

Supporting information

Energetics of Saddling Versus Ruffling in Metalloporphyrins: Unusual Ruffled Dodecasubstituted Porphyrins

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Table S1. Experimental structural data for selected saddled porphyrins: average M-N distances (Å), saddled angles (χ , deg), and α and β carbon displacement (Å) above the N₄ plane, along with respective CCSD codes.

Ligand type	Complex	[M-N] _{ave}	χ _{ave}	(z _{α}) _{ave}	(z _{β}) _{ave}	CCSD code
TPP	Ni[TPP]	1.958	5.7	0.085	0.181	TATLOR
TPP	Cu[TPP]	1.983	7.4	0.201	0.426	UBOJIE
TPP	Zn[TPP]	2.025	7.0	0.242	0.530	SEMPAB
TPP	Pt[TPP]	2.012	8.1	0.095	0.227	CEZKEX01
Cl ₈ TPP	Ni[Cl ₈ TPP]	1.905	24.5	0.368	0.893	MUJRIS
Cl ₈ TPP	Ni[Cl ₈ TPP]	1.907	25.5	0.368	0.899	MUJRIS02
Cl ₈ TPP	Cu[Cl ₈ TPFPFPP]	2.007	18.8	0.292	0.701	LALROF
Cl ₈ TPP	Zn[Cl ₈ TPFPFPP]	2.033	31.0	0.283	0.735	ZALJAX
Br ₈ TPP	Ni[Br ₈ TPFPFPP]	1.903	32.0	0.491	1.175	PAHKOY01
Br ₈ TPP	Ni[Br ₈ TPFPFPP]	1.900	32.0	0.487	1.164	PAHKOY
Br ₈ TPP	Ni[Br ₈ TMP]	1.916	14.3	0.446	0.998	PAHKIS
Br ₈ TPP	Cu[Br ₈ TPFPFPP]	1.971	37.9	0.456	1.120	LATSEE
Br ₈ TPP	Zn[Br ₈ TPFPFPP]	2.040	42.5	0.324	0.888	LALRIZ
I ₈ TPP	NiI ₈ T[P-CF ₃ -P]P	1.914	34.4	0.499	1.200	JUZQEC
I ₈ TPP	Cu[I ₈ TpCF ₃ PP]	1.970	48.5	0.466	1.184	JUZQIG
(CF ₃) ₈ TPP	Ni[(CF ₃) ₈ TPP]	1.885	59.4	0.559	1.433	TAWVOD
DPP	Ni[pFPF ₈ TPFP]P	1.914	24.9	0.429	1.104	TEZXEB
DPP	Ni[DPP]	1.832	34.8	0.398	1.020	XAWROC
DPP	Zn[Ph ₈ TpOHPP]	2.025	20.6	0.243	0.610	ODIPIC
DPP	Zn[DPP]	2.037	39.0	0.367	0.953	XAWRES
DPP	Zn[DPP]	2.018	44.9	0.382	1.015	XAWSAP
Ph ₄ TBP	Cu[Ph ₄ TBP]	1.982	30.0	0.390	0.962	SASVEP
Ph ₄ TBP	Ni[Ph ₄ TBP] ^b	1.915	22.0	0.375	0.895	BAYWOO
Ph ₄ TBP	Ni[Ph ₄ TBP]	1.913	28.8	0.449	1.078	SULDEI
Ph ₄ TBP	Pt[Ph ₄ TBP]	2.011	29.0	0.373	0.921	SEWCUT

^a Abbreviations:

^b One benzo group has a NO₂ group on it.

Table S2. Total energies for the indicated dodecasubstituted metalloporphyrins.

Complex	M		Total bonding energy E (eV)	$E_{\text{sad}} - E_{\text{ruf}}$
DPP	Cu	saddled	-1072.63	0.02
		ruffled	-1072.65	
	Ni	saddled	-1075.39	0.15
		ruffled	-1075.54	
	Pd	saddled	-1073.38	0.00
		ruffled	-1073.38	
	Pt	saddled	-1076.18	0.05
		ruffled	-1076.23	
	Zn	saddled	-1070.88	0.01
		ruffled	-1070.89	
Br ₈ TPP	Cu	saddled	-510.70	-0.65
		ruffled	-510.06	
	Ni	saddled	-513.39	-0.57
		ruffled	-512.81	
	Pd	saddled	-511.38	-0.62
		ruffled	-510.76	
	Pt	saddled	-514.13	-0.58
		ruffled	-513.55	
	Zn	saddled	-509.00	-0.58
		ruffled	-508.42	
Cl ₈ TPP	Cu	saddled	-515.22	-0.47
		ruffled	-514.76	
	Ni	saddled	-517.89	-0.42
		ruffled	-517.47	
	Pd	saddled	-515.92	-0.43
		ruffled	-515.49	
	Pt	saddled	-518.68	-0.39
		ruffled	-518.29	
	Zn	saddled	-513.55	-0.37
		ruffled	-513.18	
(CF ₃) ₈ TPP	Cu	saddled	-667.91	-0.88
		ruffled	-667.02	
	Ni	saddled	-670.71	-0.56
		ruffled	-670.15	
	Pd	saddled	-668.44	-0.91
		ruffled	-667.53	
	Pt	saddled	-671.15	-0.85
		ruffled	-670.30	
	Zn	saddled	-666.04	-1.00
		ruffled	-665.04	
Me ₈ TPP	Cu	saddled	-660.09	-0.40
		ruffled	-659.69	
	Ni	saddled	-662.83	-0.32
		ruffled	-662.51	
	Pd	saddled	-660.84	-0.38
		ruffled	-660.46	

	Pt	saddled	-663.65	-0.36
		ruffled	-663.30	
	Zn	saddled	-658.39	-0.38
		ruffled	-658.01	
A ₄ Br ₈	Cu	saddled	-552.39	0.03
		ruffled	-552.42	
	Ni	saddled	-555.01	0.25
		ruffled	-555.26	
	Pd	saddled	-552.98	0.06
		ruffled	-553.04	
	Pt	saddled	-555.70	0.10
		ruffled	-555.80	
	Zn	saddled	-550.70	-0.01
		ruffled	-550.70	
Ph ₄ Bz ₄	Cu	saddled	-701.40	-0.25
		ruffled	-701.16	
	Ni	saddled	-704.11	-0.15
		ruffled	-703.96	
	Pd	saddled	-702.23	-0.24
		ruffled	-701.99	
	Pt	saddled	-705.06	-0.24
		ruffled	-704.83	
	Zn	saddled	-699.76	-0.26
		ruffled	-699.50	
A ₄ Bz ₄	Cu	saddled	-743.30	-0.03
		ruffled	-743.27	
	Ni	saddled	-746.09	0.02
		ruffled	-746.10	
	Pd	saddled	-744.05	-0.02
		ruffled	-744.03	
	Pt	saddled	-746.86	-0.01
		ruffled	-746.84	
	Zn	saddled	-741.65	-0.10
		ruffled	-741.55	
TPP	Cu	saddled	-528.92	-0.05
		ruffled	-528.87	
	Ni	saddled	-531.53	-0.03
		ruffled	-531.51	
	Pd	saddled	-529.74	-0.03
		ruffled	-529.71	
	Pt	saddled	-532.61	-0.03
		ruffled	-532.58	
	Zn	saddled	-527.33	-0.06
		ruffled	-527.27	
I ₈ TPP	Cu	saddled	-506.14	-0.92
		ruffled	-505.22	
	Ni	saddled	-508.85	-0.81
		ruffled	-508.05	
	Pd	saddled	-506.79	-0.95
		ruffled	-505.84	

	Pt	saddled	-509.52	-0.90
		ruffled	-508.62	
	Zn	saddled	-504.39	-0.93
		ruffled	-503.46	
A ₄ Me ₈	Cu	saddled	-702.16	0.05
		ruffled	-702.21	
	Ni	saddled	-704.86	0.18
		ruffled	-705.04	
	Pd	saddled	-702.86	0.07
		ruffled	-702.93	
	Pt	saddled	-705.65	0.08
		ruffled	-705.74	
	Zn	saddled	-700.50	0.00
		ruffled	-700.50	

Table S3. Total energies and zero-point vibrational energies for MTPP.

M		Total bonding energy E (eV)	$E_{\text{sadd}} - E_{\text{ruff}}$ (eV)^a	Total free energy G (eV)	$G_{\text{sadd}} - G_{\text{ruff}}$ (eV)^a	Zero-point vibrational energy (eV)
Cu	saddled	-528.92	-0.05	-514.91	0.10	15.79
	ruffled	-528.87		-515.01		15.77
Ni	saddled	-531.53	-0.03	-517.43	-0.06	15.83
	ruffled	-531.51		-517.36		15.80
Pd	saddled	-529.74	-0.03	-515.72	-0.15	15.83
	ruffled	-529.71		-515.56		15.81
Pt	saddled	-532.61	-0.03	-518.45	0.13	15.83
	ruffled	-532.58		-518.58		15.82
Zn	saddled	-527.33	-0.06	-513.43	0.08	15.78
	ruffled	-527.27		-513.51		15.74

a Note: The free energy differences between ruffling and saddling complexes, $G_{\text{sadd}} - G_{\text{ruff}}$, showed the same trend than $E_{\text{sadd}} - E_{\text{ruff}}$, namely near zero difference for TPP complexes. We conclude that the ZPE cancels out energy differences between ruff and sadd and therefore will not change the trends and relationships obtained in the ms.

Optimized coordinates

1. Cu(DPP); S = ½ (saddled)

Cu	0.000000000	0.000000000	-0.028556000
C	0.000000000	0.000000000	3.374373000
C	0.000000000	0.000000000	4.863203000
C	0.000000000	0.000000000	7.668017000
C	0.000000000	0.000000000	-3.461024000
C	0.000000000	0.000000000	-4.946103000
C	0.000000000	0.000000000	-7.752763000
C	0.630477000	-1.030738000	6.967325000
C	0.638510000	-1.024024000	5.574024000
C	1.030109000	0.631330000	-7.051572000
C	1.031535000	0.626187000	-5.658710000
C	1.098319000	-0.557109000	-2.783090000
C	1.226196000	-2.971680000	-4.930438000
C	1.226544000	0.159909000	2.708911000
C	1.267667000	-3.738852000	-6.093479000
C	2.209062000	-1.287582000	-3.378390000
C	2.231174000	-2.030137000	-4.653401000
C	2.235179000	2.447540000	4.814023000
C	2.315813000	-3.579635000	-7.003866000
C	2.498051000	0.467476000	3.346347000
C	2.518147000	3.176279000	5.968566000
C	2.660877000	-0.711370000	-1.226116000
C	2.736883000	1.146468000	4.641214000
C	2.798808000	-0.109943000	1.163768000
C	3.193608000	-1.353462000	-2.412004000
C	3.274870000	-1.877154000	-5.577950000
C	3.308342000	2.615888000	6.975294000
C	3.318390000	-2.643509000	-6.741679000
C	3.399898000	-0.430555000	-0.059911000
C	3.477060000	0.241518000	2.402754000
C	3.523892000	0.594405000	5.660607000
C	3.806570000	1.321111000	6.817166000
C	4.421745000	-2.179165000	-2.473313000
C	4.437629000	-3.414395000	-1.805770000
C	4.876533000	-0.302370000	-0.249842000
C	4.925525000	0.341364000	2.697216000
C	5.334947000	0.792451000	-0.998719000
C	5.555666000	-0.702295000	3.391847000
C	5.562982000	-1.784688000	-3.182363000
C	5.568487000	-4.230096000	-1.842136000
C	5.676191000	1.473365000	2.357757000
C	5.808573000	-1.216093000	0.253733000
C	6.696655000	-2.596270000	-3.215905000
C	6.698923000	0.980152000	-1.224735000
C	6.704077000	-3.821845000	-2.545928000
C	6.907538000	-0.628127000	3.724112000

C	7.029760000	1.549323000	2.687133000
C	7.170984000	-1.036187000	0.020244000
C	7.620659000	0.063663000	-0.715426000
C	7.650806000	0.499458000	3.368640000
C	-0.630477000	1.030738000	6.967325000
C	-0.638510000	1.024024000	5.574024000
C	-1.030109000	-0.631330000	-7.051572000
C	-1.031535000	-0.626187000	-5.658710000
C	-1.098319000	0.557109000	-2.783090000
C	-1.226196000	2.971680000	-4.930438000
C	-1.226544000	-0.159909000	2.708911000
C	-1.267667000	3.738852000	-6.093479000
C	-2.209062000	1.287582000	-3.378390000
C	-2.231174000	2.030137000	-4.653401000
C	-2.235179000	-2.447540000	4.814023000
C	-2.315813000	3.579635000	-7.003866000
C	-2.498051000	-0.467476000	3.346347000
C	-2.518147000	-3.176279000	5.968566000
C	-2.660877000	0.711370000	-1.226116000
C	-2.736883000	-1.146468000	4.641214000
C	-2.798808000	0.109943000	1.163768000
C	-3.193608000	1.353462000	-2.412004000
C	-3.274870000	1.877154000	-5.577950000
C	-3.308342000	-2.615888000	6.975294000
C	-3.318390000	2.643509000	-6.741679000
C	-3.399898000	0.430555000	-0.059911000
C	-3.477060000	-0.241518000	2.402754000
C	-3.523892000	-0.594405000	5.660607000
C	-3.806570000	-1.321111000	6.817166000
C	-4.421745000	2.179165000	-2.473313000
C	-4.437629000	3.414395000	-1.805770000
C	-4.876533000	0.302370000	-0.249842000
C	-4.925525000	-0.341364000	2.697216000
C	-5.334947000	-0.792451000	-0.998719000
C	-5.555666000	0.702295000	3.391847000
C	-5.562982000	1.784688000	-3.182363000
C	-5.568487000	4.230096000	-1.842136000
C	-5.676191000	-1.473365000	2.357757000
C	-5.808573000	1.216093000	0.253733000
C	-6.696655000	2.596270000	-3.215905000
C	-6.698923000	-0.980152000	-1.224735000
C	-6.704077000	3.821845000	-2.545928000
C	-6.907538000	0.628127000	3.724112000
C	-7.029760000	-1.549323000	2.687133000
C	-7.170984000	1.036187000	0.020244000
C	-7.620659000	-0.063663000	-0.715426000
C	-7.650806000	-0.499458000	3.368640000
H	0.000000000	0.000000000	8.757760000
H	0.000000000	0.000000000	-8.842474000
H	0.409935000	-3.097192000	-4.218834000
H	0.478772000	-4.464592000	-6.288918000

H	1.120296000	-1.839565000	7.508481000
H	1.134591000	-1.821227000	5.019921000
H	1.621078000	2.884568000	4.025978000
H	1.833706000	1.114925000	-5.105587000
H	1.835104000	1.127791000	-7.592242000
H	2.121405000	4.185001000	6.080668000
H	2.348732000	-4.179336000	-7.913216000
H	3.532447000	3.183967000	7.877998000
H	3.551389000	-3.726132000	-1.252767000
H	3.906399000	-0.417623000	5.549528000
H	4.045045000	-1.133260000	-5.389073000
H	4.136375000	-2.505512000	-7.448146000
H	4.418286000	0.871474000	7.598644000
H	4.607221000	1.499152000	-1.398878000
H	4.973268000	-1.585534000	3.653911000
H	5.193071000	2.290318000	1.823517000
H	5.456888000	-2.077816000	0.817906000
H	5.561968000	-5.186594000	-1.320160000
H	5.571482000	-0.814716000	-3.676397000
H	7.039542000	1.840286000	-1.800813000
H	7.380726000	-1.451416000	4.258735000
H	7.580484000	-2.265542000	-3.760364000
H	7.590530000	-4.455292000	-2.572182000
H	7.601934000	2.433924000	2.410093000
H	7.883778000	-1.759562000	0.413326000
H	8.687030000	0.202578000	-0.892974000
H	8.708707000	0.561655000	3.622865000
H	-0.409935000	3.097192000	-4.218834000
H	-0.478772000	4.464592000	-6.288918000
H	-1.120296000	1.839565000	7.508481000
H	-1.134591000	1.821227000	5.019921000
H	-1.621078000	-2.884568000	4.025978000
H	-1.833706000	-1.114925000	-5.105587000
H	-1.835104000	-1.127791000	-7.592242000
H	-2.121405000	-4.185001000	6.080668000
H	-2.348732000	4.179336000	-7.913216000
H	-3.532447000	-3.183967000	7.877998000
H	-3.551389000	3.726132000	-1.252767000
H	-3.906399000	0.417623000	5.549528000
H	-4.045045000	1.133260000	-5.389073000
H	-4.136375000	2.505512000	-7.448146000
H	-4.418286000	-0.871474000	7.598644000
H	-4.607221000	-1.499152000	-1.398878000
H	-4.973268000	1.585534000	3.653911000
H	-5.193071000	-2.290318000	1.823517000
H	-5.456888000	2.077816000	0.817906000
H	-5.561968000	5.186594000	-1.320160000
H	-5.571482000	0.814716000	-3.676397000
H	-7.039542000	-1.840286000	-1.800813000
H	-7.380726000	1.451416000	4.258735000
H	-7.580484000	2.265542000	-3.760364000

H	-7.590530000	4.455292000	-2.572182000
H	-7.601934000	-2.433924000	2.410093000
H	-7.883778000	1.759562000	0.413326000
H	-8.687030000	-0.202578000	-0.892974000
H	-8.708707000	-0.561655000	3.622865000
N	1.363937000	-0.317995000	-1.448732000
N	1.430729000	-0.119733000	1.375750000
N	-1.363937000	0.317995000	-1.448732000
N	-1.430729000	0.119733000	1.375750000

2. Cu(DPP]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
C	0.135004000	2.534255000	-7.373381000
C	0.135004000	-2.534255000	7.373381000
C	0.136477000	7.373732000	-2.533961000
C	0.136477000	-7.373732000	2.533961000
C	0.221979000	6.189608000	1.889749000
C	0.221979000	-6.189608000	-1.889749000
C	0.222910000	1.890163000	6.189010000
C	0.222910000	-1.890163000	-6.189010000
C	0.352565000	0.594016000	-4.135836000
C	0.352565000	-0.594016000	4.135836000
C	0.352770000	4.135972000	-0.593929000
C	0.352770000	-4.135972000	0.593929000
C	0.501773000	0.997947000	-2.744855000
C	0.501773000	-0.997947000	2.744855000
C	0.502028000	2.744990000	-0.997833000
C	0.502028000	-2.744990000	0.997833000
C	0.753000000	1.298501000	-5.373897000
C	0.753000000	-1.298501000	5.373897000
C	0.753588000	5.373908000	-1.298344000
C	0.753588000	-5.373908000	1.298344000
C	0.886530000	2.269975000	-2.269931000
C	0.886530000	-2.269975000	2.269931000
C	1.210151000	4.058199000	-4.058259000
C	1.210151000	-4.058199000	4.058259000
C	1.474247000	2.583200000	-7.766822000
C	1.474247000	-2.583200000	7.766822000
C	1.475940000	7.766387000	-2.583265000
C	1.475940000	-7.766387000	2.583265000
C	1.733220000	3.140319000	-3.140722000
C	1.733220000	-3.140319000	3.140722000
C	2.061793000	4.838220000	-4.838635000
C	2.061793000	-4.838220000	4.838635000
C	2.091742000	1.335173000	-5.787303000
C	2.091742000	-1.335173000	5.787303000
C	2.092569000	5.786529000	-1.335343000
C	2.092569000	-5.786529000	1.335343000
C	2.450742000	1.975771000	-6.972481000

C	2.450742000	-1.975771000	6.972481000
C	2.452106000	6.971500000	-1.976008000
C	2.452106000	-6.971500000	1.976008000
C	3.123467000	3.016519000	-3.017691000
C	3.123467000	-3.016519000	3.017691000
C	3.447646000	4.709960000	-4.711159000
C	3.447646000	-4.709960000	4.711159000
C	3.978512000	3.797092000	-3.798681000
C	3.978512000	-3.797092000	3.798681000
C	-0.135004000	2.534255000	7.373381000
C	-0.135004000	-2.534255000	-7.373381000
C	-0.136477000	7.373732000	2.533961000
C	-0.136477000	-7.373732000	-2.533961000
C	-0.221979000	6.189608000	-1.889749000
C	-0.221979000	-6.189608000	1.889749000
C	-0.222910000	1.890163000	-6.189010000
C	-0.222910000	-1.890163000	6.189010000
C	-0.352565000	0.594016000	4.135836000
C	-0.352565000	-0.594016000	-4.135836000
C	-0.352770000	4.135972000	0.593929000
C	-0.352770000	-4.135972000	-0.593929000
C	-0.501773000	0.997947000	2.744855000
C	-0.501773000	-0.997947000	-2.744855000
C	-0.502028000	2.744990000	0.997833000
C	-0.502028000	-2.744990000	-0.997833000
C	-0.753000000	1.298501000	5.373897000
C	-0.753000000	-1.298501000	-5.373897000
C	-0.753588000	5.373908000	1.298344000
C	-0.753588000	-5.373908000	-1.298344000
C	-0.886530000	2.269975000	2.269931000
C	-0.886530000	-2.269975000	-2.269931000
C	-1.210151000	4.058199000	4.058259000
C	-1.210151000	-4.058199000	-4.058259000
C	-1.474247000	2.583200000	7.766822000
C	-1.474247000	-2.583200000	-7.766822000
C	-1.475940000	7.766387000	2.583265000
C	-1.475940000	-7.766387000	-2.583265000
C	-1.733220000	3.140319000	3.140722000
C	-1.733220000	-3.140319000	-3.140722000
C	-2.061793000	4.838220000	4.838635000
C	-2.061793000	-4.838220000	-4.838635000
C	-2.091742000	1.335173000	5.787303000
C	-2.091742000	-1.335173000	-5.787303000
C	-2.092569000	5.786529000	1.335343000
C	-2.092569000	-5.786529000	-1.335343000
C	-2.450742000	1.975771000	6.972481000
C	-2.450742000	-1.975771000	-6.972481000
C	-2.452106000	6.971500000	1.976008000
C	-2.452106000	-6.971500000	-1.976008000
C	-3.123467000	3.016519000	3.017691000
C	-3.123467000	-3.016519000	-3.017691000

C	-3.447646000	4.709960000	4.711159000
C	-3.447646000	-4.709960000	-4.711159000
C	-3.978512000	3.797092000	3.798681000
C	-3.978512000	-3.797092000	-3.798681000
H	0.130661000	4.156695000	-4.156066000
H	0.130661000	-4.156695000	4.156066000
H	0.632869000	7.992397000	2.995016000
H	0.632869000	-7.992397000	-2.995016000
H	0.634563000	2.995514000	7.991627000
H	0.634563000	-2.995514000	-7.991627000
H	1.265861000	5.880241000	1.845812000
H	1.265861000	-5.880241000	-1.845812000
H	1.266600000	1.846608000	5.878922000
H	1.266600000	-1.846608000	-5.878922000
H	1.640608000	5.548326000	-5.548408000
H	1.640608000	-5.548326000	5.548408000
H	1.756069000	3.088122000	-8.690672000
H	1.756069000	-3.088122000	8.690672000
H	1.758190000	8.690048000	-3.088275000
H	1.758190000	-8.690048000	3.088275000
H	2.853098000	0.871075000	-5.161314000
H	2.853098000	-0.871075000	5.161314000
H	2.853611000	5.160126000	-0.871328000
H	2.853611000	-5.160126000	0.871328000
H	3.497249000	2.005681000	-7.273747000
H	3.497249000	-2.005681000	7.273747000
H	3.498757000	7.272188000	-2.006093000
H	3.498757000	-7.272188000	2.006093000
H	3.530016000	2.300879000	-2.302317000
H	3.530016000	-2.300879000	2.302317000
H	4.111179000	5.321289000	-5.322727000
H	4.111179000	-5.321289000	5.322727000
H	5.057838000	3.690148000	-3.692301000
H	5.057838000	-3.690148000	3.692301000
H	-0.130661000	4.156695000	4.156066000
H	-0.130661000	-4.156695000	-4.156066000
H	-0.632869000	7.992397000	-2.995016000
H	-0.632869000	-7.992397000	2.995016000
H	-0.634563000	2.995514000	-7.991627000
H	-0.634563000	-2.995514000	7.991627000
H	-1.265861000	5.880241000	-1.845812000
H	-1.265861000	-5.880241000	1.845812000
H	-1.266600000	1.846608000	-5.878922000
H	-1.266600000	-1.846608000	5.878922000
H	-1.640608000	5.548326000	5.548408000
H	-1.640608000	-5.548326000	-5.548408000
H	-1.756069000	3.088122000	8.690672000
H	-1.756069000	-3.088122000	-8.690672000
H	-1.758190000	8.690048000	3.088275000
H	-1.758190000	-8.690048000	-3.088275000
H	-2.853098000	0.871075000	5.161314000

H	-2.853098000	-0.871075000	-5.161314000
H	-2.853611000	5.160126000	0.871328000
H	-2.853611000	-5.160126000	-0.871328000
H	-3.497249000	2.005681000	7.273747000
H	-3.497249000	-2.005681000	-7.273747000
H	-3.498757000	7.272188000	2.006093000
H	-3.498757000	-7.272188000	-2.006093000
H	-3.530016000	2.300879000	2.302317000
H	-3.530016000	-2.300879000	-2.302317000
H	-4.111179000	5.321289000	5.322727000
H	-4.111179000	-5.321289000	-5.322727000
H	-5.057838000	3.690148000	3.692301000
H	-5.057838000	-3.690148000	-3.692301000
N	0.000000000	0.000000000	1.946175000
N	0.000000000	0.000000000	-1.946175000
N	0.000000000	1.946347000	0.000000000
N	0.000000000	-1.946347000	0.000000000

3. Ni(DPP]; S = 0 (saddled)

Ni	0.000000000	0.000000000	-0.028280000
C	0.000000000	0.000000000	3.349456000
C	0.000000000	0.000000000	4.837384000
C	0.000000000	0.000000000	7.642445000
C	0.000000000	0.000000000	-3.419385000
C	0.000000000	0.000000000	-4.904378000
C	0.000000000	0.000000000	-7.711004000
C	0.728538000	-0.963939000	6.941612000
C	0.735410000	-0.956887000	5.548242000
C	0.971946000	-3.847597000	-5.964831000
C	0.996485000	-3.057964000	-4.816747000
C	1.036364000	-0.635360000	-2.726024000
C	1.077035000	0.547320000	-7.009743000
C	1.077856000	0.542592000	-5.616679000
C	1.192613000	0.252597000	2.665956000
C	1.984250000	2.643426000	4.661582000
C	2.027321000	-3.791868000	-6.879213000
C	2.076534000	-2.197093000	-4.557850000
C	2.111416000	-1.426820000	-3.301487000
C	2.180471000	3.443301000	5.786166000
C	2.447399000	0.643777000	3.279763000
C	2.599448000	-0.799260000	-1.174399000
C	2.623026000	1.396921000	4.541356000
C	2.765559000	-0.023224000	1.128514000
C	3.018428000	3.010095000	6.816889000
C	3.097026000	-1.500930000	-2.338187000
C	3.103602000	-2.935987000	-6.636040000
C	3.126167000	-2.146602000	-5.487164000
C	3.367980000	-0.443572000	-0.057453000
C	3.431814000	0.414407000	2.343153000

C	3.456064000	0.972050000	5.584927000
C	3.651843000	1.770193000	6.712086000
C	4.280664000	-3.548486000	-1.589561000
C	4.294747000	-2.371187000	-2.355277000
C	4.842948000	-0.356072000	-0.270101000
C	4.877841000	0.590137000	2.606700000
C	5.312968000	0.653961000	-1.123688000
C	5.382813000	-4.402897000	-1.574527000
C	5.438981000	-2.072924000	-3.105305000
C	5.549874000	-0.350520000	3.401767000
C	5.590911000	1.694964000	2.125111000
C	5.763390000	-1.232810000	0.313445000
C	6.520631000	-4.091513000	-2.323050000
C	6.544466000	-2.923133000	-3.087820000
C	6.677379000	0.794661000	-1.377006000
C	6.903409000	-0.201135000	3.700114000
C	6.946064000	1.846119000	2.420130000
C	7.126655000	-1.100079000	0.053597000
C	7.588149000	-0.084898000	-0.788565000
C	7.607303000	0.899339000	3.206815000
C	-0.728538000	0.963939000	6.941612000
C	-0.735410000	0.956887000	5.548242000
C	-0.971946000	3.847597000	-5.964831000
C	-0.996485000	3.057964000	-4.816747000
C	-1.036364000	0.635360000	-2.726024000
C	-1.077035000	-0.547320000	-7.009743000
C	-1.077856000	-0.542592000	-5.616679000
C	-1.192613000	-0.252597000	2.665956000
C	-1.984250000	-2.643426000	4.661582000
C	-2.027321000	3.791868000	-6.879213000
C	-2.076534000	2.197093000	-4.557850000
C	-2.111416000	1.426820000	-3.301487000
C	-2.180471000	-3.443301000	5.786166000
C	-2.447399000	-0.643777000	3.279763000
C	-2.599448000	0.799260000	-1.174399000
C	-2.623026000	-1.396921000	4.541356000
C	-2.765559000	0.023224000	1.128514000
C	-3.018428000	-3.010095000	6.816889000
C	-3.097026000	1.500930000	-2.338187000
C	-3.103602000	2.935987000	-6.636040000
C	-3.126167000	2.146602000	-5.487164000
C	-3.367980000	0.443572000	-0.057453000
C	-3.431814000	-0.414407000	2.343153000
C	-3.456064000	-0.972050000	5.584927000
C	-3.651843000	-1.770193000	6.712086000
C	-4.280664000	3.548486000	-1.589561000
C	-4.294747000	2.371187000	-2.355277000
C	-4.842948000	0.356072000	-0.270101000
C	-4.877841000	-0.590137000	2.606700000
C	-5.312968000	-0.653961000	-1.123688000
C	-5.382813000	4.402897000	-1.574527000

C	-5.438981000	2.072924000	-3.105305000
C	-5.549874000	0.350520000	3.401767000
C	-5.590911000	-1.694964000	2.125111000
C	-5.763390000	1.232810000	0.313445000
C	-6.520631000	4.091513000	-2.323050000
C	-6.544466000	2.923133000	-3.087820000
C	-6.677379000	-0.794661000	-1.377006000
C	-6.903409000	0.201135000	3.700114000
C	-6.946064000	-1.846119000	2.420130000
C	-7.126655000	1.100079000	0.053597000
C	-7.588149000	0.084898000	-0.788565000
C	-7.607303000	-0.899339000	3.206815000
H	0.000000000	0.000000000	8.732191000
H	0.000000000	0.000000000	-8.800746000
H	0.125837000	-4.509822000	-6.145773000
H	0.174763000	-3.102715000	-4.101843000
H	1.294951000	-1.721158000	7.482721000
H	1.306525000	-1.702011000	4.994064000
H	1.331852000	2.980369000	3.855440000
H	1.678137000	4.407739000	5.856601000
H	1.916407000	0.965904000	-5.063549000
H	1.919047000	0.978002000	-7.550407000
H	2.008479000	-4.408816000	-7.777356000
H	3.174072000	3.633467000	7.697212000
H	3.393326000	-3.783821000	-1.001677000
H	3.927488000	-2.877670000	-7.346674000
H	3.940734000	0.001194000	5.519685000
H	3.953418000	-1.462592000	-5.316019000
H	4.300538000	1.418348000	7.513640000
H	4.593324000	1.331239000	-1.584551000
H	4.999827000	-1.217590000	3.766859000
H	5.076419000	2.430887000	1.508612000
H	5.352342000	-5.313800000	-0.977292000
H	5.401980000	-2.028909000	0.962014000
H	5.474905000	-1.144063000	-3.671470000
H	7.027472000	1.589093000	-2.035782000
H	7.384965000	-4.755170000	-2.309382000
H	7.408935000	-0.945640000	4.314582000
H	7.431111000	-2.666397000	-3.666499000
H	7.488054000	2.708329000	2.033470000
H	7.831072000	-1.794141000	0.509752000
H	8.655058000	0.017158000	-0.986575000
H	8.666307000	1.019780000	3.433941000
H	-0.125837000	4.509822000	-6.145773000
H	-0.174763000	3.102715000	-4.101843000
H	-1.294951000	1.721158000	7.482721000
H	-1.306525000	1.702011000	4.994064000
H	-1.331852000	-2.980369000	3.855440000
H	-1.678137000	-4.407739000	5.856601000
H	-1.916407000	-0.965904000	-5.063549000
H	-1.919047000	-0.978002000	-7.550407000

H	-2.008479000	4.408816000	-7.777356000
H	-3.174072000	-3.633467000	7.697212000
H	-3.393326000	3.783821000	-1.001677000
H	-3.927488000	2.877670000	-7.346674000
H	-3.940734000	-0.001194000	5.519685000
H	-3.953418000	1.462592000	-5.316019000
H	-4.300538000	-1.418348000	7.513640000
H	-4.593324000	-1.331239000	-1.584551000
H	-4.999827000	1.217590000	3.766859000
H	-5.076419000	-2.430887000	1.508612000
H	-5.352342000	5.313800000	-0.977292000
H	-5.401980000	2.028909000	0.962014000
H	-5.474905000	1.144063000	-3.671470000
H	-7.027472000	-1.589093000	-2.035782000
H	-7.384965000	4.755170000	-2.309382000
H	-7.408935000	0.945640000	4.314582000
H	-7.431111000	2.666397000	-3.666499000
H	-7.488054000	-2.708329000	2.033470000
H	-7.831072000	1.794141000	0.509752000
H	-8.655058000	-0.017158000	-0.986575000
H	-8.666307000	-1.019780000	3.433941000
N	1.299597000	-0.387443000	-1.386460000
N	1.391040000	-0.053869000	1.332568000
N	-1.299597000	0.387443000	-1.386460000
N	-1.391040000	0.053869000	1.332568000

4. Ni(DPP]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
C	0.017322000	1.837068000	-6.153098000
C	0.017322000	-1.837068000	6.153098000
C	0.020054000	6.153926000	-1.836966000
C	0.020054000	-6.153926000	1.836966000
C	0.417461000	0.550813000	-4.050930000
C	0.417461000	-0.550813000	4.050930000
C	0.417789000	4.051140000	-0.550628000
C	0.417789000	-4.051140000	0.550628000
C	0.473178000	2.442304000	-7.324192000
C	0.473178000	-2.442304000	7.324192000
C	0.477381000	7.324405000	-2.442316000
C	0.477381000	-7.324405000	2.442316000
C	0.599662000	0.942686000	-2.663669000
C	0.599662000	-0.942686000	2.663669000
C	0.599999000	2.663815000	-0.942442000
C	0.599999000	-2.663815000	0.942442000
C	0.914667000	1.208141000	-5.277816000
C	0.914667000	-1.208141000	5.277816000
C	0.916225000	5.277809000	-1.207520000
C	0.916225000	-5.277809000	1.207520000
C	1.047848000	2.188826000	-2.188691000

C	1.047848000	-2.188826000	2.188691000
C	1.515251000	3.958347000	-3.957899000
C	1.515251000	-3.958347000	3.957899000
C	1.832649000	2.415125000	-7.643699000
C	1.832649000	-2.415125000	7.643699000
C	1.837153000	7.642534000	-2.414699000
C	1.837153000	-7.642534000	2.414699000
C	1.964826000	3.021015000	-3.021013000
C	1.964826000	-3.021015000	3.021013000
C	2.274694000	1.169571000	-5.616633000
C	2.274694000	-1.169571000	5.616633000
C	2.276579000	5.615376000	-1.168371000
C	2.276579000	-5.615376000	1.168371000
C	2.427726000	4.703224000	-4.702861000
C	2.427726000	-4.703224000	4.702861000
C	2.731307000	1.770997000	-6.788521000
C	2.731307000	-1.770997000	6.788521000
C	2.734654000	6.786642000	-1.769912000
C	2.734654000	-6.786642000	1.769912000
C	3.342771000	2.841605000	-2.842487000
C	3.342771000	-2.841605000	2.842487000
C	3.801234000	4.519849000	-4.520306000
C	3.801234000	-4.519849000	4.520306000
C	4.258543000	3.587032000	-3.588165000
C	4.258543000	-3.587032000	3.588165000
C	-0.017322000	1.837068000	6.153098000
C	-0.017322000	-1.837068000	-6.153098000
C	-0.020054000	6.153926000	1.836966000
C	-0.020054000	-6.153926000	-1.836966000
C	-0.417461000	0.550813000	4.050930000
C	-0.417461000	-0.550813000	-4.050930000
C	-0.417789000	4.051140000	0.550628000
C	-0.417789000	-4.051140000	-0.550628000
C	-0.473178000	2.442304000	7.324192000
C	-0.473178000	-2.442304000	-7.324192000
C	-0.477381000	7.324405000	2.442316000
C	-0.477381000	-7.324405000	-2.442316000
C	-0.599662000	0.942686000	2.663669000
C	-0.599662000	-0.942686000	-2.663669000
C	-0.599999000	2.663815000	0.942442000
C	-0.599999000	-2.663815000	-0.942442000
C	-0.914667000	1.208141000	5.277816000
C	-0.914667000	-1.208141000	-5.277816000
C	-0.916225000	5.277809000	1.207520000
C	-0.916225000	-5.277809000	-1.207520000
C	-1.047848000	2.188826000	2.188691000
C	-1.047848000	-2.188826000	-2.188691000
C	-1.515251000	3.958347000	3.957899000
C	-1.515251000	-3.958347000	-3.957899000
C	-1.832649000	2.415125000	7.643699000
C	-1.832649000	-2.415125000	-7.643699000

C	-1.837153000	7.642534000	2.414699000
C	-1.837153000	-7.642534000	-2.414699000
C	-1.964826000	3.021015000	3.021013000
C	-1.964826000	-3.021015000	-3.021013000
C	-2.274694000	1.169571000	5.616633000
C	-2.274694000	-1.169571000	-5.616633000
C	-2.276579000	5.615376000	1.168371000
C	-2.276579000	-5.615376000	-1.168371000
C	-2.427726000	4.703224000	4.702861000
C	-2.427726000	-4.703224000	-4.702861000
C	-2.731307000	1.770997000	6.788521000
C	-2.731307000	-1.770997000	-6.788521000
C	-2.734654000	6.786642000	1.769912000
C	-2.734654000	-6.786642000	-1.769912000
C	-3.342771000	2.841605000	2.842487000
C	-3.342771000	-2.841605000	-2.842487000
C	-3.801234000	4.519849000	4.520306000
C	-3.801234000	-4.519849000	-4.520306000
C	-4.258543000	3.587032000	3.588165000
C	-4.258543000	-3.587032000	-3.588165000
H	0.230822000	7.990402000	2.934258000
H	0.230822000	-7.990402000	-2.934258000
H	0.236012000	2.933668000	7.989604000
H	0.236012000	-2.933668000	-7.989604000
H	0.445196000	4.099364000	-4.098353000
H	0.445196000	-4.099364000	4.098353000
H	1.039937000	5.902556000	1.853496000
H	1.039937000	-5.902556000	-1.853496000
H	1.042454000	1.853063000	5.900731000
H	1.042454000	-1.853063000	-5.900731000
H	2.063895000	5.429093000	-5.428237000
H	2.063895000	-5.429093000	5.428237000
H	2.190638000	2.890197000	-8.556936000
H	2.190638000	-2.890197000	8.556936000
H	2.196241000	8.555258000	-2.889969000
H	2.196241000	-8.555258000	2.889969000
H	2.975109000	0.677119000	-4.942910000
H	2.975109000	-0.677119000	4.942910000
H	2.976128000	4.941056000	-0.675510000
H	2.976128000	-4.941056000	0.675510000
H	3.691141000	2.110732000	-2.112089000
H	3.691141000	-2.110732000	2.112089000
H	3.792878000	1.742103000	-7.031373000
H	3.792878000	-1.742103000	7.031373000
H	3.796478000	7.028421000	-1.740703000
H	3.796478000	-7.028421000	1.740703000
H	4.512625000	5.103720000	-5.104277000
H	4.512625000	-5.103720000	5.104277000
H	5.327704000	3.437368000	-3.439063000
H	5.327704000	-3.437368000	3.439063000
H	-0.230822000	7.990402000	-2.934258000

H	-0.230822000	-7.990402000	2.934258000
H	-0.236012000	2.933668000	-7.989604000
H	-0.236012000	-2.933668000	7.989604000
H	-0.445196000	4.099364000	4.098353000
H	-0.445196000	-4.099364000	-4.098353000
H	-1.039937000	5.902556000	-1.853496000
H	-1.039937000	-5.902556000	1.853496000
H	-1.042454000	1.853063000	-5.900731000
H	-1.042454000	-1.853063000	5.900731000
H	-2.063895000	5.429093000	5.428237000
H	-2.063895000	-5.429093000	-5.428237000
H	-2.190638000	2.890197000	8.556936000
H	-2.190638000	-2.890197000	-8.556936000
H	-2.196241000	8.555258000	2.889969000
H	-2.196241000	-8.555258000	-2.889969000
H	-2.975109000	0.677119000	4.942910000
H	-2.975109000	-0.677119000	-4.942910000
H	-2.976128000	4.941056000	0.675510000
H	-2.976128000	-4.941056000	-0.675510000
H	-3.691141000	2.110732000	2.112089000
H	-3.691141000	-2.110732000	-2.112089000
H	-3.792878000	1.742103000	7.031373000
H	-3.792878000	-1.742103000	-7.031373000
H	-3.796478000	7.028421000	1.740703000
H	-3.796478000	-7.028421000	-1.740703000
H	-4.512625000	5.103720000	5.104277000
H	-4.512625000	-5.103720000	-5.104277000
H	-5.327704000	3.437368000	3.439063000
H	-5.327704000	-3.437368000	-3.439063000
N	0.000000000	0.000000000	1.859497000
N	0.000000000	0.000000000	-1.859497000
N	0.000000000	1.859623000	0.000000000
N	0.000000000	-1.859623000	0.000000000

5. Pd(DPP]; S = 0 (saddled)

Pd	0.000000000	0.000000000	-0.029914000
C	0.000000000	0.000000000	3.390036000
C	0.000000000	0.000000000	4.879458000
C	0.000000000	0.000000000	7.682987000
C	0.000000000	0.000000000	-3.470765000
C	0.000000000	0.000000000	-4.957715000
C	0.000000000	0.000000000	-7.762842000
C	0.597460000	-1.050258000	6.982423000
C	0.605186000	-1.044023000	5.589209000
C	0.989248000	0.693600000	-7.061872000
C	0.990955000	0.688518000	-5.668890000
C	1.117388000	-0.529995000	-2.804953000
C	1.232950000	0.128673000	2.733064000
C	1.375044000	-2.911480000	-5.007680000
C	1.469147000	-3.651671000	-6.185291000

C	2.256631000	-1.208644000	-3.411951000
C	2.319455000	-1.916760000	-4.706569000
C	2.324768000	2.349806000	4.883172000
C	2.510296000	-3.411370000	-7.085797000
C	2.514222000	0.391287000	3.372543000
C	2.645205000	3.045833000	6.048172000
C	2.688631000	-0.689143000	-1.236740000
C	2.780482000	1.036640000	4.679835000
C	2.809664000	-0.156348000	1.177748000
C	3.238617000	-1.275047000	-2.444822000
C	3.356649000	-1.682408000	-5.621240000
C	3.409360000	-0.440929000	-0.054469000
C	3.428048000	2.440047000	7.034150000
C	3.452749000	-2.421460000	-6.799435000
C	3.488287000	0.152760000	2.428261000
C	3.560872000	0.438812000	5.678370000
C	3.881308000	1.132901000	6.845008000
C	4.487523000	-2.067898000	-2.536606000
C	4.525495000	-3.338020000	-1.939702000
C	4.888198000	-0.292089000	-0.225659000
C	4.937372000	0.188948000	2.739674000
C	5.342217000	0.855262000	-0.893128000
C	5.526111000	-0.919213000	3.367702000
C	5.623340000	-1.610141000	-3.215328000
C	5.674260000	-4.125788000	-2.012603000
C	5.723233000	1.321095000	2.495517000
C	5.823036000	-1.231395000	0.221051000
C	6.706397000	1.067616000	-1.096206000
C	6.774632000	-2.394206000	-3.285642000
C	6.804987000	-3.654445000	-2.684031000
C	6.873462000	-0.907385000	3.725251000
C	7.072569000	1.334759000	2.850567000
C	7.185693000	-1.025859000	0.011062000
C	7.631655000	0.125091000	-0.644117000
C	7.653026000	0.221473000	3.463462000
C	-0.597460000	1.050258000	6.982423000
C	-0.605186000	1.044023000	5.589209000
C	-0.989248000	-0.693600000	-7.061872000
C	-0.990955000	-0.688518000	-5.668890000
C	-1.117388000	0.529995000	-2.804953000
C	-1.232950000	-0.128673000	2.733064000
C	-1.375044000	2.911480000	-5.007680000
C	-1.469147000	3.651671000	-6.185291000
C	-2.256631000	1.208644000	-3.411951000
C	-2.319455000	1.916760000	-4.706569000
C	-2.324768000	-2.349806000	4.883172000
C	-2.510296000	3.411370000	-7.085797000
C	-2.514222000	-0.391287000	3.372543000
C	-2.645205000	-3.045833000	6.048172000
C	-2.688631000	0.689143000	-1.236740000
C	-2.780482000	-1.036640000	4.679835000

C	-2.809664000	0.156348000	1.177748000
C	-3.238617000	1.275047000	-2.444822000
C	-3.356649000	1.682408000	-5.621240000
C	-3.409360000	0.440929000	-0.054469000
C	-3.428048000	-2.440047000	7.034150000
C	-3.452749000	2.421460000	-6.799435000
C	-3.488287000	-0.152760000	2.428261000
C	-3.560872000	-0.438812000	5.678370000
C	-3.881308000	-1.132901000	6.845008000
C	-4.487523000	2.067898000	-2.536606000
C	-4.525495000	3.338020000	-1.939702000
C	-4.888198000	0.292089000	-0.225659000
C	-4.937372000	-0.188948000	2.739674000
C	-5.342217000	-0.855262000	-0.893128000
C	-5.526111000	0.919213000	3.367702000
C	-5.623340000	1.610141000	-3.215328000
C	-5.674260000	4.125788000	-2.012603000
C	-5.723233000	-1.321095000	2.495517000
C	-5.823036000	1.231395000	0.221051000
C	-6.706397000	-1.067616000	-1.096206000
C	-6.774632000	2.394206000	-3.285642000
C	-6.804987000	3.654445000	-2.684031000
C	-6.873462000	0.907385000	3.725251000
C	-7.072569000	-1.334759000	2.850567000
C	-7.185693000	1.025859000	0.011062000
C	-7.631655000	-0.125091000	-0.644117000
C	-7.653026000	-0.221473000	3.463462000
H	0.000000000	0.000000000	8.772686000
H	0.000000000	0.000000000	-8.852545000
H	0.564875000	-3.101319000	-4.303323000
H	0.727145000	-4.420296000	-6.399514000
H	1.061808000	-1.873984000	7.523481000
H	1.076096000	-1.856094000	5.034879000
H	1.717567000	2.822861000	4.110739000
H	1.762277000	1.224257000	-5.115417000
H	1.762405000	1.238271000	-7.602580000
H	2.283762000	4.064802000	6.184436000
H	2.584419000	-3.990477000	-8.006013000
H	3.642350000	-3.699698000	-1.412767000
H	3.681762000	2.982882000	7.944524000
H	3.910702000	-0.582021000	5.541183000
H	4.080277000	-0.898146000	-5.411339000
H	4.264918000	-2.220589000	-7.497487000
H	4.487712000	0.648274000	7.609553000
H	4.611719000	1.582430000	-1.249118000
H	4.913817000	-1.800178000	3.560733000
H	5.271160000	2.188197000	2.016099000
H	5.474257000	-2.132148000	0.722296000
H	5.612183000	-0.615319000	-3.657331000
H	5.685207000	-5.110135000	-1.545334000
H	7.044170000	1.967689000	-1.609456000

H	7.314598000	-1.779445000	4.207303000
H	7.653934000	-2.015353000	-3.805552000
H	7.673089000	2.220753000	2.647962000
H	7.705187000	-4.266338000	-2.739009000
H	7.901138000	-1.769171000	0.359451000
H	8.698112000	0.283788000	-0.803777000
H	8.707520000	0.235555000	3.738308000
H	-0.564875000	3.101319000	-4.303323000
H	-0.727145000	4.420296000	-6.399514000
H	-1.061808000	1.873984000	7.523481000
H	-1.076096000	1.856094000	5.034879000
H	-1.717567000	-2.822861000	4.110739000
H	-1.762277000	-1.224257000	-5.115417000
H	-1.762405000	-1.238271000	-7.602580000
H	-2.283762000	-4.064802000	6.184436000
H	-2.584419000	3.990477000	-8.006013000
H	-3.642350000	3.699698000	-1.412767000
H	-3.681762000	-2.982882000	7.944524000
H	-3.910702000	0.582021000	5.541183000
H	-4.080277000	0.898146000	-5.411339000
H	-4.264918000	2.220589000	-7.497487000
H	-4.487712000	-0.648274000	7.609553000
H	-4.611719000	-1.582430000	-1.249118000
H	-4.913817000	1.800178000	3.560733000
H	-5.271160000	-2.188197000	2.016099000
H	-5.474257000	2.132148000	0.722296000
H	-5.612183000	0.615319000	-3.657331000
H	-5.685207000	5.110135000	-1.545334000
H	-7.044170000	-1.967689000	-1.609456000
H	-7.314598000	1.779445000	4.207303000
H	-7.653934000	2.015353000	-3.805552000
H	-7.673089000	-2.220753000	2.647962000
H	-7.705187000	4.266338000	-2.739009000
H	-7.901138000	1.769171000	0.359451000
H	-8.698112000	-0.283788000	-0.803777000
H	-8.707520000	-0.235555000	3.738308000
N	1.380853000	-0.324821000	-1.462109000
N	1.440849000	-0.140624000	1.395415000
N	-1.380853000	0.324821000	-1.462109000
N	-1.440849000	0.140624000	1.395415000

6. Pd(DPP]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
C	0.086085000	7.381684000	2.582926000
C	0.086085000	-7.381684000	-2.582926000
C	0.090871000	2.586024000	7.379151000
C	0.090871000	-2.586024000	-7.379151000
C	0.309355000	0.616746000	-4.176534000
C	0.309355000	-0.616746000	4.176534000

C	0.309816000	4.176645000	-0.616513000
C	0.309816000	-4.176645000	0.616513000
C	0.378508000	6.190340000	1.918641000
C	0.378508000	-6.190340000	-1.918641000
C	0.381683000	1.919962000	6.188403000
C	0.381683000	-1.919962000	-6.188403000
C	0.442984000	1.031634000	-2.786496000
C	0.442984000	-1.031634000	2.786496000
C	0.443293000	2.786629000	-1.031504000
C	0.443293000	-2.786629000	1.031504000
C	0.643049000	1.350130000	-5.419310000
C	0.643049000	-1.350130000	5.419310000
C	0.644999000	5.419793000	-1.348623000
C	0.644999000	-5.419793000	1.348623000
C	0.786408000	2.314605000	-2.314516000
C	0.786408000	-2.314605000	2.314516000
C	1.022975000	4.112201000	-4.110842000
C	1.022975000	-4.112201000	4.110842000
C	1.229510000	2.678941000	-7.824507000
C	1.229510000	-2.678941000	7.824507000
C	1.234708000	7.826111000	-2.673989000
C	1.234708000	-7.826111000	2.673989000
C	1.589079000	3.207082000	-3.206861000
C	1.589079000	-3.207082000	3.206861000
C	1.837473000	4.912291000	-4.910415000
C	1.837473000	-4.912291000	4.910415000
C	1.962233000	1.430063000	-5.885032000
C	1.962233000	-1.430063000	5.885032000
C	1.964646000	5.884592000	-1.426638000
C	1.964646000	-5.884592000	1.426638000
C	2.254344000	2.093128000	-7.076312000
C	2.254344000	-2.093128000	7.076312000
C	2.258361000	7.076404000	-2.088037000
C	2.258361000	-7.076404000	2.088037000
C	2.984322000	3.115772000	-3.116122000
C	2.984322000	-3.115772000	3.116122000
C	3.228520000	4.816767000	-4.815396000
C	3.228520000	-4.816767000	4.815396000
C	3.802126000	3.916580000	-3.916298000
C	3.802126000	-3.916580000	3.916298000
C	-0.086085000	7.381684000	-2.582926000
C	-0.086085000	-7.381684000	2.582926000
C	-0.090871000	2.586024000	-7.379151000
C	-0.090871000	-2.586024000	7.379151000
C	-0.309355000	0.616746000	4.176534000
C	-0.309355000	-0.616746000	-4.176534000
C	-0.309816000	4.176645000	0.616513000
C	-0.309816000	-4.176645000	-0.616513000
C	-0.378508000	6.190340000	-1.918641000
C	-0.378508000	-6.190340000	1.918641000
C	-0.381683000	1.919962000	-6.188403000

C	-0.381683000	-1.919962000	6.188403000
C	-0.442984000	1.031634000	2.786496000
C	-0.442984000	-1.031634000	-2.786496000
C	-0.443293000	2.786629000	1.031504000
C	-0.443293000	-2.786629000	-1.031504000
C	-0.643049000	1.350130000	5.419310000
C	-0.643049000	-1.350130000	-5.419310000
C	-0.644999000	5.419793000	1.348623000
C	-0.644999000	-5.419793000	-1.348623000
C	-0.786408000	2.314605000	2.314516000
C	-0.786408000	-2.314605000	-2.314516000
C	-1.022975000	4.112201000	4.110842000
C	-1.022975000	-4.112201000	-4.110842000
C	-1.229510000	2.678941000	7.824507000
C	-1.229510000	-2.678941000	-7.824507000
C	-1.234708000	7.826111000	2.673989000
C	-1.234708000	-7.826111000	-2.673989000
C	-1.589079000	3.207082000	3.206861000
C	-1.589079000	-3.207082000	-3.206861000
C	-1.837473000	4.912291000	4.910415000
C	-1.837473000	-4.912291000	-4.910415000
C	-1.962233000	1.430063000	5.885032000
C	-1.962233000	-1.430063000	-5.885032000
C	-1.964646000	5.884592000	1.426638000
C	-1.964646000	-5.884592000	-1.426638000
C	-2.254344000	2.093128000	7.076312000
C	-2.254344000	-2.093128000	-7.076312000
C	-2.258361000	7.076404000	2.088037000
C	-2.258361000	-7.076404000	-2.088037000
C	-2.984322000	3.115772000	3.116122000
C	-2.984322000	-3.115772000	-3.116122000
C	-3.228520000	4.816767000	4.815396000
C	-3.228520000	-4.816767000	-4.815396000
C	-3.802126000	3.916580000	3.916298000
C	-3.802126000	-3.916580000	-3.916298000
H	0.060423000	4.185112000	4.183400000
H	0.060423000	-4.185112000	-4.183400000
H	0.892138000	7.965274000	3.026710000
H	0.892138000	-7.965274000	-3.026710000
H	0.897824000	3.029753000	7.961539000
H	0.897824000	-3.029753000	-7.961539000
H	1.383150000	5.612361000	-5.609618000
H	1.383150000	-5.612361000	5.609618000
H	1.407470000	5.839959000	1.842268000
H	1.407470000	-5.839959000	-1.842268000
H	1.410308000	1.842186000	5.837294000
H	1.410308000	-1.842186000	-5.837294000
H	1.459270000	3.200859000	-8.753301000
H	1.459270000	-3.200859000	8.753301000
H	1.465735000	8.755395000	-3.194484000
H	1.465735000	-8.755395000	3.194484000

H	2.761279000	0.982396000	-5.295124000
H	2.761279000	-0.982396000	5.295124000
H	2.762764000	5.293545000	-0.978811000
H	2.762764000	-5.293545000	0.978811000
H	3.286543000	2.156955000	-7.418843000
H	3.286543000	-2.156955000	7.418843000
H	3.290882000	7.418227000	-2.150396000
H	3.290882000	-7.418227000	2.150396000
H	3.424052000	2.409684000	-2.410861000
H	3.424052000	-2.409684000	2.410861000
H	3.862803000	5.443806000	-5.441938000
H	3.862803000	-5.443806000	5.441938000
H	4.885883000	3.835180000	-3.835257000
H	4.885883000	-3.835180000	3.835257000
H	-0.060423000	4.185112000	-4.183400000
H	-0.060423000	-4.185112000	4.183400000
H	-0.892138000	7.965274000	-3.026710000
H	-0.892138000	-7.965274000	3.026710000
H	-0.897824000	3.029753000	-7.961539000
H	-0.897824000	-3.029753000	7.961539000
H	-1.383150000	5.612361000	5.609618000
H	-1.383150000	-5.612361000	-5.609618000
H	-1.407470000	5.839959000	-1.842268000
H	-1.407470000	-5.839959000	1.842268000
H	-1.410308000	1.842186000	-5.837294000
H	-1.410308000	-1.842186000	5.837294000
H	-1.459270000	3.200859000	8.753301000
H	-1.459270000	-3.200859000	-8.753301000
H	-1.465735000	8.755395000	3.194484000
H	-1.465735000	-8.755395000	-3.194484000
H	-2.761279000	0.982396000	5.295124000
H	-2.761279000	-0.982396000	-5.295124000
H	-2.762764000	5.293545000	0.978811000
H	-2.762764000	-5.293545000	-0.978811000
H	-3.286543000	2.156955000	7.418843000
H	-3.286543000	-2.156955000	-7.418843000
H	-3.290882000	7.418227000	2.150396000
H	-3.290882000	-7.418227000	-2.150396000
H	-3.424052000	2.409684000	2.410861000
H	-3.424052000	-2.409684000	-2.410861000
H	-3.862803000	5.443806000	5.441938000
H	-3.862803000	-5.443806000	-5.441938000
H	-4.885883000	3.835180000	3.835257000
H	-4.885883000	-3.835180000	-3.835257000
N	0.000000000	0.000000000	1.990182000
N	0.000000000	0.000000000	-1.990182000
N	0.000000000	1.990359000	0.000000000
N	0.000000000	-1.990359000	0.000000000

7. Pt(DPP]; S = 0 (saddled)

Pt	0.000000000	0.000000000	-0.030573000
C	0.000000000	0.000000000	3.397325000
C	0.000000000	0.000000000	4.887768000
C	0.000000000	0.000000000	7.690670000
C	0.000000000	0.000000000	-3.474396000
C	0.000000000	0.000000000	-4.962725000
C	0.000000000	0.000000000	-7.767307000
C	0.562150000	-1.069576000	6.990229000
C	0.569245000	-1.064057000	5.596977000
C	0.956602000	0.737914000	-7.066411000
C	0.958414000	0.733021000	-5.673313000
C	1.127038000	-0.512487000	-2.813242000
C	1.234669000	0.114564000	2.742910000
C	1.475195000	-2.861093000	-5.050433000
C	1.603943000	-3.583457000	-6.235942000
C	2.284582000	-1.145962000	-3.429750000
C	2.375194000	-1.830344000	-4.735890000
C	2.400462000	2.261976000	4.940471000
C	2.519990000	0.331744000	3.385787000
C	2.636002000	-3.288689000	-7.130653000
C	2.703038000	-0.666029000	-1.243808000
C	2.755962000	2.923446000	6.115499000
C	2.809852000	-0.181087000	1.182847000
C	2.811891000	0.939739000	4.705531000
C	3.267057000	-1.204645000	-2.464768000
C	3.403954000	-1.541748000	-5.644416000
C	3.413414000	-0.438342000	-0.053346000
C	3.488502000	0.081548000	2.440139000
C	3.530400000	2.273329000	7.079623000
C	3.534465000	-2.262590000	-6.830551000
C	3.584212000	0.297069000	5.682363000
C	3.939722000	0.956637000	6.858820000
C	4.537184000	-1.959254000	-2.585155000
C	4.604363000	-3.257012000	-2.054781000
C	4.893283000	-0.267553000	-0.208507000
C	4.934671000	0.048443000	2.766319000
C	5.337172000	0.924528000	-0.799300000
C	5.477070000	-1.121133000	3.320521000
C	5.662026000	-1.439404000	-3.236479000
C	5.757702000	1.170611000	2.621202000
C	5.772768000	-4.011187000	-2.163229000
C	5.836393000	-1.223413000	0.182000000
C	6.700088000	1.163209000	-0.983083000
C	6.817100000	-1.178209000	3.700171000
C	6.832645000	-2.190036000	-3.342419000
C	6.893051000	-3.478002000	-2.805191000
C	7.099957000	1.115368000	2.998595000
C	7.197646000	-0.990362000	-0.007218000
C	7.633714000	0.204143000	-0.586729000

C	7.635042000	-0.057946000	3.535976000
C	-0.562150000	1.069576000	6.990229000
C	-0.569245000	1.064057000	5.596977000
C	-0.956602000	-0.737914000	-7.066411000
C	-0.958414000	-0.733021000	-5.673313000
C	-1.127038000	0.512487000	-2.813242000
C	-1.234669000	-0.114564000	2.742910000
C	-1.475195000	2.861093000	-5.050433000
C	-1.603943000	3.583457000	-6.235942000
C	-2.284582000	1.145962000	-3.429750000
C	-2.375194000	1.830344000	-4.735890000
C	-2.400462000	-2.261976000	4.940471000
C	-2.519990000	-0.331744000	3.385787000
C	-2.636002000	3.288689000	-7.130653000
C	-2.703038000	0.666029000	-1.243808000
C	-2.755962000	-2.923446000	6.115499000
C	-2.809852000	0.181087000	1.182847000
C	-2.811891000	-0.939739000	4.705531000
C	-3.267057000	1.204645000	-2.464768000
C	-3.403954000	1.541748000	-5.644416000
C	-3.413414000	0.438342000	-0.053346000
C	-3.488502000	-0.081548000	2.440139000
C	-3.530400000	-2.273329000	7.079623000
C	-3.534465000	2.262590000	-6.830551000
C	-3.584212000	-0.297069000	5.682363000
C	-3.939722000	-0.956637000	6.858820000
C	-4.537184000	1.959254000	-2.585155000
C	-4.604363000	3.257012000	-2.054781000
C	-4.893283000	0.267553000	-0.208507000
C	-4.934671000	-0.048443000	2.766319000
C	-5.337172000	-0.924528000	-0.799300000
C	-5.477070000	1.121133000	3.320521000
C	-5.662026000	1.439404000	-3.236479000
C	-5.757702000	-1.170611000	2.621202000
C	-5.772768000	4.011187000	-2.163229000
C	-5.836393000	1.223413000	0.182000000
C	-6.700088000	-1.163209000	-0.983083000
C	-6.817100000	1.178209000	3.700171000
C	-6.832645000	2.190036000	-3.342419000
C	-6.893051000	3.478002000	-2.805191000
C	-7.099957000	-1.115368000	2.998595000
C	-7.197646000	0.990362000	-0.007218000
C	-7.633714000	-0.204143000	-0.586729000
C	-7.635042000	0.057946000	3.535976000
H	0.000000000	0.000000000	8.780365000
H	0.000000000	0.000000000	-8.857017000
H	0.672344000	-3.093106000	-4.350364000
H	0.896122000	-4.380765000	-6.460826000
H	0.999382000	-1.907984000	7.531341000
H	1.013098000	-1.891270000	5.042630000
H	1.704382000	1.316932000	-7.607166000

H	1.704887000	1.302853000	-5.119707000
H	1.800565000	2.769661000	4.184551000
H	2.428485000	3.950251000	6.276604000
H	2.737231000	-3.853867000	-8.056977000
H	3.728745000	-3.666748000	-1.551004000
H	3.811688000	2.789293000	7.997504000
H	3.902335000	-0.730338000	5.518681000
H	4.094027000	-0.730835000	-5.422350000
H	4.339283000	-2.019544000	-7.523683000
H	4.539669000	0.437833000	7.605779000
H	4.600248000	1.665575000	-1.110743000
H	4.833357000	-1.992649000	3.441237000
H	5.340302000	2.084825000	2.201816000
H	5.495859000	-2.157744000	0.623671000
H	5.625526000	-0.424653000	-3.629150000
H	5.807096000	-5.017694000	-1.747108000
H	7.030017000	2.097319000	-1.437186000
H	7.222399000	-2.096602000	4.124145000
H	7.703263000	-1.763824000	-3.839706000
H	7.730381000	1.994853000	2.873368000
H	7.808421000	-4.063747000	-2.887847000
H	7.919513000	-1.746440000	0.297672000
H	8.683974000	-0.097178000	3.829084000
H	8.699020000	0.384039000	-0.730927000
H	-0.672344000	3.093106000	-4.350364000
H	-0.896122000	4.380765000	-6.460826000
H	-0.999382000	1.907984000	7.531341000
H	-1.013098000	1.891270000	5.042630000
H	-1.704382000	-1.316932000	-7.607166000
H	-1.704887000	-1.302853000	-5.119707000
H	-1.800565000	-2.769661000	4.184551000
H	-2.428485000	-3.950251000	6.276604000
H	-2.737231000	3.853867000	-8.056977000
H	-3.728745000	3.666748000	-1.551004000
H	-3.811688000	-2.789293000	7.997504000
H	-3.902335000	0.730338000	5.518681000
H	-4.094027000	0.730835000	-5.422350000
H	-4.339283000	2.019544000	-7.523683000
H	-4.539669000	-0.437833000	7.605779000
H	-4.600248000	-1.665575000	-1.110743000
H	-4.833357000	1.992649000	3.441237000
H	-5.340302000	-2.084825000	2.201816000
H	-5.495859000	2.157744000	0.623671000
H	-5.625526000	0.424653000	-3.629150000
H	-5.807096000	5.017694000	-1.747108000
H	-7.030017000	-2.097319000	-1.437186000
H	-7.222399000	2.096602000	4.124145000
H	-7.703263000	1.763824000	-3.839706000
H	-7.730381000	-1.994853000	2.873368000
H	-7.808421000	4.063747000	-2.887847000
H	-7.919513000	1.746440000	0.297672000

H	-8.683974000	0.097178000	3.829084000
H	-8.699020000	-0.384039000	-0.730927000
N	1.380790000	-0.335862000	-1.461152000
N	1.438253000	-0.131099000	1.395991000
N	-1.380790000	0.335862000	-1.461152000
N	-1.438253000	0.131099000	1.395991000

8. Pt(DPP]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
C	0.121349000	2.592330000	7.377856000
C	0.121349000	-2.592330000	-7.377856000
C	0.128746000	7.374092000	2.597150000
C	0.128746000	-7.374092000	-2.597150000
C	0.301179000	4.180208000	-0.620308000
C	0.301179000	-4.180208000	0.620308000
C	0.302009000	0.619932000	-4.180294000
C	0.302009000	-0.619932000	4.180294000
C	0.403711000	1.924329000	6.186111000
C	0.403711000	-1.924329000	-6.186111000
C	0.408419000	6.182334000	1.928057000
C	0.408419000	-6.182334000	-1.928057000
C	0.432427000	2.793586000	-1.037833000
C	0.432427000	-2.793586000	1.037833000
C	0.433138000	1.037552000	-2.793669000
C	0.433138000	-1.037552000	2.793669000
C	0.623414000	5.424076000	-1.356913000
C	0.623414000	-5.424076000	1.356913000
C	0.626609000	1.355504000	-5.424086000
C	0.626609000	-1.355504000	5.424086000
C	0.770321000	2.322079000	-2.322174000
C	0.770321000	-2.322079000	2.322174000
C	1.003208000	4.119885000	-4.121168000
C	1.003208000	-4.119885000	4.121168000
C	1.187521000	7.831006000	-2.691813000
C	1.187521000	-7.831006000	2.691813000
C	1.196144000	2.688200000	-7.830976000
C	1.196144000	-2.688200000	7.830976000
C	1.570078000	3.216502000	-3.215926000
C	1.570078000	-3.216502000	3.215926000
C	1.817246000	4.920491000	-4.920769000
C	1.817246000	-4.920491000	4.920769000
C	1.938191000	5.901471000	-1.438269000
C	1.938191000	-5.901471000	1.438269000
C	1.942724000	1.438111000	-5.897660000
C	1.942724000	-1.438111000	5.897660000
C	2.219298000	7.093584000	-2.104599000
C	2.219298000	-7.093584000	2.104599000
C	2.226510000	2.103310000	-7.089731000
C	2.226510000	-2.103310000	7.089731000

C	2.965498000	3.127295000	-3.123931000
C	2.965498000	-3.127295000	3.123931000
C	3.208358000	4.827072000	-4.824632000
C	3.208358000	-4.827072000	4.824632000
C	3.782688000	3.928545000	-3.924303000
C	3.782688000	-3.928545000	3.924303000
C	-0.121349000	2.592330000	-7.377856000
C	-0.121349000	-2.592330000	7.377856000
C	-0.128746000	7.374092000	-2.597150000
C	-0.128746000	-7.374092000	2.597150000
C	-0.301179000	4.180208000	0.620308000
C	-0.301179000	-4.180208000	-0.620308000
C	-0.302009000	0.619932000	4.180294000
C	-0.302009000	-0.619932000	-4.180294000
C	-0.403711000	1.924329000	-6.186111000
C	-0.403711000	-1.924329000	6.186111000
C	-0.408419000	6.182334000	-1.928057000
C	-0.408419000	-6.182334000	1.928057000
C	-0.432427000	2.793586000	1.037833000
C	-0.432427000	-2.793586000	-1.037833000
C	-0.433138000	1.037552000	2.793669000
C	-0.433138000	-1.037552000	-2.793669000
C	-0.623414000	5.424076000	1.356913000
C	-0.623414000	-5.424076000	-1.356913000
C	-0.626609000	1.355504000	5.424086000
C	-0.626609000	-1.355504000	-5.424086000
C	-0.770321000	2.322079000	2.322174000
C	-0.770321000	-2.322079000	-2.322174000
C	-1.003208000	4.119885000	4.121168000
C	-1.003208000	-4.119885000	-4.121168000
C	-1.187521000	7.831006000	2.691813000
C	-1.187521000	-7.831006000	-2.691813000
C	-1.196144000	2.688200000	7.830976000
C	-1.196144000	-2.688200000	-7.830976000
C	-1.570078000	3.216502000	3.215926000
C	-1.570078000	-3.216502000	-3.215926000
C	-1.817246000	4.920491000	4.920769000
C	-1.817246000	-4.920491000	-4.920769000
C	-1.938191000	5.901471000	1.438269000
C	-1.938191000	-5.901471000	-1.438269000
C	-1.942724000	1.438111000	5.897660000
C	-1.942724000	-1.438111000	-5.897660000
C	-2.219298000	7.093584000	2.104599000
C	-2.219298000	-7.093584000	-2.104599000
C	-2.226510000	2.103310000	7.089731000
C	-2.226510000	-2.103310000	-7.089731000
C	-2.965498000	3.127295000	3.123931000
C	-2.965498000	-3.127295000	-3.123931000
C	-3.208358000	4.827072000	4.824632000
C	-3.208358000	-4.827072000	-4.824632000
C	-3.782688000	3.928545000	3.924303000

C	-3.782688000	-3.928545000	-3.924303000
H	0.080227000	4.191229000	4.194693000
H	0.080227000	-4.191229000	-4.194693000
H	0.932563000	3.035254000	7.954922000
H	0.932563000	-3.035254000	-7.954922000
H	0.941100000	7.948156000	3.041935000
H	0.941100000	-7.948156000	-3.041935000
H	1.362485000	5.619340000	-5.620971000
H	1.362485000	-5.619340000	5.620971000
H	1.408695000	8.760541000	-3.216113000
H	1.408695000	-8.760541000	3.216113000
H	1.419349000	3.211634000	-8.760505000
H	1.419349000	-3.211634000	8.760505000
H	1.429880000	1.844482000	5.828463000
H	1.429880000	-1.844482000	-5.828463000
H	1.433620000	5.821657000	1.849180000
H	1.433620000	-5.821657000	-1.849180000
H	2.742564000	5.319636000	-0.989641000
H	2.742564000	-5.319636000	0.989641000
H	2.745967000	0.991333000	-5.312854000
H	2.745967000	-0.991333000	5.312854000
H	3.248326000	7.445199000	-2.169841000
H	3.248326000	-7.445199000	2.169841000
H	3.256504000	2.169539000	-7.438288000
H	3.256504000	-2.169539000	7.438288000
H	3.405223000	2.422377000	-2.417505000
H	3.405223000	-2.422377000	2.417505000
H	3.842193000	5.454446000	-5.451278000
H	3.842193000	-5.454446000	5.451278000
H	4.866532000	3.848864000	-3.842420000
H	4.866532000	-3.848864000	3.842420000
H	-0.080227000	4.191229000	-4.194693000
H	-0.080227000	-4.191229000	4.194693000
H	-0.932563000	3.035254000	-7.954922000
H	-0.932563000	-3.035254000	7.954922000
H	-0.941100000	7.948156000	-3.041935000
H	-0.941100000	-7.948156000	3.041935000
H	-1.362485000	5.619340000	5.620971000
H	-1.362485000	-5.619340000	-5.620971000
H	-1.408695000	8.760541000	3.216113000
H	-1.408695000	-8.760541000	-3.216113000
H	-1.419349000	3.211634000	8.760505000
H	-1.419349000	-3.211634000	-8.760505000
H	-1.429880000	1.844482000	-5.828463000
H	-1.429880000	-1.844482000	5.828463000
H	-1.433620000	5.821657000	-1.849180000
H	-1.433620000	-5.821657000	1.849180000
H	-2.742564000	5.319636000	0.989641000
H	-2.742564000	-5.319636000	-0.989641000
H	-2.745967000	0.991333000	5.312854000
H	-2.745967000	-0.991333000	-5.312854000

H	-3.248326000	7.445199000	2.169841000
H	-3.248326000	-7.445199000	-2.169841000
H	-3.256504000	2.169539000	7.438288000
H	-3.256504000	-2.169539000	-7.438288000
H	-3.405223000	2.422377000	2.417505000
H	-3.405223000	-2.422377000	-2.417505000
H	-3.842193000	5.454446000	5.451278000
H	-3.842193000	-5.454446000	-5.451278000
H	-4.866532000	3.848864000	3.842420000
H	-4.866532000	-3.848864000	-3.842420000
N	0.000000000	0.000000000	1.994187000
N	0.000000000	0.000000000	-1.994187000
N	0.000000000	1.994103000	0.000000000
N	0.000000000	-1.994103000	0.000000000

9. Zn(DPP]; S = 0 (saddled)

Zn	0.000000000	0.000000000	-0.023670000
C	0.000000000	0.000000000	3.406913000
C	0.000000000	0.000000000	4.897366000
C	0.000000000	0.000000000	7.701430000
C	0.000000000	0.000000000	-3.488451000
C	0.000000000	0.000000000	-4.976242000
C	0.000000000	0.000000000	-7.781883000
C	0.509612000	-1.095362000	7.000775000
C	0.515841000	-1.090406000	5.607515000
C	0.928373000	0.772940000	-7.080837000
C	0.930369000	0.767808000	-5.687826000
C	1.155134000	-0.473559000	-2.831390000
C	1.251051000	0.064619000	2.759509000
C	1.600433000	-2.795378000	-5.118935000
C	1.767738000	-3.489287000	-6.316828000
C	2.325374000	-1.076373000	-3.460614000
C	2.451146000	-1.731412000	-4.780023000
C	2.538041000	2.094632000	5.059321000
C	2.541216000	0.228166000	3.418186000
C	2.723056000	-0.618936000	-1.266065000
C	2.790139000	-3.132189000	-7.199619000
C	2.817929000	-0.214309000	1.198092000
C	2.869374000	0.763023000	4.762002000
C	2.940841000	2.681204000	6.258946000
C	3.308347000	-1.129504000	-2.492055000
C	3.422107000	-0.425106000	-0.053857000
C	3.471470000	-1.381122000	-5.676525000
C	3.506869000	-0.010718000	2.462838000
C	3.612531000	0.034505000	5.700974000
C	3.640208000	-2.072744000	-6.875029000
C	3.684490000	1.945548000	7.184851000
C	4.015665000	0.618803000	6.901361000
C	4.600580000	-1.840380000	-2.640670000

C	4.704017000	-3.163043000	-2.183070000
C	4.901693000	-0.233571000	-0.192612000
C	4.950198000	-0.092350000	2.793658000
C	5.337233000	0.994880000	-0.710909000
C	5.469623000	-1.307342000	3.266484000
C	5.712463000	-1.252547000	-3.256115000
C	5.792347000	1.023589000	2.734335000
C	5.853679000	-1.200480000	0.146269000
C	5.895647000	-3.874569000	-2.324062000
C	6.698693000	1.257765000	-0.872967000
C	6.806215000	-1.413751000	3.647679000
C	6.905813000	-1.960537000	-3.394492000
C	7.002787000	-3.273548000	-2.927456000
C	7.131211000	0.918741000	3.112879000
C	7.213388000	-0.943550000	-0.021352000
C	7.640316000	0.286930000	-0.527695000
C	7.643833000	-0.298827000	3.567401000
C	-0.509612000	1.095362000	7.000775000
C	-0.515841000	1.090406000	5.607515000
C	-0.928373000	-0.772940000	-7.080837000
C	-0.930369000	-0.767808000	-5.687826000
C	-1.155134000	0.473559000	-2.831390000
C	-1.251051000	-0.064619000	2.759509000
C	-1.600433000	2.795378000	-5.118935000
C	-1.767738000	3.489287000	-6.316828000
C	-2.325374000	1.076373000	-3.460614000
C	-2.451146000	1.731412000	-4.780023000
C	-2.538041000	-2.094632000	5.059321000
C	-2.541216000	-0.228166000	3.418186000
C	-2.723056000	0.618936000	-1.266065000
C	-2.790139000	3.132189000	-7.199619000
C	-2.817929000	0.214309000	1.198092000
C	-2.869374000	-0.763023000	4.762002000
C	-2.940841000	-2.681204000	6.258946000
C	-3.308347000	1.129504000	-2.492055000
C	-3.422107000	0.425106000	-0.053857000
C	-3.471470000	1.381122000	-5.676525000
C	-3.506869000	0.010718000	2.462838000
C	-3.612531000	-0.034505000	5.700974000
C	-3.640208000	2.072744000	-6.875029000
C	-3.684490000	-1.945548000	7.184851000
C	-4.015665000	-0.618803000	6.901361000
C	-4.600580000	1.840380000	-2.640670000
C	-4.704017000	3.163043000	-2.183070000
C	-4.901693000	0.233571000	-0.192612000
C	-4.950198000	0.092350000	2.793658000
C	-5.337233000	-0.994880000	-0.710909000
C	-5.469623000	1.307342000	3.266484000
C	-5.712463000	1.252547000	-3.256115000
C	-5.792347000	-1.023589000	2.734335000
C	-5.853679000	1.200480000	0.146269000

C	-5.895647000	3.874569000	-2.324062000
C	-6.698693000	-1.257765000	-0.872967000
C	-6.806215000	1.413751000	3.647679000
C	-6.905813000	1.960537000	-3.394492000
C	-7.002787000	3.273548000	-2.927456000
C	-7.131211000	-0.918741000	3.112879000
C	-7.213388000	0.943550000	-0.021352000
C	-7.640316000	-0.286930000	-0.527695000
C	-7.643833000	0.298827000	3.567401000
H	0.000000000	0.000000000	8.791155000
H	0.000000000	0.000000000	-8.871594000
H	0.804612000	-3.075908000	-4.428718000
H	0.906738000	-1.953548000	7.541805000
H	0.918881000	-1.938531000	5.053552000
H	1.097309000	-4.312911000	-6.560738000
H	1.654274000	1.379218000	-7.621512000
H	1.655081000	1.365294000	-5.134479000
H	1.962679000	2.669969000	4.333442000
H	2.674174000	3.716758000	6.468944000
H	2.921752000	-3.675093000	-8.135382000
H	3.838445000	-3.626912000	-1.709769000
H	3.871748000	-1.000318000	5.486678000
H	4.002960000	2.403179000	8.121345000
H	4.125359000	-0.546248000	-5.433989000
H	4.437709000	-1.781752000	-7.558096000
H	4.592184000	0.033922000	7.617342000
H	4.594994000	1.746109000	-0.983090000
H	4.810945000	-2.174216000	3.322670000
H	5.392763000	1.972546000	2.379730000
H	5.521239000	-2.162441000	0.530716000
H	5.646321000	-0.220100000	-3.595569000
H	5.958271000	-4.901003000	-1.963590000
H	7.020867000	2.220046000	-1.270387000
H	7.193574000	-2.366716000	4.007314000
H	7.765486000	-1.481870000	-3.862246000
H	7.776822000	1.794129000	3.053645000
H	7.936010000	-3.826060000	-3.035384000
H	7.941025000	-1.709196000	0.243225000
H	8.690250000	-0.376628000	3.861823000
H	8.704401000	0.485675000	-0.655122000
H	-0.804612000	3.075908000	-4.428718000
H	-0.906738000	1.953548000	7.541805000
H	-0.918881000	1.938531000	5.053552000
H	-1.097309000	4.312911000	-6.560738000
H	-1.654274000	-1.379218000	-7.621512000
H	-1.655081000	-1.365294000	-5.134479000
H	-1.962679000	-2.669969000	4.333442000
H	-2.674174000	-3.716758000	6.468944000
H	-2.921752000	3.675093000	-8.135382000
H	-3.838445000	3.626912000	-1.709769000
H	-3.871748000	1.000318000	5.486678000

H	-4.002960000	-2.403179000	8.121345000
H	-4.125359000	0.546248000	-5.433989000
H	-4.437709000	1.781752000	-7.558096000
H	-4.592184000	-0.033922000	7.617342000
H	-4.594994000	-1.746109000	-0.983090000
H	-4.810945000	2.174216000	3.322670000
H	-5.392763000	-1.972546000	2.379730000
H	-5.521239000	2.162441000	0.530716000
H	-5.646321000	0.220100000	-3.595569000
H	-5.958271000	4.901003000	-1.963590000
H	-7.020867000	-2.220046000	-1.270387000
H	-7.193574000	2.366716000	4.007314000
H	-7.765486000	1.481870000	-3.862246000
H	-7.776822000	-1.794129000	3.053645000
H	-7.936010000	3.826060000	-3.035384000
H	-7.941025000	1.709196000	0.243225000
H	-8.690250000	0.376628000	3.861823000
H	-8.704401000	-0.485675000	-0.655122000
N	1.405037000	-0.294289000	-1.485003000
N	1.452759000	-0.152219000	1.412400000
N	-1.405037000	0.294289000	-1.485003000
N	-1.452759000	0.152219000	1.412400000

10. Zn(DPP]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
C	0.247410000	2.602673000	7.389006000
C	0.247410000	-2.602673000	-7.389006000
C	0.261975000	7.382930000	2.609100000
C	0.261975000	-7.382930000	-2.609100000
C	0.275942000	4.205531000	-0.632838000
C	0.275942000	-4.205531000	0.632838000
C	0.277153000	0.632327000	-4.205380000
C	0.277153000	-0.632327000	4.205380000
C	0.392847000	2.813777000	-1.046487000
C	0.392847000	-2.813777000	1.046487000
C	0.393655000	1.046218000	-2.813657000
C	0.393655000	-1.046218000	2.813657000
C	0.491981000	1.926155000	6.193860000
C	0.491981000	-1.926155000	-6.193860000
C	0.501188000	6.188272000	1.929796000
C	0.501188000	-6.188272000	-1.929796000
C	0.559102000	5.452727000	-1.380585000
C	0.559102000	-5.452727000	1.380585000
C	0.564949000	1.377860000	-5.452845000
C	0.564949000	-1.377860000	5.452845000
C	0.709992000	2.340732000	-2.340747000
C	0.709992000	-2.340732000	2.340747000
C	0.876480000	4.141851000	-4.144309000
C	0.876480000	-4.141851000	4.144309000

C	1.042008000	7.866574000	-2.736061000
C	1.042008000	-7.866574000	2.736061000
C	1.058605000	2.727709000	-7.867661000
C	1.058605000	-2.727709000	7.867661000
C	1.476697000	3.249844000	-3.249306000
C	1.476697000	-3.249844000	3.249306000
C	1.659571000	4.957450000	-4.959540000
C	1.659571000	-4.957450000	4.959540000
C	1.861211000	5.957197000	-1.493953000
C	1.861211000	-5.957197000	1.493953000
C	1.869200000	1.489302000	-5.952285000
C	1.869200000	-1.489302000	5.952285000
C	2.101870000	7.152490000	-2.170608000
C	2.101870000	-7.152490000	2.170608000
C	2.115213000	2.163187000	-7.148036000
C	2.115213000	-2.163187000	7.148036000
C	2.875179000	3.188632000	-3.184253000
C	2.875179000	-3.188632000	3.184253000
C	3.053756000	4.891220000	-4.889767000
C	3.053756000	-4.891220000	4.889767000
C	3.661924000	4.004708000	-3.999934000
C	3.661924000	-4.004708000	3.999934000
C	-0.247410000	2.602673000	-7.389006000
C	-0.247410000	-2.602673000	7.389006000
C	-0.261975000	7.382930000	-2.609100000
C	-0.261975000	-7.382930000	2.609100000
C	-0.275942000	4.205531000	0.632838000
C	-0.275942000	-4.205531000	-0.632838000
C	-0.277153000	0.632327000	4.205380000
C	-0.277153000	-0.632327000	-4.205380000
C	-0.392847000	2.813777000	1.046487000
C	-0.392847000	-2.813777000	-1.046487000
C	-0.393655000	1.046218000	2.813657000
C	-0.393655000	-1.046218000	-2.813657000
C	-0.491981000	1.926155000	-6.193860000
C	-0.491981000	-1.926155000	6.193860000
C	-0.501188000	6.188272000	-1.929796000
C	-0.501188000	-6.188272000	1.929796000
C	-0.559102000	5.452727000	1.380585000
C	-0.559102000	-5.452727000	-1.380585000
C	-0.564949000	1.377860000	5.452845000
C	-0.564949000	-1.377860000	-5.452845000
C	-0.709992000	2.340732000	2.340747000
C	-0.709992000	-2.340732000	-2.340747000
C	-0.876480000	4.141851000	4.144309000
C	-0.876480000	-4.141851000	-4.144309000
C	-1.042008000	7.866574000	2.736061000
C	-1.042008000	-7.866574000	-2.736061000
C	-1.058605000	2.727709000	7.867661000
C	-1.058605000	-2.727709000	-7.867661000
C	-1.476697000	3.249844000	3.249306000

C	-1.476697000	-3.249844000	-3.249306000
C	-1.659571000	4.957450000	4.959540000
C	-1.659571000	-4.957450000	-4.959540000
C	-1.861211000	5.957197000	1.493953000
C	-1.861211000	-5.957197000	-1.493953000
C	-1.869200000	1.489302000	5.952285000
C	-1.869200000	-1.489302000	-5.952285000
C	-2.101870000	7.152490000	2.170608000
C	-2.101870000	-7.152490000	-2.170608000
C	-2.115213000	2.163187000	7.148036000
C	-2.115213000	-2.163187000	-7.148036000
C	-2.875179000	3.188632000	3.184253000
C	-2.875179000	-3.188632000	-3.184253000
C	-3.053756000	4.891220000	4.889767000
C	-3.053756000	-4.891220000	-4.889767000
C	-3.661924000	4.004708000	3.999934000
C	-3.661924000	-4.004708000	-3.999934000
H	0.209305000	4.192467000	4.197700000
H	0.209305000	-4.192467000	-4.197700000
H	1.079155000	3.029185000	7.949028000
H	1.079155000	-3.029185000	-7.949028000
H	1.096317000	7.938576000	3.036272000
H	1.096317000	-7.938576000	-3.036272000
H	1.178067000	5.646713000	-5.651269000
H	1.178067000	-5.646713000	5.651269000
H	1.231706000	8.798611000	-3.268191000
H	1.231706000	-8.798611000	3.268191000
H	1.252420000	3.257636000	-8.800102000
H	1.252420000	-3.257636000	8.800102000
H	1.509329000	1.823614000	5.816950000
H	1.509329000	-1.823614000	-5.816950000
H	1.516929000	5.807419000	1.825792000
H	1.516929000	-5.807419000	-1.825792000
H	2.687969000	5.394284000	-1.062184000
H	2.687969000	-5.394284000	1.062184000
H	2.693384000	1.058243000	-5.385046000
H	2.693384000	-1.058243000	5.385046000
H	3.121638000	7.525132000	-2.260662000
H	3.121638000	-7.525132000	2.260662000
H	3.136582000	2.251780000	-7.516677000
H	3.136582000	-2.251780000	7.516677000
H	3.342771000	2.493245000	-2.486239000
H	3.342771000	-2.493245000	2.486239000
H	3.663359000	5.530286000	-5.528506000
H	3.663359000	-5.530286000	5.528506000
H	4.748425000	3.945875000	-3.938148000
H	4.748425000	-3.945875000	3.938148000
H	-0.209305000	4.192467000	-4.197700000
H	-0.209305000	-4.192467000	4.197700000
H	-1.079155000	3.029185000	-7.949028000
H	-1.079155000	-3.029185000	7.949028000

H	-1.096317000	7.938576000	-3.036272000
H	-1.096317000	-7.938576000	3.036272000
H	-1.178067000	5.646713000	5.651269000
H	-1.178067000	-5.646713000	-5.651269000
H	-1.231706000	8.798611000	3.268191000
H	-1.231706000	-8.798611000	-3.268191000
H	-1.252420000	3.257636000	8.800102000
H	-1.252420000	-3.257636000	-8.800102000
H	-1.509329000	1.823614000	-5.816950000
H	-1.509329000	-1.823614000	5.816950000
H	-1.516929000	5.807419000	-1.825792000
H	-1.516929000	-5.807419000	1.825792000
H	-2.687969000	5.394284000	1.062184000
H	-2.687969000	-5.394284000	-1.062184000
H	-2.693384000	1.058243000	5.385046000
H	-2.693384000	-1.058243000	-5.385046000
H	-3.121638000	7.525132000	2.260662000
H	-3.121638000	-7.525132000	-2.260662000
H	-3.136582000	2.251780000	7.516677000
H	-3.136582000	-2.251780000	-7.516677000
H	-3.342771000	2.493245000	2.486239000
H	-3.342771000	-2.493245000	-2.486239000
H	-3.663359000	5.530286000	5.528506000
H	-3.663359000	-5.530286000	-5.528506000
H	-4.748425000	3.945875000	3.938148000
H	-4.748425000	-3.945875000	-3.938148000
N	0.000000000	0.000000000	2.012617000
N	0.000000000	0.000000000	-2.012617000
N	0.000000000	2.012823000	0.000000000
N	0.000000000	-2.012823000	0.000000000

11. Cu[Br₈TPP]; S = ½ (saddled)

Cu	0.000000000	0.000000000	0.000000000
Br	2.416674000	4.893563000	2.092269000
Br	2.416674000	-4.893563000	-2.092269000
Br	4.893563000	2.416674000	2.092269000
Br	4.893563000	-2.416674000	-2.092269000
Br	-2.416674000	4.893563000	-2.092269000
Br	-2.416674000	-4.893563000	2.092269000
Br	-4.893563000	2.416674000	-2.092269000
Br	-4.893563000	-2.416674000	2.092269000
C	0.000000000	3.404387000	0.000000000
C	0.000000000	4.887632000	0.000000000
C	0.000000000	7.686848000	0.000000000
C	0.000000000	-3.404387000	0.000000000
C	0.000000000	-4.887632000	0.000000000
C	0.000000000	-7.686848000	0.000000000
C	0.885498000	6.987003000	-0.824346000

C	0.885498000	-6.987003000	0.824346000
C	0.891629000	5.594356000	-0.817074000
C	0.891629000	-5.594356000	0.817074000
C	1.143840000	2.721803000	0.446208000
C	1.143840000	-2.721803000	-0.446208000
C	2.289280000	3.262520000	1.154182000
C	2.289280000	-3.262520000	-1.154182000
C	2.721803000	1.143840000	0.446208000
C	2.721803000	-1.143840000	-0.446208000
C	3.262520000	2.289280000	1.154182000
C	3.262520000	-2.289280000	-1.154182000
C	3.404387000	0.000000000	0.000000000
C	4.887632000	0.000000000	0.000000000
C	5.594356000	0.891629000	-0.817074000
C	5.594356000	-0.891629000	0.817074000
C	6.987003000	0.885498000	-0.824346000
C	6.987003000	-0.885498000	0.824346000
C	7.686848000	0.000000000	0.000000000
C	-0.885498000	6.987003000	0.824346000
C	-0.885498000	-6.987003000	-0.824346000
C	-0.891629000	5.594356000	0.817074000
C	-0.891629000	-5.594356000	-0.817074000
C	-1.143840000	2.721803000	-0.446208000
C	-1.143840000	-2.721803000	0.446208000
C	-2.289280000	3.262520000	-1.154182000
C	-2.289280000	-3.262520000	1.154182000
C	-2.721803000	1.143840000	-0.446208000
C	-2.721803000	-1.143840000	0.446208000
C	-3.262520000	2.289280000	-1.154182000
C	-3.262520000	-2.289280000	1.154182000
C	-3.404387000	0.000000000	0.000000000
C	-4.887632000	0.000000000	0.000000000
C	-5.594356000	0.891629000	0.817074000
C	-5.594356000	-0.891629000	-0.817074000
C	-6.987003000	0.885498000	0.824346000
C	-6.987003000	-0.885498000	-0.824346000
C	-7.686848000	0.000000000	0.000000000
H	0.000000000	8.776444000	0.000000000
H	0.000000000	-8.776444000	0.000000000
H	1.575451000	7.528271000	-1.470060000
H	1.575451000	-7.528271000	1.470060000
H	1.582908000	5.040059000	-1.450634000
H	1.582908000	-5.040059000	1.450634000
H	5.040059000	1.582908000	-1.450634000
H	5.040059000	-1.582908000	1.450634000
H	7.528271000	1.575451000	-1.470060000
H	7.528271000	-1.575451000	1.470060000
H	8.776444000	0.000000000	0.000000000
H	-1.575451000	7.528271000	1.470060000
H	-1.575451000	-7.528271000	-1.470060000
H	-1.582908000	5.040059000	1.450634000

H	-1.582908000	-5.040059000	-1.450634000
H	-5.040059000	1.582908000	1.450634000
H	-5.040059000	-1.582908000	-1.450634000
H	-7.528271000	1.575451000	1.470060000
H	-7.528271000	-1.575451000	-1.470060000
H	-8.776444000	0.000000000	0.000000000
N	1.405813000	1.405813000	0.127111000
N	1.405813000	-1.405813000	-0.127111000
N	-1.405813000	1.405813000	-0.127111000
N	-1.405813000	-1.405813000	0.127111000

12. Cu[Br₈TPP]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
Br	1.398683000	5.759657000	-0.964169000
Br	1.398683000	-5.759657000	0.964169000
Br	5.759657000	1.398683000	-0.964169000
Br	5.759657000	-1.398683000	0.964169000
Br	-1.398683000	5.759657000	0.964169000
Br	-1.398683000	-5.759657000	-0.964169000
Br	-5.759657000	1.398683000	0.964169000
Br	-5.759657000	-1.398683000	-0.964169000
C	0.603556000	4.169245000	-0.329204000
C	0.603556000	-4.169245000	0.329204000
C	1.032968000	2.781743000	-0.441025000
C	1.032968000	-2.781743000	0.441025000
C	2.331106000	2.331106000	-0.739645000
C	2.331106000	-2.331106000	0.739645000
C	2.781743000	1.032968000	-0.441025000
C	2.781743000	-1.032968000	0.441025000
C	3.325727000	3.325727000	-1.236384000
C	3.325727000	-3.325727000	1.236384000
C	3.508525000	3.508525000	-2.608970000
C	3.508525000	-3.508525000	2.608970000
C	4.081133000	4.081133000	-0.331546000
C	4.081133000	-4.081133000	0.331546000
C	4.169245000	0.603556000	-0.329204000
C	4.169245000	-0.603556000	0.329204000
C	4.438415000	4.438415000	-3.074058000
C	4.438415000	-4.438415000	3.074058000
C	5.009317000	5.009317000	-0.793947000
C	5.009317000	-5.009317000	0.793947000
C	5.190038000	5.190038000	-2.167704000
C	5.190038000	-5.190038000	2.167704000
C	-0.603556000	4.169245000	0.329204000
C	-0.603556000	-4.169245000	-0.329204000
C	-1.032968000	2.781743000	0.441025000
C	-1.032968000	-2.781743000	-0.441025000
C	-2.331106000	2.331106000	0.739645000
C	-2.331106000	-2.331106000	-0.739645000

C	-2.781743000	1.032968000	0.441025000
C	-2.781743000	-1.032968000	-0.441025000
C	-3.325727000	3.325727000	1.236384000
C	-3.325727000	-3.325727000	-1.236384000
C	-3.508525000	3.508525000	2.608970000
C	-3.508525000	-3.508525000	-2.608970000
C	-4.081133000	4.081133000	0.331546000
C	-4.081133000	-4.081133000	-0.331546000
C	-4.169245000	0.603556000	0.329204000
C	-4.169245000	-0.603556000	-0.329204000
C	-4.438415000	4.438415000	3.074058000
C	-4.438415000	-4.438415000	-3.074058000
C	-5.009317000	5.009317000	0.793947000
C	-5.009317000	-5.009317000	-0.793947000
C	-5.190038000	5.190038000	2.167704000
C	-5.190038000	-5.190038000	-2.167704000
H	2.918637000	2.918637000	-3.309282000
H	2.918637000	-2.918637000	3.309282000
H	3.932028000	3.932028000	0.737000000
H	3.932028000	-3.932028000	-0.737000000
H	4.576349000	4.576349000	-4.145488000
H	4.576349000	-4.576349000	4.145488000
H	5.592538000	5.592538000	-0.083021000
H	5.592538000	-5.592538000	0.083021000
H	5.916168000	5.916168000	-2.532075000
H	5.916168000	-5.916168000	2.532075000
H	-2.918637000	2.918637000	3.309282000
H	-2.918637000	-2.918637000	-3.309282000
H	-3.932028000	3.932028000	-0.737000000
H	-3.932028000	-3.932028000	0.737000000
H	-4.576349000	4.576349000	4.145488000
H	-4.576349000	-4.576349000	-4.145488000
H	-5.592538000	5.592538000	0.083021000
H	-5.592538000	-5.592538000	-0.083021000
H	-5.916168000	5.916168000	2.532075000
H	-5.916168000	-5.916168000	-2.532075000
N	0.000000000	1.979136000	0.000000000
N	0.000000000	-1.979136000	0.000000000
N	1.979136000	0.000000000	0.000000000
N	-1.979136000	0.000000000	0.000000000

13. Ni[Br₃TPP]; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.000000000
Br	2.320972000	4.815410000	2.210905000
Br	2.320972000	-4.815410000	-2.210905000
Br	4.815410000	2.320972000	2.210905000
Br	4.815410000	-2.320972000	-2.210905000
Br	-2.320972000	4.815410000	-2.210905000
Br	-2.320972000	-4.815410000	2.210905000

Br	-4.815410000	2.320972000	-2.210905000
Br	-4.815410000	-2.320972000	2.210905000
C	0.000000000	3.365618000	0.000000000
C	0.000000000	4.849269000	0.000000000
C	0.000000000	7.648167000	0.000000000
C	0.000000000	-3.365618000	0.000000000
C	0.000000000	-4.849269000	0.000000000
C	0.000000000	-7.648167000	0.000000000
C	0.922279000	6.948255000	-0.782786000
C	0.922279000	-6.948255000	0.782786000
C	0.927383000	5.55285000	-0.776014000
C	0.927383000	-5.55285000	0.776014000
C	1.091666000	2.666228000	0.520625000
C	1.091666000	-2.666228000	-0.520625000
C	2.220710000	3.191941000	1.260623000
C	2.220710000	-3.191941000	-1.260623000
C	2.666228000	1.091666000	0.520625000
C	2.666228000	-1.091666000	-0.520625000
C	3.191941000	2.220710000	1.260623000
C	3.191941000	-2.220710000	-1.260623000
C	3.365618000	0.000000000	0.000000000
C	4.849269000	0.000000000	0.000000000
C	5.55285000	0.927383000	-0.776014000
C	5.55285000	-0.927383000	0.776014000
C	6.948255000	0.922279000	-0.782786000
C	6.948255000	-0.922279000	0.782786000
C	7.648167000	0.000000000	0.000000000
C	-0.922279000	6.948255000	0.782786000
C	-0.922279000	-6.948255000	-0.782786000
C	-0.927383000	5.55285000	0.776014000
C	-0.927383000	-5.55285000	-0.776014000
C	-1.091666000	2.666228000	-0.520625000
C	-1.091666000	-2.666228000	0.520625000
C	-2.220710000	3.191941000	-1.260623000
C	-2.220710000	-3.191941000	1.260623000
C	-2.666228000	1.091666000	-0.520625000
C	-2.666228000	-1.091666000	0.520625000
C	-3.191941000	2.220710000	-1.260623000
C	-3.191941000	-2.220710000	1.260623000
C	-3.365618000	0.000000000	0.000000000
C	-4.849269000	0.000000000	0.000000000
C	-5.55285000	0.927383000	0.776014000
C	-5.55285000	-0.927383000	-0.776014000
C	-6.948255000	0.922279000	0.782786000
C	-6.948255000	-0.922279000	-0.782786000
C	-7.648167000	0.000000000	0.000000000
H	0.000000000	8.737764000	0.000000000
H	0.000000000	-8.737764000	0.000000000
H	1.641615000	7.489454000	-1.395757000
H	1.641615000	-7.489454000	1.395757000
H	1.646856000	5.000888000	-1.377355000

H	1.646856000	-5.000888000	1.377355000
H	5.000888000	1.646856000	-1.377355000
H	5.000888000	-1.646856000	1.377355000
H	7.489454000	1.641615000	-1.395757000
H	7.489454000	-1.641615000	1.395757000
H	8.737764000	0.000000000	0.000000000
H	-1.641615000	7.489454000	1.395757000
H	-1.641615000	-7.489454000	-1.395757000
H	-1.646856000	5.000888000	1.377355000
H	-1.646856000	-5.000888000	-1.377355000
H	-5.000888000	1.646856000	1.377355000
H	-5.000888000	-1.646856000	-1.377355000
H	-7.489454000	1.641615000	1.395757000
H	-7.489454000	-1.641615000	-1.395757000
H	-8.737764000	0.000000000	0.000000000
N	1.339515000	1.339515000	0.208541000
N	1.339515000	-1.339515000	-0.208541000
N	-1.339515000	1.339515000	-0.208541000
N	-1.339515000	-1.339515000	0.208541000

14. Ni[Br₈TPP]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
Br	1.277132000	5.656320000	-1.148397000
Br	1.277132000	-5.656320000	1.148397000
Br	5.656320000	1.277132000	-1.148397000
Br	5.656320000	-1.277132000	1.148397000
Br	-1.277132000	5.656320000	1.148397000
Br	-1.277132000	-5.656320000	-1.148397000
Br	-5.656320000	1.277132000	1.148397000
Br	-5.656320000	-1.277132000	-1.148397000
C	0.556900000	4.081426000	-0.401969000
C	0.556900000	-4.081426000	0.401969000
C	0.976162000	2.697062000	-0.553047000
C	0.976162000	-2.697062000	0.553047000
C	2.249135000	2.249135000	-0.932388000
C	2.249135000	-2.249135000	0.932388000
C	2.697062000	0.976162000	-0.553047000
C	2.697062000	-0.976162000	0.553047000
C	3.206258000	3.206258000	-1.556079000
C	3.206258000	-3.206258000	1.556079000
C	3.297140000	3.297140000	-2.946758000
C	3.297140000	-3.297140000	2.946758000
C	4.019167000	4.019167000	-0.756526000
C	4.019167000	-4.019167000	0.756526000
C	4.081426000	0.556900000	-0.401969000
C	4.081426000	-0.556900000	0.401969000
C	4.192402000	4.192402000	-3.533943000
C	4.192402000	-4.192402000	3.533943000
C	4.912337000	4.912337000	-1.340169000

C	4.912337000	-4.912337000	1.340169000
C	5.001054000	5.001054000	-2.732039000
C	5.001054000	-5.001054000	2.732039000
C	-0.556900000	4.081426000	0.401969000
C	-0.556900000	-4.081426000	-0.401969000
C	-0.976162000	2.697062000	0.553047000
C	-0.976162000	-2.697062000	-0.553047000
C	-2.249135000	2.249135000	0.932388000
C	-2.249135000	-2.249135000	-0.932388000
C	-2.697062000	0.976162000	0.553047000
C	-2.697062000	-0.976162000	-0.553047000
C	-3.206258000	3.206258000	1.556079000
C	-3.206258000	-3.206258000	-1.556079000
C	-3.297140000	3.297140000	2.946758000
C	-3.297140000	-3.297140000	-2.946758000
C	-4.019167000	4.019167000	0.756526000
C	-4.019167000	-4.019167000	-0.756526000
C	-4.081426000	0.556900000	0.401969000
C	-4.081426000	-0.556900000	-0.401969000
C	-4.192402000	4.192402000	3.533943000
C	-4.192402000	-4.192402000	-3.533943000
C	-4.912337000	4.912337000	1.340169000
C	-4.912337000	-4.912337000	-1.340169000
C	-5.001054000	5.001054000	2.732039000
C	-5.001054000	-5.001054000	-2.732039000
H	2.663425000	2.663425000	-3.565864000
H	2.663425000	-2.663425000	3.565864000
H	3.942055000	3.942055000	0.327158000
H	3.942055000	-3.942055000	-0.327158000
H	4.258088000	4.258088000	-4.619076000
H	4.258088000	-4.258088000	4.619076000
H	5.540079000	5.540079000	-0.709584000
H	5.540079000	-5.540079000	0.709584000
H	5.699696000	5.699696000	-3.191528000
H	5.699696000	-5.699696000	3.191528000
H	-2.663425000	2.663425000	3.565864000
H	-2.663425000	-2.663425000	-3.565864000
H	-3.942055000	3.942055000	-0.327158000
H	-3.942055000	-3.942055000	0.327158000
H	-4.258088000	4.258088000	4.619076000
H	-4.258088000	-4.258088000	-4.619076000
H	-5.540079000	5.540079000	0.709584000
H	-5.540079000	-5.540079000	-0.709584000
H	-5.699696000	5.699696000	3.191528000
H	-5.699696000	-5.699696000	-3.191528000
N	0.000000000	1.888373000	0.000000000
N	0.000000000	-1.888373000	0.000000000
N	1.888373000	0.000000000	0.000000000
N	-1.888373000	0.000000000	0.000000000

15. Pd[Br₈TPP]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.000000000
Br	2.467241000	4.936350000	2.012843000
Br	2.467241000	-4.936350000	-2.012843000
Br	4.936350000	2.467241000	2.012843000
Br	4.936350000	-2.467241000	-2.012843000
Br	-2.467241000	4.936350000	-2.012843000
Br	-2.467241000	-4.936350000	2.012843000
Br	-4.936350000	2.467241000	-2.012843000
Br	-4.936350000	-2.467241000	2.012843000
C	0.000000000	3.416723000	0.000000000
C	0.000000000	4.901518000	0.000000000
C	0.000000000	7.699561000	0.000000000
C	0.000000000	-3.416723000	0.000000000
C	0.000000000	-4.901518000	0.000000000
C	0.000000000	-7.699561000	0.000000000
C	0.851997000	6.999868000	-0.858946000
C	0.851997000	-6.999868000	0.858946000
C	0.858247000	5.607184000	-0.851992000
C	0.858247000	-5.607184000	0.851992000
C	1.156803000	2.744662000	0.424282000
C	1.156803000	-2.744662000	-0.424282000
C	2.319954000	3.292370000	1.101706000
C	2.319954000	-3.292370000	-1.101706000
C	2.744662000	1.156803000	0.424282000
C	2.744662000	-1.156803000	-0.424282000
C	3.292370000	2.319954000	1.101706000
C	3.292370000	-2.319954000	-1.101706000
C	3.416723000	0.000000000	0.000000000
C	4.901518000	0.000000000	0.000000000
C	5.607184000	0.858247000	-0.851992000
C	5.607184000	-0.858247000	0.851992000
C	6.999868000	0.851997000	-0.858946000
C	6.999868000	-0.851997000	0.858946000
C	7.699561000	0.000000000	0.000000000
C	-0.851997000	6.999868000	0.858946000
C	-0.851997000	-6.999868000	-0.858946000
C	-0.858247000	5.607184000	0.851992000
C	-0.858247000	-5.607184000	-0.851992000
C	-1.156803000	2.744662000	-0.424282000
C	-1.156803000	-2.744662000	0.424282000
C	-2.319954000	3.292370000	-1.101706000
C	-2.319954000	-3.292370000	1.101706000
C	-2.744662000	1.156803000	-0.424282000
C	-2.744662000	-1.156803000	0.424282000
C	-3.292370000	2.319954000	-1.101706000
C	-3.292370000	-2.319954000	1.101706000
C	-3.416723000	0.000000000	0.000000000
C	-4.901518000	0.000000000	0.000000000
C	-5.607184000	0.858247000	0.851992000

C	-5.607184000	-0.858247000	-0.851992000
C	-6.999868000	0.851997000	0.858946000
C	-6.999868000	-0.851997000	-0.858946000
C	-7.699561000	0.000000000	0.000000000
H	0.000000000	8.789161000	0.000000000
H	0.000000000	-8.789161000	0.000000000
H	1.515891000	7.541118000	-1.531394000
H	1.515891000	-7.541118000	1.531394000
H	1.523785000	5.052455000	-1.512158000
H	1.523785000	-5.052455000	1.512158000
H	5.052455000	1.523785000	-1.512158000
H	5.052455000	-1.523785000	1.512158000
H	7.541118000	1.515891000	-1.531394000
H	7.541118000	-1.515891000	1.531394000
H	8.789161000	0.000000000	0.000000000
H	-1.515891000	7.541118000	1.531394000
H	-1.515891000	-7.541118000	-1.531394000
H	-1.523785000	5.052455000	1.512158000
H	-1.523785000	-5.052455000	-1.512158000
H	-5.052455000	1.523785000	1.512158000
H	-5.052455000	-1.523785000	-1.512158000
H	-7.541118000	1.515891000	1.531394000
H	-7.541118000	-1.515891000	-1.531394000
H	-8.789161000	0.000000000	0.000000000
N	1.422609000	1.422609000	0.123027000
N	1.422609000	-1.422609000	-0.123027000
N	-1.422609000	1.422609000	-0.123027000
N	-1.422609000	-1.422609000	0.123027000

16. Pd[Br₈TPP]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
Br	1.463985000	5.803931000	-0.841311000
Br	1.463985000	-5.803931000	0.841311000
Br	5.803931000	1.463985000	-0.841311000
Br	5.803931000	-1.463985000	0.841311000
Br	-1.463985000	5.803931000	0.841311000
Br	-1.463985000	-5.803931000	-0.841311000
Br	-5.803931000	1.463985000	0.841311000
Br	-5.803931000	-1.463985000	-0.841311000
C	0.624808000	4.207229000	-0.284351000
C	0.624808000	-4.207229000	0.284351000
C	1.062457000	2.818718000	-0.378332000
C	1.062457000	-2.818718000	0.378332000
C	2.369490000	2.369490000	-0.629424000
C	2.369490000	-2.369490000	0.629424000
C	2.818718000	1.062457000	-0.378332000
C	2.818718000	-1.062457000	0.378332000
C	3.381700000	3.381700000	-1.051473000
C	3.381700000	-3.381700000	1.051473000

C	3.615299000	3.615299000	-2.408555000
C	3.615299000	-3.615299000	2.408555000
C	4.101199000	4.101199000	-0.090556000
C	4.101199000	-4.101199000	0.090556000
C	4.207229000	0.624808000	-0.284351000
C	4.207229000	-0.624808000	0.284351000
C	4.561126000	4.561126000	-2.802809000
C	4.561126000	-4.561126000	2.802809000
C	5.045505000	5.045505000	-0.482541000
C	5.045505000	-5.045505000	0.482541000
C	5.277468000	5.277468000	-1.840824000
C	5.277468000	-5.277468000	1.840824000
C	-0.624808000	4.207229000	0.284351000
C	-0.624808000	-4.207229000	-0.284351000
C	-1.062457000	2.818718000	0.378332000
C	-1.062457000	-2.818718000	-0.378332000
C	-2.369490000	2.369490000	0.629424000
C	-2.369490000	-2.369490000	-0.629424000
C	-2.818718000	1.062457000	0.378332000
C	-2.818718000	-1.062457000	-0.378332000
C	-3.381700000	3.381700000	1.051473000
C	-3.381700000	-3.381700000	-1.051473000
C	-3.615299000	3.615299000	2.408555000
C	-3.615299000	-3.615299000	-2.408555000
C	-4.101199000	4.101199000	0.090556000
C	-4.101199000	-4.101199000	-0.090556000
C	-4.207229000	0.624808000	0.284351000
C	-4.207229000	-0.624808000	-0.284351000
C	-4.561126000	4.561126000	2.802809000
C	-4.561126000	-4.561126000	-2.802809000
\C	-5.045505000	5.045505000	0.482541000
C	-5.045505000	-5.045505000	-0.482541000
C	-5.277468000	5.277468000	1.840824000
C	-5.277468000	-5.277468000	-1.840824000
H	3.052246000	3.052246000	-3.151650000
H	3.052246000	-3.052246000	3.151650000
H	3.911837000	3.911837000	0.965141000
H	3.911837000	-3.911837000	-0.965141000
H	4.739353000	4.739353000	-3.862242000
H	4.739353000	-4.739353000	3.862242000
H	5.601240000	5.601240000	0.271083000
H	5.601240000	-5.601240000	-0.271083000
H	6.016290000	6.016290000	-2.149964000
H	6.016290000	-6.016290000	2.149964000
H	-3.052246000	3.052246000	3.151650000
H	-3.052246000	-3.052246000	-3.151650000
H	-3.911837000	3.911837000	-0.965141000
H	-3.911837000	-3.911837000	0.965141000
H	-4.739353000	4.739353000	3.862242000
H	-4.739353000	-4.739353000	-3.862242000
H	-5.601240000	5.601240000	-0.271083000

H	-5.601240000	-5.601240000	0.271083000
H	-6.016290000	6.016290000	2.149964000
H	-6.016290000	-6.016290000	-2.149964000
N	0.000000000	2.018677000	0.000000000
N	0.000000000	-2.018677000	0.000000000
N	2.018677000	0.000000000	0.000000000
N	-2.018677000	0.000000000	0.000000000

17. Pt[Br₈TPP]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.000000000
Br	2.505941000	4.967165000	1.944216000
Br	2.505941000	-4.967165000	-1.944216000
Br	4.967165000	2.505941000	1.944216000
Br	4.967165000	-2.505941000	-1.944216000
Br	-2.505941000	4.967165000	-1.944216000
Br	-2.505941000	-4.967165000	1.944216000
Br	-4.967165000	2.505941000	-1.944216000
Br	-4.967165000	-2.505941000	1.944216000
C	0.000000000	3.419163000	0.000000000
C	0.000000000	4.905627000	0.000000000
C	0.000000000	7.703212000	0.000000000
C	0.000000000	-3.419163000	0.000000000
C	0.000000000	-4.905627000	0.000000000
C	0.000000000	-7.703212000	0.000000000
C	0.820473000	7.003564000	-0.889058000
C	0.820473000	-7.003564000	0.889058000
C	0.826556000	5.610778000	-0.882674000
C	0.826556000	-5.610778000	0.882674000
C	1.160409000	2.751602000	0.420037000
C	1.160409000	-2.751602000	-0.420037000
C	2.336543000	3.308206000	1.064923000
C	2.336543000	-3.308206000	-1.064923000
C	2.751602000	1.160409000	0.420037000
C	2.751602000	-1.160409000	-0.420037000
C	3.308206000	2.336543000	1.064923000
C	3.308206000	-2.336543000	-1.064923000
C	3.419163000	0.000000000	0.000000000
C	4.905627000	0.000000000	0.000000000
C	5.610778000	0.826556000	-0.882674000
C	5.610778000	-0.826556000	0.882674000
C	7.003564000	0.820473000	-0.889058000
C	7.003564000	-0.820473000	0.889058000
C	7.703212000	0.000000000	0.000000000
C	-0.820473000	7.003564000	0.889058000
C	-0.820473000	-7.003564000	-0.889058000
C	-0.826556000	5.610778000	0.882674000
C	-0.826556000	-5.610778000	-0.882674000
C	-1.160409000	2.751602000	-0.420037000
C	-1.160409000	-2.751602000	0.420037000

C	-2.336543000	3.308206000	-1.064923000
C	-2.336543000	-3.308206000	1.064923000
C	-2.751602000	1.160409000	-0.420037000
C	-2.751602000	-1.160409000	0.420037000
C	-3.308206000	2.336543000	-1.064923000
C	-3.308206000	-2.336543000	1.064923000
C	-3.419163000	0.000000000	0.000000000
C	-4.905627000	0.000000000	0.000000000
C	-5.610778000	0.826556000	0.882674000
C	-5.610778000	-0.826556000	-0.882674000
C	-7.003564000	0.820473000	0.889058000
C	-7.003564000	-0.820473000	-0.889058000
C	-7.703212000	0.000000000	0.000000000
H	0.000000000	8.792780000	0.000000000
H	0.000000000	-8.792780000	0.000000000
H	1.460030000	7.544830000	-1.584655000
H	1.460030000	-7.544830000	1.584655000
H	1.467470000	5.055977000	-1.566709000
H	1.467470000	-5.055977000	1.566709000
H	5.055977000	1.467470000	-1.566709000
H	5.055977000	-1.467470000	1.566709000
H	7.544830000	1.460030000	-1.584655000
H	7.544830000	-1.460030000	1.584655000
H	8.792780000	0.000000000	0.000000000
H	-1.460030000	7.544830000	1.584655000
H	-1.460030000	-7.544830000	-1.584655000
H	-1.467470000	5.055977000	1.566709000
H	-1.467470000	-5.055977000	-1.566709000
H	-5.055977000	1.467470000	1.566709000
H	-5.055977000	-1.467470000	-1.566709000
H	-7.544830000	1.460030000	1.584655000
H	-7.544830000	-1.460030000	-1.584655000
H	-8.792780000	0.000000000	0.000000000
N	1.418074000	1.418074000	0.149964000
N	1.418074000	-1.418074000	-0.149964000
N	-1.418074000	1.418074000	-0.149964000
N	-1.418074000	-1.418074000	0.149964000

18. Pt[Br₈TPP]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
Br	1.472291000	5.807558000	-0.821927000
Br	1.472291000	-5.807558000	0.821927000
Br	5.807558000	1.472291000	-0.821927000
Br	5.807558000	-1.472291000	0.821927000
Br	-1.472291000	5.807558000	0.821927000
Br	-1.472291000	-5.807558000	-0.821927000
Br	-5.807558000	1.472291000	0.821927000
Br	-5.807558000	-1.472291000	-0.821927000
C	0.627630000	4.209747000	-0.277069000

C	0.627630000	-4.209747000	0.277069000
C	1.067161000	2.823874000	-0.369116000
C	1.067161000	-2.823874000	0.369116000
C	2.375027000	2.375027000	-0.613794000
C	2.375027000	-2.375027000	0.613794000
C	2.823874000	1.067161000	-0.369116000
C	2.823874000	-1.067161000	0.369116000
C	3.389708000	3.389708000	-1.025205000
C	3.389708000	-3.389708000	1.025205000
C	3.630208000	3.630208000	-2.379980000
C	3.630208000	-3.630208000	2.379980000
C	4.104082000	4.104082000	-0.056640000
C	4.104082000	-4.104082000	0.056640000
C	4.209747000	0.627630000	-0.277069000
C	4.209747000	-0.627630000	0.277069000
C	4.578062000	4.578062000	-2.764338000
C	4.578062000	-4.578062000	2.764338000
C	5.050395000	5.050395000	-0.438921000
C	5.050395000	-5.050395000	0.438921000
C	5.289349000	5.289349000	-1.794811000
C	5.289349000	-5.289349000	1.794811000
C	-0.627630000	4.209747000	0.277069000
C	-0.627630000	-4.209747000	-0.277069000
C	-1.067161000	2.823874000	0.369116000
C	-1.067161000	-2.823874000	-0.369116000
C	-2.375027000	2.375027000	0.613794000
C	-2.375027000	-2.375027000	-0.613794000
C	-2.823874000	1.067161000	0.369116000
C	-2.823874000	-1.067161000	-0.369116000
C	-3.389708000	3.389708000	1.025205000
C	-3.389708000	-3.389708000	-1.025205000
C	-3.630208000	3.630208000	2.379980000
C	-3.630208000	-3.630208000	-2.379980000
C	-4.104082000	4.104082000	0.056640000
C	-4.104082000	-4.104082000	-0.056640000
C	-4.209747000	0.627630000	0.277069000
C	-4.209747000	-0.627630000	-0.277069000
C	-4.578062000	4.578062000	2.764338000
C	-4.578062000	-4.578062000	-2.764338000
C	-5.050395000	5.050395000	0.438921000
C	-5.050395000	-5.050395000	-0.438921000
C	-5.289349000	5.289349000	1.794811000
C	-5.289349000	-5.289349000	-1.794811000
H	3.070861000	3.070861000	-3.128673000
H	3.070861000	-3.070861000	3.128673000
H	3.909119000	3.909119000	0.997036000
H	3.909119000	-3.909119000	-0.997036000
H	4.761897000	4.761897000	-3.821864000
H	4.761897000	-4.761897000	3.821864000
H	5.602304000	5.602304000	0.320310000
H	5.602304000	-5.602304000	-0.320310000

H	6.029783000	6.029783000	-2.096222000
H	6.029783000	-6.029783000	2.096222000
H	-3.070861000	3.070861000	3.128673000
H	-3.070861000	-3.070861000	-3.128673000
H	-3.909119000	3.909119000	-0.997036000
H	-3.909119000	-3.909119000	0.997036000
H	-4.761897000	4.761897000	3.821864000
H	-4.761897000	-4.761897000	-3.821864000
H	-5.602304000	5.602304000	-0.320310000
H	-5.602304000	-5.602304000	0.320310000
H	-6.029783000	6.029783000	2.096222000
H	-6.029783000	-6.029783000	-2.096222000
N	0.000000000	2.020007000	0.000000000
N	0.000000000	-2.020007000	0.000000000
N	2.020007000	0.000000000	0.000000000
N	-2.020007000	0.000000000	0.000000000

19. Zn[Br₈TPP]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.000000000
Br	2.522443000	4.980079000	1.935999000
Br	2.522443000	-4.980079000	-1.935999000
Br	4.980079000	2.522443000	1.935999000
Br	4.980079000	-2.522443000	-1.935999000
Br	-2.522443000	4.980079000	-1.935999000
Br	-2.522443000	-4.980079000	1.935999000
Br	-4.980079000	2.522443000	-1.935999000
Br	-4.980079000	-2.522443000	1.935999000
C	0.000000000	3.424408000	0.000000000
C	0.000000000	4.909992000	0.000000000
C	0.000000000	7.708984000	0.000000000
C	0.000000000	-3.424408000	0.000000000
C	0.000000000	-4.909992000	0.000000000
C	0.000000000	-7.708984000	0.000000000
C	0.821150000	7.009136000	-0.888330000
C	0.821150000	-7.009136000	0.888330000
C	0.827255000	5.616438000	-0.881738000
C	0.827255000	-5.616438000	0.881738000
C	1.174412000	2.758881000	0.406837000
C	1.174412000	-2.758881000	-0.406837000
C	2.346679000	3.321386000	1.054669000
C	2.346679000	-3.321386000	-1.054669000
C	2.758881000	1.174412000	0.406837000
C	2.758881000	-1.174412000	-0.406837000
C	3.321386000	2.346679000	1.054669000
C	3.321386000	-2.346679000	-1.054669000
C	3.424408000	0.000000000	0.000000000
C	4.909992000	0.000000000	0.000000000
C	5.616438000	0.827255000	-0.881738000
C	5.616438000	-0.827255000	0.881738000

C	7.009136000	0.821150000	-0.888330000
C	7.009136000	-0.821150000	0.888330000
C	7.708984000	0.000000000	0.000000000
C	-0.821150000	7.009136000	0.888330000
C	-0.821150000	-7.009136000	-0.888330000
C	-0.827255000	5.616438000	0.881738000
C	-0.827255000	-5.616438000	-0.881738000
C	-1.174412000	2.758881000	-0.406837000
C	-1.174412000	-2.758881000	0.406837000
C	-2.346679000	3.321386000	-1.054669000
C	-2.346679000	-3.321386000	1.054669000
C	-2.758881000	1.174412000	-0.406837000
C	-2.758881000	-1.174412000	0.406837000
C	-3.321386000	2.346679000	-1.054669000
C	-3.321386000	-2.346679000	1.054669000
C	-3.424408000	0.000000000	0.000000000
C	-4.909992000	0.000000000	0.000000000
C	-5.616438000	0.827255000	0.881738000
C	-5.616438000	-0.827255000	-0.881738000
C	-7.009136000	0.821150000	0.888330000
C	-7.009136000	-0.821150000	-0.888330000
C	-7.708984000	0.000000000	0.000000000
H	0.000000000	8.798581000	0.000000000
H	0.000000000	-8.798581000	0.000000000
H	1.461018000	7.550377000	-1.583732000
H	1.461018000	-7.550377000	1.583732000
H	1.468826000	5.062102000	-1.565527000
H	1.468826000	-5.062102000	1.565527000
H	5.062102000	1.468826000	-1.565527000
H	5.062102000	-1.468826000	1.565527000
H	7.550377000	1.461018000	-1.583732000
H	7.550377000	-1.461018000	1.583732000
H	8.798581000	0.000000000	0.000000000
H	-1.461018000	7.550377000	1.583732000
H	-1.461018000	-7.550377000	-1.583732000
H	-1.468826000	5.062102000	1.565527000
H	-1.468826000	-5.062102000	-1.565527000
H	-5.062102000	1.468826000	1.565527000
H	-5.062102000	-1.468826000	-1.565527000
H	-7.550377000	1.461018000	1.583732000
H	-7.550377000	-1.461018000	-1.583732000
H	-8.798581000	0.000000000	0.000000000
N	1.435327000	1.435327000	0.123335000
N	1.435327000	-1.435327000	-0.123335000
N	-1.435327000	1.435327000	-0.123335000
N	-1.435327000	-1.435327000	0.123335000

20. Zn[Br₈TPP]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
Br	1.502098000	5.843852000	-0.748869000
Br	1.502098000	-5.843852000	0.748869000
Br	5.843852000	1.502098000	-0.748869000
Br	5.843852000	-1.502098000	0.748869000
Br	-1.502098000	5.843852000	0.748869000
Br	-1.502098000	-5.843852000	-0.748869000
Br	-5.843852000	1.502098000	0.748869000
Br	-5.843852000	-1.502098000	-0.748869000
C	0.641718000	4.237708000	-0.247867000
C	0.641718000	-4.237708000	0.247867000
C	1.077878000	2.848899000	-0.323798000
C	1.077878000	-2.848899000	0.323798000
C	2.394552000	2.394552000	-0.540687000
C	2.394552000	-2.394552000	0.540687000
C	2.848899000	1.077878000	-0.323798000
C	2.848899000	-1.077878000	0.323798000
C	3.418485000	3.418485000	-0.904607000
C	3.418485000	-3.418485000	0.904607000
C	3.691569000	3.691569000	-2.247197000
C	3.691569000	-3.691569000	2.247197000
C	4.109663000	4.109663000	0.096819000
C	4.109663000	-4.109663000	-0.096819000
C	4.237708000	0.641718000	-0.247867000
C	4.237708000	-0.641718000	0.247867000
C	4.647706000	4.647706000	-2.586800000
C	4.647706000	-4.647706000	2.586800000
C	5.064606000	5.064606000	-0.240608000
C	5.064606000	-5.064606000	0.240608000
C	5.335692000	5.335692000	-1.584232000
C	5.335692000	-5.335692000	1.584232000
C	-0.641718000	4.237708000	0.247867000
C	-0.641718000	-4.237708000	-0.247867000
C	-1.077878000	2.848899000	0.323798000
C	-1.077878000	-2.848899000	-0.323798000
C	-2.394552000	2.394552000	0.540687000
C	-2.394552000	-2.394552000	-0.540687000
C	-2.848899000	1.077878000	0.323798000
C	-2.848899000	-1.077878000	-0.323798000
C	-3.418485000	3.418485000	0.904607000
C	-3.418485000	-3.418485000	-0.904607000
C	-3.691569000	3.691569000	2.247197000
C	-3.691569000	-3.691569000	-2.247197000
C	-4.109663000	4.109663000	-0.096819000
C	-4.109663000	-4.109663000	0.096819000
C	-4.237708000	0.641718000	0.247867000
C	-4.237708000	-0.641718000	-0.247867000
C	-4.647706000	4.647706000	2.586800000

C	-4.647706000	-4.647706000	-2.586800000
C	-5.064606000	5.064606000	0.240608000
C	-5.064606000	-5.064606000	-0.240608000
C	-5.335692000	5.335692000	1.584232000
C	-5.335692000	-5.335692000	-1.584232000
H	3.150533000	3.150533000	-3.022296000
H	3.150533000	-3.150533000	3.022296000
H	3.890220000	3.890220000	1.140790000
H	3.890220000	-3.890220000	-1.140790000
H	4.856363000	4.856363000	-3.635115000
H	4.856363000	-4.856363000	3.635115000
H	5.598215000	5.598215000	0.544378000
H	5.598215000	-5.598215000	-0.544378000
H	6.082861000	6.082861000	-1.850285000
H	6.082861000	-6.082861000	1.850285000
H	-3.150533000	3.150533000	3.022296000
H	-3.150533000	-3.150533000	-3.022296000
H	-3.890220000	3.890220000	-1.140790000
H	-3.890220000	-3.890220000	1.140790000
H	-4.856363000	4.856363000	3.635115000
H	-4.856363000	-4.856363000	-3.635115000
H	-5.598215000	5.598215000	-0.544378000
H	-5.598215000	-5.598215000	0.544378000
H	-6.082861000	6.082861000	1.850285000
H	-6.082861000	-6.082861000	-1.850285000
N	0.000000000	2.045410000	0.000000000
N	0.000000000	-2.045410000	0.000000000
N	2.045410000	0.000000000	0.000000000
N	-2.045410000	0.000000000	0.000000000

21. Cu[Cl₈TPP]; S = ½ (saddled)

Cu	0.000000000	0.000000000	0.000000000
C	0.000000000	3.412854000	0.000000000
C	0.000000000	4.897934000	0.000000000
C	0.000000000	7.697475000	0.000000000
C	0.000000000	-3.412854000	0.000000000
C	0.000000000	-4.897934000	0.000000000
C	0.000000000	-7.697475000	0.000000000
C	0.838970000	6.997427000	-0.871333000
C	0.838970000	-6.997427000	0.871333000
C	0.844376000	5.604352000	-0.865409000
C	0.844376000	-5.604352000	0.865409000
C	1.155408000	2.731889000	0.412408000
C	1.155408000	-2.731889000	-0.412408000
C	2.320174000	3.292289000	1.068583000
C	2.320174000	-3.292289000	-1.068583000
C	2.731889000	1.155408000	0.412408000
C	2.731889000	-1.155408000	-0.412408000
C	3.292289000	2.320174000	1.068583000

C	3.292289000	-2.320174000	-1.068583000
C	3.412854000	0.000000000	0.000000000
C	4.897934000	0.000000000	0.000000000
C	5.604352000	0.844376000	-0.865409000
C	5.604352000	-0.844376000	0.865409000
C	6.997427000	0.838970000	-0.871333000
C	6.997427000	-0.838970000	0.871333000
C	7.697475000	0.000000000	0.000000000
C	-0.838970000	6.997427000	0.871333000
C	-0.838970000	-6.997427000	-0.871333000
C	-0.844376000	5.604352000	0.865409000
C	-0.844376000	-5.604352000	-0.865409000
C	-1.155408000	2.731889000	-0.412408000
C	-1.155408000	-2.731889000	0.412408000
C	-2.320174000	3.292289000	-1.068583000
C	-2.320174000	-3.292289000	1.068583000
C	-2.731889000	1.155408000	-0.412408000
C	-2.731889000	-1.155408000	0.412408000
C	-3.292289000	2.320174000	-1.068583000
C	-3.292289000	-2.320174000	1.068583000
C	-3.412854000	0.000000000	0.000000000
C	-4.897934000	0.000000000	0.000000000
C	-5.604352000	0.844376000	0.865409000
C	-5.604352000	-0.844376000	-0.865409000
C	-6.997427000	0.838970000	0.871333000
C	-6.997427000	-0.838970000	-0.871333000
C	-7.697475000	0.000000000	0.000000000
C1	2.474166000	4.813402000	1.849153000
C1	2.474166000	-4.813402000	-1.849153000
C1	4.813402000	2.474166000	1.849153000
C1	4.813402000	-2.474166000	-1.849153000
C1	-2.474166000	4.813402000	-1.849153000
C1	-2.474166000	-4.813402000	1.849153000
C1	-4.813402000	2.474166000	-1.849153000
C1	-4.813402000	-2.474166000	1.849153000
H	0.000000000	8.787037000	0.000000000
H	0.000000000	-8.787037000	0.000000000
H	1.492635000	7.538342000	-1.554050000
H	1.492635000	-7.538342000	1.554050000
H	1.500380000	5.050472000	-1.536140000
H	1.500380000	-5.050472000	1.536140000
H	5.050472000	1.500380000	-1.536140000
H	5.050472000	-1.500380000	1.536140000
H	7.538342000	1.492635000	-1.554050000
H	7.538342000	-1.492635000	1.554050000
H	8.787037000	0.000000000	0.000000000
H	-1.492635000	7.538342000	1.554050000
H	-1.492635000	-7.538342000	-1.554050000
H	-1.500380000	5.050472000	1.536140000
H	-1.500380000	-5.050472000	-1.536140000
H	-5.050472000	1.500380000	1.536140000

H	-5.050472000	-1.500380000	-1.536140000
H	-7.538342000	1.492635000	1.554050000
H	-7.538342000	-1.492635000	-1.554050000
H	-8.787037000	0.000000000	0.000000000
N	1.408687000	1.408687000	0.117203000
N	1.408687000	-1.408687000	-0.117203000
N	-1.408687000	1.408687000	-0.117203000
N	-1.408687000	-1.408687000	0.117203000

22. Cu[Cl₈TPP]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
C	0.622653000	4.182152000	-0.288540000
C	0.622653000	-4.182152000	0.288540000
C	1.051099000	2.796314000	-0.388781000
C	1.051099000	-2.796314000	0.388781000
C	2.357049000	2.357049000	-0.655968000
C	2.357049000	-2.357049000	0.655968000
C	2.796314000	1.051099000	-0.388781000
C	2.796314000	-1.051099000	0.388781000
C	3.362987000	3.362987000	-1.109088000
C	3.362987000	-3.362987000	1.109088000
C	3.572891000	3.572891000	-2.473696000
C	3.572891000	-3.572891000	2.473696000
C	4.100011000	4.100011000	-0.174932000
C	4.100011000	-4.100011000	0.174932000
C	4.182152000	0.622653000	-0.288540000
C	4.182152000	-0.622653000	0.288540000
C	4.511954000	4.511954000	-2.902476000
C	4.511954000	-4.511954000	2.902476000
C	5.036876000	5.036876000	-0.600817000
C	5.036876000	-5.036876000	0.600817000
C	5.245205000	5.245205000	-1.967246000
C	5.245205000	-5.245205000	1.967246000
C	-0.622653000	4.182152000	0.288540000
C	-0.622653000	-4.182152000	-0.288540000
C	-1.051099000	2.796314000	0.388781000
C	-1.051099000	-2.796314000	-0.388781000
C	-2.357049000	2.357049000	0.655968000
C	-2.357049000	-2.357049000	-0.655968000
C	-2.796314000	1.051099000	0.388781000
C	-2.796314000	-1.051099000	-0.388781000
C	-3.362987000	3.362987000	1.109088000
C	-3.362987000	-3.362987000	-1.109088000
C	-3.572891000	3.572891000	2.473696000
C	-3.572891000	-3.572891000	-2.473696000
C	-4.100011000	4.100011000	0.174932000
C	-4.100011000	-4.100011000	-0.174932000
C	-4.182152000	0.622653000	0.288540000
C	-4.182152000	-0.622653000	-0.288540000

C	-4.511954000	4.511954000	2.902476000
C	-4.511954000	-4.511954000	-2.902476000
C	-5.036876000	5.036876000	0.600817000
C	-5.036876000	-5.036876000	-0.600817000
C	-5.245205000	5.245205000	1.967246000
C	-5.245205000	-5.245205000	-1.967246000
Cl	1.413574000	5.629531000	-0.765805000
Cl	1.413574000	-5.629531000	0.765805000
Cl	5.629531000	1.413574000	-0.765805000
Cl	5.629531000	-1.413574000	0.765805000
Cl	-1.413574000	5.629531000	0.765805000
Cl	-1.413574000	-5.629531000	-0.765805000
Cl	-5.629531000	1.413574000	0.765805000
Cl	-5.629531000	-1.413574000	-0.765805000
H	2.997119000	2.997119000	-3.197470000
H	2.997119000	-2.997119000	3.197470000
H	3.930429000	3.930429000	0.887651000
H	3.930429000	-3.930429000	-0.887651000
H	4.670526000	4.670526000	-3.968236000
H	4.670526000	-4.670526000	3.968236000
H	5.605792000	5.605792000	0.133066000
H	5.605792000	-5.605792000	-0.133066000
H	5.978324000	5.978324000	-2.302294000
H	5.978324000	-5.978324000	2.302294000
H	-2.997119000	2.997119000	3.197470000
H	-2.997119000	-2.997119000	-3.197470000
H	-3.930429000	3.930429000	-0.887651000
H	-3.930429000	-3.930429000	0.887651000
H	-4.670526000	4.670526000	3.968236000
H	-4.670526000	-4.670526000	-3.968236000
H	-5.605792000	5.605792000	-0.133066000
H	-5.605792000	-5.605792000	0.133066000
H	-5.978324000	5.978324000	2.302294000
H	-5.978324000	-5.978324000	-2.302294000
N	0.000000000	1.989719000	0.000000000
N	0.000000000	-1.989719000	0.000000000
N	1.989719000	0.000000000	0.000000000
N	-1.989719000	0.000000000	0.000000000

23. Ni[Cl₈TPP]; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	3.375073000	0.000000000
C	0.000000000	4.860166000	0.000000000
C	0.000000000	7.659527000	0.000000000
C	0.000000000	-3.375073000	0.000000000
C	0.000000000	-4.860166000	0.000000000
C	0.000000000	-7.659527000	0.000000000
C	0.889757000	6.959401000	-0.819242000
C	0.889757000	-6.959401000	0.819242000

C	0.894153000	5.566054000	-0.813687000
C	0.894153000	-5.566054000	0.813687000
C	1.103355000	2.676353000	0.492433000
C	1.103355000	-2.676353000	-0.492433000
C	2.247687000	3.217989000	1.193158000
C	2.247687000	-3.217989000	-1.193158000
C	2.676353000	1.103355000	0.492433000
C	2.676353000	-1.103355000	-0.492433000
C	3.217989000	2.247687000	1.193158000
C	3.217989000	-2.247687000	-1.193158000
C	3.375073000	0.000000000	0.000000000
C	4.860166000	0.000000000	0.000000000
C	5.566054000	0.894153000	-0.813687000
C	5.566054000	-0.894153000	0.813687000
C	6.959401000	0.889757000	-0.819242000
C	6.959401000	-0.889757000	0.819242000
C	7.659527000	0.000000000	0.000000000
C	-0.889757000	6.959401000	0.819242000
C	-0.889757000	-6.959401000	-0.819242000
C	-0.894153000	5.566054000	0.813687000
C	-0.894153000	-5.566054000	-0.813687000
C	-1.103355000	2.676353000	-0.492433000
C	-1.103355000	-2.676353000	0.492433000
C	-2.247687000	3.217989000	-1.193158000
C	-2.247687000	-3.217989000	1.193158000
C	-2.676353000	1.103355000	-0.492433000
C	-2.676353000	-1.103355000	0.492433000
C	-3.217989000	2.247687000	-1.193158000
C	-3.217989000	-2.247687000	1.193158000
C	-3.375073000	0.000000000	0.000000000
C	-4.860166000	0.000000000	0.000000000
C	-5.566054000	0.894153000	0.813687000
C	-5.566054000	-0.894153000	-0.813687000
C	-6.959401000	0.889757000	0.819242000
C	-6.959401000	-0.889757000	-0.819242000
C	-7.659527000	0.000000000	0.000000000
C1	2.371307000	4.728356000	1.996839000
C1	2.371307000	-4.728356000	-1.996839000
C1	4.728356000	2.371307000	1.996839000
C1	4.728356000	-2.371307000	-1.996839000
C1	-2.371307000	4.728356000	-1.996839000
C1	-2.371307000	-4.728356000	1.996839000
C1	-4.728356000	2.371307000	-1.996839000
C1	-4.728356000	-2.371307000	1.996839000
H	0.000000000	8.749081000	0.000000000
H	0.000000000	-8.749081000	0.000000000
H	1.583660000	7.500274000	-1.461113000
H	1.583660000	-7.500274000	1.461113000
H	1.588932000	5.012107000	-1.444088000
H	1.588932000	-5.012107000	1.444088000
H	5.012107000	1.588932000	-1.444088000

H	5.012107000	-1.588932000	1.444088000
H	7.500274000	1.583660000	-1.461113000
H	7.500274000	-1.583660000	1.461113000
H	8.749081000	0.000000000	0.000000000
H	-1.583660000	7.500274000	1.461113000
H	-1.583660000	-7.500274000	-1.461113000
H	-1.588932000	5.012107000	1.444088000
H	-1.588932000	-5.012107000	-1.444088000
H	-5.012107000	1.588932000	1.444088000
H	-5.012107000	-1.588932000	-1.444088000
H	-7.500274000	1.583660000	1.461113000
H	-7.500274000	-1.583660000	-1.461113000
H	-8.749081000	0.000000000	0.000000000
N	1.345020000	1.345020000	0.196700000
N	1.345020000	-1.345020000	-0.196700000
N	-1.345020000	1.345020000	-0.196700000
N	-1.345020000	-1.345020000	0.196700000

24. Ni[Cl₈TPP]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
C	0.571832000	4.088052000	-0.378787000
C	0.571832000	-4.088052000	0.378787000
C	0.988964000	2.705531000	-0.525557000
C	0.988964000	-2.705531000	0.525557000
C	2.265976000	2.265976000	-0.892932000
C	2.265976000	-2.265976000	0.892932000
C	2.705531000	0.988964000	-0.525557000
C	2.705531000	-0.988964000	0.525557000
C	3.223780000	3.223780000	-1.517406000
C	3.223780000	-3.223780000	1.517406000
C	3.308587000	3.308587000	-2.908776000
C	3.308587000	-3.308587000	2.908776000
C	4.040105000	4.040105000	-0.725510000
C	4.040105000	-4.040105000	0.725510000
C	4.088052000	0.571832000	-0.378787000
C	4.088052000	-0.571832000	0.378787000
C	4.201509000	4.201509000	-3.504841000
C	4.201509000	-4.201509000	3.504841000
C	4.930461000	4.930461000	-1.317579000
C	4.930461000	-4.930461000	1.317579000
C	5.013427000	5.013427000	-2.710726000
C	5.013427000	-5.013427000	2.710726000
C	-0.571832000	4.088052000	0.378787000
C	-0.571832000	-4.088052000	-0.378787000
C	-0.988964000	2.705531000	0.525557000
C	-0.988964000	-2.705531000	-0.525557000
C	-2.265976000	2.265976000	0.892932000
C	-2.265976000	-2.265976000	-0.892932000
C	-2.705531000	0.988964000	0.525557000

C	-2.705531000	-0.988964000	-0.525557000
C	-3.223780000	3.223780000	1.517406000
C	-3.223780000	-3.223780000	-1.517406000
C	-3.308587000	3.308587000	2.908776000
C	-3.308587000	-3.308587000	-2.908776000
C	-4.040105000	4.040105000	0.725510000
C	-4.040105000	-4.040105000	-0.725510000
C	-4.088052000	0.571832000	0.378787000
C	-4.088052000	-0.571832000	-0.378787000
C	-4.201509000	4.201509000	3.504841000
C	-4.201509000	-4.201509000	-3.504841000
C	-4.930461000	4.930461000	1.317579000
C	-4.930461000	-4.930461000	-1.317579000
C	-5.013427000	5.013427000	2.710726000
C	-5.013427000	-5.013427000	-2.710726000
C1	1.295489000	5.521913000	-0.981957000
C1	1.295489000	-5.521913000	0.981957000
C1	5.521913000	1.295489000	-0.981957000
C1	5.521913000	-1.295489000	0.981957000
C1	-1.295489000	5.521913000	0.981957000
C1	-1.295489000	-5.521913000	-0.981957000
C1	-5.521913000	1.295489000	0.981957000
C1	-5.521913000	-1.295489000	-0.981957000
H	2.672108000	2.672108000	-3.522575000
H	2.672108000	-2.672108000	3.522575000
H	3.968660000	3.968660000	0.359029000
H	3.968660000	-3.968660000	-0.359029000
H	4.261692000	4.261692000	-4.590583000
H	4.261692000	-4.261692000	4.590583000
H	5.561026000	5.561026000	-0.692514000
H	5.561026000	-5.561026000	0.692514000
H	5.710101000	5.710101000	-3.175986000
H	5.710101000	-5.710101000	3.175986000
H	-2.672108000	2.672108000	3.522575000
H	-2.672108000	-2.672108000	-3.522575000
H	-3.968660000	3.968660000	-0.359029000
H	-3.968660000	-3.968660000	0.359029000
H	-4.261692000	4.261692000	4.590583000
H	-4.261692000	-4.261692000	-4.590583000
H	-5.561026000	5.561026000	0.692514000
H	-5.561026000	-5.561026000	-0.692514000
H	-5.710101000	5.710101000	3.175986000
H	-5.710101000	-5.710101000	-3.175986000
N	0.000000000	1.894139000	0.000000000
N	0.000000000	-1.894139000	0.000000000
N	1.894139000	0.000000000	0.000000000
N	-1.894139000	0.000000000	0.000000000

25. Pd[Cl₈TPP]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.000000000
C	0.000000000	3.424764000	0.000000000
C	0.000000000	4.911455000	0.000000000
C	0.000000000	7.709696000	0.000000000
C	0.000000000	-3.424764000	0.000000000
C	0.000000000	-4.911455000	0.000000000
C	0.000000000	-7.709696000	0.000000000
C	0.796018000	7.009795000	-0.910799000
C	0.796018000	-7.009795000	0.910799000
C	0.801610000	5.616663000	-0.905140000
C	0.801610000	-5.616663000	0.905140000
C	1.168075000	2.754152000	0.388325000
C	1.168075000	-2.754152000	-0.388325000
C	2.350764000	3.322000000	1.009233000
C	2.350764000	-3.322000000	-1.009233000
C	2.754152000	1.168075000	0.388325000
C	2.754152000	-1.168075000	-0.388325000
C	3.322000000	2.350764000	1.009233000
C	3.322000000	-2.350764000	-1.009233000
C	3.424764000	0.000000000	0.000000000
C	4.911455000	0.000000000	0.000000000
C	5.616663000	0.801610000	-0.905140000
C	5.616663000	-0.801610000	0.905140000
C	7.009795000	0.796018000	-0.910799000
C	7.009795000	-0.796018000	0.910799000
C	7.709696000	0.000000000	0.000000000
C	-0.796018000	7.009795000	0.910799000
C	-0.796018000	-7.009795000	-0.910799000
C	-0.801610000	5.616663000	0.905140000
C	-0.801610000	-5.616663000	-0.905140000
C	-1.168075000	2.754152000	-0.388325000
C	-1.168075000	-2.754152000	0.388325000
C	-2.350764000	3.322000000	-1.009233000
C	-2.350764000	-3.322000000	1.009233000
C	-2.754152000	1.168075000	-0.388325000
C	-2.754152000	-1.168075000	0.388325000
C	-3.322000000	2.350764000	-1.009233000
C	-3.322000000	-2.350764000	1.009233000
C	-3.424764000	0.000000000	0.000000000
C	-4.911455000	0.000000000	0.000000000
C	-5.616663000	0.801610000	0.905140000
C	-5.616663000	-0.801610000	-0.905140000
C	-7.009795000	0.796018000	0.910799000
C	-7.009795000	-0.796018000	-0.910799000
C	-7.709696000	0.000000000	0.000000000
Cl	2.524087000	4.856650000	1.757805000
Cl	2.524087000	-4.856650000	-1.757805000
Cl	4.856650000	2.524087000	1.757805000

C1	4.856650000	-2.524087000	-1.757805000
C1	-2.524087000	4.856650000	-1.757805000
C1	-2.524087000	-4.856650000	1.757805000
C1	-4.856650000	2.524087000	-1.757805000
C1	-4.856650000	-2.524087000	1.757805000
H	0.000000000	8.799235000	0.000000000
H	0.000000000	-8.799235000	0.000000000
H	1.416247000	7.550677000	-1.624020000
H	1.416247000	-7.550677000	1.624020000
H	1.424646000	5.062389000	-1.606225000
H	1.424646000	-5.062389000	1.606225000
H	5.062389000	1.424646000	-1.606225000
H	5.062389000	-1.424646000	1.606225000
H	7.550677000	1.416247000	-1.624020000
H	7.550677000	-1.416247000	1.624020000
H	8.799235000	0.000000000	0.000000000
H	-1.416247000	7.550677000	1.624020000
H	-1.416247000	-7.550677000	-1.624020000
H	-1.424646000	5.062389000	1.606225000
H	-1.424646000	-5.062389000	-1.606225000
H	-5.062389000	1.424646000	1.606225000
H	-5.062389000	-1.424646000	-1.606225000
H	-7.550677000	1.416247000	1.624020000
H	-7.550677000	-1.416247000	-1.624020000
H	-8.799235000	0.000000000	0.000000000
N	1.425004000	1.425004000	0.112717000
N	1.425004000	-1.425004000	-0.112717000
N	-1.425004000	1.425004000	-0.112717000
N	-1.425004000	-1.425004000	0.112717000

26. Pd[Cl₃TPP]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
C	0.644682000	4.218940000	-0.231834000
C	0.644682000	-4.218940000	0.231834000
C	1.081011000	2.832468000	-0.310849000
C	1.081011000	-2.832468000	0.310849000
C	2.396101000	2.396101000	-0.520275000
C	2.396101000	-2.396101000	0.520275000
C	2.832468000	1.081011000	-0.310849000
C	2.832468000	-1.081011000	0.310849000
C	3.421594000	3.421594000	-0.877419000
C	3.421594000	-3.421594000	0.877419000
C	3.696318000	3.696318000	-2.218745000
C	3.696318000	-3.696318000	2.218745000
C	4.110797000	4.110797000	0.126341000
C	4.110797000	-4.110797000	-0.126341000
C	4.218940000	0.644682000	-0.231834000
C	4.218940000	-0.644682000	0.231834000
C	4.653587000	4.653587000	-2.555466000

C	4.653587000	-4.653587000	2.555466000
C	5.066170000	5.066170000	-0.208069000
C	5.066170000	-5.066170000	0.208069000
C	5.339854000	5.339854000	-1.551162000
C	5.339854000	-5.339854000	1.551162000
C	-0.644682000	4.218940000	0.231834000
C	-0.644682000	-4.218940000	-0.231834000
C	-1.081011000	2.832468000	0.310849000
C	-1.081011000	-2.832468000	-0.310849000
C	-2.396101000	2.396101000	0.520275000
C	-2.396101000	-2.396101000	-0.520275000
C	-2.832468000	1.081011000	0.310849000
C	-2.832468000	-1.081011000	-0.310849000
C	-3.421594000	3.421594000	0.877419000
C	-3.421594000	-3.421594000	-0.877419000
C	-3.696318000	3.696318000	2.218745000
C	-3.696318000	-3.696318000	-2.218745000
C	-4.110797000	4.110797000	-0.126341000
C	-4.110797000	-4.110797000	0.126341000
C	-4.218940000	0.644682000	0.231834000
C	-4.218940000	-0.644682000	-0.231834000
C	-4.653587000	4.653587000	2.555466000
C	-4.653587000	-4.653587000	-2.555466000
C	-5.066170000	5.066170000	0.208069000
C	-5.066170000	-5.066170000	-0.208069000
C	-5.339854000	5.339854000	1.551162000
C	-5.339854000	-5.339854000	-1.551162000
C1	1.475850000	5.670522000	-0.618543000
C1	1.475850000	-5.670522000	0.618543000
C1	5.670522000	1.475850000	-0.618543000
C1	5.670522000	-1.475850000	0.618543000
C1	-1.475850000	5.670522000	0.618543000
C1	-1.475850000	-5.670522000	-0.618543000
C1	-5.670522000	1.475850000	0.618543000
C1	-5.670522000	-1.475850000	-0.618543000
H	3.156502000	3.156502000	-2.995839000
H	3.156502000	-3.156502000	2.995839000
H	3.889953000	3.889953000	1.169920000
H	3.889953000	-3.889953000	-1.169920000
H	4.863558000	4.863558000	-3.603267000
H	4.863558000	-4.863558000	3.603267000
H	5.598439000	5.598439000	0.578845000
H	5.598439000	-5.598439000	-0.578845000
H	6.087450000	6.087450000	-1.814548000
H	6.087450000	-6.087450000	1.814548000
H	-3.156502000	3.156502000	2.995839000
H	-3.156502000	-3.156502000	-2.995839000
H	-3.889953000	3.889953000	-1.169920000
H	-3.889953000	-3.889953000	1.169920000
H	-4.863558000	4.863558000	3.603267000
H	-4.863558000	-4.863558000	-3.603267000

H	-5.598439000	5.598439000	-0.578845000
H	-5.598439000	-5.598439000	0.578845000
H	-6.087450000	6.087450000	1.814548000
H	-6.087450000	-6.087450000	-1.814548000
N	0.000000000	2.027486000	0.000000000
N	0.000000000	-2.027486000	0.000000000
N	2.027486000	0.000000000	0.000000000
N	-2.027486000	0.000000000	0.000000000

27. Pt[Cl₈TPP]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.000000000
C	0.000000000	3.427560000	0.000000000
C	0.000000000	4.916076000	0.000000000
C	0.000000000	7.713729000	0.000000000
C	0.000000000	-3.427560000	0.000000000
C	0.000000000	-4.916076000	0.000000000
C	0.000000000	-7.713729000	0.000000000
C	0.754341000	7.013874000	-0.945556000
C	0.754341000	-7.013874000	0.945556000
C	0.759529000	5.620608000	-0.940691000
C	0.759529000	-5.620608000	0.940691000
C	1.172099000	2.761277000	0.381043000
C	1.172099000	-2.761277000	-0.381043000
C	2.367673000	3.338077000	0.965223000
C	2.367673000	-3.338077000	-0.965223000
C	2.761277000	1.172099000	0.381043000
C	2.761277000	-1.172099000	-0.381043000
C	3.338077000	2.367673000	0.965223000
C	3.338077000	-2.367673000	-0.965223000
C	3.427560000	0.000000000	0.000000000
C	4.916076000	0.000000000	0.000000000
C	5.620608000	0.759529000	-0.940691000
C	5.620608000	-0.759529000	0.940691000
C	7.013874000	0.754341000	-0.945556000
C	7.013874000	-0.754341000	0.945556000
C	7.713729000	0.000000000	0.000000000
C	-0.754341000	7.013874000	0.945556000
C	-0.754341000	-7.013874000	-0.945556000
C	-0.759529000	5.620608000	0.940691000
C	-0.759529000	-5.620608000	-0.940691000
C	-1.172099000	2.761277000	-0.381043000
C	-1.172099000	-2.761277000	0.381043000
C	-2.367673000	3.338077000	-0.965223000
C	-2.367673000	-3.338077000	0.965223000
C	-2.761277000	1.172099000	-0.381043000
C	-2.761277000	-1.172099000	0.381043000
C	-3.338077000	2.367673000	-0.965223000
C	-3.338077000	-2.367673000	0.965223000
C	-3.427560000	0.000000000	0.000000000

C	-4.916076000	0.000000000	0.000000000
C	-5.620608000	0.759529000	0.940691000
C	-5.620608000	-0.759529000	-0.940691000
C	-7.013874000	0.754341000	0.945556000
C	-7.013874000	-0.754341000	-0.945556000
C	-7.713729000	0.000000000	0.000000000
Cl	2.562015000	4.887529000	1.676690000
Cl	2.562015000	-4.887529000	-1.676690000
Cl	4.887529000	2.562015000	1.676690000
Cl	4.887529000	-2.562015000	-1.676690000
Cl	-2.562015000	4.887529000	-1.676690000
Cl	-2.562015000	-4.887529000	1.676690000
Cl	-4.887529000	2.562015000	-1.676690000
Cl	-4.887529000	-2.562015000	1.676690000
H	0.000000000	8.803266000	0.000000000
H	0.000000000	-8.803266000	0.000000000
H	1.342068000	7.554815000	-1.685794000
H	1.342068000	-7.554815000	1.685794000
H	1.349743000	5.066260000	-1.669593000
H	1.349743000	-5.066260000	1.669593000
H	5.066260000	1.349743000	-1.669593000
H	5.066260000	-1.349743000	1.669593000
H	7.554815000	1.342068000	-1.685794000
H	7.554815000	-1.342068000	1.685794000
H	8.803266000	0.000000000	0.000000000
H	-1.342068000	7.554815000	1.685794000
H	-1.342068000	-7.554815000	-1.685794000
H	-1.349743000	5.066260000	1.669593000
H	-1.349743000	-5.066260000	-1.669593000
H	-5.066260000	1.349743000	1.669593000
H	-5.066260000	-1.349743000	-1.669593000
H	-7.554815000	1.342068000	1.685794000
H	-7.554815000	-1.342068000	-1.685794000
H	-8.803266000	0.000000000	0.000000000
N	1.421301000	1.421301000	0.136661000
N	1.421301000	-1.421301000	-0.136661000
N	-1.421301000	1.421301000	-0.136661000
N	-1.421301000	-1.421301000	0.136661000

28. Pt[Cl₈TPP]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
C	0.647422000	4.221104000	-0.222723000
C	0.647422000	-4.221104000	0.222723000
C	1.085739000	2.837401000	-0.299174000
C	1.085739000	-2.837401000	0.299174000
C	2.401545000	2.401545000	-0.500571000
C	2.401545000	-2.401545000	0.500571000
C	2.837401000	1.085739000	-0.299174000
C	2.837401000	-1.085739000	0.299174000

C	3.429675000	3.429675000	-0.843845000
C	3.429675000	-3.429675000	0.843845000
C	3.713427000	3.713427000	-2.181447000
C	3.713427000	-3.713427000	2.181447000
C	4.111770000	4.111770000	0.169544000
C	4.111770000	-4.111770000	-0.169544000
C	4.221104000	0.647422000	-0.222723000
C	4.221104000	-0.647422000	0.222723000
C	4.672949000	4.672949000	-2.504901000
C	4.672949000	-4.672949000	2.504901000
C	5.069401000	5.069401000	-0.151811000
C	5.069401000	-5.069401000	0.151811000
C	5.352253000	5.352253000	-1.491117000
C	5.352253000	-5.352253000	1.491117000
C	-0.647422000	4.221104000	0.222723000
C	-0.647422000	-4.221104000	-0.222723000
C	-1.085739000	2.837401000	0.299174000
C	-1.085739000	-2.837401000	-0.299174000
C	-2.401545000	2.401545000	0.500571000
C	-2.401545000	-2.401545000	-0.500571000
C	-2.837401000	1.085739000	0.299174000
C	-2.837401000	-1.085739000	-0.299174000
C	-3.429675000	3.429675000	0.843845000
C	-3.429675000	-3.429675000	-0.843845000
C	-3.713427000	3.713427000	2.181447000
C	-3.713427000	-3.713427000	-2.181447000
C	-4.111770000	4.111770000	-0.169544000
C	-4.111770000	-4.111770000	0.169544000
C	-4.221104000	0.647422000	0.222723000
C	-4.221104000	-0.647422000	-0.222723000
C	-4.672949000	4.672949000	2.504901000
C	-4.672949000	-4.672949000	-2.504901000
C	-5.069401000	5.069401000	0.151811000
C	-5.069401000	-5.069401000	-0.151811000
C	-5.352253000	5.352253000	1.491117000
C	-5.352253000	-5.352253000	-1.491117000
C1	1.483339000	5.673554000	-0.595232000
C1	1.483339000	-5.673554000	0.595232000
C1	5.673554000	1.483339000	-0.595232000
C1	5.673554000	-1.483339000	0.595232000
C1	-1.483339000	5.673554000	0.595232000
C1	-1.483339000	-5.673554000	-0.595232000
C1	-5.673554000	1.483339000	0.595232000
C1	-5.673554000	-1.483339000	-0.595232000
H	3.178831000	3.178831000	-2.965733000
H	3.178831000	-3.178831000	2.965733000
H	3.883628000	3.883628000	1.209981000
H	3.883628000	-3.883628000	-1.209981000
H	4.890147000	4.890147000	-3.549740000
H	4.890147000	-4.890147000	3.549740000
H	5.596287000	5.596287000	0.642333000

H	5.596287000	-5.596287000	-0.642333000
H	6.101646000	6.101646000	-1.744187000
H	6.101646000	-6.101646000	1.744187000
H	-3.178831000	3.178831000	2.965733000
H	-3.178831000	-3.178831000	-2.965733000
H	-3.883628000	3.883628000	-1.209981000
H	-3.883628000	-3.883628000	1.209981000
H	-4.890147000	4.890147000	3.549740000
H	-4.890147000	-4.890147000	-3.549740000
H	-5.596287000	5.596287000	-0.642333000
H	-5.596287000	-5.596287000	0.642333000
H	-6.101646000	6.101646000	1.744187000
H	-6.101646000	-6.101646000	-1.744187000
N	0.000000000	2.028486000	0.000000000
N	0.000000000	-2.028486000	0.000000000
N	2.028486000	0.000000000	0.000000000
N	-2.028486000	0.000000000	0.000000000

29. Zn[Cl₂TPP]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.000000000
C	0.000000000	3.433360000	0.000000000
C	0.000000000	4.921250000	0.000000000
C	0.000000000	7.720176000	0.000000000
C	0.000000000	-3.433360000	0.000000000
C	0.000000000	-4.921250000	0.000000000
C	0.000000000	-7.720176000	0.000000000
C	0.749235000	7.020163000	-0.949468000
C	0.749235000	-7.020163000	0.949468000
C	0.754739000	5.626987000	-0.944204000
C	0.754739000	-5.626987000	0.944204000
C	1.187341000	2.770371000	0.364662000
C	1.187341000	-2.770371000	-0.364662000
C	2.382098000	3.355498000	0.944256000
C	2.382098000	-3.355498000	-0.944256000
C	2.770371000	1.187341000	0.364662000
C	2.770371000	-1.187341000	-0.364662000
C	3.355498000	2.382098000	0.944256000
C	3.355498000	-2.382098000	-0.944256000
C	3.433360000	0.000000000	0.000000000
C	4.921250000	0.000000000	0.000000000
C	5.626987000	0.754739000	-0.944204000
C	5.626987000	-0.754739000	0.944204000
C	7.020163000	0.749235000	-0.949468000
C	7.020163000	-0.749235000	0.949468000
C	7.720176000	0.000000000	0.000000000
C	-0.749235000	7.020163000	0.949468000
C	-0.749235000	-7.020163000	-0.949468000
C	-0.754739000	5.626987000	0.944204000
C	-0.754739000	-5.626987000	-0.944204000

C	-1.187341000	2.770371000	-0.364662000
C	-1.187341000	-2.770371000	0.364662000
C	-2.382098000	3.355498000	-0.944256000
C	-2.382098000	-3.355498000	0.944256000
C	-2.770371000	1.187341000	-0.364662000
C	-2.770371000	-1.187341000	0.364662000
C	-3.355498000	2.382098000	-0.944256000
C	-3.355498000	-2.382098000	0.944256000
C	-3.433360000	0.000000000	0.000000000
C	-4.921250000	0.000000000	0.000000000
C	-5.626987000	0.754739000	0.944204000
C	-5.626987000	-0.754739000	-0.944204000
C	-7.020163000	0.749235000	0.949468000
C	-7.020163000	-0.749235000	-0.949468000
C	-7.720176000	0.000000000	0.000000000
C1	2.586312000	4.906191000	1.652611000
C1	2.586312000	-4.906191000	-1.652611000
C1	4.906191000	2.586312000	1.652611000
C1	4.906191000	-2.586312000	-1.652611000
C1	-2.586312000	4.906191000	-1.652611000
C1	-2.586312000	-4.906191000	1.652611000
C1	-4.906191000	2.586312000	-1.652611000
C1	-4.906191000	-2.586312000	1.652611000
H	0.000000000	8.809737000	0.000000000
H	0.000000000	-8.809737000	0.000000000
H	1.332974000	7.561109000	-1.692872000
H	1.332974000	-7.561109000	1.692872000
H	1.341420000	5.072980000	-1.676191000
H	1.341420000	-5.072980000	1.676191000
H	5.072980000	1.341420000	-1.676191000
H	5.072980000	-1.341420000	1.676191000
H	7.561109000	1.332974000	-1.692872000
H	7.561109000	-1.332974000	1.692872000
H	8.809737000	0.000000000	0.000000000
H	-1.332974000	7.561109000	1.692872000
H	-1.332974000	-7.561109000	-1.692872000
H	-1.341420000	5.072980000	1.676191000
H	-1.341420000	-5.072980000	-1.676191000
H	-5.072980000	1.341420000	1.676191000
H	-5.072980000	-1.341420000	-1.676191000
H	-7.561109000	1.332974000	1.692872000
H	-7.561109000	-1.332974000	-1.692872000
H	-8.809737000	0.000000000	0.000000000
N	1.438154000	1.438154000	0.112702000
N	1.438154000	-1.438154000	-0.112702000
N	-1.438154000	1.438154000	-0.112702000
N	-1.438154000	-1.438154000	0.112702000

30. Zn[Cl₈TPP]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
C	0.666539000	4.255953000	-0.163704000
C	0.666539000	-4.255953000	0.163704000
C	1.101555000	2.869062000	-0.215109000
C	1.101555000	-2.869062000	0.215109000
C	2.428891000	2.428891000	-0.361584000
C	2.428891000	-2.428891000	0.361584000
C	2.869062000	1.101555000	-0.215109000
C	2.869062000	-1.101555000	0.215109000
C	3.470755000	3.470755000	-0.610131000
C	3.470755000	-3.470755000	0.610131000
C	3.816796000	3.816796000	-1.918504000
C	3.816796000	-3.816796000	1.918504000
C	4.104252000	4.104252000	0.464110000
C	4.104252000	-4.104252000	-0.464110000
C	4.255953000	0.666539000	-0.163704000
C	4.255953000	-0.666539000	0.163704000
C	4.788849000	4.788849000	-2.152257000
C	4.788849000	-4.788849000	2.152257000
C	5.075016000	5.075016000	0.232411000
C	5.075016000	-5.075016000	-0.232411000
C	5.419634000	5.419634000	-1.077387000
C	5.419634000	-5.419634000	1.077387000
C	-0.666539000	4.255953000	0.163704000
C	-0.666539000	-4.255953000	-0.163704000
C	-1.101555000	2.869062000	0.215109000
C	-1.101555000	-2.869062000	-0.215109000
C	-2.428891000	2.428891000	0.361584000
C	-2.428891000	-2.428891000	-0.361584000
C	-2.869062000	1.101555000	0.215109000
C	-2.869062000	-1.101555000	-0.215109000
C	-3.470755000	3.470755000	0.610131000
C	-3.470755000	-3.470755000	-0.610131000
C	-3.816796000	3.816796000	1.918504000
C	-3.816796000	-3.816796000	-1.918504000
C	-4.104252000	4.104252000	-0.464110000
C	-4.104252000	-4.104252000	0.464110000
C	-4.255953000	0.666539000	0.163704000
C	-4.255953000	-0.666539000	-0.163704000
C	-4.788849000	4.788849000	2.152257000
C	-4.788849000	-4.788849000	-2.152257000
C	-5.075016000	5.075016000	-0.232411000
C	-5.075016000	-5.075016000	0.232411000
C	-5.419634000	5.419634000	1.077387000
C	-5.419634000	-5.419634000	-1.077387000
Cl	1.525389000	5.717078000	-0.445801000
Cl	1.525389000	-5.717078000	0.445801000
Cl	5.717078000	1.525389000	-0.445801000

C1	5.717078000	-1.525389000	0.445801000
C1	-1.525389000	5.717078000	0.445801000
C1	-1.525389000	-5.717078000	-0.445801000
C1	-5.717078000	1.525389000	0.445801000
C1	-5.717078000	-1.525389000	-0.445801000
H	3.320031000	3.320031000	-2.751129000
H	3.320031000	-3.320031000	2.751129000
H	3.828529000	3.828529000	1.481239000
H	3.828529000	-3.828529000	-1.481239000
H	5.054162000	5.054162000	-3.174660000
H	5.054162000	-5.054162000	3.174660000
H	5.563862000	5.563862000	1.073834000
H	5.563862000	-5.563862000	-1.073834000
H	6.179197000	6.179197000	-1.260044000
H	6.179197000	-6.179197000	1.260044000
H	-3.320031000	3.320031000	2.751129000
H	-3.320031000	-3.320031000	-2.751129000
H	-3.828529000	3.828529000	-1.481239000
H	-3.828529000	-3.828529000	1.481239000
H	-5.054162000	5.054162000	3.174660000
H	-5.054162000	-5.054162000	-3.174660000
H	-5.563862000	5.563862000	-1.073834000
H	-5.563862000	-5.563862000	1.073834000
H	-6.179197000	6.179197000	1.260044000
H	-6.179197000	-6.179197000	-1.260044000
N	0.000000000	2.059916000	0.000000000
N	0.000000000	-2.059916000	0.000000000
N	2.059916000	0.000000000	0.000000000
N	-2.059916000	0.000000000	0.000000000

31. Cu[(CF₃)₈TPP]; S = ½ (saddled)

C	0.000000000	0.000000000	3.387892000
C	0.000000000	0.000000000	4.856074000
C	0.000000000	0.000000000	7.657429000
C	0.000000000	0.000000000	-3.387892000
C	0.000000000	0.000000000	-4.856074000
C	0.000000000	0.000000000	-7.657429000
C	1.084283000	0.576831000	-2.670281000
C	1.084283000	-0.576831000	2.670281000
C	1.116974000	0.465525000	6.958373000
C	1.116974000	-0.465525000	-6.958373000
C	1.122546000	0.454355000	5.567737000
C	1.122546000	-0.454355000	-5.567737000
C	2.057560000	2.426538000	-4.299652000
C	2.057560000	-2.426538000	4.299652000
C	2.079493000	1.559696000	-3.058854000
C	2.079493000	-1.559696000	3.058854000
C	2.619052000	0.620116000	-1.056197000
C	2.619052000	-0.620116000	1.056197000

C	3.016998000	1.611657000	-2.031300000
C	3.016998000	-1.611657000	2.031300000
C	3.340853000	0.000000000	0.000000000
C	4.054929000	2.699303000	-1.833002000
C	4.054929000	-2.699303000	1.833002000
C	4.803684000	0.000000000	0.000000000
C	5.519179000	0.214893000	1.193052000
C	5.519179000	-0.214893000	-1.193052000
C	6.909296000	0.218120000	1.190596000
C	6.909296000	-0.218120000	-1.190596000
C	7.609327000	0.000000000	0.000000000
C	-1.084283000	0.576831000	2.670281000
C	-1.084283000	-0.576831000	-2.670281000
C	-1.116974000	0.465525000	-6.958373000
C	-1.116974000	-0.465525000	6.958373000
C	-1.122546000	0.454355000	-5.567737000
C	-1.122546000	-0.454355000	5.567737000
C	-2.057560000	2.426538000	4.299652000
C	-2.057560000	-2.426538000	-4.299652000
C	-2.079493000	1.559696000	3.058854000
C	-2.079493000	-1.559696000	-3.058854000
C	-2.619052000	0.620116000	1.056197000
C	-2.619052000	-0.620116000	-1.056197000
C	-3.016998000	1.611657000	2.031300000
C	-3.016998000	-1.611657000	-2.031300000
C	-3.340853000	0.000000000	0.000000000
C	-4.054929000	2.699303000	1.833002000
C	-4.054929000	-2.699303000	-1.833002000
C	-4.803684000	0.000000000	0.000000000
C	-5.519179000	0.214893000	-1.193052000
C	-5.519179000	-0.214893000	1.193052000
C	-6.909296000	0.218120000	-1.190596000
C	-6.909296000	-0.218120000	1.190596000
C	-7.609327000	0.000000000	0.000000000
Cu	0.000000000	0.000000000	0.000000000
F	0.796569000	2.648994000	-4.742306000
F	0.796569000	-2.648994000	4.742306000
F	2.610773000	3.646766000	-4.103636000
F	2.610773000	-3.646766000	4.103636000
F	2.765508000	1.851745000	-5.317332000
F	2.765508000	-1.851745000	5.317332000
F	3.456142000	3.917696000	-1.725492000
F	3.456142000	-3.917696000	1.725492000
F	4.778738000	2.558314000	-0.700797000
F	4.778738000	-2.558314000	0.700797000
F	4.933428000	2.759222000	-2.873040000
F	4.933428000	-2.759222000	2.873040000
F	-0.796569000	2.648994000	4.742306000
F	-0.796569000	-2.648994000	-4.742306000
F	-2.610773000	3.646766000	4.103636000
F	-2.610773000	-3.646766000	-4.103636000

F	-2.765508000	1.851745000	5.317332000
F	-2.765508000	-1.851745000	-5.317332000
F	-3.456142000	3.917696000	1.725492000
F	-3.456142000	-3.917696000	-1.725492000
F	-4.778738000	2.558314000	0.700797000
F	-4.778738000	-2.558314000	-0.700797000
F	-4.933428000	2.759222000	2.873040000
F	-4.933428000	-2.759222000	-2.873040000
H	0.000000000	0.000000000	8.746847000
H	0.000000000	0.000000000	-8.746847000
H	1.986620000	0.834994000	7.498890000
H	1.986620000	-0.834994000	-7.498890000
H	1.987411000	0.820806000	5.017549000
H	1.987411000	-0.820806000	-5.017549000
H	4.972684000	0.406358000	2.115364000
H	4.972684000	-0.406358000	-2.115364000
H	7.450186000	0.397512000	2.118201000
H	7.450186000	-0.397512000	-2.118201000
H	8.698621000	0.000000000	0.000000000
H	-1.986620000	0.834994000	-7.498890000
H	-1.986620000	-0.834994000	7.498890000
H	-1.987411000	0.820806000	-5.017549000
H	-1.987411000	-0.820806000	5.017549000
H	-4.972684000	0.406358000	-2.115364000
H	-4.972684000	-0.406358000	2.115364000
H	-7.450186000	0.397512000	-2.118201000
H	-7.450186000	-0.397512000	2.118201000
H	-8.698621000	0.000000000	0.000000000
N	1.390072000	0.124441000	-1.410669000
N	1.390072000	-0.124441000	1.410669000
N	-1.390072000	0.124441000	1.410669000
N	-1.390072000	-0.124441000	-1.410669000

32. Cu[(CF₃)₈TPP]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
C	0.519799000	4.086691000	0.457870000
C	0.519799000	-4.086691000	-0.457870000
C	0.940463000	2.695455000	0.622886000
C	0.940463000	-2.695455000	-0.622886000
C	0.949211000	5.323037000	1.230133000
C	0.949211000	-5.323037000	-1.230133000
C	2.193635000	2.193635000	1.071039000
C	2.193635000	-2.193635000	-1.071039000
C	2.695455000	0.940463000	0.622886000
C	2.695455000	-0.940463000	-0.622886000
C	2.926522000	2.926522000	3.324977000
C	2.926522000	-2.926522000	-3.324977000
C	3.051419000	3.051419000	1.934105000
C	3.051419000	-3.051419000	-1.934105000

C	3.707816000	3.707816000	4.170292000
C	3.707816000	-3.707816000	-4.170292000
C	3.962774000	3.962774000	1.401759000
C	3.962774000	-3.962774000	-1.401759000
C	4.086691000	0.519799000	0.457870000
C	4.086691000	-0.519799000	-0.457870000
C	4.620640000	4.620640000	3.632794000
C	4.620640000	-4.620640000	-3.632794000
C	4.746359000	4.746359000	2.250236000
C	4.746359000	-4.746359000	-2.250236000
C	5.323037000	0.949211000	1.230133000
C	5.323037000	-0.949211000	-1.230133000
C	-0.519799000	4.086691000	-0.457870000
C	-0.519799000	-4.086691000	0.457870000
C	-0.940463000	2.695455000	-0.622886000
C	-0.940463000	-2.695455000	0.622886000
C	-0.949211000	5.323037000	-1.230133000
C	-0.949211000	-5.323037000	1.230133000
C	-2.193635000	2.193635000	-1.071039000
C	-2.193635000	-2.193635000	1.071039000
C	-2.695455000	0.940463000	-0.622886000
C	-2.695455000	-0.940463000	0.622886000
C	-2.926522000	2.926522000	-3.324977000
C	-2.926522000	-2.926522000	3.324977000
C	-3.051419000	3.051419000	-1.934105000
C	-3.051419000	-3.051419000	1.934105000
C	-3.707816000	3.707816000	-4.170292000
C	-3.707816000	-3.707816000	4.170292000
C	-3.962774000	3.962774000	-1.401759000
C	-3.962774000	-3.962774000	1.401759000
C	-4.086691000	0.519799000	-0.457870000
C	-4.086691000	-0.519799000	0.457870000
C	-4.620640000	4.620640000	-3.632794000
C	-4.620640000	-4.620640000	3.632794000
C	-4.746359000	4.746359000	-2.250236000
C	-4.746359000	-4.746359000	2.250236000
C	-5.323037000	0.949211000	-1.230133000
C	-5.323037000	-0.949211000	1.230133000
F	0.060309000	6.237307000	-1.276978000
F	0.060309000	-6.237307000	1.276978000
F	1.215735000	5.024100000	2.522220000
F	1.215735000	-5.024100000	-2.522220000
F	2.031538000	5.952135000	0.706808000
F	2.031538000	-5.952135000	-0.706808000
F	5.024100000	1.215735000	2.522220000
F	5.024100000	-1.215735000	-2.522220000
F	5.952135000	2.031538000	0.706808000
F	5.952135000	-2.031538000	-0.706808000
F	6.237307000	0.060309000	-1.276978000
F	6.237307000	-0.060309000	1.276978000
F	-0.060309000	6.237307000	1.276978000

F	-0.060309000	-6.237307000	-1.276978000
F	-1.215735000	5.024100000	-2.522220000
F	-1.215735000	-5.024100000	2.522220000
F	-2.031538000	5.952135000	-0.706808000
F	-2.031538000	-5.952135000	0.706808000
F	-5.024100000	1.215735000	-2.522220000
F	-5.024100000	-1.215735000	2.522220000
F	-5.952135000	2.031538000	-0.706808000
F	-5.952135000	-2.031538000	0.706808000
F	-6.237307000	0.060309000	1.276978000
F	-6.237307000	-0.060309000	-1.276978000
H	2.213126000	2.213126000	3.735478000
H	2.213126000	-2.213126000	-3.735478000
H	3.605409000	3.605409000	5.249455000
H	3.605409000	-3.605409000	-5.249455000
H	4.057554000	4.057554000	0.322057000
H	4.057554000	-4.057554000	-0.322057000
H	5.232735000	5.232735000	4.294220000
H	5.232735000	-5.232735000	-4.294220000
H	5.454982000	5.454982000	1.825238000
H	5.454982000	-5.454982000	-1.825238000
H	-2.213126000	2.213126000	-3.735478000
H	-2.213126000	-2.213126000	3.735478000
H	-3.605409000	3.605409000	-5.249455000
H	-3.605409000	-3.605409000	5.249455000
H	-4.057554000	4.057554000	-0.322057000
H	-4.057554000	-4.057554000	0.322057000
H	-5.232735000	5.232735000	-4.294220000
H	-5.232735000	-5.232735000	4.294220000
H	-5.454982000	5.454982000	-1.825238000
H	-5.454982000	-5.454982000	1.825238000
N	0.000000000	1.918601000	0.000000000
N	0.000000000	-1.918601000	0.000000000
N	1.918601000	0.000000000	0.000000000
N	-1.918601000	0.000000000	0.000000000

33. Ni[(CF₃)₈TPP]; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.345188000
C	0.000000000	0.000000000	4.818864000
C	0.000000000	0.000000000	7.618427000
C	0.000000000	0.000000000	-3.345188000
C	0.000000000	0.000000000	-4.818864000
C	0.000000000	0.000000000	-7.618427000
C	1.037367000	0.627808000	-2.620187000
C	1.037367000	-0.627808000	2.620187000
C	1.102127000	0.498636000	6.919439000
C	1.102127000	-0.498636000	-6.919439000
C	1.107701000	0.487551000	5.527981000

C	1.107701000	-0.487551000	-5.527981000
C	2.047798000	2.424128000	-4.279879000
C	2.047798000	-2.424128000	4.279879000
C	2.050070000	1.586345000	-3.019827000
C	2.050070000	-1.586345000	3.019827000
C	2.574017000	0.674699000	-1.002388000
C	2.574017000	-0.674699000	1.002388000
C	2.983926000	1.642901000	-1.992788000
C	2.983926000	-1.642901000	1.992788000
C	3.304423000	0.000000000	0.000000000
C	4.045303000	2.709253000	-1.805529000
C	4.045303000	-2.709253000	1.805529000
C	4.772216000	0.000000000	0.000000000
C	5.485026000	0.207548000	1.193562000
C	5.485026000	-0.207548000	-1.193562000
C	6.875916000	0.210718000	1.191493000
C	6.875916000	-0.210718000	-1.191493000
C	7.575882000	0.000000000	0.000000000
C	-1.037367000	0.627808000	2.620187000
C	-1.037367000	-0.627808000	-2.620187000
C	-1.102127000	0.498636000	-6.919439000
C	-1.102127000	-0.498636000	6.919439000
C	-1.107701000	0.487551000	-5.527981000
C	-1.107701000	-0.487551000	5.527981000
C	-2.047798000	2.424128000	4.279879000
C	-2.047798000	-2.424128000	-4.279879000
C	-2.050070000	1.586345000	3.019827000
C	-2.050070000	-1.586345000	-3.019827000
C	-2.574017000	0.674699000	1.002388000
C	-2.574017000	-0.674699000	-1.002388000
C	-2.983926000	1.642901000	1.992788000
C	-2.983926000	-1.642901000	-1.992788000
C	-3.304423000	0.000000000	0.000000000
C	-4.045303000	2.709253000	1.805529000
C	-4.045303000	-2.709253000	-1.805529000
C	-4.772216000	0.000000000	0.000000000
C	-5.485026000	0.207548000	-1.193562000
C	-5.485026000	-0.207548000	1.193562000
C	-6.875916000	0.210718000	-1.191493000
C	-6.875916000	-0.210718000	1.191493000
C	-7.575882000	0.000000000	0.000000000
F	0.791892000	2.666001000	-4.726276000
F	0.791892000	-2.666001000	4.726276000
F	2.629625000	3.634591000	-4.106408000
F	2.629625000	-3.634591000	4.106408000
F	2.742610000	1.814264000	-5.285074000
F	2.742610000	-1.814264000	5.285074000
F	3.473452000	3.942945000	-1.732797000
F	3.473452000	-3.942945000	1.732797000
F	4.747498000	2.574432000	-0.659240000
F	4.747498000	-2.574432000	0.659240000

F	4.938703000	2.727282000	-2.833779000
F	4.938703000	-2.727282000	2.833779000
F	-0.791892000	2.666001000	4.726276000
F	-0.791892000	-2.666001000	-4.726276000
F	-2.629625000	3.634591000	4.106408000
F	-2.629625000	-3.634591000	-4.106408000
F	-2.742610000	1.814264000	5.285074000
F	-2.742610000	-1.814264000	-5.285074000
F	-3.473452000	3.942945000	1.732797000
F	-3.473452000	-3.942945000	-1.732797000
F	-4.747498000	2.574432000	0.659240000
F	-4.747498000	-2.574432000	-0.659240000
F	-4.938703000	2.727282000	2.833779000
F	-4.938703000	-2.727282000	-2.833779000
H	0.000000000	0.000000000	8.707867000
H	0.000000000	0.000000000	-8.707867000
H	1.961135000	0.892869000	7.459532000
H	1.961135000	-0.892869000	-7.459532000
H	1.962663000	0.876150000	4.977326000
H	1.962663000	-0.876150000	-4.977326000
H	4.937934000	0.389137000	2.117612000
H	4.937934000	-0.389137000	-2.117612000
H	7.416476000	0.382942000	2.120633000
H	7.416476000	-0.382942000	-2.120633000
H	8.665192000	0.000000000	0.000000000
H	-1.961135000	0.892869000	-7.459532000
H	-1.961135000	-0.892869000	7.459532000
H	-1.962663000	0.876150000	-4.977326000
H	-1.962663000	-0.876150000	4.977326000
H	-4.937934000	0.389137000	-2.117612000
H	-4.937934000	-0.389137000	2.117612000
H	-7.416476000	0.382942000	-2.120633000
H	-7.416476000	-0.382942000	2.120633000
H	-8.665192000	0.000000000	0.000000000
N	1.311788000	0.222816000	-1.328768000
N	1.311788000	-0.222816000	1.328768000
N	-1.311788000	0.222816000	1.328768000
N	-1.311788000	-0.222816000	-1.328768000

34. Ni[(CF₃)₈TPP]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
C	0.491632000	4.014967000	0.486852000
C	0.491632000	-4.014967000	-0.486852000
C	0.895544000	5.246986000	1.275639000
C	0.895544000	-5.246986000	-1.275639000
C	0.901334000	2.628662000	0.677052000
C	0.901334000	-2.628662000	-0.677052000
C	2.134229000	2.134229000	1.166667000
C	2.134229000	-2.134229000	-1.166667000

C	2.628662000	0.901334000	0.677052000
C	2.628662000	-0.901334000	-0.677052000
C	2.797150000	2.797150000	3.461156000
C	2.797150000	-2.797150000	-3.461156000
C	2.964593000	2.964593000	2.079581000
C	2.964593000	-2.964593000	-2.079581000
C	3.552356000	3.552356000	4.353149000
C	3.552356000	-3.552356000	-4.353149000
C	3.891337000	3.891337000	1.602914000
C	3.891337000	-3.891337000	-1.602914000
C	4.014967000	0.491632000	0.486852000
C	4.014967000	-0.491632000	-0.486852000
C	4.480613000	4.480613000	3.871772000
C	4.480613000	-4.480613000	-3.871772000
C	4.648193000	4.648193000	2.497954000
C	4.648193000	-4.648193000	-2.497954000
C	5.246986000	0.895544000	1.275639000
C	5.246986000	-0.895544000	-1.275639000
C	-0.491632000	4.014967000	-0.486852000
C	-0.491632000	-4.014967000	0.486852000
C	-0.895544000	5.246986000	-1.275639000
C	-0.895544000	-5.246986000	1.275639000
C	-0.901334000	2.628662000	-0.677052000
C	-0.901334000	-2.628662000	0.677052000
C	-2.134229000	2.134229000	-1.166667000
C	-2.134229000	-2.134229000	1.166667000
C	-2.628662000	0.901334000	-0.677052000
C	-2.628662000	-0.901334000	0.677052000
C	-2.797150000	2.797150000	-3.461156000
C	-2.797150000	-2.797150000	3.461156000
C	-2.964593000	2.964593000	-2.079581000
C	-2.964593000	-2.964593000	2.079581000
C	-3.552356000	3.552356000	-4.353149000
C	-3.552356000	-3.552356000	4.353149000
C	-3.891337000	3.891337000	-1.602914000
C	-3.891337000	-3.891337000	1.602914000
C	-4.014967000	0.491632000	-0.486852000
C	-4.014967000	-0.491632000	0.486852000
C	-4.480613000	4.480613000	-3.871772000
C	-4.480613000	-4.480613000	3.871772000
C	-4.648193000	4.648193000	-2.497954000
C	-4.648193000	-4.648193000	2.497954000
C	-5.246986000	0.895544000	-1.275639000
C	-5.246986000	-0.895544000	1.275639000
F	0.111115000	6.164810000	-1.281402000
F	0.111115000	-6.164810000	1.281402000
F	1.114171000	4.946650000	2.576424000
F	1.114171000	-4.946650000	-2.576424000
F	1.999810000	5.871962000	0.792769000
F	1.999810000	-5.871962000	-0.792769000
F	4.946650000	1.114171000	2.576424000

F	4.946650000	-1.114171000	-2.576424000
F	5.871962000	1.999810000	0.792769000
F	5.871962000	-1.999810000	-0.792769000
F	6.164810000	0.111115000	-1.281402000
F	6.164810000	-0.111115000	1.281402000
F	-0.111115000	6.164810000	1.281402000
F	-0.111115000	-6.164810000	-1.281402000
F	-1.114171000	4.946650000	-2.576424000
F	-1.114171000	-4.946650000	2.576424000
F	-1.999810000	5.871962000	-0.792769000
F	-1.999810000	-5.871962000	0.792769000
F	-4.946650000	1.114171000	-2.576424000
F	-4.946650000	-1.114171000	2.576424000
F	-5.871962000	1.999810000	-0.792769000
F	-5.871962000	-1.999810000	0.792769000
F	-6.164810000	0.111115000	1.281402000
F	-6.164810000	-0.111115000	-1.281402000
H	2.071905000	2.071905000	3.827648000
H	2.071905000	-2.071905000	-3.827648000
H	3.417255000	3.417255000	5.425084000
H	3.417255000	-3.417255000	-5.425084000
H	4.018767000	4.018767000	0.530245000
H	4.018767000	-4.018767000	-0.530245000
H	5.072015000	5.072015000	4.569795000
H	5.072015000	-5.072015000	-4.569795000
H	5.369026000	5.369026000	2.116389000
H	5.369026000	-5.369026000	-2.116389000
H	-2.071905000	2.071905000	-3.827648000
H	-2.071905000	-2.071905000	3.827648000
H	-3.417255000	3.417255000	-5.425084000
H	-3.417255000	-3.417255000	5.425084000
H	-4.018767000	4.018767000	-0.530245000
H	-4.018767000	-4.018767000	0.530245000
H	-5.072015000	5.072015000	-4.569795000
H	-5.072015000	-5.072015000	4.569795000
H	-5.369026000	5.369026000	-2.116389000
H	-5.369026000	-5.369026000	2.116389000
N	0.000000000	1.842268000	0.000000000
N	0.000000000	-1.842268000	0.000000000
N	1.842268000	0.000000000	0.000000000
N	-1.842268000	0.000000000	0.000000000

35. Pd[(CF₃)₈TPP]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.406456000
C	0.000000000	0.000000000	4.882611000
C	0.000000000	0.000000000	7.681320000
C	0.000000000	0.000000000	-3.406456000
C	0.000000000	0.000000000	-4.882611000

C	0.000000000	0.000000000	-7.681320000
C	1.030861000	0.633318000	6.982766000
C	1.030861000	-0.633318000	-6.982766000
C	1.039710000	0.619184000	5.591336000
C	1.039710000	-0.619184000	-5.591336000
C	1.104002000	0.552641000	-2.705170000
C	1.104002000	-0.552641000	2.705170000
C	2.142387000	1.488236000	-3.113803000
C	2.142387000	-1.488236000	3.113803000
C	2.165608000	2.295379000	-4.394569000
C	2.165608000	-2.295379000	4.394569000
C	2.644806000	0.606962000	-1.069344000
C	2.644806000	-0.606962000	1.069344000
C	3.067176000	1.556076000	-2.077527000
C	3.067176000	-1.556076000	2.077527000
C	3.351372000	0.000000000	0.000000000
C	4.122313000	2.631019000	-1.885122000
C	4.122313000	-2.631019000	1.885122000
C	4.819107000	0.000000000	0.000000000
C	5.533165000	0.257208000	1.183965000
C	5.533165000	-0.257208000	-1.183965000
C	6.923685000	0.259377000	1.181921000
C	6.923685000	-0.259377000	-1.181921000
C	7.623734000	0.000000000	0.000000000
C	-1.030861000	0.633318000	-6.982766000
C	-1.030861000	-0.633318000	6.982766000
C	-1.039710000	0.619184000	-5.591336000
C	-1.039710000	-0.619184000	5.591336000
C	-1.104002000	0.552641000	2.705170000
C	-1.104002000	-0.552641000	-2.705170000
C	-2.142387000	1.488236000	3.113803000
C	-2.142387000	-1.488236000	-3.113803000
C	-2.165608000	2.295379000	4.394569000
C	-2.165608000	-2.295379000	-4.394569000
C	-2.644806000	0.606962000	1.069344000
C	-2.644806000	-0.606962000	-1.069344000
C	-3.067176000	1.556076000	2.077527000
C	-3.067176000	-1.556076000	-2.077527000
C	-3.351372000	0.000000000	0.000000000
C	-4.122313000	2.631019000	1.885122000
C	-4.122313000	-2.631019000	-1.885122000
C	-4.819107000	0.000000000	0.000000000
C	-5.533165000	0.257208000	-1.183965000
C	-5.533165000	-0.257208000	1.183965000
C	-6.923685000	0.259377000	-1.181921000
C	-6.923685000	-0.259377000	1.181921000
C	-7.623734000	0.000000000	0.000000000
F	0.918248000	2.664098000	-4.778350000
F	0.918248000	-2.664098000	4.778350000
F	2.731232000	1.588244000	-5.415474000
F	2.731232000	-1.588244000	5.415474000

F	2.886420000	3.436245000	-4.295268000
F	2.886420000	-3.436245000	4.295268000
F	3.554595000	3.868188000	-1.907852000
F	3.554595000	-3.868188000	1.907852000
F	4.749346000	2.553001000	-0.689673000
F	4.749346000	-2.553001000	0.689673000
F	5.080462000	2.594430000	-2.851571000
F	5.080462000	-2.594430000	2.851571000
F	-0.918248000	2.664098000	4.778350000
F	-0.918248000	-2.664098000	-4.778350000
F	-2.731232000	1.588244000	5.415474000
F	-2.731232000	-1.588244000	-5.415474000
F	-2.886420000	3.436245000	4.295268000
F	-2.886420000	-3.436245000	-4.295268000
F	-3.554595000	3.868188000	1.907852000
F	-3.554595000	-3.868188000	-1.907852000
F	-4.749346000	2.553001000	0.689673000
F	-4.749346000	-2.553001000	-0.689673000
F	-5.080462000	2.594430000	2.851571000
F	-5.080462000	-2.594430000	-2.851571000
H	0.000000000	0.000000000	8.770710000
H	0.000000000	0.000000000	-8.770710000
H	1.833279000	1.132649000	7.522929000
H	1.833279000	-1.132649000	-7.522929000
H	1.841285000	1.107371000	5.039470000
H	1.841285000	-1.107371000	-5.039470000
H	4.986822000	0.482100000	2.098757000
H	4.986822000	-0.482100000	-2.098757000
H	7.464170000	0.470512000	2.102989000
H	7.464170000	-0.470512000	-2.102989000
H	8.713063000	0.000000000	0.000000000
H	-1.833279000	1.132649000	-7.522929000
H	-1.833279000	-1.132649000	7.522929000
H	-1.841285000	1.107371000	-5.039470000
H	-1.841285000	-1.107371000	5.039470000
H	-4.986822000	0.482100000	-2.098757000
H	-4.986822000	-0.482100000	2.098757000
H	-7.464170000	0.470512000	-2.102989000
H	-7.464170000	-0.470512000	2.102989000
H	-8.713063000	0.000000000	0.000000000
N	1.398212000	0.141702000	-1.422878000
N	1.398212000	-0.141702000	1.422878000
N	-1.398212000	0.141702000	1.422878000
N	-1.398212000	-0.141702000	-1.422878000

36. Pd[(CF₃)₈TPP]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
C	0.538825000	4.129086000	0.435110000
C	0.538825000	-4.129086000	-0.435110000

C	0.971915000	2.738159000	0.586795000
C	0.971915000	-2.738159000	-0.586795000
C	0.990212000	5.368558000	1.192783000
C	0.990212000	-5.368558000	-1.192783000
C	2.235773000	2.235773000	1.003119000
C	2.235773000	-2.235773000	-1.003119000
C	2.738159000	0.971915000	0.586795000
C	2.738159000	-0.971915000	-0.586795000
C	3.018331000	3.018331000	3.223992000
C	3.018331000	-3.018331000	-3.223992000
C	3.112913000	3.112913000	1.828254000
C	3.112913000	-3.112913000	-1.828254000
C	3.817584000	3.817584000	4.034517000
C	3.817584000	-3.817584000	-4.034517000
C	4.011796000	4.011796000	1.255896000
C	4.011796000	-4.011796000	-1.255896000
C	4.129086000	0.538825000	0.435110000
C	4.129086000	-0.538825000	-0.435110000
C	4.718173000	4.718173000	3.457011000
C	4.718173000	-4.718173000	-3.457011000
C	4.813705000	4.813705000	2.069758000
C	4.813705000	-4.813705000	-2.069758000
C	5.368558000	0.990212000	1.192783000
C	5.368558000	-0.990212000	-1.192783000
C	-0.538825000	4.129086000	-0.435110000
C	-0.538825000	-4.129086000	0.435110000
C	-0.971915000	2.738159000	-0.586795000
C	-0.971915000	-2.738159000	0.586795000
C	-0.990212000	5.368558000	-1.192783000
C	-0.990212000	-5.368558000	1.192783000
C	-2.235773000	2.235773000	-1.003119000
C	-2.235773000	-2.235773000	1.003119000
C	-2.738159000	0.971915000	-0.586795000
C	-2.738159000	-0.971915000	0.586795000
C	-3.018331000	3.018331000	-3.223992000
C	-3.018331000	-3.018331000	3.223992000
C	-3.112913000	3.112913000	-1.828254000
C	-3.112913000	-3.112913000	1.828254000
C	-3.817584000	3.817584000	-4.034517000
C	-3.817584000	-3.817584000	4.034517000
C	-4.011796000	4.011796000	-1.255896000
C	-4.011796000	-4.011796000	1.255896000
C	-4.129086000	0.538825000	-0.435110000
C	-4.129086000	-0.538825000	0.435110000
C	-4.718173000	4.718173000	-3.457011000
C	-4.718173000	-4.718173000	3.457011000
C	-4.813705000	4.813705000	-2.069758000
C	-4.813705000	-4.813705000	2.069758000
C	-5.368558000	0.990212000	-1.192783000
C	-5.368558000	-0.990212000	1.192783000
F	0.019457000	6.280645000	-1.268826000

F	0.019457000	-6.280645000	1.268826000
F	1.291988000	5.073480000	2.477710000
F	1.291988000	-5.073480000	-2.477710000
F	2.055611000	5.998680000	0.638331000
F	2.055611000	-5.998680000	-0.638331000
F	5.073480000	1.291988000	2.477710000
F	5.073480000	-1.291988000	-2.477710000
F	5.998680000	2.055611000	0.638331000
F	5.998680000	-2.055611000	-0.638331000
F	6.280645000	0.019457000	-1.268826000
F	6.280645000	-0.019457000	1.268826000
F	-0.019457000	6.280645000	1.268826000
F	-0.019457000	-6.280645000	-1.268826000
F	-1.291988000	5.073480000	-2.477710000
F	-1.291988000	-5.073480000	2.477710000
F	-2.055611000	5.998680000	-0.638331000
F	-2.055611000	-5.998680000	0.638331000
F	-5.073480000	1.291988000	-2.477710000
F	-5.073480000	-1.291988000	2.477710000
F	-5.998680000	2.055611000	-0.638331000
F	-5.998680000	-2.055611000	0.638331000
F	-6.280645000	0.019457000	1.268826000
F	-6.280645000	-0.019457000	-1.268826000
H	2.314126000	2.314126000	3.665088000
H	2.314126000	-2.314126000	-3.665088000
H	3.738822000	3.738822000	5.117614000
H	3.738822000	-3.738822000	-5.117614000
H	4.082807000	4.082807000	0.172419000
H	4.082807000	-4.082807000	-0.172419000
H	5.344524000	5.344524000	4.091229000
H	5.344524000	-5.344524000	-4.091229000
H	5.512662000	5.512662000	1.614056000
H	5.512662000	-5.512662000	-1.614056000
H	-2.314126000	2.314126000	-3.665088000
H	-2.314126000	-2.314126000	3.665088000
H	-3.738822000	3.738822000	-5.117614000
H	-3.738822000	-3.738822000	5.117614000
H	-4.082807000	4.082807000	-0.172419000
H	-4.082807000	-4.082807000	0.172419000
H	-5.344524000	5.344524000	-4.091229000
H	-5.344524000	-5.344524000	4.091229000
H	-5.512662000	5.512662000	-1.614056000
H	-5.512662000	-5.512662000	1.614056000
N	0.000000000	1.965902000	0.000000000
N	0.000000000	-1.965902000	0.000000000
N	1.965902000	0.000000000	0.000000000
N	-1.965902000	0.000000000	0.000000000

37. Pt[(CF₃)₈TPP]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.421202000
C	0.000000000	0.000000000	4.909577000
C	0.000000000	0.000000000	7.704256000
C	0.000000000	0.000000000	-3.421202000
C	0.000000000	0.000000000	-4.909577000
C	0.000000000	0.000000000	-7.704256000
C	0.714324000	0.975654000	7.005914000
C	0.714324000	-0.975654000	-7.005914000
C	0.726021000	0.967397000	5.612911000
C	0.726021000	-0.967397000	-5.612911000
C	1.130129000	0.512113000	-2.736954000
C	1.130129000	-0.512113000	2.736954000
C	2.239468000	1.348401000	-3.192274000
C	2.239468000	-1.348401000	3.192274000
C	2.344649000	2.072071000	-4.518265000
C	2.344649000	-2.072071000	4.518265000
C	2.662776000	0.582275000	-1.086247000
C	2.662776000	-0.582275000	1.086247000
C	3.140162000	1.448126000	-2.142715000
C	3.140162000	-1.448126000	2.142715000
C	3.356811000	0.000000000	0.000000000
C	4.211979000	2.510185000	-1.954971000
C	4.211979000	-2.510185000	1.954971000
C	4.829759000	0.000000000	0.000000000
C	5.543554000	0.338691000	1.162449000
C	5.543554000	-0.338691000	-1.162449000
C	6.934545000	0.341334000	1.160305000
C	6.934545000	-0.341334000	-1.160305000
C	7.634638000	0.000000000	0.000000000
C	-0.714324000	0.975654000	-7.005914000
C	-0.714324000	-0.975654000	7.005914000
C	-0.726021000	0.967397000	-5.612911000
C	-0.726021000	-0.967397000	5.612911000
C	-1.130129000	0.512113000	2.736954000
C	-1.130129000	-0.512113000	-2.736954000
C	-2.239468000	1.348401000	3.192274000
C	-2.239468000	-1.348401000	-3.192274000
C	-2.344649000	2.072071000	4.518265000
C	-2.344649000	-2.072071000	-4.518265000
C	-2.662776000	0.582275000	1.086247000
C	-2.662776000	-0.582275000	-1.086247000
C	-3.140162000	1.448126000	2.142715000
C	-3.140162000	-1.448126000	-2.142715000
C	-3.356811000	0.000000000	0.000000000
C	-4.211979000	2.510185000	1.954971000
C	-4.211979000	-2.510185000	-1.954971000
C	-4.829759000	0.000000000	0.000000000

C	-5.543554000	0.338691000	-1.162449000
C	-5.543554000	-0.338691000	1.162449000
C	-6.934545000	0.341334000	-1.160305000
C	-6.934545000	-0.341334000	1.160305000
C	-7.634638000	0.000000000	0.000000000
F	1.254161000	2.858311000	-4.736705000
F	1.254161000	-2.858311000	4.736705000
F	2.465054000	1.215846000	-5.562685000
F	2.465054000	-1.215846000	5.562685000
F	3.428982000	2.880567000	-4.592054000
F	3.428982000	-2.880567000	4.592054000
F	3.711365000	3.744113000	-2.241780000
F	3.711365000	-3.744113000	2.241780000
F	4.630740000	2.587573000	-0.668884000
F	4.630740000	-2.587573000	0.668884000
F	5.310212000	2.317480000	-2.729958000
F	5.310212000	-2.317480000	2.729958000
F	-1.254161000	2.858311000	4.736705000
F	-1.254161000	-2.858311000	-4.736705000
F	-2.465054000	1.215846000	5.562685000
F	-2.465054000	-1.215846000	-5.562685000
F	-3.428982000	2.880567000	4.592054000
F	-3.428982000	-2.880567000	-4.592054000
F	-3.711365000	3.744113000	2.241780000
F	-3.711365000	-3.744113000	-2.241780000
F	-4.630740000	2.587573000	0.668884000
F	-4.630740000	-2.587573000	-0.668884000
F	-5.310212000	2.317480000	2.729958000
F	-5.310212000	-2.317480000	-2.729958000
H	0.000000000	0.000000000	8.793709000
H	0.000000000	0.000000000	-8.793709000
H	1.269826000	1.740634000	7.545747000
H	1.269826000	-1.740634000	-7.545747000
H	1.287351000	1.719248000	5.060803000
H	1.287351000	-1.719248000	-5.060803000
H	4.997952000	0.627760000	2.059424000
H	4.997952000	-0.627760000	-2.059424000
H	7.474330000	0.615723000	2.064927000
H	7.474330000	-0.615723000	-2.064927000
H	8.723961000	0.000000000	0.000000000
H	-1.269826000	1.740634000	-7.545747000
H	-1.269826000	-1.740634000	7.545747000
H	-1.287351000	1.719248000	-5.060803000
H	-1.287351000	-1.719248000	5.060803000
H	-4.997952000	0.627760000	-2.059424000
H	-4.997952000	-0.627760000	2.059424000
H	-7.474330000	0.615723000	-2.064927000
H	-7.474330000	-0.615723000	2.064927000
H	-8.723961000	0.000000000	0.000000000
N	1.387165000	0.182135000	-1.418765000
N	1.387165000	-0.182135000	1.418765000

N	-1.387165000	0.182135000	1.418765000
N	-1.387165000	-0.182135000	-1.418765000

38. Pt[(CF₃)₈TPP]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
C	0.543653000	4.136571000	0.428801000
C	0.543653000	-4.136571000	-0.428801000
C	0.980062000	2.748740000	0.576843000
C	0.980062000	-2.748740000	-0.576843000
C	0.999548000	5.376649000	1.182741000
C	0.999548000	-5.376649000	-1.182741000
C	2.246730000	2.246730000	0.986216000
C	2.246730000	-2.246730000	-0.986216000
C	2.748740000	0.980062000	0.576843000
C	2.748740000	-0.980062000	-0.576843000
C	3.039565000	3.039565000	3.199588000
C	3.039565000	-3.039565000	-3.199588000
C	3.128048000	3.128048000	1.802955000
C	3.128048000	-3.128048000	-1.802955000
C	3.842362000	3.842362000	4.002957000
C	3.842362000	-3.842362000	-4.002957000
C	4.024294000	4.024294000	1.222539000
C	4.024294000	-4.024294000	-1.222539000
C	4.136571000	0.543653000	0.428801000
C	4.136571000	-0.543653000	-0.428801000
C	4.740346000	4.740346000	3.417363000
C	4.740346000	-4.740346000	-3.417363000
C	4.829793000	4.829793000	2.029337000
C	4.829793000	-4.829793000	-2.029337000
C	5.376649000	0.999548000	1.182741000
C	5.376649000	-0.999548000	-1.182741000
C	-0.543653000	4.136571000	-0.428801000
C	-0.543653000	-4.136571000	0.428801000
C	-0.980062000	2.748740000	-0.576843000
C	-0.980062000	-2.748740000	0.576843000
C	-0.999548000	5.376649000	-1.182741000
C	-0.999548000	-5.376649000	1.182741000
C	-2.246730000	2.246730000	-0.986216000
C	-2.246730000	-2.246730000	0.986216000
C	-2.748740000	0.980062000	-0.576843000
C	-2.748740000	-0.980062000	0.576843000
C	-3.039565000	3.039565000	-3.199588000
C	-3.039565000	-3.039565000	3.199588000
C	-3.128048000	3.128048000	-1.802955000
C	-3.128048000	-3.128048000	1.802955000
C	-3.842362000	3.842362000	-4.002957000
C	-3.842362000	-3.842362000	4.002957000
C	-4.024294000	4.024294000	-1.222539000
C	-4.024294000	-4.024294000	1.222539000

C	-4.136571000	0.543653000	-0.428801000
C	-4.136571000	-0.543653000	0.428801000
C	-4.740346000	4.740346000	-3.417363000
C	-4.740346000	-4.740346000	3.417363000
C	-4.829793000	4.829793000	-2.029337000
C	-4.829793000	-4.829793000	2.029337000
C	-5.376649000	0.999548000	-1.182741000
C	-5.376649000	-0.999548000	1.182741000
F	0.010457000	6.287701000	-1.266230000
F	0.010457000	-6.287701000	1.266230000
F	1.310162000	5.082774000	2.465781000
F	1.310162000	-5.082774000	-2.465781000
F	2.060455000	6.007792000	0.620842000
F	2.060455000	-6.007792000	-0.620842000
F	5.082774000	1.310162000	2.465781000
F	5.082774000	-1.310162000	-2.465781000
F	6.007792000	2.060455000	0.620842000
F	6.007792000	-2.060455000	-0.620842000
F	6.287701000	0.010457000	-1.266230000
F	6.287701000	-0.010457000	1.266230000
F	-0.010457000	6.287701000	1.266230000
F	-0.010457000	-6.287701000	-1.266230000
F	-1.310162000	5.082774000	-2.465781000
F	-1.310162000	-5.082774000	2.465781000
F	-2.060455000	6.007792000	-0.620842000
F	-2.060455000	-6.007792000	0.620842000
F	-5.082774000	1.310162000	-2.465781000
F	-5.082774000	-1.310162000	2.465781000
F	-6.007792000	2.060455000	-0.620842000
F	-6.007792000	-2.060455000	0.620842000
F	-6.287701000	0.010457000	1.266230000
F	-6.287701000	-0.010457000	-1.266230000
H	2.337178000	2.337178000	3.646378000
H	2.337178000	-2.337178000	-3.646378000
H	3.768537000	3.768537000	5.086720000
H	3.768537000	-3.768537000	-5.086720000
H	4.090354000	4.090354000	0.138401000
H	4.090354000	-4.090354000	-0.138401000
H	5.369495000	5.369495000	4.045988000
H	5.369495000	-5.369495000	-4.045988000
H	5.526762000	5.526762000	1.567567000
H	5.526762000	-5.526762000	-1.567567000
H	-2.337178000	2.337178000	-3.646378000
H	-2.337178000	-2.337178000	3.646378000
H	-3.768537000	3.768537000	-5.086720000
H	-3.768537000	-3.768537000	5.086720000
H	-4.090354000	4.090354000	-0.138401000
H	-4.090354000	-4.090354000	0.138401000
H	-5.369495000	5.369495000	-4.045988000
H	-5.369495000	-5.369495000	4.045988000
H	-5.526762000	5.526762000	-1.567567000

H	-5.526762000	-5.526762000	1.567567000
N	0.000000000	1.973353000	0.000000000
N	0.000000000	-1.973353000	0.000000000
N	1.973353000	0.000000000	0.000000000
N	-1.973353000	0.000000000	0.000000000

39. Zn[(CF₃)₈TPP]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.408437000
C	0.000000000	0.000000000	4.878070000
C	0.000000000	0.000000000	7.680413000
C	0.000000000	0.000000000	-3.408437000
C	0.000000000	0.000000000	-4.878070000
C	0.000000000	0.000000000	-7.680413000
C	1.095060000	0.514458000	6.981105000
C	1.095060000	-0.514458000	-6.981105000
C	1.100722000	0.503664000	5.590402000
C	1.100722000	-0.503664000	-5.590402000
C	1.111380000	0.552566000	-2.703214000
C	1.111380000	-0.552566000	2.703214000
C	2.125557000	1.513527000	-3.104863000
C	2.125557000	-1.513527000	3.104863000
C	2.125606000	2.360285000	-4.360990000
C	2.125606000	-2.360285000	4.360990000
C	2.650607000	0.596421000	-1.083824000
C	2.650607000	-0.596421000	1.083824000
C	3.062838000	1.567921000	-2.074681000
C	3.062838000	-1.567921000	2.074681000
C	3.360290000	0.000000000	0.000000000
C	4.108079000	2.652260000	-1.887570000
C	4.108079000	-2.652260000	1.887570000
C	4.823564000	0.000000000	0.000000000
C	5.540319000	0.248867000	1.186190000
C	5.540319000	-0.248867000	-1.186190000
C	6.930398000	0.250498000	1.184012000
C	6.930398000	-0.250498000	-1.184012000
C	7.630780000	0.000000000	0.000000000
C	-1.095060000	0.514458000	-6.981105000
C	-1.095060000	-0.514458000	6.981105000
C	-1.100722000	0.503664000	-5.590402000
C	-1.100722000	-0.503664000	5.590402000
C	-1.111380000	0.552566000	2.703214000
C	-1.111380000	-0.552566000	-2.703214000
C	-2.125557000	1.513527000	3.104863000
C	-2.125557000	-1.513527000	-3.104863000
C	-2.125606000	2.360285000	4.360990000
C	-2.125606000	-2.360285000	-4.360990000
C	-2.650607000	0.596421000	1.083824000
C	-2.650607000	-0.596421000	-1.083824000

C	-3.062838000	1.567921000	2.074681000
C	-3.062838000	-1.567921000	-2.074681000
C	-3.360290000	0.000000000	0.000000000
C	-4.108079000	2.652260000	1.887570000
C	-4.108079000	-2.652260000	-1.887570000
C	-4.823564000	0.000000000	0.000000000
C	-5.540319000	0.248867000	-1.186190000
C	-5.540319000	-0.248867000	1.186190000
C	-6.930398000	0.250498000	-1.184012000
C	-6.930398000	-0.250498000	1.184012000
C	-7.630780000	0.000000000	0.000000000
F	0.869923000	2.621930000	-4.797093000
F	0.869923000	-2.621930000	4.797093000
F	2.724214000	3.563028000	-4.193630000
F	2.724214000	-3.563028000	4.193630000
F	2.804299000	1.741799000	-5.372250000
F	2.804299000	-1.741799000	5.372250000
F	3.515177000	3.876704000	-1.815183000
F	3.515177000	-3.876704000	1.815183000
F	4.814097000	2.534778000	-0.741875000
F	4.814097000	-2.534778000	0.741875000
F	5.001931000	2.682234000	-2.914941000
F	5.001931000	-2.682234000	2.914941000
F	-0.869923000	2.621930000	4.797093000
F	-0.869923000	-2.621930000	-4.797093000
F	-2.724214000	3.563028000	4.193630000
F	-2.724214000	-3.563028000	-4.193630000
F	-2.804299000	1.741799000	5.372250000
F	-2.804299000	-1.741799000	-5.372250000
F	-3.515177000	3.876704000	1.815183000
F	-3.515177000	-3.876704000	-1.815183000
F	-4.814097000	2.534778000	0.741875000
F	-4.814097000	-2.534778000	-0.741875000
F	-5.001931000	2.682234000	2.914941000
F	-5.001931000	-2.682234000	-2.914941000
H	0.000000000	0.000000000	8.769843000
H	0.000000000	0.000000000	-8.769843000
H	1.947658000	0.922122000	7.521363000
H	1.947658000	-0.922122000	-7.521363000
H	1.948364000	0.908436000	5.040219000
H	1.948364000	-0.908436000	-5.040219000
H	4.994367000	0.469688000	2.102188000
H	4.994367000	-0.469688000	-2.102188000
H	7.471183000	0.455847000	2.106322000
H	7.471183000	-0.455847000	-2.106322000
H	8.720092000	0.000000000	0.000000000
H	-1.947658000	0.922122000	-7.521363000
H	-1.947658000	-0.922122000	7.521363000
H	-1.948364000	0.908436000	-5.040219000
H	-1.948364000	-0.908436000	5.040219000
H	-4.994367000	0.469688000	-2.102188000

H	-4.994367000	-0.469688000	2.102188000
H	-7.471183000	0.455847000	-2.106322000
H	-7.471183000	-0.455847000	2.106322000
H	-8.720092000	0.000000000	0.000000000
N	1.419222000	0.116365000	-1.440795000
N	1.419222000	-0.116365000	1.440795000
N	-1.419222000	0.116365000	1.440795000
N	-1.419222000	-0.116365000	-1.440795000

40. Zn[(CF₃)₈TPP]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
C	0.544148000	4.145322000	0.429586000
C	0.544148000	-4.145322000	-0.429586000
C	0.974640000	2.751993000	0.571702000
C	0.974640000	-2.751993000	-0.571702000
C	0.995323000	5.385510000	1.186117000
C	0.995323000	-5.385510000	-1.186117000
C	2.244801000	2.244801000	0.980668000
C	2.244801000	-2.244801000	-0.980668000
C	2.751993000	0.974640000	0.571702000
C	2.751993000	-0.974640000	-0.571702000
C	3.051561000	3.051561000	3.186671000
C	3.051561000	-3.051561000	-3.186671000
C	3.130178000	3.130178000	1.788981000
C	3.130178000	-3.130178000	-1.788981000
C	3.859311000	3.859311000	3.980056000
C	3.859311000	-3.859311000	-3.980056000
C	4.023070000	4.023070000	1.197836000
C	4.023070000	-4.023070000	-1.197836000
C	4.145322000	0.544148000	0.429586000
C	4.145322000	-0.544148000	-0.429586000
C	4.753540000	4.753540000	3.383272000
C	4.753540000	-4.753540000	-3.383272000
C	4.833804000	4.833804000	1.994179000
C	4.833804000	-4.833804000	-1.994179000
C	5.385510000	0.995323000	1.186117000
C	5.385510000	-0.995323000	-1.186117000
C	-0.544148000	4.145322000	-0.429586000
C	-0.544148000	-4.145322000	0.429586000
C	-0.974640000	2.751993000	-0.571702000
C	-0.974640000	-2.751993000	0.571702000
C	-0.995323000	5.385510000	-1.186117000
C	-0.995323000	-5.385510000	1.186117000
C	-2.244801000	2.244801000	-0.980668000
C	-2.244801000	-2.244801000	0.980668000
C	-2.751993000	0.974640000	-0.571702000
C	-2.751993000	-0.974640000	0.571702000
C	-3.051561000	3.051561000	-3.186671000
C	-3.051561000	-3.051561000	3.186671000

C	-3.130178000	3.130178000	-1.788981000
C	-3.130178000	-3.130178000	1.788981000
C	-3.859311000	3.859311000	-3.980056000
C	-3.859311000	-3.859311000	3.980056000
C	-4.023070000	4.023070000	-1.197836000
C	-4.023070000	-4.023070000	1.197836000
C	-4.145322000	0.544148000	-0.429586000
C	-4.145322000	-0.544148000	0.429586000
C	-4.753540000	4.753540000	-3.383272000
C	-4.753540000	-4.753540000	3.383272000
C	-4.833804000	4.833804000	-1.994179000
C	-4.833804000	-4.833804000	1.994179000
C	-5.385510000	0.995323000	-1.186117000
C	-5.385510000	-0.995323000	1.186117000
F	0.015068000	6.296707000	-1.269985000
F	0.015068000	-6.296707000	1.269985000
F	1.303337000	5.087894000	2.469426000
F	1.303337000	-5.087894000	-2.469426000
F	2.057076000	6.018346000	0.628421000
F	2.057076000	-6.018346000	-0.628421000
F	5.087894000	1.303337000	2.469426000
F	5.087894000	-1.303337000	-2.469426000
F	6.018346000	2.057076000	0.628421000
F	6.018346000	-2.057076000	-0.628421000
F	6.296707000	0.015068000	-1.269985000
F	6.296707000	-0.015068000	1.269985000
F	-0.015068000	6.296707000	1.269985000
F	-0.015068000	-6.296707000	-1.269985000
F	-1.303337000	5.087894000	-2.469426000
F	-1.303337000	-5.087894000	2.469426000
F	-2.057076000	6.018346000	-0.628421000
F	-2.057076000	-6.018346000	0.628421000
F	-5.087894000	1.303337000	-2.469426000
F	-5.087894000	-1.303337000	2.469426000
F	-6.018346000	2.057076000	-0.628421000
F	-6.018346000	-2.057076000	0.628421000
F	-6.296707000	0.015068000	1.269985000
F	-6.296707000	-0.015068000	-1.269985000
H	2.352457000	2.352457000	3.643625000
H	2.352457000	-2.352457000	-3.643625000
H	3.792179000	3.792179000	5.064711000
H	3.792179000	-3.792179000	-5.064711000
H	4.082492000	4.082492000	0.112878000
H	4.082492000	-4.082492000	-0.112878000
H	5.386715000	5.386715000	4.003789000
H	5.386715000	-5.386715000	-4.003789000
H	5.527690000	5.527690000	1.523224000
H	5.527690000	-5.527690000	-1.523224000
H	-2.352457000	2.352457000	-3.643625000
H	-2.352457000	-2.352457000	3.643625000
H	-3.792179000	3.792179000	-5.064711000

H	-3.792179000	-3.792179000	5.064711000
H	-4.082492000	4.082492000	-0.112878000
H	-4.082492000	-4.082492000	0.112878000
H	-5.386715000	5.386715000	-4.003789000
H	-5.386715000	-5.386715000	4.003789000
H	-5.527690000	5.527690000	-1.523224000
H	-5.527690000	-5.527690000	1.523224000
N	0.000000000	1.977195000	0.000000000
N	0.000000000	-1.977195000	0.000000000
N	1.977195000	0.000000000	0.000000000
N	-1.977195000	0.000000000	0.000000000

41. Cu[Me₈TPP]; S = ½ (saddled)

Cu	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.396883000
C	0.000000000	0.000000000	4.882326000
C	0.000000000	0.000000000	7.694377000
C	0.000000000	0.000000000	-3.396883000
C	0.000000000	0.000000000	-4.882326000
C	0.000000000	0.000000000	-7.694377000
C	0.917189000	0.786674000	6.991614000
C	0.917189000	-0.786674000	-6.991614000
C	0.919198000	0.781796000	5.597199000
C	0.919198000	-0.781796000	-5.597199000
C	1.158702000	0.428754000	-2.724021000
C	1.158702000	-0.428754000	2.724021000
C	2.314574000	1.105658000	-3.289446000
C	2.314574000	-1.105658000	3.289446000
C	2.436940000	1.792755000	-4.617432000
C	2.436940000	-1.792755000	4.617432000
C	2.723997000	0.428709000	-1.158710000
C	2.723997000	-0.428709000	1.158710000
C	3.289446000	1.105560000	-2.314571000
C	3.289446000	-1.105560000	2.314571000
C	3.396825000	0.000000000	0.000000000
C	4.617462000	1.792596000	-2.436808000
C	4.617462000	-1.792596000	2.436808000
C	4.882225000	0.000000000	0.000000000
C	5.597062000	0.782370000	0.918715000
C	5.597062000	-0.782370000	-0.918715000
C	6.991460000	0.787387000	0.916581000
C	6.991460000	-0.787387000	-0.916581000
C	7.694217000	0.000000000	0.000000000
C	-0.917189000	0.786674000	-6.991614000
C	-0.917189000	-0.786674000	6.991614000
C	-0.919198000	0.781796000	-5.597199000
C	-0.919198000	-0.781796000	5.597199000
C	-1.158702000	0.428754000	2.724021000
C	-1.158702000	-0.428754000	-2.724021000

C	-2.314574000	1.105658000	3.289446000
C	-2.314574000	-1.105658000	-3.289446000
C	-2.436940000	1.792755000	4.617432000
C	-2.436940000	-1.792755000	-4.617432000
C	-2.723997000	0.428709000	1.158710000
C	-2.723997000	-0.428709000	-1.158710000
C	-3.289446000	1.105560000	2.314571000
C	-3.289446000	-1.105560000	-2.314571000
C	-3.396825000	0.000000000	0.000000000
C	-4.617462000	1.792596000	2.436808000
C	-4.617462000	-1.792596000	-2.436808000
C	-4.882225000	0.000000000	0.000000000
C	-5.597062000	0.782370000	-0.918715000
C	-5.597062000	-0.782370000	0.918715000
C	-6.991460000	0.787387000	-0.916581000
C	-6.991460000	-0.787387000	0.916581000
C	-7.694217000	0.000000000	0.000000000
H	0.000000000	0.000000000	8.784005000
H	0.000000000	0.000000000	-8.784005000
H	1.467262000	2.126647000	-5.002129000
H	1.467262000	-2.126647000	5.002129000
H	1.632701000	1.405548000	7.531969000
H	1.632701000	-1.405548000	-7.531969000
H	1.633483000	1.389261000	5.041988000
H	1.633483000	-1.389261000	-5.041988000
H	2.880076000	1.140484000	-5.384552000
H	2.880076000	-1.140484000	5.384552000
H	3.087603000	2.672746000	-4.526726000
H	3.087603000	-2.672746000	4.526726000
H	4.526863000	2.672605000	-3.087462000
H	4.526863000	-2.672605000	3.087462000
H	5.002089000	2.126453000	-1.467091000
H	5.002089000	-2.126453000	1.467091000
H	5.041836000	1.390319000	1.632585000
H	5.041836000	-1.390319000	-1.632585000
H	5.384589000	1.140290000	-2.879870000
H	5.384589000	-1.140290000	2.879870000
H	7.531787000	1.406927000	1.631511000
H	7.531787000	-1.406927000	-1.631511000
H	8.783844000	0.000000000	0.000000000
H	-1.467262000	2.126647000	5.002129000
H	-1.467262000	-2.126647000	-5.002129000
H	-1.632701000	1.405548000	-7.531969000
H	-1.632701000	-1.405548000	7.531969000
H	-1.633483000	1.389261000	-5.041988000
H	-1.633483000	-1.389261000	5.041988000
H	-2.880076000	1.140484000	5.384552000
H	-2.880076000	-1.140484000	-5.384552000
H	-3.087603000	2.672746000	4.526726000
H	-3.087603000	-2.672746000	-4.526726000
H	-4.526863000	2.672605000	3.087462000

H	-4.526863000	-2.672605000	-3.087462000
H	-5.002089000	2.126453000	1.467091000
H	-5.002089000	-2.126453000	-1.467091000
H	-5.041836000	1.390319000	-1.632585000
H	-5.041836000	-1.390319000	1.632585000
H	-5.384589000	1.140290000	2.879870000
H	-5.384589000	-1.140290000	-2.879870000
H	-7.531787000	1.406927000	-1.631511000
H	-7.531787000	-1.406927000	1.631511000
H	-8.783844000	0.000000000	0.000000000
N	1.402231000	0.126000000	-1.402239000
N	1.402231000	-0.126000000	1.402239000
N	-1.402231000	0.126000000	1.402239000
N	-1.402231000	-0.126000000	-1.402239000

42. Cu[Me₃TPP]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
C	0.617749000	4.186902000	0.302882000
C	0.617749000	-4.186902000	-0.302882000
C	1.034840000	2.792934000	0.407667000
C	1.034840000	-2.792934000	-0.407667000
C	1.312005000	5.446966000	0.739371000
C	1.312005000	-5.446966000	-0.739371000
C	2.333161000	2.333161000	0.694636000
C	2.333161000	-2.333161000	-0.694636000
C	2.792934000	1.034840000	0.407667000
C	2.792934000	-1.034840000	-0.407667000
C	3.324039000	3.324039000	1.211382000
C	3.324039000	-3.324039000	-1.211382000
C	3.488522000	3.488522000	2.591874000
C	3.488522000	-3.488522000	-2.591874000
C	4.097718000	4.097718000	0.339656000
C	4.097718000	-4.097718000	-0.339656000
C	4.186902000	0.617749000	0.302882000
C	4.186902000	-0.617749000	-0.302882000
C	4.410193000	4.410193000	3.092129000
C	4.410193000	-4.410193000	-3.092129000
C	5.019509000	5.019509000	0.834664000
C	5.019509000	-5.019509000	-0.834664000
C	5.178667000	5.178667000	2.213611000
C	5.178667000	-5.178667000	-2.213611000
C	5.446966000	1.312005000	0.739371000
C	5.446966000	-1.312005000	-0.739371000
C	-0.617749000	4.186902000	-0.302882000
C	-0.617749000	-4.186902000	0.302882000
C	-1.034840000	2.792934000	-0.407667000
C	-1.034840000	-2.792934000	0.407667000
C	-1.312005000	5.446966000	-0.739371000
C	-1.312005000	-5.446966000	0.739371000

C	-2.333161000	2.333161000	-0.694636000
C	-2.333161000	-2.333161000	0.694636000
C	-2.792934000	1.034840000	-0.407667000
C	-2.792934000	-1.034840000	0.407667000
C	-3.324039000	3.324039000	-1.211382000
C	-3.324039000	-3.324039000	1.211382000
C	-3.488522000	3.488522000	-2.591874000
C	-3.488522000	-3.488522000	2.591874000
C	-4.097718000	4.097718000	-0.339656000
C	-4.097718000	-4.097718000	0.339656000
C	-4.186902000	0.617749000	-0.302882000
C	-4.186902000	-0.617749000	0.302882000
C	-4.410193000	4.410193000	-3.092129000
C	-4.410193000	-4.410193000	3.092129000
C	-5.019509000	5.019509000	-0.834664000
C	-5.019509000	-5.019509000	0.834664000
C	-5.178667000	5.178667000	-2.213611000
C	-5.178667000	-5.178667000	2.213611000
C	-5.446966000	1.312005000	-0.739371000
C	-5.446966000	-1.312005000	0.739371000
H	0.576656000	6.248658000	0.874352000
H	0.576656000	-6.248658000	-0.874352000
H	1.840723000	5.323970000	1.689921000
H	1.840723000	-5.323970000	-1.689921000
H	2.052796000	5.795537000	0.004857000
H	2.052796000	-5.795537000	-0.004857000
H	2.885429000	2.885429000	3.269870000
H	2.885429000	-2.885429000	-3.269870000
H	3.966831000	3.966831000	-0.734178000
H	3.966831000	-3.966831000	0.734178000
H	4.528589000	4.528589000	4.168490000
H	4.528589000	-4.528589000	-4.168490000
H	5.323970000	1.840723000	1.689921000
H	5.323970000	-1.840723000	-1.689921000
H	5.615167000	5.615167000	0.143772000
H	5.615167000	-5.615167000	-0.143772000
H	5.795537000	2.052796000	0.004857000
H	5.795537000	-2.052796000	-0.004857000
H	5.898372000	5.898372000	2.602456000
H	5.898372000	-5.898372000	-2.602456000
H	6.248658000	0.576656000	0.874352000
H	6.248658000	-0.576656000	-0.874352000
H	-0.576656000	6.248658000	-0.874352000
H	-0.576656000	-6.248658000	0.874352000
H	-1.840723000	5.323970000	-1.689921000
H	-1.840723000	-5.323970000	1.689921000
H	-2.052796000	5.795537000	-0.004857000
H	-2.052796000	-5.795537000	0.004857000
H	-2.885429000	2.885429000	-3.269870000
H	-2.885429000	-2.885429000	3.269870000
H	-3.966831000	3.966831000	0.734178000

H	-3.966831000	-3.966831000	-0.734178000
H	-4.528589000	4.528589000	-4.168490000
H	-4.528589000	-4.528589000	4.168490000
H	-5.323970000	1.840723000	-1.689921000
H	-5.323970000	-1.840723000	1.689921000
H	-5.615167000	5.615167000	-0.143772000
H	-5.615167000	-5.615167000	0.143772000
H	-5.795537000	2.052796000	-0.004857000
H	-5.795537000	-2.052796000	0.004857000
H	-5.898372000	5.898372000	-2.602456000
H	-5.898372000	-5.898372000	2.602456000
H	-6.248658000	0.576656000	-0.874352000
H	-6.248658000	-0.576656000	0.874352000
N	0.000000000	1.979388000	0.000000000
N	0.000000000	-1.979388000	0.000000000
N	1.979388000	0.000000000	0.000000000
N	-1.979388000	0.000000000	0.000000000

43. Ni[Me₃TPP]; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.358514000
C	0.000000000	0.000000000	4.843853000
C	0.000000000	0.000000000	7.655338000
C	0.000000000	0.000000000	-3.358514000
C	0.000000000	0.000000000	-4.843853000
C	0.000000000	0.000000000	-7.655338000
C	0.958030000	0.736332000	6.952658000
C	0.958030000	-0.736332000	-6.952658000
C	0.959502000	0.731662000	5.558039000
C	0.959502000	-0.731662000	-5.558039000
C	1.106273000	0.506669000	-2.668717000
C	1.106273000	-0.506669000	2.668717000
C	2.242440000	1.222520000	-3.215763000
C	2.242440000	-1.222520000	3.215763000
C	2.344126000	1.926817000	-4.535975000
C	2.344126000	-1.926817000	4.535975000
C	2.668724000	0.506731000	-1.106167000
C	2.668724000	-0.506731000	1.106167000
C	3.215805000	1.222630000	-2.242230000
C	3.215805000	-1.222630000	2.242230000
C	3.358567000	0.000000000	0.000000000
C	4.535917000	1.927104000	-2.343632000
C	4.535917000	-1.927104000	2.343632000
C	4.843918000	0.000000000	0.000000000
C	5.558118000	0.731793000	0.959394000
C	5.558118000	-0.731793000	-0.959394000
C	6.952743000	0.736450000	0.957937000
C	6.952743000	-0.736450000	-0.957937000
C	7.655436000	0.000000000	0.000000000

C	-0.958030000	0.736332000	-6.952658000
C	-0.958030000	-0.736332000	6.952658000
C	-0.959502000	0.731662000	-5.558039000
C	-0.959502000	-0.731662000	5.558039000
C	-1.106273000	0.506669000	2.668717000
C	-1.106273000	-0.506669000	-2.668717000
C	-2.242440000	1.222520000	3.215763000
C	-2.242440000	-1.222520000	-3.215763000
C	-2.344126000	1.926817000	4.535975000
C	-2.344126000	-1.926817000	-4.535975000
C	-2.668724000	0.506731000	1.106167000
C	-2.668724000	-0.506731000	-1.106167000
C	-3.215805000	1.222630000	2.242230000
C	-3.215805000	-1.222630000	-2.242230000
C	-3.358567000	0.000000000	0.000000000
C	-4.535917000	1.927104000	2.343632000
C	-4.535917000	-1.927104000	-2.343632000
C	-4.843918000	0.000000000	0.000000000
C	-5.558118000	0.731793000	-0.959394000
C	-5.558118000	-0.731793000	0.959394000
C	-6.952743000	0.736450000	-0.957937000
C	-6.952743000	-0.736450000	0.957937000
C	-7.655436000	0.000000000	0.000000000
H	0.000000000	0.000000000	8.744941000
H	0.000000000	0.000000000	-8.744941000
H	1.363959000	2.232562000	-4.917912000
H	1.363959000	-2.232562000	4.917912000
H	1.705443000	1.299741000	5.002650000
H	1.705443000	-1.299741000	-5.002650000
H	1.705793000	1.315804000	7.493049000
H	1.705793000	-1.315804000	-7.493049000
H	2.809638000	1.298242000	-5.309699000
H	2.809638000	-1.298242000	5.309699000
H	2.965422000	2.826689000	-4.433105000
H	2.965422000	-2.826689000	4.433105000
H	4.433142000	2.826769000	-2.965242000
H	4.433142000	-2.826769000	2.965242000
H	4.917412000	2.233228000	-1.363400000
H	4.917412000	-2.233228000	1.363400000
H	5.002745000	1.299887000	1.705330000
H	5.002745000	-1.299887000	-1.705330000
H	5.309940000	1.298516000	-2.808634000
H	5.309940000	-1.298516000	2.808634000
H	7.493108000	1.315982000	1.705668000
H	7.493108000	-1.315982000	-1.705668000
H	8.745048000	0.000000000	0.000000000
H	-1.363959000	2.232562000	4.917912000
H	-1.363959000	-2.232562000	-4.917912000
H	-1.705443000	1.299741000	-5.002650000
H	-1.705443000	-1.299741000	5.002650000
H	-1.705793000	1.315804000	-7.493049000

H	-1.705793000	-1.315804000	7.493049000
H	-2.809638000	1.298242000	5.309699000
H	-2.809638000	-1.298242000	-5.309699000
H	-2.965422000	2.826689000	4.433105000
H	-2.965422000	-2.826689000	-4.433105000
H	-4.433142000	2.826769000	2.965242000
H	-4.433142000	-2.826769000	-2.965242000
H	-4.917412000	2.233228000	1.363400000
H	-4.917412000	-2.233228000	-1.363400000
H	-5.002745000	1.299887000	-1.705330000
H	-5.002745000	-1.299887000	1.705330000
H	-5.309940000	1.298516000	2.808634000
H	-5.309940000	-1.298516000	-2.808634000
H	-7.493108000	1.315982000	-1.705668000
H	-7.493108000	-1.315982000	1.705668000
H	-8.745048000	0.000000000	0.000000000
N	1.338197000	0.204529000	-1.338158000
N	1.338197000	-0.204529000	1.338158000
N	-1.338197000	0.204529000	1.338158000
N	-1.338197000	-0.204529000	-1.338158000

44. Ni[Me₈TPP]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
C	0.574534000	4.099357000	0.377605000
C	0.574534000	-4.099357000	-0.377605000
C	0.981193000	2.709979000	0.521886000
C	0.981193000	-2.709979000	-0.521886000
C	1.214291000	5.352698000	0.904949000
C	1.214291000	-5.352698000	-0.904949000
C	2.254284000	2.254284000	0.889949000
C	2.254284000	-2.254284000	-0.889949000
C	2.709979000	0.981193000	0.521886000
C	2.709979000	-0.981193000	-0.521886000
C	3.208212000	3.208212000	1.526815000
C	3.208212000	-3.208212000	-1.526815000
C	3.285673000	3.285673000	2.922164000
C	3.285673000	-3.285673000	-2.922164000
C	4.033849000	4.033849000	0.755228000
C	4.033849000	-4.033849000	-0.755228000
C	4.099357000	0.574534000	0.377605000
C	4.099357000	-0.574534000	-0.377605000
C	4.172794000	4.172794000	3.535672000
C	4.172794000	-4.172794000	-3.535672000
C	4.920836000	4.920836000	1.363275000
C	4.920836000	-4.920836000	-1.363275000
C	4.993093000	4.993093000	2.757010000
C	4.993093000	-4.993093000	-2.757010000
C	5.352698000	1.214291000	0.904949000
C	5.352698000	-1.214291000	-0.904949000

C	-0.574534000	4.099357000	-0.377605000
C	-0.574534000	-4.099357000	0.377605000
C	-0.981193000	2.709979000	-0.521886000
C	-0.981193000	-2.709979000	0.521886000
C	-1.214291000	5.352698000	-0.904949000
C	-1.214291000	-5.352698000	0.904949000
C	-2.254284000	2.254284000	-0.889949000
C	-2.254284000	-2.254284000	0.889949000
C	-2.709979000	0.981193000	-0.521886000
C	-2.709979000	-0.981193000	0.521886000
C	-3.208212000	3.208212000	-1.526815000
C	-3.208212000	-3.208212000	1.526815000
C	-3.285673000	3.285673000	-2.922164000
C	-3.285673000	-3.285673000	2.922164000
C	-4.033849000	4.033849000	-0.755228000
C	-4.033849000	-4.033849000	0.755228000
C	-4.099357000	0.574534000	-0.377605000
C	-4.099357000	-0.574534000	0.377605000
C	-4.172794000	4.172794000	-3.535672000
C	-4.172794000	-4.172794000	3.535672000
C	-4.920836000	4.920836000	-1.363275000
C	-4.920836000	-4.920836000	1.363275000
C	-4.993093000	4.993093000	-2.757010000
C	-4.993093000	-4.993093000	2.757010000
C	-5.352698000	1.214291000	-0.904949000
C	-5.352698000	-1.214291000	0.904949000
H	0.459826000	6.143937000	0.992517000
H	0.459826000	-6.143937000	-0.992517000
H	1.657810000	5.207702000	1.895583000
H	1.657810000	-5.207702000	-1.895583000
H	2.013292000	5.727668000	0.248245000
H	2.013292000	-5.727668000	-0.248245000
H	2.642665000	2.642665000	3.522283000
H	2.642665000	-2.642665000	-3.522283000
H	3.970393000	3.970393000	-0.330674000
H	3.970393000	-3.970393000	0.330674000
H	4.223201000	4.223201000	4.622667000
H	4.223201000	-4.223201000	-4.622667000
H	5.207702000	1.657810000	1.895583000
H	5.207702000	-1.657810000	-1.895583000
H	5.557301000	5.557301000	0.749527000
H	5.557301000	-5.557301000	-0.749527000
H	5.685634000	5.685634000	3.234416000
H	5.685634000	-5.685634000	-3.234416000
H	5.727668000	2.013292000	0.248245000
H	5.727668000	-2.013292000	-0.248245000
H	6.143937000	0.459826000	0.992517000
H	6.143937000	-0.459826000	-0.992517000
H	-0.459826000	6.143937000	-0.992517000
H	-0.459826000	-6.143937000	0.992517000
H	-1.657810000	5.207702000	-1.895583000

H	-1.657810000	-5.207702000	1.895583000
H	-2.013292000	5.727668000	-0.248245000
H	-2.013292000	-5.727668000	0.248245000
H	-2.642665000	2.642665000	-3.522283000
H	-2.642665000	-2.642665000	3.522283000
H	-3.970393000	3.970393000	0.330674000
H	-3.970393000	-3.970393000	-0.330674000
H	-4.223201000	4.223201000	-4.622667000
H	-4.223201000	-4.223201000	4.622667000
H	-5.207702000	1.657810000	-1.895583000
H	-5.207702000	-1.657810000	1.895583000
H	-5.557301000	5.557301000	-0.749527000
H	-5.557301000	-5.557301000	0.749527000
H	-5.685634000	5.685634000	-3.234416000
H	-5.685634000	-5.685634000	3.234416000
H	-5.727668000	2.013292000	-0.248245000
H	-5.727668000	-2.013292000	0.248245000
H	-6.143937000	0.459826000	-0.992517000
H	-6.143937000	-0.459826000	0.992517000
N	0.000000000	1.889557000	0.000000000
N	0.000000000	-1.889557000	0.000000000
N	1.889557000	0.000000000	0.000000000
N	-1.889557000	0.000000000	0.000000000

45. Pd[Me₈TPP]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.408516000
C	0.000000000	0.000000000	4.895752000
C	0.000000000	0.000000000	7.706414000
C	0.000000000	0.000000000	-3.408516000
C	0.000000000	0.000000000	-4.895752000
C	0.000000000	0.000000000	-7.706414000
C	0.879250000	0.828926000	7.003850000
C	0.879250000	-0.828926000	-7.003850000
C	0.881830000	0.823573000	5.609379000
C	0.881830000	-0.823573000	-5.609379000
C	1.171232000	0.407341000	-2.746648000
C	1.171232000	-0.407341000	2.746648000
C	2.342781000	1.056073000	-3.317305000
C	2.342781000	-1.056073000	3.317305000
C	2.475498000	1.719912000	-4.656386000
C	2.475498000	-1.719912000	4.656386000
C	2.746738000	0.407228000	-1.171293000
C	2.746738000	-0.407228000	1.171293000
C	3.317356000	1.055810000	-2.342958000
C	3.317356000	-1.055810000	2.342958000
C	3.408632000	0.000000000	0.000000000
C	4.656514000	1.719519000	-2.475791000
C	4.656514000	-1.719519000	2.475791000

C	4.895859000	0.000000000	0.000000000
C	5.609506000	0.824054000	0.881379000
C	5.609506000	-0.824054000	-0.881379000
C	7.003979000	0.829478000	0.878728000
C	7.003979000	-0.829478000	-0.878728000
C	7.706553000	0.000000000	0.000000000
C	-0.879250000	0.828926000	-7.003850000
C	-0.879250000	-0.828926000	7.003850000
C	-0.881830000	0.823573000	-5.609379000
C	-0.881830000	-0.823573000	5.609379000
C	-1.171232000	0.407341000	2.746648000
C	-1.171232000	-0.407341000	-2.746648000
C	-2.342781000	1.056073000	3.317305000
C	-2.342781000	-1.056073000	-3.317305000
C	-2.475498000	1.719912000	4.656386000
C	-2.475498000	-1.719912000	-4.656386000
C	-2.746738000	0.407228000	1.171293000
C	-2.746738000	-0.407228000	-1.171293000
C	-3.317356000	1.055810000	2.342958000
C	-3.317356000	-1.055810000	-2.342958000
C	-3.408632000	0.000000000	0.000000000
C	-4.656514000	1.719519000	2.475791000
C	-4.656514000	-1.719519000	-2.475791000
C	-4.895859000	0.000000000	0.000000000
C	-5.609506000	0.824054000	-0.881379000
C	-5.609506000	-0.824054000	0.881379000
C	-7.003979000	0.829478000	-0.878728000
C	-7.003979000	-0.829478000	0.878728000
C	-7.706553000	0.000000000	0.000000000
H	0.000000000	0.000000000	8.796013000
H	0.000000000	0.000000000	-8.796013000
H	1.516671000	2.099122000	-5.026463000
H	1.516671000	-2.099122000	5.026463000
H	1.565030000	1.480597000	7.544094000
H	1.565030000	-1.480597000	-7.544094000
H	1.567557000	1.462715000	5.053689000
H	1.567557000	-1.462715000	-5.053689000
H	2.868401000	1.037256000	-5.424331000
H	2.868401000	-1.037256000	5.424331000
H	3.171171000	2.566362000	-4.589465000
H	3.171171000	-2.566362000	4.589465000
H	4.589224000	2.566840000	-3.170379000
H	4.589224000	-2.566840000	3.170379000
H	5.027302000	2.097506000	-1.516758000
H	5.027302000	-2.097506000	1.516758000
H	5.053827000	1.463534000	1.566793000
H	5.053827000	-1.463534000	-1.566793000
H	5.424048000	1.037181000	-2.870061000
H	5.424048000	-1.037181000	2.870061000
H	7.544220000	1.481542000	1.564143000
H	7.544220000	-1.481542000	-1.564143000

H	8.796163000	0.000000000	0.000000000
H	-1.516671000	2.099122000	5.026463000
H	-1.516671000	-2.099122000	-5.026463000
H	-1.565030000	1.480597000	-7.544094000
H	-1.565030000	-1.480597000	7.544094000
H	-1.567557000	1.462715000	-5.053689000
H	-1.567557000	-1.462715000	5.053689000
H	-2.868401000	1.037256000	5.424331000
H	-2.868401000	-1.037256000	-5.424331000
H	-3.171171000	2.566362000	4.589465000
H	-3.171171000	-2.566362000	-4.589465000
H	-4.589224000	2.566840000	3.170379000
H	-4.589224000	-2.566840000	-3.170379000
H	-5.027302000	2.097506000	1.516758000
H	-5.027302000	-2.097506000	-1.516758000
H	-5.053827000	1.463534000	-1.566793000
H	-5.053827000	-1.463534000	1.566793000
H	-5.424048000	1.037181000	2.870061000
H	-5.424048000	-1.037181000	-2.870061000
H	-7.544220000	1.481542000	-1.564143000
H	-7.544220000	-1.481542000	1.564143000
H	-8.796163000	0.000000000	0.000000000
N	1.420043000	0.119909000	-1.419994000
N	1.420043000	-0.119909000	1.419994000
N	-1.420043000	0.119909000	1.419994000
N	-1.420043000	-0.119909000	-1.419994000

46. Pd[Me₃TPP]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
C	0.633368000	4.217948000	0.267672000
C	0.633368000	-4.217948000	-0.267672000
C	1.058619000	2.823653000	0.358838000
C	1.058619000	-2.823653000	-0.358838000
C	1.353190000	5.478723000	0.659304000
C	1.353190000	-5.478723000	-0.659304000
C	2.363179000	2.363179000	0.608227000
C	2.363179000	-2.363179000	-0.608227000
C	2.823653000	1.058619000	0.358838000
C	2.823653000	-1.058619000	-0.358838000
C	3.367172000	3.367172000	1.073703000
C	3.367172000	-3.367172000	-1.073703000
C	3.565773000	3.565773000	2.445106000
C	3.565773000	-3.565773000	-2.445106000
C	4.117789000	4.117789000	0.163428000
C	4.117789000	-4.117789000	-0.163428000
C	4.217948000	0.633368000	0.267672000
C	4.217948000	-0.633368000	-0.267672000
C	4.499255000	4.499255000	2.898738000
C	4.499255000	-4.499255000	-2.898738000

C	5.051526000	5.051526000	0.611904000
C	5.051526000	-5.051526000	-0.611904000
C	5.245138000	5.245138000	1.981884000
C	5.245138000	-5.245138000	-1.981884000
C	5.478723000	1.353190000	0.659304000
C	5.478723000	-1.353190000	-0.659304000
C	-0.633368000	4.217948000	-0.267672000
C	-0.633368000	-4.217948000	0.267672000
C	-1.058619000	2.823653000	-0.358838000
C	-1.058619000	-2.823653000	0.358838000
C	-1.353190000	5.478723000	-0.659304000
C	-1.353190000	-5.478723000	0.659304000
C	-2.363179000	2.363179000	-0.608227000
C	-2.363179000	-2.363179000	0.608227000
C	-2.823653000	1.058619000	-0.358838000
C	-2.823653000	-1.058619000	0.358838000
C	-3.367172000	3.367172000	-1.073703000
C	-3.367172000	-3.367172000	1.073703000
C	-3.565773000	3.565773000	-2.445106000
C	-3.565773000	-3.565773000	2.445106000
C	-4.117789000	4.117789000	-0.163428000
C	-4.117789000	-4.117789000	0.163428000
C	-4.217948000	0.633368000	-0.267672000
C	-4.217948000	-0.633368000	0.267672000
C	-4.499255000	4.499255000	-2.898738000
C	-4.499255000	-4.499255000	2.898738000
C	-5.051526000	5.051526000	-0.611904000
C	-5.051526000	-5.051526000	0.611904000
C	-5.245138000	5.245138000	-1.981884000
C	-5.245138000	-5.245138000	1.981884000
C	-5.478723000	1.353190000	-0.659304000
C	-5.478723000	-1.353190000	0.659304000
H	0.630542000	6.289868000	0.801918000
H	0.630542000	-6.289868000	-0.801918000
H	1.907869000	5.368602000	1.596593000
H	1.907869000	-5.368602000	-1.596593000
H	2.075471000	5.806148000	-0.102533000
H	2.075471000	-5.806148000	0.102533000
H	2.979841000	2.979841000	3.152581000
H	2.979841000	-2.979841000	-3.152581000
H	3.960035000	3.960035000	-0.903118000
H	3.960035000	-3.960035000	0.903118000
H	4.644552000	4.644552000	3.968459000
H	4.644552000	-4.644552000	-3.968459000
H	5.368602000	1.907869000	1.596593000
H	5.368602000	-1.907869000	-1.596593000
H	5.629436000	5.629436000	-0.108456000
H	5.629436000	-5.629436000	0.108456000
H	5.806148000	2.075471000	-0.102533000
H	5.806148000	-2.075471000	0.102533000
H	5.974184000	5.974184000	2.334174000

H	5.974184000	-5.974184000	-2.334174000
H	6.289868000	0.630542000	0.801918000
H	6.289868000	-0.630542000	-0.801918000
H	-0.630542000	6.289868000	-0.801918000
H	-0.630542000	-6.289868000	0.801918000
H	-1.907869000	5.368602000	-1.596593000
H	-1.907869000	-5.368602000	1.596593000
H	-2.075471000	5.806148000	0.102533000
H	-2.075471000	-5.806148000	-0.102533000
H	-2.979841000	2.979841000	-3.152581000
H	-2.979841000	-2.979841000	3.152581000
H	-3.960035000	3.960035000	0.903118000
H	-3.960035000	-3.960035000	-0.903118000
H	-4.644552000	4.644552000	-3.968459000
H	-4.644552000	-4.644552000	3.968459000
H	-5.368602000	1.907869000	-1.596593000
H	-5.368602000	-1.907869000	1.596593000
H	-5.629436000	5.629436000	0.108456000
H	-5.629436000	-5.629436000	-0.108456000
H	-5.806148000	2.075471000	0.102533000
H	-5.806148000	-2.075471000	-0.102533000
H	-5.974184000	5.974184000	-2.334174000
H	-5.974184000	-5.974184000	2.334174000
H	-6.289868000	0.630542000	-0.801918000
H	-6.289868000	-0.630542000	0.801918000
N	0.000000000	2.014030000	0.000000000
N	0.000000000	-2.014030000	0.000000000
N	2.014030000	0.000000000	0.000000000
N	-2.014030000	0.000000000	0.000000000

47. Pt[Me₈TPP]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.411643000
C	0.000000000	0.000000000	4.900280000
C	0.000000000	0.000000000	7.710689000
C	0.000000000	0.000000000	-3.411643000
C	0.000000000	0.000000000	-4.900280000
C	0.000000000	0.000000000	-7.710689000
C	0.850806000	0.858049000	7.008159000
C	0.850806000	-0.858049000	-7.008159000
C	0.853554000	0.852715000	5.613559000
C	0.853554000	-0.852715000	-5.613559000
C	1.175408000	0.401009000	-2.753878000
C	1.175408000	-0.401009000	2.753878000
C	2.357617000	1.020370000	-3.331254000
C	2.357617000	-1.020370000	3.331254000
C	2.504344000	1.659069000	-4.680889000
C	2.504344000	-1.659069000	4.680889000
C	2.754112000	0.401200000	-1.175147000

C	2.754112000	-0.401200000	1.175147000
C	3.331429000	1.020835000	-2.357169000
C	3.331429000	-1.020835000	2.357169000
C	3.412037000	0.000000000	0.000000000
C	4.680988000	1.659801000	-2.503540000
C	4.680988000	-1.659801000	2.503540000
C	4.900677000	0.000000000	0.000000000
C	5.614020000	0.852268000	0.854022000
C	5.614020000	-0.852268000	-0.854022000
C	7.008615000	0.857676000	0.851156000
C	7.008615000	-0.857676000	-0.851156000
C	7.711144000	0.000000000	0.000000000
C	-0.850806000	0.858049000	-7.008159000
C	-0.850806000	-0.858049000	7.008159000
C	-0.853554000	0.852715000	-5.613559000
C	-0.853554000	-0.852715000	5.613559000
C	-1.175408000	0.401009000	2.753878000
C	-1.175408000	-0.401009000	-2.753878000
C	-2.357617000	1.020370000	3.331254000
C	-2.357617000	-1.020370000	-3.331254000
C	-2.504344000	1.659069000	4.680889000
C	-2.504344000	-1.659069000	-4.680889000
C	-2.754112000	0.401200000	1.175147000
C	-2.754112000	-0.401200000	-1.175147000
C	-3.331429000	1.020835000	2.357169000
C	-3.331429000	-1.020835000	-2.357169000
C	-3.412037000	0.000000000	0.000000000
C	-4.680988000	1.659801000	2.503540000
C	-4.680988000	-1.659801000	-2.503540000
C	-4.900677000	0.000000000	0.000000000
C	-5.614020000	0.852268000	-0.854022000
C	-5.614020000	-0.852268000	0.854022000
C	-7.008615000	0.857676000	-0.851156000
C	-7.008615000	-0.857676000	0.851156000
C	-7.711144000	0.000000000	0.000000000
H	0.000000000	0.000000000	8.800302000
H	0.000000000	0.000000000	-8.800302000
H	1.514478000	1.532205000	7.548451000
H	1.514478000	-1.532205000	-7.548451000
H	1.517631000	1.514276000	5.057821000
H	1.517631000	-1.514276000	-5.057821000
H	1.555580000	2.059236000	-5.054208000
H	1.555580000	-2.059236000	5.054208000
H	2.875889000	0.954412000	-5.439391000
H	2.875889000	-0.954412000	5.439391000
H	3.222968000	2.486891000	-4.628804000
H	3.222968000	-2.486891000	4.628804000
H	4.629080000	2.487572000	-3.222234000
H	4.629080000	-2.487572000	3.222234000
H	5.053857000	2.060102000	-1.554625000
H	5.053857000	-2.060102000	1.554625000

H	5.058501000	1.513509000	1.518666000
H	5.058501000	-1.513509000	-1.518666000
H	5.439821000	0.955298000	-2.874696000
H	5.439821000	-0.955298000	2.874696000
H	7.548890000	1.531404000	1.515245000
H	7.548890000	-1.531404000	-1.515245000
H	8.800744000	0.000000000	0.000000000
H	-1.514478000	1.532205000	-7.548451000
H	-1.514478000	-1.532205000	7.548451000
H	-1.517631000	1.514276000	-5.057821000
H	-1.517631000	-1.514276000	5.057821000
H	-1.555580000	2.059236000	5.054208000
H	-1.555580000	-2.059236000	-5.054208000
H	-2.875889000	0.954412000	5.439391000
H	-2.875889000	-0.954412000	-5.439391000
H	-3.222968000	2.486891000	4.628804000
H	-3.222968000	-2.486891000	-4.628804000
H	-4.629080000	2.487572000	3.222234000
H	-4.629080000	-2.487572000	-3.222234000
H	-5.053857000	2.060102000	1.554625000
H	-5.053857000	-2.060102000	-1.554625000
H	-5.058501000	1.513509000	-1.518666000
H	-5.058501000	-1.513509000	1.518666000
H	-5.439821000	0.955298000	2.874696000
H	-5.439821000	-0.955298000	-2.874696000
H	-7.548890000	1.531404000	-1.515245000
H	-7.548890000	-1.531404000	1.515245000
H	-8.800744000	0.000000000	0.000000000
N	1.417844000	0.140231000	-1.417594000
N	1.417844000	-0.140231000	1.417594000
N	-1.417844000	0.140231000	1.417594000
N	-1.417844000	-0.140231000	-1.417594000

48. Pt[Me₃TPP]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
C	0.634693000	4.218585000	0.263798000
C	0.634693000	-4.218585000	-0.263798000
C	1.061805000	2.827339000	0.354388000
C	1.061805000	-2.827339000	-0.354388000
C	1.357190000	5.479358000	0.649570000
C	1.357190000	-5.479358000	-0.649570000
C	2.366252000	2.366252000	0.601585000
C	2.366252000	-2.366252000	-0.601585000
C	2.827339000	1.061805000	0.354388000
C	2.827339000	-1.061805000	-0.354388000
C	3.369837000	3.369837000	1.069749000
C	3.369837000	-3.369837000	-1.069749000
C	3.565445000	3.565445000	2.442074000
C	3.565445000	-3.565445000	-2.442074000

C	4.122281000	4.122281000	0.162480000
C	4.122281000	-4.122281000	-0.162480000
C	4.218585000	0.634693000	0.263798000
C	4.218585000	-0.634693000	-0.263798000
C	4.497974000	4.497974000	2.899647000
C	4.497974000	-4.497974000	-2.899647000
C	5.055038000	5.055038000	0.615069000
C	5.055038000	-5.055038000	-0.615069000
C	5.245740000	5.245740000	1.985894000
C	5.245740000	-5.245740000	-1.985894000
C	5.479358000	1.357190000	0.649570000
C	5.479358000	-1.357190000	-0.649570000
C	-0.634693000	4.218585000	-0.263798000
C	-0.634693000	-4.218585000	0.263798000
C	-1.061805000	2.827339000	-0.354388000
C	-1.061805000	-2.827339000	0.354388000
C	-1.357190000	5.479358000	-0.649570000
C	-1.357190000	-5.479358000	0.649570000
C	-2.366252000	2.366252000	-0.601585000
C	-2.366252000	-2.366252000	0.601585000
C	-2.827339000	1.061805000	-0.354388000
C	-2.827339000	-1.061805000	0.354388000
C	-3.369837000	3.369837000	-1.069749000
C	-3.369837000	-3.369837000	1.069749000
C	-3.565445000	3.565445000	-2.442074000
C	-3.565445000	-3.565445000	2.442074000
C	-4.122281000	4.122281000	-0.162480000
C	-4.122281000	-4.122281000	0.162480000
C	-4.218585000	0.634693000	-0.263798000
C	-4.218585000	-0.634693000	0.263798000
C	-4.497974000	4.497974000	-2.899647000
C	-4.497974000	-4.497974000	2.899647000
C	-5.055038000	5.055038000	-0.615069000
C	-5.055038000	-5.055038000	0.615069000
C	-5.245740000	5.245740000	-1.985894000
C	-5.245740000	-5.245740000	1.985894000
C	-5.479358000	1.357190000	-0.649570000
C	-5.479358000	-1.357190000	0.649570000
H	0.636156000	6.291728000	0.792676000
H	0.636156000	-6.291728000	-0.792676000
H	1.914961000	5.371206000	1.585172000
H	1.914961000	-5.371206000	-1.585172000
H	2.077142000	5.803847000	-0.115679000
H	2.077142000	-5.803847000	0.115679000
H	2.977869000	2.977869000	3.146821000
H	2.977869000	-2.977869000	-3.146821000
H	3.966708000	3.966708000	-0.904715000
H	3.966708000	-3.966708000	0.904715000
H	4.641079000	4.641079000	3.969975000
H	4.641079000	-4.641079000	-3.969975000
H	5.371206000	1.914961000	1.585172000

H	5.371206000	-1.914961000	-1.585172000
H	5.634501000	5.634501000	-0.102697000
H	5.634501000	-5.634501000	0.102697000
H	5.803847000	2.077142000	-0.115679000
H	5.803847000	-2.077142000	0.115679000
H	5.974045000	5.974045000	2.341298000
H	5.974045000	-5.974045000	-2.341298000
H	6.291728000	0.636156000	0.792676000
H	6.291728000	-0.636156000	-0.792676000
H	-0.636156000	6.291728000	-0.792676000
H	-0.636156000	-6.291728000	0.792676000
H	-1.914961000	5.371206000	-1.585172000
H	-1.914961000	-5.371206000	1.585172000
H	-2.077142000	5.803847000	0.115679000
H	-2.077142000	-5.803847000	-0.115679000
H	-2.977869000	2.977869000	-3.146821000
H	-2.977869000	-2.977869000	3.146821000
H	-3.966708000	3.966708000	0.904715000
H	-3.966708000	-3.966708000	-0.904715000
H	-4.641079000	4.641079000	-3.969975000
H	-4.641079000	-4.641079000	3.969975000
H	-5.371206000	1.914961000	-1.585172000
H	-5.371206000	-1.914961000	1.585172000
H	-5.634501000	5.634501000	0.102697000
H	-5.634501000	-5.634501000	-0.102697000
H	-5.803847000	2.077142000	0.115679000
H	-5.803847000	-2.077142000	-0.115679000
H	-5.974045000	5.974045000	-2.341298000
H	-5.974045000	-5.974045000	2.341298000
H	-6.291728000	0.636156000	-0.792676000
H	-6.291728000	-0.636156000	0.792676000
N	0.000000000	2.015082000	0.000000000
N	0.000000000	-2.015082000	0.000000000
N	2.015082000	0.000000000	0.000000000
N	-2.015082000	0.000000000	0.000000000

49. Zn[Me₈TPP]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	3.417965000
C	0.000000000	0.000000000	4.904525000
C	0.000000000	0.000000000	7.716857000
C	0.000000000	0.000000000	-3.417965000
C	0.000000000	0.000000000	-4.904525000
C	0.000000000	0.000000000	-7.716857000
C	0.874747000	0.833509000	7.013986000
C	0.874747000	-0.833509000	-7.013986000
C	0.876930000	0.828548000	5.619653000
C	0.876930000	-0.828548000	-5.619653000
C	1.190130000	0.383817000	-2.760204000

C	1.190130000	-0.383817000	2.760204000
C	2.364729000	1.018117000	-3.340986000
C	2.364729000	-1.018117000	3.340986000
C	2.510011000	1.675298000	-4.682232000
C	2.510011000	-1.675298000	4.682232000
C	2.760153000	0.383921000	-1.190115000
C	2.760153000	-0.383921000	1.190115000
C	3.340991000	1.018081000	-2.364794000
C	3.340991000	-1.018081000	2.364794000
C	3.417891000	0.000000000	0.000000000
C	4.682210000	1.675298000	-2.510189000
C	4.682210000	-1.675298000	2.510189000
C	4.904435000	0.000000000	0.000000000
C	5.619552000	0.828424000	0.877051000
C	5.619552000	-0.828424000	-0.877051000
C	7.013878000	0.833579000	0.874680000
C	7.013878000	-0.833579000	-0.874680000
C	7.716738000	0.000000000	0.000000000
C	-0.874747000	0.833509000	-7.013986000
C	-0.874747000	-0.833509000	7.013986000
C	-0.876930000	0.828548000	-5.619653000
C	-0.876930000	-0.828548000	5.619653000
C	-1.190130000	0.383817000	2.760204000
C	-1.190130000	-0.383817000	-2.760204000
C	-2.364729000	1.018117000	3.340986000
C	-2.364729000	-1.018117000	-3.340986000
C	-2.510011000	1.675298000	4.682232000
C	-2.510011000	-1.675298000	-4.682232000
C	-2.760153000	0.383921000	1.190115000
C	-2.760153000	-0.383921000	-1.190115000
C	-3.340991000	1.018081000	2.364794000
C	-3.340991000	-1.018081000	-2.364794000
C	-3.417891000	0.000000000	0.000000000
C	-4.682210000	1.675298000	2.510189000
C	-4.682210000	-1.675298000	-2.510189000
C	-4.904435000	0.000000000	0.000000000
C	-5.619552000	0.828424000	-0.877051000
C	-5.619552000	-0.828424000	0.877051000
C	-7.013878000	0.833579000	-0.874680000
C	-7.013878000	-0.833579000	0.874680000
C	-7.716738000	0.000000000	0.000000000
H	0.000000000	0.000000000	8.806473000
H	0.000000000	0.000000000	-8.806473000
H	1.552899000	2.037870000	-5.072085000
H	1.552899000	-2.037870000	5.072085000
H	1.556920000	1.489027000	7.554209000
H	1.556920000	-1.489027000	-7.554209000
H	1.558536000	1.472411000	5.064433000
H	1.558536000	-1.472411000	-5.064433000
H	2.926421000	0.992230000	-5.437380000
H	2.926421000	-0.992230000	5.437380000

H	3.193224000	2.531885000	-4.610640000
H	3.193224000	-2.531885000	4.610640000
H	4.610270000	2.532533000	-3.192554000
H	4.610270000	-2.532533000	3.192554000
H	5.064363000	1.472340000	1.558635000
H	5.064363000	-1.472340000	-1.558635000
H	5.072611000	2.036991000	-1.552984000
H	5.072611000	-2.036991000	1.552984000
H	5.437072000	0.992564000	-2.927686000
H	5.437072000	-0.992564000	2.927686000
H	7.554081000	1.489148000	1.556833000
H	7.554081000	-1.489148000	-1.556833000
H	8.806330000	0.000000000	0.000000000
H	-1.552899000	2.037870000	5.072085000
H	-1.552899000	-2.037870000	-5.072085000
H	-1.556920000	1.489027000	-7.554209000
H	-1.556920000	-1.489027000	7.554209000
H	-1.558536000	1.472411000	-5.064433000
H	-1.558536000	-1.472411000	5.064433000
H	-2.926421000	0.992230000	5.437380000
H	-2.926421000	-0.992230000	-5.437380000
H	-3.193224000	2.531885000	4.610640000
H	-3.193224000	-2.531885000	-4.610640000
H	-4.610270000	2.532533000	3.192554000
H	-4.610270000	-2.532533000	-3.192554000
H	-5.064363000	1.472340000	-1.558635000
H	-5.064363000	-1.472340000	1.558635000
H	-5.072611000	2.036991000	1.552984000
H	-5.072611000	-2.036991000	-1.552984000
H	-5.437072000	0.992564000	2.927686000
H	-5.437072000	-0.992564000	-2.927686000
H	-7.554081000	1.489148000	-1.556833000
H	-7.554081000	-1.489148000	1.556833000
H	-8.806330000	0.000000000	0.000000000
N	1.435783000	0.101449000	-1.435812000
N	1.435783000	-0.101449000	1.435812000
N	-1.435783000	0.101449000	1.435812000
N	-1.435783000	-0.101449000	-1.435812000

50. Zn[Me₈TPP]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
C	0.648891000	4.249393000	0.230472000
C	0.648891000	-4.249393000	-0.230472000
C	1.072313000	2.853073000	0.302595000
C	1.072313000	-2.853073000	-0.302595000
C	1.387611000	5.513552000	0.574172000
C	1.387611000	-5.513552000	-0.574172000
C	2.387508000	2.387508000	0.516516000
C	2.387508000	-2.387508000	-0.516516000

C	2.853073000	1.072313000	0.302595000
C	2.853073000	-1.072313000	-0.302595000
C	3.404237000	3.404237000	0.925167000
C	3.404237000	-3.404237000	-0.925167000
C	3.641605000	3.641605000	2.284327000
C	3.641605000	-3.641605000	-2.284327000
C	4.128975000	4.128975000	-0.025874000
C	4.128975000	-4.128975000	0.025874000
C	4.249393000	0.648891000	0.230472000
C	4.249393000	-0.648891000	-0.230472000
C	4.586744000	4.586744000	2.686010000
C	4.586744000	-4.586744000	-2.686010000
C	5.074661000	5.074661000	0.370326000
C	5.074661000	-5.074661000	-0.370326000
C	5.306530000	5.306530000	1.728265000
C	5.306530000	-5.306530000	-1.728265000
C	5.513552000	1.387611000	0.574172000
C	5.513552000	-1.387611000	-0.574172000
C	-0.648891000	4.249393000	-0.230472000
C	-0.648891000	-4.249393000	0.230472000
C	-1.072313000	2.853073000	-0.302595000
C	-1.072313000	-2.853073000	0.302595000
C	-1.387611000	5.513552000	-0.574172000
C	-1.387611000	-5.513552000	0.574172000
C	-2.387508000	2.387508000	-0.516516000
C	-2.387508000	-2.387508000	0.516516000
C	-2.853073000	1.072313000	-0.302595000
C	-2.853073000	-1.072313000	0.302595000
C	-3.404237000	3.404237000	-0.925167000
C	-3.404237000	-3.404237000	0.925167000
C	-3.641605000	3.641605000	-2.284327000
C	-3.641605000	-3.641605000	2.284327000
C	-4.128975000	4.128975000	0.025874000
C	-4.128975000	-4.128975000	-0.025874000
C	-4.249393000	0.648891000	-0.230472000
C	-4.249393000	-0.648891000	0.230472000
C	-4.586744000	4.586744000	-2.686010000
C	-4.586744000	-4.586744000	2.686010000
C	-5.074661000	5.074661000	-0.370326000
C	-5.074661000	-5.074661000	0.370326000
C	-5.306530000	5.306530000	-1.728265000
C	-5.306530000	-5.306530000	1.728265000
C	-5.513552000	1.387611000	-0.574172000
C	-5.513552000	-1.387611000	0.574172000
H	0.676491000	6.330773000	0.737339000
H	0.676491000	-6.330773000	-0.737339000
H	1.983094000	5.414637000	1.487001000
H	1.983094000	-5.414637000	-1.487001000
H	2.077178000	5.826351000	-0.223299000
H	2.077178000	-5.826351000	0.223299000
H	3.075951000	3.075951000	3.023988000

H	3.075951000	-3.075951000	-3.023988000
H	3.941827000	3.941827000	-1.082891000
H	3.941827000	-3.941827000	1.082891000
H	4.761699000	4.761699000	3.746834000
H	4.761699000	-4.761699000	-3.746834000
H	5.414637000	1.983094000	1.487001000
H	5.414637000	-1.983094000	-1.487001000
H	5.632046000	5.632046000	-0.381660000
H	5.632046000	-5.632046000	0.381660000
H	5.826351000	2.077178000	-0.223299000
H	5.826351000	-2.077178000	0.223299000
H	6.044837000	6.044837000	2.039531000
H	6.044837000	-6.044837000	-2.039531000
H	6.330773000	0.676491000	0.737339000
H	6.330773000	-0.676491000	-0.737339000
H	-0.676491000	6.330773000	-0.737339000
H	-0.676491000	-6.330773000	0.737339000
H	-1.983094000	5.414637000	-1.487001000
H	-1.983094000	-5.414637000	1.487001000
H	-2.077178000	5.826351000	0.223299000
H	-2.077178000	-5.826351000	-0.223299000
H	-3.075951000	3.075951000	-3.023988000
H	-3.075951000	-3.075951000	3.023988000
H	-3.941827000	3.941827000	1.082891000
H	-3.941827000	-3.941827000	-1.082891000
H	-4.761699000	4.761699000	-3.746834000
H	-4.761699000	-4.761699000	3.746834000
H	-5.414637000	1.983094000	-1.487001000
H	-5.414637000	-1.983094000	1.487001000
H	-5.632046000	5.632046000	0.381660000
H	-5.632046000	-5.632046000	-0.381660000
H	-5.826351000	2.077178000	0.223299000
H	-5.826351000	-2.077178000	-0.223299000
H	-6.044837000	6.044837000	-2.039531000
H	-6.044837000	-6.044837000	2.039531000
H	-6.330773000	0.676491000	-0.737339000
H	-6.330773000	-0.676491000	0.737339000
N	0.000000000	2.040300000	0.000000000
N	0.000000000	-2.040300000	0.000000000
N	2.040300000	0.000000000	0.000000000
N	-2.040300000	0.000000000	0.000000000

51. Cu[A₄Br₈]; S = ½ (saddled)

Cu	0.000000000	0.000000000	0.004317000
Br	1.484323000	-5.512787000	-1.417179000
Br	1.881957000	5.114076000	-2.216799000
Br	5.130773000	-1.913377000	2.168092000
Br	5.549443000	1.452838000	1.382950000
Br	-1.484323000	5.512787000	-1.417179000

Br	-1.881957000	-5.114076000	-2.216799000
Br	-5.130773000	1.913377000	2.168092000
Br	-5.549443000	-1.452838000	1.382950000
C	0.437484000	-4.042480000	-0.874493000
C	0.860211000	-2.846535000	-0.187057000
C	0.890863000	3.872268000	-1.205906000
C	1.297848000	2.588732000	-0.674258000
C	2.100995000	-2.602683000	0.462844000
C	2.590423000	-1.296331000	0.674596000
C	2.606403000	2.107907000	-0.449556000
C	2.832375000	-3.723055000	0.896085000
C	2.853585000	0.861828000	0.188194000
C	3.188249000	-7.233439000	2.973121000
C	3.393162000	-4.731045000	1.302803000
C	3.718920000	2.870748000	-0.847650000
C	3.879985000	-0.897601000	1.194976000
C	4.054008000	0.430445000	0.865045000
C	4.707561000	3.484857000	-1.223026000
C	4.750885000	-7.200476000	0.306356000
C	5.840752000	-5.630426000	2.763440000
C	6.013386000	6.169844000	-0.971502000
C	6.139428000	4.578255000	-3.622240000
C	7.703433000	3.568462000	-1.131630000
C	-0.437484000	4.042480000	-0.874493000
C	-0.860211000	2.846535000	-0.187057000
C	-0.890863000	-3.872268000	-1.205906000
C	-1.297848000	-2.588732000	-0.674258000
C	-2.100995000	2.602683000	0.462844000
C	-2.590423000	1.296331000	0.674596000
C	-2.606403000	-2.107907000	-0.449556000
C	-2.832375000	3.723055000	0.896085000
C	-2.853585000	-0.861828000	0.188194000
C	-3.188249000	7.233439000	2.973121000
C	-3.393162000	4.731045000	1.302803000
C	-3.718920000	-2.870748000	-0.847650000
C	-3.879985000	0.897601000	1.194976000
C	-4.054008000	-0.430445000	0.865045000
C	-4.707561000	-3.484857000	-1.223026000
C	-4.750885000	7.200476000	0.306356000
C	-5.840752000	5.630426000	2.763440000
C	-6.013386000	-6.169844000	-0.971502000
C	-6.139428000	-4.578255000	-3.622240000
C	-7.703433000	-3.568462000	-1.131630000
H	2.274138000	-7.530944000	2.439793000
H	2.892091000	-6.655545000	3.859967000
H	3.703327000	-8.145641000	3.310929000
H	3.840055000	-7.495935000	-0.233997000
H	5.075905000	6.651532000	-1.284554000
H	5.208581000	5.051116000	-3.966634000
H	5.305108000	-8.113802000	0.570822000
H	5.371926000	-6.601004000	-0.373718000

H	5.559052000	-5.020108000	3.633614000
H	6.008512000	6.101796000	0.125598000
H	6.201788000	3.580228000	-4.078349000
H	6.440552000	-6.481224000	3.119958000
H	6.470491000	-5.015244000	2.104883000
H	6.852772000	6.813665000	-1.275287000
H	6.986714000	5.179383000	-3.985754000
H	7.701106000	3.500957000	-0.034365000
H	7.744125000	2.545615000	-1.531637000
H	8.615912000	4.099882000	-1.441537000
H	-2.274138000	7.530944000	2.439793000
H	-2.892091000	6.655545000	3.859967000
H	-3.703327000	8.145641000	3.310929000
H	-3.840055000	7.495935000	-0.233997000
H	-5.075905000	-6.651532000	-1.284554000
H	-5.208581000	-5.051116000	-3.966634000
H	-5.305108000	8.113802000	0.570822000
H	-5.371926000	6.601004000	-0.373718000
H	-5.559052000	5.020108000	3.633614000
H	-6.008512000	-6.101796000	0.125598000
H	-6.201788000	-3.580228000	-4.078349000
H	-6.440552000	6.481224000	3.119958000
H	-6.470491000	5.015244000	2.104883000
H	-6.852772000	-6.813665000	-1.275287000
H	-6.986714000	-5.179383000	-3.985754000
H	-7.701106000	-3.500957000	-0.034365000
H	-7.744125000	-2.545615000	-1.531637000
H	-8.615912000	-4.099882000	-1.441537000
N	0.185894000	1.962870000	-0.150693000
N	1.966195000	-0.182560000	0.154049000
N	-0.185894000	-1.962870000	-0.150693000
N	-1.966195000	0.182560000	0.154049000
Si	4.305820000	-6.221276000	1.850286000
Si	6.166610000	4.462034000	-1.744948000
Si	-4.305820000	6.221276000	1.850286000
Si	-6.166610000	-4.462034000	-1.744948000

52. Cu[A₄Br₈]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
Br	1.585989000	5.727948000	-0.690920000
Br	1.585989000	-5.727948000	0.690920000
Br	5.727948000	1.585989000	-0.690920000
Br	5.727948000	-1.585989000	0.690920000
Br	-1.585989000	5.727948000	0.690920000
Br	-1.585989000	-5.727948000	-0.690920000
Br	-5.727948000	1.585989000	0.690920000
Br	-5.727948000	-1.585989000	-0.690920000
C	0.620408000	4.157000000	-0.302178000
C	0.620408000	-4.157000000	0.302178000

C	1.021046000	2.775800000	-0.448184000
C	1.021046000	-2.775800000	0.448184000
C	2.293379000	2.293379000	-0.844551000
C	2.293379000	-2.293379000	0.844551000
C	2.775800000	1.021046000	-0.448184000
C	2.775800000	-1.021046000	0.448184000
C	3.109924000	3.109924000	-1.645327000
C	3.109924000	-3.109924000	1.645327000
C	3.756609000	5.960676000	-4.489885000
C	3.756609000	-5.960676000	4.489885000
C	3.772672000	3.772672000	-2.431473000
C	3.772672000	-3.772672000	2.431473000
C	4.157000000	0.620408000	-0.302178000
C	4.157000000	-0.620408000	0.302178000
C	5.873404000	5.873404000	-2.226640000
C	5.873404000	-5.873404000	2.226640000
C	5.960676000	3.756609000	-4.489885000
C	5.960676000	-3.756609000	4.489885000
C	-0.620408000	4.157000000	0.302178000
C	-0.620408000	-4.157000000	-0.302178000
C	-1.021046000	2.775800000	0.448184000
C	-1.021046000	-2.775800000	-0.448184000
C	-2.293379000	2.293379000	0.844551000
C	-2.293379000	-2.293379000	-0.844551000
C	-2.775800000	1.021046000	0.448184000
C	-2.775800000	-1.021046000	-0.448184000
C	-3.109924000	3.109924000	1.645327000
C	-3.109924000	-3.109924000	-1.645327000
C	-3.756609000	5.960676000	4.489885000
C	-3.756609000	-5.960676000	-4.489885000
C	-3.772672000	3.772672000	2.431473000
C	-3.772672000	-3.772672000	-2.431473000
C	-4.157000000	0.620408000	0.302178000
C	-4.157000000	-0.620408000	-0.302178000
C	-5.873404000	5.873404000	2.226640000
C	-5.873404000	-5.873404000	-2.226640000
C	-5.960676000	3.756609000	4.489885000
C	-5.960676000	-3.756609000	-4.489885000
H	3.069927000	6.536174000	-3.852335000
H	3.069927000	-6.536174000	3.852335000
H	3.150426000	5.363372000	-5.185597000
H	3.150426000	-5.363372000	5.185597000
H	4.359913000	6.669342000	-5.077192000
H	4.359913000	-6.669342000	5.077192000
H	5.218271000	6.475126000	-1.580796000
H	5.218271000	-6.475126000	1.580796000
H	5.363372000	3.150426000	-5.185597000
H	5.363372000	-3.150426000	5.185597000
H	6.475126000	5.218271000	-1.580796000
H	6.475126000	-5.218271000	1.580796000
H	6.536174000	3.069927000	-3.852335000

H	6.536174000	-3.069927000	3.852335000
H	6.553403000	6.553403000	-2.762107000
H	6.553403000	-6.553403000	2.762107000
H	6.669342000	4.359913000	-5.077192000
H	6.669342000	-4.359913000	5.077192000
H	-3.069927000	6.536174000	3.852335000
H	-3.069927000	-6.536174000	-3.852335000
H	-3.150426000	5.363372000	5.185597000
H	-3.150426000	-5.363372000	-5.185597000
H	-4.359913000	6.669342000	5.077192000
H	-4.359913000	-6.669342000	-5.077192000
H	-5.218271000	6.475126000	1.580796000
H	-5.218271000	-6.475126000	-1.580796000
H	-5.363372000	3.150426000	5.185597000
H	-5.363372000	-3.150426000	-5.185597000
H	-6.475126000	5.218271000	1.580796000
H	-6.475126000	-5.218271000	-1.580796000
H	-6.536174000	3.069927000	3.852335000
H	-6.536174000	-3.069927000	-3.852335000
H	-6.553403000	6.553403000	2.762107000
H	-6.553403000	-6.553403000	-2.762107000
H	-6.669342000	4.359913000	5.077192000
H	-6.669342000	-4.359913000	-5.077192000
N	0.000000000	1.975142000	0.000000000
N	0.000000000	-1.975142000	0.000000000
N	1.975142000	0.000000000	0.000000000
N	-1.975142000	0.000000000	0.000000000
Si	4.854702000	4.854702000	-3.438577000
Si	4.854702000	-4.854702000	3.438577000
Si	-4.854702000	4.854702000	3.438577000
Si	-4.854702000	-4.854702000	-3.438577000

53. Ni[A₄Br₈]; S = 0 (saddled)

Ni	-0.001197000	-0.001614000	0.000000000
Br	1.501014000	-2.456367000	5.013586000
Br	1.501014000	-2.456367000	-5.013586000
Br	5.305193000	1.586484000	1.750299000
Br	5.305193000	1.586484000	-1.750299000
Br	-1.997026000	-2.074184000	5.013666000
Br	-1.997026000	-2.074184000	-5.013666000
Br	-4.845488000	2.687232000	1.749663000
Br	-4.845488000	2.687232000	-1.749663000
C	0.538762000	-1.400035000	3.788899000
C	0.538762000	-1.400035000	-3.788899000
C	1.039880000	-0.698414000	2.631920000
C	1.039880000	-0.698414000	-2.631920000
C	2.352784000	-0.256655000	2.375076000
C	2.352784000	-0.256655000	-2.375076000
C	2.688525000	0.264678000	1.111443000

C	2.688525000	0.264678000	-1.111443000
C	3.315195000	-0.321722000	3.399477000
C	3.315195000	-0.321722000	-3.399477000
C	3.933956000	0.857985000	0.688079000
C	3.933956000	0.857985000	-0.688079000
C	4.129303000	-0.372066000	4.309830000
C	4.129303000	-0.372066000	-4.309830000
C	4.771877000	0.620319000	7.079511000
C	4.771877000	0.620319000	-7.079511000
C	5.458010000	-2.266067000	6.205029000
C	5.458010000	-2.266067000	-6.205029000
C	7.002059000	0.144705000	4.978580000
C	7.002059000	0.144705000	-4.978580000
C	-0.829307000	-1.250446000	3.789065000
C	-0.829307000	-1.250446000	-3.789065000
C	-1.167203000	-0.457214000	2.632162000
C	-1.167203000	-0.457214000	-2.632162000
C	-2.354067000	0.257357000	2.375602000
C	-2.354067000	0.257357000	-2.375602000
C	-2.571004000	0.836886000	1.111489000
C	-2.571004000	0.836886000	-1.111489000
C	-3.304775000	0.405037000	3.402333000
C	-3.304775000	0.405037000	-3.402333000
C	-3.660305000	1.683412000	0.688052000
C	-3.660305000	1.683412000	-0.688052000
C	-4.105992000	0.535928000	4.316092000
C	-4.105992000	0.535928000	-4.316092000
C	-4.498855000	1.643366000	7.088599000
C	-4.498855000	1.643366000	-7.088599000
C	-5.827596000	-1.008863000	6.212352000
C	-5.827596000	-1.008863000	-6.212352000
C	-6.783115000	1.693000000	4.992492000
C	-6.783115000	1.693000000	-4.992492000
H	3.790494000	0.284818000	7.443849000
H	3.790494000	0.284818000	-7.443849000
H	4.474271000	-2.614495000	6.551387000
H	4.474271000	-2.614495000	-6.551387000
H	4.675290000	1.666473000	6.756204000
H	4.675290000	1.666473000	-6.756204000
H	5.483953000	0.582155000	7.918038000
H	5.483953000	0.582155000	-7.918038000
H	5.773851000	-2.911061000	5.373218000
H	5.773851000	-2.911061000	-5.373218000
H	6.175319000	-2.386432000	7.030942000
H	6.175319000	-2.386432000	-7.030942000
H	6.919040000	1.194330000	4.661495000
H	6.919040000	1.194330000	-4.661495000
H	7.307222000	-0.449445000	4.105800000
H	7.307222000	-0.449445000	-4.105800000
H	7.794456000	0.078801000	5.739327000
H	7.794456000	0.078801000	-5.739327000

H	-3.618830000	1.092416000	7.449746000
H	-3.618830000	1.092416000	-7.449746000
H	-4.167139000	2.640483000	6.766066000
H	-4.167139000	2.640483000	-6.766066000
H	-4.948385000	-1.573525000	6.554789000
H	-4.948385000	-1.573525000	-6.554789000
H	-5.198713000	1.767128000	7.929147000
H	-5.198713000	1.767128000	-7.929147000
H	-6.284980000	-1.562880000	5.380741000
H	-6.284980000	-1.562880000	-5.380741000
H	-6.463183000	2.696960000	4.678113000
H	-6.463183000	2.696960000	-4.678113000
H	-6.550912000	-0.963911000	7.040583000
H	-6.550912000	-0.963911000	-7.040583000
H	-7.216670000	1.186580000	4.118721000
H	-7.216670000	1.186580000	-4.118721000
H	-7.568798000	1.807345000	5.754444000
H	-7.568798000	1.807345000	-5.754444000
N	1.902014000	0.030063000	0.000000000
N	-0.028466000	-0.254356000	1.878448000
N	-0.028466000	-0.254356000	-1.878448000
N	-1.853367000	0.438683000	0.000000000
Si	5.360274000	-0.467190000	5.662741000
Si	5.360274000	-0.467190000	-5.662741000
Si	-5.323060000	0.721173000	5.672143000
Si	-5.323060000	0.721173000	-5.672143000

54. Ni[A₄Br₈]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	-0.000713000
Br	0.854314000	-5.719999000	1.101841000
Br	2.124929000	5.450277000	-0.706116000
Br	5.452853000	-2.130707000	0.686629000
Br	5.718992000	0.845545000	-1.119303000
Br	-0.854314000	5.719999000	1.101841000
Br	-2.124929000	-5.450277000	-0.706116000
Br	-5.452853000	2.130707000	0.686629000
Br	-5.718992000	-0.845545000	-1.119303000
C	0.128866000	-4.093531000	0.494489000
C	0.678924000	-2.763658000	0.606848000
C	1.023692000	3.991848000	-0.255592000
C	1.244100000	2.587129000	-0.504044000
C	1.982653000	-2.413572000	1.018791000
C	2.414449000	1.983984000	-1.018918000
C	2.587205000	-1.244712000	0.501342000
C	2.704823000	-3.241091000	1.893625000
C	2.764068000	0.678662000	-0.609742000
C	3.237504000	-5.731820000	5.117060000
C	3.251049000	2.707720000	-1.884502000
C	3.315858000	-3.885516000	2.735158000

C	3.920013000	3.308933000	-2.713766000
C	3.991453000	-1.025892000	0.250383000
C	4.093883000	0.126589000	-0.499981000
C	4.533003000	4.072630000	-5.577027000
C	4.881777000	6.083188000	-3.245536000
C	5.215688000	-6.181448000	2.770936000
C	5.604419000	-3.761477000	4.667415000
C	6.782885000	3.631975000	-3.490719000
C	-0.128866000	4.093531000	0.494489000
C	-0.678924000	2.763658000	0.606848000
C	-1.023692000	-3.991848000	-0.255592000
C	-1.244100000	-2.587129000	-0.504044000
C	-1.982653000	2.413572000	1.018791000
C	-2.414449000	-1.983984000	-1.018918000
C	-2.587205000	1.244712000	0.501342000
C	-2.704823000	3.241091000	1.893625000
C	-2.764068000	-0.678662000	-0.609742000
C	-3.237504000	5.731820000	5.117060000
C	-3.251049000	-2.707720000	-1.884502000
C	-3.315858000	3.885516000	2.735158000
C	-3.920013000	-3.308933000	-2.713766000
C	-3.991453000	1.025892000	0.250383000
C	-4.093883000	-0.126589000	-0.499981000
C	-4.533003000	-4.072630000	-5.577027000
C	-4.881777000	-6.083188000	-3.245536000
C	-5.215688000	6.181448000	2.770936000
C	-5.604419000	3.761477000	4.667415000
C	-6.782885000	-3.631975000	-3.490719000
H	2.479330000	-6.352671000	4.618702000
H	2.713946000	-4.982197000	5.727197000
H	3.501622000	4.418781000	-5.734381000
H	3.823231000	-6.376331000	5.789996000
H	3.847909000	6.432203000	-3.379476000
H	4.479987000	-6.818499000	2.259895000
H	4.588221000	3.016505000	-5.876773000
H	5.099727000	-3.008572000	5.289194000
H	5.145703000	6.197300000	-2.184461000
H	5.196062000	4.653466000	-6.236219000
H	5.544443000	6.730958000	-3.838942000
H	5.826640000	-5.687105000	2.002237000
H	5.872330000	-6.825412000	3.375594000
H	6.192804000	-3.230067000	3.905527000
H	6.296681000	-4.330515000	5.306274000
H	6.843896000	2.569103000	-3.765190000
H	7.061309000	3.727472000	-2.431468000
H	7.517812000	4.186564000	-4.093290000
H	-2.479330000	6.352671000	4.618702000
H	-2.713946000	4.982197000	5.727197000
H	-3.501622000	-4.418781000	-5.734381000
H	-3.823231000	6.376331000	5.789996000
H	-3.847909000	-6.432203000	-3.379476000

H	-4.479987000	6.818499000	2.259895000
H	-4.588221000	-3.016505000	-5.876773000
H	-5.099727000	3.008572000	5.289194000
H	-5.145703000	-6.197300000	-2.184461000
H	-5.196062000	-4.653466000	-6.236219000
H	-5.544443000	-6.730958000	-3.838942000
H	-5.826640000	5.687105000	2.002237000
H	-5.872330000	6.825412000	3.375594000
H	-6.192804000	3.230067000	3.905527000
H	-6.296681000	4.330515000	5.306274000
H	-6.843896000	-2.569103000	-3.765190000
H	-7.061309000	-3.727472000	-2.431468000
H	-7.517812000	-4.186564000	-4.093290000
N	0.192579000	1.874462000	0.020133000
N	1.874982000	-0.192609000	-0.022544000
N	-0.192579000	-1.874462000	0.020133000
N	-1.874982000	0.192609000	-0.022544000
Si	4.353458000	-4.903387000	3.851140000
Si	5.042724000	4.286391000	-3.780423000
Si	-4.353458000	4.903387000	3.851140000
Si	-5.042724000	-4.286391000	-3.780423000

55. Pd[A₄Br₈]; S = 0 (saddled)

Pd	0.000000000	0.000000000	-0.030946000
Br	1.219210000	-5.392690000	-2.025292000
Br	2.241430000	5.000543000	-2.155942000
Br	5.140532000	-2.255643000	1.861846000
Br	5.527324000	1.174810000	1.755830000
Br	-1.219210000	5.392690000	-2.025292000
Br	-2.241430000	-5.000543000	-2.155942000
Br	-5.140532000	2.255643000	1.861846000
Br	-5.527324000	-1.174810000	1.755830000
C	0.281464000	-4.006629000	-1.160225000
C	0.819791000	-2.853860000	-0.472023000
C	1.086488000	3.850616000	-1.211131000
C	1.401271000	2.604408000	-0.545162000
C	2.125553000	-2.666079000	0.044479000
C	2.623820000	-1.405251000	0.439910000
C	2.658243000	2.140360000	-0.089633000
C	2.874619000	0.820541000	0.369424000
C	2.925914000	-3.814204000	0.200258000
C	3.564606000	-4.844094000	0.359640000
C	3.570472000	-7.562098000	1.656085000
C	3.721940000	3.062617000	-0.059058000
C	3.895640000	-1.094250000	1.057790000
C	4.051469000	0.273080000	1.010839000
C	4.614830000	3.896083000	-0.019588000
C	4.870711000	-7.098512000	-1.111531000
C	5.376175000	6.602190000	1.052873000

C	6.159421000	-5.865934000	1.441672000
C	6.331736000	5.650315000	-1.730674000
C	7.450936000	4.305001000	0.845409000
C	-0.281464000	4.006629000	-1.160225000
C	-0.819791000	2.853860000	-0.472023000
C	-1.086488000	-3.850616000	-1.211131000
C	-1.401271000	-2.604408000	-0.545162000
C	-2.125553000	2.666079000	0.044479000
C	-2.623820000	1.405251000	0.439910000
C	-2.658243000	-2.140360000	-0.089633000
C	-2.874619000	-0.820541000	0.369424000
C	-2.925914000	3.814204000	0.200258000
C	-3.564606000	4.844094000	0.359640000
C	-3.570472000	7.562098000	1.656085000
C	-3.721940000	-3.062617000	-0.059058000
C	-3.895640000	1.094250000	1.057790000
C	-4.051469000	-0.273080000	1.010839000
C	-4.614830000	-3.896083000	-0.019588000
C	-4.870711000	7.098512000	-1.111531000
C	-5.376175000	-6.602190000	1.052873000
C	-6.159421000	5.865934000	1.441672000
C	-6.331736000	-5.650315000	-1.730674000
C	-7.450936000	-4.305001000	0.845409000
H	2.614009000	-7.809554000	1.173962000
H	3.351945000	-7.123388000	2.640022000
H	3.917756000	-7.331375000	-1.608238000
H	4.131793000	-8.496172000	1.811061000
H	4.477067000	7.046084000	0.602256000
H	5.126530000	6.296032000	2.078700000
H	5.422906000	-6.392761000	-1.747599000
H	5.432153000	6.076402000	-2.197912000
H	5.454271000	-8.028398000	-1.034482000
H	5.949982000	-5.424831000	2.427028000
H	6.156808000	7.376540000	1.103401000
H	6.653160000	4.789936000	-2.334040000
H	6.701869000	-5.120478000	0.843139000
H	6.815385000	-6.737010000	1.589286000
H	7.126322000	6.411297000	-1.757596000
H	7.211811000	4.005622000	1.876186000
H	7.745301000	3.403830000	0.289312000
H	8.311734000	4.989664000	0.879404000
H	-2.614009000	7.809554000	1.173962000
H	-3.351945000	7.123388000	2.640022000
H	-3.917756000	7.331375000	-1.608238000
H	-4.131793000	8.496172000	1.811061000
H	-4.477067000	-7.046084000	0.602256000
H	-5.126530000	-6.296032000	2.078700000
H	-5.422906000	6.392761000	-1.747599000
H	-5.432153000	-6.076402000	-2.197912000
H	-5.454271000	8.028398000	-1.034482000
H	-5.949982000	5.424831000	2.427028000

H	-6.156808000	-7.376540000	1.103401000
H	-6.653160000	-4.789936000	-2.334040000
H	-6.701869000	5.120478000	0.843139000
H	-6.815385000	6.737010000	1.589286000
H	-7.126322000	-6.411297000	-1.757596000
H	-7.211811000	-4.005622000	1.876186000
H	-7.745301000	-3.403830000	0.289312000
H	-8.311734000	-4.989664000	0.879404000
N	0.216462000	1.989409000	-0.204287000
N	2.004309000	-0.216954000	0.110916000
N	-0.216462000	-1.989409000	-0.204287000
N	-2.004309000	0.216954000	0.110916000
Si	4.556781000	-6.365912000	0.592426000
Si	5.965386000	5.131771000	0.040042000
Si	-4.556781000	6.365912000	0.592426000
Si	-5.965386000	-5.131771000	0.040042000

56. Pd[A₄Br₈]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
Br	1.629144000	5.765043000	-0.568686000
Br	1.629144000	-5.765043000	0.568686000
Br	5.765043000	1.629144000	-0.568686000
Br	5.765043000	-1.629144000	0.568686000
Br	-1.629144000	5.765043000	0.568686000
Br	-1.629144000	-5.765043000	-0.568686000
Br	-5.765043000	1.629144000	0.568686000
Br	-5.765043000	-1.629144000	-0.568686000
C	0.637483000	4.192787000	-0.261833000
C	0.637483000	-4.192787000	0.261833000
C	1.048385000	2.810810000	-0.393436000
C	1.048385000	-2.810810000	0.393436000
C	2.331812000	2.331812000	-0.751588000
C	2.331812000	-2.331812000	0.751588000
C	2.810810000	1.048385000	-0.393436000
C	2.810810000	-1.048385000	0.393436000
C	3.168551000	3.168551000	-1.511670000
C	3.168551000	-3.168551000	1.511670000
C	3.847693000	3.847693000	-2.268801000
C	3.847693000	-3.847693000	2.268801000
C	3.871166000	6.075702000	-4.282819000
C	3.871166000	-6.075702000	4.282819000
C	4.192787000	0.637483000	-0.261833000
C	4.192787000	-0.637483000	0.261833000
C	5.943757000	5.943757000	-1.981135000
C	5.943757000	-5.943757000	1.981135000
C	6.075702000	3.871166000	-4.282819000
C	6.075702000	-3.871166000	4.282819000
C	-0.637483000	4.192787000	0.261833000
C	-0.637483000	-4.192787000	-0.261833000

C	-1.048385000	2.810810000	0.393436000
C	-1.048385000	-2.810810000	-0.393436000
C	-2.331812000	2.331812000	0.751588000
C	-2.331812000	-2.331812000	-0.751588000
C	-2.810810000	1.048385000	0.393436000
C	-2.810810000	-1.048385000	-0.393436000
C	-3.168551000	3.168551000	1.511670000
C	-3.168551000	-3.168551000	-1.511670000
C	-3.847693000	3.847693000	2.268801000
C	-3.847693000	-3.847693000	-2.268801000
C	-3.871166000	6.075702000	4.282819000
C	-3.871166000	-6.075702000	-4.282819000
C	-4.192787000	0.637483000	0.261833000
C	-4.192787000	-0.637483000	-0.261833000
C	-5.943757000	5.943757000	1.981135000
C	-5.943757000	-5.943757000	-1.981135000
C	-6.075702000	3.871166000	4.282819000
C	-6.075702000	-3.871166000	-4.282819000
H	3.171606000	6.637809000	-3.647307000
H	3.171606000	-6.637809000	3.647307000
H	3.279104000	5.492091000	-5.001898000
H	3.279104000	-5.492091000	5.001898000
H	4.485185000	6.796265000	-4.843962000
H	4.485185000	-6.796265000	4.843962000
H	5.275998000	6.532844000	-1.336560000
H	5.275998000	-6.532844000	1.336560000
H	5.492091000	3.279104000	-5.001898000
H	5.492091000	-3.279104000	5.001898000
H	6.532844000	5.275998000	-1.336560000
H	6.532844000	-5.275998000	1.336560000
H	6.634099000	6.634099000	-2.489435000
H	6.634099000	-6.634099000	2.489435000
H	6.637809000	3.171606000	-3.647307000
H	6.637809000	-3.171606000	3.647307000
H	6.796265000	4.485185000	-4.843962000
H	6.796265000	-4.485185000	4.843962000
H	-3.171606000	6.637809000	3.647307000
H	-3.171606000	-6.637809000	-3.647307000
H	-3.279104000	5.492091000	5.001898000
H	-3.279104000	-5.492091000	-5.001898000
H	-4.485185000	6.796265000	4.843962000
H	-4.485185000	-6.796265000	-4.843962000
H	-5.275998000	6.532844000	1.336560000
H	-5.275998000	-6.532844000	-1.336560000
H	-5.492091000	3.279104000	5.001898000
H	-5.492091000	-3.279104000	-5.001898000
H	-6.532844000	5.275998000	1.336560000
H	-6.532844000	-5.275998000	-1.336560000
H	-6.634099000	6.634099000	2.489435000
H	-6.634099000	-6.634099000	-2.489435000
H	-6.637809000	3.171606000	3.647307000

H	-6.637809000	-3.171606000	-3.647307000
H	-6.796265000	4.485185000	4.843962000
H	-6.796265000	-4.485185000	-4.843962000
N	0.000000000	2.012863000	0.000000000
N	0.000000000	-2.012863000	0.000000000
N	2.012863000	0.000000000	0.000000000
N	-2.012863000	0.000000000	0.000000000
Si	4.949243000	4.949243000	-3.232641000
Si	4.949243000	-4.949243000	3.232641000
Si	-4.949243000	4.949243000	3.232641000
Si	-4.949243000	-4.949243000	-3.232641000

57. Pt[A₄Br₈]; S = 0 (saddled)

Pt	0.000000000	0.000000000	-0.042922000
Br	1.210259000	-5.425172000	-1.988173000
Br	2.244675000	5.034344000	-2.116860000
Br	5.186658000	-2.260476000	1.767276000
Br	5.571603000	1.160061000	1.667423000
Br	-1.210259000	5.425172000	-1.988173000
Br	-2.244675000	-5.034344000	-2.116860000
Br	-5.186658000	2.260476000	1.767276000
Br	-5.571603000	-1.160061000	1.667423000
C	0.276993000	-4.027171000	-1.138128000
C	0.819813000	-2.863000000	-0.476039000
C	1.090016000	3.871405000	-1.188351000
C	1.404426000	2.613151000	-0.548098000
C	2.125394000	-2.670689000	0.037425000
C	2.631718000	-1.409251000	0.418880000
C	2.659808000	2.144394000	-0.094243000
C	2.883006000	0.821198000	0.350167000
C	2.917685000	-3.823374000	0.210854000
C	3.521376000	-7.565301000	1.710063000
C	3.541520000	-4.859286000	0.387665000
C	3.717064000	3.075158000	-0.044196000
C	3.916400000	-1.098562000	1.005507000
C	4.071910000	0.267975000	0.960228000
C	4.597261000	3.920480000	0.017087000
C	4.845528000	-7.135989000	-1.051532000
C	5.315715000	6.619846000	1.134542000
C	6.121475000	-5.884636000	1.498001000
C	6.323032000	5.713907000	-1.645911000
C	7.415815000	4.344810000	0.928116000
C	-0.276993000	4.027171000	-1.138128000
C	-0.819813000	2.863000000	-0.476039000
C	-1.090016000	-3.871405000	-1.188351000
C	-1.404426000	-2.613151000	-0.548098000
C	-2.125394000	2.670689000	0.037425000
C	-2.631718000	1.409251000	0.418880000
C	-2.659808000	-2.144394000	-0.094243000

C	-2.883006000	-0.821198000	0.350167000
C	-2.917685000	3.823374000	0.210854000
C	-3.521376000	7.565301000	1.710063000
C	-3.541520000	4.859286000	0.387665000
C	-3.717064000	-3.075158000	-0.044196000
C	-3.916400000	1.098562000	1.005507000
C	-4.071910000	-0.267975000	0.960228000
C	-4.597261000	-3.920480000	0.017087000
C	-4.845528000	7.135989000	-1.051532000
C	-5.315715000	-6.619846000	1.134542000
C	-6.121475000	5.884636000	1.498001000
C	-6.323032000	-5.713907000	-1.645911000
C	-7.415815000	-4.344810000	0.928116000
H	2.566982000	-7.811543000	1.223230000
H	3.298317000	-7.116374000	2.688351000
H	3.895385000	-7.369036000	-1.553514000
H	4.075952000	-8.501230000	1.877467000
H	4.418643000	7.060163000	0.676332000
H	5.054317000	6.298161000	2.152645000
H	5.406168000	-6.439081000	-1.689992000
H	5.423854000	-8.067925000	-0.960966000
H	5.426904000	6.137845000	-2.121629000
H	5.907210000	-5.426190000	2.474323000
H	6.087353000	7.401489000	1.206179000
H	6.661975000	4.864588000	-2.255340000
H	6.675121000	-5.153404000	0.892046000
H	6.769270000	-6.758349000	1.664776000
H	7.110692000	6.482489000	-1.650481000
H	7.163555000	4.026708000	1.950131000
H	7.728822000	3.455944000	0.362332000
H	8.268680000	5.037678000	0.986556000
H	-2.566982000	7.811543000	1.223230000
H	-3.298317000	7.116374000	2.688351000
H	-3.895385000	7.369036000	-1.553514000
H	-4.075952000	8.501230000	1.877467000
H	-4.418643000	-7.060163000	0.676332000
H	-5.054317000	-6.298161000	2.152645000
H	-5.406168000	6.439081000	-1.689992000
H	-5.423854000	8.067925000	-0.960966000
H	-5.426904000	-6.137845000	-2.121629000
H	-5.907210000	5.426190000	2.474323000
H	-6.087353000	-7.401489000	1.206179000
H	-6.661975000	-4.864588000	-2.255340000
H	-6.675121000	5.153404000	0.892046000
H	-6.769270000	6.758349000	1.664776000
H	-7.110692000	-6.482489000	-1.650481000
H	-7.163555000	-4.026708000	1.950131000
H	-7.728822000	-3.455944000	0.362332000
H	-8.268680000	-5.037678000	0.986556000
N	0.215589000	1.985541000	-0.233849000
N	2.000914000	-0.216434000	0.114747000

N	-0.215589000	-1.985541000	-0.233849000
N	-2.000914000	0.216434000	0.114747000
Si	4.522074000	-6.384802000	0.642525000
Si	5.934219000	5.168460000	0.111835000
Si	-4.522074000	6.384802000	0.642525000
Si	-5.934219000	-5.168460000	0.111835000

58. Pt[A₄Br₈]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
Br	1.634003000	5.765038000	-0.554910000
Br	1.634003000	-5.765038000	0.554910000
Br	5.765038000	1.634003000	-0.554910000
Br	5.765038000	-1.634003000	0.554910000
Br	-1.634003000	5.765038000	0.554910000
Br	-1.634003000	-5.765038000	-0.554910000
Br	-5.765038000	1.634003000	0.554910000
Br	-5.765038000	-1.634003000	-0.554910000
C	0.638904000	4.193514000	-0.257538000
C	0.638904000	-4.193514000	0.257538000
C	1.051568000	2.814214000	-0.388426000
C	1.051568000	-2.814214000	0.388426000
C	2.335173000	2.335173000	-0.744980000
C	2.335173000	-2.335173000	0.744980000
C	2.814214000	1.051568000	-0.388426000
C	2.814214000	-1.051568000	0.388426000
C	3.172213000	3.172213000	-1.505374000
C	3.172213000	-3.172213000	1.505374000
C	3.849996000	3.849996000	-2.264888000
C	3.849996000	-3.849996000	2.264888000
C	3.868793000	6.073245000	-4.283946000
C	3.868793000	-6.073245000	4.283946000
C	4.193514000	0.638904000	-0.257538000
C	4.193514000	-0.638904000	0.257538000
C	5.946784000	5.946784000	-1.986607000
C	5.946784000	-5.946784000	1.986607000
C	6.073245000	3.868793000	-4.283946000
C	6.073245000	-3.868793000	4.283946000
C	-0.638904000	4.193514000	0.257538000
C	-0.638904000	-4.193514000	-0.257538000
C	-1.051568000	2.814214000	0.388426000
C	-1.051568000	-2.814214000	-0.388426000
C	-2.335173000	2.335173000	0.744980000
C	-2.335173000	-2.335173000	-0.744980000
C	-2.814214000	1.051568000	0.388426000
C	-2.814214000	-1.051568000	-0.388426000
C	-3.172213000	3.172213000	1.505374000
C	-3.172213000	-3.172213000	-1.505374000
C	-3.849996000	3.849996000	2.264888000
C	-3.849996000	-3.849996000	-2.264888000

C	-3.868793000	6.073245000	4.283946000
C	-3.868793000	-6.073245000	-4.283946000
C	-4.193514000	0.638904000	0.257538000
C	-4.193514000	-0.638904000	-0.257538000
C	-5.946784000	5.946784000	1.986607000
C	-5.946784000	-5.946784000	-1.986607000
C	-6.073245000	3.868793000	4.283946000
C	-6.073245000	-3.868793000	-4.283946000
H	3.170583000	6.636673000	-3.648130000
H	3.170583000	-6.636673000	3.648130000
H	3.275190000	5.487703000	-5.000218000
H	3.275190000	-5.487703000	5.000218000
H	4.481233000	6.792644000	-4.848294000
H	4.481233000	-6.792644000	4.848294000
H	5.280589000	6.537450000	-1.341832000
H	5.280589000	-6.537450000	1.341832000
H	5.487703000	3.275190000	-5.000218000
H	5.487703000	-3.275190000	5.000218000
H	6.537450000	5.280589000	-1.341832000
H	6.537450000	-5.280589000	1.341832000
H	6.635941000	6.635941000	-2.498139000
H	6.635941000	-6.635941000	2.498139000
H	6.636673000	3.170583000	-3.648130000
H	6.636673000	-3.170583000	3.648130000
H	6.792644000	4.481233000	-4.848294000
H	6.792644000	-4.481233000	4.848294000
H	-3.170583000	6.636673000	3.648130000
H	-3.170583000	-6.636673000	-3.648130000
H	-3.275190000	5.487703000	5.000218000
H	-3.275190000	-5.487703000	-5.000218000
H	-4.481233000	6.792644000	4.848294000
H	-4.481233000	-6.792644000	-4.848294000
H	-5.280589000	6.537450000	1.341832000
H	-5.280589000	-6.537450000	-1.341832000
H	-5.487703000	3.275190000	5.000218000
H	-5.487703000	-3.275190000	-5.000218000
H	-6.537450000	5.280589000	1.341832000
H	-6.537450000	-5.280589000	-1.341832000
H	-6.635941000	6.635941000	2.498139000
H	-6.635941000	-6.635941000	-2.498139000
H	-6.636673000	3.170583000	3.648130000
H	-6.636673000	-3.170583000	-3.648130000
H	-6.792644000	4.481233000	4.848294000
H	-6.792644000	-4.481233000	-4.848294000
N	0.000000000	2.013189000	0.000000000
N	0.000000000	-2.013189000	0.000000000
N	2.013189000	0.000000000	0.000000000
N	-2.013189000	0.000000000	0.000000000
Si	4.949410000	4.949410000	-3.233585000
Si	4.949410000	-4.949410000	3.233585000
Si	-4.949410000	4.949410000	3.233585000

Si -4.949410000 -4.949410000 -3.233585000

59. Zn[A₄Br₈]; S = 0 (saddled)

Zn	0.000000000	0.000000000	-0.005049000
Br	1.142292000	-5.407794000	-2.064042000
Br	2.310027000	5.027177000	-2.051324000
Br	5.211928000	-2.315276000	1.734345000
Br	5.595719000	1.107077000	1.734083000
Br	-1.142292000	5.407794000	-2.064042000
Br	-2.310027000	-5.027177000	-2.051324000
Br	-5.211928000	2.315276000	1.734345000
Br	-5.595719000	-1.107077000	1.734083000
C	0.247168000	-4.012909000	-1.166292000
C	0.805098000	-2.857999000	-0.499980000
C	1.126028000	3.861092000	-1.162010000
C	1.414186000	2.611929000	-0.494554000
C	2.129940000	-2.671094000	-0.014159000
C	2.649623000	-1.420017000	0.410441000
C	2.664352000	2.138119000	-0.005332000
C	2.896843000	0.801938000	0.413893000
C	2.941957000	-3.817239000	0.080828000
C	3.601823000	-4.841537000	0.182715000
C	3.675605000	-7.611028000	1.360614000
C	3.705370000	3.080086000	0.099354000
C	3.937715000	-1.134381000	1.004920000
C	4.090744000	0.238064000	1.006449000
C	4.569654000	3.937738000	0.210896000
C	4.890852000	-7.015205000	-1.419762000
C	5.226574000	6.623729000	1.400399000
C	6.240077000	-5.877961000	1.144729000
C	6.308396000	5.787951000	-1.373098000
C	7.361070000	4.380466000	1.196041000
C	-0.247168000	4.012909000	-1.166292000
C	-0.805098000	2.857999000	-0.499980000
C	-1.126028000	-3.861092000	-1.162010000
C	-1.414186000	-2.611929000	-0.494554000
C	-2.129940000	2.671094000	-0.014159000
C	-2.649623000	1.420017000	0.410441000
C	-2.664352000	-2.138119000	-0.005332000
C	-2.896843000	-0.801938000	0.413893000
C	-2.941957000	3.817239000	0.080828000
C	-3.601823000	4.841537000	0.182715000
C	-3.675605000	7.611028000	1.360614000
C	-3.705370000	-3.080086000	0.099354000
C	-3.937715000	1.134381000	1.004920000
C	-4.090744000	-0.238064000	1.006449000
C	-4.569654000	-3.937738000	0.210896000
C	-4.890852000	7.015205000	-1.419762000
C	-5.226574000	-6.623729000	1.400399000

C	-6.240077000	5.877961000	1.144729000
C	-6.308396000	-5.787951000	-1.373098000
C	-7.361070000	-4.380466000	1.196041000
H	2.707418000	-7.846908000	0.896417000
H	3.482663000	-7.218267000	2.368999000
H	3.927001000	-7.238581000	-1.899477000
H	4.250014000	-8.544980000	1.457313000
H	4.335329000	7.062680000	0.929755000
H	4.945550000	6.279282000	2.405735000
H	5.416820000	-6.276533000	-2.040522000
H	5.418698000	6.213437000	-1.859340000
H	5.486719000	-7.940234000	-1.398452000
H	5.987009000	7.412612000	1.505072000
H	6.056529000	-5.483153000	2.154539000
H	6.669559000	4.955439000	-1.992834000
H	6.756687000	-5.100871000	0.563839000
H	6.908771000	-6.747330000	1.233592000
H	7.088023000	6.564159000	-1.343272000
H	7.088208000	4.029055000	2.201681000
H	7.704773000	3.513776000	0.613836000
H	8.199446000	5.086163000	1.295853000
H	-2.707418000	7.846908000	0.896417000
H	-3.482663000	7.218267000	2.368999000
H	-3.927001000	7.238581000	-1.899477000
H	-4.250014000	8.544980000	1.457313000
H	-4.335329000	-7.062680000	0.929755000
H	-4.945550000	-6.279282000	2.405735000
H	-5.416820000	6.276533000	-2.040522000
H	-5.418698000	-6.213437000	-1.859340000
H	-5.486719000	7.940234000	-1.398452000
H	-5.987009000	-7.412612000	1.505072000
H	-6.056529000	5.483153000	2.154539000
H	-6.669559000	-4.955439000	-1.992834000
H	-6.756687000	5.100871000	0.563839000
H	-6.908771000	6.747330000	1.233592000
H	-7.088023000	-6.564159000	-1.343272000
H	-7.088208000	-4.029055000	2.201681000
H	-7.704773000	-3.513776000	0.613836000
H	-8.199446000	-5.086163000	1.295853000
N	0.221607000	1.992492000	-0.203515000
N	2.022125000	-0.225059000	0.145175000
N	-0.221607000	-1.992492000	-0.203515000
N	-2.022125000	0.225059000	0.145175000
Si	4.617784000	-6.358493000	0.321972000
Si	5.886554000	5.200670000	0.363752000
Si	-4.617784000	6.358493000	0.321972000
Si	-5.886554000	-5.200670000	0.363752000

60. Zn[A₄Br₈]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
Br	1.653840000	5.804802000	-0.461906000
Br	1.653840000	-5.804802000	0.461906000
Br	5.804802000	1.653840000	-0.461906000
Br	5.804802000	-1.653840000	0.461906000
Br	-1.653840000	5.804802000	0.461906000
Br	-1.653840000	-5.804802000	-0.461906000
Br	-5.804802000	1.653840000	0.461906000
Br	-5.804802000	-1.653840000	-0.461906000
C	0.653382000	4.224223000	-0.222894000
C	0.653382000	-4.224223000	0.222894000
C	1.065111000	2.842332000	-0.335937000
C	1.065111000	-2.842332000	0.335937000
C	2.361759000	2.361759000	-0.661176000
C	2.361759000	-2.361759000	0.661176000
C	2.842332000	1.065111000	-0.335937000
C	2.842332000	-1.065111000	0.335937000
C	3.217112000	3.217112000	-1.379646000
C	3.217112000	-3.217112000	1.379646000
C	3.914203000	3.914203000	-2.103690000
C	3.914203000	-3.914203000	2.103690000
C	3.992672000	6.197538000	-4.053184000
C	3.992672000	-6.197538000	4.053184000
C	4.224223000	0.653382000	-0.222894000
C	4.224223000	-0.653382000	0.222894000
C	5.999524000	5.999524000	-1.698335000
C	5.999524000	-5.999524000	1.698335000
C	6.197538000	3.992672000	-4.053184000
C	6.197538000	-3.992672000	4.053184000
C	-0.653382000	4.224223000	0.222894000
C	-0.653382000	-4.224223000	-0.222894000
C	-1.065111000	2.842332000	0.335937000
C	-1.065111000	-2.842332000	-0.335937000
C	-2.361759000	2.361759000	0.661176000
C	-2.361759000	-2.361759000	-0.661176000
C	-2.842332000	1.065111000	0.335937000
C	-2.842332000	-1.065111000	-0.335937000
C	-3.217112000	3.217112000	1.379646000
C	-3.217112000	-3.217112000	-1.379646000
C	-3.914203000	3.914203000	2.103690000
C	-3.914203000	-3.914203000	-2.103690000
C	-3.992672000	6.197538000	4.053184000
C	-3.992672000	-6.197538000	-4.053184000
C	-4.224223000	0.653382000	0.222894000
C	-4.224223000	-0.653382000	-0.222894000
C	-5.999524000	5.999524000	1.698335000
C	-5.999524000	-5.999524000	-1.698335000
C	-6.197538000	3.992672000	4.053184000

C	-6.197538000	-3.992672000	-4.053184000
H	3.273702000	6.739328000	-3.421649000
H	3.273702000	-6.739328000	3.421649000
H	3.422862000	5.634951000	-4.806225000
H	3.422862000	-5.634951000	4.806225000
H	4.621141000	6.935305000	-4.574537000
H	4.621141000	-6.935305000	4.574537000
H	5.313074000	6.569913000	-1.056566000
H	5.313074000	-6.569913000	1.056566000
H	5.634951000	3.422862000	-4.806225000
H	5.634951000	-3.422862000	4.806225000
H	6.569913000	5.313074000	-1.056566000
H	6.569913000	-5.313074000	1.056566000
H	6.703910000	6.703910000	-2.166494000
H	6.703910000	-6.703910000	2.166494000
H	6.739328000	3.273702000	-3.421649000
H	6.739328000	-3.273702000	3.421649000
H	6.935305000	4.621141000	-4.574537000
H	6.935305000	-4.621141000	4.574537000
H	-3.273702000	6.739328000	3.421649000
H	-3.273702000	-6.739328000	-3.421649000
H	-3.422862000	5.634951000	4.806225000
H	-3.422862000	-5.634951000	-4.806225000
H	-4.621141000	6.935305000	4.574537000
H	-4.621141000	-6.935305000	-4.574537000
H	-5.313074000	6.569913000	1.056566000
H	-5.313074000	-6.569913000	-1.056566000
H	-5.634951000	3.422862000	4.806225000
H	-5.634951000	-3.422862000	-4.806225000
H	-6.569913000	5.313074000	1.056566000
H	-6.569913000	-5.313074000	-1.056566000
H	-6.703910000	6.703910000	2.166494000
H	-6.703910000	-6.703910000	-2.166494000
H	-6.739328000	3.273702000	3.421649000
H	-6.739328000	-3.273702000	-3.421649000
H	-6.935305000	4.621141000	4.574537000
H	-6.935305000	-4.621141000	-4.574537000
N	0.000000000	2.040294000	0.000000000
N	0.000000000	-2.040294000	0.000000000
N	2.040294000	0.000000000	0.000000000
N	-2.040294000	0.000000000	0.000000000
Si	5.041422000	5.041422000	-3.005452000
Si	5.041422000	-5.041422000	3.005452000
Si	-5.041422000	5.041422000	3.005452000
Si	-5.041422000	-5.041422000	-3.005452000

61. Cu[Ph₄Bz₈]; S = ½ (saddled)

C	0.000000000	3.402148000	0.000000000
C	0.000000000	4.891312000	0.000000000
C	0.000000000	7.696899000	0.000000000
C	0.000000000	-3.402148000	0.000000000
C	0.000000000	-4.891312000	0.000000000
C	0.000000000	-7.696899000	0.000000000
C	0.781663000	6.995481000	-0.922122000
C	0.781663000	-6.995481000	0.922122000
C	0.783650000	5.600646000	-0.918384000
C	0.783650000	-5.600646000	0.918384000
C	1.162675000	2.743363000	0.415038000
C	1.162675000	-2.743363000	-0.415038000
C	2.349462000	3.350681000	1.003298000
C	2.349462000	-3.350681000	-1.003298000
C	2.601540000	4.604938000	1.583657000
C	2.601540000	-4.604938000	-1.583657000
C	2.743363000	1.162675000	0.415038000
C	2.743363000	-1.162675000	-0.415038000
C	3.350681000	2.349462000	1.003298000
C	3.350681000	-2.349462000	-1.003298000
C	3.402148000	0.000000000	0.000000000
C	3.849361000	4.842772000	2.148171000
C	3.849361000	-4.842772000	-2.148171000
C	4.604938000	2.601540000	1.583657000
C	4.604938000	-2.601540000	-1.583657000
C	4.842772000	3.849361000	2.148171000
C	4.842772000	-3.849361000	-2.148171000
C	4.891312000	0.000000000	0.000000000
C	5.600646000	0.783650000	-0.918384000
C	5.600646000	-0.783650000	0.918384000
C	6.995481000	0.781663000	-0.922122000
C	6.995481000	-0.781663000	0.922122000
C	7.696899000	0.000000000	0.000000000
C	-0.781663000	6.995481000	0.922122000
C	-0.781663000	-6.995481000	-0.922122000
C	-0.783650000	5.600646000	0.918384000
C	-0.783650000	-5.600646000	-0.918384000
C	-1.162675000	2.743363000	-0.415038000
C	-1.162675000	-2.743363000	0.415038000
C	-2.349462000	3.350681000	-1.003298000
C	-2.349462000	-3.350681000	1.003298000
C	-2.601540000	4.604938000	-1.583657000
C	-2.601540000	-4.604938000	1.583657000
C	-2.743363000	1.162675000	-0.415038000
C	-2.743363000	-1.162675000	0.415038000
C	-3.350681000	2.349462000	-1.003298000
C	-3.350681000	-2.349462000	1.003298000

C	-3.402148000	0.000000000	0.000000000
C	-3.849361000	4.842772000	-2.148171000
C	-3.849361000	-4.842772000	2.148171000
C	-4.604938000	2.601540000	-1.583657000
C	-4.604938000	-2.601540000	1.583657000
C	-4.842772000	3.849361000	-2.148171000
C	-4.842772000	-3.849361000	2.148171000
C	-4.891312000	0.000000000	0.000000000
C	-5.600646000	0.783650000	0.918384000
C	-5.600646000	-0.783650000	-0.918384000
C	-6.995481000	0.781663000	0.922122000
C	-6.995481000	-0.781663000	-0.922122000
C	-7.696899000	0.000000000	0.000000000
Cu	0.000000000	0.000000000	0.000000000
H	0.000000000	8.786403000	0.000000000
H	0.000000000	-8.786403000	0.000000000
H	1.392944000	7.535499000	-1.643785000
H	1.392944000	-7.535499000	1.643785000
H	1.396283000	5.046001000	-1.627794000
H	1.396283000	-5.046001000	1.627794000
H	1.838586000	5.377259000	1.617842000
H	1.838586000	-5.377259000	-1.617842000
H	4.051298000	5.808205000	2.609962000
H	4.051298000	-5.808205000	-2.609962000
H	5.046001000	1.396283000	-1.627794000
H	5.046001000	-1.396283000	1.627794000
H	5.377259000	1.838586000	1.617842000
H	5.377259000	-1.838586000	-1.617842000
H	5.808205000	4.051298000	2.609962000
H	5.808205000	-4.051298000	-2.609962000
H	7.535499000	1.392944000	-1.643785000
H	7.535499000	-1.392944000	1.643785000
H	8.786403000	0.000000000	0.000000000
H	-1.392944000	7.535499000	1.643785000
H	-1.392944000	-7.535499000	-1.643785000
H	-1.396283000	5.046001000	1.627794000
H	-1.396283000	-5.046001000	-1.627794000
H	-1.838586000	5.377259000	-1.617842000
H	-1.838586000	-5.377259000	1.617842000
H	-4.051298000	5.808205000	-2.609962000
H	-4.051298000	-5.808205000	2.609962000
H	-5.046001000	1.396283000	1.627794000
H	-5.046001000	-1.396283000	-1.627794000
H	-5.377259000	1.838586000	-1.617842000
H	-5.377259000	-1.838586000	1.617842000
H	-5.808205000	4.051298000	-2.609962000
H	-5.808205000	-4.051298000	2.609962000
H	-7.535499000	1.392944000	1.643785000
H	-7.535499000	-1.392944000	-1.643785000
H	-8.786403000	0.000000000	0.000000000
N	1.407067000	1.407067000	0.181882000

N	1.407067000	-1.407067000	-0.181882000
N	-1.407067000	1.407067000	-0.181882000
N	-1.407067000	-1.407067000	0.181882000

62. Cu[Ph₄Bz₈]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.001551000
C	0.000000000	3.275141000	-0.751673000
C	0.000000000	4.676255000	-1.261726000
C	0.000000000	4.925682000	-2.636527000
C	0.000000000	5.755875000	-0.369428000
C	0.000000000	6.237568000	-3.116849000
C	0.000000000	7.065646000	-0.845127000
C	0.000000000	7.309979000	-2.221798000
C	0.000000000	-3.275141000	-0.751673000
C	0.000000000	-4.676255000	-1.261726000
C	0.000000000	-4.925682000	-2.636527000
C	0.000000000	-5.755875000	-0.369428000
C	0.000000000	-6.237568000	-3.116849000
C	0.000000000	-7.065646000	-0.845127000
C	0.000000000	-7.309979000	-2.221798000
C	1.239163000	2.692502000	-0.448832000
C	1.239163000	-2.692502000	-0.448832000
C	2.517486000	3.393642000	-0.345065000
C	2.517486000	-3.393642000	-0.345065000
C	2.692782000	1.239146000	0.450633000
C	2.692782000	-1.239146000	0.450633000
C	2.970392000	4.660261000	-0.752829000
C	2.970392000	-4.660261000	-0.752829000
C	3.275560000	0.000000000	0.753271000
C	3.394119000	2.517257000	0.345612000
C	3.394119000	-2.517257000	0.345612000
C	4.247899000	5.071791000	-0.390148000
C	4.247899000	-5.071791000	-0.390148000
C	4.661219000	2.970039000	0.752021000
C	4.661219000	-2.970039000	0.752021000
C	4.677106000	0.000000000	1.262191000
C	4.927853000	0.000000000	2.636752000
C	5.072952000	4.247073000	0.387913000
C	5.072952000	-4.247073000	0.387913000
C	5.755897000	0.000000000	0.368863000
C	6.240209000	0.000000000	3.115804000
C	7.066138000	0.000000000	0.843289000
C	7.311780000	0.000000000	2.219733000
C	-1.239163000	2.692502000	-0.448832000
C	-1.239163000	-2.692502000	-0.448832000
C	-2.517486000	3.393642000	-0.345065000
C	-2.517486000	-3.393642000	-0.345065000
C	-2.692782000	1.239146000	0.450633000
C	-2.692782000	-1.239146000	0.450633000

C	-2.970392000	4.660261000	-0.752829000
C	-2.970392000	-4.660261000	-0.752829000
C	-3.275560000	0.000000000	0.753271000
C	-3.394119000	2.517257000	0.345612000
C	-3.394119000	-2.517257000	0.345612000
C	-4.247899000	5.071791000	-0.390148000
C	-4.247899000	-5.071791000	-0.390148000
C	-4.661219000	2.970039000	0.752021000
C	-4.661219000	-2.970039000	0.752021000
C	-4.677106000	0.000000000	1.262191000
C	-4.927853000	0.000000000	2.636752000
C	-5.072952000	4.247073000	0.387913000
C	-5.072952000	-4.247073000	0.387913000
C	-5.755897000	0.000000000	0.368863000
C	-6.240209000	0.000000000	3.115804000
C	-7.066138000	0.000000000	0.843289000
C	-7.311780000	0.000000000	2.219733000
H	0.000000000	4.083670000	-3.327392000
H	0.000000000	5.554013000	0.700435000
H	0.000000000	6.420973000	-4.190289000
H	0.000000000	7.896814000	-0.141621000
H	0.000000000	8.333272000	-2.595785000
H	0.000000000	-4.083670000	-3.327392000
H	0.000000000	-5.554013000	0.700435000
H	0.000000000	-6.420973000	-4.190289000
H	0.000000000	-7.896814000	-0.141621000
H	0.000000000	-8.333272000	-2.595785000
H	2.353177000	5.319006000	-1.353759000
H	2.353177000	-5.319006000	-1.353759000
H	4.086536000	0.000000000	3.328470000
H	4.602299000	6.051666000	-0.706969000
H	4.602299000	-6.051666000	-0.706969000
H	5.320279000	2.353016000	1.352807000
H	5.320279000	-2.353016000	1.352807000
H	5.552998000	0.000000000	-0.700805000
H	6.053231000	4.601367000	0.703622000
H	6.053231000	-4.601367000	0.703622000
H	6.424636000	0.000000000	4.189075000
H	7.896658000	0.000000000	0.138964000
H	8.335436000	0.000000000	2.592739000
H	-2.353177000	5.319006000	-1.353759000
H	-2.353177000	-5.319006000	-1.353759000
H	-4.086536000	0.000000000	3.328470000
H	-4.602299000	6.051666000	-0.706969000
H	-4.602299000	-6.051666000	-0.706969000
H	-5.320279000	2.353016000	1.352807000
H	-5.320279000	-2.353016000	1.352807000
H	-5.552998000	0.000000000	-0.700805000
H	-6.053231000	4.601367000	0.703622000
H	-6.053231000	-4.601367000	0.703622000
H	-6.424636000	0.000000000	4.189075000

H	-7.896658000	0.000000000	0.138964000
H	-8.335436000	0.000000000	2.592739000
N	1.402286000	1.402224000	0.001190000
N	1.402286000	-1.402224000	0.001190000
N	-1.402286000	1.402224000	0.001190000
N	-1.402286000	-1.402224000	0.001190000

63. Ni[Ph₄Bz₈]; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	3.370803000	0.000000000
C	0.000000000	4.858951000	0.000000000
C	0.000000000	7.664358000	0.000000000
C	0.000000000	-3.370803000	0.000000000
C	0.000000000	-4.858951000	0.000000000
C	0.000000000	-7.664358000	0.000000000
C	0.849179000	6.962944000	-0.860290000
C	0.849179000	-6.962944000	0.860290000
C	0.850864000	5.568055000	-0.856617000
C	0.850864000	-5.568055000	0.856617000
C	1.116231000	2.694199000	0.484814000
C	1.116231000	-2.694199000	-0.484814000
C	2.278456000	3.278046000	1.131670000
C	2.278456000	-3.278046000	-1.131670000
C	2.511158000	4.517151000	1.749936000
C	2.511158000	-4.517151000	-1.749936000
C	2.694199000	1.116231000	0.484814000
C	2.694199000	-1.116231000	-0.484814000
C	3.278046000	2.278456000	1.131670000
C	3.278046000	-2.278456000	-1.131670000
C	3.370803000	0.000000000	0.000000000
C	3.743436000	4.737470000	2.355176000
C	3.743436000	-4.737470000	-2.355176000
C	4.517151000	2.511158000	1.749936000
C	4.517151000	-2.511158000	-1.749936000
C	4.737470000	3.743436000	2.355176000
C	4.737470000	-3.743436000	-2.355176000
C	4.858951000	0.000000000	0.000000000
C	5.568055000	0.850864000	-0.856617000
C	5.568055000	-0.850864000	0.856617000
C	6.962944000	0.849179000	-0.860290000
C	6.962944000	-0.849179000	0.860290000
C	7.664358000	0.000000000	0.000000000
C	-0.849179000	6.962944000	0.860290000
C	-0.849179000	-6.962944000	-0.860290000
C	-0.850864000	5.568055000	0.856617000
C	-0.850864000	-5.568055000	-0.856617000
C	-1.116231000	2.694199000	-0.484814000
C	-1.116231000	-2.694199000	0.484814000
C	-2.278456000	3.278046000	-1.131670000

C	-2.278456000	-3.278046000	1.131670000
C	-2.511158000	4.517151000	-1.749936000
C	-2.511158000	-4.517151000	1.749936000
C	-2.694199000	1.116231000	-0.484814000
C	-2.694199000	-1.116231000	0.484814000
C	-3.278046000	2.278456000	-1.131670000
C	-3.278046000	-2.278456000	1.131670000
C	-3.370803000	0.000000000	0.000000000
C	-3.743436000	4.737470000	-2.355176000
C	-3.743436000	-4.737470000	2.355176000
C	-4.517151000	2.511158000	-1.749936000
C	-4.517151000	-2.511158000	1.749936000
C	-4.737470000	3.743436000	-2.355176000
C	-4.737470000	-3.743436000	2.355176000
C	-4.858951000	0.000000000	0.000000000
C	-5.568055000	0.850864000	0.856617000
C	-5.568055000	-0.850864000	-0.856617000
C	-6.962944000	0.849179000	0.860290000
C	-6.962944000	-0.849179000	-0.860290000
C	-7.664358000	0.000000000	0.000000000
H	0.000000000	8.753881000	0.000000000
H	0.000000000	-8.753881000	0.000000000
H	1.513415000	7.502898000	-1.533580000
H	1.513415000	-7.502898000	1.533580000
H	1.515577000	5.013452000	-1.517581000
H	1.515577000	-5.013452000	1.517581000
H	1.745716000	5.287775000	1.779762000
H	1.745716000	-5.287775000	-1.779762000
H	3.933385000	5.689461000	2.848751000
H	3.933385000	-5.689461000	-2.848751000
H	5.013452000	1.515577000	-1.517581000
H	5.013452000	-1.515577000	1.517581000
H	5.287775000	1.745716000	1.779762000
H	5.287775000	-1.745716000	-1.779762000
H	5.689461000	3.933385000	2.848751000
H	5.689461000	-3.933385000	-2.848751000
H	7.502898000	1.513415000	-1.533580000
H	7.502898000	-1.513415000	1.533580000
H	8.753881000	0.000000000	0.000000000
H	-1.513415000	7.502898000	1.533580000
H	-1.513415000	-7.502898000	-1.533580000
H	-1.515577000	5.013452000	1.517581000
H	-1.515577000	-5.013452000	-1.517581000
H	-1.745716000	5.287775000	-1.779762000
H	-1.745716000	-5.287775000	1.779762000
H	-3.933385000	5.689461000	-2.848751000
H	-3.933385000	-5.689461000	2.848751000
H	-5.013452000	1.515577000	1.517581000
H	-5.013452000	-1.515577000	-1.517581000
H	-5.287775000	1.745716000	-1.779762000
H	-5.287775000	-1.745716000	1.779762000

H	-5.689461000	3.933385000	-2.848751000
H	-5.689461000	-3.933385000	2.848751000
H	-7.502898000	1.513415000	1.533580000
H	-7.502898000	-1.513415000	-1.533580000
H	-8.753881000	0.000000000	0.000000000
N	1.352837000	1.352837000	0.235308000
N	1.352837000	-1.352837000	-0.235308000
N	-1.352837000	1.352837000	-0.235308000
N	-1.352837000	-1.352837000	0.235308000

64. Ni[Ph₄Bz₈]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000288000
C	0.000000000	3.157193000	-0.945346000
C	0.000000000	4.508158000	-1.573001000
C	0.000000000	4.639245000	-2.964100000
C	0.000000000	5.660952000	-0.776529000
C	0.000000000	5.905591000	-3.554997000
C	0.000000000	6.924975000	-1.362719000
C	0.000000000	7.050603000	-2.755310000
C	0.000000000	-3.157193000	-0.945346000
C	0.000000000	-4.508158000	-1.573001000
C	0.000000000	-4.639245000	-2.964100000
C	0.000000000	-5.660952000	-0.776529000
C	0.000000000	-5.905591000	-3.554997000
C	0.000000000	-6.924975000	-1.362719000
C	0.000000000	-7.050603000	-2.755310000
C	1.218218000	2.590263000	-0.561958000
C	1.218218000	-2.590263000	-0.561958000
C	2.485796000	3.294687000	-0.418831000
C	2.485796000	-3.294687000	-0.418831000
C	2.590273000	1.218190000	0.562597000
C	2.590273000	-1.218190000	0.562597000
C	2.973630000	4.522577000	-0.895264000
C	2.973630000	-4.522577000	-0.895264000
C	3.157259000	0.000000000	0.945904000
C	3.294878000	2.485599000	0.419099000
C	3.294878000	-2.485599000	0.419099000
C	4.217111000	4.967639000	-0.458645000
C	4.217111000	-4.967639000	-0.458645000
C	4.508468000	0.000000000	1.573035000
C	4.523107000	2.973108000	0.895006000
C	4.523107000	-2.973108000	0.895006000
C	4.639768000	0.000000000	2.964109000
C	4.968403000	4.216374000	0.458029000
C	4.968403000	-4.216374000	0.458029000
C	5.661159000	0.000000000	0.776412000
C	5.906185000	0.000000000	3.554836000
C	6.925260000	0.000000000	1.362435000
C	7.051091000	0.000000000	2.755007000

C	-1.218218000	2.590263000	-0.561958000
C	-1.218218000	-2.590263000	-0.561958000
C	-2.485796000	3.294687000	-0.418831000
C	-2.485796000	-3.294687000	-0.418831000
C	-2.590273000	1.218190000	0.562597000
C	-2.590273000	-1.218190000	0.562597000
C	-2.973630000	4.522577000	-0.895264000
C	-2.973630000	-4.522577000	-0.895264000
C	-3.157259000	0.000000000	0.945904000
C	-3.294878000	2.485599000	0.419099000
C	-3.294878000	-2.485599000	0.419099000
C	-4.217111000	4.967639000	-0.458645000
C	-4.217111000	-4.967639000	-0.458645000
C	-4.508468000	0.000000000	1.573035000
C	-4.523107000	2.973108000	0.895006000
C	-4.523107000	-2.973108000	0.895006000
C	-4.639768000	0.000000000	2.964109000
C	-4.968403000	4.216374000	0.458029000
C	-4.968403000	-4.216374000	0.458029000
C	-5.661159000	0.000000000	0.776412000
C	-5.906185000	0.000000000	3.554836000
C	-6.925260000	0.000000000	1.362435000
C	-7.051091000	0.000000000	2.755007000
H	0.000000000	3.741392000	-3.580805000
H	0.000000000	5.551676000	0.306705000
H	0.000000000	5.996329000	-4.640266000
H	0.000000000	7.813192000	-0.732735000
H	0.000000000	8.038135000	-3.215548000
H	0.000000000	-3.741392000	-3.580805000
H	0.000000000	-5.551676000	0.306705000
H	0.000000000	-5.996329000	-4.640266000
H	0.000000000	-7.813192000	-0.732735000
H	0.000000000	-8.038135000	-3.215548000
H	2.409048000	5.120897000	-1.603008000
H	2.409048000	-5.120897000	-1.603008000
H	3.741998000	0.000000000	3.580940000
H	4.603086000	5.917100000	-0.826900000
H	4.603086000	-5.917100000	-0.826900000
H	5.121432000	2.408502000	1.602721000
H	5.121432000	-2.408502000	1.602721000
H	5.551769000	0.000000000	-0.306811000
H	5.918081000	4.602163000	0.825953000
H	5.918081000	-4.602163000	0.825953000
H	5.997038000	0.000000000	4.640078000
H	7.813373000	0.000000000	0.732332000
H	8.038693000	0.000000000	3.215139000
H	-2.409048000	5.120897000	-1.603008000
H	-2.409048000	-5.120897000	-1.603008000
H	-3.741998000	0.000000000	3.580940000
H	-4.603086000	5.917100000	-0.826900000
H	-4.603086000	-5.917100000	-0.826900000

H	-5.121432000	2.408502000	1.602721000
H	-5.121432000	-2.408502000	1.602721000
H	-5.551769000	0.000000000	-0.306811000
H	-5.918081000	4.602163000	0.825953000
H	-5.918081000	-4.602163000	0.825953000
H	-5.997038000	0.000000000	4.640078000
H	-7.813373000	0.000000000	0.732332000
H	-8.038693000	0.000000000	3.215139000
N	1.335707000	1.335717000	0.000348000
N	1.335707000	-1.335717000	0.000348000
N	-1.335707000	1.335717000	0.000348000
N	-1.335707000	-1.335717000	0.000348000

65. Pd[Ph₄Bz₈]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.000000000
C	0.000000000	3.415323000	0.000000000
C	0.000000000	4.904955000	0.000000000
C	0.000000000	7.709213000	0.000000000
C	0.000000000	-3.415323000	0.000000000
C	0.000000000	-4.904955000	0.000000000
C	0.000000000	-7.709213000	0.000000000
C	0.754562000	7.007981000	-0.944578000
C	0.754562000	-7.007981000	0.944578000
C	0.756676000	5.613214000	-0.940905000
C	0.756676000	-5.613214000	0.940905000
C	1.175946000	2.764722000	0.384637000
C	1.175946000	-2.764722000	-0.384637000
C	2.372262000	3.373725000	0.953536000
C	2.372262000	-3.373725000	-0.953536000
C	2.629972000	4.632140000	1.521923000
C	2.629972000	-4.632140000	-1.521923000
C	2.764722000	1.175946000	0.384637000
C	2.764722000	-1.175946000	-0.384637000
C	3.373725000	2.372262000	0.953536000
C	3.373725000	-2.372262000	-0.953536000
C	3.415323000	0.000000000	0.000000000
C	3.882877000	4.875572000	2.073686000
C	3.882877000	-4.875572000	-2.073686000
C	4.632140000	2.629972000	1.521923000
C	4.632140000	-2.629972000	-1.521923000
C	4.875572000	3.882877000	2.073686000
C	4.875572000	-3.882877000	-2.073686000
C	4.904955000	0.000000000	0.000000000
C	5.613214000	0.756676000	-0.940905000
C	5.613214000	-0.756676000	0.940905000
C	7.007981000	0.754562000	-0.944578000
C	7.007981000	-0.754562000	0.944578000
C	7.709213000	0.000000000	0.000000000
C	-0.754562000	7.007981000	0.944578000

C	-0.754562000	-7.007981000	-0.944578000
C	-0.756676000	5.613214000	0.940905000
C	-0.756676000	-5.613214000	-0.940905000
C	-1.175946000	2.764722000	-0.384637000
C	-1.175946000	-2.764722000	0.384637000
C	-2.372262000	3.373725000	-0.953536000
C	-2.372262000	-3.373725000	0.953536000
C	-2.629972000	4.632140000	-1.521923000
C	-2.629972000	-4.632140000	1.521923000
C	-2.764722000	1.175946000	-0.384637000
C	-2.764722000	-1.175946000	0.384637000
C	-3.373725000	2.372262000	-0.953536000
C	-3.373725000	-2.372262000	0.953536000
C	-3.415323000	0.000000000	0.000000000
C	-3.882877000	4.875572000	-2.073686000
C	-3.882877000	-4.875572000	2.073686000
C	-4.632140000	2.629972000	-1.521923000
C	-4.632140000	-2.629972000	1.521923000
C	-4.875572000	3.882877000	-2.073686000
C	-4.875572000	-3.882877000	2.073686000
C	-4.904955000	0.000000000	0.000000000
C	-5.613214000	0.756676000	0.940905000
C	-5.613214000	-0.756676000	-0.940905000
C	-7.007981000	0.754562000	0.944578000
C	-7.007981000	-0.754562000	-0.944578000
C	-7.709213000	0.000000000	0.000000000
H	0.000000000	8.798717000	0.000000000
H	0.000000000	-8.798717000	0.000000000
H	1.344431000	7.548028000	-1.683753000
H	1.344431000	-7.548028000	1.683753000
H	1.348400000	5.058149000	-1.667383000
H	1.348400000	-5.058149000	1.667383000
H	1.868203000	5.405223000	1.557904000
H	1.868203000	-5.405223000	-1.557904000
H	4.087769000	5.845312000	2.525005000
H	4.087769000	-5.845312000	-2.525005000
H	5.058149000	1.348400000	-1.667383000
H	5.058149000	-1.348400000	1.667383000
H	5.405223000	1.868203000	1.557904000
H	5.405223000	-1.868203000	-1.557904000
H	5.845312000	4.087769000	2.525005000
H	5.845312000	-4.087769000	-2.525005000
H	7.548028000	1.344431000	-1.683753000
H	7.548028000	-1.344431000	1.683753000
H	8.798717000	0.000000000	0.000000000
H	-1.344431000	7.548028000	1.683753000
H	-1.344431000	-7.548028000	-1.683753000
H	-1.348400000	5.058149000	1.667383000
H	-1.348400000	-5.058149000	-1.667383000
H	-1.868203000	5.405223000	-1.557904000
H	-1.868203000	-5.405223000	1.557904000

H	-4.087769000	5.845312000	-2.525005000
H	-4.087769000	-5.845312000	2.525005000
H	-5.058149000	1.348400000	1.667383000
H	-5.058149000	-1.348400000	-1.667383000
H	-5.405223000	1.868203000	-1.557904000
H	-5.405223000	-1.868203000	1.557904000
H	-5.845312000	4.087769000	-2.525005000
H	-5.845312000	-4.087769000	2.525005000
H	-7.548028000	1.344431000	1.683753000
H	-7.548028000	-1.344431000	-1.683753000
H	-8.798717000	0.000000000	0.000000000
N	1.426738000	1.426738000	0.154872000
N	1.426738000	-1.426738000	-0.154872000
N	-1.426738000	1.426738000	-0.154872000
N	-1.426738000	-1.426738000	0.154872000

66. Pd[Ph₄Bz₈]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000911000
C	0.000000000	3.321156000	-0.664300000
C	0.000000000	4.741916000	-1.118012000
C	0.000000000	5.045206000	-2.481791000
C	0.000000000	5.783830000	-0.182766000
C	0.000000000	6.375096000	-2.908979000
C	0.000000000	7.111641000	-0.605598000
C	0.000000000	7.410716000	-1.971365000
C	0.000000000	-3.321156000	-0.664300000
C	0.000000000	-4.741916000	-1.118012000
C	0.000000000	-5.045206000	-2.481791000
C	0.000000000	-5.783830000	-0.182766000
C	0.000000000	-6.375096000	-2.908979000
C	0.000000000	-7.111641000	-0.605598000
C	0.000000000	-7.410716000	-1.971365000
C	1.243577000	2.733417000	-0.399329000
C	1.243577000	-2.733417000	-0.399329000
C	2.526565000	3.429407000	-0.308831000
C	2.526565000	-3.429407000	-0.308831000
C	2.733535000	1.243571000	0.400592000
C	2.733535000	-1.243571000	0.400592000
C	2.964075000	4.712936000	-0.679786000
C	2.964075000	-4.712936000	-0.679786000
C	3.321383000	0.000000000	0.665356000
C	3.429526000	2.526539000	0.309770000
C	3.429526000	-2.526539000	0.309770000
C	4.255549000	5.111007000	-0.353191000
C	4.255549000	-5.111007000	-0.353191000
C	4.713144000	2.964085000	0.680383000
C	4.713144000	-2.964085000	0.680383000
C	4.742614000	0.000000000	1.117583000
C	5.047418000	0.000000000	2.481017000

C	5.111156000	4.255515000	0.353528000
C	5.111156000	-4.255515000	0.353528000
C	5.783496000	0.000000000	0.181176000
C	6.377798000	0.000000000	2.906696000
C	7.111777000	0.000000000	0.602502000
C	7.412367000	0.000000000	1.967928000
C	-1.243577000	2.733417000	-0.399329000
C	-1.243577000	-2.733417000	-0.399329000
C	-2.526565000	3.429407000	-0.308831000
C	-2.526565000	-3.429407000	-0.308831000
C	-2.733535000	1.243571000	0.400592000
C	-2.733535000	-1.243571000	0.400592000
C	-2.964075000	4.712936000	-0.679786000
C	-2.964075000	-4.712936000	-0.679786000
C	-3.321383000	0.000000000	0.665356000
C	-3.429526000	2.526539000	0.309770000
C	-3.429526000	-2.526539000	0.309770000
C	-4.255549000	5.111007000	-0.353191000
C	-4.255549000	-5.111007000	-0.353191000
C	-4.713144000	2.964085000	0.680383000
C	-4.713144000	-2.964085000	0.680383000
C	-4.742614000	0.000000000	1.117583000
C	-5.047418000	0.000000000	2.481017000
C	-5.111156000	4.255515000	0.353528000
C	-5.111156000	-4.255515000	0.353528000
C	-5.783496000	0.000000000	0.181176000
C	-6.377798000	0.000000000	2.906696000
C	-7.111777000	0.000000000	0.602502000
C	-7.412367000	0.000000000	1.967928000
H	0.000000000	4.231191000	-3.205323000
H	0.000000000	5.539023000	0.878048000
H	0.000000000	6.601555000	-3.974155000
H	0.000000000	7.914006000	0.130482000
H	0.000000000	8.448196000	-2.303940000
H	0.000000000	-4.231191000	-3.205323000
H	0.000000000	-5.539023000	0.878048000
H	0.000000000	-6.601555000	-3.974155000
H	0.000000000	-7.914006000	0.130482000
H	0.000000000	-8.448196000	-2.303940000
H	2.325608000	5.397514000	-1.226276000
H	2.325608000	-5.397514000	-1.226276000
H	4.234221000	0.000000000	3.205472000
H	4.595927000	6.104081000	-0.643108000
H	4.595927000	-6.104081000	-0.643108000
H	5.397797000	2.325711000	1.226890000
H	5.397797000	-2.325711000	1.226890000
H	5.537493000	0.000000000	-0.879360000
H	6.104306000	4.595924000	0.643166000
H	6.104306000	-4.595924000	0.643166000
H	6.605471000	0.000000000	3.971610000
H	7.913297000	0.000000000	-0.134497000

H	8.450200000	0.000000000	2.299364000
H	-2.325608000	5.397514000	-1.226276000
H	-2.325608000	-5.397514000	-1.226276000
H	-4.234221000	0.000000000	3.205472000
H	-4.595927000	6.104081000	-0.643108000
H	-4.595927000	-6.104081000	-0.643108000
H	-5.397797000	2.325711000	1.226890000
H	-5.397797000	-2.325711000	1.226890000
H	-5.537493000	0.000000000	-0.879360000
H	-6.104306000	4.595924000	0.643166000
H	-6.104306000	-4.595924000	0.643166000
H	-6.605471000	0.000000000	3.971610000
H	-7.913297000	0.000000000	-0.134497000
H	-8.450200000	0.000000000	2.299364000
N	1.426713000	1.426692000	0.000789000
N	1.426713000	-1.426692000	0.000789000
N	-1.426713000	1.426692000	0.000789000
N	-1.426713000	-1.426692000	0.000789000

67. Pt[Ph₄Bz₈]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.000000000
C	0.000000000	3.417675000	0.000000000
C	0.000000000	4.907931000	0.000000000
C	0.000000000	7.711763000	0.000000000
C	0.000000000	-3.417675000	0.000000000
C	0.000000000	-4.907931000	0.000000000
C	0.000000000	-7.711763000	0.000000000
C	0.731812000	7.010593000	-0.962357000
C	0.731812000	-7.010593000	0.962357000
C	0.733877000	5.615774000	-0.958887000
C	0.733877000	-5.615774000	0.958887000
C	1.178689000	2.769678000	0.378681000
C	1.178689000	-2.769678000	-0.378681000
C	2.380627000	3.381650000	0.926967000
C	2.380627000	-3.381650000	-0.926967000
C	2.645870000	4.646855000	1.476903000
C	2.645870000	-4.646855000	-1.476903000
C	2.769678000	1.178689000	0.378681000
C	2.769678000	-1.178689000	-0.378681000
C	3.381650000	2.380627000	0.926967000
C	3.381650000	-2.380627000	-0.926967000
C	3.417675000	0.000000000	0.000000000
C	3.905006000	4.897526000	2.010259000
C	3.905006000	-4.897526000	-2.010259000
C	4.646855000	2.645870000	1.476903000
C	4.646855000	-2.645870000	-1.476903000
C	4.897526000	3.905006000	2.010259000
C	4.897526000	-3.905006000	-2.010259000
C	4.907931000	0.000000000	0.000000000

C	5.615774000	0.733877000	-0.958887000
C	5.615774000	-0.733877000	0.958887000
C	7.010593000	0.731812000	-0.962357000
C	7.010593000	-0.731812000	0.962357000
C	7.711763000	0.000000000	0.000000000
C	-0.731812000	7.010593000	0.962357000
C	-0.731812000	-7.010593000	-0.962357000
C	-0.733877000	5.615774000	0.958887000
C	-0.733877000	-5.615774000	-0.958887000
C	-1.178689000	2.769678000	-0.378681000
C	-1.178689000	-2.769678000	0.378681000
C	-2.380627000	3.381650000	-0.926967000
C	-2.380627000	-3.381650000	0.926967000
C	-2.645870000	4.646855000	-1.476903000
C	-2.645870000	-4.646855000	1.476903000
C	-2.769678000	1.178689000	-0.378681000
C	-2.769678000	-1.178689000	0.378681000
C	-3.381650000	2.380627000	-0.926967000
C	-3.381650000	-2.380627000	0.926967000
C	-3.417675000	0.000000000	0.000000000
C	-3.905006000	4.897526000	-2.010259000
C	-3.905006000	-4.897526000	2.010259000
C	-4.646855000	2.645870000	-1.476903000
C	-4.646855000	-2.645870000	1.476903000
C	-4.897526000	3.905006000	-2.010259000
C	-4.897526000	-3.905006000	2.010259000
C	-4.907931000	0.000000000	0.000000000
C	-5.615774000	0.733877000	0.958887000
C	-5.615774000	-0.733877000	-0.958887000
C	-7.010593000	0.731812000	0.962357000
C	-7.010593000	-0.731812000	-0.962357000
C	-7.711763000	0.000000000	0.000000000
H	0.000000000	8.801258000	0.000000000
H	0.000000000	-8.801258000	0.000000000
H	1.303982000	7.550692000	-1.715273000
H	1.303982000	-7.550692000	1.715273000
H	1.307715000	5.060729000	-1.699644000
H	1.307715000	-5.060729000	1.699644000
H	1.884680000	5.420055000	1.513705000
H	1.884680000	-5.420055000	-1.513705000
H	4.114738000	5.872646000	2.447500000
H	4.114738000	-5.872646000	-2.447500000
H	5.060729000	1.307715000	-1.699644000
H	5.060729000	-1.307715000	1.699644000
H	5.420055000	1.884680000	1.513705000
H	5.420055000	-1.884680000	-1.513705000
H	5.872646000	4.114738000	2.447500000
H	5.872646000	-4.114738000	-2.447500000
H	7.550692000	1.303982000	-1.715273000
H	7.550692000	-1.303982000	1.715273000
H	8.801258000	0.000000000	0.000000000

H	-1.303982000	7.550692000	1.715273000
H	-1.303982000	-7.550692000	-1.715273000
H	-1.307715000	5.060729000	1.699644000
H	-1.307715000	-5.060729000	-1.699644000
H	-1.884680000	5.420055000	-1.513705000
H	-1.884680000	-5.420055000	1.513705000
H	-4.114738000	5.872646000	-2.447500000
H	-4.114738000	-5.872646000	2.447500000
H	-5.060729000	1.307715000	1.699644000
H	-5.060729000	-1.307715000	-1.699644000
H	-5.420055000	1.884680000	-1.513705000
H	-5.420055000	-1.884680000	1.513705000
H	-5.872646000	4.114738000	-2.447500000
H	-5.872646000	-4.114738000	2.447500000
H	-7.550692000	1.303982000	1.715273000
H	-7.550692000	-1.303982000	-1.715273000
H	-8.801258000	0.000000000	0.000000000
N	1.424679000	1.424679000	0.165749000
N	1.424679000	-1.424679000	-0.165749000
N	-1.424679000	1.424679000	-0.165749000
N	-1.424679000	-1.424679000	0.165749000

68. Pt[Ph₄Bz₈]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	-0.000179000
C	0.000000000	3.327637000	-0.653737000
C	0.000000000	4.750820000	-1.100428000
C	0.000000000	5.060477000	-2.462823000
C	0.000000000	5.788037000	-0.159947000
C	0.000000000	6.392455000	-2.883447000
C	0.000000000	7.117867000	-0.576418000
C	0.000000000	7.423472000	-1.940749000
C	0.000000000	-3.327637000	-0.653737000
C	0.000000000	-4.750820000	-1.100428000
C	0.000000000	-5.060477000	-2.462823000
C	0.000000000	-5.788037000	-0.159947000
C	0.000000000	-6.392455000	-2.883447000
C	0.000000000	-7.117867000	-0.576418000
C	0.000000000	-7.423472000	-1.940749000
C	1.243710000	2.739143000	-0.393126000
C	1.243710000	-2.739143000	-0.393126000
C	2.525663000	3.431805000	-0.303862000
C	2.525663000	-3.431805000	-0.303862000
C	2.739194000	1.243688000	0.392706000
C	2.739194000	-1.243688000	0.392706000
C	2.961492000	4.717382000	-0.669905000
C	2.961492000	-4.717382000	-0.669905000
C	3.327684000	0.000000000	0.653400000
C	3.431877000	2.525612000	0.303360000
C	3.431877000	-2.525612000	0.303360000

C	4.254646000	5.113905000	-0.348954000
C	4.254646000	-5.113905000	-0.348954000
C	4.717565000	2.961377000	0.669119000
C	4.717565000	-2.961377000	0.669119000
C	4.750663000	0.000000000	1.100725000
C	5.059377000	0.000000000	2.463360000
C	5.114198000	4.254406000	0.347831000
C	5.114198000	-4.254406000	0.347831000
C	5.788549000	0.000000000	0.160973000
C	6.391037000	0.000000000	2.884950000
C	7.118091000	0.000000000	0.578431000
C	7.422715000	0.000000000	1.942979000
C	-1.243710000	2.739143000	-0.393126000
C	-1.243710000	-2.739143000	-0.393126000
C	-2.525663000	3.431805000	-0.303862000
C	-2.525663000	-3.431805000	-0.303862000
C	-2.739194000	1.243688000	0.392706000
C	-2.739194000	-1.243688000	0.392706000
C	-2.961492000	4.717382000	-0.669905000
C	-2.961492000	-4.717382000	-0.669905000
C	-3.327684000	0.000000000	0.653400000
C	-3.431877000	2.525612000	0.303360000
C	-3.431877000	-2.525612000	0.303360000
C	-4.254646000	5.113905000	-0.348954000
C	-4.254646000	-5.113905000	-0.348954000
C	-4.717565000	2.961377000	0.669119000
C	-4.717565000	-2.961377000	0.669119000
C	-4.750663000	0.000000000	1.100725000
C	-5.059377000	0.000000000	2.463360000
C	-5.114198000	4.254406000	0.347831000
C	-5.114198000	-4.254406000	0.347831000
C	-5.788549000	0.000000000	0.160973000
C	-6.391037000	0.000000000	2.884950000
C	-7.118091000	0.000000000	0.578431000
C	-7.422715000	0.000000000	1.942979000
H	0.000000000	4.249803000	-3.190117000
H	0.000000000	5.537772000	0.899594000
H	0.000000000	6.624223000	-3.947458000
H	0.000000000	7.916786000	0.163406000
H	0.000000000	8.462560000	-2.268290000
H	0.000000000	-4.249803000	-3.190117000
H	0.000000000	-5.537772000	0.899594000
H	0.000000000	-6.624223000	-3.947458000
H	0.000000000	-7.916786000	0.163406000
H	0.000000000	-8.462560000	-2.268290000
H	2.319964000	5.404988000	-1.208536000
H	2.319964000	-5.404988000	-1.208536000
H	4.248156000	0.000000000	3.190045000
H	4.593005000	6.108682000	-0.635239000
H	4.593005000	-6.108682000	-0.635239000
H	5.405108000	2.319880000	1.207865000

H	5.405108000	-2.319880000	1.207865000
H	5.539187000	0.000000000	-0.898807000
H	6.109053000	4.592727000	0.633897000
H	6.109053000	-4.592727000	0.633897000
H	6.622040000	0.000000000	3.949146000
H	7.917517000	0.000000000	-0.160868000
H	8.461536000	0.000000000	2.271304000
H	-2.319964000	5.404988000	-1.208536000
H	-2.319964000	-5.404988000	-1.208536000
H	-4.248156000	0.000000000	3.190045000
H	-4.593005000	6.108682000	-0.635239000
H	-4.593005000	-6.108682000	-0.635239000
H	-5.405108000	2.319880000	1.207865000
H	-5.405108000	-2.319880000	1.207865000
H	-5.539187000	0.000000000	-0.898807000
H	-6.109053000	4.592727000	0.633897000
H	-6.109053000	-4.592727000	0.633897000
H	-6.622040000	0.000000000	3.949146000
H	-7.917517000	0.000000000	-0.160868000
H	-8.461536000	0.000000000	2.271304000
N	1.427097000	1.427053000	-0.000207000
N	1.427097000	-1.427053000	-0.000207000
N	-1.427097000	1.427053000	-0.000207000
N	-1.427097000	-1.427053000	-0.000207000

69. Zn[Ph₄Bz₈]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.000000000
C	0.000000000	3.422310000	0.000000000
C	0.000000000	4.912946000	0.000000000
C	0.000000000	7.718227000	0.000000000
C	0.000000000	-3.422310000	0.000000000
C	0.000000000	-4.912946000	0.000000000
C	0.000000000	-7.718227000	0.000000000
C	0.709938000	7.016804000	-0.978415000
C	0.709938000	-7.016804000	0.978415000
C	0.711917000	5.621954000	-0.974752000
C	0.711917000	-5.621954000	0.974752000
C	1.195026000	2.780785000	0.367688000
C	1.195026000	-2.780785000	-0.367688000
C	2.404096000	3.407194000	0.894316000
C	2.404096000	-3.407194000	-0.894316000
C	2.678236000	4.679052000	1.425848000
C	2.678236000	-4.679052000	-1.425848000
C	2.780785000	1.195026000	0.367688000
C	2.780785000	-1.195026000	-0.367688000
C	3.407194000	2.404096000	0.894316000
C	3.407194000	-2.404096000	-0.894316000
C	3.422310000	0.000000000	0.000000000
C	3.943103000	4.935879000	1.941578000

C	3.943103000	-4.935879000	-1.941578000
C	4.679052000	2.678236000	1.425848000
C	4.679052000	-2.678236000	-1.425848000
C	4.912946000	0.000000000	0.000000000
C	4.935879000	3.943103000	1.941578000
C	4.935879000	-3.943103000	-1.941578000
C	5.621954000	0.711917000	-0.974752000
C	5.621954000	-0.711917000	0.974752000
C	7.016804000	0.709938000	-0.978415000
C	7.016804000	-0.709938000	0.978415000
C	7.718227000	0.000000000	0.000000000
C	-0.709938000	7.016804000	0.978415000
C	-0.709938000	-7.016804000	-0.978415000
C	-0.711917000	5.621954000	0.974752000
C	-0.711917000	-5.621954000	-0.974752000
C	-1.195026000	2.780785000	-0.367688000
C	-1.195026000	-2.780785000	0.367688000
C	-2.404096000	3.407194000	-0.894316000
C	-2.404096000	-3.407194000	0.894316000
C	-2.678236000	4.679052000	-1.425848000
C	-2.678236000	-4.679052000	1.425848000
C	-2.780785000	1.195026000	-0.367688000
C	-2.780785000	-1.195026000	0.367688000
C	-3.407194000	2.404096000	-0.894316000
C	-3.407194000	-2.404096000	0.894316000
C	-3.422310000	0.000000000	0.000000000
C	-3.943103000	4.935879000	-1.941578000
C	-3.943103000	-4.935879000	1.941578000
C	-4.679052000	2.678236000	-1.425848000
C	-4.679052000	-2.678236000	1.425848000
C	-4.912946000	0.000000000	0.000000000
C	-4.935879000	3.943103000	-1.941578000
C	-4.935879000	-3.943103000	1.941578000
C	-5.621954000	0.711917000	0.974752000
C	-5.621954000	-0.711917000	-0.974752000
C	-7.016804000	0.709938000	0.978415000
C	-7.016804000	-0.709938000	-0.978415000
C	-7.718227000	0.000000000	0.000000000
H	0.000000000	8.807713000	0.000000000
H	0.000000000	-8.807713000	0.000000000
H	1.265117000	7.556748000	-1.744066000
H	1.265117000	-7.556748000	1.744066000
H	1.269115000	5.067147000	-1.728259000
H	1.269115000	-5.067147000	1.728259000
H	1.918470000	5.453844000	1.462308000
H	1.918470000	-5.453844000	-1.462308000
H	4.158281000	5.916100000	2.364778000
H	4.158281000	-5.916100000	-2.364778000
H	5.067147000	1.269115000	-1.728259000
H	5.067147000	-1.269115000	1.728259000
H	5.453844000	1.918470000	1.462308000

H	5.453844000	-1.918470000	-1.462308000
H	5.916100000	4.158281000	2.364778000
H	5.916100000	-4.158281000	-2.364778000
H	7.556748000	1.265117000	-1.744066000
H	7.556748000	-1.265117000	1.744066000
H	8.807713000	0.000000000	0.000000000
H	-1.265117000	7.556748000	1.744066000
H	-1.265117000	-7.556748000	-1.744066000
H	-1.269115000	5.067147000	1.728259000
H	-1.269115000	-5.067147000	-1.728259000
H	-1.918470000	5.453844000	-1.462308000
H	-1.918470000	-5.453844000	1.462308000
H	-4.158281000	5.916100000	-2.364778000
H	-4.158281000	-5.916100000	2.364778000
H	-5.067147000	1.269115000	1.728259000
H	-5.067147000	-1.269115000	-1.728259000
H	-5.453844000	1.918470000	-1.462308000
H	-5.453844000	-1.918470000	1.462308000
H	-5.916100000	4.158281000	-2.364778000
H	-5.916100000	-4.158281000	2.364778000
H	-7.556748000	1.265117000	1.744066000
H	-7.556748000	-1.265117000	-1.744066000
H	-8.807713000	0.000000000	0.000000000
N	1.441094000	1.441094000	0.163841000
N	1.441094000	-1.441094000	-0.163841000
N	-1.441094000	1.441094000	-0.163841000
N	-1.441094000	-1.441094000	0.163841000

70. Zn[Ph₄Bz₈]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.001272000
C	0.000000000	3.363373000	-0.561528000
C	0.000000000	4.804303000	-0.949395000
C	0.000000000	5.171180000	-2.297684000
C	0.000000000	5.802024000	0.032586000
C	0.000000000	6.519117000	-2.663107000
C	0.000000000	7.148208000	-0.328218000
C	0.000000000	7.510384000	-1.678556000
C	0.000000000	-3.363373000	-0.561528000
C	0.000000000	-4.804303000	-0.949395000
C	0.000000000	-5.171180000	-2.297684000
C	0.000000000	-5.802024000	0.032586000
C	0.000000000	-6.519117000	-2.663107000
C	0.000000000	-7.148208000	-0.328218000
C	0.000000000	-7.510384000	-1.678556000
C	1.255202000	2.770903000	-0.335940000
C	1.255202000	-2.770903000	-0.335940000
C	2.539057000	3.470172000	-0.264717000
C	2.539057000	-3.470172000	-0.264717000
C	2.771043000	1.255191000	0.337318000

C	2.771043000	-1.255191000	0.337318000
C	2.962106000	4.771689000	-0.591581000
C	2.962106000	-4.771689000	-0.591581000
C	3.363619000	0.000000000	0.562677000
C	3.470294000	2.539034000	0.265708000
C	3.470294000	-2.539034000	0.265708000
C	4.267178000	5.156058000	-0.309358000
C	4.267178000	-5.156058000	-0.309358000
C	4.771910000	2.962119000	0.592140000
C	4.771910000	-2.962119000	0.592140000
C	4.804980000	0.000000000	0.948932000
C	5.156170000	4.267188000	0.309735000
C	5.156170000	-4.267188000	0.309735000
C	5.173266000	0.000000000	2.296837000
C	5.801679000	0.000000000	-0.034080000
C	6.521580000	0.000000000	2.660862000
C	7.148234000	0.000000000	0.325318000
C	7.511822000	0.000000000	1.675276000
C	-1.255202000	2.770903000	-0.335940000
C	-1.255202000	-2.770903000	-0.335940000
C	-2.539057000	3.470172000	-0.264717000
C	-2.539057000	-3.470172000	-0.264717000
C	-2.771043000	1.255191000	0.337318000
C	-2.771043000	-1.255191000	0.337318000
C	-2.962106000	4.771689000	-0.591581000
C	-2.962106000	-4.771689000	-0.591581000
C	-3.363619000	0.000000000	0.562677000
C	-3.470294000	2.539034000	0.265708000
C	-3.470294000	-2.539034000	0.265708000
C	-4.267178000	5.156058000	-0.309358000
C	-4.267178000	-5.156058000	-0.309358000
C	-4.771910000	2.962119000	0.592140000
C	-4.771910000	-2.962119000	0.592140000
C	-4.804980000	0.000000000	0.948932000
C	-5.156170000	4.267188000	0.309735000
C	-5.156170000	-4.267188000	0.309735000
C	-5.173266000	0.000000000	2.296837000
C	-5.801679000	0.000000000	-0.034080000
C	-6.521580000	0.000000000	2.660862000
C	-7.148234000	0.000000000	0.325318000
C	-7.511822000	0.000000000	1.675276000
H	0.000000000	4.391623000	-3.058120000
H	0.000000000	5.508503000	1.080958000
H	0.000000000	6.794585000	-3.716658000
H	0.000000000	7.915685000	0.444203000
H	0.000000000	8.562135000	-1.962681000
H	0.000000000	-4.391623000	-3.058120000
H	0.000000000	-5.508503000	1.080958000
H	0.000000000	-6.794585000	-3.716658000
H	0.000000000	-7.915685000	0.444203000
H	0.000000000	-8.562135000	-1.962681000

H	2.299922000	5.483963000	-1.069446000
H	2.299922000	-5.483963000	-1.069446000
H	4.394517000	0.000000000	3.058091000
H	4.592860000	6.163645000	-0.564188000
H	4.592860000	-6.163645000	-0.564188000
H	5.484340000	2.299960000	1.069810000
H	5.484340000	-2.299960000	1.069810000
H	5.507062000	0.000000000	-1.082141000
H	6.163804000	4.592931000	0.564291000
H	6.163804000	-4.592931000	0.564291000
H	6.798128000	0.000000000	3.714131000
H	7.914915000	0.000000000	-0.447886000
H	8.563875000	0.000000000	1.958281000
H	-2.299922000	5.483963000	-1.069446000
H	-2.299922000	-5.483963000	-1.069446000
H	-4.394517000	0.000000000	3.058091000
H	-4.592860000	6.163645000	-0.564188000
H	-4.592860000	-6.163645000	-0.564188000
H	-5.484340000	2.299960000	1.069810000
H	-5.484340000	-2.299960000	1.069810000
H	-5.507062000	0.000000000	-1.082141000
H	-6.163804000	4.592931000	0.564291000
H	-6.163804000	-4.592931000	0.564291000
H	-6.798128000	0.000000000	3.714131000
H	-7.914915000	0.000000000	-0.447886000
H	-8.563875000	0.000000000	1.958281000
N	1.449069000	1.449017000	0.000848000
N	1.449069000	-1.449017000	0.000848000
N	-1.449069000	1.449017000	0.000848000
N	-1.449069000	-1.449017000	0.000848000

71. Cu[A₄Bz₈]; S = ½ (saddled)

Cu	0.000000000	0.000000000	0.003401000
C	0.193723000	-5.208026000	-1.788268000
C	0.301707000	2.903864000	-0.635086000
C	0.499530000	-4.017736000	-1.112603000
C	1.231136000	-6.068934000	-2.130006000
C	1.688972000	2.900030000	-0.392921000
C	1.819513000	-2.380704000	-0.190008000
C	1.844303000	-3.700256000	-0.795212000
C	2.379072000	1.818188000	0.198227000
C	2.433944000	4.056964000	-0.715371000
C	2.563034000	-5.757580000	-1.809916000
C	2.809022000	7.617717000	-2.510103000
C	2.881408000	-4.577317000	-1.146717000
C	2.902001000	-1.689214000	0.398218000
C	2.902896000	-0.302451000	0.644212000
C	3.084800000	5.048267000	-1.016125000

C	3.696688000	1.844292000	0.807130000
C	4.014233000	0.499902000	1.125856000
C	4.065495000	-2.428586000	0.710450000
C	4.430752000	7.477482000	0.131863000
C	4.569757000	2.882916000	1.163882000
C	5.065482000	-3.070939000	1.000640000
C	5.200362000	0.195940000	1.809605000
C	5.533344000	6.125234000	-2.418039000
C	5.746536000	2.566295000	1.834046000
C	6.057531000	1.234791000	2.156531000
C	6.154322000	-5.595628000	2.243203000
C	7.552750000	-2.846013000	2.637543000
C	7.596635000	-4.239752000	-0.130072000
C	-0.193723000	5.208026000	-1.788268000
C	-0.301707000	-2.903864000	-0.635086000
C	-0.499530000	4.017736000	-1.112603000
C	-1.231136000	6.068934000	-2.130006000
C	-1.688972000	-2.900030000	-0.392921000
C	-1.819513000	2.380704000	-0.190008000
C	-1.844303000	3.700256000	-0.795212000
C	-2.379072000	-1.818188000	0.198227000
C	-2.433944000	-4.056964000	-0.715371000
C	-2.563034000	5.757580000	-1.809916000
C	-2.809022000	-7.617717000	-2.510103000
C	-2.881408000	4.577317000	-1.146717000
C	-2.902001000	1.689214000	0.398218000
C	-2.902896000	0.302451000	0.644212000
C	-3.084800000	-5.048267000	-1.016125000
C	-3.696688000	-1.844292000	0.807130000
C	-4.014233000	-0.499902000	1.125856000
C	-4.065495000	2.428586000	0.710450000
C	-4.430752000	-7.477482000	0.131863000
C	-4.569757000	-2.882916000	1.163882000
C	-5.065482000	3.070939000	1.000640000
C	-5.200362000	-0.195940000	1.809605000
C	-5.533344000	-6.125234000	-2.418039000
C	-5.746536000	-2.566295000	1.834046000
C	-6.057531000	-1.234791000	2.156531000
C	-6.154322000	5.595628000	2.243203000
C	-7.552750000	2.846013000	2.637543000
C	-7.596635000	4.239752000	-0.130072000
H	0.827993000	5.445893000	-2.058546000
H	1.006160000	-6.990106000	-2.665866000
H	1.889613000	7.847695000	-1.952855000
H	2.527912000	7.080257000	-3.427252000
H	3.280864000	8.567975000	-2.802151000
H	3.360008000	-6.442431000	-2.096579000
H	3.529243000	7.717892000	0.712861000
H	3.913700000	-4.335152000	-0.918565000
H	4.326675000	3.914990000	0.935256000
H	4.963614000	8.415582000	-0.086174000

H	5.082985000	6.852726000	0.759265000
H	5.282342000	5.578794000	-3.338093000
H	5.436954000	-0.825240000	2.083187000
H	5.555819000	-5.439710000	3.151771000
H	5.561926000	-6.211140000	1.550908000
H	6.099878000	7.027571000	-2.694344000
H	6.185889000	5.481643000	-1.810675000
H	6.428208000	3.364329000	2.125319000
H	6.957789000	-2.643690000	3.539708000
H	6.975087000	1.011632000	2.699308000
H	7.029129000	-4.855212000	-0.843038000
H	7.059535000	-6.159020000	2.516366000
H	7.794452000	-1.883818000	2.163606000
H	7.833366000	-3.284568000	-0.619681000
H	8.495496000	-3.320920000	2.948530000
H	8.541313000	-4.758667000	0.093341000
H	-0.827993000	-5.445893000	-2.058546000
H	-1.006160000	6.990106000	-2.665866000
H	-1.889613000	-7.847695000	-1.952855000
H	-2.527912000	-7.080257000	-3.427252000
H	-3.280864000	-8.567975000	-2.802151000
H	-3.360008000	6.442431000	-2.096579000
H	-3.529243000	-7.717892000	0.712861000
H	-3.913700000	4.335152000	-0.918565000
H	-4.326675000	-3.914990000	0.935256000
H	-4.963614000	-8.415582000	-0.086174000
H	-5.082985000	-6.852726000	0.759265000
H	-5.282342000	-5.578794000	-3.338093000
H	-5.436954000	0.825240000	2.083187000
H	-5.555819000	5.439710000	3.151771000
H	-5.561926000	6.211140000	1.550908000
H	-6.099878000	-7.027571000	-2.694344000
H	-6.185889000	-5.481643000	-1.810675000
H	-6.428208000	-3.364329000	2.125319000
H	-6.957789000	2.643690000	3.539708000
H	-6.975087000	-1.011632000	2.699308000
H	-7.029129000	4.855212000	-0.843038000
H	-7.059535000	6.159020000	2.516366000
H	-7.794452000	1.883818000	2.163606000
H	-7.833366000	3.284568000	-0.619681000
H	-8.495496000	3.320920000	2.948530000
H	-8.541313000	4.758667000	0.093341000
N	0.534428000	-1.904481000	-0.190030000
N	1.903510000	0.533166000	0.197908000
N	-0.534428000	1.904481000	-0.190030000
N	-1.903510000	-0.533166000	0.197908000
Si	3.980815000	6.580665000	-1.460742000
Si	6.605572000	-3.954685000	1.444292000
Si	-3.980815000	-6.580665000	-1.460742000
Si	-6.605572000	3.954685000	1.444292000

72. Cu[A₄Bz₈]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.012244000
C	0.000000000	3.252018000	-0.795667000
C	0.000000000	4.484105000	-1.485580000
C	0.000000000	5.520089000	-2.136735000
C	0.000000000	6.872952000	-4.868389000
C	0.000000000	-3.252018000	-0.795667000
C	0.000000000	-4.484105000	-1.485580000
C	0.000000000	-5.520089000	-2.136735000
C	0.000000000	-6.872952000	-4.868389000
C	1.244750000	2.692340000	-0.432896000
C	1.244750000	-2.692340000	-0.432896000
C	1.554141000	8.044589000	-2.444612000
C	1.554141000	-8.044589000	-2.444612000
C	2.504226000	3.406259000	-0.300856000
C	2.504226000	-3.406259000	-0.300856000
C	2.693663000	1.244927000	0.454968000
C	2.693663000	-1.244927000	0.454968000
C	2.911187000	4.714550000	-0.605263000
C	2.911187000	-4.714550000	-0.605263000
C	3.254863000	0.000000000	0.815136000
C	3.406832000	2.504870000	0.320896000
C	3.406832000	-2.504870000	0.320896000
C	4.208600000	5.105754000	-0.294919000
C	4.208600000	-5.105754000	-0.294919000
C	4.492923000	0.000000000	1.494012000
C	4.714673000	2.914015000	0.624356000
C	4.714673000	-2.914015000	0.624356000
C	5.104109000	4.211619000	0.312608000
C	5.104109000	-4.211619000	0.312608000
C	5.537341000	0.000000000	2.131355000
C	6.947852000	0.000000000	4.814733000
C	8.072391000	1.556092000	2.384923000
C	8.072391000	-1.556092000	2.384923000
C	-1.244750000	2.692340000	-0.432896000
C	-1.244750000	-2.692340000	-0.432896000
C	-1.554141000	8.044589000	-2.444612000
C	-1.554141000	-8.044589000	-2.444612000
C	-2.504226000	3.406259000	-0.300856000
C	-2.504226000	-3.406259000	-0.300856000
C	-2.693663000	1.244927000	0.454968000
C	-2.693663000	-1.244927000	0.454968000
C	-2.911187000	4.714550000	-0.605263000
C	-2.911187000	-4.714550000	-0.605263000
C	-3.254863000	0.000000000	0.815136000
C	-3.406832000	2.504870000	0.320896000
C	-3.406832000	-2.504870000	0.320896000
C	-4.208600000	5.105754000	-0.294919000
C	-4.208600000	-5.105754000	-0.294919000
C	-4.492923000	0.000000000	1.494012000

C	-4.714673000	2.914015000	0.624356000
C	-4.714673000	-2.914015000	0.624356000
C	-5.104109000	4.211619000	0.312608000
C	-5.104109000	-4.211619000	0.312608000
C	-5.537341000	0.000000000	2.131355000
C	-6.947852000	0.000000000	4.814733000
C	-8.072391000	1.556092000	2.384923000
C	-8.072391000	-1.556092000	2.384923000
H	0.000000000	5.802023000	-5.112367000
H	0.000000000	-5.802023000	-5.112367000
H	0.890020000	7.325935000	-5.328756000
H	0.890020000	-7.325935000	-5.328756000
H	1.569878000	8.171393000	-1.352840000
H	1.569878000	-8.171393000	-1.352840000
H	1.610878000	9.040281000	-2.910014000
H	1.610878000	-9.040281000	-2.910014000
H	2.229529000	5.410474000	-1.078989000
H	2.229529000	-5.410474000	-1.078989000
H	2.452185000	7.481235000	-2.737261000
H	2.452185000	-7.481235000	-2.737261000
H	4.531686000	6.119098000	-0.529268000
H	4.531686000	-6.119098000	-0.529268000
H	5.411590000	2.233946000	1.098591000
H	5.411590000	-2.233946000	1.098591000
H	6.117217000	4.536032000	0.546217000
H	6.117217000	-4.536032000	0.546217000
H	6.389469000	0.889312000	5.139884000
H	6.389469000	-0.889312000	5.139884000
H	7.516237000	2.454188000	2.690335000
H	7.516237000	-2.454188000	2.690335000
H	7.924094000	0.000000000	5.323273000
H	8.175517000	1.573981000	1.290660000
H	8.175517000	-1.573981000	1.290660000
H	9.078360000	1.611723000	2.827442000
H	9.078360000	-1.611723000	2.827442000
H	-0.890020000	7.325935000	-5.328756000
H	-0.890020000	-7.325935000	-5.328756000
H	-1.569878000	8.171393000	-1.352840000
H	-1.569878000	-8.171393000	-1.352840000
H	-1.610878000	9.040281000	-2.910014000
H	-1.610878000	-9.040281000	-2.910014000
H	-2.229529000	5.410474000	-1.078989000
H	-2.229529000	-5.410474000	-1.078989000
H	-2.452185000	7.481235000	-2.737261000
H	-2.452185000	-7.481235000	-2.737261000
H	-4.531686000	6.119098000	-0.529268000
H	-4.531686000	-6.119098000	-0.529268000
H	-5.411590000	2.233946000	1.098591000
H	-5.411590000	-2.233946000	1.098591000
H	-6.117217000	4.536032000	0.546217000
H	-6.117217000	-4.536032000	0.546217000

H	-6.389469000	0.889312000	5.139884000
H	-6.389469000	-0.889312000	5.139884000
H	-7.516237000	2.454188000	2.690335000
H	-7.516237000	-2.454188000	2.690335000
H	-7.924094000	0.000000000	5.323273000
H	-8.175517000	1.573981000	1.290660000
H	-8.175517000	-1.573981000	1.290660000
H	-9.078360000	1.611723000	2.827442000
H	-9.078360000	-1.611723000	2.827442000
N	1.405274000	1.404878000	0.012111000
N	1.405274000	-1.404878000	0.012111000
N	-1.405274000	1.404878000	0.012111000
N	-1.405274000	-1.404878000	0.012111000
Si	0.000000000	7.135096000	-2.996820000
Si	0.000000000	-7.135096000	-2.996820000
Si	7.173820000	0.000000000	2.949290000
Si	-7.173820000	0.000000000	2.949290000

73. Ni[A₄Bz₈]; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.002568000
C	0.210984000	2.781247000	-0.801051000
C	0.454402000	-5.080021000	-1.866322000
C	0.643648000	-3.907119000	-1.122133000
C	1.506805000	-5.985368000	-1.961004000
C	1.613341000	2.777235000	-0.780759000
C	1.780536000	-2.327081000	0.092179000
C	1.886483000	-3.648955000	-0.490799000
C	2.326883000	1.779321000	-0.089112000
C	2.328047000	3.849356000	-1.356341000
C	2.608629000	7.101862000	-3.703157000
C	2.734378000	-5.736879000	-1.323995000
C	2.779327000	-1.613853000	0.783023000
C	2.782231000	-0.211464000	0.804682000
C	2.937205000	-4.572987000	-0.589428000
C	2.954971000	4.762756000	-1.875256000
C	3.649106000	1.886081000	0.492919000
C	3.854187000	-2.327604000	1.354939000
C	3.907968000	0.643747000	1.124942000
C	4.428439000	7.288423000	-1.199653000
C	4.572629000	2.937351000	0.590585000
C	4.770807000	-2.952437000	1.870846000
C	5.080983000	0.455768000	1.869320000
C	5.303262000	5.552096000	-3.601600000
C	5.572134000	-5.394088000	3.451613000
C	5.736915000	2.735563000	1.324793000
C	5.985982000	1.508591000	1.962791000
C	6.999938000	-2.658247000	3.843220000
C	7.394441000	-4.264915000	1.224587000
C	-0.210984000	-2.781247000	-0.801051000

C	-0.454402000	5.080021000	-1.866322000
C	-0.643648000	3.907119000	-1.122133000
C	-1.506805000	5.985368000	-1.961004000
C	-1.613341000	-2.777235000	-0.780759000
C	-1.780536000	2.327081000	0.092179000
C	-1.886483000	3.648955000	-0.490799000
C	-2.326883000	-1.779321000	-0.089112000
C	-2.328047000	-3.849356000	-1.356341000
C	-2.608629000	-7.101862000	-3.703157000
C	-2.734378000	5.736879000	-1.323995000
C	-2.779327000	1.613853000	0.783023000
C	-2.782231000	0.211464000	0.804682000
C	-2.937205000	4.572987000	-0.589428000
C	-2.954971000	-4.762756000	-1.875256000
C	-3.649106000	-1.886081000	0.492919000
C	-3.854187000	2.327604000	1.354939000
C	-3.907968000	-0.643747000	1.124942000
C	-4.428439000	-7.288423000	-1.199653000
C	-4.572629000	-2.937351000	0.590585000
C	-4.770807000	2.952437000	1.870846000
C	-5.080983000	-0.455768000	1.869320000
C	-5.303262000	-5.552096000	-3.601600000
C	-5.572134000	5.394088000	3.451613000
C	-5.736915000	-2.735563000	1.324793000
C	-5.985982000	-1.508591000	1.962791000
C	-6.999938000	2.658247000	3.843220000
C	-7.394441000	4.264915000	1.224587000
H	0.483870000	5.269046000	-2.375445000
H	1.379299000	-6.894017000	-2.547773000
H	1.755523000	7.462822000	-3.110875000
H	2.222235000	6.440689000	-4.491986000
H	3.082046000	7.970566000	-4.185068000
H	3.543796000	-6.459921000	-1.415596000
H	3.578937000	7.632572000	-0.592974000
H	3.891486000	-4.380633000	-0.110301000
H	4.379342000	3.891483000	0.111533000
H	4.851590000	-5.153139000	4.245796000
H	4.957189000	8.171685000	-1.589305000
H	4.972189000	4.885935000	-4.410677000
H	5.067937000	-6.048156000	2.725626000
H	5.117363000	6.741631000	-0.539661000
H	5.269701000	-0.481783000	2.379964000
H	5.863580000	6.387771000	-4.047872000
H	5.988863000	4.984491000	-2.955975000
H	6.282842000	-2.355519000	4.619492000
H	6.406448000	-5.955595000	3.898876000
H	6.459522000	3.545470000	1.415665000
H	6.894825000	1.382146000	2.549510000
H	6.915747000	-4.921034000	0.483360000
H	7.360302000	-1.750629000	3.337892000
H	7.732082000	-3.356900000	0.705235000

H	7.859000000	-3.137383000	4.336743000
H	8.278528000	-4.785929000	1.622798000
H	-0.483870000	-5.269046000	-2.375445000
H	-1.379299000	6.894017000	-2.547773000
H	-1.755523000	-7.462822000	-3.110875000
H	-2.222235000	-6.440689000	-4.491986000
H	-3.082046000	-7.970566000	-4.185068000
H	-3.543796000	6.459921000	-1.415596000
H	-3.578937000	-7.632572000	-0.592974000
H	-3.891486000	4.380633000	-0.110301000
H	-4.379342000	-3.891483000	0.111533000
H	-4.851590000	5.153139000	4.245796000
H	-4.957189000	-8.171685000	-1.589305000
H	-4.972189000	-4.885935000	-4.410677000
H	-5.067937000	6.048156000	2.725626000
H	-5.117363000	-6.741631000	-0.539661000
H	-5.269701000	0.481783000	2.379964000
H	-5.863580000	-6.387771000	-4.047872000
H	-5.988863000	-4.984491000	-2.955975000
H	-6.282842000	2.355519000	4.619492000
H	-6.406448000	5.955595000	3.898876000
H	-6.459522000	-3.545470000	1.415665000
H	-6.894825000	-1.382146000	2.549510000
H	-6.915747000	4.921034000	0.483360000
H	-7.360302000	1.750629000	3.337892000
H	-7.732082000	3.356900000	0.705235000
H	-7.859000000	3.137383000	4.336743000
H	-8.278528000	4.785929000	1.622798000
N	0.538959000	-1.807151000	-0.168771000
N	1.807138000	0.538196000	0.173417000
N	-0.538959000	1.807151000	-0.168771000
N	-1.807138000	-0.538196000	0.173417000
Si	3.839133000	6.187991000	-2.608695000
Si	6.195794000	-3.832894000	2.610083000
Si	-3.839133000	-6.187991000	-2.608695000
Si	-6.195794000	3.832894000	2.610083000

74. Ni[A₄Bz₈]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.017026000
C	0.000000000	3.119639000	-0.992637000
C	0.000000000	4.296517000	-1.769179000
C	0.000000000	5.289295000	-2.484512000
C	0.000000000	6.474613000	-5.293231000
C	0.000000000	-3.119639000	-0.992637000
C	0.000000000	-4.296517000	-1.769179000
C	0.000000000	-5.289295000	-2.484512000
C	0.000000000	-6.474613000	-5.293231000
C	1.223611000	2.582894000	-0.551059000
C	1.223611000	-2.582894000	-0.551059000

C	1.553946000	7.790922000	-2.944920000
C	1.553946000	-7.790922000	-2.944920000
C	2.470466000	3.303287000	-0.382382000
C	2.470466000	-3.303287000	-0.382382000
C	2.585002000	1.223908000	0.580635000
C	2.585002000	-1.223908000	0.580635000
C	2.911315000	4.573920000	-0.780830000
C	2.911315000	-4.573920000	-0.780830000
C	3.124475000	0.000000000	1.018343000
C	3.304103000	2.471468000	0.409443000
C	3.304103000	-2.471468000	0.409443000
C	4.174154000	4.999481000	-0.382280000
C	4.174154000	-4.999481000	-0.382280000
C	4.311168000	0.000000000	1.779675000
C	4.573993000	2.915567000	0.806751000
C	4.573993000	-2.915567000	0.806751000
C	4.996771000	4.178890000	0.406759000
C	4.996771000	-4.178890000	0.406759000
C	5.317096000	0.000000000	2.476182000
C	6.580656000	0.000000000	5.231756000
C	7.835365000	1.555673000	2.866227000
C	7.835365000	-1.555673000	2.866227000
C	-1.223611000	2.582894000	-0.551059000
C	-1.223611000	-2.582894000	-0.551059000
C	-1.553946000	7.790922000	-2.944920000
C	-1.553946000	-7.790922000	-2.944920000
C	-2.470466000	3.303287000	-0.382382000
C	-2.470466000	-3.303287000	-0.382382000
C	-2.585002000	1.223908000	0.580635000
C	-2.585002000	-1.223908000	0.580635000
C	-2.911315000	4.573920000	-0.780830000
C	-2.911315000	-4.573920000	-0.780830000
C	-3.124475000	0.000000000	1.018343000
C	-3.304103000	2.471468000	0.409443000
C	-3.304103000	-2.471468000	0.409443000
C	-4.174154000	4.999481000	-0.382280000
C	-4.174154000	-4.999481000	-0.382280000
C	-4.311168000	0.000000000	1.779675000
C	-4.573993000	2.915567000	0.806751000
C	-4.573993000	-2.915567000	0.806751000
C	-4.996771000	4.178890000	0.406759000
C	-4.996771000	-4.178890000	0.406759000
C	-5.317096000	0.000000000	2.476182000
C	-6.580656000	0.000000000	5.231756000
C	-7.835365000	1.555673000	2.866227000
C	-7.835365000	-1.555673000	2.866227000
H	0.000000000	5.390990000	-5.472445000
H	0.000000000	-5.390990000	-5.472445000
H	0.889961000	6.899078000	-5.780146000
H	0.889961000	-6.899078000	-5.780146000
H	1.571601000	7.978878000	-1.862060000

H	1.571601000	-7.978878000	-1.862060000
H	1.607912000	8.758852000	-3.465938000
H	1.607912000	-8.758852000	-3.465938000
H	2.283511000	5.211718000	-1.392693000
H	2.283511000	-5.211718000	-1.392693000
H	2.452387000	7.213432000	-3.207379000
H	2.452387000	-7.213432000	-3.207379000
H	4.527885000	5.983079000	-0.688039000
H	4.527885000	-5.983079000	-0.688039000
H	5.213403000	2.289925000	1.418890000
H	5.213403000	-2.289925000	1.418890000
H	5.979834000	4.534771000	0.711769000
H	5.979834000	-4.534771000	0.711769000
H	6.005669000	0.889308000	5.526528000
H	6.005669000	-0.889308000	5.526528000
H	7.266338000	2.454387000	3.144974000
H	7.266338000	-2.454387000	3.144974000
H	7.528025000	0.000000000	5.792239000
H	7.992910000	1.574974000	1.778523000
H	7.992910000	-1.574974000	1.778523000
H	8.818022000	1.608547000	3.358708000
H	8.818022000	-1.608547000	3.358708000
H	-0.889961000	6.899078000	-5.780146000
H	-0.889961000	-6.899078000	-5.780146000
H	-1.571601000	7.978878000	-1.862060000
H	-1.571601000	-7.978878000	-1.862060000
H	-1.607912000	8.758852000	-3.465938000
H	-1.607912000	-8.758852000	-3.465938000
H	-2.283511000	5.211718000	-1.392693000
H	-2.283511000	-5.211718000	-1.392693000
H	-2.452387000	7.213432000	-3.207379000
H	-2.452387000	-7.213432000	-3.207379000
H	-4.527885000	5.983079000	-0.688039000
H	-4.527885000	-5.983079000	-0.688039000
H	-5.213403000	2.289925000	1.418890000
H	-5.213403000	-2.289925000	1.418890000
H	-5.979834000	4.534771000	0.711769000
H	-5.979834000	-4.534771000	0.711769000
H	-6.005669000	0.889308000	5.526528000
H	-6.005669000	-0.889308000	5.526528000
H	-7.266338000	2.454387000	3.144974000
H	-7.266338000	-2.454387000	3.144974000
H	-7.528025000	0.000000000	5.792239000
H	-7.992910000	1.574974000	1.778523000
H	-7.992910000	-1.574974000	1.778523000
H	-8.818022000	1.608547000	3.358708000
H	-8.818022000	-1.608547000	3.358708000
N	1.336497000	1.336112000	0.016411000
N	1.336497000	-1.336112000	0.016411000
N	-1.336497000	1.336112000	0.016411000
N	-1.336497000	-1.336112000	0.016411000

Si	0.000000000	6.849749000	-3.440821000
Si	0.000000000	-6.849749000	-3.440821000
Si	6.907491000	0.000000000	3.381206000
Si	-6.907491000	0.000000000	3.381206000

75. Pd[A₄Bz₈]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.008976000
C	0.133556000	-5.267519000	-1.686436000
C	0.320681000	2.948226000	-0.550531000
C	0.466513000	-4.064514000	-1.047207000
C	1.156841000	-6.122983000	-2.081397000
C	1.701328000	2.932423000	-0.281432000
C	1.824613000	-3.729288000	-0.818261000
C	1.827780000	-2.402105000	-0.227479000
C	2.400758000	1.826595000	0.246349000
C	2.443921000	4.109546000	-0.532679000
C	2.501708000	-5.792561000	-1.851681000
C	2.846960000	-4.599338000	-1.225386000
C	2.849101000	7.736413000	-2.181100000
C	2.934574000	-1.701134000	0.295932000
C	2.947727000	-0.321191000	0.570035000
C	3.094198000	5.117210000	-0.772065000
C	3.726227000	1.824675000	0.840416000
C	4.061886000	0.466862000	1.070321000
C	4.119372000	-2.436562000	0.532331000
C	4.416717000	7.504622000	0.488261000
C	4.591796000	2.848407000	1.253449000
C	5.138079000	-3.075412000	0.755174000
C	5.260863000	0.135383000	1.717893000
C	5.570218000	6.237664000	-2.083405000
C	5.781857000	2.504601000	1.886418000
C	6.112436000	1.159939000	2.118145000
C	6.288491000	-5.624640000	1.881262000
C	7.619043000	-4.203507000	-0.519497000
C	7.695184000	-2.879785000	2.283238000
C	-0.133556000	5.267519000	-1.686436000
C	-0.320681000	-2.948226000	-0.550531000
C	-0.466513000	4.064514000	-1.047207000
C	-1.156841000	6.122983000	-2.081397000
C	-1.701328000	-2.932423000	-0.281432000
C	-1.824613000	3.729288000	-0.818261000
C	-1.827780000	2.402105000	-0.227479000
C	-2.400758000	-1.826595000	0.246349000
C	-2.443921000	-4.109546000	-0.532679000
C	-2.501708000	5.792561000	-1.851681000
C	-2.846960000	4.599338000	-1.225386000
C	-2.849101000	-7.736413000	-2.181100000
C	-2.934574000	1.701134000	0.295932000
C	-2.947727000	0.321191000	0.570035000

C	-3.094198000	-5.117210000	-0.772065000
C	-3.726227000	-1.824675000	0.840416000
C	-4.061886000	-0.466862000	1.070321000
C	-4.119372000	2.436562000	0.532331000
C	-4.416717000	-7.504622000	0.488261000
C	-4.591796000	-2.848407000	1.253449000
C	-5.138079000	3.075412000	0.755174000
C	-5.260863000	-0.135383000	1.717893000
C	-5.570218000	-6.237664000	-2.083405000
C	-5.781857000	-2.504601000	1.886418000
C	-6.112436000	-1.159939000	2.118145000
C	-6.288491000	5.624640000	1.881262000
C	-7.619043000	4.203507000	-0.519497000
C	-7.695184000	2.879785000	2.283238000
H	0.899696000	5.520813000	-1.889014000
H	0.907990000	-7.054110000	-2.588653000
H	1.917164000	7.945932000	-1.636800000
H	2.589154000	7.230829000	-3.122295000
H	3.287636000	-6.471363000	-2.180118000
H	3.325796000	8.696556000	-2.429692000
H	3.503800000	7.726001000	1.058905000
H	3.888739000	-4.342594000	-1.069373000
H	4.333565000	3.890023000	1.097680000
H	4.954506000	8.448990000	0.313806000
H	5.055680000	6.857580000	1.106686000
H	5.336711000	5.723858000	-3.026584000
H	5.513022000	-0.897504000	1.924198000
H	5.664022000	-6.222696000	1.201989000
H	5.733437000	-5.493218000	2.820773000
H	6.144542000	7.147123000	-2.316915000
H	6.208414000	5.571336000	-1.485405000
H	6.457337000	3.291388000	2.219674000
H	7.021064000	-4.803208000	-1.220908000
H	7.040080000	0.912609000	2.632517000
H	7.141364000	-2.706799000	3.217164000
H	7.205650000	-6.193690000	2.096672000
H	7.830138000	-3.235410000	-0.995247000
H	7.908041000	-1.903126000	1.825360000
H	8.574520000	-4.723998000	-0.352943000
H	8.654288000	-3.355803000	2.537272000
H	-0.899696000	-5.520813000	-1.889014000
H	-0.907990000	7.054110000	-2.588653000
H	-1.917164000	-7.945932000	-1.636800000
H	-2.589154000	-7.230829000	-3.122295000
H	-3.287636000	6.471363000	-2.180118000
H	-3.325796000	-8.696556000	-2.429692000
H	-3.503800000	-7.726001000	1.058905000
H	-3.888739000	4.342594000	-1.069373000
H	-4.333565000	-3.890023000	1.097680000
H	-4.954506000	-8.448990000	0.313806000
H	-5.055680000	-6.857580000	1.106686000

H	-5.336711000	-5.723858000	-3.026584000
H	-5.513022000	0.897504000	1.924198000
H	-5.664022000	6.222696000	1.201989000
H	-5.733437000	5.493218000	2.820773000
H	-6.144542000	-7.147123000	-2.316915000
H	-6.208414000	-5.571336000	-1.485405000
H	-6.457337000	-3.291388000	2.219674000
H	-7.021064000	4.803208000	-1.220908000
H	-7.040080000	-0.912609000	2.632517000
H	-7.141364000	2.706799000	3.217164000
H	-7.205650000	6.193690000	2.096672000
H	-7.830138000	3.235410000	-0.995247000
H	-7.908041000	1.903126000	1.825360000
H	-8.574520000	4.723998000	-0.352943000
H	-8.654288000	3.355803000	2.537272000
N	0.536131000	-1.940259000	-0.159747000
N	1.939409000	0.535119000	0.179132000
N	-0.536131000	1.940259000	-0.159747000
N	-1.939409000	-0.535119000	0.179132000
Si	3.999274000	6.664359000	-1.143250000
Si	6.700616000	-3.962675000	1.105208000
Si	-3.999274000	-6.664359000	-1.143250000
Si	-6.700616000	3.962675000	1.105208000

76. Pd[A₄Bz₈]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.017306000
C	0.000000000	3.301717000	-0.702332000
C	0.000000000	4.557088000	-1.350903000
C	0.000000000	5.611415000	-1.971073000
C	0.000000000	7.036455000	-4.664887000
C	0.000000000	-3.301717000	-0.702332000
C	0.000000000	-4.557088000	-1.350903000
C	0.000000000	-5.611415000	-1.971073000
C	0.000000000	-7.036455000	-4.664887000
C	1.248991000	2.733721000	-0.375659000
C	1.248991000	-2.733721000	-0.375659000
C	1.554598000	8.142147000	-2.210020000
C	1.554598000	-8.142147000	-2.210020000
C	2.513949000	3.441683000	-0.256324000
C	2.513949000	-3.441683000	-0.256324000
C	2.735569000	1.249253000	0.405838000
C	2.735569000	-1.249253000	0.405838000
C	2.906837000	4.764499000	-0.513166000
C	2.906837000	-4.764499000	-0.513166000
C	3.305599000	0.000000000	0.728691000
C	3.442307000	2.515034000	0.283815000
C	3.442307000	-2.515034000	0.283815000
C	4.217573000	5.143525000	-0.246163000
C	4.217573000	-5.143525000	-0.246163000

C	4.568740000	0.000000000	1.361738000
C	4.764475000	2.911138000	0.539288000
C	4.764475000	-2.911138000	0.539288000
C	5.140839000	4.222243000	0.270302000
C	5.140839000	-4.222243000	0.270302000
C	5.634056000	0.000000000	1.962606000
C	7.131228000	0.000000000	4.598039000
C	8.174865000	1.556414000	2.131773000
C	8.174865000	-1.556414000	2.131773000
C	-1.248991000	2.733721000	-0.375659000
C	-1.248991000	-2.733721000	-0.375659000
C	-1.554598000	8.142147000	-2.210020000
C	-1.554598000	-8.142147000	-2.210020000
C	-2.513949000	3.441683000	-0.256324000
C	-2.513949000	-3.441683000	-0.256324000
C	-2.735569000	1.249253000	0.405838000
C	-2.735569000	-1.249253000	0.405838000
C	-2.906837000	4.764499000	-0.513166000
C	-2.906837000	-4.764499000	-0.513166000
C	-3.305599000	0.000000000	0.728691000
C	-3.442307000	2.515034000	0.283815000
C	-3.442307000	-2.515034000	0.283815000
C	-4.217573000	5.143525000	-0.246163000
C	-4.217573000	-5.143525000	-0.246163000
C	-4.568740000	0.000000000	1.361738000
C	-4.764475000	2.911138000	0.539288000
C	-4.764475000	-2.911138000	0.539288000
C	-5.140839000	4.222243000	0.270302000
C	-5.140839000	-4.222243000	0.270302000
C	-5.634056000	0.000000000	1.962606000
C	-7.131228000	0.000000000	4.598039000
C	-8.174865000	1.556414000	2.131773000
C	-8.174865000	-1.556414000	2.131773000
H	0.000000000	5.972228000	-4.936587000
H	0.000000000	-5.972228000	-4.936587000
H	0.890077000	7.501254000	-5.113197000
H	0.890077000	-7.501254000	-5.113197000
H	1.569929000	8.240073000	-1.115261000
H	1.569929000	-8.240073000	-1.115261000
H	1.612925000	9.149748000	-2.648792000
H	1.612925000	-9.149748000	-2.648792000
H	2.204662000	5.482402000	-0.918132000
H	2.204662000	-5.482402000	-0.918132000
H	2.451979000	7.585395000	-2.516941000
H	2.451979000	-7.585395000	-2.516941000
H	4.528050000	6.168362000	-0.444769000
H	4.528050000	-6.168362000	-0.444769000
H	5.483937000	2.211198000	0.944869000
H	5.483937000	-2.211198000	0.944869000
H	6.165316000	4.534679000	0.467820000
H	6.165316000	-4.534679000	0.467820000

H	6.583506000	0.889314000	4.940820000
H	6.583506000	-0.889314000	4.940820000
H	7.627707000	2.453990000	2.454385000
H	7.627707000	-2.453990000	2.454385000
H	8.123327000	0.000000000	5.074895000
H	8.242433000	1.573613000	1.034722000
H	8.242433000	-1.573613000	1.034722000
H	9.194616000	1.613645000	2.541267000
H	9.194616000	-1.613645000	2.541267000
H	-0.890077000	7.501254000	-5.113197000
H	-0.890077000	-7.501254000	-5.113197000
H	-1.569929000	8.240073000	-1.115261000
H	-1.569929000	-8.240073000	-1.115261000
H	-1.612925000	9.149748000	-2.648792000
H	-1.612925000	-9.149748000	-2.648792000
H	-2.204662000	5.482402000	-0.918132000
H	-2.204662000	-5.482402000	-0.918132000
H	-2.451979000	7.585395000	-2.516941000
H	-2.451979000	-7.585395000	-2.516941000
H	-4.528050000	6.168362000	-0.444769000
H	-4.528050000	-6.168362000	-0.444769000
H	-5.483937000	2.211198000	0.944869000
H	-5.483937000	-2.211198000	0.944869000
H	-6.165316000	4.534679000	0.467820000
H	-6.165316000	-4.534679000	0.467820000
H	-6.583506000	0.889314000	4.940820000
H	-6.583506000	-0.889314000	4.940820000
H	-7.627707000	2.453990000	2.454385000
H	-7.627707000	-2.453990000	2.454385000
H	-8.123327000	0.000000000	5.074895000
H	-8.242433000	1.573613000	1.034722000
H	-8.242433000	-1.573613000	1.034722000
H	-9.194616000	1.613645000	2.541267000
H	-9.194616000	-1.613645000	2.541267000
N	1.429470000	1.428906000	0.016777000
N	1.429470000	-1.428906000	0.016777000
N	-1.429470000	1.428906000	0.016777000
N	-1.429470000	-1.428906000	0.016777000
Si	0.000000000	7.249296000	-2.787366000
Si	0.000000000	-7.249296000	-2.787366000
Si	7.296776000	0.000000000	2.726527000
Si	-7.296776000	0.000000000	2.726527000

77. Pt[A₄Bz₈]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.005780000
C	0.134074000	-5.285573000	-1.651934000
C	0.322610000	2.954295000	-0.548032000
C	0.465701000	-4.075445000	-1.025331000
C	1.156805000	-6.148973000	-2.029938000

C	1.704828000	2.933604000	-0.289090000
C	1.822732000	-3.740832000	-0.792754000
C	1.828304000	-2.408579000	-0.219075000
C	2.407475000	1.827391000	0.232430000
C	2.447249000	4.111126000	-0.543251000
C	2.500934000	-5.819178000	-1.796115000
C	2.840892000	7.740381000	-2.188552000
C	2.844847000	-4.618986000	-1.183074000
C	2.935289000	-1.704443000	0.298599000
C	2.953356000	-0.322954000	0.562293000
C	3.095539000	5.119626000	-0.783970000
C	3.737865000	1.822699000	0.810191000
C	4.072223000	0.465859000	1.044170000
C	4.120021000	-2.440226000	0.538745000
C	4.408878000	7.510379000	0.479897000
C	4.611944000	2.845791000	1.206926000
C	5.138689000	-3.078151000	0.763894000
C	5.277658000	0.135187000	1.680257000
C	5.567936000	6.250448000	-2.092667000
C	5.808253000	2.502820000	1.828065000
C	6.137257000	1.158833000	2.064498000
C	6.291458000	-5.624434000	1.892469000
C	7.623126000	-4.202695000	-0.507687000
C	7.694770000	-2.876889000	2.293247000
C	-0.134074000	5.285573000	-1.651934000
C	-0.322610000	-2.954295000	-0.548032000
C	-0.465701000	4.075445000	-1.025331000
C	-1.156805000	6.148973000	-2.029938000
C	-1.704828000	-2.933604000	-0.289090000
C	-1.822732000	3.740832000	-0.792754000
C	-1.828304000	2.408579000	-0.219075000
C	-2.407475000	-1.827391000	0.232430000
C	-2.447249000	-4.111126000	-0.543251000
C	-2.500934000	5.819178000	-1.796115000
C	-2.840892000	-7.740381000	-2.188552000
C	-2.844847000	4.618986000	-1.183074000
C	-2.935289000	1.704443000	0.298599000
C	-2.953356000	0.322954000	0.562293000
C	-3.095539000	-5.119626000	-0.783970000
C	-3.737865000	-1.822699000	0.810191000
C	-4.072223000	-0.465859000	1.044170000
C	-4.120021000	2.440226000	0.538745000
C	-4.408878000	-7.510379000	0.479897000
C	-4.611944000	-2.845791000	1.206926000
C	-5.138689000	3.078151000	0.763894000
C	-5.277658000	-0.135187000	1.680257000
C	-5.567936000	-6.250448000	-2.092667000
C	-5.808253000	-2.502820000	1.828065000
C	-6.137257000	-1.158833000	2.064498000
C	-6.291458000	5.624434000	1.892469000
C	-7.623126000	4.202695000	-0.507687000

C	-7.694770000	2.876889000	2.293247000
H	0.898245000	5.537792000	-1.858834000
H	0.908085000	-7.085315000	-2.527571000
H	1.909609000	7.947894000	-1.642311000
H	2.580109000	7.234646000	-3.129424000
H	3.287438000	-6.503594000	-2.111114000
H	3.315016000	8.701696000	-2.437469000
H	3.494870000	7.728068000	1.050205000
H	3.886078000	-4.362609000	-1.024668000
H	4.354817000	3.886972000	1.048504000
H	4.943514000	8.456767000	0.306662000
H	5.049564000	6.864902000	1.098167000
H	5.336925000	5.738160000	-3.037251000
H	5.528053000	-0.896871000	1.891208000
H	5.668814000	-6.223669000	1.212541000
H	5.734671000	-5.493063000	2.830934000
H	6.140069000	7.161991000	-2.323355000
H	6.207331000	5.584508000	-1.495468000
H	6.489432000	3.289865000	2.148701000
H	7.026525000	-4.802278000	-1.210334000
H	7.069491000	0.911319000	2.570404000
H	7.139506000	-2.701679000	3.225862000
H	7.208948000	-6.192235000	2.109665000
H	7.834541000	-3.234305000	-0.982704000
H	7.908470000	-1.901329000	1.833397000
H	8.578621000	-4.722752000	-0.339826000
H	8.653670000	-3.352049000	2.549653000
H	-0.898245000	-5.537792000	-1.858834000
H	-0.908085000	7.085315000	-2.527571000
H	-1.909609000	-7.947894000	-1.642311000
H	-2.580109000	-7.234646000	-3.129424000
H	-3.287438000	6.503594000	-2.111114000
H	-3.315016000	-8.701696000	-2.437469000
H	-3.494870000	-7.728068000	1.050205000
H	-3.886078000	4.362609000	-1.024668000
H	-4.354817000	-3.886972000	1.048504000
H	-4.943514000	-8.456767000	0.306662000
H	-5.049564000	-6.864902000	1.098167000
H	-5.336925000	-5.738160000	-3.037251000
H	-5.528053000	0.896871000	1.891208000
H	-5.668814000	6.223669000	1.212541000
H	-5.734671000	5.493063000	2.830934000
H	-6.140069000	-7.161991000	-2.323355000
H	-6.207331000	-5.584508000	-1.495468000
H	-6.489432000	-3.289865000	2.148701000
H	-7.026525000	4.802278000	-1.210334000
H	-7.069491000	-0.911319000	2.570404000
H	-7.139506000	2.701679000	3.225862000
H	-7.208948000	6.192235000	2.109665000
H	-7.834541000	3.234305000	-0.982704000
H	-7.908470000	1.901329000	1.833397000

H	-8.578621000	4.722752000	-0.339826000
H	-8.653670000	3.352049000	2.549653000
N	0.535513000	-1.938807000	-0.168382000
N	1.938053000	0.534836000	0.181682000
N	-0.535513000	1.938807000	-0.168382000
N	-1.938053000	-0.534836000	0.181682000
Si	3.995166000	6.670683000	-1.152774000
Si	6.702534000	-3.962583000	1.115821000
Si	-3.995166000	-6.670683000	-1.152774000
Si	-6.702534000	3.962583000	1.115821000

78. Pt[A₄Bz₈]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.015130000
C	0.000000000	3.305804000	-0.699144000
C	0.000000000	4.562152000	-1.346691000
C	0.000000000	5.616715000	-1.966430000
C	0.000000000	7.045170000	-4.658627000
C	0.000000000	-3.305804000	-0.699144000
C	0.000000000	-4.562152000	-1.346691000
C	0.000000000	-5.616715000	-1.966430000
C	0.000000000	-7.045170000	-4.658627000
C	1.248971000	2.737635000	-0.373747000
C	1.248971000	-2.737635000	-0.373747000
C	1.554738000	8.147203000	-2.201999000
C	1.554738000	-8.147203000	-2.201999000
C	2.512925000	3.442241000	-0.254311000
C	2.512925000	-3.442241000	-0.254311000
C	2.739018000	1.249261000	0.400533000
C	2.739018000	-1.249261000	0.400533000
C	2.905126000	4.765975000	-0.507211000
C	2.905126000	-4.765975000	-0.507211000
C	3.308858000	0.000000000	0.722501000
C	3.442673000	2.513852000	0.278807000
C	3.442673000	-2.513852000	0.278807000
C	4.216771000	5.144017000	-0.244010000
C	4.216771000	-5.144017000	-0.244010000
C	4.572035000	0.000000000	1.356333000
C	4.765906000	2.908704000	0.530423000
C	4.765906000	-2.908704000	0.530423000
C	5.141899000	4.220501000	0.265050000
C	5.141899000	-4.220501000	0.265050000
C	5.636423000	0.000000000	1.958858000
C	7.128107000	0.000000000	4.596956000
C	8.176484000	1.556731000	2.132999000
C	8.176484000	-1.556731000	2.132999000
C	-1.248971000	2.737635000	-0.373747000
C	-1.248971000	-2.737635000	-0.373747000
C	-1.554738000	8.147203000	-2.201999000
C	-1.554738000	-8.147203000	-2.201999000

C	-2.512925000	3.442241000	-0.254311000
C	-2.512925000	-3.442241000	-0.254311000
C	-2.739018000	1.249261000	0.400533000
C	-2.739018000	-1.249261000	0.400533000
C	-2.905126000	4.765975000	-0.507211000
C	-2.905126000	-4.765975000	-0.507211000
C	-3.308858000	0.000000000	0.722501000
C	-3.442673000	2.513852000	0.278807000
C	-3.442673000	-2.513852000	0.278807000
C	-4.216771000	5.144017000	-0.244010000
C	-4.216771000	-5.144017000	-0.244010000
C	-4.572035000	0.000000000	1.356333000
C	-4.765906000	2.908704000	0.530423000
C	-4.765906000	-2.908704000	0.530423000
C	-5.141899000	4.220501000	0.265050000
C	-5.141899000	-4.220501000	0.265050000
C	-5.636423000	0.000000000	1.958858000
C	-7.128107000	0.000000000	4.596956000
C	-8.176484000	1.556731000	2.132999000
C	-8.176484000	-1.556731000	2.132999000
H	0.000000000	5.981272000	-4.931643000
H	0.000000000	-5.981272000	-4.931643000
H	0.890088000	7.510524000	-5.106307000
H	0.890088000	-7.510524000	-5.106307000
H	1.569817000	8.243399000	-1.107085000
H	1.569817000	-8.243399000	-1.107085000
H	1.613593000	9.155438000	-2.639178000
H	1.613593000	-9.155438000	-2.639178000
H	2.201298000	5.485224000	-0.906657000
H	2.201298000	-5.485224000	-0.906657000
H	2.451932000	7.590488000	-2.509526000
H	2.451932000	-7.590488000	-2.509526000
H	4.526351000	6.169598000	-0.439896000
H	4.526351000	-6.169598000	-0.439896000
H	5.486512000	2.206756000	0.930287000
H	5.486512000	-2.206756000	0.930287000
H	6.167334000	4.531539000	0.459518000
H	6.167334000	-4.531539000	0.459518000
H	6.579629000	0.889316000	4.938466000
H	6.579629000	-0.889316000	4.938466000
H	7.627955000	2.453828000	2.454555000
H	7.627955000	-2.453828000	2.454555000
H	8.119120000	0.000000000	5.076053000
H	8.246639000	1.574119000	1.036146000
H	8.246639000	-1.574119000	1.036146000
H	9.195235000	1.614543000	2.544841000
H	9.195235000	-1.614543000	2.544841000
H	-0.890088000	7.510524000	-5.106307000
H	-0.890088000	-7.510524000	-5.106307000
H	-1.569817000	8.243399000	-1.107085000
H	-1.569817000	-8.243399000	-1.107085000

H	-1.613593000	9.155438000	-2.639178000
H	-1.613593000	-9.155438000	-2.639178000
H	-2.201298000	5.485224000	-0.906657000
H	-2.201298000	-5.485224000	-0.906657000
H	-2.451932000	7.590488000	-2.509526000
H	-2.451932000	-7.590488000	-2.509526000
H	-4.526351000	6.169598000	-0.439896000
H	-4.526351000	-6.169598000	-0.439896000
H	-5.486512000	2.206756000	0.930287000
H	-5.486512000	-2.206756000	0.930287000
H	-6.167334000	4.531539000	0.459518000
H	-6.167334000	-4.531539000	0.459518000
H	-6.579629000	0.889316000	4.938466000
H	-6.579629000	-0.889316000	4.938466000
H	-7.627955000	2.453828000	2.454555000
H	-7.627955000	-2.453828000	2.454555000
H	-8.119120000	0.000000000	5.076053000
H	-8.246639000	1.574119000	1.036146000
H	-8.246639000	-1.574119000	1.036146000
H	-9.195235000	1.614543000	2.544841000
H	-9.195235000	-1.614543000	2.544841000
N	1.429147000	1.428786000	0.014696000
N	1.429147000	-1.428786000	0.014696000
N	-1.429147000	1.428786000	0.014696000
N	-1.429147000	-1.428786000	0.014696000
Si	0.000000000	7.255599000	-2.780842000
Si	0.000000000	-7.255599000	-2.780842000
Si	7.297733000	0.000000000	2.725838000
Si	-7.297733000	0.000000000	2.725838000

79. Zn[A₄Bz₈]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.010375000
C	0.025556000	-5.346251000	-1.550884000
C	0.349518000	2.982804000	-0.469585000
C	0.399846000	-4.118722000	-0.983906000
C	1.017037000	-6.209347000	-2.003695000
C	1.720172000	2.945823000	-0.118907000
C	1.771618000	-3.768196000	-0.883762000
C	1.810000000	-2.424531000	-0.329081000
C	2.374116000	-5.863089000	-1.903590000
C	2.422025000	1.808789000	0.353292000
C	2.456469000	4.147195000	-0.246489000
C	2.761150000	-4.647794000	-1.349469000
C	2.860070000	7.896704000	-1.597201000
C	2.947101000	-1.719874000	0.138176000
C	2.980361000	-0.350470000	0.494958000
C	3.095373000	5.182444000	-0.375661000
C	3.763649000	1.770633000	0.912516000
C	4.113730000	0.398996000	1.014483000

C	4.156550000	-2.445954000	0.247391000
C	4.327281000	7.492023000	1.108309000
C	4.639294000	2.760419000	1.385054000
C	5.203086000	-3.070225000	0.355596000
C	5.336171000	0.024436000	1.592260000
C	5.598690000	6.433033000	-1.500411000
C	5.850429000	2.373343000	1.948111000
C	6.195609000	1.016082000	2.051606000
C	6.480450000	-5.636035000	1.285647000
C	7.603358000	-4.096225000	-1.146647000
C	7.866165000	-2.882340000	1.693854000
C	-0.025556000	5.346251000	-1.550884000
C	-0.349518000	-2.982804000	-0.469585000
C	-0.399846000	4.118722000	-0.983906000
C	-1.017037000	6.209347000	-2.003695000
C	-1.720172000	-2.945823000	-0.118907000
C	-1.771618000	3.768196000	-0.883762000
C	-1.810000000	2.424531000	-0.329081000
C	-2.374116000	5.863089000	-1.903590000
C	-2.422025000	-1.808789000	0.353292000
C	-2.456469000	-4.147195000	-0.246489000
C	-2.761150000	4.647794000	-1.349469000
C	-2.860070000	-7.896704000	-1.597201000
C	-2.947101000	1.719874000	0.138176000
C	-2.980361000	0.350470000	0.494958000
C	-3.095373000	-5.182444000	-0.375661000
C	-3.763649000	-1.770633000	0.912516000
C	-4.113730000	-0.398996000	1.014483000
C	-4.156550000	2.445954000	0.247391000
C	-4.327281000	-7.492023000	1.108309000
C	-4.639294000	-2.760419000	1.385054000
C	-5.203086000	3.070225000	0.355596000
C	-5.336171000	-0.024436000	1.592260000
C	-5.598690000	-6.433033000	-1.500411000
C	-5.850429000	-2.373343000	1.948111000
C	-6.195609000	-1.016082000	2.051606000
C	-6.480450000	5.636035000	1.285647000
C	-7.603358000	4.096225000	-1.146647000
C	-7.866165000	2.882340000	1.693854000
H	0.732922000	-7.159252000	-2.454591000
H	1.018900000	5.612765000	-1.653473000
H	1.898455000	8.042136000	-1.084606000
H	2.657187000	7.465432000	-2.588161000
H	3.134534000	-6.547662000	-2.277225000
H	3.325457000	8.883104000	-1.743426000
H	3.390335000	7.659323000	1.657994000
H	3.809958000	-4.379482000	-1.294711000
H	4.370479000	3.809231000	1.329854000
H	4.856020000	8.453610000	1.022762000
H	4.952862000	6.810532000	1.702981000
H	5.409543000	5.988794000	-2.487827000

H	5.600604000	-1.020218000	1.699525000
H	5.815754000	-6.219364000	0.632189000
H	5.996675000	-5.552471000	2.269032000
H	6.166768000	7.365013000	-1.642456000
H	6.224328000	5.731739000	-0.929723000
H	6.531900000	3.133619000	2.327603000
H	6.964275000	-4.678328000	-1.826330000
H	7.141172000	0.732287000	2.511789000
H	7.388710000	-2.769287000	2.677831000
H	7.420721000	-6.194949000	1.407682000
H	7.764514000	-3.106663000	-1.597110000
H	8.015768000	-1.879450000	1.268843000
H	8.576104000	-4.605833000	-1.071329000
H	8.854360000	-3.342632000	1.844209000
H	-0.732922000	7.159252000	-2.454591000
H	-1.018900000	-5.612765000	-1.653473000
H	-1.898455000	-8.042136000	-1.084606000
H	-2.657187000	-7.465432000	-2.588161000
H	-3.134534000	6.547662000	-2.277225000
H	-3.325457000	-8.883104000	-1.743426000
H	-3.390335000	-7.659323000	1.657994000
H	-3.809958000	4.379482000	-1.294711000
H	-4.370479000	-3.809231000	1.329854000
H	-4.856020000	-8.453610000	1.022762000
H	-4.952862000	-6.810532000	1.702981000
H	-5.409543000	-5.988794000	-2.487827000
H	-5.600604000	1.020218000	1.699525000
H	-5.815754000	6.219364000	0.632189000
H	-5.996675000	5.552471000	2.269032000
H	-6.166768000	-7.365013000	-1.642456000
H	-6.224328000	-5.731739000	-0.929723000
H	-6.531900000	-3.133619000	2.327603000
H	-6.964275000	4.678328000	-1.826330000
H	-7.141172000	-0.732287000	2.511789000
H	-7.388710000	2.769287000	2.677831000
H	-7.420721000	6.194949000	1.407682000
H	-7.764514000	3.106663000	-1.597110000
H	-8.015768000	1.879450000	1.268843000
H	-8.576104000	4.605833000	-1.071329000
H	-8.854360000	3.342632000	1.844209000
N	0.525853000	-1.961654000	-0.184861000
N	1.959360000	0.524725000	0.208785000
N	-0.525853000	1.961654000	-0.184861000
N	-1.959360000	-0.524725000	0.208785000
Si	3.985379000	6.766202000	-0.594123000
Si	6.803437000	-3.936343000	0.549102000
Si	-3.985379000	-6.766202000	-0.594123000
Si	-6.803437000	3.936343000	0.549102000

80. Zn[A₄Bz₈]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.014209000
C	0.000000000	3.362061000	-0.563928000
C	0.000000000	4.651776000	-1.144363000
C	0.000000000	5.735107000	-1.712931000
C	0.000000000	7.278609000	-4.340752000
C	0.000000000	-3.362061000	-0.563928000
C	0.000000000	-4.651776000	-1.144363000
C	0.000000000	-5.735107000	-1.712931000
C	0.000000000	-7.278609000	-4.340752000
C	1.261387000	2.781062000	-0.289831000
C	1.261387000	-2.781062000	-0.289831000
C	1.554750000	8.274734000	-1.840433000
C	1.554750000	-8.274734000	-1.840433000
C	2.529183000	3.489570000	-0.192645000
C	2.529183000	-3.489570000	-0.192645000
C	2.782471000	1.261648000	0.317273000
C	2.782471000	-1.261648000	0.317273000
C	2.907237000	4.830343000	-0.373735000
C	2.907237000	-4.830343000	-0.373735000
C	3.365061000	0.000000000	0.587454000
C	3.489380000	2.530790000	0.220445000
C	3.489380000	-2.530790000	0.220445000
C	4.232735000	5.194460000	-0.171437000
C	4.232735000	-5.194460000	-0.171437000
C	4.661116000	0.000000000	1.153227000
C	4.828816000	2.912612000	0.403855000
C	4.828816000	-2.912612000	0.403855000
C	5.189746000	4.239212000	0.203112000
C	5.189746000	-4.239212000	0.203112000
C	5.753741000	0.000000000	1.703477000
C	7.363062000	0.000000000	4.271585000
C	8.300616000	1.556620000	1.764355000
C	8.300616000	-1.556620000	1.764355000
C	-1.261387000	2.781062000	-0.289831000
C	-1.261387000	-2.781062000	-0.289831000
C	-1.554750000	8.274734000	-1.840433000
C	-1.554750000	-8.274734000	-1.840433000
C	-2.529183000	3.489570000	-0.192645000
C	-2.529183000	-3.489570000	-0.192645000
C	-2.782471000	1.261648000	0.317273000
C	-2.782471000	-1.261648000	0.317273000
C	-2.907237000	4.830343000	-0.373735000
C	-2.907237000	-4.830343000	-0.373735000
C	-3.365061000	0.000000000	0.587454000
C	-3.489380000	2.530790000	0.220445000
C	-3.489380000	-2.530790000	0.220445000
C	-4.232735000	5.194460000	-0.171437000
C	-4.232735000	-5.194460000	-0.171437000
C	-4.661116000	0.000000000	1.153227000

C	-4.828816000	2.912612000	0.403855000
C	-4.828816000	-2.912612000	0.403855000
C	-5.189746000	4.239212000	0.203112000
C	-5.189746000	-4.239212000	0.203112000
C	-5.753741000	0.000000000	1.703477000
C	-7.363062000	0.000000000	4.271585000
C	-8.300616000	1.556620000	1.764355000
C	-8.300616000	-1.556620000	1.764355000
H	0.000000000	6.227585000	-4.659659000
H	0.000000000	-6.227585000	-4.659659000
H	0.890108000	7.762998000	-4.767776000
H	0.890108000	-7.762998000	-4.767776000
H	1.570372000	8.326877000	-0.742519000
H	1.570372000	-8.326877000	-0.742519000
H	1.613612000	9.299815000	-2.236565000
H	1.613612000	-9.299815000	-2.236565000
H	2.180035000	5.575243000	-0.670179000
H	2.180035000	-5.575243000	-0.670179000
H	2.451768000	7.730708000	-2.170408000
H	2.451768000	-7.730708000	-2.170408000
H	4.528681000	6.233367000	-0.310577000
H	4.528681000	-6.233367000	-0.310577000
H	5.575127000	2.187472000	0.701088000
H	5.575127000	-2.187472000	0.701088000
H	6.227765000	4.537541000	0.344046000
H	6.227765000	-4.537541000	0.344046000
H	6.830575000	0.889334000	4.637520000
H	6.830575000	-0.889334000	4.637520000
H	7.767730000	2.453957000	2.110694000
H	7.767730000	-2.453957000	2.110694000
H	8.322303000	1.575338000	0.665465000
H	8.322303000	-1.575338000	0.665465000
H	8.374823000	0.000000000	4.705195000
H	9.336682000	1.613028000	2.130741000
H	9.336682000	-1.613028000	2.130741000
H	-0.890108000	7.762998000	-4.767776000
H	-0.890108000	-7.762998000	-4.767776000
H	-1.570372000	8.326877000	-0.742519000
H	-1.570372000	-8.326877000	-0.742519000
H	-1.613612000	9.299815000	-2.236565000
H	-1.613612000	-9.299815000	-2.236565000
H	-2.180035000	5.575243000	-0.670179000
H	-2.180035000	-5.575243000	-0.670179000
H	-2.451768000	7.730708000	-2.170408000
H	-2.451768000	-7.730708000	-2.170408000
H	-4.528681000	6.233367000	-0.310577000
H	-4.528681000	-6.233367000	-0.310577000
H	-5.575127000	2.187472000	0.701088000
H	-5.575127000	-2.187472000	0.701088000
H	-6.227765000	4.537541000	0.344046000
H	-6.227765000	-4.537541000	0.344046000

H	-6.830575000	0.889334000	4.637520000
H	-6.830575000	-0.889334000	4.637520000
H	-7.767730000	2.453957000	2.110694000
H	-7.767730000	-2.453957000	2.110694000
H	-8.322303000	1.575338000	0.665465000
H	-8.322303000	-1.575338000	0.665465000
H	-8.374823000	0.000000000	4.705195000
H	-9.336682000	1.613028000	2.130741000
H	-9.336682000	-1.613028000	2.130741000
N	1.456296000	1.455556000	0.014448000
N	1.456296000	-1.455556000	0.014448000
N	-1.456296000	1.455556000	0.014448000
N	-1.456296000	-1.455556000	0.014448000
Si	0.000000000	7.407014000	-2.455381000
Si	0.000000000	-7.407014000	-2.455381000
Si	7.447334000	0.000000000	2.394530000
Si	-7.447334000	0.000000000	2.394530000

81. Cu(TPP]; S = ½ (saddled)

Cu	0.000000000	0.000000000	0.000000000
C	0.000000000	3.447753000	0.000000000
C	0.000000000	4.937665000	0.000000000
C	0.000000000	7.751261000	0.000000000
C	0.000000000	-3.447753000	0.000000000
C	0.000000000	-4.937665000	0.000000000
C	0.000000000	-7.751261000	0.000000000
C	0.601259000	7.048517000	-1.047379000
C	0.601259000	-7.048517000	1.047379000
C	0.601431000	5.652989000	-1.046089000
C	0.601431000	-5.652989000	1.046089000
C	1.229221000	2.786903000	0.074506000
C	1.229221000	-2.786903000	-0.074506000
C	2.494387000	3.456791000	0.243538000
C	2.494387000	-3.456791000	-0.243538000
C	2.786903000	1.229221000	0.074506000
C	2.786903000	-1.229221000	-0.074506000
C	3.447753000	0.000000000	0.000000000
C	3.456791000	2.494387000	0.243538000
C	3.456791000	-2.494387000	-0.243538000
C	4.937665000	0.000000000	0.000000000
C	5.652989000	0.601431000	-1.046089000
C	5.652989000	-0.601431000	1.046089000
C	7.048517000	0.601259000	-1.047379000
C	7.048517000	-0.601259000	1.047379000
C	7.751261000	0.000000000	0.000000000
C	-0.601259000	7.048517000	1.047379000
C	-0.601259000	-7.048517000	-1.047379000
C	-0.601431000	5.652989000	1.046089000
C	-0.601431000	-5.652989000	-1.046089000

C	-1.229221000	2.786903000	-0.074506000
C	-1.229221000	-2.786903000	0.074506000
C	-2.494387000	3.456791000	-0.243538000
C	-2.494387000	-3.456791000	0.243538000
C	-2.786903000	1.229221000	-0.074506000
C	-2.786903000	-1.229221000	0.074506000
C	-3.447753000	0.000000000	0.000000000
C	-3.456791000	2.494387000	-0.243538000
C	-3.456791000	-2.494387000	0.243538000
C	-4.937665000	0.000000000	0.000000000
C	-5.652989000	0.601431000	1.046089000
C	-5.652989000	-0.601431000	-1.046089000
C	-7.048517000	0.601259000	1.047379000
C	-7.048517000	-0.601259000	-1.047379000
C	-7.751261000	0.000000000	0.000000000
H	0.000000000	8.840782000	0.000000000
H	0.000000000	-8.840782000	0.000000000
H	1.066162000	5.101418000	-1.862591000
H	1.066162000	-5.101418000	1.862591000
H	1.067658000	7.587542000	-1.871084000
H	1.067658000	-7.587542000	1.871084000
H	2.620758000	4.525197000	0.367767000
H	2.620758000	-4.525197000	-0.367767000
H	4.525197000	2.620758000	0.367767000
H	4.525197000	-2.620758000	-0.367767000
H	5.101418000	1.066162000	-1.862591000
H	5.101418000	-1.066162000	1.862591000
H	7.587542000	1.067658000	-1.871084000
H	7.587542000	-1.067658000	1.871084000
H	8.840782000	0.000000000	0.000000000
H	-1.066162000	5.101418000	1.862591000
H	-1.066162000	-5.101418000	-1.862591000
H	-1.067658000	7.587542000	1.871084000
H	-1.067658000	-7.587542000	-1.871084000
H	-2.620758000	4.525197000	-0.367767000
H	-2.620758000	-4.525197000	0.367767000
H	-4.525197000	2.620758000	-0.367767000
H	-4.525197000	-2.620758000	0.367767000
H	-5.101418000	1.066162000	1.862591000
H	-5.101418000	-1.066162000	-1.862591000
H	-7.587542000	1.067658000	1.871084000
H	-7.587542000	-1.067658000	-1.871084000
H	-8.840782000	0.000000000	0.000000000
N	1.422824000	1.422824000	-0.003837000
N	1.422824000	-1.422824000	0.003837000
N	-1.422824000	1.422824000	0.003837000
N	-1.422824000	-1.422824000	-0.003837000

82. Cu(TPP]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
C	0.680799000	4.220153000	-0.007468000
C	0.680799000	-4.220153000	0.007468000
C	1.100110000	2.840178000	-0.010735000
C	1.100110000	-2.840178000	0.010735000
C	2.433903000	2.433903000	-0.018773000
C	2.433903000	-2.433903000	0.018773000
C	2.840178000	1.100110000	-0.010735000
C	2.840178000	-1.100110000	0.010735000
C	3.490858000	3.490858000	-0.032401000
C	3.490858000	-3.490858000	0.032401000
C	3.984818000	3.984818000	-1.245871000
C	3.984818000	-3.984818000	1.245871000
C	4.000697000	4.000697000	1.167821000
C	4.000697000	-4.000697000	-1.167821000
C	4.220153000	0.680799000	-0.007468000
C	4.220153000	-0.680799000	0.007468000
C	4.972426000	4.972426000	-1.260063000
C	4.972426000	-4.972426000	1.260063000
C	4.988298000	4.988298000	1.156032000
C	4.988298000	-4.988298000	-1.156032000
C	5.476562000	5.476562000	-0.058540000
C	5.476562000	-5.476562000	0.058540000
C	-0.680799000	4.220153000	0.007468000
C	-0.680799000	-4.220153000	-0.007468000
C	-1.100110000	2.840178000	0.010735000
C	-1.100110000	-2.840178000	-0.010735000
C	-2.433903000	2.433903000	0.018773000
C	-2.433903000	-2.433903000	-0.018773000
C	-2.840178000	1.100110000	0.010735000
C	-2.840178000	-1.100110000	-0.010735000
C	-3.490858000	3.490858000	0.032401000
C	-3.490858000	-3.490858000	-0.032401000
C	-3.984818000	3.984818000	1.245871000
C	-3.984818000	-3.984818000	-1.245871000
C	-4.000697000	4.000697000	-1.167821000
C	-4.000697000	-4.000697000	1.167821000
C	-4.220153000	0.680799000	0.007468000
C	-4.220153000	-0.680799000	-0.007468000
C	-4.972426000	4.972426000	1.260063000
C	-4.972426000	-4.972426000	-1.260063000
C	-4.988298000	4.988298000	-1.156032000
C	-4.988298000	-4.988298000	1.156032000
C	-5.476562000	5.476562000	0.058540000
C	-5.476562000	-5.476562000	-0.058540000
H	1.353203000	5.070105000	-0.014688000
H	1.353203000	-5.070105000	0.014688000
H	3.587189000	3.587189000	-2.179270000

H	3.587189000	-3.587189000	2.179270000
H	3.615368000	3.615368000	2.111468000
H	3.615368000	-3.615368000	-2.111468000
H	5.070105000	1.353203000	-0.014688000
H	5.070105000	-1.353203000	0.014688000
H	5.347866000	5.347866000	-2.211250000
H	5.347866000	-5.347866000	2.211250000
H	5.376168000	5.376168000	2.097161000
H	5.376168000	-5.376168000	-2.097161000
H	6.246956000	6.246956000	-0.068652000
H	6.246956000	-6.246956000	0.068652000
H	-1.353203000	5.070105000	0.014688000
H	-1.353203000	-5.070105000	-0.014688000
H	-3.587189000	3.587189000	2.179270000
H	-3.587189000	-3.587189000	-2.179270000
H	-3.615368000	3.615368000	-2.111468000
H	-3.615368000	-3.615368000	2.111468000
H	-5.070105000	1.353203000	0.014688000
H	-5.070105000	-1.353203000	-0.014688000
H	-5.347866000	5.347866000	2.211250000
H	-5.347866000	-5.347866000	-2.211250000
H	-5.376168000	5.376168000	-2.097161000
H	-5.376168000	-5.376168000	2.097161000
H	-6.246956000	6.246956000	0.068652000
H	-6.246956000	-6.246956000	-0.068652000
N	0.000000000	2.008300000	0.000000000
N	0.000000000	-2.008300000	0.000000000
N	2.008300000	0.000000000	0.000000000
N	-2.008300000	0.000000000	0.000000000

83. Ni (TPP]; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	3.419657000	0.000000000
C	0.000000000	4.907593000	0.000000000
C	0.000000000	7.720939000	0.000000000
C	0.000000000	-3.419657000	0.000000000
C	0.000000000	-4.907593000	0.000000000
C	0.000000000	-7.720939000	0.000000000
C	0.762020000	7.018378000	-0.937103000
C	0.762020000	-7.018378000	0.937103000
C	0.762353000	5.622844000	-0.935608000
C	0.762353000	-5.622844000	0.935608000
C	1.187824000	2.739823000	0.239071000
C	1.187824000	-2.739823000	-0.239071000
C	2.426528000	3.387891000	0.573471000
C	2.426528000	-3.387891000	-0.573471000
C	2.739823000	1.187824000	0.239071000
C	2.739823000	-1.187824000	-0.239071000
C	3.387891000	2.426528000	0.573471000

C	3.387891000	-2.426528000	-0.573471000
C	3.419657000	0.000000000	0.000000000
C	4.907593000	0.000000000	0.000000000
C	5.622844000	0.762353000	-0.935608000
C	5.622844000	-0.762353000	0.935608000
C	7.018378000	0.762020000	-0.937103000
C	7.018378000	-0.762020000	0.937103000
C	7.720939000	0.000000000	0.000000000
C	-0.762020000	7.018378000	0.937103000
C	-0.762020000	-7.018378000	-0.937103000
C	-0.762353000	5.622844000	0.935608000
C	-0.762353000	-5.622844000	-0.935608000
C	-1.187824000	2.739823000	-0.239071000
C	-1.187824000	-2.739823000	0.239071000
C	-2.426528000	3.387891000	-0.573471000
C	-2.426528000	-3.387891000	0.573471000
C	-2.739823000	1.187824000	-0.239071000
C	-2.739823000	-1.187824000	0.239071000
C	-3.387891000	2.426528000	-0.573471000
C	-3.387891000	-2.426528000	0.573471000
C	-3.419657000	0.000000000	0.000000000
C	-4.907593000	0.000000000	0.000000000
C	-5.622844000	0.762353000	0.935608000
C	-5.622844000	-0.762353000	-0.935608000
C	-7.018378000	0.762020000	0.937103000
C	-7.018378000	-0.762020000	-0.937103000
C	-7.720939000	0.000000000	0.000000000
H	0.000000000	8.810441000	0.000000000
H	0.000000000	-8.810441000	0.000000000
H	1.352452000	5.071113000	-1.666486000
H	1.352452000	-5.071113000	1.666486000
H	1.354530000	7.557515000	-1.675235000
H	1.354530000	-7.557515000	1.675235000
H	2.532054000	4.445474000	0.781154000
H	2.532054000	-4.445474000	-0.781154000
H	4.445474000	2.532054000	0.781154000
H	4.445474000	-2.532054000	-0.781154000
H	5.071113000	1.352452000	-1.666486000
H	5.071113000	-1.352452000	1.666486000
H	7.557515000	1.354530000	-1.675235000
H	7.557515000	-1.354530000	1.675235000
H	8.810441000	0.000000000	0.000000000
H	-1.352452000	5.071113000	1.666486000
H	-1.352452000	-5.071113000	-1.666486000
H	-1.354530000	7.557515000	1.675235000
H	-1.354530000	-7.557515000	-1.675235000
H	-2.532054000	4.445474000	-0.781154000
H	-2.532054000	-4.445474000	0.781154000
H	-4.445474000	2.532054000	-0.781154000
H	-4.445474000	-2.532054000	0.781154000
H	-5.071113000	1.352452000	1.666486000

H	-5.071113000	-1.352452000	-1.666486000
H	-7.557515000	1.354530000	1.675235000
H	-7.557515000	-1.354530000	-1.675235000
H	-8.810441000	0.000000000	0.000000000
N	1.373222000	1.373222000	0.098972000
N	1.373222000	-1.373222000	-0.098972000
N	-1.373222000	1.373222000	-0.098972000
N	-1.373222000	-1.373222000	0.098972000

84. Ni(TPP]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
C	0.649189000	4.149495000	0.204537000
C	0.649189000	-4.149495000	-0.204537000
C	1.058748000	2.772913000	0.296290000
C	1.058748000	-2.772913000	-0.296290000
C	2.370475000	2.370475000	0.514160000
C	2.370475000	-2.370475000	-0.514160000
C	2.772913000	1.058748000	0.296290000
C	2.772913000	-1.058748000	-0.296290000
C	3.396669000	3.396669000	0.862528000
C	3.396669000	-3.396669000	-0.862528000
C	3.681396000	3.681396000	2.203258000
C	3.681396000	-3.681396000	-2.203258000
C	4.086996000	4.086996000	-0.141843000
C	4.086996000	-4.086996000	0.141843000
C	4.149495000	0.649189000	0.204537000
C	4.149495000	-0.649189000	-0.204537000
C	4.640886000	4.640886000	2.535510000
C	4.640886000	-4.640886000	-2.535510000
C	5.046368000	5.046368000	0.188199000
C	5.046368000	-5.046368000	-0.188199000
C	5.325529000	5.325529000	1.528652000
C	5.325529000	-5.325529000	-1.528652000
C	-0.649189000	4.149495000	-0.204537000
C	-0.649189000	-4.149495000	0.204537000
C	-1.058748000	2.772913000	-0.296290000
C	-1.058748000	-2.772913000	0.296290000
C	-2.370475000	2.370475000	-0.514160000
C	-2.370475000	-2.370475000	0.514160000
C	-2.772913000	1.058748000	-0.296290000
C	-2.772913000	-1.058748000	0.296290000
C	-3.396669000	3.396669000	-0.862528000
C	-3.396669000	-3.396669000	0.862528000
C	-3.681396000	3.681396000	-2.203258000
C	-3.681396000	-3.681396000	2.203258000
C	-4.086996000	4.086996000	0.141843000
C	-4.086996000	-4.086996000	-0.141843000
C	-4.149495000	0.649189000	-0.204537000
C	-4.149495000	-0.649189000	0.204537000

C	-4.640886000	4.640886000	-2.535510000
C	-4.640886000	-4.640886000	2.535510000
C	-5.046368000	5.046368000	-0.188199000
C	-5.046368000	-5.046368000	0.188199000
C	-5.325529000	5.325529000	-1.528652000
C	-5.325529000	-5.325529000	1.528652000
H	1.296504000	4.996291000	0.400153000
H	1.296504000	-4.996291000	-0.400153000
H	3.143992000	3.143992000	2.984171000
H	3.143992000	-3.143992000	-2.984171000
H	3.863282000	3.863282000	-1.184531000
H	3.863282000	-3.863282000	1.184531000
H	4.852885000	4.852885000	3.582746000
H	4.852885000	-4.852885000	-3.582746000
H	4.996291000	1.296504000	0.400153000
H	4.996291000	-1.296504000	-0.400153000
H	5.575964000	5.575964000	-0.602824000
H	5.575964000	-5.575964000	0.602824000
H	6.073933000	6.073933000	1.787285000
H	6.073933000	-6.073933000	-1.787285000
H	-1.296504000	4.996291000	-0.400153000
H	-1.296504000	-4.996291000	0.400153000
H	-3.143992000	3.143992000	-2.984171000
H	-3.143992000	-3.143992000	2.984171000
H	-3.863282000	3.863282000	1.184531000
H	-3.863282000	-3.863282000	-1.184531000
H	-4.852885000	4.852885000	-3.582746000
H	-4.852885000	-4.852885000	3.582746000
H	-4.996291000	1.296504000	-0.400153000
H	-4.996291000	-1.296504000	0.400153000
H	-5.575964000	5.575964000	0.602824000
H	-5.575964000	-5.575964000	-0.602824000
H	-6.073933000	6.073933000	-1.787285000
H	-6.073933000	-6.073933000	1.787285000
N	0.000000000	1.932680000	0.000000000
N	0.000000000	-1.932680000	0.000000000
N	1.932680000	0.000000000	0.000000000
N	-1.932680000	0.000000000	0.000000000

85. Pd(TPP)]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.000000000
C	0.000000000	3.452342000	0.000000000
C	0.000000000	4.942876000	0.000000000
C	0.000000000	7.755811000	0.000000000
C	0.000000000	-3.452342000	0.000000000
C	0.000000000	-4.942876000	0.000000000
C	0.000000000	-7.755811000	0.000000000
C	0.604308000	5.657555000	-1.044476000
C	0.604308000	-5.657555000	1.044476000

C	0.604835000	7.053129000	-1.045357000
C	0.604835000	-7.053129000	1.045357000
C	1.231392000	2.797683000	0.082878000
C	1.231392000	-2.797683000	-0.082878000
C	2.500788000	3.463116000	0.247666000
C	2.500788000	-3.463116000	-0.247666000
C	2.797683000	1.231392000	0.082878000
C	2.797683000	-1.231392000	-0.082878000
C	3.452342000	0.000000000	0.000000000
C	3.463116000	2.500788000	0.247666000
C	3.463116000	-2.500788000	-0.247666000
C	4.942876000	0.000000000	0.000000000
C	5.657555000	0.604308000	-1.044476000
C	5.657555000	-0.604308000	1.044476000
C	7.053129000	0.604835000	-1.045357000
C	7.053129000	-0.604835000	1.045357000
C	7.755811000	0.000000000	0.000000000
C	-0.604308000	5.657555000	1.044476000
C	-0.604308000	-5.657555000	-1.044476000
C	-0.604835000	7.053129000	1.045357000
C	-0.604835000	-7.053129000	-1.045357000
C	-1.231392000	2.797683000	-0.082878000
C	-1.231392000	-2.797683000	0.082878000
C	-2.500788000	3.463116000	-0.247666000
C	-2.500788000	-3.463116000	0.247666000
C	-2.797683000	1.231392000	-0.082878000
C	-2.797683000	-1.231392000	0.082878000
C	-3.452342000	0.000000000	0.000000000
C	-3.463116000	2.500788000	-0.247666000
C	-3.463116000	-2.500788000	0.247666000
C	-4.942876000	0.000000000	0.000000000
C	-5.657555000	0.604308000	1.044476000
C	-5.657555000	-0.604308000	-1.044476000
C	-7.053129000	0.604835000	1.045357000
C	-7.053129000	-0.604835000	-1.045357000
C	-7.755811000	0.000000000	0.000000000
H	0.000000000	8.845232000	0.000000000
H	0.000000000	-8.845232000	0.000000000
H	1.071419000	5.105786000	-1.859463000
H	1.071419000	-5.105786000	1.859463000
H	1.074194000	7.592074000	-1.867417000
H	1.074194000	-7.592074000	1.867417000
H	2.628703000	4.531842000	0.367467000
H	2.628703000	-4.531842000	-0.367467000
H	4.531842000	2.628703000	0.367467000
H	4.531842000	-2.628703000	-0.367467000
H	5.105786000	1.071419000	-1.859463000
H	5.105786000	-1.071419000	1.859463000
H	7.592074000	1.074194000	-1.867417000
H	7.592074000	-1.074194000	1.867417000
H	8.845232000	0.000000000	0.000000000

H	-1.071419000	5.105786000	1.859463000
H	-1.071419000	-5.105786000	-1.859463000
H	-1.074194000	7.592074000	1.867417000
H	-1.074194000	-7.592074000	-1.867417000
H	-2.628703000	4.531842000	-0.367467000
H	-2.628703000	-4.531842000	0.367467000
H	-4.531842000	2.628703000	-0.367467000
H	-4.531842000	-2.628703000	0.367467000
H	-5.105786000	1.071419000	1.859463000
H	-5.105786000	-1.071419000	-1.859463000
H	-7.592074000	1.074194000	1.867417000
H	-7.592074000	-1.074194000	-1.867417000
H	-8.845232000	0.000000000	0.000000000
N	1.433368000	1.433368000	0.011653000
N	1.433368000	-1.433368000	-0.011653000
N	-1.433368000	1.433368000	-0.011653000
N	-1.433368000	-1.433368000	0.011653000

86. Pd(TPP]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
C	0.680818000	4.229569000	-0.006889000
C	0.680818000	-4.229569000	0.006889000
C	1.106195000	2.850311000	-0.009967000
C	1.106195000	-2.850311000	0.009967000
C	2.437641000	2.437641000	-0.017311000
C	2.437641000	-2.437641000	0.017311000
C	2.850311000	1.106195000	-0.009967000
C	2.850311000	-1.106195000	0.009967000
C	3.494763000	3.494763000	-0.030437000
C	3.494763000	-3.494763000	0.030437000
C	3.988515000	3.988515000	-1.243809000
C	3.988515000	-3.988515000	1.243809000
C	4.003893000	4.003893000	1.170132000
C	4.003893000	-4.003893000	-1.170132000
C	4.229569000	0.680818000	-0.006889000
C	4.229569000	-0.680818000	0.006889000
C	4.976105000	4.976105000	-1.257539000
C	4.976105000	-4.976105000	1.257539000
C	4.991482000	4.991482000	1.158689000
C	4.991482000	-4.991482000	-1.158689000
C	5.479914000	5.479914000	-0.055755000
C	5.479914000	-5.479914000	0.055755000
C	-0.680818000	4.229569000	0.006889000
C	-0.680818000	-4.229569000	-0.006889000
C	-1.106195000	2.850311000	0.009967000
C	-1.106195000	-2.850311000	-0.009967000
C	-2.437641000	2.437641000	0.017311000
C	-2.437641000	-2.437641000	-0.017311000
C	-2.850311000	1.106195000	0.009967000

C	-2.850311000	-1.106195000	-0.009967000
C	-3.494763000	3.494763000	0.030437000
C	-3.494763000	-3.494763000	-0.030437000
C	-3.988515000	3.988515000	1.243809000
C	-3.988515000	-3.988515000	-1.243809000
C	-4.003893000	4.003893000	-1.170132000
C	-4.003893000	-4.003893000	1.170132000
C	-4.229569000	0.680818000	0.006889000
C	-4.229569000	-0.680818000	-0.006889000
C	-4.976105000	4.976105000	1.257539000
C	-4.976105000	-4.976105000	-1.257539000
C	-4.991482000	4.991482000	-1.158689000
C	-4.991482000	-4.991482000	1.158689000
C	-5.479914000	5.479914000	0.055755000
C	-5.479914000	-5.479914000	-0.055755000
H	1.352369000	5.080302000	-0.013667000
H	1.352369000	-5.080302000	0.013667000
H	3.590933000	3.590933000	-2.177218000
H	3.590933000	-3.590933000	2.177218000
H	3.618241000	3.618241000	2.113487000
H	3.618241000	-3.618241000	-2.113487000
H	5.080302000	1.352369000	-0.013667000
H	5.080302000	-1.352369000	0.013667000
H	5.351727000	5.351727000	-2.208528000
H	5.351727000	-5.351727000	2.208528000
H	5.379191000	5.379191000	2.099927000
H	5.379191000	-5.379191000	-2.099927000
H	6.250294000	6.250294000	-0.065544000
H	6.250294000	-6.250294000	0.065544000
H	-1.352369000	5.080302000	0.013667000
H	-1.352369000	-5.080302000	-0.013667000
H	-3.590933000	3.590933000	2.177218000
H	-3.590933000	-3.590933000	-2.177218000
H	-3.618241000	3.618241000	-2.113487000
H	-3.618241000	-3.618241000	2.113487000
H	-5.080302000	1.352369000	0.013667000
H	-5.080302000	-1.352369000	-0.013667000
H	-5.351727000	5.351727000	2.208528000
H	-5.351727000	-5.351727000	-2.208528000
H	-5.379191000	5.379191000	-2.099927000
H	-5.379191000	-5.379191000	2.099927000
H	-6.250294000	6.250294000	0.065544000
H	-6.250294000	-6.250294000	-0.065544000
N	0.000000000	2.024861000	0.000000000
N	0.000000000	-2.024861000	0.000000000
N	2.024861000	0.000000000	0.000000000
N	-2.024861000	0.000000000	0.000000000

87. Pt(TPP]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.000000000
C	0.000000000	3.454272000	0.000000000
C	0.000000000	4.945842000	0.000000000
C	0.000000000	7.758495000	0.000000000
C	0.000000000	-3.454272000	0.000000000
C	0.000000000	-4.945842000	0.000000000
C	0.000000000	-7.758495000	0.000000000
C	0.573345000	5.660154000	-1.061848000
C	0.573345000	-5.660154000	1.061848000
C	0.573614000	7.055902000	-1.062811000
C	0.573614000	-7.055902000	1.062811000
C	1.232326000	2.801214000	0.069961000
C	1.232326000	-2.801214000	-0.069961000
C	2.503142000	3.465206000	0.208030000
C	2.503142000	-3.465206000	-0.208030000
C	2.801214000	1.232326000	0.069961000
C	2.801214000	-1.232326000	-0.069961000
C	3.454272000	0.000000000	0.000000000
C	3.465206000	2.503142000	0.208030000
C	3.465206000	-2.503142000	-0.208030000
C	4.945842000	0.000000000	0.000000000
C	5.660154000	0.573345000	-1.061848000
C	5.660154000	-0.573345000	1.061848000
C	7.055902000	0.573614000	-1.062811000
C	7.055902000	-0.573614000	1.062811000
C	7.758495000	0.000000000	0.000000000
C	-0.573345000	5.660154000	1.061848000
C	-0.573345000	-5.660154000	-1.061848000
C	-0.573614000	7.055902000	1.062811000
C	-0.573614000	-7.055902000	-1.062811000
C	-1.232326000	2.801214000	-0.069961000
C	-1.232326000	-2.801214000	0.069961000
C	-2.503142000	3.465206000	-0.208030000
C	-2.503142000	-3.465206000	0.208030000
C	-2.801214000	1.232326000	-0.069961000
C	-2.801214000	-1.232326000	0.069961000
C	-3.454272000	0.000000000	0.000000000
C	-3.465206000	2.503142000	-0.208030000
C	-3.465206000	-2.503142000	0.208030000
C	-4.945842000	0.000000000	0.000000000
C	-5.660154000	0.573345000	1.061848000
C	-5.660154000	-0.573345000	-1.061848000
C	-7.055902000	0.573614000	1.062811000
C	-7.055902000	-0.573614000	-1.062811000
C	-7.758495000	0.000000000	0.000000000
H	0.000000000	8.847978000	0.000000000
H	0.000000000	-8.847978000	0.000000000
H	1.016559000	5.108245000	-1.890050000

H	1.016559000	-5.108245000	1.890050000
H	1.018590000	7.595014000	-1.898220000
H	1.018590000	-7.595014000	1.898220000
H	2.632457000	4.535360000	0.309932000
H	2.632457000	-4.535360000	-0.309932000
H	4.535360000	2.632457000	0.309932000
H	4.535360000	-2.632457000	-0.309932000
H	5.108245000	1.016559000	-1.890050000
H	5.108245000	-1.016559000	1.890050000
H	7.595014000	1.018590000	-1.898220000
H	7.595014000	-1.018590000	1.898220000
H	8.847978000	0.000000000	0.000000000
H	-1.016559000	5.108245000	1.890050000
H	-1.016559000	-5.108245000	-1.890050000
H	-1.018590000	7.595014000	1.898220000
H	-1.018590000	-7.595014000	-1.898220000
H	-2.632457000	4.535360000	-0.309932000
H	-2.632457000	-4.535360000	0.309932000
H	-4.535360000	2.632457000	-0.309932000
H	-4.535360000	-2.632457000	0.309932000
H	-5.108245000	1.016559000	1.890050000
H	-5.108245000	-1.016559000	-1.890050000
H	-7.595014000	1.018590000	1.898220000
H	-7.595014000	-1.018590000	-1.898220000
H	-8.847978000	0.000000000	0.000000000
N	1.432727000	1.432727000	0.014557000
N	1.432727000	-1.432727000	-0.014557000
N	-1.432727000	1.432727000	-0.014557000
N	-1.432727000	-1.432727000	0.014557000

88. Pt(TPP]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
C	0.680663000	4.228743000	-0.005013000
C	0.680663000	-4.228743000	0.005013000
C	1.108052000	2.852416000	-0.007190000
C	1.108052000	-2.852416000	0.007190000
C	2.438763000	2.438763000	-0.012628000
C	2.438763000	-2.438763000	0.012628000
C	2.852416000	1.108052000	-0.007190000
C	2.852416000	-1.108052000	0.007190000
C	3.496097000	3.496097000	-0.022725000
C	3.496097000	-3.496097000	0.022725000
C	3.991486000	3.991486000	-1.234789000
C	3.991486000	-3.991486000	1.234789000
C	4.003383000	4.003383000	1.179455000
C	4.003383000	-4.003383000	-1.179455000
C	4.228743000	0.680663000	-0.005013000
C	4.228743000	-0.680663000	0.005013000
C	4.979096000	4.979096000	-1.245597000

C	4.979096000	-4.979096000	1.245597000
C	4.991006000	4.991006000	1.170773000
C	4.991006000	-4.991006000	-1.170773000
C	5.481144000	5.481144000	-0.042308000
C	5.481144000	-5.481144000	0.042308000
C	-0.680663000	4.228743000	0.005013000
C	-0.680663000	-4.228743000	-0.005013000
C	-1.108052000	2.852416000	0.007190000
C	-1.108052000	-2.852416000	-0.007190000
C	-2.438763000	2.438763000	0.012628000
C	-2.438763000	-2.438763000	-0.012628000
C	-2.852416000	1.108052000	0.007190000
C	-2.852416000	-1.108052000	-0.007190000
C	-3.496097000	3.496097000	0.022725000
C	-3.496097000	-3.496097000	-0.022725000
C	-3.991486000	3.991486000	1.234789000
C	-3.991486000	-3.991486000	-1.234789000
C	-4.003383000	4.003383000	-1.179455000
C	-4.003383000	-4.003383000	1.179455000
C	-4.228743000	0.680663000	0.005013000
C	-4.228743000	-0.680663000	-0.005013000
C	-4.979096000	4.979096000	1.245597000
C	-4.979096000	-4.979096000	-1.245597000
C	-4.991006000	4.991006000	-1.170773000
C	-4.991006000	-4.991006000	1.170773000
C	-5.481144000	5.481144000	0.042308000
C	-5.481144000	-5.481144000	-0.042308000
H	1.352018000	5.079247000	-0.009795000
H	1.352018000	-5.079247000	0.009795000
H	3.595108000	3.595108000	-2.169256000
H	3.595108000	-3.595108000	2.169256000
H	3.616240000	3.616240000	2.121609000
H	3.616240000	-3.616240000	-2.121609000
H	5.079247000	1.352018000	-0.009795000
H	5.079247000	-1.352018000	0.009795000
H	5.356144000	5.356144000	-2.195482000
H	5.356144000	-5.356144000	2.195482000
H	5.377391000	5.377391000	2.113090000
H	5.377391000	-5.377391000	-2.113090000
H	6.251565000	6.251565000	-0.049898000
H	6.251565000	-6.251565000	0.049898000
H	-1.352018000	5.079247000	0.009795000
H	-1.352018000	-5.079247000	-0.009795000
H	-3.595108000	3.595108000	2.169256000
H	-3.595108000	-3.595108000	-2.169256000
H	-3.616240000	3.616240000	-2.121609000
H	-3.616240000	-3.616240000	2.121609000
H	-5.079247000	1.352018000	0.009795000
H	-5.079247000	-1.352018000	-0.009795000
H	-5.356144000	5.356144000	2.195482000
H	-5.356144000	-5.356144000	-2.195482000

H	-5.377391000	5.377391000	-2.113090000
H	-5.377391000	-5.377391000	2.113090000
H	-6.251565000	6.251565000	0.049898000
H	-6.251565000	-6.251565000	-0.049898000
N	0.000000000	2.024295000	0.000000000
N	0.000000000	-2.024295000	0.000000000
N	2.024295000	0.000000000	0.000000000
N	-2.024295000	0.000000000	0.000000000

89. Zn(TPP]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.000000000
C	0.000000000	3.459022000	0.000000000
C	0.000000000	4.949751000	0.000000000
C	0.000000000	7.764432000	0.000000000
C	0.000000000	-3.459022000	0.000000000
C	0.000000000	-4.949751000	0.000000000
C	0.000000000	-7.764432000	0.000000000
C	0.578285000	5.665925000	-1.058730000
C	0.578285000	-5.665925000	1.058730000
C	0.578691000	7.061448000	-1.059833000
C	0.578691000	-7.061448000	1.059833000
C	1.245880000	2.810070000	0.032986000
C	1.245880000	-2.810070000	-0.032986000
C	2.517293000	3.481422000	0.162605000
C	2.517293000	-3.481422000	-0.162605000
C	2.810070000	1.245880000	0.032986000
C	2.810070000	-1.245880000	-0.032986000
C	3.459022000	0.000000000	0.000000000
C	3.481422000	2.517293000	0.162605000
C	3.481422000	-2.517293000	-0.162605000
C	4.949751000	0.000000000	0.000000000
C	5.665925000	0.578285000	-1.058730000
C	5.665925000	-0.578285000	1.058730000
C	7.061448000	0.578691000	-1.059833000
C	7.061448000	-0.578691000	1.059833000
C	7.764432000	0.000000000	0.000000000
C	-0.578285000	5.665925000	1.058730000
C	-0.578285000	-5.665925000	-1.058730000
C	-0.578691000	7.061448000	1.059833000
C	-0.578691000	-7.061448000	-1.059833000
C	-1.245880000	2.810070000	-0.032986000
C	-1.245880000	-2.810070000	0.032986000
C	-2.517293000	3.481422000	-0.162605000
C	-2.517293000	-3.481422000	0.162605000
C	-2.810070000	1.245880000	-0.032986000
C	-2.810070000	-1.245880000	0.032986000
C	-3.459022000	0.000000000	0.000000000
C	-3.481422000	2.517293000	-0.162605000
C	-3.481422000	-2.517293000	0.162605000

C	-4.949751000	0.000000000	0.000000000
C	-5.665925000	0.578285000	1.058730000
C	-5.665925000	-0.578285000	-1.058730000
C	-7.061448000	0.578691000	1.059833000
C	-7.061448000	-0.578691000	-1.059833000
C	-7.764432000	0.000000000	0.000000000
H	0.000000000	8.853922000	0.000000000
H	0.000000000	-8.853922000	0.000000000
H	1.024249000	5.114843000	-1.885906000
H	1.024249000	-5.114843000	1.885906000
H	1.027250000	7.600336000	-1.893495000
H	1.027250000	-7.600336000	1.893495000
H	2.652913000	4.550975000	0.267465000
H	2.652913000	-4.550975000	-0.267465000
H	4.550975000	2.652913000	0.267465000
H	4.550975000	-2.652913000	-0.267465000
H	5.114843000	1.024249000	-1.885906000
H	5.114843000	-1.024249000	1.885906000
H	7.600336000	1.027250000	-1.893495000
H	7.600336000	-1.027250000	1.893495000
H	8.853922000	0.000000000	0.000000000
H	-1.024249000	5.114843000	1.885906000
H	-1.024249000	-5.114843000	-1.885906000
H	-1.027250000	7.600336000	1.893495000
H	-1.027250000	-7.600336000	-1.893495000
H	-2.652913000	4.550975000	-0.267465000
H	-2.652913000	-4.550975000	0.267465000
H	-4.550975000	2.652913000	-0.267465000
H	-4.550975000	-2.652913000	0.267465000
H	-5.114843000	1.024249000	1.885906000
H	-5.114843000	-1.024249000	-1.885906000
H	-7.600336000	1.027250000	1.893495000
H	-7.600336000	-1.027250000	-1.893495000
H	-8.853922000	0.000000000	0.000000000
N	1.447878000	1.447878000	-0.029455000
N	1.447878000	-1.447878000	0.029455000
N	-1.447878000	1.447878000	0.029455000
N	-1.447878000	-1.447878000	-0.029455000

90. Zn(TPP]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
C	0.682283000	4.246927000	-0.001831000
C	0.682283000	-4.246927000	0.001831000
C	1.104765000	2.865577000	-0.002626000
C	1.104765000	-2.865577000	0.002626000
C	2.440541000	2.440541000	-0.004597000
C	2.440541000	-2.440541000	0.004597000
C	2.865577000	1.104765000	-0.002626000
C	2.865577000	-1.104765000	0.002626000

C	3.498211000	3.498211000	-0.008190000
C	3.498211000	-3.498211000	0.008190000
C	3.998181000	3.998181000	-1.216638000
C	3.998181000	-3.998181000	1.216638000
C	4.002423000	4.002423000	1.196715000
C	4.002423000	-4.002423000	-1.196715000
C	4.246927000	0.682283000	-0.001831000
C	4.246927000	-0.682283000	0.001831000
C	4.985833000	4.985833000	-1.221450000
C	4.985833000	-4.985833000	1.221450000
C	4.990094000	4.990094000	1.194606000
C	4.990094000	-4.990094000	-1.194606000
C	5.484257000	5.484257000	-0.015161000
C	5.484257000	-5.484257000	0.015161000
C	-0.682283000	4.246927000	0.001831000
C	-0.682283000	-4.246927000	-0.001831000
C	-1.104765000	2.865577000	0.002626000
C	-1.104765000	-2.865577000	-0.002626000
C	-2.440541000	2.440541000	0.004597000
C	-2.440541000	-2.440541000	-0.004597000
C	-2.865577000	1.104765000	0.002626000
C	-2.865577000	-1.104765000	-0.002626000
C	-3.498211000	3.498211000	0.008190000
C	-3.498211000	-3.498211000	-0.008190000
C	-3.998181000	3.998181000	1.216638000
C	-3.998181000	-3.998181000	-1.216638000
C	-4.002423000	4.002423000	-1.196715000
C	-4.002423000	-4.002423000	1.196715000
C	-4.246927000	0.682283000	0.001831000
C	-4.246927000	-0.682283000	-0.001831000
C	-4.985833000	4.985833000	1.221450000
C	-4.985833000	-4.985833000	-1.221450000
C	-4.990094000	4.990094000	-1.194606000
C	-4.990094000	-4.990094000	1.194606000
C	-5.484257000	5.484257000	0.015161000
C	-5.484257000	-5.484257000	-0.015161000
H	1.349570000	5.101294000	-0.003662000
H	1.349570000	-5.101294000	0.003662000
H	3.605145000	3.605145000	-2.153923000
H	3.605145000	-3.605145000	2.153923000
H	3.612688000	3.612688000	2.136739000
H	3.612688000	-3.612688000	-2.136739000
H	5.101294000	1.349570000	-0.003662000
H	5.101294000	-1.349570000	0.003662000
H	5.365736000	5.365736000	-2.169070000
H	5.365736000	-5.365736000	2.169070000
H	5.373349000	5.373349000	2.139538000
H	5.373349000	-5.373349000	-2.139538000
H	6.254679000	6.254679000	-0.017849000
H	6.254679000	-6.254679000	0.017849000
H	-1.349570000	5.101294000	0.003662000

H	-1.349570000	-5.101294000	-0.003662000
H	-3.605145000	3.605145000	2.153923000
H	-3.605145000	-3.605145000	-2.153923000
H	-3.612688000	3.612688000	-2.136739000
H	-3.612688000	-3.612688000	2.136739000
H	-5.101294000	1.349570000	0.003662000
H	-5.101294000	-1.349570000	-0.003662000
H	-5.365736000	5.365736000	2.169070000
H	-5.365736000	-5.365736000	-2.169070000
H	-5.373349000	5.373349000	-2.139538000
H	-5.373349000	-5.373349000	2.139538000
H	-6.254679000	6.254679000	0.017849000
H	-6.254679000	-6.254679000	-0.017849000
N	0.000000000	2.042671000	0.000000000
N	0.000000000	-2.042671000	0.000000000
N	2.042671000	0.000000000	0.000000000
N	-2.042671000	0.000000000	0.000000000

91. Cu(I₈TPP] ; S = ½ (saddled)

Cu	0.000000000	0.000000000	0.000000000
C	0.000000000	3.391355000	0.000000000
C	0.000000000	4.870805000	0.000000000
C	0.000000000	7.670509000	0.000000000
C	0.000000000	-3.391355000	0.000000000
C	0.000000000	-4.870805000	0.000000000
C	0.000000000	-7.670509000	0.000000000
C	0.965343000	6.971221000	-0.729577000
C	0.965343000	-6.971221000	0.729577000
C	0.972222000	5.579246000	-0.720172000
C	0.972222000	-5.579246000	0.720172000
C	1.127364000	2.704112000	0.489683000
C	1.127364000	-2.704112000	-0.489683000
C	2.238317000	3.215370000	1.273915000
C	2.238317000	-3.215370000	-1.273915000
C	2.704112000	1.127364000	0.489683000
C	2.704112000	-1.127364000	-0.489683000
C	3.215370000	2.238317000	1.273915000
C	3.215370000	-2.238317000	-1.273915000
C	3.391355000	0.000000000	0.000000000
C	4.870805000	0.000000000	0.000000000
C	5.579246000	0.972222000	-0.720172000
C	5.579246000	-0.972222000	0.720172000
C	6.971221000	0.965343000	-0.729577000
C	6.971221000	-0.965343000	0.729577000
C	7.670509000	0.000000000	0.000000000
C	-0.965343000	6.971221000	0.729577000
C	-0.965343000	-6.971221000	-0.729577000
C	-0.972222000	5.579246000	0.720172000
C	-0.972222000	-5.579246000	-0.720172000

C	-1.127364000	2.704112000	-0.489683000
C	-1.127364000	-2.704112000	0.489683000
C	-2.238317000	3.215370000	-1.273915000
C	-2.238317000	-3.215370000	1.273915000
C	-2.704112000	1.127364000	-0.489683000
C	-2.704112000	-1.127364000	0.489683000
C	-3.215370000	2.238317000	-1.273915000
C	-3.215370000	-2.238317000	1.273915000
C	-3.391355000	0.000000000	0.000000000
C	-4.870805000	0.000000000	0.000000000
C	-5.579246000	0.972222000	0.720172000
C	-5.579246000	-0.972222000	-0.720172000
C	-6.971221000	0.965343000	0.729577000
C	-6.971221000	-0.965343000	-0.729577000
C	-7.670509000	0.000000000	0.000000000
H	0.000000000	8.760070000	0.000000000
H	0.000000000	-8.760070000	0.000000000
H	1.717578000	7.512598000	-1.301155000
H	1.717578000	-7.512598000	1.301155000
H	1.724186000	5.024565000	-1.279682000
H	1.724186000	-5.024565000	1.279682000
H	5.024565000	1.724186000	-1.279682000
H	5.024565000	-1.724186000	1.279682000
H	7.512598000	1.717578000	-1.301155000
H	7.512598000	-1.717578000	1.301155000
H	8.760070000	0.000000000	0.000000000
H	-1.717578000	7.512598000	1.301155000
H	-1.717578000	-7.512598000	-1.301155000
H	-1.724186000	5.024565000	1.279682000
H	-1.724186000	-5.024565000	-1.279682000
H	-5.024565000	1.724186000	1.279682000
H	-5.024565000	-1.724186000	-1.279682000
H	-7.512598000	1.717578000	1.301155000
H	-7.512598000	-1.717578000	-1.301155000
H	-8.760070000	0.000000000	0.000000000
I	2.284179000	4.946826000	2.450327000
I	2.284179000	-4.946826000	-2.450327000
I	4.946826000	2.284179000	2.450327000
I	4.946826000	-2.284179000	-2.450327000
I	-2.284179000	4.946826000	-2.450327000
I	-2.284179000	-4.946826000	2.450327000
I	-4.946826000	2.284179000	-2.450327000
I	-4.946826000	-2.284179000	2.450327000
N	1.401628000	1.401628000	0.133829000
N	1.401628000	-1.401628000	-0.133829000
N	-1.401628000	1.401628000	-0.133829000
N	-1.401628000	-1.401628000	0.133829000

92. Cu(I₈TPP]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
C	0.569342000	4.139799000	-0.391757000
C	0.569342000	-4.139799000	0.391757000
C	0.996695000	2.749965000	-0.522324000
C	0.996695000	-2.749965000	0.522324000
C	2.280655000	2.280655000	-0.874038000
C	2.280655000	-2.280655000	0.874038000
C	2.749965000	0.996695000	-0.522324000
C	2.749965000	-0.996695000	0.522324000
C	3.249494000	3.249494000	-1.460105000
C	3.249494000	-3.249494000	1.460105000
C	3.370012000	3.370012000	-2.847604000
C	3.370012000	-3.370012000	2.847604000
C	4.045217000	4.045217000	-0.626343000
C	4.045217000	-4.045217000	0.626343000
C	4.139799000	0.569342000	-0.391757000
C	4.139799000	-0.569342000	0.391757000
C	4.276344000	4.276344000	-3.395953000
C	4.276344000	-4.276344000	3.395953000
C	4.950759000	4.950759000	-1.173129000
C	4.950759000	-4.950759000	1.173129000
C	5.067794000	5.067794000	-2.559658000
C	5.067794000	-5.067794000	2.559658000
C	-0.569342000	4.139799000	0.391757000
C	-0.569342000	-4.139799000	-0.391757000
C	-0.996695000	2.749965000	0.522324000
C	-0.996695000	-2.749965000	-0.522324000
C	-2.280655000	2.280655000	0.874038000
C	-2.280655000	-2.280655000	-0.874038000
C	-2.749965000	0.996695000	0.522324000
C	-2.749965000	-0.996695000	-0.522324000
C	-3.249494000	3.249494000	1.460105000
C	-3.249494000	-3.249494000	-1.460105000
C	-3.370012000	3.370012000	2.847604000
C	-3.370012000	-3.370012000	-2.847604000
C	-4.045217000	4.045217000	0.626343000
C	-4.045217000	-4.045217000	-0.626343000
C	-4.139799000	0.569342000	0.391757000
C	-4.139799000	-0.569342000	-0.391757000
C	-4.276344000	4.276344000	3.395953000
C	-4.276344000	-4.276344000	-3.395953000
C	-4.950759000	4.950759000	1.173129000
C	-4.950759000	-4.950759000	-1.173129000
C	-5.067794000	5.067794000	2.559658000
C	-5.067794000	-5.067794000	-2.559658000
H	2.749342000	2.749342000	-3.492276000
H	2.749342000	-2.749342000	3.492276000
H	3.944898000	3.944898000	0.453463000

H	3.944898000	-3.944898000	-0.453463000
H	4.365131000	4.365131000	-4.477660000
H	4.365131000	-4.365131000	4.477660000
H	5.564891000	5.564891000	-0.516704000
H	5.564891000	-5.564891000	0.516704000
H	5.775675000	5.775675000	-2.989784000
H	5.775675000	-5.775675000	2.989784000
H	-2.749342000	2.749342000	3.492276000
H	-2.749342000	-2.749342000	-3.492276000
H	-3.944898000	3.944898000	-0.453463000
H	-3.944898000	-3.944898000	0.453463000
H	-4.365131000	4.365131000	4.477660000
H	-4.365131000	-4.365131000	-4.477660000
H	-5.564891000	5.564891000	0.516704000
H	-5.564891000	-5.564891000	-0.516704000
H	-5.775675000	5.775675000	2.989784000
H	-5.775675000	-5.775675000	-2.989784000
I	1.284597000	5.887364000	-1.308786000
I	1.284597000	-5.887364000	1.308786000
I	5.887364000	1.284597000	-1.308786000
I	5.887364000	-1.284597000	1.308786000
I	-1.284597000	5.887364000	1.308786000
I	-1.284597000	-5.887364000	-1.308786000
I	-5.887364000	1.284597000	1.308786000
I	-5.887364000	-1.284597000	-1.308786000
N	0.000000000	1.954777000	0.000000000
N	0.000000000	-1.954777000	0.000000000
N	1.954777000	0.000000000	0.000000000
N	-1.954777000	0.000000000	0.000000000

93. Ni (I₈TPP] ; S = 0 (saddled)

Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	3.351965000	0.000000000
C	0.000000000	4.832573000	0.000000000
C	0.000000000	7.631649000	0.000000000
C	0.000000000	-3.351965000	0.000000000
C	0.000000000	-4.832573000	0.000000000
C	0.000000000	-7.631649000	0.000000000
C	0.986546000	6.932319000	-0.700384000
C	0.986546000	-6.932319000	0.700384000
C	0.992323000	5.539964000	-0.691784000
C	0.992323000	-5.539964000	0.691784000
C	1.075902000	2.649841000	0.556809000
C	1.075902000	-2.649841000	-0.556809000
C	2.176977000	3.151823000	1.356846000
C	2.176977000	-3.151823000	-1.356846000
C	2.649841000	1.075902000	0.556809000
C	2.649841000	-1.075902000	-0.556809000
C	3.151823000	2.176977000	1.356846000

C	3.151823000	-2.176977000	-1.356846000
C	3.351965000	0.000000000	0.000000000
C	4.832573000	0.000000000	0.000000000
C	5.539964000	0.992323000	-0.691784000
C	5.539964000	-0.992323000	0.691784000
C	6.932319000	0.986546000	-0.700384000
C	6.932319000	-0.986546000	0.700384000
C	7.631649000	0.000000000	0.000000000
C	-0.986546000	6.932319000	0.700384000
C	-0.986546000	-6.932319000	-0.700384000
C	-0.992323000	5.539964000	0.691784000
C	-0.992323000	-5.539964000	-0.691784000
C	-1.075902000	2.649841000	-0.556809000
C	-1.075902000	-2.649841000	0.556809000
C	-2.176977000	3.151823000	-1.356846000
C	-2.176977000	-3.151823000	1.356846000
C	-2.649841000	1.075902000	-0.556809000
C	-2.649841000	-1.075902000	0.556809000
C	-3.151823000	2.176977000	-1.356846000
C	-3.151823000	-2.176977000	1.356846000
C	-3.351965000	0.000000000	0.000000000
C	-4.832573000	0.000000000	0.000000000
C	-5.539964000	0.992323000	0.691784000
C	-5.539964000	-0.992323000	-0.691784000
C	-6.932319000	0.986546000	0.700384000
C	-6.932319000	-0.986546000	-0.700384000
C	-7.631649000	0.000000000	0.000000000
H	0.000000000	8.721185000	0.000000000
H	0.000000000	-8.721185000	0.000000000
H	1.755740000	7.473613000	-1.248986000
H	1.755740000	-7.473613000	1.248986000
H	1.760564000	4.985118000	-1.228614000
H	1.760564000	-4.985118000	1.228614000
H	4.985118000	1.760564000	-1.228614000
H	4.985118000	-1.760564000	1.228614000
H	7.473613000	1.755740000	-1.248986000
H	7.473613000	-1.755740000	1.248986000
H	8.721185000	0.000000000	0.000000000
H	-1.755740000	7.473613000	1.248986000
H	-1.755740000	-7.473613000	-1.248986000
H	-1.760564000	4.985118000	1.228614000
H	-1.760564000	-4.985118000	-1.228614000
H	-4.985118000	1.760564000	1.228614000
H	-4.985118000	-1.760564000	-1.228614000
H	-7.473613000	1.755740000	1.248986000
H	-7.473613000	-1.755740000	-1.248986000
H	-8.721185000	0.000000000	0.000000000
I	2.202796000	4.881422000	2.531861000
I	2.202796000	-4.881422000	-2.531861000
I	4.881422000	2.202796000	2.531861000
I	4.881422000	-2.202796000	-2.531861000

I	-2.202796000	4.881422000	-2.531861000
I	-2.202796000	-4.881422000	2.531861000
I	-4.881422000	2.202796000	-2.531861000
I	-4.881422000	-2.202796000	2.531861000
N	1.332467000	1.332467000	0.219060000
N	1.332467000	-1.332467000	-0.219060000
N	-1.332467000	1.332467000	-0.219060000
N	-1.332467000	-1.332467000	0.219060000

94. Ni(I₈TPP]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
C	0.531034000	4.062327000	-0.440550000
C	0.531034000	-4.062327000	0.440550000
C	0.948796000	2.675390000	-0.601442000
C	0.948796000	-2.675390000	0.601442000
C	2.212020000	2.212020000	-1.010474000
C	2.212020000	-2.212020000	1.010474000
C	2.675390000	0.948796000	-0.601442000
C	2.675390000	-0.948796000	0.601442000
C	3.153708000	3.153708000	-1.675724000
C	3.153708000	-3.153708000	1.675724000
C	3.215855000	3.215855000	-3.070668000
C	3.215855000	-3.215855000	3.070668000
C	3.983295000	3.983295000	-0.910324000
C	3.983295000	-3.983295000	0.910324000
C	4.062327000	0.531034000	-0.440550000
C	4.062327000	-0.531034000	0.440550000
C	4.097896000	4.097896000	-3.694013000
C	4.097896000	-4.097896000	3.694013000
C	4.864287000	4.864287000	-1.531747000
C	4.864287000	-4.864287000	1.531747000
C	4.923089000	4.923089000	-2.925657000
C	4.923089000	-4.923089000	2.925657000
C	-0.531034000	4.062327000	0.440550000
C	-0.531034000	-4.062327000	-0.440550000
C	-0.948796000	2.675390000	0.601442000
C	-0.948796000	-2.675390000	-0.601442000
C	-2.212020000	2.212020000	1.010474000
C	-2.212020000	-2.212020000	-1.010474000
C	-2.675390000	0.948796000	0.601442000
C	-2.675390000	-0.948796000	-0.601442000
C	-3.153708000	3.153708000	1.675724000
C	-3.153708000	-3.153708000	-1.675724000
C	-3.215855000	3.215855000	3.070668000
C	-3.215855000	-3.215855000	-3.070668000
C	-3.983295000	3.983295000	0.910324000
C	-3.983295000	-3.983295000	-0.910324000
C	-4.062327000	0.531034000	0.440550000
C	-4.062327000	-0.531034000	-0.440550000

C	-4.097896000	4.097896000	3.694013000
C	-4.097896000	-4.097896000	-3.694013000
C	-4.864287000	4.864287000	1.531747000
C	-4.864287000	-4.864287000	-1.531747000
C	-4.923089000	4.923089000	2.925657000
C	-4.923089000	-4.923089000	-2.925657000
H	2.569244000	2.569244000	-3.662138000
H	2.569244000	-2.569244000	3.662138000
H	3.928390000	3.928390000	0.176020000
H	3.928390000	-3.928390000	-0.176020000
H	4.141213000	4.141213000	-4.781280000
H	4.141213000	-4.141213000	4.781280000
H	5.504764000	5.504764000	-0.927750000
H	5.504764000	-5.504764000	0.927750000
H	5.611642000	5.611642000	-3.414525000
H	5.611642000	-5.611642000	3.414525000
H	-2.569244000	2.569244000	3.662138000
H	-2.569244000	-2.569244000	-3.662138000
H	-3.928390000	3.928390000	-0.176020000
H	-3.928390000	-3.928390000	0.176020000
H	-4.141213000	4.141213000	4.781280000
H	-4.141213000	-4.141213000	-4.781280000
H	-5.504764000	5.504764000	0.927750000
H	-5.504764000	-5.504764000	-0.927750000
H	-5.611642000	5.611642000	3.414525000
H	-5.611642000	-5.611642000	-3.414525000
I	1.173930000	5.792971000	-1.432247000
I	1.173930000	-5.792971000	1.432247000
I	5.792971000	1.173930000	-1.432247000
I	5.792971000	-1.173930000	1.432247000
I	-1.173930000	5.792971000	1.432247000
I	-1.173930000	-5.792971000	-1.432247000
I	-5.792971000	1.173930000	1.432247000
I	-5.792971000	-1.173930000	-1.432247000
N	0.000000000	1.872522000	0.000000000
N	0.000000000	-1.872522000	0.000000000
N	1.872522000	0.000000000	0.000000000
N	-1.872522000	0.000000000	0.000000000

95. Pd(I₈TPP]; S = 0 (saddled)

Pd	0.000000000	0.000000000	0.000000000
C	0.000000000	3.404352000	0.000000000
C	0.000000000	4.885655000	0.000000000
C	0.000000000	7.684202000	0.000000000
C	0.000000000	-3.404352000	0.000000000
C	0.000000000	-4.885655000	0.000000000
C	0.000000000	-7.684202000	0.000000000
C	0.936132000	6.985097000	-0.766739000
C	0.936132000	-6.985097000	0.766739000

C	0.943321000	5.593024000	-0.757509000
C	0.943321000	-5.593024000	0.757509000
C	1.141166000	2.728506000	0.469817000
C	1.141166000	-2.728506000	-0.469817000
C	2.271190000	3.247470000	1.225364000
C	2.271190000	-3.247470000	-1.225364000
C	2.728506000	1.141166000	0.469817000
C	2.728506000	-1.141166000	-0.469817000
C	3.247470000	2.271190000	1.225364000
C	3.247470000	-2.271190000	-1.225364000
C	3.404352000	0.000000000	0.000000000
C	4.885655000	0.000000000	0.000000000
C	5.593024000	0.943321000	-0.757509000
C	5.593024000	-0.943321000	0.757509000
C	6.985097000	0.936132000	-0.766739000
C	6.985097000	-0.936132000	0.766739000
C	7.684202000	0.000000000	0.000000000
C	-0.936132000	6.985097000	0.766739000
C	-0.936132000	-6.985097000	-0.766739000
C	-0.943321000	5.593024000	0.757509000
C	-0.943321000	-5.593024000	-0.757509000
C	-1.141166000	2.728506000	-0.469817000
C	-1.141166000	-2.728506000	0.469817000
C	-2.271190000	3.247470000	-1.225364000
C	-2.271190000	-3.247470000	1.225364000
C	-2.728506000	1.141166000	-0.469817000
C	-2.728506000	-1.141166000	0.469817000
C	-3.247470000	2.271190000	-1.225364000
C	-3.247470000	-2.271190000	1.225364000
C	-3.404352000	0.000000000	0.000000000
C	-4.885655000	0.000000000	0.000000000
C	-5.593024000	0.943321000	0.757509000
C	-5.593024000	-0.943321000	-0.757509000
C	-6.985097000	0.936132000	0.766739000
C	-6.985097000	-0.936132000	-0.766739000
C	-7.684202000	0.000000000	0.000000000
H	0.000000000	8.773770000	0.000000000
H	0.000000000	-8.773770000	0.000000000
H	1.665517000	7.526502000	-1.367099000
H	1.665517000	-7.526502000	1.367099000
H	1.673036000	5.037897000	-1.345247000
H	1.673036000	-5.037897000	1.345247000
H	5.037897000	1.673036000	-1.345247000
H	5.037897000	-1.673036000	1.345247000
H	7.526502000	1.665517000	-1.367099000
H	7.526502000	-1.665517000	1.367099000
H	8.773770000	0.000000000	0.000000000
H	-1.665517000	7.526502000	1.367099000
H	-1.665517000	-7.526502000	-1.367099000
H	-1.673036000	5.037897000	1.345247000
H	-1.673036000	-5.037897000	-1.345247000

H	-5.037897000	1.673036000	1.345247000
H	-5.037897000	-1.673036000	-1.345247000
H	-7.526502000	1.665517000	1.367099000
H	-7.526502000	-1.665517000	-1.367099000
H	-8.773770000	0.000000000	0.000000000
I	2.341673000	4.994847000	2.376183000
I	2.341673000	-4.994847000	-2.376183000
I	4.994847000	2.341673000	2.376183000
I	4.994847000	-2.341673000	-2.376183000
I	-2.341673000	4.994847000	-2.376183000
I	-2.341673000	-4.994847000	2.376183000
I	-4.994847000	2.341673000	-2.376183000
I	-4.994847000	-2.341673000	2.376183000
N	1.418713000	1.418713000	0.132745000
N	1.418713000	-1.418713000	-0.132745000
N	-1.418713000	1.418713000	-0.132745000
N	-1.418713000	-1.418713000	0.132745000

96. Pd(I₈TPP]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
C	0.590525000	4.181422000	-0.357417000
C	0.590525000	-4.181422000	0.357417000
C	1.027147000	2.790293000	-0.472496000
C	1.027147000	-2.790293000	0.472496000
C	2.320708000	2.320708000	-0.784947000
C	2.320708000	-2.320708000	0.784947000
C	2.790293000	1.027147000	-0.472496000
C	2.790293000	-1.027147000	0.472496000
C	3.305660000	3.305660000	-1.316739000
C	3.305660000	-3.305660000	1.316739000
C	3.463903000	3.463903000	-2.696695000
C	3.463903000	-3.463903000	2.696695000
C	4.077365000	4.077365000	-0.439477000
C	4.077365000	-4.077365000	0.439477000
C	4.181422000	0.590525000	-0.357417000
C	4.181422000	-0.590525000	0.357417000
C	4.384490000	4.384490000	-3.194681000
C	4.384490000	-4.384490000	3.194681000
C	4.997300000	4.997300000	-0.936122000
C	4.997300000	-4.997300000	0.936122000
C	5.152226000	5.152226000	-2.315249000
C	5.152226000	-5.152226000	2.315249000
C	-0.590525000	4.181422000	0.357417000
C	-0.590525000	-4.181422000	-0.357417000
C	-1.027147000	2.790293000	0.472496000
C	-1.027147000	-2.790293000	-0.472496000
C	-2.320708000	2.320708000	0.784947000
C	-2.320708000	-2.320708000	-0.784947000
C	-2.790293000	1.027147000	0.472496000

C	-2.790293000	-1.027147000	-0.472496000
C	-3.305660000	3.305660000	1.316739000
C	-3.305660000	-3.305660000	-1.316739000
C	-3.463903000	3.463903000	2.696695000
C	-3.463903000	-3.463903000	-2.696695000
C	-4.077365000	4.077365000	0.439477000
C	-4.077365000	-4.077365000	-0.439477000
C	-4.181422000	0.590525000	0.357417000
C	-4.181422000	-0.590525000	-0.357417000
C	-4.384490000	4.384490000	3.194681000
C	-4.384490000	-4.384490000	-3.194681000
C	-4.997300000	4.997300000	0.936122000
C	-4.997300000	-4.997300000	-0.936122000
C	-5.152226000	5.152226000	2.315249000
C	-5.152226000	-5.152226000	-2.315249000
H	2.861143000	2.861143000	-3.374442000
H	2.861143000	-2.861143000	3.374442000
H	3.947262000	3.947262000	0.633924000
H	3.947262000	-3.947262000	-0.633924000
H	4.503065000	4.503065000	-4.270568000
H	4.503065000	-4.503065000	4.270568000
H	5.592989000	5.592989000	-0.246615000
H	5.592989000	-5.592989000	0.246615000
H	5.871416000	5.871416000	-2.706059000
H	5.871416000	-5.871416000	2.706059000
H	-2.861143000	2.861143000	3.374442000
H	-2.861143000	-2.861143000	-3.374442000
H	-3.947262000	3.947262000	-0.633924000
H	-3.947262000	-3.947262000	0.633924000
H	-4.503065000	4.503065000	4.270568000
H	-4.503065000	-4.503065000	-4.270568000
H	-5.592989000	5.592989000	0.246615000
H	-5.592989000	-5.592989000	-0.246615000
H	-5.871416000	5.871416000	2.706059000
H	-5.871416000	-5.871416000	-2.706059000
I	1.357754000	5.935927000	-1.216319000
I	1.357754000	-5.935927000	1.216319000
I	5.935927000	1.357754000	-1.216319000
I	5.935927000	-1.357754000	1.216319000
I	-1.357754000	5.935927000	1.216319000
I	-1.357754000	-5.935927000	-1.216319000
I	-5.935927000	1.357754000	1.216319000
I	-5.935927000	-1.357754000	-1.216319000
N	0.000000000	1.999111000	0.000000000
N	0.000000000	-1.999111000	0.000000000
N	1.999111000	0.000000000	0.000000000
N	-1.999111000	0.000000000	0.000000000

97. Pt(I₈TPP]; S = 0 (saddled)

Pt	0.000000000	0.000000000	0.000000000
C	0.000000000	3.406586000	0.000000000
C	0.000000000	4.889677000	0.000000000
C	0.000000000	7.687884000	0.000000000
C	0.000000000	-3.406586000	0.000000000
C	0.000000000	-4.889677000	0.000000000
C	0.000000000	-7.687884000	0.000000000
C	0.913005000	6.988815000	-0.794039000
C	0.913005000	-6.988815000	0.794039000
C	0.920010000	5.596616000	-0.785486000
C	0.920010000	-5.596616000	0.785486000
C	1.144719000	2.735711000	0.467747000
C	1.144719000	-2.735711000	-0.467747000
C	2.289107000	3.264726000	1.192737000
C	2.289107000	-3.264726000	-1.192737000
C	2.735711000	1.144719000	0.467747000
C	2.735711000	-1.144719000	-0.467747000
C	3.264726000	2.289107000	1.192737000
C	3.264726000	-2.289107000	-1.192737000
C	3.406586000	0.000000000	0.000000000
C	4.889677000	0.000000000	0.000000000
C	5.596616000	0.920010000	-0.785486000
C	5.596616000	-0.920010000	0.785486000
C	6.988815000	0.913005000	-0.794039000
C	6.988815000	-0.913005000	0.794039000
C	7.687884000	0.000000000	0.000000000
C	-0.913005000	6.988815000	0.794039000
C	-0.913005000	-6.988815000	-0.794039000
C	-0.920010000	5.596616000	0.785486000
C	-0.920010000	-5.596616000	-0.785486000
C	-1.144719000	2.735711000	-0.467747000
C	-1.144719000	-2.735711000	0.467747000
C	-2.289107000	3.264726000	-1.192737000
C	-2.289107000	-3.264726000	1.192737000
C	-2.735711000	1.144719000	-0.467747000
C	-2.735711000	-1.144719000	0.467747000
C	-3.264726000	2.289107000	-1.192737000
C	-3.264726000	-2.289107000	1.192737000
C	-3.406586000	0.000000000	0.000000000
C	-4.889677000	0.000000000	0.000000000
C	-5.596616000	0.920010000	0.785486000
C	-5.596616000	-0.920010000	-0.785486000
C	-6.988815000	0.913005000	0.794039000
C	-6.988815000	-0.913005000	-0.794039000
C	-7.687884000	0.000000000	0.000000000
H	0.000000000	8.777447000	0.000000000
H	0.000000000	-8.777447000	0.000000000
H	1.624591000	7.530202000	-1.415388000

H	1.624591000	-7.530202000	1.415388000
H	1.631755000	5.041426000	-1.394844000
H	1.631755000	-5.041426000	1.394844000
H	5.041426000	1.631755000	-1.394844000
H	5.041426000	-1.631755000	1.394844000
H	7.530202000	1.624591000	-1.415388000
H	7.530202000	-1.624591000	1.415388000
H	8.777447000	0.000000000	0.000000000
H	-1.624591000	7.530202000	1.415388000
H	-1.624591000	-7.530202000	-1.415388000
H	-1.631755000	5.041426000	1.394844000
H	-1.631755000	-5.041426000	-1.394844000
H	-5.041426000	1.631755000	1.394844000
H	-5.041426000	-1.631755000	-1.394844000
H	-7.530202000	1.624591000	1.415388000
H	-7.530202000	-1.624591000	-1.415388000
H	-8.777447000	0.000000000	0.000000000
I	2.382785000	5.027539000	2.318059000
I	2.382785000	-5.027539000	-2.318059000
I	5.027539000	2.382785000	2.318059000
I	5.027539000	-2.382785000	-2.318059000
I	-2.382785000	5.027539000	-2.318059000
I	-2.382785000	-5.027539000	2.318059000
I	-5.027539000	2.382785000	-2.318059000
I	-5.027539000	-2.382785000	2.318059000
N	1.412916000	1.412916000	0.163626000
N	1.412916000	-1.412916000	-0.163626000
N	-1.412916000	1.412916000	-0.163626000
N	-1.412916000	-1.412916000	0.163626000

98. Pt(I₈TPP]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
C	0.594076000	4.185465000	-0.350631000
C	0.594076000	-4.185465000	0.350631000
C	1.032792000	2.796954000	-0.463469000
C	1.032792000	-2.796954000	0.463469000
C	2.327714000	2.327714000	-0.769619000
C	2.327714000	-2.327714000	0.769619000
C	2.796954000	1.032792000	-0.463469000
C	2.796954000	-1.032792000	0.463469000
C	3.315487000	3.315487000	-1.291833000
C	3.315487000	-3.315487000	1.291833000
C	3.480076000	3.480076000	-2.670394000
C	3.480076000	-3.480076000	2.670394000
C	4.082972000	4.082972000	-0.407174000
C	4.082972000	-4.082972000	0.407174000
C	4.185465000	0.594076000	-0.350631000
C	4.185465000	-0.594076000	0.350631000
C	4.402981000	4.402981000	-3.159689000

C	4.402981000	-4.402981000	3.159689000
C	5.005212000	5.005212000	-0.895285000
C	5.005212000	-5.005212000	0.895285000
C	5.166541000	5.166541000	-2.272964000
C	5.166541000	-5.166541000	2.272964000
C	-0.594076000	4.185465000	0.350631000
C	-0.594076000	-4.185465000	-0.350631000
C	-1.032792000	2.796954000	0.463469000
C	-1.032792000	-2.796954000	-0.463469000
C	-2.327714000	2.327714000	0.769619000
C	-2.327714000	-2.327714000	-0.769619000
C	-2.796954000	1.032792000	0.463469000
C	-2.796954000	-1.032792000	-0.463469000
C	-3.315487000	3.315487000	1.291833000
C	-3.315487000	-3.315487000	-1.291833000
C	-3.480076000	3.480076000	2.670394000
C	-3.480076000	-3.480076000	-2.670394000
C	-4.082972000	4.082972000	0.407174000
C	-4.082972000	-4.082972000	-0.407174000
C	-4.185465000	0.594076000	0.350631000
C	-4.185465000	-0.594076000	-0.350631000
C	-4.402981000	4.402981000	3.159689000
C	-4.402981000	-4.402981000	-3.159689000
C	-5.005212000	5.005212000	0.895285000
C	-5.005212000	-5.005212000	-0.895285000
C	-5.166541000	5.166541000	2.272964000
C	-5.166541000	-5.166541000	-2.272964000
H	2.880344000	2.880344000	-3.353506000
H	2.880344000	-2.880344000	3.353506000
H	3.947685000	3.947685000	0.664950000
H	3.947685000	-3.947685000	-0.664950000
H	4.526703000	4.526703000	-4.234414000
H	4.526703000	-4.526703000	4.234414000
H	5.597752000	5.597752000	-0.200345000
H	5.597752000	-5.597752000	0.200345000
H	5.887573000	5.887573000	-2.657001000
H	5.887573000	-5.887573000	2.657001000
H	-2.880344000	2.880344000	3.353506000
H	-2.880344000	-2.880344000	-3.353506000
H	-3.947685000	3.947685000	-0.664950000
H	-3.947685000	-3.947685000	0.664950000
H	-4.526703000	4.526703000	4.234414000
H	-4.526703000	-4.526703000	-4.234414000
H	-5.597752000	5.597752000	0.200345000
H	-5.597752000	-5.597752000	-0.200345000
H	-5.887573000	5.887573000	2.657001000
H	-5.887573000	-5.887573000	-2.657001000
I	1.370170000	5.941512000	-1.198420000
I	1.370170000	-5.941512000	1.198420000
I	5.941512000	1.370170000	-1.198420000
I	5.941512000	-1.370170000	1.198420000

I	-1.370170000	5.941512000	1.198420000
I	-1.370170000	-5.941512000	-1.198420000
I	-5.941512000	1.370170000	1.198420000
I	-5.941512000	-1.370170000	-1.198420000
N	0.000000000	2.002190000	0.000000000
N	0.000000000	-2.002190000	0.000000000
N	2.002190000	0.000000000	0.000000000
N	-2.002190000	0.000000000	0.000000000

99. Zn(I₈TPP]; S = 0 (saddled)

Zn	0.000000000	0.000000000	0.000000000
C	0.000000000	3.411249000	0.000000000
C	0.000000000	4.892780000	0.000000000
C	0.000000000	7.692654000	0.000000000
C	0.000000000	-3.411249000	0.000000000
C	0.000000000	-4.892780000	0.000000000
C	0.000000000	-7.692654000	0.000000000
C	0.922493000	6.993294000	-0.782904000
C	0.922493000	-6.993294000	0.782904000
C	0.929321000	5.601267000	-0.774193000
C	0.929321000	-5.601267000	0.774193000
C	1.156893000	2.739852000	0.456748000
C	1.156893000	-2.739852000	-0.456748000
C	2.291593000	3.270138000	1.196391000
C	2.291593000	-3.270138000	-1.196391000
C	2.739852000	1.156893000	0.456748000
C	2.739852000	-1.156893000	-0.456748000
C	3.270138000	2.291593000	1.196391000
C	3.270138000	-2.291593000	-1.196391000
C	3.411249000	0.000000000	0.000000000
C	4.892780000	0.000000000	0.000000000
C	5.601267000	0.929321000	-0.774193000
C	5.601267000	-0.929321000	0.774193000
C	6.993294000	0.922493000	-0.782904000
C	6.993294000	-0.922493000	0.782904000
C	7.692654000	0.000000000	0.000000000
C	-0.922493000	6.993294000	0.782904000
C	-0.922493000	-6.993294000	-0.782904000
C	-0.929321000	5.601267000	0.774193000
C	-0.929321000	-5.601267000	-0.774193000
C	-1.156893000	2.739852000	-0.456748000
C	-1.156893000	-2.739852000	0.456748000
C	-2.291593000	3.270138000	-1.196391000
C	-2.291593000	-3.270138000	1.196391000
C	-2.739852000	1.156893000	-0.456748000
C	-2.739852000	-1.156893000	0.456748000
C	-3.270138000	2.291593000	-1.196391000
C	-3.270138000	-2.291593000	1.196391000
C	-3.411249000	0.000000000	0.000000000

C	-4.892780000	0.000000000	0.000000000
C	-5.601267000	0.929321000	0.774193000
C	-5.601267000	-0.929321000	-0.774193000
C	-6.993294000	0.922493000	0.782904000
C	-6.993294000	-0.922493000	-0.782904000
C	-7.692654000	0.000000000	0.000000000
H	0.000000000	8.782219000	0.000000000
H	0.000000000	-8.782219000	0.000000000
H	1.641331000	7.534614000	-1.395988000
H	1.641331000	-7.534614000	1.395988000
H	1.648025000	5.046588000	-1.375757000
H	1.648025000	-5.046588000	1.375757000
H	5.046588000	1.648025000	-1.375757000
H	5.046588000	-1.648025000	1.375757000
H	7.534614000	1.641331000	-1.395988000
H	7.534614000	-1.641331000	1.395988000
H	8.782219000	0.000000000	0.000000000
H	-1.641331000	7.534614000	1.395988000
H	-1.641331000	-7.534614000	-1.395988000
H	-1.648025000	5.046588000	1.375757000
H	-1.648025000	-5.046588000	-1.375757000
H	-5.046588000	1.648025000	1.375757000
H	-5.046588000	-1.648025000	-1.375757000
H	-7.534614000	1.641331000	1.395988000
H	-7.534614000	-1.641331000	-1.395988000
H	-8.782219000	0.000000000	0.000000000
I	2.382525000	5.026849000	2.333404000
I	2.382525000	-5.026849000	-2.333404000
I	5.026849000	2.382525000	2.333404000
I	5.026849000	-2.382525000	-2.333404000
I	-2.382525000	5.026849000	-2.333404000
I	-2.382525000	-5.026849000	2.333404000
I	-5.026849000	2.382525000	-2.333404000
I	-5.026849000	-2.382525000	2.333404000
N	1.431361000	1.431361000	0.129191000
N	1.431361000	-1.431361000	-0.129191000
N	-1.431361000	1.431361000	-0.129191000
N	-1.431361000	-1.431361000	0.129191000

100. Zn(I₈TPP]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
C	0.602176000	4.203095000	-0.340533000
C	0.602176000	-4.203095000	0.340533000
C	1.036837000	2.812091000	-0.443401000
C	1.036837000	-2.812091000	0.443401000
C	2.337280000	2.337280000	-0.739656000
C	2.337280000	-2.337280000	0.739656000
C	2.812091000	1.036837000	-0.443401000
C	2.812091000	-1.036837000	0.443401000

C	3.329744000	3.329744000	-1.244875000
C	3.329744000	-3.329744000	1.244875000
C	3.507354000	3.507354000	-2.620229000
C	3.507354000	-3.507354000	2.620229000
C	4.089425000	4.089425000	-0.346973000
C	4.089425000	-4.089425000	0.346973000
C	4.203095000	0.602176000	-0.340533000
C	4.203095000	-0.602176000	0.340533000
C	4.434398000	4.434398000	-3.093252000
C	4.434398000	-4.434398000	3.093252000
C	5.016041000	5.016041000	-0.818553000
C	5.016041000	-5.016041000	0.818553000
C	5.189967000	5.189967000	-2.193138000
C	5.189967000	-5.189967000	2.193138000
C	-0.602176000	4.203095000	0.340533000
C	-0.602176000	-4.203095000	-0.340533000
C	-1.036837000	2.812091000	0.443401000
C	-1.036837000	-2.812091000	-0.443401000
C	-2.337280000	2.337280000	0.739656000
C	-2.337280000	-2.337280000	-0.739656000
C	-2.812091000	1.036837000	0.443401000
C	-2.812091000	-1.036837000	-0.443401000
C	-3.329744000	3.329744000	1.244875000
C	-3.329744000	-3.329744000	-1.244875000
C	-3.507354000	3.507354000	2.620229000
C	-3.507354000	-3.507354000	-2.620229000
C	-4.089425000	4.089425000	0.346973000
C	-4.089425000	-4.089425000	-0.346973000
C	-4.203095000	0.602176000	0.340533000
C	-4.203095000	-0.602176000	-0.340533000
C	-4.434398000	4.434398000	3.093252000
C	-4.434398000	-4.434398000	-3.093252000
C	-5.016041000	5.016041000	0.818553000
C	-5.016041000	-5.016041000	-0.818553000
C	-5.189967000	5.189967000	2.193138000
C	-5.189967000	-5.189967000	-2.193138000
H	2.914182000	2.914182000	-3.314697000
H	2.914182000	-2.914182000	3.314697000
H	3.944923000	3.944923000	0.722724000
H	3.944923000	-3.944923000	-0.722724000
H	4.567518000	4.567518000	-4.165714000
H	4.567518000	-4.567518000	4.165714000
H	5.602242000	5.602242000	-0.112863000
H	5.602242000	-5.602242000	0.112863000
H	5.914410000	5.914410000	-2.564050000
H	5.914410000	-5.914410000	2.564050000
H	-2.914182000	2.914182000	3.314697000
H	-2.914182000	-2.914182000	-3.314697000
H	-3.944923000	3.944923000	-0.722724000
H	-3.944923000	-3.944923000	0.722724000
H	-4.567518000	4.567518000	4.165714000

H	-4.567518000	-4.567518000	-4.165714000
H	-5.602242000	5.602242000	0.112863000
H	-5.602242000	-5.602242000	-0.112863000
H	-5.914410000	5.914410000	2.564050000
H	-5.914410000	-5.914410000	-2.564050000
I	1.384605000	5.964709000	-1.175941000
I	1.384605000	-5.964709000	1.175941000
I	5.964709000	1.384605000	-1.175941000
I	5.964709000	-1.384605000	1.175941000
I	-1.384605000	5.964709000	1.175941000
I	-1.384605000	-5.964709000	-1.175941000
I	-5.964709000	1.384605000	1.175941000
I	-5.964709000	-1.384605000	-1.175941000
N	0.000000000	2.017293000	0.000000000
N	0.000000000	-2.017293000	0.000000000
N	2.017293000	0.000000000	0.000000000
N	-2.017293000	0.000000000	0.000000000

101. Cu[A₄Me₈]; S = ½ (saddled)

Cu	0.006651000	0.058588000	0.000000000
C	0.581469000	-1.042934000	4.013680000
C	0.581469000	-1.042934000	-4.013680000
C	1.055124000	-0.497036000	2.754935000
C	1.055124000	-0.497036000	-2.754935000
C	1.390752000	-1.682265000	5.100584000
C	1.390752000	-1.682265000	-5.100584000
C	2.392585000	-0.203242000	2.398519000
C	2.392585000	-0.203242000	-2.398519000
C	2.786609000	0.205011000	1.101807000
C	2.786609000	0.205011000	-1.101807000
C	3.395882000	-0.338052000	3.385300000
C	3.395882000	-0.338052000	-3.385300000
C	4.099349000	0.664669000	0.689522000
C	4.099349000	0.664669000	-0.689522000
C	4.268288000	-0.466082000	4.234962000
C	4.268288000	-0.466082000	-4.234962000
C	5.127583000	0.314999000	7.019992000
C	5.127583000	0.314999000	-7.019992000
C	5.234812000	1.104264000	1.561884000
C	5.234812000	1.104264000	-1.561884000
C	5.641957000	-2.527601000	5.935125000
C	5.641957000	-2.527601000	-5.935125000
C	7.203139000	-0.117315000	4.760518000
C	7.203139000	-0.117315000	-4.760518000
C	-0.789756000	-0.895747000	4.013539000
C	-0.789756000	-0.895747000	-4.013539000
C	-1.136531000	-0.261891000	2.754668000
C	-1.136531000	-0.261891000	-2.754668000
C	-1.716376000	-1.348612000	5.100439000

C	-1.716376000	-1.348612000	-5.100439000
C	-2.381027000	0.309171000	2.398083000
C	-2.381027000	0.309171000	-2.398083000
C	-2.678525000	0.793132000	1.101715000
C	-2.678525000	0.793132000	-1.101715000
C	-3.391237000	0.388281000	3.383820000
C	-3.391237000	0.388281000	-3.383820000
C	-3.862954000	1.522307000	0.689524000
C	-3.862954000	1.522307000	-0.689524000
C	-4.272056000	0.445509000	4.232517000
C	-4.272056000	0.445509000	-4.232517000
C	-4.878022000	2.194320000	1.562175000
C	-4.878022000	2.194320000	-1.562175000
C	-4.939285000	1.366557000	7.027030000
C	-4.939285000	1.366557000	-7.027030000
C	-6.063667000	-1.282854000	5.915223000
C	-6.063667000	-1.282854000	-5.915223000
C	-7.059572000	1.422124000	4.767595000
C	-7.059572000	1.422124000	-4.767595000
H	0.746475000	-2.278117000	5.757970000
H	0.746475000	-2.278117000	-5.757970000
H	1.901951000	-0.932388000	5.719996000
H	1.901951000	-0.932388000	-5.719996000
H	2.168094000	-2.339188000	4.693818000
H	2.168094000	-2.339188000	-4.693818000
H	4.160789000	-0.007657000	7.432733000
H	4.160789000	-0.007657000	-7.432733000
H	4.674293000	-2.868232000	6.331055000
H	4.674293000	-2.868232000	-6.331055000
H	4.883709000	1.679843000	2.425840000
H	4.883709000	1.679843000	-2.425840000
H	5.050655000	1.383549000	6.773700000
H	5.050655000	1.383549000	-6.773700000
H	5.797181000	0.248627000	1.960246000
H	5.797181000	0.248627000	-1.960246000
H	5.878089000	-3.133819000	5.049074000
H	5.878089000	-3.133819000	-5.049074000
H	5.891747000	0.194660000	7.803073000
H	5.891747000	0.194660000	-7.803073000
H	5.934407000	1.728909000	0.993455000
H	5.934407000	1.728909000	-0.993455000
H	6.411252000	-2.716542000	6.699415000
H	6.411252000	-2.716542000	-6.699415000
H	7.138836000	0.935675000	4.451116000
H	7.138836000	0.935675000	-4.451116000
H	7.467034000	-0.715272000	3.876429000
H	7.467034000	-0.715272000	-3.876429000
H	8.018311000	-0.211199000	5.493983000
H	8.018311000	-0.211199000	-5.493983000
H	-1.212902000	-2.066426000	5.758863000
H	-1.212902000	-2.066426000	-5.758863000

H	-2.057946000	-0.507065000	5.718847000
H	-2.057946000	-0.507065000	-5.718847000
H	-2.614737000	-1.826929000	4.693713000
H	-2.614737000	-1.826929000	-4.693713000
H	-4.066876000	0.835253000	7.434207000
H	-4.066876000	0.835253000	-7.434207000
H	-4.411781000	2.681030000	2.426351000
H	-4.411781000	2.681030000	-2.426351000
H	-4.629701000	2.394665000	6.791437000
H	-4.629701000	2.394665000	-6.791437000
H	-5.194149000	-1.830706000	6.306335000
H	-5.194149000	-1.830706000	-6.306335000
H	-5.427737000	2.954507000	0.994110000
H	-5.427737000	2.954507000	-0.994110000
H	-5.610454000	1.478705000	1.960305000
H	-5.610454000	1.478705000	-1.960305000
H	-5.711142000	1.408650000	7.810684000
H	-5.711142000	1.408650000	-7.810684000
H	-6.426108000	-1.814064000	5.023726000
H	-6.426108000	-1.814064000	-5.023726000
H	-6.766574000	2.438601000	4.468354000
H	-6.766574000	2.438601000	-4.468354000
H	-6.856099000	-1.306478000	6.678869000
H	-6.856099000	-1.306478000	-6.678869000
H	-7.447645000	0.905172000	3.878239000
H	-7.447645000	0.905172000	-3.878239000
H	-7.875698000	1.501325000	5.501695000
H	-7.875698000	1.501325000	-5.501695000
N	1.985231000	0.028146000	0.000000000
N	-0.012488000	-0.117452000	1.978221000
N	-0.012488000	-0.117452000	-1.978221000
N	-1.933009000	0.449992000	0.000000000
Si	5.568949000	-0.697695000	5.495361000
Si	5.568949000	-0.697695000	-5.495361000
Si	-5.591997000	0.491056000	5.493284000
Si	-5.591997000	0.491056000	-5.493284000

102. Cu[A₄Me₈]; S = ½ (ruffled)

Cu	0.000000000	0.000000000	0.000000000
C	0.635265000	4.187980000	0.268891000
C	0.635265000	-4.187980000	-0.268891000
C	1.030786000	2.796083000	0.393367000
C	1.030786000	-2.796083000	-0.393367000
C	1.448740000	5.406212000	0.584019000
C	1.448740000	-5.406212000	-0.584019000
C	2.322336000	2.322336000	0.731024000
C	2.322336000	-2.322336000	-0.731024000
C	2.796083000	1.030786000	0.393367000
C	2.796083000	-1.030786000	-0.393367000

C	3.197235000	3.197235000	1.413108000
C	3.197235000	-3.197235000	-1.413108000
C	3.930033000	3.930033000	2.065802000
C	3.930033000	-3.930033000	-2.065802000
C	4.030087000	6.226963000	4.008295000
C	4.030087000	-6.226963000	-4.008295000
C	4.187980000	0.635265000	0.268891000
C	4.187980000	-0.635265000	-0.268891000
C	5.406212000	1.448740000	0.584019000
C	5.406212000	-1.448740000	-0.584019000
C	6.035596000	6.035596000	1.664965000
C	6.035596000	-6.035596000	-1.664965000
C	6.226963000	4.030087000	4.008295000
C	6.226963000	-4.030087000	-4.008295000
C	-0.635265000	4.187980000	-0.268891000
C	-0.635265000	-4.187980000	0.268891000
C	-1.030786000	2.796083000	-0.393367000
C	-1.030786000	-2.796083000	0.393367000
C	-1.448740000	5.406212000	-0.584019000
C	-1.448740000	-5.406212000	0.584019000
C	-2.322336000	2.322336000	-0.731024000
C	-2.322336000	-2.322336000	0.731024000
C	-2.796083000	1.030786000	-0.393367000
C	-2.796083000	-1.030786000	0.393367000
C	-3.197235000	3.197235000	-1.413108000
C	-3.197235000	-3.197235000	1.413108000
C	-3.930033000	3.930033000	-2.065802000
C	-3.930033000	-3.930033000	2.065802000
C	-4.030087000	6.226963000	-4.008295000
C	-4.030087000	-6.226963000	4.008295000
C	-4.187980000	0.635265000	-0.268891000
C	-4.187980000	-0.635265000	0.268891000
C	-5.406212000	1.448740000	-0.584019000
C	-5.406212000	-1.448740000	0.584019000
C	-6.035596000	6.035596000	-1.664965000
C	-6.035596000	-6.035596000	1.664965000
C	-6.226963000	4.030087000	-4.008295000
C	-6.226963000	-4.030087000	4.008295000
H	0.944249000	6.311374000	0.228724000
H	0.944249000	-6.311374000	-0.228724000
H	1.622105000	5.510005000	1.663183000
H	1.622105000	-5.510005000	-1.663183000
H	2.437608000	5.364069000	0.110290000
H	2.437608000	-5.364069000	-0.110290000
H	3.343287000	6.813924000	3.381325000
H	3.343287000	-6.813924000	-3.381325000
H	3.428349000	5.665796000	4.737217000
H	3.428349000	-5.665796000	-4.737217000
H	4.674760000	6.928730000	4.559064000
H	4.674760000	-6.928730000	-4.559064000
H	5.359790000	6.617541000	1.021977000

H	5.359790000	-6.617541000	-1.021977000
H	5.364069000	2.437608000	0.110290000
H	5.364069000	-2.437608000	-0.110290000
H	5.510005000	1.622105000	1.663183000
H	5.510005000	-1.622105000	-1.663183000
H	5.665796000	3.428349000	4.737217000
H	5.665796000	-3.428349000	-4.737217000
H	6.311374000	0.944249000	0.228724000
H	6.311374000	-0.944249000	-0.228724000
H	6.617541000	5.359790000	1.021977000
H	6.617541000	-5.359790000	-1.021977000
H	6.733764000	6.733764000	2.151729000
H	6.733764000	-6.733764000	-2.151729000
H	6.813924000	3.343287000	3.381325000
H	6.813924000	-3.343287000	-3.381325000
H	6.928730000	4.674760000	4.559064000
H	6.928730000	-4.674760000	-4.559064000
H	-0.944249000	6.311374000	-0.228724000
H	-0.944249000	-6.311374000	0.228724000
H	-1.622105000	5.510005000	-1.663183000
H	-1.622105000	-5.510005000	1.663183000
H	-2.437608000	5.364069000	-0.110290000
H	-2.437608000	-5.364069000	0.110290000
H	-3.343287000	6.813924000	-3.381325000
H	-3.343287000	-6.813924000	3.381325000
H	-3.428349000	5.665796000	-4.737217000
H	-3.428349000	-5.665796000	4.737217000
H	-4.674760000	6.928730000	-4.559064000
H	-4.674760000	-6.928730000	4.559064000
H	-5.359790000	6.617541000	-1.021977000
H	-5.359790000	-6.617541000	1.021977000
H	-5.364069000	2.437608000	-0.110290000
H	-5.364069000	-2.437608000	0.110290000
H	-5.510005000	1.622105000	-1.663183000
H	-5.510005000	-1.622105000	1.663183000
H	-5.665796000	3.428349000	-4.737217000
H	-5.665796000	-3.428349000	4.737217000
H	-6.311374000	0.944249000	-0.228724000
H	-6.311374000	-0.944249000	0.228724000
H	-6.617541000	5.359790000	-1.021977000
H	-6.617541000	-5.359790000	1.021977000
H	-6.733764000	6.733764000	-2.151729000
H	-6.733764000	-6.733764000	2.151729000
H	-6.813924000	3.343287000	-3.381325000
H	-6.813924000	-3.343287000	3.381325000
H	-6.928730000	4.674760000	-4.559064000
H	-6.928730000	-4.674760000	4.559064000
N	0.000000000	1.981277000	0.000000000
N	0.000000000	-1.981277000	0.000000000
N	1.981277000	0.000000000	0.000000000
N	-1.981277000	0.000000000	0.000000000

Si	5.060523000	5.060523000	2.949212000
Si	5.060523000	-5.060523000	-2.949212000
Si	-5.060523000	5.060523000	-2.949212000
Si	-5.060523000	-5.060523000	2.949212000

103. Ni [A₄Me₈]; S = 0 (saddled)

Ni	0.005051000	0.049561000	0.000000000
C	0.564433000	-1.203191000	3.890328000
C	0.564433000	-1.203191000	-3.890328000
C	1.043296000	-0.587474000	2.671413000
C	1.043296000	-0.587474000	-2.671413000
C	1.378035000	-1.890016000	4.943999000
C	1.378035000	-1.890016000	-4.943999000
C	2.364012000	-0.207374000	2.370112000
C	2.364012000	-0.207374000	-2.370112000
C	2.715359000	0.284815000	1.099424000
C	2.715359000	0.284815000	-1.099424000
C	3.365071000	-0.334501000	3.359444000
C	3.365071000	-0.334501000	-3.359444000
C	3.998407000	0.812385000	0.688571000
C	3.998407000	0.812385000	-0.688571000
C	4.235511000	-0.454147000	4.211916000
C	4.235511000	-0.454147000	-4.211916000
C	5.108860000	1.294106000	1.570353000
C	5.108860000	1.294106000	-1.570353000
C	5.122465000	0.336100000	6.989155000
C	5.122465000	0.336100000	-6.989155000
C	5.631258000	-2.507435000	5.901569000
C	5.631258000	-2.507435000	-5.901569000
C	7.172351000	-0.092406000	4.707721000
C	7.172351000	-0.092406000	-4.707721000
C	-0.805064000	-1.057625000	3.890420000
C	-0.805064000	-1.057625000	-3.890420000
C	-1.143882000	-0.354954000	2.671543000
C	-1.143882000	-0.354954000	-2.671543000
C	-1.744951000	-1.557950000	4.944102000
C	-1.744951000	-1.557950000	-4.944102000
C	-2.355115000	0.294463000	2.370241000
C	-2.355115000	0.294463000	-2.370241000
C	-2.595065000	0.849380000	1.099454000
C	-2.595065000	0.849380000	-1.099454000
C	-3.360225000	0.381712000	3.359816000
C	-3.360225000	0.381712000	-3.359816000
C	-3.738102000	1.635528000	0.688577000
C	-3.738102000	1.635528000	-0.688577000
C	-4.236342000	0.448968000	4.212223000
C	-4.236342000	0.448968000	-4.212223000
C	-4.721881000	2.340776000	1.570312000
C	-4.721881000	2.340776000	-1.570312000

C	-4.925047000	1.392227000	6.997489000
C	-4.925047000	1.392227000	-6.997489000
C	-6.051259000	-1.259140000	5.889043000
C	-6.051259000	-1.259140000	-5.889043000
C	-7.020580000	1.446179000	4.717639000
C	-7.020580000	1.446179000	-4.717639000
H	0.742926000	-2.554012000	5.543067000
H	0.742926000	-2.554012000	-5.543067000
H	1.849564000	-1.169341000	5.626702000
H	1.849564000	-1.169341000	-5.626702000
H	2.186092000	-2.487770000	4.507021000
H	2.186092000	-2.487770000	-4.507021000
H	4.161347000	0.012902000	7.414365000
H	4.161347000	0.012902000	-7.414365000
H	4.667428000	-2.851575000	6.303754000
H	4.667428000	-2.851575000	-6.303754000
H	4.727219000	1.828624000	2.447775000
H	4.727219000	1.828624000	-2.447775000
H	5.040927000	1.404074000	6.741764000
H	5.040927000	1.404074000	-6.741764000
H	5.719835000	0.462248000	1.947513000
H	5.719835000	0.462248000	-1.947513000
H	5.770257000	1.970401000	1.014900000
H	5.770257000	1.970401000	-1.014900000
H	5.863904000	-3.112982000	5.014109000
H	5.863904000	-3.112982000	-5.014109000
H	5.896621000	0.218726000	7.762834000
H	5.896621000	0.218726000	-7.762834000
H	6.406190000	-2.693434000	6.660826000
H	6.406190000	-2.693434000	-6.660826000
H	7.101714000	0.961755000	4.403502000
H	7.101714000	0.961755000	-4.403502000
H	7.425218000	-0.686426000	3.817780000
H	7.425218000	-0.686426000	-3.817780000
H	7.997430000	-0.187257000	5.429881000
H	7.997430000	-0.187257000	-5.429881000
H	-1.263918000	-2.341001000	5.542905000
H	-1.263918000	-2.341001000	-5.542905000
H	-2.054025000	-0.754249000	5.627009000
H	-2.054025000	-0.754249000	-5.627009000
H	-2.660802000	-1.971926000	4.507006000
H	-2.660802000	-1.971926000	-4.507006000
H	-4.058935000	0.860866000	7.417645000
H	-4.058935000	0.860866000	-7.417645000
H	-4.235920000	2.783333000	2.447360000
H	-4.235920000	2.783333000	-2.447360000
H	-4.609408000	2.417701000	6.758324000
H	-4.609408000	2.417701000	-6.758324000
H	-5.187601000	-1.811096000	6.287261000
H	-5.187601000	-1.811096000	-6.287261000
H	-5.226118000	3.140950000	1.014634000

H	-5.226118000	3.140950000	-1.014634000
H	-5.494283000	1.656537000	1.948101000
H	-5.494283000	1.656537000	-1.948101000
H	-5.705370000	1.442598000	7.772231000
H	-5.705370000	1.442598000	-7.772231000
H	-6.411857000	-1.791320000	4.997336000
H	-6.411857000	-1.791320000	-4.997336000
H	-6.718852000	2.460912000	4.420936000
H	-6.718852000	2.460912000	-4.420936000
H	-6.848395000	-1.274932000	6.647968000
H	-6.848395000	-1.274932000	-6.647968000
H	-7.399442000	0.929706000	3.824041000
H	-7.399442000	0.929706000	-3.824041000
H	-7.845555000	1.530532000	5.441207000
H	-7.845555000	1.530532000	-5.441207000
N	1.906124000	0.087693000	0.000000000
N	-0.020073000	-0.186796000	1.889497000
N	-0.020073000	-0.186796000	-1.889497000
N	-1.845545000	0.486228000	0.000000000
Si	5.548475000	-0.678044000	5.461207000
Si	5.548475000	-0.678044000	-5.461207000
Si	-5.565840000	0.510026000	5.462646000
Si	-5.565840000	0.510026000	-5.462646000

104. Ni [A₄Me₈]; S = 0 (ruffled)

Ni	0.000000000	0.000000000	0.000000000
C	0.592060000	4.099409000	0.353554000
C	0.592060000	-4.099409000	-0.353554000
C	0.974897000	2.710827000	0.515097000
C	0.974897000	-2.710827000	-0.515097000
C	1.357349000	5.308501000	0.796136000
C	1.357349000	-5.308501000	-0.796136000
C	2.237454000	2.237454000	0.931392000
C	2.237454000	-2.237454000	-0.931392000
C	2.710827000	0.974897000	0.515097000
C	2.710827000	-0.974897000	-0.515097000
C	3.074460000	3.074460000	1.699763000
C	3.074460000	-3.074460000	-1.699763000
C	3.776677000	3.776677000	2.416358000
C	3.776677000	-3.776677000	-2.416358000
C	3.783145000	5.980167000	4.466674000
C	3.783145000	-5.980167000	-4.466674000
C	4.099409000	0.592060000	0.353554000
C	4.099409000	-0.592060000	-0.353554000
C	5.308501000	1.357349000	0.796136000
C	5.308501000	-1.357349000	-0.796136000
C	5.896245000	5.896245000	2.213277000
C	5.896245000	-5.896245000	-2.213277000
C	5.980167000	3.783145000	4.466674000

C	5.980167000	-3.783145000	-4.466674000
C	-0.592060000	4.099409000	-0.353554000
C	-0.592060000	-4.099409000	0.353554000
C	-0.974897000	2.710827000	-0.515097000
C	-0.974897000	-2.710827000	0.515097000
C	-1.357349000	5.308501000	-0.796136000
C	-1.357349000	-5.308501000	0.796136000
C	-2.237454000	2.237454000	-0.931392000
C	-2.237454000	-2.237454000	0.931392000
C	-2.710827000	0.974897000	-0.515097000
C	-2.710827000	-0.974897000	0.515097000
C	-3.074460000	3.074460000	-1.699763000
C	-3.074460000	-3.074460000	1.699763000
C	-3.776677000	3.776677000	-2.416358000
C	-3.776677000	-3.776677000	2.416358000
C	-3.783145000	5.980167000	-4.466674000
C	-3.783145000	-5.980167000	4.466674000
C	-4.099409000	0.592060000	-0.353554000
C	-4.099409000	-0.592060000	0.353554000
C	-5.308501000	1.357349000	-0.796136000
C	-5.308501000	-1.357349000	0.796136000
C	-5.896245000	5.896245000	-2.213277000
C	-5.896245000	-5.896245000	2.213277000
C	-5.980167000	3.783145000	-4.466674000
C	-5.980167000	-3.783145000	4.466674000
H	0.865583000	6.225546000	0.453411000
H	0.865583000	-6.225546000	-0.453411000
H	1.443075000	5.353297000	1.889544000
H	1.443075000	-5.353297000	-1.889544000
H	2.381712000	5.305782000	0.400910000
H	2.381712000	-5.305782000	-0.400910000
H	3.123585000	6.594204000	3.836375000
H	3.123585000	-6.594204000	-3.836375000
H	3.150798000	5.386276000	5.141718000
H	3.150798000	-5.386276000	-5.141718000
H	4.400512000	6.656748000	5.077005000
H	4.400512000	-6.656748000	-5.077005000
H	5.250486000	6.508271000	1.567327000
H	5.250486000	-6.508271000	-1.567327000
H	5.305782000	2.381712000	0.400910000
H	5.305782000	-2.381712000	-0.400910000
H	5.353297000	1.443075000	1.889544000
H	5.353297000	-1.443075000	-1.889544000
H	5.386276000	3.150798000	5.141718000
H	5.386276000	-3.150798000	-5.141718000
H	6.225546000	0.865583000	0.453411000
H	6.225546000	-0.865583000	-0.453411000
H	6.508271000	5.250486000	1.567327000
H	6.508271000	-5.250486000	-1.567327000
H	6.570190000	6.570190000	2.764054000
H	6.570190000	-6.570190000	-2.764054000

H	6.594204000	3.123585000	3.836375000
H	6.594204000	-3.123585000	-3.836375000
H	6.656748000	4.400512000	5.077005000
H	6.656748000	-4.400512000	-5.077005000
H	-0.865583000	6.225546000	-0.453411000
H	-0.865583000	-6.225546000	0.453411000
H	-1.443075000	5.353297000	-1.889544000
H	-1.443075000	-5.353297000	1.889544000
H	-2.381712000	5.305782000	-0.400910000
H	-2.381712000	-5.305782000	0.400910000
H	-3.123585000	6.594204000	-3.836375000
H	-3.123585000	-6.594204000	3.836375000
H	-3.150798000	5.386276000	-5.141718000
H	-3.150798000	-5.386276000	5.141718000
H	-4.400512000	6.656748000	-5.077005000
H	-4.400512000	-6.656748000	5.077005000
H	-5.250486000	6.508271000	-1.567327000
H	-5.250486000	-6.508271000	1.567327000
H	-5.305782000	2.381712000	-0.400910000
H	-5.305782000	-2.381712000	0.400910000
H	-5.353297000	1.443075000	-1.889544000
H	-5.353297000	-1.443075000	1.889544000
H	-5.386276000	3.150798000	-5.141718000
H	-5.386276000	-3.150798000	5.141718000
H	-6.225546000	0.865583000	-0.453411000
H	-6.225546000	-0.865583000	0.453411000
H	-6.508271000	5.250486000	-1.567327000
H	-6.508271000	-5.250486000	1.567327000
H	-6.570190000	6.570190000	-2.764054000
H	-6.570190000	-6.570190000	2.764054000
H	-6.594204000	3.123585000	-3.836375000
H	-6.594204000	-3.123585000	3.836375000
H	-6.656748000	4.400512000	-5.077005000
H	-6.656748000	-4.400512000	5.077005000
N	0.000000000	1.890381000	0.000000000
N	0.000000000	-1.890381000	0.000000000
N	1.890381000	0.000000000	0.000000000
N	-1.890381000	0.000000000	0.000000000
Si	4.863447000	4.863447000	3.403864000
Si	4.863447000	-4.863447000	-3.403864000
Si	-4.863447000	4.863447000	-3.403864000
Si	-4.863447000	-4.863447000	3.403864000

105. Pd[A₄Me₈]; S = 0 (saddled)

Pd	0.005500000	0.054075000	0.000000000
C	0.587638000	-0.981586000	4.055890000
C	0.587638000	-0.981586000	-4.055890000
C	1.064862000	-0.463166000	2.785186000
C	1.064862000	-0.463166000	-2.785186000

C	1.396469000	-1.605380000	5.152652000
C	1.396469000	-1.605380000	-5.152652000
C	2.404008000	-0.206900000	2.410351000
C	2.404008000	-0.206900000	-2.410351000
C	2.814073000	0.161665000	1.107940000
C	2.814073000	0.161665000	-1.107940000
C	3.406850000	-0.340896000	3.399205000
C	3.406850000	-0.340896000	-3.399205000
C	4.135259000	0.595873000	0.689112000
C	4.135259000	0.595873000	-0.689112000
C	4.277436000	-0.467673000	4.250088000
C	4.277436000	-0.467673000	-4.250088000
C	5.119106000	0.320552000	7.036757000
C	5.119106000	0.320552000	-7.036757000
C	5.277750000	1.021949000	1.559600000
C	5.277750000	1.021949000	-1.559600000
C	5.644989000	-2.523908000	5.961792000
C	5.644989000	-2.523908000	-5.961792000
C	7.208973000	-0.114443000	4.789369000
C	7.208973000	-0.114443000	-4.789369000
C	-0.782772000	-0.834780000	4.055925000
C	-0.782772000	-0.834780000	-4.055925000
C	-1.139482000	-0.227155000	2.785186000
C	-1.139482000	-0.227155000	-2.785186000
C	-1.705127000	-1.272431000	5.153145000
C	-1.705127000	-1.272431000	-5.153145000
C	-2.394092000	0.306523000	2.410234000
C	-2.394092000	0.306523000	-2.410234000
C	-2.716578000	0.753963000	1.107910000
C	-2.716578000	0.753963000	-1.107910000
C	-3.402968000	0.386937000	3.398753000
C	-3.402968000	0.386937000	-3.398753000
C	-3.915723000	1.458318000	0.689117000
C	-3.915723000	1.458318000	-0.689117000
C	-4.280904000	0.445934000	4.249481000
C	-4.280904000	0.445934000	-4.249481000
C	-4.925095000	1.372520000	7.045700000
C	-4.925095000	1.372520000	-7.045700000
C	-4.941649000	2.117036000	1.559792000
C	-4.941649000	2.117036000	-1.559792000
C	-6.064755000	-1.276278000	5.947054000
C	-6.064755000	-1.276278000	-5.947054000
C	-7.062934000	1.428656000	4.801578000
C	-7.062934000	1.428656000	-4.801578000
H	0.748502000	-2.174927000	5.828960000
H	0.748502000	-2.174927000	-5.828960000
H	1.923820000	-0.848814000	5.749732000
H	1.923820000	-0.848814000	-5.749732000
H	2.159816000	-2.284972000	4.756665000
H	2.159816000	-2.284972000	-4.756665000
H	4.150539000	-0.003557000	7.444240000

H	4.150539000	-0.003557000	-7.444240000
H	4.676068000	-2.864542000	6.354679000
H	4.676068000	-2.864542000	-6.354679000
H	4.937460000	1.622300000	2.411067000
H	4.937460000	1.622300000	-2.411067000
H	5.040982000	1.388226000	6.787119000
H	5.040982000	1.388226000	-6.787119000
H	5.817149000	0.160356000	1.976029000
H	5.817149000	0.160356000	-1.976029000
H	5.878461000	0.204202000	7.825069000
H	5.878461000	0.204202000	-7.825069000
H	5.885245000	-3.131985000	5.078119000
H	5.885245000	-3.131985000	-5.078119000
H	5.994791000	1.618934000	0.983793000
H	5.994791000	1.618934000	-0.983793000
H	6.411396000	-2.710327000	6.729594000
H	6.411396000	-2.710327000	-6.729594000
H	7.144440000	0.937112000	4.475229000
H	7.144440000	0.937112000	-4.475229000
H	7.478999000	-0.715457000	3.909230000
H	7.478999000	-0.715457000	-3.909230000
H	8.020193000	-0.203942000	5.527697000
H	8.020193000	-0.203942000	-5.527697000
H	-1.191801000	-1.964230000	5.831036000
H	-1.191801000	-1.964230000	-5.831036000
H	-2.061594000	-0.420667000	5.748460000
H	-2.061594000	-0.420667000	-5.748460000
H	-2.594298000	-1.776876000	4.757841000
H	-2.594298000	-1.776876000	-4.757841000
H	-4.050707000	0.839552000	7.446430000
H	-4.050707000	0.839552000	-7.446430000
H	-4.481525000	2.631534000	2.411156000
H	-4.481525000	2.631534000	-2.411156000
H	-4.614749000	2.399358000	6.805645000
H	-4.614749000	2.399358000	-6.805645000
H	-5.193960000	-1.824930000	6.334184000
H	-5.193960000	-1.824930000	-6.334184000
H	-5.515875000	2.852555000	0.984120000
H	-5.515875000	2.852555000	-0.984120000
H	-5.651385000	1.389479000	1.976453000
H	-5.651385000	1.389479000	-1.976453000
H	-5.690073000	1.417979000	7.835852000
H	-5.690073000	1.417979000	-7.835852000
H	-6.433356000	-1.808599000	5.058746000
H	-6.433356000	-1.808599000	-5.058746000
H	-6.769652000	2.443415000	4.496887000
H	-6.769652000	2.443415000	-4.496887000
H	-6.852761000	-1.296976000	6.715354000
H	-6.852761000	-1.296976000	-6.715354000
H	-7.459251000	0.910061000	3.916846000
H	-7.459251000	0.910061000	-3.916846000

H	-7.873178000	1.512095000	5.541690000
H	-7.873178000	1.512095000	-5.541690000
N	2.017059000	-0.009751000	0.000000000
N	-0.010082000	-0.090796000	2.011108000
N	-0.010082000	-0.090796000	-2.011108000
N	-1.973900000	0.417723000	0.000000000
Si	5.572192000	-0.695199000	5.517746000
Si	5.572192000	-0.695199000	-5.517746000
Si	-5.592623000	0.495890000	5.519129000
Si	-5.592623000	0.495890000	-5.519129000

106. Pd[A₄Me₈]; S = 0 (ruffled)

Pd	0.000000000	0.000000000	0.000000000
C	0.650570000	4.219655000	0.227352000
C	0.650570000	-4.219655000	-0.227352000
C	1.055597000	2.827864000	0.338511000
C	1.055597000	-2.827864000	-0.338511000
C	1.482193000	5.441882000	0.474890000
C	1.482193000	-5.441882000	-0.474890000
C	2.356147000	2.356147000	0.636155000
C	2.356147000	-2.356147000	-0.636155000
C	2.827864000	1.055597000	0.338511000
C	2.827864000	-1.055597000	-0.338511000
C	3.250211000	3.250211000	1.269434000
C	3.250211000	-3.250211000	-1.269434000
C	3.999354000	3.999354000	1.883157000
C	3.999354000	-3.999354000	-1.883157000
C	4.146754000	6.343694000	3.764646000
C	4.146754000	-6.343694000	-3.764646000
C	4.219655000	0.650570000	0.227352000
C	4.219655000	-0.650570000	-0.227352000
C	5.441882000	1.482193000	0.474890000
C	5.441882000	-1.482193000	-0.474890000
C	6.093676000	6.093676000	1.377604000
C	6.093676000	-6.093676000	-1.377604000
C	6.343694000	4.146754000	3.764646000
C	6.343694000	-4.146754000	-3.764646000
C	-0.650570000	4.219655000	-0.227352000
C	-0.650570000	-4.219655000	0.227352000
C	-1.055597000	2.827864000	-0.338511000
C	-1.055597000	-2.827864000	0.338511000
C	-1.482193000	5.441882000	-0.474890000
C	-1.482193000	-5.441882000	0.474890000
C	-2.356147000	2.356147000	-0.636155000
C	-2.356147000	-2.356147000	0.636155000
C	-2.827864000	1.055597000	-0.338511000
C	-2.827864000	-1.055597000	0.338511000
C	-3.250211000	3.250211000	-1.269434000
C	-3.250211000	-3.250211000	1.269434000

C	-3.999354000	3.999354000	-1.883157000
C	-3.999354000	-3.999354000	1.883157000
C	-4.146754000	6.343694000	-3.764646000
C	-4.146754000	-6.343694000	3.764646000
C	-4.219655000	0.650570000	-0.227352000
C	-4.219655000	-0.650570000	0.227352000
C	-5.441882000	1.482193000	-0.474890000
C	-5.441882000	-1.482193000	0.474890000
C	-6.093676000	6.093676000	-1.377604000
C	-6.093676000	-6.093676000	1.377604000
C	-6.343694000	4.146754000	-3.764646000
C	-6.343694000	-4.146754000	3.764646000
H	0.966313000	6.338176000	0.113948000
H	0.966313000	-6.338176000	-0.113948000
H	1.701587000	5.576688000	1.542248000
H	1.701587000	-5.576688000	-1.542248000
H	2.449216000	5.381705000	-0.039589000
H	2.449216000	-5.381705000	0.039589000
H	3.445584000	6.916327000	3.140341000
H	3.445584000	-6.916327000	-3.140341000
H	3.562262000	5.800674000	4.520804000
H	3.562262000	-5.800674000	-4.520804000
H	4.804644000	7.057781000	4.283004000
H	4.804644000	-7.057781000	-4.283004000
H	5.381705000	2.449216000	-0.039589000
H	5.381705000	-2.449216000	0.039589000
H	5.401897000	6.659655000	0.737346000
H	5.401897000	-6.659655000	-0.737346000
H	5.576688000	1.701587000	1.542248000
H	5.576688000	-1.701587000	-1.542248000
H	5.800674000	3.562262000	4.520804000
H	5.800674000	-3.562262000	-4.520804000
H	6.338176000	0.966313000	0.113948000
H	6.338176000	-0.966313000	-0.113948000
H	6.659655000	5.401897000	0.737346000
H	6.659655000	-5.401897000	-0.737346000
H	6.803538000	6.803538000	1.829257000
H	6.803538000	-6.803538000	-1.829257000
H	6.916327000	3.445584000	3.140341000
H	6.916327000	-3.445584000	-3.140341000
H	7.057781000	4.804644000	4.283004000
H	7.057781000	-4.804644000	-4.283004000
H	-0.966313000	6.338176000	-0.113948000
H	-0.966313000	-6.338176000	0.113948000
H	-1.701587000	5.576688000	-1.542248000
H	-1.701587000	-5.576688000	1.542248000
H	-2.449216000	5.381705000	0.039589000
H	-2.449216000	-5.381705000	-0.039589000
H	-3.445584000	6.916327000	-3.140341000
H	-3.445584000	-6.916327000	3.140341000
H	-3.562262000	5.800674000	-4.520804000

H	-3.562262000	-5.800674000	4.520804000
H	-4.804644000	7.057781000	-4.283004000
H	-4.804644000	-7.057781000	4.283004000
H	-5.381705000	2.449216000	0.039589000
H	-5.381705000	-2.449216000	-0.039589000
H	-5.401897000	6.659655000	-0.737346000
H	-5.401897000	-6.659655000	0.737346000
H	-5.576688000	1.701587000	-1.542248000
H	-5.576688000	-1.701587000	1.542248000
H	-5.800674000	3.562262000	-4.520804000
H	-5.800674000	-3.562262000	4.520804000
H	-6.338176000	0.966313000	-0.113948000
H	-6.338176000	-0.966313000	0.113948000
H	-6.659655000	5.401897000	-0.737346000
H	-6.659655000	-5.401897000	0.737346000
H	-6.803538000	6.803538000	-1.829257000
H	-6.803538000	-6.803538000	1.829257000
H	-6.916327000	3.445584000	-3.140341000
H	-6.916327000	-3.445584000	3.140341000
H	-7.057781000	4.804644000	-4.283004000
H	-7.057781000	-4.804644000	4.283004000
N	0.000000000	2.016092000	0.000000000
N	0.000000000	-2.016092000	0.000000000
N	2.016092000	0.000000000	0.000000000
N	-2.016092000	0.000000000	0.000000000
Si	5.151355000	5.151355000	2.709687000
Si	5.151355000	-5.151355000	-2.709687000
Si	-5.151355000	5.151355000	-2.709687000
Si	-5.151355000	-5.151355000	2.709687000

107. Pt[A₄Me₈]; S = 0 (saddled)

Pt	0.005007000	0.048972000	0.000000000
C	0.590082000	-0.955907000	4.069700000
C	0.590082000	-0.955907000	-4.069700000
C	1.067301000	-0.459676000	2.792478000
C	1.067301000	-0.459676000	-2.792478000
C	1.398403000	-1.562868000	5.176119000
C	1.398403000	-1.562868000	-5.176119000
C	2.406400000	-0.211995000	2.413151000
C	2.406400000	-0.211995000	-2.413151000
C	2.820422000	0.146926000	1.109859000
C	2.820422000	0.146926000	-1.109859000
C	3.409283000	-0.344000000	3.403798000
C	3.409283000	-0.344000000	-3.403798000
C	4.145466000	0.560054000	0.688737000
C	4.145466000	0.560054000	-0.688737000
C	4.278830000	-0.467363000	4.256101000
C	4.278830000	-0.467363000	-4.256101000
C	5.113262000	0.330793000	7.041643000

C	5.113262000	0.330793000	-7.041643000
C	5.295137000	0.970477000	1.557074000
C	5.295137000	0.970477000	-1.557074000
C	5.649499000	-2.515431000	5.976502000
C	5.649499000	-2.515431000	-5.976502000
C	7.208615000	-0.105215000	4.799844000
C	7.208615000	-0.105215000	-4.799844000
C	-0.779571000	-0.808790000	4.069854000
C	-0.779571000	-0.808790000	-4.069854000
C	-1.140920000	-0.222908000	2.792552000
C	-1.140920000	-0.222908000	-2.792552000
C	-1.697974000	-1.229573000	5.176794000
C	-1.697974000	-1.229573000	-5.176794000
C	-2.397193000	0.302496000	2.413075000
C	-2.397193000	0.302496000	-2.413075000
C	-2.725677000	0.741287000	1.109829000
C	-2.725677000	0.741287000	-1.109829000
C	-3.405761000	0.384997000	3.403283000
C	-3.405761000	0.384997000	-3.403283000
C	-3.933139000	1.425675000	0.688747000
C	-3.933139000	1.425675000	-0.688747000
C	-4.282338000	0.446857000	4.255059000
C	-4.282338000	0.446857000	-4.255059000
C	-4.917421000	1.381147000	7.049997000
C	-4.917421000	1.381147000	-7.049997000
C	-4.969734000	2.070392000	1.557088000
C	-4.969734000	2.070392000	-1.557088000
C	-6.067448000	-1.267155000	5.961089000
C	-6.067448000	-1.267155000	-5.961089000
C	-7.060720000	1.437400000	4.811022000
C	-7.060720000	1.437400000	-4.811022000
H	0.749025000	-2.116943000	5.863563000
H	0.749025000	-2.116943000	-5.863563000
H	1.930323000	-0.798404000	5.758612000
H	1.930323000	-0.798404000	-5.758612000
H	2.157336000	-2.253348000	4.791084000
H	2.157336000	-2.253348000	-4.791084000
H	4.144884000	0.005328000	7.448486000
H	4.144884000	0.005328000	-7.448486000
H	4.681293000	-2.857591000	6.369786000
H	4.681293000	-2.857591000	-6.369786000
H	4.965466000	1.583291000	2.403621000
H	4.965466000	1.583291000	-2.403621000
H	5.032743000	1.397455000	6.788514000
H	5.032743000	1.397455000	-6.788514000
H	5.818478000	0.102430000	1.979989000
H	5.818478000	0.102430000	-1.979989000
H	5.871499000	0.218978000	7.831682000
H	5.871499000	0.218978000	-7.831682000
H	5.892108000	-3.125745000	5.095025000
H	5.892108000	-3.125745000	-5.095025000

H	6.023129000	1.549991000	0.977566000
H	6.023129000	1.549991000	-0.977566000
H	6.415855000	-2.697241000	6.745472000
H	6.415855000	-2.697241000	-6.745472000
H	7.141879000	0.945218000	4.482513000
H	7.141879000	0.945218000	-4.482513000
H	7.482454000	-0.707918000	3.922057000
H	7.482454000	-0.707918000	-3.922057000
H	8.018412000	-0.190340000	5.540253000
H	8.018412000	-0.190340000	-5.540253000
H	-1.179986000	-1.905840000	5.866425000
H	-1.179986000	-1.905840000	-5.866425000
H	-2.057641000	-0.368837000	5.756773000
H	-2.057641000	-0.368837000	-5.756773000
H	-2.584908000	-1.746094000	4.792605000
H	-2.584908000	-1.746094000	-4.792605000
H	-4.043451000	0.846815000	7.449865000
H	-4.043451000	0.846815000	-7.449865000
H	-4.517807000	2.598044000	2.404567000
H	-4.517807000	2.598044000	-2.404567000
H	-4.604946000	2.406539000	6.806515000
H	-4.604946000	2.406539000	-6.806515000
H	-5.197419000	-1.817267000	6.347884000
H	-5.197419000	-1.817267000	-6.347884000
H	-5.557260000	2.792263000	0.977954000
H	-5.557260000	2.792263000	-0.977954000
H	-5.666149000	1.333137000	1.978696000
H	-5.666149000	1.333137000	-1.978696000
H	-5.680172000	1.430664000	7.842056000
H	-5.680172000	1.430664000	-7.842056000
H	-6.439465000	-1.800895000	5.075057000
H	-6.439465000	-1.800895000	-5.075057000
H	-6.765438000	2.450503000	4.502840000
H	-6.765438000	2.450503000	-4.502840000
H	-6.853849000	-1.283493000	6.731141000
H	-6.853849000	-1.283493000	-6.731141000
H	-7.460826000	0.917673000	3.928664000
H	-7.460826000	0.917673000	-3.928664000
H	-7.868837000	1.525017000	5.552968000
H	-7.868837000	1.525017000	-5.552968000
N	2.017365000	-0.006602000	0.000000000
N	-0.011460000	-0.104717000	2.010277000
N	-0.011460000	-0.104717000	-2.010277000
N	-1.973335000	0.421150000	0.000000000
Si	5.571912000	-0.688391000	5.526571000
Si	5.571912000	-0.688391000	-5.526571000
Si	-5.591179000	0.502433000	5.527336000
Si	-5.591179000	0.502433000	-5.527336000

108. Pt[A₄Me₈]; S = 0 (ruffled)

Pt	0.000000000	0.000000000	0.000000000
C	0.650865000	0.225769000	-4.218660000
C	0.650865000	-0.225769000	4.218660000
C	1.057555000	0.337466000	-2.830009000
C	1.057555000	-0.337466000	2.830009000
C	1.483409000	0.470443000	-5.440564000
C	1.483409000	-0.470443000	5.440564000
C	2.357484000	0.635586000	-2.357584000
C	2.357484000	-0.635586000	2.357584000
C	2.829845000	0.337394000	-1.057644000
C	2.829845000	-0.337394000	1.057644000
C	3.250755000	1.272513000	-3.250542000
C	3.250755000	-1.272513000	3.250542000
C	3.998386000	1.891006000	-3.997300000
C	3.998386000	-1.891006000	3.997300000
C	4.140989000	3.756043000	-6.354620000
C	4.140989000	-3.756043000	6.354620000
C	4.218446000	0.225803000	-0.650854000
C	4.218446000	-0.225803000	0.650854000
C	5.440391000	0.470093000	-1.483356000
C	5.440391000	-0.470093000	1.483356000
C	6.118770000	1.397965000	-6.067836000
C	6.118770000	-1.397965000	6.067836000
C	6.318130000	3.803912000	-4.138704000
C	6.318130000	-3.803912000	4.138704000
C	-0.650865000	0.225769000	4.218660000
C	-0.650865000	-0.225769000	-4.218660000
C	-1.057555000	0.337466000	2.830009000
C	-1.057555000	-0.337466000	-2.830009000
C	-1.483409000	0.470443000	5.440564000
C	-1.483409000	-0.470443000	-5.440564000
C	-2.357484000	0.635586000	2.357584000
C	-2.357484000	-0.635586000	-2.357584000
C	-2.829845000	0.337394000	1.057644000
C	-2.829845000	-0.337394000	-1.057644000
C	-3.250755000	1.272513000	3.250542000
C	-3.250755000	-1.272513000	-3.250542000
C	-3.998386000	1.891006000	3.997300000
C	-3.998386000	-1.891006000	-3.997300000
C	-4.140989000	3.756043000	6.354620000
C	-4.140989000	-3.756043000	-6.354620000
C	-4.218446000	0.225803000	0.650854000
C	-4.218446000	-0.225803000	-0.650854000
C	-5.440391000	0.470093000	1.483356000
C	-5.440391000	-0.470093000	-1.483356000
C	-6.118770000	1.397965000	6.067836000
C	-6.118770000	-1.397965000	-6.067836000
C	-6.318130000	3.803912000	4.138704000
C	-6.318130000	-3.803912000	-4.138704000

H	0.969098000	0.105737000	-6.336166000
H	0.969098000	-0.105737000	6.336166000
H	1.701843000	1.537566000	-5.578637000
H	1.701843000	-1.537566000	5.578637000
H	2.450766000	0.042758000	5.377153000
H	2.450766000	-0.042758000	-5.377153000
H	3.452572000	3.117765000	-6.927356000
H	3.452572000	-3.117765000	6.927356000
H	3.542440000	4.509194000	-5.822782000
H	3.542440000	-4.509194000	5.822782000
H	4.797749000	4.276820000	-7.067950000
H	4.797749000	-4.276820000	7.067950000
H	5.376796000	0.043070000	2.450720000
H	5.376796000	-0.043070000	-2.450720000
H	5.441425000	0.745355000	-6.637127000
H	5.441425000	-0.745355000	6.637127000
H	5.578886000	1.537175000	-1.701730000
H	5.578886000	-1.537175000	1.701730000
H	5.759456000	4.556455000	-3.564413000
H	5.759456000	-4.556455000	3.564413000
H	6.335745000	0.105075000	-0.968962000
H	6.335745000	-0.105075000	0.968962000
H	6.684754000	0.769560000	-5.365257000
H	6.684754000	-0.769560000	5.365257000
H	6.831000000	1.853669000	-6.772677000
H	6.831000000	-1.853669000	6.772677000
H	6.893874000	3.193245000	-3.428118000
H	6.893874000	-3.193245000	3.428118000
H	7.030166000	4.327569000	-4.794607000
H	7.030166000	-4.327569000	4.794607000
H	-0.969098000	0.105737000	6.336166000
H	-0.969098000	-0.105737000	-6.336166000
H	-1.701843000	1.537566000	5.578637000
H	-1.701843000	-1.537566000	-5.578637000
H	-2.450766000	0.042758000	-5.377153000
H	-2.450766000	-0.042758000	5.377153000
H	-3.452572000	3.117765000	6.927356000
H	-3.452572000	-3.117765000	-6.927356000
H	-3.542440000	4.509194000	5.822782000
H	-3.542440000	-4.509194000	-5.822782000
H	-4.797749000	4.276820000	7.067950000
H	-4.797749000	-4.276820000	-7.067950000
H	-5.376796000	0.043070000	-2.450720000
H	-5.376796000	-0.043070000	2.450720000
H	-5.441425000	0.745355000	6.637127000
H	-5.441425000	-0.745355000	-6.637127000
H	-5.578886000	1.537175000	1.701730000
H	-5.578886000	-1.537175000	-1.701730000
H	-5.759456000	4.556455000	3.564413000
H	-5.759456000	-4.556455000	-3.564413000
H	-6.335745000	0.105075000	0.968962000

H	-6.335745000	-0.105075000	-0.968962000
H	-6.684754000	0.769560000	5.365257000
H	-6.684754000	-0.769560000	-5.365257000
H	-6.831000000	1.853669000	6.772677000
H	-6.831000000	-1.853669000	-6.772677000
H	-6.893874000	3.193245000	3.428118000
H	-6.893874000	-3.193245000	-3.428118000
H	-7.030166000	4.327569000	4.794607000
H	-7.030166000	-4.327569000	-4.794607000
N	0.000000000	0.000000000	2.016066000
N	0.000000000	0.000000000	-2.016066000
N	2.016011000	0.000000000	0.000000000
N	-2.016011000	0.000000000	0.000000000
Si	5.149476000	2.724532000	-5.145146000
Si	5.149476000	-2.724532000	5.145146000
Si	-5.149476000	2.724532000	5.145146000
Si	-5.149476000	-2.724532000	-5.145146000

109. Zn[A₄Me₈]; S = 0 (saddled)

Zn	0.009160000	0.074872000	0.000000000
C	0.597562000	-0.909611000	4.098546000
C	0.597562000	-0.909611000	-4.098546000
C	1.066870000	-0.424955000	2.810844000
C	1.066870000	-0.424955000	-2.810844000
C	1.405215000	-1.499671000	5.214656000
C	1.405215000	-1.499671000	-5.214656000
C	2.411550000	-0.188072000	2.415557000
C	2.411550000	-0.188072000	-2.415557000
C	2.833406000	0.168814000	1.105174000
C	2.833406000	0.168814000	-1.105174000
C	3.418378000	-0.336208000	3.397941000
C	3.418378000	-0.336208000	-3.397941000
C	4.165167000	0.573259000	0.690547000
C	4.165167000	0.573259000	-0.690547000
C	4.292699000	-0.479212000	4.243213000
C	4.292699000	-0.479212000	-4.243213000
C	5.140302000	0.272501000	7.037070000
C	5.140302000	0.272501000	-7.037070000
C	5.321029000	0.972899000	1.555900000
C	5.321029000	0.972899000	-1.555900000
C	5.640186000	-2.565559000	5.936193000
C	5.640186000	-2.565559000	-5.936193000
C	7.228906000	-0.161830000	4.788007000
C	7.228906000	-0.161830000	-4.788007000
C	-0.775510000	-0.761603000	4.098638000
C	-0.775510000	-0.761603000	-4.098638000
C	-1.131048000	-0.188603000	2.810792000
C	-1.131048000	-0.188603000	-2.810792000
C	-1.690126000	-1.164865000	5.215300000

C	-1.690126000	-1.164865000	-5.215300000
C	-2.394578000	0.328475000	2.415350000
C	-2.394578000	0.328475000	-2.415350000
C	-2.730361000	0.767807000	1.105117000
C	-2.730361000	0.767807000	-1.105117000
C	-3.411336000	0.395042000	3.396403000
C	-3.411336000	0.395042000	-3.396403000
C	-3.945286000	1.446765000	0.690544000
C	-3.945286000	1.446765000	-0.690544000
C	-4.298084000	0.438205000	4.239675000
C	-4.298084000	0.438205000	-4.239675000
C	-4.966128000	1.327959000	7.041295000
C	-4.966128000	1.327959000	-7.041295000
C	-4.989157000	2.083849000	1.555963000
C	-4.989157000	2.083849000	-1.555963000
C	-6.073224000	-1.320342000	5.911215000
C	-6.073224000	-1.320342000	-5.911215000
C	-7.095006000	1.383849000	4.788142000
C	-7.095006000	1.383849000	-4.788142000
H	0.756130000	-2.027624000	5.922757000
H	0.756130000	-2.027624000	-5.922757000
H	1.952382000	-0.726755000	5.771502000
H	1.952382000	-0.726755000	-5.771502000
H	2.153320000	-2.208519000	4.841309000
H	2.153320000	-2.208519000	-4.841309000
H	4.168618000	-0.047320000	7.440599000
H	4.168618000	-0.047320000	-7.440599000
H	4.668029000	-2.900209000	6.326219000
H	4.668029000	-2.900209000	-6.326219000
H	4.997960000	1.578120000	2.410482000
H	4.997960000	1.578120000	-2.410482000
H	5.071737000	1.343306000	6.798261000
H	5.071737000	1.343306000	-6.798261000
H	5.841719000	0.098092000	1.968673000
H	5.841719000	0.098092000	-1.968673000
H	5.874579000	-3.168450000	5.047404000
H	5.874579000	-3.168450000	-5.047404000
H	5.897904000	0.141368000	7.824759000
H	5.897904000	0.141368000	-7.824759000
H	6.050026000	1.554389000	0.979121000
H	6.050026000	1.554389000	-0.979121000
H	6.404697000	-2.765864000	6.702428000
H	6.404697000	-2.765864000	-6.702428000
H	7.176087000	0.892904000	4.482587000
H	7.176087000	0.892904000	-4.482587000
H	7.494976000	-0.758143000	3.903491000
H	7.494976000	-0.758143000	-3.903491000
H	8.037394000	-0.266067000	5.527411000
H	8.037394000	-0.266067000	-5.527411000
H	-1.167754000	-1.816271000	5.925408000
H	-1.167754000	-1.816271000	-5.925408000

H	-2.061676000	-0.292251000	5.769705000
H	-2.061676000	-0.292251000	-5.769705000
H	-2.571076000	-1.700385000	4.842921000
H	-2.571076000	-1.700385000	-4.842921000
H	-4.088565000	0.799132000	7.440713000
H	-4.088565000	0.799132000	-7.440713000
H	-4.544489000	2.604044000	2.411913000
H	-4.544489000	2.604044000	-2.411913000
H	-4.664624000	2.360253000	6.813706000
H	-4.664624000	2.360253000	-6.813706000
H	-5.199225000	-1.863546000	6.298824000
H	-5.199225000	-1.863546000	-6.298824000
H	-5.575638000	2.809370000	0.979831000
H	-5.575638000	2.809370000	-0.979831000
H	-5.686020000	1.340580000	1.966730000
H	-5.686020000	1.340580000	-1.966730000
H	-5.735291000	1.357479000	7.828142000
H	-5.735291000	1.357479000	-7.828142000
H	-6.430993000	-1.848510000	5.016009000
H	-6.430993000	-1.848510000	-5.016009000
H	-6.812376000	2.404545000	4.493474000
H	-6.812376000	2.404545000	-4.493474000
H	-6.865580000	-1.355943000	6.674520000
H	-6.865580000	-1.355943000	-6.674520000
H	-7.482975000	0.868898000	3.897572000
H	-7.482975000	0.868898000	-3.897572000
H	-7.908390000	1.451350000	5.526434000
H	-7.908390000	1.451350000	-5.526434000
N	2.032407000	0.017309000	0.000000000
N	-0.006832000	-0.072276000	2.031591000
N	-0.006832000	-0.072276000	-2.031591000
N	-1.979992000	0.449119000	0.000000000
Si	5.584723000	-0.732302000	5.507955000
Si	5.584723000	-0.732302000	-5.507955000
Si	-5.616827000	0.460532000	5.501967000
Si	-5.616827000	0.460532000	-5.501967000

110. Zn[A₄Me₈]; S = 0 (ruffled)

Zn	0.000000000	0.000000000	0.000000000
C	0.668261000	4.255504000	0.170982000
C	0.668261000	-4.255504000	-0.170982000
C	1.074281000	2.862822000	0.258615000
C	1.074281000	-2.862822000	-0.258615000
C	1.510933000	5.484847000	0.334476000
C	1.510933000	-5.484847000	-0.334476000
C	2.391094000	2.391094000	0.505906000
C	2.391094000	-2.391094000	-0.505906000
C	2.862822000	1.074281000	0.258615000
C	2.862822000	-1.074281000	-0.258615000

C	3.309243000	3.309243000	1.067765000
C	3.309243000	-3.309243000	-1.067765000
C	4.081718000	4.081718000	1.621345000
C	4.081718000	-4.081718000	-1.621345000
C	4.255504000	0.668261000	0.170982000
C	4.255504000	-0.668261000	-0.170982000
C	4.306099000	6.502738000	3.396147000
C	4.306099000	-6.502738000	-3.396147000
C	5.484847000	1.510933000	0.334476000
C	5.484847000	-1.510933000	-0.334476000
C	6.151809000	6.151809000	0.943165000
C	6.151809000	-6.151809000	-0.943165000
C	6.502738000	4.306099000	3.396147000
C	6.502738000	-4.306099000	-3.396147000
C	-0.668261000	4.255504000	-0.170982000
C	-0.668261000	-4.255504000	0.170982000
C	-1.074281000	2.862822000	-0.258615000
C	-1.074281000	-2.862822000	0.258615000
C	-1.510933000	5.484847000	-0.334476000
C	-1.510933000	-5.484847000	0.334476000
C	-2.391094000	2.391094000	-0.505906000
C	-2.391094000	-2.391094000	0.505906000
C	-2.862822000	1.074281000	-0.258615000
C	-2.862822000	-1.074281000	0.258615000
C	-3.309243000	3.309243000	-1.067765000
C	-3.309243000	-3.309243000	1.067765000
C	-4.081718000	4.081718000	-1.621345000
C	-4.081718000	-4.081718000	1.621345000
C	-4.255504000	0.668261000	-0.170982000
C	-4.255504000	-0.668261000	0.170982000
C	-4.306099000	6.502738000	-3.396147000
C	-4.306099000	-6.502738000	3.396147000
C	-5.484847000	1.510933000	-0.334476000
C	-5.484847000	-1.510933000	0.334476000
C	-6.151809000	6.151809000	-0.943165000
C	-6.151809000	-6.151809000	0.943165000
C	-6.502738000	4.306099000	-3.396147000
C	-6.502738000	-4.306099000	3.396147000
H	0.976097000	6.369491000	-0.028073000
H	0.976097000	-6.369491000	0.028073000
H	1.787248000	5.654707000	1.383627000
H	1.787248000	-5.654707000	-1.383627000
H	2.448899000	5.406472000	-0.228119000
H	2.448899000	-5.406472000	0.228119000
H	3.581486000	7.052200000	2.777816000
H	3.581486000	-7.052200000	-2.777816000
H	3.751504000	5.992606000	4.196430000
H	3.751504000	-5.992606000	-4.196430000
H	4.985431000	7.234980000	3.858489000
H	4.985431000	-7.234980000	-3.858489000
H	5.406472000	2.448899000	-0.228119000

H	5.406472000	-2.448899000	0.228119000
H	5.433826000	6.691557000	0.309114000
H	5.433826000	-6.691557000	-0.309114000
H	5.654707000	1.787248000	1.383627000
H	5.654707000	-1.787248000	-1.383627000
H	5.992606000	3.751504000	4.196430000
H	5.992606000	-3.751504000	-4.196430000
H	6.369491000	0.976097000	-0.028073000
H	6.369491000	-0.976097000	0.028073000
H	6.691557000	5.433826000	0.309114000
H	6.691557000	-5.433826000	-0.309114000
H	6.879069000	6.879069000	1.335654000
H	6.879069000	-6.879069000	-1.335654000
H	7.052200000	3.581486000	2.777816000
H	7.052200000	-3.581486000	-2.777816000
H	7.234980000	4.985431000	3.858489000
H	7.234980000	-4.985431000	-3.858489000
H	-0.976097000	6.369491000	0.028073000
H	-0.976097000	-6.369491000	-0.028073000
H	-1.787248000	5.654707000	-1.383627000
H	-1.787248000	-5.654707000	1.383627000
H	-2.448899000	5.406472000	0.228119000
H	-2.448899000	-5.406472000	-0.228119000
H	-3.581486000	7.052200000	-2.777816000
H	-3.581486000	-7.052200000	2.777816000
H	-3.751504000	5.992606000	-4.196430000
H	-3.751504000	-5.992606000	4.196430000
H	-4.985431000	7.234980000	-3.858489000
H	-4.985431000	-7.234980000	3.858489000
H	-5.406472000	2.448899000	0.228119000
H	-5.406472000	-2.448899000	-0.228119000
H	-5.433826000	6.691557000	-0.309114000
H	-5.433826000	-6.691557000	0.309114000
H	-5.654707000	1.787248000	-1.383627000
H	-5.654707000	-1.787248000	1.383627000
H	-5.992606000	3.751504000	-4.196430000
H	-5.992606000	-3.751504000	4.196430000
H	-6.369491000	0.976097000	0.028073000
H	-6.369491000	-0.976097000	-0.028073000
H	-6.691557000	5.433826000	-0.309114000
H	-6.691557000	-5.433826000	0.309114000
H	-6.879069000	6.879069000	-1.335654000
H	-6.879069000	-6.879069000	1.335654000
H	-7.052200000	3.581486000	-2.777816000
H	-7.052200000	-3.581486000	2.777816000
H	-7.234980000	4.985431000	-3.858489000
H	-7.234980000	-4.985431000	3.858489000
N	0.000000000	2.046561000	0.000000000
N	0.000000000	-2.046561000	0.000000000
N	2.046561000	0.000000000	0.000000000
N	-2.046561000	0.000000000	0.000000000

Si	5.265731000	5.265731000	2.350414000
Si	5.265731000	-5.265731000	-2.350414000
Si	-5.265731000	5.265731000	-2.350414000
Si	-5.265731000	-5.265731000	2.350414000