
Mo 2.732455 0.242280 -0.000022
S 4.454892 -1.177330 -0.990335
S 3.318474 2.241692 0.000070
S 4.454798 -1.177330 0.990456
S -1.570868 -1.748728 -0.000384
Mo -3.116517 -0.049610 -0.000192
S -5.179881 -0.102743 -1.020957

S -5.178568 -0.102708 1.022925
S -1.609086 1.698248 -0.000330

[Mo3S9]+ II
E= -3788.861298
S -1.596183 -0.006789 1.730818
Mo -0.000199 -0.688454 0.000002
S -1.596215 -0.006756 -1.730811
Mo -2.964258 0.344800 0.000013
S -4.725116 -0.904788 0.000003
S -3.876761 2.256767 0.000025
S 1.596513 -0.006842 -1.730890
S -0.000140 -2.762361 -0.000034
S 1.596582 -0.007030 1.730904
Mo 2.964236 0.344822 -0.000002
S 3.876970 2.298228 0.000084
S 4.724932 -0.904982 -0.000134

E= -3788.860593
S 1.595930 0.013872 1.733413
Mo -0.000003 0.695651 -0.000001
S 1.595612 0.013486 -1.733367
Mo 2.957068 -0.347106 -0.000030
S 4.724586 0.891337 -0.000258
S 3.860137 -2.304960 0.000104
S -1.595886 0.013840 -1.733419
S -0.000191 2.769084 0.000151
S -1.595494 0.012967 1.733354
Mo -2.957043 -0.347155 0.000012
S -3.860414 -2.304875 -0.000349
S -4.724337 0.891599 0.000423

[Mo3S9]+ III
E= -3788.885944
S 1.690189 0.328703 1.776493
Mo 0.127769 0.159878 0.197856
S 1.365838 -0.304268 -1.624124
Mo 3.130716 -0.155367 -0.056793
S 4.465719 1.404941 -0.507767
S 4.147271 -1.973024 0.229017
S -1.915757 1.331644 -1.336899
S -0.803187 2.258943 0.145449
S -1.228212 -1.542217 0.865215
Mo -3.008250 -0.273379 -0.013279
S -4.167687 -1.385613 -1.363259
S -4.211042 0.586670 1.480463

E= -3788.819064
S 0.940801 -0.597989 1.543828
Mo -0.084018 0.594249 -0.131698
S 1.687352 0.737887 -1.540746
Mo 2.744922 -0.589728 0.073092
S 4.452030 0.398510 0.812176
S 3.198351 -2.542455 -0.571871
S -0.913790 2.838227 -1.043247
S -0.155416 2.839539 0.774900
S -1.415583 -0.820940 -1.508746
Mo -3.148431 -0.451074 -0.103419
S -4.318835 -2.124119 0.338163
S -2.195150 0.443543 1.620859

[Mo3S9]+ IV
E= -3788.904249
S -1.270894 3.549552 0.848128
Mo -0.475168 1.835690 -0.090572
S 1.556135 1.738694 -1.226819
Mo 1.580474 -0.257914 -0.100546
S 0.045280 0.341091 1.628165
Mo -1.172483 -0.817674 -0.063867
S -2.059913 0.798390 -1.383368
S -2.621171 -1.972257 1.456318
S 0.451340 -1.880812 -1.262278
S 3.289383 -0.831409 1.475724
S 3.743976 -1.248321 -0.426609
S -2.957795 -2.490196 -0.439924

E= -3788.900603
S -1.084399 3.599450 0.841903
Mo -0.382686 1.841510 -0.093778
S 1.667867 1.647465 -1.212526
Mo 1.522709 -0.314346 -0.060878
S 0.012590 0.325613 1.651832

Mo -1.221204 -0.776067 -0.064383
S -2.003574 0.880634 -1.401908
S -2.750305 -1.863487 1.428454
S 0.384523 -1.887503 -1.259651
S 3.249929 -1.020908 1.449937
S 3.788001 -1.271146 -0.448495
S -3.051532 -2.381746 -0.474570

[Mo3S9]+ V
E= -3788.865319
S 0.997110 -0.074185 -1.727352
Mo -0.487967 0.710796 -0.025496
S -0.479084 2.782244 -0.183404
Mo 2.235202 -0.169593 0.097862
S 4.511765 -0.912605 -0.707907
S 3.342008 -2.164338 0.482179
S 0.968726 0.272882 1.837064
S 4.251658 0.964793 0.170765
S -2.127857 -0.081584 -1.761332
Mo -3.472899 -0.175998 -0.021323
S -2.143817 0.058531 1.728325
S -4.790641 -1.804401 0.027675

E= -3788.803582
S -0.763310 -1.074697 -1.614001
Mo 0.628854 -0.611226 0.295814
S 0.671269 -2.383739 1.376489
Mo -2.139924 -0.053533 -0.249026
S -4.553760 0.632559 -0.892559
S -5.025870 2.184479 0.220903
S -0.987627 0.770914 1.426677
S -4.125640 -1.106496 0.248448
S 2.363965 -0.816036 -1.491042
Mo 3.580050 0.298621 -0.025945
S 2.129634 0.995804 1.484262
S 4.860266 1.758324 -0.813890

[Mo3S9]+ VI
E= -3788.857198
S -1.524305 0.071672 1.728096
Mo 0.091729 0.706752 -0.000033
S 0.147351 2.779926 -0.000168
Mo -2.891167 -0.241821 0.000006
S -4.629039 -1.727802 0.000093
S -5.118393 0.282979 -0.000136
S -1.524210 0.071279 -1.728086
S 1.671773 -0.016123 1.731027
Mo 3.027798 -0.407784 0.000041
S 4.822742 0.791693 0.000054
S 1.671866 -0.016197 -1.731021
S 3.882769 -2.387438 0.000105

E= -3788.856844
S 1.520839 0.071581 -1.728014
Mo -0.091456 0.710406 0.000000
S -0.142618 2.783448 -0.000120
Mo 2.887656 -0.245278 0.000009
S 4.628304 -1.728705 0.000076
S 5.113859 0.282789 -0.000069
S 1.520860 0.071841 1.728031
S -1.674296 -0.010507 -1.733588
Mo -3.023484 -0.408568 0.000012
S -4.823397 0.782155 -0.000078
S -1.674322 -0.010297 1.733599
S -3.872633 -2.390778 0.000105

[Mo3S9]+ VII
E= -3788.819184
S -1.627060 -0.514627 1.687354
Mo -0.342583 0.572538 -0.002370
S -1.246298 2.629796 -0.651058
S 0.207294 2.718024 0.750864
Mo -2.980410 -1.075250 -0.009996
S -5.011620 -0.651276 0.255131
S -2.054522 -0.150193 -1.763728
S 1.403627 0.042829 1.771861
Mo 2.594281 -0.356675 -0.032914
S 1.076779 -0.185854 -1.707164
S 4.810303 0.187735 -0.207277
S 4.354366 -1.820542 -0.017123

E= -3788.818965

S -1.646538 -0.456640 1.706319
Mo -0.330074 0.564952 0.000890
S -1.235183 2.618670 -0.667806
S 0.226905 2.722132 0.718388
Mo -2.989823 -1.040711 0.004626
S -5.043568 -0.702164 0.227444
S -2.054420 -0.158062 -1.764592
S 1.404870 0.041248 1.773203
Mo 2.596206 -0.368232 -0.031132
S 1.068596 -0.234557 -1.700453
S 4.806249 0.197139 -0.221871
S 4.372777 -1.812287 -0.003394

[Mo3S9]+ VIII
E= -3788.856634
S -1.546674 0.044403 1.764555
Mo -2.817338 -0.289824 -0.000740
S -5.123332 0.143268 0.000891
S -4.609094 -1.816467 -0.000729
Mo 0.000357 0.719794 0.000430
S 0.001509 2.798821 0.002008
S 1.545966 0.045666 -1.764832
Mo 2.816489 -0.291522 0.000018
S 1.545766 0.043688 1.765110
S -1.546256 0.047289 -1.765274
S 4.611529 -1.815294 -0.000159
S 5.121878 0.145201 -0.000804

E= -3788.853640
S 1.564759 0.052989 -1.770932
Mo 0.020622 0.668610 0.000043
S -1.550885 -0.028072 1.755106
Mo -2.880503 -0.300458 -0.000031
S -5.101258 0.271108 0.000269
S -4.658747 -1.749908 -0.000229
Mo 2.802696 -0.240667 -0.000072
S 1.564949 0.052976 1.770893
S 4.664295 -1.787156 0.000027
S 5.185298 0.132506 -0.000065
S -1.551107 -0.027329 -1.755191
S 0.032805 2.748237 0.000278

[Mo3S9]+ IX
E= -3788.825841
Mo 0.202205 0.524358 0.071163
S -1.335724 -0.662507 1.733231
Mo -2.627850 -0.650471 -0.102439
S -3.660563 -2.467709 -0.310627
S -3.971519 1.030817 -0.161228
S -1.145242 2.253647 0.811148
S 0.378838 2.816376 -0.381828
S -0.925166 -0.395780 -1.692736
Mo 3.292534 -0.162543 0.103503
S 4.530038 -1.809673 -0.228949
S 1.735129 -0.461030 1.679931
S 2.118624 0.453582 -1.638537

E= -3788.870840
Mo -1.887291 -0.456401 -0.150131
S 0.112292 -0.161651 1.302452
Mo 2.155087 -0.857066 0.133058
S 3.746481 -0.667194 1.487619
S 2.154530 -2.768426 -0.761991
S -3.244589 -0.912059 1.832854
S -4.236419 -0.117237 0.312411
S -1.708807 -2.086762 -1.416687
Mo 0.410430 1.618531 -0.225088
S 0.803485 3.476090 0.652748
S 2.184376 0.897598 -1.435814
S -1.591693 1.538847 -1.337919

[Mo3S9]+ X
E= -3788.893344
S 1.687266 1.686955 -0.136482
Mo 0.281274 -0.036775 0.003157
S -1.158971 -0.173519 -1.727952
Mo -2.747441 0.266821 -0.021082
S -4.405964 -1.287176 -0.892090
S -4.413520 -1.119904 1.084204
Mo 3.313579 -0.053635 0.004406
S 1.667136 -1.776161 0.143643
S 4.494980 -0.199488 -1.730893

S 4.494836 0.079567 1.740823
S -1.159510 0.105140 1.733814
S -3.430713 2.221507 -0.179580

E= -3788.885443
S 1.712417 -1.711840 -0.019261
Mo 0.159253 -0.005549 -0.000151
S -1.152460 0.043887 1.798560
Mo -2.638371 -0.245896 -0.002746
S -4.360034 1.162151 1.003487
S -4.361404 1.182538 -0.976817
Mo 3.178005 0.064004 0.000723
S 1.646619 1.773652 0.019641
S 4.528020 0.081707 1.675634
S 4.528181 0.120065 -1.673243
S -1.152793 0.084698 -1.797134
S -3.223124 -2.244824 -0.025161

[Mo3S9]+ XI
E= -3788.834412
S 1.281124 -1.106936 0.000324
Mo -0.342646 0.442687 0.000040
S -1.844293 0.107860 -1.724339
Mo -3.319682 -0.183118 0.000021
S -5.158266 -1.557250 0.000105
S -5.529174 0.457584 -0.000208
Mo 3.569105 -0.300542 0.000004
S 4.852567 -2.008860 0.000371
S 4.078591 0.844110 1.735191
S 4.078458 0.843243 -1.735798
S 0.330110 2.419442 -0.000221
S -1.844407 0.108362 1.724406

E= -3788.834466
S 1.281783 -1.108453 0.000022
Mo -0.342425 0.440726 0.000003
S -1.843288 0.105937 -1.724686
Mo -3.318873 -0.183270 -0.000047
S -5.160023 -1.554288 0.000045
S -5.527636 0.460918 0.000045
Mo 3.568219 -0.299398 0.000003
S 4.855159 -2.005906 0.000155
S 4.075373 0.844454 1.736124
S 4.075459 0.844197 -1.736265
S 0.330864 2.417324 0.000031
S -1.843359 0.105916 1.724637

[Mo3S8H]+ I
E= -3391.186299
S -2.271658 -0.368264 1.750756
Mo -0.441586 0.375936 0.481604
S -0.505768 2.460641 0.348652
Mo -2.862494 -0.666415 -0.382502
S -0.969014 -0.573497 -1.582971
S -4.119338 0.893669 -0.960673
S 1.088220 -0.416018 2.119480
Mo 2.332911 -0.456556 0.258692
S 4.408136 0.717278 -0.717085
S 2.465786 1.394447 -1.108731
S 2.157789 -2.242413 -0.809059
H 4.720979 1.521981 0.326767

E= -3391.197409
S 1.941564 1.742806 -0.317247
Mo 0.315603 0.033936 0.475775
S 0.395672 0.153010 2.548568
Mo 3.176053 -0.045304 -0.701649
S 1.927442 -1.767973 -0.116498
S 5.148407 -0.013120 0.010467
S -1.203662 1.775174 -0.188694
Mo -2.468120 -0.009290 -0.292396
S -4.854224 -0.193482 -1.260448
S -4.522246 0.060099 0.776800
S -1.204909 -1.770520 0.010642
H -5.037261 1.091767 -1.650112

[Mo3S8H]+ II
E= -3391.248394
S -1.390601 1.746474 0.351168
Mo -2.944622 -0.024631 0.024356
S -4.707853 0.495001 -0.994813
Mo 0.030346 0.049264 -0.158997

S 1.496286 0.783880 -1.689098
Mo 2.823233 0.027355 0.072324
S 3.754281 1.672865 0.945695
S -1.386776 -1.389270 -1.178471
S 1.260864 -0.837448 1.528519
S -3.402995 -0.945406 1.852508
S 4.277192 -1.602834 -0.632432
H 5.417463 -0.955702 -0.311921

E= -3391.252908
S -1.431929 1.723412 -0.000139
Mo -3.074207 -0.013800 0.000022
S -4.252880 -0.021200 -1.742510
Mo -0.041251 -0.009947 -0.000056
S 1.466361 -0.002294 -1.728834
Mo 2.988159 0.051477 0.000018
S 4.042492 1.842468 -0.000066
S -1.421920 -1.746337 0.000099
S 1.466255 -0.002045 1.728797
S -4.252892 -0.020992 1.742547
S 4.371181 -1.774760 0.000147
H 5.559876 -1.136750 0.000024

[Mo3S8H]+ III
E= -3391.231575
S -3.549310 2.398739 -0.000138
Mo -2.527151 0.340306 -0.000109
S -1.172980 0.039430 1.741367
S 0.231692 -2.823973 0.000193
Mo 0.376680 -0.750642 0.000061
S 3.530519 2.246311 -0.000193
S -1.172986 0.038744 -1.741465
S -4.118185 -1.013451 0.000210
S 1.916248 -0.257761 -1.781136
Mo 3.128908 0.195434 0.000029
S 1.916048 -0.257413 1.781230
H -2.391046 3.095877 -0.000313

E= -3391.225896
S -3.627822 -2.445644 -0.000415
Mo -2.693559 -0.351075 0.000025
S -1.323922 0.018616 -1.725812
S 0.246806 2.778747 0.000114
Mo 0.245839 0.704749 -0.000149
S 4.602616 -1.721931 0.000135
S -1.323282 0.017436 1.725633
S -4.345861 0.921785 0.000767
S 1.885461 -0.001920 1.725977
Mo 3.268050 -0.114252 -0.000043
S 1.885157 -0.002248 -1.725978
H -2.440303 -3.093185 0.000255

[Mo3S8H]+ IV
E= -3391.260377
S -1.070677 0.071861 1.805411
Mo -1.206284 -1.280144 -0.019665
S -1.373725 0.096993 -1.818824
Mo -0.931713 1.465653 -0.020196
S -2.315156 3.036548 0.093247
S 1.227426 2.126759 -0.124965
Mo 2.001841 -0.134053 -0.006229
S 3.068770 -0.256469 1.789145
S 3.361906 -0.280897 -1.587100
S 0.787198 -2.243236 -0.138308
S -3.073576 -2.581900 0.095929
H -4.076122 -1.675696 0.103193

E= -3391.232805
S -0.044730 0.016376 -1.544771
Mo 1.663872 -0.663749 -0.063340
S 2.050304 1.098640 1.311140
Mo 0.096365 1.646493 0.214659
S 0.079955 3.549794 -0.675149
S -1.721252 1.087107 1.503162
Mo -1.756643 -0.587736 -0.080842
S -3.530004 -0.472575 -1.166879
S -1.259119 -2.781193 0.425562
S 0.608863 -2.210210 1.244967
S 3.557725 -1.317735 -1.181373
H 3.981177 -0.113592 -1.626568

[Mo3S8H]+ V

E= -3391.170573
Mo 1.937133 0.490563 -0.339101
S 3.533952 1.347413 1.080086
S 4.507326 0.351971 -0.474460
S 1.176727 -1.507672 0.257661
S 0.092932 1.738627 -0.771629
S 5.096087 -1.547355 0.124890
Mo -0.758692 -0.230900 0.005970
S -2.197786 -1.239610 -1.440261
Mo -3.517131 -0.428321 0.228738
S -4.459171 1.321834 -0.399691
S -2.010182 0.053053 1.877405
H 6.386834 -1.208538 0.320439

E= -3391.175515
Mo 1.948506 0.462476 -0.221607
S 3.670310 1.399792 1.010777
S 4.477226 0.360137 -0.600612
S 1.103315 -1.512930 0.459253
S 0.087343 1.656710 -0.796616
S 5.133122 -1.526284 -0.012402
Mo -0.765875 -0.261577 0.042988
S -2.208977 -1.284490 -1.422289
Mo -3.537341 -0.387416 0.183048
S -4.389060 1.376318 -0.524734
S -2.094551 0.095064 1.874090
H 6.438184 -1.186978 0.014493

[Mo3S8H]+ VI
E= -3391.189065
S 0.369884 -1.964020 -0.416783
Mo -0.778745 1.130158 -0.003173
S -1.495667 3.233227 0.601755
Mo -1.813843 -1.455796 -0.352899
S -2.597903 -1.881554 1.537676
S -2.626107 0.435963 -1.255826
S 0.478690 0.511439 1.847557
Mo 1.727874 0.021011 0.020926
S 3.949150 0.396020 0.334804
S 3.525980 -1.517300 -0.231993
S 0.842548 1.397181 -1.571200
H -2.827178 3.019060 0.540305

E= -3391.184399
S 1.820473 -0.720502 -1.622397
Mo 0.317737 0.434259 -0.076354
S 0.474527 2.639510 -0.631467
Mo 3.100751 -0.763340 0.179560
S 5.037617 -0.016576 -0.093651
S 1.888488 0.210213 1.764413
S -1.177091 -0.254376 -1.738120
Mo -2.560970 -0.156575 0.033987
S -4.763201 0.494988 -0.040539
S -4.429816 -1.504481 0.226058
S -1.173344 0.237001 1.745659
H 1.141748 3.025123 0.478556

[Mo3S8H]+ VII
E= -3391.222270
S -1.379411 0.230301 1.727724
Mo -0.042457 -0.001815 -0.011576
S 1.378139 1.726473 -0.182917
Mo 3.030502 0.032298 -0.001780
S 4.274228 -0.075712 -1.690657
Mo -3.049844 0.004885 0.004631
S -4.167420 -1.769715 0.158625
S -4.287733 1.696555 -0.139684
S 1.512179 -1.890723 0.199703
S -1.398067 -0.082678 -1.751338
S 4.138778 0.216986 1.769229
H 1.464506 -2.309248 -1.084512

E= -3391.224732
S 1.406464 -0.109248 1.713841
Mo 0.049361 0.004582 -0.026226
S -1.413530 -1.709948 -0.093577
Mo -3.070244 -0.033866 0.004398
S -4.308582 -0.005078 -1.691352
Mo 3.086834 -0.005548 0.003826
S 4.223349 1.763444 0.081479
S 4.302391 -1.719555 -0.034373
S -1.548246 1.881618 0.110820

S 1.443567 -0.011612 -1.743612
S -4.184343 -0.137976 1.778585
H -1.507081 2.236646 -1.192924

[Mo3S8H]+ VIII
E= -3391.133835
S -0.628881 -1.065136 -1.492706
Mo 0.768771 -0.652479 0.262146
S 2.578686 -2.185469 0.438640
Mo 2.732012 -0.149020 -0.608193
S 2.723140 0.966446 1.371264
S 3.043013 2.266837 -0.154510
Mo -2.076416 0.251928 -0.231779
S -3.773804 -1.379755 -0.087625
S -4.156863 0.155715 1.243550
S -2.568063 1.888554 -1.441556
S -0.729164 0.817730 1.490845
H -3.632426 -0.357104 2.382281

E= -3391.211807
S -1.914811 2.015317 0.465358
Mo 0.104085 1.931578 0.561003
S 0.188144 -0.112341 -1.689239
Mo 1.448349 -0.246738 0.285728
S 2.448285 -2.491123 0.179768
S 3.514580 -1.011071 -0.653279
Mo -1.360246 -0.214660 0.095384
S -3.643243 -0.859516 0.275022
S -2.559704 -2.309061 -0.729817
S -0.215055 -0.904269 1.860074
S 1.853326 1.937095 0.890601
H -2.816261 -1.988039 -2.020375

[Mo3S8H]+ IX
E= -3391.191053
S 2.629639 0.443778 -1.255542
Mo 0.764962 1.124056 -0.013876
S -0.862517 1.398720 1.580405
Mo -1.735083 0.023341 0.020026
S -3.518825 -1.534149 -0.214037
S -3.960602 0.381685 0.329558
Mo 1.826347 -1.448365 -0.351433
S -0.361900 -1.949869 -0.413187
S 2.610851 -1.863759 1.540730
S 1.667153 3.140296 0.590687
S -0.486106 0.536646 1.845836
H 0.555429 3.787055 1.003649

E= -3391.184399
S -1.888507 0.210504 1.764377
Mo -0.317737 0.434247 -0.076415
S 1.173329 0.237233 1.745632
Mo 2.560967 -0.156574 0.034018
S 4.429824 -1.504446 0.226252
S 4.763194 0.494990 -0.040603
Mo -3.100753 -0.763313 0.179676
S -1.820456 -0.720773 -1.622277
S -5.037612 -0.016586 -0.093683
S -0.474514 2.639418 -0.631854
S 1.177101 -0.254612 -1.738082
H -1.141744 3.025204 0.478103

[Mo3S8H]+ X
E= -3391.254481
S 2.107510 2.855942 1.220078
Mo 1.178705 1.319949 -0.214353
S -0.681594 1.868392 -1.427641
Mo -1.308045 0.129228 -0.081659
S -3.740436 0.312542 -0.390182
S -3.110290 0.228223 1.499417
S 2.444061 -0.281607 -1.285213
Mo 0.912277 -1.527416 -0.051791
S 1.374397 -3.301518 0.988896
S 0.389634 0.064139 1.591990
S -1.002116 -1.763857 -1.295762
H 2.617992 3.569954 0.182416

E= -3391.254413
S 1.900952 2.975016 1.230155
Mo 1.085861 1.386530 -0.216561
S -0.787190 1.831948 -1.446652
Mo -1.311153 0.070152 -0.085437

S -3.745937 0.138890 -0.386976
S -3.111142 0.045871 1.501559
S 2.459548 -0.150248 -1.265060
Mo 1.005852 -1.483102 -0.038765
S 1.588926 -3.258617 0.935037
S 0.388728 0.068646 1.596451
S -0.892381 -1.814622 -1.282843
H 2.392440 3.719500 0.205336

[Mo3S8H]+ XI
E= -3391.243299
S 0.628354 3.484297 0.903509
Mo 0.673309 1.676360 -0.151489
S -1.119112 1.394605 -1.600939
Mo -1.286793 -0.316908 -0.168432
S -3.326222 -1.473538 -0.267462
S -3.471486 0.074160 1.120089
S 2.598556 0.592421 -0.969396
Mo 1.475464 -1.132640 0.076572
S 2.540472 -2.699935 0.983772
S 0.221561 0.073082 1.604369
S -0.131733 -2.003376 -1.277437
H -3.249367 -0.593565 2.276578

E= -3391.241633
S 1.150815 3.318674 1.154657
Mo 0.801422 1.569676 0.032610
S -0.956708 1.766698 -1.415843
Mo -1.379433 -0.141211 -0.212367
S -3.670498 0.222767 -0.160959
S -3.261769 -1.280955 1.218708
S 2.550808 0.461315 -1.036448
Mo 1.386557 -1.279727 -0.083725
S 2.557412 -2.804991 0.759932
S 0.192931 -0.100690 1.571997
S -0.465814 -1.824992 -1.428993
H -3.513756 -2.372213 0.457451

[Mo3S8H]+ XII
E= -3391.258378
S 1.514312 3.290900 0.886758
Mo 1.069970 1.494422 -0.099439
S -0.814552 1.798834 -1.366449
Mo -1.264728 -0.009773 -0.052664
S -3.813067 -0.008119 -0.454958
S -3.018201 -0.011528 1.469902
S 2.651409 0.027018 -1.030540
Mo 1.117191 -1.464304 -0.083003
S 1.632747 -3.253839 0.881596
S 0.438215 0.007333 1.618033
S -0.758306 -1.820930 -1.349162
H -4.063103 -1.329211 -0.608423

E= -3391.252214
S 0.968369 3.476940 0.830019
Mo 0.681288 1.607421 -0.093021
S -1.222652 1.541701 -1.380327
Mo -1.345671 -0.291508 -0.042662
S -3.853373 -0.703196 -0.463388
S -3.108078 -0.425039 1.460316
S 2.401939 0.551964 -1.232285
Mo 1.485127 -1.208928 -0.042122
S 2.901038 -2.513868 0.790046
S 0.363955 0.013896 1.611995
S -0.361434 -2.094716 -1.118880
H -3.893028 -2.056305 -0.492189

[Mo3S8]+ I
E= -3390.650077
S 2.385028 0.000024 -1.418471
Mo 1.145408 1.380393 -0.083124
S 2.301358 2.788952 0.960374
Mo 1.145427 -1.380401 -0.083133
S 0.129275 -0.000023 1.529389
S 2.301514 -2.788865 0.960333
S -0.854009 1.949176 -1.134246
Mo -1.609795 0.000028 -0.167134
S -3.271974 -0.000033 1.509529
S -3.924918 -0.000067 -0.397596
S -0.854004 -1.949215 -1.134158

E= -3390.647867

S 2.470721 0.006406 -1.123502
Mo 1.055395 1.483655 -0.031455
S 1.950459 3.194433 0.793873
Mo 1.064448 -1.478840 -0.030866
S 0.311185 0.000348 1.603097
S 1.971389 -3.183555 0.793923
S -0.799994 1.853991 -1.336420
Mo -1.425221 -0.003762 -0.143731
S -3.128695 -0.004943 1.517366
S -3.808037 -0.009044 -0.373729
S -0.790410 -1.860401 -1.333722

[Mo3S8]+ II
E= -3390.629858
S -1.255918 1.691201 -0.002003
Mo -3.012283 0.080348 -0.000156
S -4.202262 0.081619 -1.729760
Mo 0.012633 -0.160645 0.000468
S 1.437818 -0.416500 -1.736372
Mo 3.006698 0.031661 -0.000181
S 3.536135 2.061392 -0.003333
S -1.498184 -1.791569 0.003633
S 1.438117 -0.410860 1.737816
S -4.204521 0.087435 1.727903
S 4.730310 -1.175050 0.001774

E= -3390.626541
S -1.420119 -0.000296 1.732771
Mo -3.072581 -0.000051 0.000038
S -4.250573 1.742891 0.000389
Mo -0.037031 0.000067 -0.000201
S 1.487089 1.736393 0.000077
Mo 2.989390 -0.000023 0.000016
S 4.341455 -0.000330 1.670142
S -1.420405 0.000185 -1.732960
S 1.486968 -1.736344 -0.000471
S -4.251055 -1.742674 -0.000047
S 4.342222 0.000195 -1.669516

[Mo3S8]+ III
E= -3390.590806
S -2.641314 -2.541344 -0.492844
Mo -2.639453 -0.510243 0.064768
S -1.745844 0.982917 -1.476509
S 0.583835 2.974692 -0.011463
Mo 0.132229 0.940389 -0.156238
S 4.138236 -2.065572 0.188503
S -0.964298 -0.104973 1.637167
S -4.572148 0.116628 0.619772
S 2.083289 0.440781 1.684237
Mo 3.116694 -0.266415 -0.082952
S 1.518387 -0.232924 -1.691003

E= -3390.600803
S -3.544861 -2.380601 0.000371
Mo -2.689598 -0.401083 -0.000059
S -1.332176 -0.007686 -1.731177
S 0.225437 2.781531 0.000035
Mo 0.238438 0.708613 0.000166
S 4.586451 -1.722966 -0.000245
S -1.332961 -0.006468 1.731359
S -4.483718 0.795445 -0.000818
S 1.876168 0.007431 1.724473
Mo 3.262216 -0.107513 0.000081
S 1.876639 0.008267 -1.724492

[Mo3S8]+ IV
E= -3390.643957
S 0.207918 0.055495 -1.595362
Mo 1.028588 -1.433200 0.016376
S 1.881579 -0.125313 1.670303
Mo 1.034242 1.385074 0.154461
S 2.491740 2.733188 -0.521102
S -0.964853 2.166809 0.913011
Mo -1.780603 0.217366 -0.142103
S -3.464452 0.780979 -1.228123
S -2.164754 -1.254605 1.607080
S -1.257289 -2.314018 0.054216
S 2.529265 -2.486792 -0.975449

E= -3390.618112
S -1.500292 0.000015 1.771970

Mo -1.123614 -1.430099 -0.000069
S -1.500187 0.000026 -1.772111
Mo -1.123511 1.430150 -0.000062
S -2.510328 2.998944 0.000160
S 1.005476 2.179916 0.000129
Mo 1.974401 -0.000028 0.000013
S 3.363295 -0.000068 1.632939
S 3.362990 -0.000066 -1.633066
S 1.005360 -2.179916 0.000127
S -2.510415 -2.998909 0.000162

[Mo3S8]+ V
E= -3390.616456
Mo 2.136082 -0.090679 0.000014
S 3.770103 -0.005800 1.622063
S 4.318324 1.196196 -0.000152
S 0.934516 -2.008526 0.000281
S 0.543495 1.542748 -0.000268
S 3.770140 -0.006275 -1.622024
Mo -0.663768 -0.377181 0.000014
S -2.088049 -0.526182 -1.782353
Mo -3.438342 -0.122379 0.000046
S -3.999752 1.882879 -0.000233
S -2.087953 -0.525660 1.782492

E= -3390.593336
Mo -2.269640 -0.051085 0.095613
S -3.944281 -1.368577 0.938654
S -4.476942 -0.552800 -0.935113
S -0.847932 1.347178 1.315668
S -0.585149 -1.044925 -1.169448
S -3.903013 1.422134 -0.685647
Mo 0.768006 0.201627 0.167668
S 2.140775 1.660524 -0.869922
Mo 3.524004 0.126892 0.147619
S 4.217570 -1.245446 -1.261901
S 2.090253 -0.946353 1.589095

[Mo3S8]+ VI
E= -3390.609552
S 1.818449 1.782911 -0.547233
Mo 0.515422 0.000045 0.349763
S 0.864605 0.000397 2.396600
Mo 3.104535 -0.000159 -0.804895
S 4.567171 0.000237 0.681940
S 1.818578 -1.783181 -0.546405
S -1.234857 1.738954 -0.012718
Mo -2.601822 0.000018 -0.098218
S -4.556325 -0.000034 -1.287281
S -4.715434 -0.000054 0.780193
S -1.234790 -1.738878 -0.012553

E= -3390.595915
S 1.897467 1.760196 -0.231884
Mo 0.317808 -0.000067 0.526654
S 0.474260 -0.000304 2.598818
Mo 3.124632 0.000093 -0.752764
S 5.111195 0.000025 -0.081548
S 1.897485 -1.760139 -0.232283
S -1.239565 1.770562 -0.021608
Mo -2.508845 0.000002 -0.142981
S -4.492279 0.000206 -1.539748
S -4.859694 -0.000032 0.412694
S -1.239553 -1.770589 0.021207

[Mo3S8]+ VII
E= -3390.612778
S 2.501328 1.444708 0.675319
Mo 1.732813 -0.641261 0.111140
S 0.448934 -0.022019 -1.766338
S 3.057952 -2.173067 -0.465694
Mo 0.376829 1.853684 -0.317434
S -1.382748 1.667376 1.291939
S -2.127277 1.829450 -0.632302
S 0.245235 -1.388012 1.692617
Mo -1.039907 -0.393790 0.064658
S -2.423702 -1.964118 -1.116825
S -3.127776 -1.543231 0.693076

E= -3390.611976
S 2.529011 1.415733 0.662532
Mo 1.718426 -0.664665 0.119558

S 0.444924 -0.026171 -1.759989
S 2.997509 -2.227192 -0.477327
Mo 0.413635 1.855433 -0.320554
S -1.354038 1.692338 1.286203
S -2.087076 1.849102 -0.643432
S 0.219757 -1.372292 1.708337
Mo -1.048200 -0.384233 0.068623
S -2.441681 -1.952075 -1.114343
S -3.153542 -1.496596 0.685499

[Mo3S8]+ VIII
E= -3390.582892
S 0.000001 -0.317512 -1.235774
Mo -0.000002 1.634598 0.131203
S -1.992741 1.295233 1.283559
Mo -2.019466 -0.517095 -0.045964
S -4.010990 -1.278085 -0.883260
S -3.216139 -2.334684 0.681487
Mo 2.019469 -0.517092 -0.045964
S 1.992742 1.295238 1.283555
S 3.216144 -2.334679 0.681487
S 4.010992 -1.278080 -0.883261
S -0.000011 3.376487 -1.030891

E= -3390.589851
S 0.000012 -0.323334 -1.244469
Mo -0.000021 1.616483 0.123325
S -1.964787 1.307257 1.303532
Mo -2.030050 -0.520205 -0.030474
S -3.275341 -2.335060 0.653625
S -4.043943 -1.237651 -0.884877
Mo 2.030078 -0.520171 -0.030472
S 1.964792 1.307333 1.303481
S 3.275416 -2.334991 0.653638
S 4.043963 -1.237599 -0.884904
S -0.000131 3.341762 -1.063771

[Mo3S8]+ IX
E= -3390.629859
S -1.255991 1.691226 -0.003004
Mo 0.012626 -0.160579 0.000544
S 1.437758 -0.417196 -1.736193
Mo 3.006715 0.031656 -0.000209
S 4.730205 -1.175228 0.002330
Mo -3.012299 0.080318 -0.000206
S -4.203971 0.088092 1.728230
S -4.202848 0.080898 -1.729426
S 1.438151 -0.409982 1.737995
S -1.498139 -1.791554 0.004011
S 3.536348 2.061333 -0.004283

E= -3390.626541
S 1.419941 -0.002688 1.732804
Mo 0.037019 -0.000377 -0.000293
S -1.487298 -1.736519 -0.002616
Mo -2.989389 0.000084 0.000033
S -4.342123 0.002549 -1.669568
Mo 3.072553 0.000092 0.000196
S 4.250282 1.743210 0.002276
S 4.251293 -1.742348 -0.002103
S -1.486737 1.736221 0.002092
S 1.420557 0.002075 -1.732927
S -4.341397 -0.001974 1.670208

[Mo3S8]+ X
E= -3390.627328
S 1.484202 -1.730379 0.002610
Mo -0.041023 -0.000154 -0.000163
S -1.424790 0.002839 1.733073
Mo -3.076549 0.000057 0.000026
S -4.254864 1.742772 -0.002499
Mo 2.998478 0.000016 0.000003
S 1.484003 1.730233 -0.003281
S 4.351436 0.002931 1.671487
S 4.352632 -0.002630 -1.670600
S -1.424980 -0.003002 -1.733233
S -4.255016 -1.742554 0.002794

E= -3390.626542
S 1.486060 -1.736464 0.001185
Mo -0.036865 -0.000119 -0.000113
S -1.421099 0.001252 1.732761

Mo -3.072742 0.000042 0.000013
S -4.250453 1.743166 -0.001080
Mo 2.989913 0.000019 -0.000016
S 1.485894 1.736359 -0.001485
S 4.342442 0.001357 1.669309
S 4.343179 -0.001139 -1.668782
S -1.421240 -0.001384 -1.732874
S -4.250588 -1.742990 0.001269

[Mo3S8]+ XI
E= -3390.615437
S -1.451415 -0.513335 -1.671828
Mo -0.091568 -0.000555 0.000463
S 1.392635 -1.747066 0.341829
Mo 2.766931 0.000111 0.000273
S 4.905805 -0.483813 -0.881311
S 4.906725 0.484585 0.879723
Mo -3.106534 0.000155 -0.000180
S -4.280000 1.699840 -0.405104
S -4.281732 -1.698513 0.404031
S -1.451917 0.512442 1.672318
S 1.391724 1.746619 -0.341117

E= -3390.624597
S -1.520064 -0.000027 -1.733743
Mo -0.132486 -0.000289 0.000954
S 1.386625 -1.719402 0.000378
Mo 2.916560 -0.000285 -0.000413
S 4.982635 0.000386 -1.019899
S 4.982423 0.000779 1.019200
Mo -3.167205 0.000142 -0.000271
S -4.345187 1.743536 -0.000965
S -4.345909 -1.742762 -0.000774
S -1.521495 -0.000166 1.734615
S 1.386692 1.718790 0.000480

[Mo3S7]+ I
E= -2992.323942
S -0.220287 0.080463 -1.868942
Mo -1.705794 -0.136115 -0.041787
S 0.576273 -1.960771 1.702496
S -1.273836 -2.253727 0.796654
Mo 1.245456 -0.980937 -0.299411
S 3.242620 -1.123773 -0.886663
Mo 0.555023 1.633296 -0.133589
S -1.201075 1.687632 1.267591
S 2.275450 2.067383 0.989988
S -3.647691 0.147651 -0.754808

E= -2992.348386
S -0.012155 -0.036647 1.687282
Mo -1.626665 0.445415 0.048850
S 0.715885 1.623367 -1.575783
S -1.062877 2.482019 -0.845101
Mo 1.723815 0.380147 0.117395
S 3.445220 1.266988 0.917151
Mo -0.051069 -1.879640 0.114472
S -1.831186 -1.498818 -1.218461
S 2.033777 -1.718145 -0.814156
S -3.409627 0.648189 1.112184

[Mo3S7]+ II
E= -2992.318492
S 0.365070 -0.000051 1.851409
Mo -0.945580 -0.000051 0.019880
S -2.415472 1.811983 -0.038453
Mo -3.710074 0.000055 -0.089013
Mo 1.879244 -0.000016 0.136544
S 3.509395 -1.620973 0.288430
S 4.216868 0.000055 -0.829098
S 3.509292 1.621031 0.288448
S 0.518545 -0.000039 -1.699206
S -2.415622 -1.811975 -0.038481

E= -2992.324238
S 0.394113 -0.000044 1.849711
Mo -0.963723 -0.000037 0.015267
S -2.366437 1.805838 -0.032303
Mo -3.722762 0.000041 -0.086082
Mo 1.866580 -0.000018 0.130155
S 3.492889 -1.624251 0.287382
S 4.220677 0.000055 -0.809738

S 3.492783 1.624301 0.287413
S 0.534772 -0.000025 -1.705913
S -2.366545 -1.805835 -0.032323

[Mo3S7]+ III
E= -2992.320595
S 2.203571 1.809293 -0.306668
Mo 3.365543 -0.000026 -0.706991
S 2.203641 -1.809319 -0.306415
Mo 0.788898 0.000027 0.455908
S -0.902223 -1.740624 -0.033611
Mo -2.266736 0.000001 -0.158361
S -4.411374 -0.000104 0.647805
S -4.182578 0.000002 -1.410465
S 1.036036 0.000081 2.517619
S -0.902299 1.740666 -0.033474

E= -2992.320606
S 2.202429 1.809849 -0.305539
Mo 3.363395 0.000000 -0.709201
S 2.202461 -1.809852 -0.305477
Mo 0.791132 0.000004 0.457752
S -0.901809 -1.739931 -0.035153
Mo -2.266298 -0.000001 -0.162351
S -4.407806 -0.000040 0.653294
S -4.189891 0.000015 -1.405121
S 1.039856 0.000007 2.519293
S -0.901841 1.739943 -0.035074

[Mo3S7]+ IV
E= -2992.403450
S 2.083947 -0.000154 -1.416357
Mo 0.887857 -1.421384 -0.074622
S -1.123407 -1.949669 -1.124475
Mo -1.815936 0.000110 -0.061556
S -3.697411 0.000293 0.839836
Mo 0.888096 1.421233 -0.074582
S -1.123057 1.949823 -1.124433
S 2.029067 2.864067 0.918728
S -0.092807 0.000010 1.541090
S 2.028622 -2.864264 0.918855

E= -2992.397932
S -1.548597 1.591931 -1.186011
Mo 0.463770 1.640535 -0.049985
S 2.152459 0.545424 -1.186447
Mo 1.188990 -1.221893 -0.049968
S 2.531751 -2.601756 0.781553
Mo -1.652844 -0.418443 -0.049814
S -0.604399 -2.137207 -1.185595
S -3.519111 -0.891156 0.782024
S -0.000081 -0.000396 1.605061
S 0.988197 3.492638 0.782553

[Mo3S7]+ V
E= -2992.340636
S 2.729469 -0.000038 -1.360903
Mo 1.203294 -1.256281 -0.159890
S -0.812777 -2.037398 -1.002193
Mo -1.594404 0.000042 -0.324368
S -3.893307 -0.000010 -0.074030
S -2.788834 0.000016 1.637807
Mo 1.203349 1.256254 -0.159876
S -0.812697 2.037455 -1.002174
S 1.723057 1.927541 1.746181
S 1.722960 -1.927607 1.746165

E= -2992.331395
S 2.682714 0.838972 -0.823302
Mo 1.635408 -1.090614 -0.161569
S -0.163287 -2.145851 -1.265150
Mo -1.233428 -0.372335 -0.399046
S -3.623924 -0.429866 0.110256
S -2.388737 -0.553077 1.674132
Mo 0.564787 1.473711 -0.132438
S -1.249977 1.621146 -1.543920
S 0.347195 2.218451 1.817187
S 1.858253 -1.578022 1.850062

[Mo3S7]+ VI
E= -2992.335159
S 1.793546 1.770380 -0.987505

Mo 1.932801 -0.218428 0.055811
S 0.944966 -1.824928 -1.196423
Mo -0.931638 -0.854691 -0.193443
S -3.224063 -1.093624 -0.863431
S -2.902955 -1.516789 1.047790
Mo -0.442977 1.429088 -0.069895
S -2.235701 2.512478 0.206635
S 0.275407 0.012809 1.744511
S 3.883564 -0.794743 0.593182

E= -2992.334433
S 2.190886 0.443697 1.706752
Mo 0.729162 1.149752 0.071484
S -1.346813 1.768366 0.948328
Mo -2.010792 -0.144622 -0.053112
S -3.804217 -1.317770 0.775679
S -4.093884 -0.351621 -1.003250
Mo 1.992137 -1.327382 0.292578
S 3.625363 -1.365889 -0.993949
S 0.027697 -0.876914 -0.990122
S 1.535889 2.546039 -1.259683

[Mo3S7]+ VII
E= -2992.392782
S -2.313075 1.272368 -0.930864
Mo -0.640286 1.715517 0.510668
S 1.181437 2.073484 -0.773592
Mo 1.222582 -0.111491 -0.039219
S 3.536458 -0.582799 -0.700306
S 3.020049 -1.185650 1.127922
Mo -1.492753 -0.761662 -0.159880
S 0.167996 -1.322468 -1.657094
S -2.883358 -2.272353 0.334156
S -0.319558 -0.193786 1.781911

E= -2992.377159
S -2.478606 1.250367 -0.738070
Mo -0.551603 1.869867 0.391312
S 1.402726 2.051882 -0.767282
Mo 1.188702 -0.125815 -0.075012
S 3.491331 -0.780423 -0.629376
S 2.883456 -1.228536 1.214854
Mo -1.526262 -0.777971 -0.146694
S 0.107688 -1.342081 -1.658059
S -2.693089 -2.451562 0.370817
S -0.379452 -0.035611 1.761938

[Mo3S7]+ VIII
E= -2992.378269
S 1.247735 -0.000172 -1.805429
Mo -0.364051 -0.000073 -0.282643
S -1.781553 -1.793586 -0.552461
Mo -3.138098 0.000014 -0.253612
S -3.772161 0.000157 1.724389
Mo 2.637485 0.000016 0.146953
S 3.804205 -1.745362 0.287857
S 3.804021 1.745535 0.287620
S 0.748936 0.000047 1.632627
S -1.781438 1.793493 -0.552682

E= -2992.360165
S 1.191662 -0.000190 -1.727317
Mo -0.227259 -0.000111 -0.035677
S -1.816550 -1.721049 -0.045030
Mo -3.242741 0.000027 -0.391165
S -4.878454 0.000139 0.901593
Mo 2.805419 0.000015 0.053361
S 3.981179 -1.744041 0.079742
S 3.980691 1.744397 0.079613
S 1.102363 -0.000051 1.736907
S -1.816366 1.720978 -0.045121

[Mo3S7]+ IX
E= -2992.297523
S -1.223678 1.779910 -0.448453
Mo 0.096317 0.000044 -0.209455
S 1.450694 -0.000447 1.587347
Mo 2.920106 0.000020 -0.235241
S 4.104805 -1.726723 -0.085141
Mo -2.781113 -0.000013 -0.014724
S -3.390226 -0.000463 1.991270
S -4.440011 0.000304 -1.305230

S -1.223621 -1.779744 -0.449180
S 4.104347 1.727029 -0.084637

E= -2992.360170
S -1.101079 0.000245 -1.735983
Mo 0.227465 0.000195 0.037875
S 1.815879 1.721047 0.046687
Mo 3.243798 -0.000215 0.390208
S 4.878326 0.000127 -0.903762
Mo -2.805770 0.000028 -0.054082
S -3.981225 1.744286 -0.081723
S -3.980165 -1.744946 -0.081273
S -1.193935 0.000239 1.728232
S 1.815283 -1.721018 0.046069

[Mo3S7]+ X
E= -2992.325387
S -3.528973 -2.031762 0.000312
Mo -2.356384 -0.218412 0.000050
S -3.926954 1.265519 -0.000056
S -0.979698 -0.067732 -1.743566
Mo 0.691399 0.459594 -0.000105
S 2.121685 -0.275925 -1.808662
Mo 3.292712 -0.650128 0.000125
S 2.121806 -0.274962 1.808773
S -0.979534 -0.067342 1.743538
S 0.898886 2.525689 -0.000522

E= -2992.325287
S 3.539493 -2.025688 0.000004

Mo 2.356918 -0.218225 0.000021
S 3.922985 1.271200 0.000149
S 0.979575 -0.073123 1.743098
Mo -0.691267 0.456264 -0.000030
S -2.124520 -0.275190 1.809213
Mo -3.295585 -0.646191 0.000034
S -2.124402 -0.275622 -1.809172
S 0.979765 -0.072944 -1.743145
S -0.894316 2.522765 -0.000213

[Mo3S7]+ XI
E= -2992.345926
Mo -2.841427 -0.325820 0.000871
Mo -0.175652 0.789448 -0.000404
S -1.659078 0.215726 1.785999
S -1.661201 0.216164 -1.785413
Mo 2.822293 -0.143674 -0.000811
S 1.473388 0.031693 -1.736972
S 1.476399 0.037373 1.736773
S 4.096396 -1.804421 0.001046
S -0.135009 2.863779 -0.001250
S -3.079581 -2.400193 0.000720

E= -2992.340382
Mo -3.006410 -0.169306 -0.000279
Mo -0.000011 0.709955 -0.000166
S -1.615668 -0.025966 1.719927
S -1.614640 -0.028813 -1.719935
Mo 3.006365 -0.169345 0.000335
S 1.615585 -0.027641 -1.719896

S 1.614737 -0.027041 1.720026
S 4.280589 -1.823683 0.000746
S 0.000016 2.782231 -0.001272
S -4.280472 -1.823759 0.000693

[Mo3S7]+ XII
E= -2992.371289
S -0.000496 -0.030217 -1.817441
Mo -1.466960 -0.463577 0.008272
S 0.000649 -2.441061 0.285647
S 0.001240 -1.196514 1.931012
Mo 1.467000 -0.462563 0.007751
S 3.356971 -1.038243 -0.706885
Mo -0.000405 1.828087 -0.372813
S -1.753056 1.687964 0.975647
S 1.752737 1.688755 0.975214
S -3.357088 -1.038293 -0.706621

E= -2992.343424
S 0.185947 0.316001 -1.728255
Mo -1.668884 -0.242847 -0.146555
S -0.284051 -2.283713 0.635404
S -1.391458 -1.162322 1.995761
Mo 1.442739 -0.745106 -0.045805
S 3.083662 -1.589987 -1.026516
Mo 0.700554 1.897001 -0.057191
S -1.496745 2.069881 0.455239
S 2.154650 0.861412 1.396581
S -3.497328 -0.597526 -1.073146