

**N<sub>2</sub>H<sub>2</sub> binding to the nitrogenase FeMo cluster**  
**studied by QM/MM methods**

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**Table S1.** Mulliken spin populations for the Fe and Mo ions in the FeMo cluster obtained from TPSS and B3LYP calculations with the def2-SV(P) basis set for the various states.

Structure	BS	TPSS							B3LYP								
		Fe1	Fe2	Fe3	Fe4	Fe5	Fe6	Fe7	Mo	Fe1	Fe2	Fe3	Fe4	Fe5	Fe6	Fe7	Mo
<b>End-on NNH<sub>2</sub> binding</b>																	
Fe1	BS7-235	1.7	-2.4	-3.2	3.0	-2.9	2.4	3.0	-0.4	2.4	-3.5	-3.7	3.7	-3.5	3.5	3.6	-1.1
Fe2	BS7-235	3.3	-2.5	-2.9	2.9	-2.6	0.4	2.2	0.1	3.7	-3.8	-3.7	3.6	-3.5	3.2	3.3	-1.0
Fe3	BS10-147	3.2	-2.6	-2.0	3.1	-2.4	-1.3	2.3	0.2	3.6	-3.4	-2.5	3.7	-3.3	-3.1	3.5	0.9
Fe4	BS7-235	3.2	-2.7	-2.8	2.3	-2.9	2.2	2.4	-0.1	3.6	-3.7	-3.6	3.1	-3.6	3.3	3.4	-0.8
Fe5	BS7-235	3.4	-3.4	-3.1	2.5	-2.5	2.3	2.1	-0.2	3.6	-3.8	-3.8	3.4	-3.5	3.4	3.4	-1.1
Fe6	BS10-147	-3.2	2.6	2.7	-3.0	2.7	1.6	-2.2	-0.3	-3.7	3.6	3.6	-3.6	3.6	2.1	-3.5	-0.7
Fe6(HCA)	BS10-135	-3.2	2.8	-3.0	2.8	-2.5	1.6	2.7	-0.2	-3.7	3.6	-3.7	3.5	-3.5	2.2	3.5	-0.9
Fe6(HNNH <sub>2</sub> )	BS10-135	-3.2	2.9	2.8	-3.0	2.8	1.8	-2.5	-0.3	-3.7	3.6	3.6	-3.6	3.6	2.7	-3.5	-0.8
Fe6(S2B)	BS10-127	-3.3	-2.8	2.9	2.8	2.2	1.5	-2.5	-0.1	-3.7	-3.5	3.5	3.4	3.0	2.6	-3.5	-0.7
Fe7	BS7-235	3.4	-2.8	-3.1	3.1	-2.6	2.7	1.0	-0.9	3.7	-3.6	-3.7	3.7	-3.5	3.6	2.1	-1.3
Fe3(S2A)	BS7-235	3.1	-3.0	-2.9	2.5	-2.8	2.2	2.1	-0.1	3.6	-3.7	-3.7	3.5	-3.6	3.3	3.3	-0.8
Fe2/4	BS7-235	2.5	-2.5	-2.8	1.8	-2.6	2.3	2.5	-0.2	3.5	-3.6	-3.6	3.4	-3.5	3.3	3.4	-1.0
Fe3/4	BS7-235	2.6	-2.9	-2.0	1.7	-2.7	2.4	2.5	-0.2	3.6	-3.7	-3.7	3.6	-3.5	3.4	3.4	-1.0
Fe2/6/7	BS7-235	3.3	-2.0	-2.8	2.8	-2.8	1.8	0.7	-0.2	3.7	-3.2	-3.7	3.5	-3.5	3.2	2.5	-1.1
Fe2/6(5)	BS10-147	3.3	-2.1	-2.7	3.1	-2.7	-0.8	2.3	0.3	3.7	-2.8	-3.5	3.6	-3.4	-2.7	3.5	1.2
Fe3/7(2)	BS5-256	3.4	-2.6	0.1	3.0	-2.7	-2.1	1.3	0.4	3.7	-3.8	2.4	3.5	-3.5	-3.5	2.1	1.1
Fe3/7(3)	BS7-235	3.3	-2.9	-2.1	3.0	-2.7	2.1	0.5	0.1	3.7	-3.7	-3.6	3.6	-3.5	3.2	2.3	-0.7
Fe4/5(2)	BS7-235	3.3	-2.8	-2.9	1.7	-2.6	2.2	2.3	-0.3	3.6	-3.7	-3.6	3.1	-3.4	3.4	3.4	-1.2
Fe4/5(5)	BS7-235	3.3	-2.7	-2.8	1.5	-2.8	2.3	2.5	-0.2	3.8	-3.6	-3.6	2.4	-3.6	3.4	3.5	-1.0
Fe2/3/6/7	BS7-235	3.3	-1.3	-2.9	2.9	-2.7	2.3	-1.1	0.1	3.7	-2.7	-3.6	3.6	-3.3	3.6	-2.3	0.6
Fe2/4/5/6	BS7-235	3.3	-3.0	-3.0	1.7	-2.1	2.4	2.3	-0.3	3.6	-3.7	-3.7	2.9	-3.2	3.4	3.4	-1.1
Fe3/4/5/7	BS7-235	3.3	-2.7	-2.8	1.6	-2.5	2.5	1.2	-0.1	3.8	-3.6	-3.6	2.4	-3.5	3.4	2.4	-0.7
<b>Side-on cis-HNNH binding</b>																	
Fe2Fe2	BS10-147	3.3	-2.3	-2.7	3.1	-2.3	-1.2	2.6	0.1	3.7	-2.6	-3.4	3.7	-3.3	-3.0	3.5	0.8
Fe4Fe4	BS10-147	-3.2	2.3	2.7	-2.6	1.8	2.1	-2.6	-0.1	-3.7	3.4	3.4	-3.4	2.8	2.8	-3.5	-0.6
Fe5Fe5	BS10-146	3.2	-2.7	-2.5	3.1	-1.6	2.7	-1.8	0.1	3.7	-3.5	-3.3	3.7	-2.5	3.5	-3.0	0.9
Fe6Fe6	BS7-235	3.4	-3.1	-2.9	3.1	-2.7	1.2	1.8	0.2	3.7	-3.6	-3.8	3.6	-3.5	3.0	3.3	-0.8
Fe7Fe7	BS5-256	3.2	-2.8	1.0	3.0	-2.7	-1.9	1.2	0.3	3.6	-3.7	2.4	3.5	-3.6	-3.5	2.7	0.7
Fe2/3Fe6/7	BS7-235	3.3	-2.3	-2.0	2.9	-2.7	0.9	0.8	-0.4	3.7	-3.8	-3.8	3.5	-3.5	2.4	3.5	-1.2

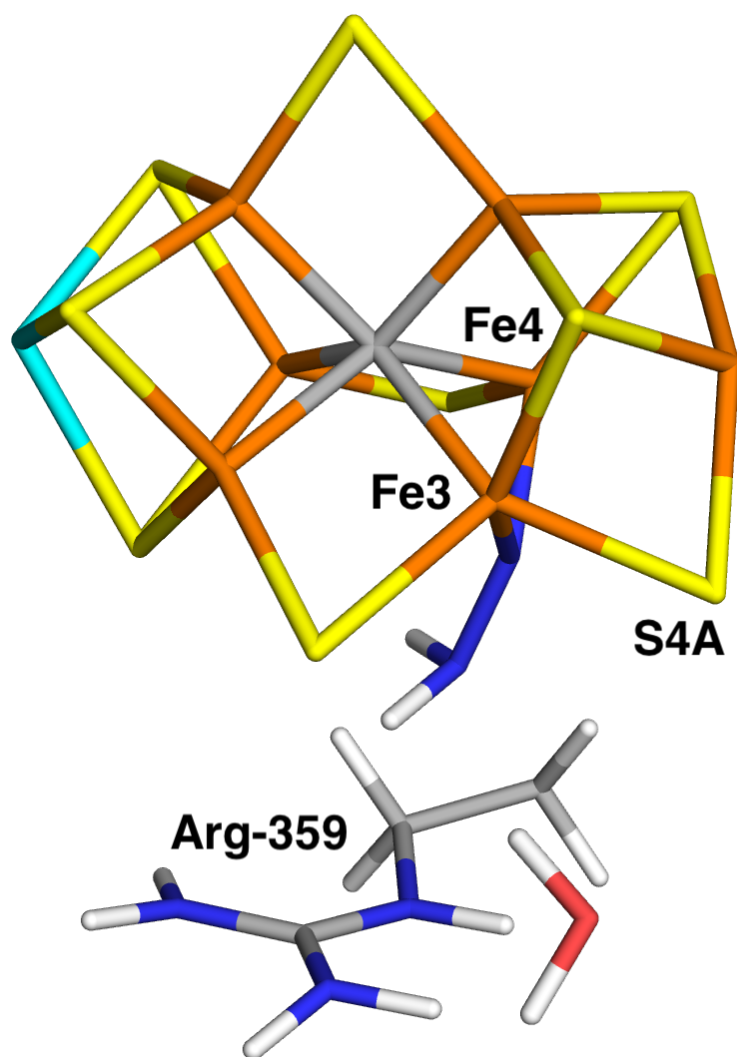
Fe2/6Fe3/7	BS7-235	3.0	-2.4	-2.1	0.9	-2.5	2.2	1.9	-0.2	3.7	-3.6	-3.6	3.5	-3.5	2.8	2.7	-0.9
Fe2/6Fe3/7tr <sup>a</sup>	BS6-156	3.1	-1.6	-1.1	-2.9	2.7	1.1	0.0	-0.4	-3.6	3.0	2.6	3.6	-3.5	-3.5	2.4	0.9
Fe2/4Fe5/6	BS2-234	3.1	-1.6	-2.7	-1.4	0.2	1.4	2.5	-0.5	3.8	-2.6	-3.5	-3.7	2.8	2.6	3.4	-2.1
Fe2/6Fe4/5	BS3-134	3.1	-1.9	1.7	1.9	-1.3	-0.5	-2.4	0.3	3.7	-3.0	3.5	2.7	-2.7	-2.7	-3.5	2.2
Fe2/6Fe4	BS7-235	3.2	-1.6	-2.8	1.4	-2.7	1.2	2.4	-0.2	3.6	-2.7	-3.7	2.8	-3.5	2.7	3.4	-1.2
Fe3/7Fe4/5	BS2-234	3.0	-2.7	-1.6	-1.8	1.1	2.4	0.8	-0.5	3.8	-3.5	-3.5	-3.5	2.7	3.5	2.7	-2.3
Fe2Fe7	BS7-235	3.3	-2.6	-3.0	3.0	-2.8	2.2	0.9	-0.2	3.7	-3.6	-3.8	3.5	-3.5	3.4	2.2	-0.8
Fe3Fe6	BS10-147	3.5	-3.3	-1.3	2.8	-2.7	-1.1	2.4	0.2	3.7	-3.7	-2.0	3.6	-3.5	-2.4	3.5	0.8
Fe2Fe6(3)	BS8-245	3.3	-2.0	-2.6	3.0	-2.7	-0.7	2.2	0.3	3.7	-2.9	-3.5	3.7	-3.4	-2.4	3.5	1.0
Fe2Fe6(5)	BS7-235	3.2	-2.8	-3.0	2.9	-2.7	1.1	2.3	-0.2	3.7	-3.6	-3.8	3.5	-3.5	2.3	3.4	-1.1
Fe3/7Fe3(2)	BS8-245	-3.5	2.9	-0.5	3.0	2.6	-2.4	-1.1	0.2	-3.8	3.6	-1.3	3.6	3.5	-3.4	-2.7	0.9
Fe3Fe7(3)	BS5-256	3.3	-2.6	1.5	3.0	-2.7	-1.8	0.3	0.5	3.7	-3.7	2.5	3.6	-3.5	-3.4	2.1	1.4
Fe45Fe5(2)	BS7-235	3.3	-2.7	-2.8	0.4	-2.0	2.3	2.5	-0.4	3.8	-3.6	-3.6	1.7	-3.4	3.4	3.4	-1.1
Fe4Fe5(5)	BS6-167	3.4	-2.8	-3.2	0.0	-1.2	2.3	2.3	-0.3	3.8	-3.5	-3.6	-1.1	-2.0	3.4	3.4	-1.3
<b>End-on trans-HNNH binding</b>																	
Fe2(trans)	BS10-147	-3.2	2.1	3.0	-3.0	2.6	2.4	-2.4	-0.3	3.7	-3.6	-3.7	3.6	3.5	-3.7	3.6	-2.4
Fe3(trans)	BS10-146	-3.3	2.9	2.0	-2.9	2.6	-2.4	2.6	-0.2	-3.7	3.7	2.3	-3.6	3.4	-3.5	3.4	-0.7
Fe4(trans)	BS7-235	3.3	-2.7	-2.8	1.2	-2.8	2.3	2.5	-0.2	3.8	-3.6	-3.6	2.0	-3.6	3.4	3.4	-1.0
Fe5(trans)	BS10-147	3.2	-2.2	-2.7	3.0	-1.5	-2.0	2.8	0.1	3.7	-3.3	-3.5	3.7	-2.1	-3.1	3.5	1.1
Fe6(trans)	BS10-147	3.2	-2.1	-2.6	3.0	-2.3	-1.3	2.7	0.1	-3.5	3.8	3.8	3.8	-3.4	-3.5	-3.4	2.3
Fe7(trans)	BS10-147	3.1	-2.1	-2.2	3.1	-2.6	-1.1	2.6	0.0	3.7	-2.7	-3.0	3.6	-3.4	-3.0	3.6	1.0
<b>End-on cis-HNNH binding</b>																	
MoFe6	BS7-235	3.0	-2.5	-2.6	2.8	-2.9	2.0	2.5	-0.6	3.5	-3.4	-3.4	3.5	-3.5	3.2	3.4	1.7
Fe2(cis)	BS10-147	-3.2	2.1	3.0	-2.9	2.5	2.4	-2.5	-0.3	3.7	-3.6	-3.7	3.6	3.5	-3.7	3.6	-2.4
Fe3(cis)	BS10-146	-3.3	2.9	2.0	-2.8	2.6	-2.5	2.6	-0.2	-3.7	3.7	2.4	-3.6	3.4	-3.5	3.4	-0.7
Fe4(cis)	BS7-235	3.3	-2.7	-2.9	1.4	-2.8	2.3	2.5	-0.2	3.8	-3.6	-3.6	2.1	-3.6	3.4	3.4	-1.0
Fe5(cis)	BS7-235	3.2	-3.0	-3.0	2.5	-2.8	1.8	2.3	0.0	3.6	-3.8	-3.8	3.4	-3.6	3.3	3.4	-1.0
Fe6(cis)	BS10-135	-3.2	2.7	-2.9	2.8	-2.5	1.4	2.7	-0.1	-3.7	3.6	-3.7	3.5	-3.5	2.1	3.5	-0.8
Fe7(cis)	BS7-235	3.2	-2.8	-2.4	2.9	-2.8	2.0	0.9	0.0	3.7	-3.7	-3.5	3.6	-3.5	3.3	2.2	-0.7

<sup>a</sup> In this structure, one of the protons of HNNH has moved to S5A, whereas the ligand has taken a proton from Arg-96 (cf. Figure S2).

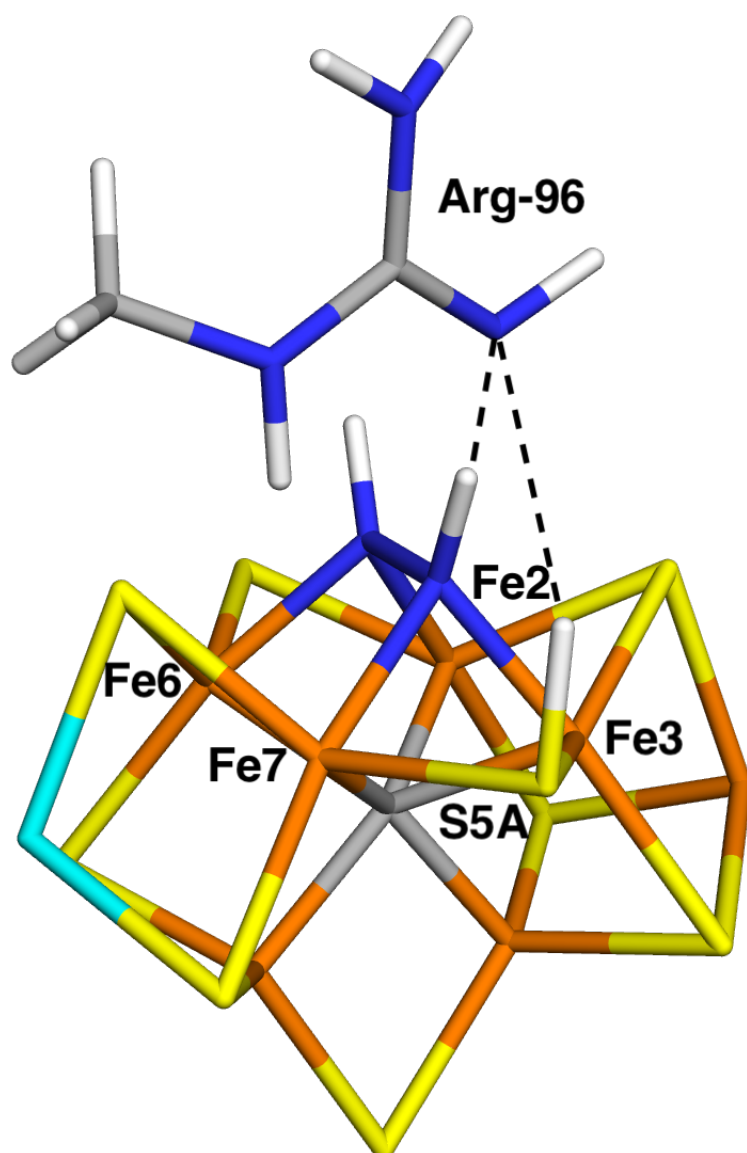
**Table S2.** Relative energies of the 35 BS states for some of the studied structures, obtained with TPSS (TP) or B3LYP(B3).

BS state	Fe2(trans)		Fe6-HNNH2		Fe6(trans)		Fe2(cis)		Fe6		Fe6(HCA)		Fe3/4	Fe4/5(5)		Fe3(S2A)	Fe3/7Fe4/5		Fe2Fe6(3)	Fe2Fe6(5)	
	TP	B3	TP	B3	TP	B3	TP	B3	TP	B3	TP	B3	TP	TP	B3	B3	TP	B3	TP	TP	TP
BS1-567	86	186	101	161		220	97	179		254	44	35	83	64	218	207			56		
BS2-234	19	2	43	22	35	0	18	3	41	50	32	50	48	4	83	18	0	70	60		26
BS3-123	55	8	5	112	37	32	55	7	47	113	58	59	72	67	119	31	57	104	56		71
BS3-124	44	14	53	67		20	55	11	66	70	44	123	66	40	101	55	61	114	48		65
BS3-134	64	32	48	30	43	11	68	44	71	78	44	36	73	28	88	73	58	69	68		39
BS4-257	79	149	55	86	58	91	80	135	71	124	53	112	25	24	76	134	44	69	67		39
BS4-356	30	64	44	74	33	68	27	69		131	54	138	55	20	80	123	45	77	51		0
BS4-467	41	95	63	95		158	38	90	78	198			64	48	216	161	38	107	0		90
BS5-256		120	44	105	58	108		137		153			54	64	140	162			69		0
BS5-267		145	68	94		167		145	90	202			50	22	132	193			53		115
BS5-357	45	89	49	74	55	127	51	86	81	155	57	122	61	47	117	148			51		60
BS5-367	53	86	77	97	32	194	46	87	90	187	80	194	54	32	113	186	53	196	37		60
BS5-456	51	93	76	110		89	50	120	77	224	71	187	63	78	200	130			56		83
BS5-457	59	94	53	97	45	96	59	96		229	56	142	84	8	201	117	77	123	56		54
BS6-156	18	72	19	62	29	69	17	69	39	118	35	159	19		110	140	20	46	16		66
BS6-157	8	62	21	33	14	75	6	55	34	150	16	91	45	4	107	138	33	147	16		37
BS6-167	22	87	36	117	34	123	17	85	69	118			53	26	105	132	18	36	0		0
BS7-235	32	24	17	10		48	34	89	51	0	8	19	0	0	0	0	19	0	3		0
BS7-247	45	27	8	8	45	56	40	29	51	92	38	124	33	8	122	47	38	62	77		49
BS7-346	3	15	5	36		41	1	14	36	85	65	87	75	50	125	53	38	67	0		67
BS8-236	28	0	11	51		51	26	0	86	58		223	52	23	83	72	67	73	40		74
BS8-237	42	79	40	24	49	64	46	97	66	45	42	85	13	9	49	66			40		40
BS8-245	49	74	45	33	55	67	48	128	87	108	54	109	49	65	94	70	38	56	62		75
BS8-246	31	15	13	87		49	32	9	122	164	64	171	53	68	139	90			52		87
BS8-345	18	18	19	9	45	18	17	16	51	113	46	79	76	61	122	70	80	51	31		43
BS8-347	17	16	14	4	41	64	16	13	41	141	46	86	76	79	156	74			33		37
BS9-126	26	28	47	86	53	87	25	26	75	109	45	140	86	60	102	107	95	143	29		90
BS9-137	33	44	38	28	45	85	34	41	73	166	42	97	71	45	79	105	25		65		68
BS9-145	29	25	38	17	37	49	26	23	72	118	37	20	43	31	96	95			54		58
BS10-125	18	18	28	6	13	29	14	17	42	59	14	12	49	22	65	41	69	50	21		38
BS10-127	15	40	24	7	15	44	16	42	32	82	14	55	53	35	75	63	66	55	25		41
BS10-135	5	20	5	4	0	32	5	15	43	79	0	0	46	12	59	60	27	76	37		64
BS10-136	33	26	29	54	56	47	32	29	46	85	67	140	38	20	38	86	48	29	74		50
BS10-146	26	20	26	46	51	60	37	18	41	99	20	84	45	3	115	91	44	44	4		37
BS10-147	0	9	0	0	6	54	0	10	0	120	8	58	22	22	112	70	24	86	0		21

**Figure S1.** The QM/MM geometry of the Fe3/4 structure.



**Figure S2.** The QM/MM geometry of the Fe2/6Fe3/7tr structure.



**Table S3.** Coordinates of the best structures in PDB format.

Fe6(HCA)				REMARK Energies (QM/MM, QM+ptch) = -17129.752558 -16290.129409 -5.284382 H		
ATOM						
ATOM	1	H	???	1	3.500	2.240 -29.687
ATOM	2	C	???	1	3.906	2.095 -30.706
ATOM	3	H	???	1	5.011	2.115 -30.641
ATOM	4	H	???	1	3.594	1.112 -31.093
ATOM	5	N	???	1	3.476	3.148 -31.617
ATOM	6	H	???	1	3.968	4.049 -31.522
ATOM	7	C	???	1	2.847	2.926 -32.785
ATOM	8	N	???	1	1.989	1.881 -32.911
ATOM	9	H	???	1	1.813	1.274 -32.108
ATOM	10	H	???	1	1.787	1.493 -33.843
ATOM	11	N	???	1	3.066	3.743 -33.817
ATOM	12	H	???	1	3.624	4.614 -33.675
ATOM	13	H	???	1	2.416	3.767 -34.609
ATOM	14	H	???	1	7.276	1.562 -41.618
ATOM	15	C	???	1	7.581	2.030 -40.684
ATOM	16	N	???	1	8.438	3.113 -40.698
ATOM	17	C	???	1	8.511	3.514 -39.434
ATOM	18	H	???	1	9.078	4.358 -39.042
ATOM	19	N	???	1	7.746	2.736 -38.622
ATOM	20	H	???	1	7.595	2.940 -37.616
ATOM	21	C	???	1	7.128	1.786 -39.401
ATOM	22	H	???	1	6.433	1.057 -38.985
ATOM	23	H	???	1	2.978	9.557 -40.118
ATOM	24	C	???	1	3.104	8.705 -39.422
ATOM	25	H	???	1	2.509	7.840 -39.762
ATOM	26	H	???	1	2.796	9.023 -38.413
ATOM	27	S	???	1	4.918	8.301 -39.430
ATOM	28	H	???	1	6.637	8.643 -42.923
ATOM	29	C	???	1	7.435	7.842 -42.957
ATOM	30	H	???	1	8.006	8.022 -43.881
ATOM	31	H	???	1	8.092	7.980 -42.081
ATOM	32	C	???	1	6.837	6.419 -43.009
ATOM	33	O	???	1	7.262	5.638 -43.871
ATOM	34	N	???	1	5.923	6.124 -42.064
ATOM	35	H	???	1	5.588	6.846 -41.409
ATOM	36	C	???	1	5.391	4.763 -41.928
ATOM	37	H	???	1	6.246	4.093 -42.128
ATOM	38	C	???	1	4.922	4.521 -40.489
ATOM	39	H	???	1	4.592	3.469 -40.417
ATOM	40	H	???	1	5.757	4.667 -39.771
ATOM	41	O	???	1	3.807	5.335 -40.100
ATOM	42	H	???	1	4.172	6.176 -39.724
ATOM	43	H	???	1	4.607	4.494 -42.656
ATOM	44	H	???	1	13.632	11.342 -31.927
ATOM	45	C	???	1	12.719	10.654 -31.970
ATOM	46	H	???	1	12.873	9.949 -31.129
ATOM	47	H	???	1	11.736	11.192 -31.788
ATOM	48	C	???	1	12.887	9.818 -33.252
ATOM	49	O	???	1	14.017	9.620 -33.703
ATOM	50	N	???	1	11.789	9.210 -33.775
ATOM	51	H	???	1	10.829	9.423 -33.469
ATOM	52	C	???	1	11.956	8.128 -34.737
ATOM	53	H	???	1	12.913	7.632 -34.528
ATOM	54	H	???	1	11.128	7.417 -34.566
ATOM	55	C	???	1	11.982	8.526 -36.221
ATOM	56	O	???	1	12.994	8.407 -36.914
ATOM	57	N	???	1	10.779	8.969 -36.715
ATOM	58	H	???	1	9.939	8.819 -36.131
ATOM	59	C	???	1	10.594	9.155 -38.142
ATOM	60	H	???	1	11.591	9.303 -38.593
ATOM	61	H	???	1	10.153	8.254 -38.606
ATOM	62	C	???	1	9.676	10.291 -38.578
ATOM	63	O	???	1	9.529	10.513 -39.786
ATOM	64	N	???	1	9.053	11.005 -37.603
ATOM	65	H	???	1	9.117	10.677 -36.631
ATOM	66	C	???	1	8.100	12.061 -37.928
ATOM	67	H	???	1	8.334	12.410 -38.945
ATOM	68	H	???	1	7.043	11.659 -37.929
ATOM	69	C	???	1	8.207	13.251 -36.958
ATOM	70	O	???	1	8.476	14.390 -37.364
ATOM	71	N	???	1	7.918	12.931 -35.677
ATOM	72	H	???	1	7.748	11.944 -35.440
ATOM	73	C	???	1	7.844	13.898 -34.572
ATOM	74	H	???	1	6.991	14.578 -34.788
ATOM	75	C	???	1	7.531	13.116 -33.288
ATOM	76	H	???	1	8.318	12.354 -33.114
ATOM	77	H	???	1	7.559	13.819 -32.433
ATOM	78	C	???	1	6.159	12.415 -33.323
ATOM	79	H	???	1	5.357	13.183 -33.320
ATOM	80	H	???	1	6.037	11.822 -34.252
ATOM	81	C	???	1	5.963	11.462 -32.142
ATOM	82	H	???	1	6.654	10.600 -32.234
ATOM	83	H	???	1	6.189	11.992 -31.195
ATOM	84	N	???	1	4.572	10.996 -32.105
ATOM	85	H	???	1	3.963	11.178 -32.917
ATOM	86	C	???	1	3.988	10.366 -31.079
ATOM	87	N	???	1	4.663	10.163 -29.937
ATOM	88	H	???	1	5.611	10.533 -29.826
ATOM	89	H	???	1	4.323	9.520 -29.215
ATOM	90	N	???	1	2.709	9.938 -31.210
ATOM	91	H	???	1	2.243	10.183 -32.094
ATOM	92	H	???	1	2.097	9.951 -30.391
ATOM	93	H	???	1	8.731	14.564 -34.480
ATOM	94	H	???	1	8.402	7.469 -28.176
ATOM	95	C	???	1	9.346	7.522 -28.725
ATOM	96	N	???	1	9.536	6.791 -29.884
ATOM	97	C	???	1	10.842	6.862 -30.166
ATOM	98	H	???	1	11.343	6.389 -31.011
ATOM	99	N	???	1	11.483	7.626 -29.249

ATOM	100	H	???	1	12.495	7.849	-29.266
ATOM	101	C	???	1	10.555	8.051	-28.319
ATOM	102	H	???	1	10.834	8.719	-27.505
ATOM	103	O	???	1	10.648	5.253	-25.654
ATOM	104	C	???	1	10.944	4.627	-26.735
ATOM	105	O	???	1	12.096	4.379	-27.167
ATOM	106	C	???	1	9.736	4.221	-27.610
ATOM	107	H	???	1	8.870	4.020	-26.953
ATOM	108	H	???	1	9.484	5.132	-28.179
ATOM	109	C	???	1	9.914	3.093	-28.634
ATOM	110	H	???	1	10.887	3.196	-29.142
ATOM	111	H	???	1	9.916	2.101	-28.137
ATOM	112	C	???	1	8.824	3.120	-29.749
ATOM	113	O	???	1	9.238	4.082	-30.746
ATOM	114	H	???	1	9.291	3.680	-31.766
ATOM	115	C	???	1	7.507	3.632	-29.121
ATOM	116	O	???	1	7.111	4.794	-29.520
ATOM	117	O	???	1	6.903	2.972	-28.247
ATOM	118	C	???	1	8.570	1.740	-30.392
ATOM	119	H	???	1	8.109	1.080	-29.636
ATOM	120	H	???	1	7.818	1.883	-31.199
ATOM	121	C	???	1	9.800	1.030	-31.019
ATOM	122	O	???	1	10.562	1.759	-31.739
ATOM	123	O	???	1	9.918	-0.201	-30.831
ATOM	124	FE	???	1	7.919	7.752	-33.107
ATOM	125	MO	???	1	7.993	5.792	-31.254
ATOM	126	FE	???	1	6.995	8.481	-35.338
ATOM	127	FE	???	1	5.813	6.429	-32.629
ATOM	128	FE	???	1	7.932	5.099	-33.834
ATOM	129	FE	???	1	6.847	5.999	-36.046
ATOM	130	FE	???	1	5.514	7.776	-37.309
ATOM	131	FE	???	1	4.871	7.134	-34.849
ATOM	132	C	???	1	6.738	6.827	-34.294
ATOM	133	S	???	1	7.736	7.663	-37.360
ATOM	134	S	???	1	9.609	6.325	-32.920
ATOM	135	S	???	1	4.739	5.702	-36.646
ATOM	136	S	???	1	7.977	4.166	-35.895
ATOM	137	S	???	1	8.510	9.631	-34.196
ATOM	138	S	???	1	6.429	4.298	-32.308
ATOM	139	S	???	1	4.914	9.276	-35.636
ATOM	140	S	???	1	6.748	7.812	-31.168
ATOM	141	S	???	1	3.666	6.744	-32.982
ATOM	142	N	???	1	8.936	3.667	-33.235
ATOM	143	H	???	1	9.852	1.950	-33.247
ATOM	144	N	???	1	9.292	2.623	-33.836
ATOM	145	H	???	1	9.065	2.536	-34.853
ATOM	146	O	???	1	4.507	5.540	-29.443
ATOM	147	H	???	1	5.462	5.257	-29.486
ATOM	148	H	???	1	4.439	6.273	-30.095
ATOM	149	O	???	1	1.061	8.394	-34.250
ATOM	150	H	???	1	1.915	8.051	-33.887
ATOM	151	H	???	1	0.548	8.690	-33.441
END							

Fe6

REMARK Energies (QM/MM, QM+ptch) = -17129.745891 -16290.117291

ATOM	1	H	???	1	3.496	2.241	-29.688
ATOM	2	C	???	1	3.896	2.098	-30.711
ATOM	3	H	???	1	5.002	2.103	-30.655
ATOM	4	H	???	1	3.569	1.120	-31.101
ATOM	5	N	???	1	3.469	3.163	-31.609
ATOM	6	H	???	1	3.961	4.062	-31.495
ATOM	7	C	???	1	2.856	2.958	-32.789
ATOM	8	N	???	1	2.001	1.913	-32.938
ATOM	9	H	???	1	1.825	1.293	-32.145
ATOM	10	H	???	1	1.805	1.535	-33.876
ATOM	11	N	???	1	3.086	3.793	-33.804
ATOM	12	H	???	1	3.634	4.667	-33.635
ATOM	13	H	???	1	2.449	3.826	-34.606
ATOM	14	H	???	1	7.279	1.558	-41.619
ATOM	15	C	???	1	7.594	2.016	-40.683
ATOM	16	N	???	1	8.457	3.094	-40.689
ATOM	17	C	???	1	8.574	3.450	-39.415
ATOM	18	H	???	1	9.155	4.281	-39.014
ATOM	19	N	???	1	7.834	2.644	-38.605
ATOM	20	H	???	1	7.699	2.821	-37.592
ATOM	21	C	???	1	7.181	1.730	-39.397
ATOM	22	H	???	1	6.491	0.995	-38.983
ATOM	23	H	???	1	2.981	9.557	-40.119
ATOM	24	C	???	1	3.115	8.706	-39.423
ATOM	25	H	???	1	2.538	7.831	-39.770
ATOM	26	H	???	1	2.783	9.021	-38.420
ATOM	27	S	???	1	4.941	8.335	-39.405
ATOM	28	H	???	1	6.638	8.643	-42.923
ATOM	29	C	???	1	7.436	7.841	-42.958
ATOM	30	H	???	1	8.006	8.022	-43.881
ATOM	31	H	???	1	8.092	7.980	-42.081
ATOM	32	C	???	1	6.837	6.419	-43.009
ATOM	33	O	???	1	7.258	5.639	-43.874
ATOM	34	N	???	1	5.924	6.124	-42.063
ATOM	35	H	???	1	5.599	6.846	-41.401
ATOM	36	C	???	1	5.390	4.764	-41.924
ATOM	37	H	???	1	6.245	4.093	-42.126
ATOM	38	C	???	1	4.930	4.525	-40.483
ATOM	39	H	???	1	4.591	3.477	-40.408
ATOM	40	H	???	1	5.774	4.662	-39.771
ATOM	41	O	???	1	3.826	5.349	-40.081
ATOM	42	H	???	1	4.200	6.184	-39.698
ATOM	43	H	???	1	4.607	4.495	-42.654
ATOM	44	H	???	1	13.632	11.344	-31.927
ATOM	45	C	???	1	12.720	10.656	-31.972
ATOM	46	H	???	1	12.875	9.950	-31.132
ATOM	47	H	???	1	11.737	11.192	-31.789
ATOM	48	C	???	1	12.894	9.821	-33.253
ATOM	49	O	???	1	14.028	9.614	-33.692



ATOM	50	N	???	1	11.797	9.223	-33.783
ATOM	51	H	???	1	10.835	9.455	-33.493
ATOM	52	C	???	1	11.955	8.139	-34.743
ATOM	53	H	???	1	12.914	7.642	-34.537
ATOM	54	H	???	1	11.124	7.433	-34.565
ATOM	55	C	???	1	11.974	8.528	-36.230
ATOM	56	O	???	1	12.987	8.407	-36.924
ATOM	57	N	???	1	10.769	8.960	-36.723
ATOM	58	H	???	1	9.931	8.817	-36.132
ATOM	59	C	???	1	10.575	9.143	-38.148
ATOM	60	H	???	1	11.571	9.264	-38.609
ATOM	61	H	???	1	10.102	8.251	-38.598
ATOM	62	C	???	1	9.680	10.299	-38.583
ATOM	63	O	???	1	9.550	10.537	-39.790
ATOM	64	N	???	1	9.050	11.004	-37.606
ATOM	65	H	???	1	9.096	10.658	-36.639
ATOM	66	C	???	1	8.099	12.061	-37.929
ATOM	67	H	???	1	8.333	12.411	-38.945
ATOM	68	H	???	1	7.043	11.659	-37.929
ATOM	69	C	???	1	8.208	13.252	-36.959
ATOM	70	O	???	1	8.477	14.391	-37.365
ATOM	71	N	???	1	7.919	12.932	-35.677
ATOM	72	H	???	1	7.751	11.946	-35.440
ATOM	73	C	???	1	7.845	13.900	-34.573
ATOM	74	H	???	1	6.992	14.579	-34.789
ATOM	75	C	???	1	7.532	13.117	-33.289
ATOM	76	H	???	1	8.316	12.350	-33.121
ATOM	77	H	???	1	7.567	13.817	-32.432
ATOM	78	C	???	1	6.156	12.424	-33.322
ATOM	79	H	???	1	5.358	13.195	-33.292
ATOM	80	H	???	1	6.019	11.855	-34.264
ATOM	81	C	???	1	5.970	11.443	-32.164
ATOM	82	H	???	1	6.652	10.577	-32.289
ATOM	83	H	???	1	6.217	11.946	-31.207
ATOM	84	N	???	1	4.575	10.993	-32.115
ATOM	85	H	???	1	3.966	11.167	-32.929
ATOM	86	C	???	1	3.996	10.357	-31.090
ATOM	87	N	???	1	4.678	10.137	-29.955
ATOM	88	H	???	1	5.628	10.505	-29.846
ATOM	89	H	???	1	4.338	9.494	-29.233
ATOM	90	N	???	1	2.713	9.940	-31.214
ATOM	91	H	???	1	2.242	10.191	-32.094
ATOM	92	H	???	1	2.106	9.946	-30.391
ATOM	93	H	???	1	8.731	14.565	-34.480
ATOM	94	H	???	1	8.405	7.460	-28.186
ATOM	95	C	???	1	9.349	7.499	-28.749
ATOM	96	N	???	1	9.550	6.767	-29.911
ATOM	97	C	???	1	10.852	6.867	-30.198
ATOM	98	H	???	1	11.354	6.417	-31.055
ATOM	99	N	???	1	11.484	7.640	-29.281
ATOM	100	H	???	1	12.492	7.877	-29.297
ATOM	101	C	???	1	10.551	8.047	-28.348
ATOM	102	H	???	1	10.823	8.714	-27.531
ATOM	103	O	???	1	10.666	5.259	-25.638
ATOM	104	C	???	1	10.949	4.627	-26.716
ATOM	105	O	???	1	12.095	4.360	-27.156
ATOM	106	C	???	1	9.735	4.236	-27.586
ATOM	107	H	???	1	8.847	4.118	-26.940
ATOM	108	H	???	1	9.543	5.120	-28.218
ATOM	109	C	???	1	9.877	3.044	-28.535
ATOM	110	H	???	1	10.864	3.075	-29.025
ATOM	111	H	???	1	9.829	2.083	-27.985
ATOM	112	C	???	1	8.806	3.075	-29.663
ATOM	113	O	???	1	9.275	3.989	-30.687
ATOM	114	H	???	1	9.879	3.365	-31.279
ATOM	115	C	???	1	7.496	3.630	-29.096
ATOM	116	O	???	1	7.133	4.779	-29.543
ATOM	117	O	???	1	6.869	2.987	-28.223
ATOM	118	C	???	1	8.555	1.715	-30.342
ATOM	119	H	???	1	8.155	0.988	-29.614
ATOM	120	H	???	1	7.788	1.875	-31.129
ATOM	121	C	???	1	9.806	1.137	-31.034
ATOM	122	O	???	1	10.551	2.014	-31.632
ATOM	123	O	???	1	9.984	-0.094	-31.005
ATOM	124	FE	???	1	5.889	6.434	-32.645
ATOM	125	MO	???	1	8.037	5.712	-31.319
ATOM	126	FE	???	1	7.788	5.100	-33.868
ATOM	127	FE	???	1	8.010	7.723	-33.148
ATOM	128	FE	???	1	4.833	7.262	-34.759
ATOM	129	FE	???	1	6.803	6.120	-36.061
ATOM	130	FE	???	1	5.342	7.875	-37.202
ATOM	131	FE	???	1	6.972	8.557	-35.337
ATOM	132	C	???	1	6.690	6.891	-34.315
ATOM	133	S	???	1	7.671	7.694	-37.367
ATOM	134	S	???	1	9.644	6.182	-33.013
ATOM	135	S	???	1	4.614	5.864	-36.541
ATOM	136	S	???	1	7.817	4.243	-35.998
ATOM	137	S	???	1	8.554	9.649	-34.178
ATOM	138	S	???	1	6.377	4.302	-32.321
ATOM	139	S	???	1	4.810	9.364	-35.501
ATOM	140	S	???	1	6.892	7.782	-31.186
ATOM	141	S	???	1	3.717	6.762	-32.889
ATOM	142	N	???	1	8.651	3.461	-33.715
ATOM	143	H	???	1	10.346	2.470	-33.658
ATOM	144	N	???	1	9.892	3.368	-33.883
ATOM	145	H	???	1	10.495	4.214	-34.016
ATOM	146	O	???	1	4.513	5.538	-29.470
ATOM	147	H	???	1	5.467	5.266	-29.533
ATOM	148	H	???	1	4.399	6.201	-30.189
ATOM	149	O	???	1	1.081	8.392	-34.244
ATOM	150	H	???	1	1.946	8.072	-33.886
ATOM	151	H	???	1	0.567	8.684	-33.433

END

Fe6-HNNH2

REMARK Energies (QM/MM, QM+ptch) = -17129.762036 -16290.139306

ATOM	1	H	???	1	3.501	2.240	-29.686
ATOM	2	C	???	1	3.912	2.095	-30.704
ATOM	3	H	???	1	5.017	2.108	-30.632
ATOM	4	H	???	1	3.597	1.114	-31.094
ATOM	5	N	???	1	3.492	3.151	-31.615
ATOM	6	H	???	1	3.966	4.059	-31.499
ATOM	7	C	???	1	2.859	2.936	-32.781
ATOM	8	N	???	1	2.000	1.892	-32.911
ATOM	9	H	???	1	1.823	1.283	-32.110
ATOM	10	H	???	1	1.798	1.506	-33.844
ATOM	11	N	???	1	3.076	3.756	-33.812
ATOM	12	H	???	1	3.640	4.622	-33.669
ATOM	13	H	???	1	2.421	3.787	-34.598
ATOM	14	H	???	1	7.275	1.561	-41.620
ATOM	15	C	???	1	7.581	2.027	-40.686
ATOM	16	N	???	1	8.439	3.110	-40.699
ATOM	17	C	???	1	8.512	3.508	-39.434
ATOM	18	H	???	1	9.080	4.350	-39.039
ATOM	19	N	???	1	7.746	2.727	-38.624
ATOM	20	H	???	1	7.592	2.931	-37.620
ATOM	21	C	???	1	7.127	1.781	-39.406
ATOM	22	H	???	1	6.431	1.052	-38.991
ATOM	23	H	???	1	2.977	9.557	-40.117
ATOM	24	C	???	1	3.101	8.705	-39.421
ATOM	25	H	???	1	2.511	7.838	-39.764
ATOM	26	H	???	1	2.784	9.023	-38.414
ATOM	27	S	???	1	4.916	8.306	-39.415
ATOM	28	H	???	1	6.637	8.643	-42.923
ATOM	29	C	???	1	7.435	7.842	-42.957
ATOM	30	H	???	1	8.006	8.022	-43.881
ATOM	31	H	???	1	8.092	7.980	-42.081
ATOM	32	C	???	1	6.837	6.419	-43.008
ATOM	33	O	???	1	7.261	5.638	-43.870
ATOM	34	N	???	1	5.923	6.124	-42.063
ATOM	35	H	???	1	5.589	6.846	-41.408
ATOM	36	C	???	1	5.390	4.763	-41.927
ATOM	37	H	???	1	6.246	4.094	-42.129
ATOM	38	C	???	1	4.924	4.520	-40.488
ATOM	39	H	???	1	4.591	3.469	-40.417
ATOM	40	H	???	1	5.762	4.661	-39.772
ATOM	41	O	???	1	3.813	5.336	-40.093
ATOM	42	H	???	1	4.180	6.175	-39.716
ATOM	43	H	???	1	4.607	4.494	-42.656
ATOM	44	H	???	1	13.632	11.342	-31.927
ATOM	45	C	???	1	12.719	10.655	-31.970
ATOM	46	H	???	1	12.873	9.949	-31.129
ATOM	47	H	???	1	11.736	11.192	-31.788
ATOM	48	C	???	1	12.891	9.820	-33.252
ATOM	49	O	???	1	14.022	9.625	-33.702
ATOM	50	N	???	1	11.796	9.212	-33.780
ATOM	51	H	???	1	10.835	9.414	-33.467
ATOM	52	C	???	1	11.970	8.131	-34.742
ATOM	53	H	???	1	12.933	7.644	-34.534
ATOM	54	H	???	1	11.151	7.411	-34.569
ATOM	55	C	???	1	11.988	8.528	-36.226
ATOM	56	O	???	1	12.995	8.405	-36.925
ATOM	57	N	???	1	10.783	8.973	-36.714
ATOM	58	H	???	1	9.946	8.824	-36.126
ATOM	59	C	???	1	10.594	9.155	-38.140
ATOM	60	H	???	1	11.590	9.305	-38.594
ATOM	61	H	???	1	10.155	8.253	-38.603
ATOM	62	C	???	1	9.672	10.289	-38.577
ATOM	63	O	???	1	9.519	10.505	-39.785
ATOM	64	N	???	1	9.054	11.007	-37.603
ATOM	65	H	???	1	9.128	10.688	-36.629
ATOM	66	C	???	1	8.100	12.062	-37.928
ATOM	67	H	???	1	8.333	12.411	-38.944
ATOM	68	H	???	1	7.043	11.659	-37.929
ATOM	69	C	???	1	8.207	13.252	-36.958
ATOM	70	O	???	1	8.476	14.390	-37.363
ATOM	71	N	???	1	7.918	12.931	-35.676
ATOM	72	H	???	1	7.746	11.945	-35.440
ATOM	73	C	???	1	7.844	13.899	-34.572
ATOM	74	H	???	1	6.991	14.578	-34.787
ATOM	75	C	???	1	7.531	13.118	-33.287
ATOM	76	H	???	1	8.319	12.357	-33.112
ATOM	77	H	???	1	7.558	13.822	-32.433
ATOM	78	C	???	1	6.160	12.415	-33.322
ATOM	79	H	???	1	5.357	13.183	-33.323
ATOM	80	H	???	1	6.040	11.819	-34.248
ATOM	81	C	???	1	5.962	11.467	-32.138
ATOM	82	H	???	1	6.654	10.605	-32.224
ATOM	83	H	???	1	6.185	12.001	-31.192
ATOM	84	N	???	1	4.572	10.999	-32.103
ATOM	85	H	???	1	3.962	11.184	-32.913
ATOM	86	C	???	1	3.990	10.365	-31.078
ATOM	87	N	???	1	4.668	10.157	-29.939
ATOM	88	H	???	1	5.617	10.525	-29.828
ATOM	89	H	???	1	4.328	9.514	-29.216
ATOM	90	N	???	1	2.710	9.939	-31.207
ATOM	91	H	???	1	2.242	10.189	-32.089
ATOM	92	H	???	1	2.100	9.949	-30.387
ATOM	93	H	???	1	8.731	14.564	-34.480
ATOM	94	H	???	1	8.402	7.472	-28.174
ATOM	95	C	???	1	9.349	7.530	-28.717
ATOM	96	N	???	1	9.553	6.787	-29.864
ATOM	97	C	???	1	10.861	6.855	-30.131
ATOM	98	H	???	1	11.373	6.366	-30.960
ATOM	99	N	???	1	11.491	7.632	-29.217
ATOM	100	H	???	1	12.501	7.858	-29.230
ATOM	101	C	???	1	10.552	8.066	-28.303
ATOM	102	H	???	1	10.820	8.743	-27.492
ATOM	103	O	???	1	10.649	5.254	-25.648
ATOM	104	C	???	1	10.943	4.629	-26.731

ATOM	105	O	???	1	12.096	4.386	-27.164
ATOM	106	C	???	1	9.734	4.220	-27.602
ATOM	107	H	???	1	8.872	4.017	-26.942
ATOM	108	H	???	1	9.478	5.131	-28.171
ATOM	109	C	???	1	9.906	3.098	-28.634
ATOM	110	H	???	1	10.884	3.196	-29.134
ATOM	111	H	???	1	9.890	2.101	-28.147
ATOM	112	C	???	1	8.827	3.170	-29.762
ATOM	113	O	???	1	9.233	4.133	-30.714
ATOM	114	H	???	1	9.387	3.678	-32.330
ATOM	115	C	???	1	7.499	3.641	-29.121
ATOM	116	O	???	1	7.081	4.794	-29.541
ATOM	117	O	???	1	6.894	2.983	-28.246
ATOM	118	C	???	1	8.557	1.789	-30.427
ATOM	119	H	???	1	8.064	1.129	-29.690
ATOM	120	H	???	1	7.828	1.970	-31.246
ATOM	121	C	???	1	9.770	1.045	-31.037
ATOM	122	O	???	1	10.513	1.725	-31.831
ATOM	123	O	???	1	9.910	-0.172	-30.782
ATOM	124	FE	???	1	7.927	7.753	-33.079
ATOM	125	MO	???	1	8.041	5.728	-31.251
ATOM	126	FE	???	1	7.005	8.481	-35.317
ATOM	127	FE	???	1	5.828	6.417	-32.614
ATOM	128	FE	???	1	8.008	5.129	-33.861
ATOM	129	FE	???	1	6.843	6.016	-36.043
ATOM	130	FE	???	1	5.506	7.801	-37.288
ATOM	131	FE	???	1	4.883	7.142	-34.820
ATOM	132	C	???	1	6.755	6.819	-34.277
ATOM	133	S	???	1	7.727	7.684	-37.352
ATOM	134	S	???	1	9.653	6.370	-32.894
ATOM	135	S	???	1	4.732	5.729	-36.623
ATOM	136	S	???	1	7.969	4.182	-35.927
ATOM	137	S	???	1	8.512	9.633	-34.179
ATOM	138	S	???	1	6.481	4.277	-32.373
ATOM	139	S	???	1	4.928	9.288	-35.600
ATOM	140	S	???	1	6.773	7.759	-31.131
ATOM	141	S	???	1	3.678	6.751	-32.962
ATOM	142	N	???	1	9.036	3.692	-33.340
ATOM	143	H	???	1	9.772	1.875	-33.241
ATOM	144	N	???	1	9.223	2.539	-33.865
ATOM	145	H	???	1	8.900	2.449	-34.845
ATOM	146	O	???	1	4.494	5.524	-29.473
ATOM	147	H	???	1	5.453	5.245	-29.496
ATOM	148	H	???	1	4.446	6.280	-30.099
ATOM	149	O	???	1	1.065	8.393	-34.246
ATOM	150	H	???	1	1.916	8.050	-33.878
ATOM	151	H	???	1	0.547	8.690	-33.440
END							

Fe3/7Fe4/5

REMARK Energies (QM/MM, QM+ptch) = -17129.751918 -16290.127014

ATOM	1	H	???	1	3.501	2.238	-29.687
ATOM	2	C	???	1	3.913	2.084	-30.706
ATOM	3	H	???	1	5.006	2.241	-30.656
ATOM	4	H	???	1	3.719	1.046	-31.024
ATOM	5	N	???	1	3.363	2.998	-31.696
ATOM	6	H	???	1	3.840	3.909	-31.813
ATOM	7	C	???	1	2.668	2.579	-32.771
ATOM	8	N	???	1	1.853	1.500	-32.697
ATOM	9	H	???	1	1.706	1.011	-31.810
ATOM	10	H	???	1	1.629	1.009	-33.571
ATOM	11	N	???	1	2.795	3.222	-33.928
ATOM	12	H	???	1	3.281	4.166	-33.903
ATOM	13	H	???	1	2.096	3.087	-34.665
ATOM	14	H	???	1	7.277	1.566	-41.610
ATOM	15	C	???	1	7.583	2.040	-40.669
ATOM	16	N	???	1	8.437	3.127	-40.697
ATOM	17	C	???	1	8.514	3.543	-39.439
ATOM	18	H	???	1	9.084	4.391	-39.061
ATOM	19	N	???	1	7.754	2.775	-38.612
ATOM	20	H	???	1	7.621	2.979	-37.604
ATOM	21	C	???	1	7.136	1.812	-39.380
ATOM	22	H	???	1	6.447	1.086	-38.951
ATOM	23	H	???	1	2.984	9.554	-40.118
ATOM	24	C	???	1	3.119	8.698	-39.423
ATOM	25	H	???	1	2.477	7.858	-39.738
ATOM	26	H	???	1	2.865	9.023	-38.400
ATOM	27	S	???	1	4.912	8.190	-39.469
ATOM	28	H	???	1	6.638	8.643	-42.924
ATOM	29	C	???	1	7.437	7.843	-42.960
ATOM	30	H	???	1	8.009	8.029	-43.882
ATOM	31	H	???	1	8.093	7.981	-42.082
ATOM	32	C	???	1	6.842	6.419	-43.017
ATOM	33	O	???	1	7.270	5.643	-43.883
ATOM	34	N	???	1	5.928	6.121	-42.075
ATOM	35	H	???	1	5.590	6.842	-41.418
ATOM	36	C	???	1	5.398	4.759	-41.938
ATOM	37	H	???	1	6.255	4.091	-42.143
ATOM	38	C	???	1	4.926	4.513	-40.502
ATOM	39	H	???	1	4.628	3.453	-40.424
ATOM	40	H	???	1	5.751	4.691	-39.777
ATOM	41	O	???	1	3.784	5.293	-40.131
ATOM	42	H	???	1	4.123	6.161	-39.790
ATOM	43	H	???	1	4.612	4.493	-42.662
ATOM	44	H	???	1	13.631	11.346	-31.927
ATOM	45	C	???	1	12.722	10.655	-31.975
ATOM	46	H	???	1	12.877	9.949	-31.135
ATOM	47	H	???	1	11.738	11.191	-31.790
ATOM	48	C	???	1	12.921	9.824	-33.259
ATOM	49	O	???	1	14.067	9.636	-33.675
ATOM	50	N	???	1	11.845	9.215	-33.814
ATOM	51	H	???	1	10.870	9.418	-33.540
ATOM	52	C	???	1	12.037	8.138	-34.779
ATOM	53	H	???	1	13.007	7.669	-34.567
ATOM	54	H	???	1	11.226	7.408	-34.603

ATOM	55	C	???	1	12.048	8.515	-36.274
ATOM	56	O	???	1	13.046	8.345	-36.981
ATOM	57	N	???	1	10.851	8.975	-36.749
ATOM	58	H	???	1	10.039	8.917	-36.098
ATOM	59	C	???	1	10.615	9.147	-38.167
ATOM	60	H	???	1	11.593	9.268	-38.666
ATOM	61	H	???	1	10.130	8.251	-38.598
ATOM	62	C	???	1	9.703	10.299	-38.587
ATOM	63	O	???	1	9.582	10.563	-39.791
ATOM	64	N	???	1	9.050	10.975	-37.603
ATOM	65	H	???	1	9.046	10.581	-36.649
ATOM	66	C	???	1	8.106	12.041	-37.923
ATOM	67	H	???	1	8.346	12.394	-38.936
ATOM	68	H	???	1	7.046	11.652	-37.927
ATOM	69	C	???	1	8.206	13.228	-36.950
ATOM	70	O	???	1	8.439	14.374	-37.359
ATOM	71	N	???	1	7.927	12.912	-35.663
ATOM	72	H	???	1	7.868	11.919	-35.391
ATOM	73	C	???	1	7.854	13.912	-34.591
ATOM	74	H	???	1	7.010	14.592	-34.834
ATOM	75	C	???	1	7.538	13.196	-33.275
ATOM	76	H	???	1	8.301	12.415	-33.078
ATOM	77	H	???	1	7.595	13.934	-32.452
ATOM	78	C	???	1	6.151	12.538	-33.268
ATOM	79	H	???	1	5.373	13.308	-33.447
ATOM	80	H	???	1	6.067	11.801	-34.093
ATOM	81	C	???	1	5.866	11.835	-31.942
ATOM	82	H	???	1	6.629	11.054	-31.746
ATOM	83	H	???	1	5.935	12.557	-31.103
ATOM	84	N	???	1	4.533	11.221	-31.988
ATOM	85	H	???	1	3.896	11.462	-32.765
ATOM	86	C	???	1	4.009	10.423	-31.040
ATOM	87	N	???	1	4.704	10.149	-29.932
ATOM	88	H	???	1	5.606	10.606	-29.761
ATOM	89	H	???	1	4.415	9.420	-29.268
ATOM	90	N	???	1	2.792	9.876	-31.266
ATOM	91	H	???	1	2.280	10.194	-32.103
ATOM	92	H	???	1	2.213	9.589	-30.476
ATOM	93	H	???	1	8.736	14.572	-34.492
ATOM	94	H	???	1	8.405	7.460	-28.187
ATOM	95	C	???	1	9.347	7.498	-28.754
ATOM	96	N	???	1	9.531	6.765	-29.918
ATOM	97	C	???	1	10.829	6.856	-30.218
ATOM	98	H	???	1	11.317	6.401	-31.081
ATOM	99	N	???	1	11.478	7.623	-29.306
ATOM	100	H	???	1	12.487	7.855	-29.331
ATOM	101	C	???	1	10.557	8.036	-28.364
ATOM	102	H	???	1	10.843	8.701	-27.549
ATOM	103	O	???	1	10.658	5.252	-25.646
ATOM	104	C	???	1	10.938	4.622	-26.727
ATOM	105	O	???	1	12.084	4.349	-27.163
ATOM	106	C	???	1	9.721	4.245	-27.601
ATOM	107	H	???	1	8.837	4.112	-26.952
ATOM	108	H	???	1	9.525	5.140	-28.216
ATOM	109	C	???	1	9.855	3.074	-28.578
ATOM	110	H	???	1	10.842	3.119	-29.069
ATOM	111	H	???	1	9.808	2.102	-28.045
ATOM	112	C	???	1	8.775	3.140	-29.703
ATOM	113	O	???	1	9.218	4.034	-30.715
ATOM	114	H	???	1	9.962	3.095	-31.499
ATOM	115	C	???	1	7.458	3.639	-29.093
ATOM	116	O	???	1	7.057	4.771	-29.544
ATOM	117	O	???	1	6.858	2.978	-28.212
ATOM	118	C	???	1	8.487	1.771	-30.376
ATOM	119	H	???	1	8.114	1.029	-29.650
ATOM	120	H	???	1	7.697	1.948	-31.136
ATOM	121	C	???	1	9.706	1.215	-31.095
ATOM	122	O	???	1	10.405	2.135	-31.760
ATOM	123	O	???	1	10.000	0.021	-31.072
ATOM	124	FE	???	1	6.873	8.455	-35.278
ATOM	125	MO	???	1	8.004	5.668	-31.307
ATOM	126	FE	???	1	4.835	7.079	-34.805
ATOM	127	FE	???	1	5.741	6.445	-32.630
ATOM	128	FE	???	1	7.772	7.800	-33.086
ATOM	129	FE	???	1	5.425	7.634	-37.351
ATOM	130	FE	???	1	6.858	5.978	-36.086
ATOM	131	FE	???	1	7.751	5.252	-33.849
ATOM	132	C	???	1	6.691	6.748	-34.351
ATOM	133	S	???	1	7.685	7.715	-37.286
ATOM	134	S	???	1	9.530	6.313	-33.029
ATOM	135	S	???	1	4.715	5.631	-36.581
ATOM	136	S	???	1	8.010	4.138	-35.694
ATOM	137	S	???	1	8.701	9.512	-34.394
ATOM	138	S	???	1	6.397	4.256	-32.386
ATOM	139	S	???	1	4.665	9.088	-35.905
ATOM	140	S	???	1	6.786	7.623	-31.082
ATOM	141	S	???	1	3.570	6.055	-33.150
ATOM	142	N	???	1	5.110	8.178	-33.215
ATOM	143	H	???	1	4.319	8.673	-32.785
ATOM	144	N	???	1	6.248	8.946	-33.472
ATOM	145	H	???	1	6.166	9.928	-33.198
ATOM	146	O	???	1	4.471	5.580	-29.439
ATOM	147	H	???	1	5.411	5.268	-29.521
ATOM	148	H	???	1	4.280	5.996	-30.311
ATOM	149	O	???	1	1.133	8.365	-34.201
ATOM	150	H	???	1	1.908	7.846	-33.863
ATOM	151	H	???	1	0.611	8.636	-33.391

END

Fe2(trans)

REMARK Energies (QM/MM, QM+ptch) = -17129.766955 -16290.137760

ATOM	1	H	???	1	3.501	2.241	-29.687
ATOM	2	C	???	1	3.909	2.098	-30.708
ATOM	3	H	???	1	5.013	2.109	-30.637
ATOM	4	H	???	1	3.592	1.118	-31.098

ATOM	5	N	???	1	3.493	3.154	-31.620
ATOM	6	H	???	1	3.981	4.057	-31.516
ATOM	7	C	???	1	2.859	2.939	-32.785
ATOM	8	N	???	1	1.997	1.896	-32.913
ATOM	9	H	???	1	1.821	1.286	-32.112
ATOM	10	H	???	1	1.794	1.510	-33.846
ATOM	11	N	???	1	3.077	3.759	-33.815
ATOM	12	H	???	1	3.633	4.630	-33.661
ATOM	13	H	???	1	2.419	3.793	-34.600
ATOM	14	H	???	1	7.285	1.552	-41.606
ATOM	15	C	???	1	7.615	1.993	-40.657
ATOM	16	N	???	1	8.576	2.984	-40.667
ATOM	17	C	???	1	8.816	3.256	-39.393
ATOM	18	H	???	1	9.514	3.996	-39.003
ATOM	19	N	???	1	8.045	2.494	-38.564
ATOM	20	H	???	1	7.996	2.635	-37.537
ATOM	21	C	???	1	7.254	1.685	-39.358
ATOM	22	H	???	1	6.524	0.996	-38.934
ATOM	23	H	???	1	2.986	9.555	-40.114
ATOM	24	C	???	1	3.127	8.704	-39.412
ATOM	25	H	???	1	2.585	7.812	-39.772
ATOM	26	H	???	1	2.759	9.010	-38.419
ATOM	27	S	???	1	4.964	8.376	-39.335
ATOM	28	H	???	1	6.631	8.637	-42.917
ATOM	29	C	???	1	7.422	7.828	-42.944
ATOM	30	H	???	1	7.988	7.991	-43.874
ATOM	31	H	???	1	8.088	7.976	-42.076
ATOM	32	C	???	1	6.816	6.407	-42.980
ATOM	33	O	???	1	7.231	5.626	-43.847
ATOM	34	N	???	1	5.901	6.112	-42.035
ATOM	35	H	???	1	5.611	6.816	-41.342
ATOM	36	C	???	1	5.368	4.750	-41.923
ATOM	37	H	???	1	6.224	4.078	-42.113
ATOM	38	C	???	1	4.828	4.450	-40.520
ATOM	39	H	???	1	4.349	3.455	-40.561
ATOM	40	H	???	1	5.647	4.398	-39.784
ATOM	41	O	???	1	3.819	5.366	-40.069
ATOM	42	H	???	1	4.267	6.157	-39.671
ATOM	43	H	???	1	4.600	4.490	-42.659
ATOM	44	H	???	1	13.633	11.343	-31.926
ATOM	45	C	???	1	12.721	10.656	-31.968
ATOM	46	H	???	1	12.875	9.952	-31.126
ATOM	47	H	???	1	11.737	11.192	-31.787
ATOM	48	C	???	1	12.895	9.816	-33.248
ATOM	49	O	???	1	14.026	9.621	-33.697
ATOM	50	N	???	1	11.798	9.207	-33.762
ATOM	51	H	???	1	10.837	9.426	-33.455
ATOM	52	C	???	1	11.952	8.124	-34.724
ATOM	53	H	???	1	12.903	7.615	-34.518
ATOM	54	H	???	1	11.115	7.424	-34.553
ATOM	55	C	???	1	11.980	8.530	-36.206
ATOM	56	O	???	1	12.991	8.409	-36.902
ATOM	57	N	???	1	10.780	8.988	-36.696
ATOM	58	H	???	1	9.936	8.822	-36.122
ATOM	59	C	???	1	10.593	9.161	-38.125
ATOM	60	H	???	1	11.590	9.301	-38.578
ATOM	61	H	???	1	10.148	8.258	-38.580
ATOM	62	C	???	1	9.677	10.296	-38.573
ATOM	63	O	???	1	9.517	10.495	-39.783
ATOM	64	N	???	1	9.073	11.034	-37.604
ATOM	65	H	???	1	9.139	10.708	-36.634
ATOM	66	C	???	1	8.103	12.072	-37.930
ATOM	67	H	???	1	8.330	12.426	-38.946
ATOM	68	H	???	1	7.045	11.663	-37.930
ATOM	69	C	???	1	8.205	13.260	-36.958
ATOM	70	O	???	1	8.478	14.400	-37.359
ATOM	71	N	???	1	7.915	12.937	-35.677
ATOM	72	H	???	1	7.727	11.953	-35.447
ATOM	73	C	???	1	7.844	13.903	-34.571
ATOM	74	H	???	1	6.992	14.584	-34.786
ATOM	75	C	???	1	7.533	13.125	-33.285
ATOM	76	H	???	1	8.316	12.358	-33.112
ATOM	77	H	???	1	7.570	13.831	-32.432
ATOM	78	C	???	1	6.158	12.434	-33.312
ATOM	79	H	???	1	5.359	13.205	-33.308
ATOM	80	H	???	1	6.027	11.840	-34.239
ATOM	81	C	???	1	5.960	11.482	-32.131
ATOM	82	H	???	1	6.650	10.619	-32.224
ATOM	83	H	???	1	6.188	12.011	-31.183
ATOM	84	N	???	1	4.568	11.023	-32.096
ATOM	85	H	???	1	3.964	11.194	-32.914
ATOM	86	C	???	1	3.995	10.360	-31.085
ATOM	87	N	???	1	4.680	10.130	-29.954
ATOM	88	H	???	1	5.623	10.512	-29.837
ATOM	89	H	???	1	4.343	9.480	-29.237
ATOM	90	N	???	1	2.718	9.929	-31.221
ATOM	91	H	???	1	2.247	10.194	-32.097
ATOM	92	H	???	1	2.110	9.911	-30.399
ATOM	93	H	???	1	8.731	14.566	-34.480
ATOM	94	H	???	1	8.407	7.459	-28.187
ATOM	95	C	???	1	9.352	7.497	-28.749
ATOM	96	N	???	1	9.563	6.751	-29.900
ATOM	97	C	???	1	10.864	6.856	-30.184
ATOM	98	H	???	1	11.370	6.393	-31.034
ATOM	99	N	???	1	11.489	7.644	-29.276
ATOM	100	H	???	1	12.496	7.886	-29.293
ATOM	101	C	???	1	10.551	8.056	-28.350
ATOM	102	H	???	1	10.816	8.735	-27.541
ATOM	103	O	???	1	10.667	5.255	-25.629
ATOM	104	C	???	1	10.946	4.622	-26.709
ATOM	105	O	???	1	12.091	4.350	-27.148
ATOM	106	C	???	1	9.730	4.240	-27.578
ATOM	107	H	???	1	8.839	4.135	-26.933
ATOM	108	H	???	1	9.550	5.120	-28.219
ATOM	109	C	???	1	9.858	3.043	-28.521

ATOM	110	H	???	1	10.850	3.065	-29.003
ATOM	111	H	???	1	9.794	2.084	-27.967
ATOM	112	C	???	1	8.797	3.110	-29.661
ATOM	113	O	???	1	9.282	3.993	-30.662
ATOM	114	H	???	1	9.994	3.075	-31.428
ATOM	115	C	???	1	7.474	3.631	-29.083
ATOM	116	O	???	1	7.090	4.765	-29.550
ATOM	117	O	???	1	6.851	2.980	-28.212
ATOM	118	C	???	1	8.508	1.742	-30.334
ATOM	119	H	???	1	8.133	0.999	-29.610
ATOM	120	H	???	1	7.718	1.918	-31.094
ATOM	121	C	???	1	9.723	1.183	-31.060
ATOM	122	O	???	1	10.430	2.097	-31.715
ATOM	123	O	???	1	9.996	-0.018	-31.050
ATOM	124	FE	???	1	5.903	6.325	-32.619
ATOM	125	MO	???	1	8.089	5.629	-31.308
ATOM	126	FE	???	1	7.776	5.238	-33.917
ATOM	127	FE	???	1	8.063	7.635	-33.073
ATOM	128	FE	???	1	4.840	7.240	-34.680
ATOM	129	FE	???	1	6.961	6.111	-36.197
ATOM	130	FE	???	1	5.342	7.983	-37.095
ATOM	131	FE	???	1	6.908	8.644	-35.101
ATOM	132	C	???	1	6.735	6.872	-34.305
ATOM	133	S	???	1	7.691	8.082	-37.135
ATOM	134	S	???	1	9.691	6.035	-33.009
ATOM	135	S	???	1	4.643	5.933	-36.503
ATOM	136	S	???	1	7.985	4.117	-35.753
ATOM	137	S	???	1	8.565	9.626	-33.964
ATOM	138	S	???	1	6.531	4.164	-32.410
ATOM	139	S	???	1	4.736	9.376	-35.350
ATOM	140	S	???	1	6.880	7.674	-31.154
ATOM	141	S	???	1	3.726	6.688	-32.828
ATOM	142	N	???	1	7.052	5.449	-38.020
ATOM	143	H	???	1	6.788	4.449	-38.087
ATOM	144	N	???	1	7.303	5.918	-39.158
ATOM	145	H	???	1	7.537	6.931	-39.000
ATOM	146	O	???	1	4.494	5.525	-29.479
ATOM	147	H	???	1	5.452	5.259	-29.529
ATOM	148	H	???	1	4.390	6.209	-30.180
ATOM	149	O	???	1	1.094	8.389	-34.237
ATOM	150	H	???	1	1.964	8.083	-33.880
ATOM	151	H	???	1	0.579	8.681	-33.428
END							

FE6(Trans)

REMARK Energies (QM/MM, QM+ptch) = -17129.761127 -16290.136624

ATOM	1	H	???	1	3.499	2.241	-29.688
ATOM	2	C	???	1	3.903	2.099	-30.709
ATOM	3	H	???	1	5.008	2.105	-30.645
ATOM	4	H	???	1	3.578	1.122	-31.102
ATOM	5	N	???	1	3.485	3.163	-31.611
ATOM	6	H	???	1	3.977	4.063	-31.495
ATOM	7	C	???	1	2.865	2.960	-32.787
ATOM	8	N	???	1	2.006	1.917	-32.933
ATOM	9	H	???	1	1.823	1.301	-32.140
ATOM	10	H	???	1	1.806	1.541	-33.871
ATOM	11	N	???	1	3.092	3.792	-33.805
ATOM	12	H	???	1	3.650	4.660	-33.644
ATOM	13	H	???	1	2.447	3.830	-34.600
ATOM	14	H	???	1	7.277	1.561	-41.617
ATOM	15	C	???	1	7.587	2.025	-40.682
ATOM	16	N	???	1	8.442	3.111	-40.695
ATOM	17	C	???	1	8.530	3.498	-39.428
ATOM	18	H	???	1	9.095	4.344	-39.036
ATOM	19	N	???	1	7.780	2.707	-38.614
ATOM	20	H	???	1	7.625	2.910	-37.609
ATOM	21	C	???	1	7.151	1.766	-39.396
ATOM	22	H	???	1	6.462	1.033	-38.979
ATOM	23	H	???	1	2.981	9.557	-40.119
ATOM	24	C	???	1	3.113	8.706	-39.423
ATOM	25	H	???	1	2.536	7.832	-39.770
ATOM	26	H	???	1	2.781	9.021	-38.420
ATOM	27	S	???	1	4.940	8.334	-39.404
ATOM	28	H	???	1	6.637	8.643	-42.923
ATOM	29	C	???	1	7.435	7.841	-42.957
ATOM	30	H	???	1	8.006	8.021	-43.881
ATOM	31	H	???	1	8.092	7.980	-42.081
ATOM	32	C	???	1	6.836	6.419	-43.008
ATOM	33	O	???	1	7.257	5.639	-43.871
ATOM	34	N	???	1	5.922	6.126	-42.062
ATOM	35	H	???	1	5.600	6.846	-41.399
ATOM	36	C	???	1	5.389	4.765	-41.923
ATOM	37	H	???	1	6.245	4.095	-42.125
ATOM	38	C	???	1	4.928	4.527	-40.482
ATOM	39	H	???	1	4.589	3.478	-40.408
ATOM	40	H	???	1	5.771	4.664	-39.771
ATOM	41	O	???	1	3.823	5.350	-40.081
ATOM	42	H	???	1	4.198	6.188	-39.704
ATOM	43	H	???	1	4.606	4.495	-42.653
ATOM	44	H	???	1	13.632	11.344	-31.927
ATOM	45	C	???	1	12.720	10.656	-31.971
ATOM	46	H	???	1	12.875	9.950	-31.130
ATOM	47	H	???	1	11.737	11.192	-31.788
ATOM	48	C	???	1	12.897	9.820	-33.253
ATOM	49	O	???	1	14.033	9.620	-33.691
ATOM	50	N	???	1	11.804	9.216	-33.782
ATOM	51	H	???	1	10.839	9.444	-33.495
ATOM	52	C	???	1	11.969	8.134	-34.743
ATOM	53	H	???	1	12.930	7.644	-34.540
ATOM	54	H	???	1	11.146	7.419	-34.565
ATOM	55	C	???	1	11.982	8.527	-36.230
ATOM	56	O	???	1	12.991	8.405	-36.929
ATOM	57	N	???	1	10.775	8.964	-36.716
ATOM	58	H	???	1	9.940	8.823	-36.121
ATOM	59	C	???	1	10.577	9.143	-38.142

ATOM	60	H	???	1	11.571	9.266	-38.606
ATOM	61	H	???	1	10.106	8.249	-38.589
ATOM	62	C	???	1	9.677	10.294	-38.578
ATOM	63	O	???	1	9.539	10.524	-39.786
ATOM	64	N	???	1	9.052	11.005	-37.602
ATOM	65	H	???	1	9.103	10.664	-36.634
ATOM	66	C	???	1	8.100	12.061	-37.927
ATOM	67	H	???	1	8.335	12.411	-38.943
ATOM	68	H	???	1	7.043	11.659	-37.929
ATOM	69	C	???	1	8.206	13.251	-36.956
ATOM	70	O	???	1	8.472	14.391	-37.363
ATOM	71	N	???	1	7.918	12.931	-35.675
ATOM	72	H	???	1	7.757	11.943	-35.437
ATOM	73	C	???	1	7.845	13.897	-34.570
ATOM	74	H	???	1	6.991	14.577	-34.785
ATOM	75	C	???	1	7.534	13.113	-33.287
ATOM	76	H	???	1	8.317	12.344	-33.123
ATOM	77	H	???	1	7.572	13.810	-32.428
ATOM	78	C	???	1	6.156	12.422	-33.319
ATOM	79	H	???	1	5.359	13.194	-33.274
ATOM	80	H	???	1	6.013	11.865	-34.267
ATOM	81	C	???	1	5.974	11.427	-32.172
ATOM	82	H	???	1	6.647	10.558	-32.316
ATOM	83	H	???	1	6.234	11.915	-31.211
ATOM	84	N	???	1	4.575	10.988	-32.115
ATOM	85	H	???	1	3.967	11.161	-32.929
ATOM	86	C	???	1	3.994	10.359	-31.087
ATOM	87	N	???	1	4.675	10.142	-29.951
ATOM	88	H	???	1	5.628	10.500	-29.846
ATOM	89	H	???	1	4.333	9.500	-29.229
ATOM	90	N	???	1	2.708	9.946	-31.209
ATOM	91	H	???	1	2.239	10.200	-32.089
ATOM	92	H	???	1	2.103	9.961	-30.385
ATOM	93	H	???	1	8.732	14.564	-34.479
ATOM	94	H	???	1	8.405	7.467	-28.180
ATOM	95	C	???	1	9.351	7.518	-28.733
ATOM	96	N	???	1	9.554	6.785	-29.891
ATOM	97	C	???	1	10.856	6.881	-30.175
ATOM	98	H	???	1	11.361	6.422	-31.027
ATOM	99	N	???	1	11.487	7.656	-29.260
ATOM	100	H	???	1	12.495	7.893	-29.277
ATOM	101	C	???	1	10.552	8.067	-28.330
ATOM	102	H	???	1	10.821	8.741	-27.517
ATOM	103	O	???	1	10.670	5.260	-25.619
ATOM	104	C	???	1	10.935	4.638	-26.708
ATOM	105	O	???	1	12.074	4.358	-27.158
ATOM	106	C	???	1	9.709	4.278	-27.573
ATOM	107	H	???	1	8.816	4.192	-26.929
ATOM	108	H	???	1	9.548	5.157	-28.221
ATOM	109	C	???	1	9.826	3.078	-28.510
ATOM	110	H	???	1	10.826	3.088	-28.974
ATOM	111	H	???	1	9.747	2.122	-27.952
ATOM	112	C	???	1	8.774	3.144	-29.660
ATOM	113	O	???	1	9.264	4.034	-30.657
ATOM	114	H	???	1	10.235	3.019	-31.189
ATOM	115	C	???	1	7.448	3.653	-29.082
ATOM	116	O	???	1	7.064	4.794	-29.525
ATOM	117	O	???	1	6.831	2.984	-28.218
ATOM	118	C	???	1	8.513	1.768	-30.329
ATOM	119	H	???	1	8.061	1.047	-29.626
ATOM	120	H	???	1	7.789	1.936	-31.155
ATOM	121	C	???	1	9.774	1.164	-30.927
ATOM	122	O	???	1	10.640	2.062	-31.407
ATOM	123	O	???	1	9.976	-0.045	-30.974
ATOM	124	FE	???	1	8.005	7.716	-33.087
ATOM	125	MO	???	1	8.042	5.732	-31.271
ATOM	126	FE	???	1	7.865	5.182	-33.898
ATOM	127	FE	???	1	5.841	6.440	-32.595
ATOM	128	FE	???	1	6.989	8.580	-35.311
ATOM	129	FE	???	1	5.349	7.891	-37.200
ATOM	130	FE	???	1	6.799	6.177	-36.013
ATOM	131	FE	???	1	4.855	7.242	-34.774
ATOM	132	C	???	1	6.732	6.901	-34.288
ATOM	133	S	???	1	7.668	7.717	-37.354
ATOM	134	S	???	1	9.649	6.221	-32.968
ATOM	135	S	???	1	4.660	5.844	-36.530
ATOM	136	S	???	1	7.782	4.302	-35.969
ATOM	137	S	???	1	8.574	9.635	-34.157
ATOM	138	S	???	1	6.433	4.298	-32.345
ATOM	139	S	???	1	4.812	9.352	-35.490
ATOM	140	S	???	1	6.853	7.788	-31.156
ATOM	141	S	???	1	3.694	6.777	-32.919
ATOM	142	N	???	1	8.845	3.602	-33.464
ATOM	143	H	???	1	9.064	3.581	-32.446
ATOM	144	N	???	1	9.268	2.581	-34.041
ATOM	145	H	???	1	8.992	2.684	-35.050
ATOM	146	O	???	1	4.469	5.542	-29.477
ATOM	147	H	???	1	5.427	5.271	-29.513
ATOM	148	H	???	1	4.385	6.232	-30.173
ATOM	149	O	???	1	1.066	8.390	-34.247
ATOM	150	H	???	1	1.928	8.067	-33.885
ATOM	151	H	???	1	0.553	8.689	-33.439

END

Fe4(trans)

REMARK Energies (QM/MM, QM+ptch) = -17129.756264 -16290.132084

ATOM	1	H	???	1	3.504	2.237	-29.684
ATOM	2	C	???	1	3.922	2.083	-30.700
ATOM	3	H	???	1	5.021	2.188	-30.635
ATOM	4	H	???	1	3.686	1.062	-31.042
ATOM	5	N	???	1	3.430	3.045	-31.674
ATOM	6	H	???	1	3.941	3.941	-31.738
ATOM	7	C	???	1	2.731	2.691	-32.767
ATOM	8	N	???	1	1.886	1.630	-32.741
ATOM	9	H	???	1	1.741	1.101	-31.878

ATOM	10	H	???	1	1.664	1.166	-33.633
ATOM	11	N	???	1	2.876	3.384	-33.894
ATOM	12	H	???	1	3.406	4.290	-33.862
ATOM	13	H	???	1	2.181	3.302	-34.642
ATOM	14	H	???	1	7.276	1.565	-41.613
ATOM	15	C	???	1	7.581	2.036	-40.674
ATOM	16	N	???	1	8.438	3.120	-40.694
ATOM	17	C	???	1	8.515	3.525	-39.432
ATOM	18	H	???	1	9.092	4.365	-39.046
ATOM	19	N	???	1	7.749	2.755	-38.613
ATOM	20	H	???	1	7.625	2.940	-37.601
ATOM	21	C	???	1	7.131	1.800	-39.388
ATOM	22	H	???	1	6.438	1.073	-38.965
ATOM	23	H	???	1	2.997	9.552	-40.121
ATOM	24	C	???	1	3.159	8.694	-39.433
ATOM	25	H	???	1	2.528	7.841	-39.737
ATOM	26	H	???	1	2.939	9.004	-38.398
ATOM	27	S	???	1	4.969	8.250	-39.578
ATOM	28	H	???	1	6.639	8.644	-42.926
ATOM	29	C	???	1	7.440	7.845	-42.963
ATOM	30	H	???	1	8.014	8.035	-43.883
ATOM	31	H	???	1	8.094	7.981	-42.083
ATOM	32	C	???	1	6.849	6.419	-43.027
ATOM	33	O	???	1	7.283	5.645	-43.891
ATOM	34	N	???	1	5.934	6.118	-42.087
ATOM	35	H	???	1	5.581	6.845	-41.443
ATOM	36	C	???	1	5.404	4.757	-41.951
ATOM	37	H	???	1	6.259	4.088	-42.154
ATOM	38	C	???	1	4.924	4.512	-40.519
ATOM	39	H	???	1	4.616	3.454	-40.442
ATOM	40	H	???	1	5.743	4.681	-39.786
ATOM	41	O	???	1	3.784	5.302	-40.155
ATOM	42	H	???	1	4.132	6.166	-39.819
ATOM	43	H	???	1	4.615	4.493	-42.669
ATOM	44	H	???	1	13.631	11.343	-31.927
ATOM	45	C	???	1	12.720	10.654	-31.972
ATOM	46	H	???	1	12.875	9.949	-31.131
ATOM	47	H	???	1	11.737	11.192	-31.789
ATOM	48	C	???	1	12.898	9.820	-33.255
ATOM	49	O	???	1	14.033	9.627	-33.695
ATOM	50	N	???	1	11.809	9.209	-33.789
ATOM	51	H	???	1	10.846	9.411	-33.486
ATOM	52	C	???	1	11.984	8.125	-34.750
ATOM	53	H	???	1	12.936	7.625	-34.527
ATOM	54	H	???	1	11.148	7.421	-34.588
ATOM	55	C	???	1	12.028	8.517	-36.240
ATOM	56	O	???	1	13.038	8.361	-36.930
ATOM	57	N	???	1	10.838	8.988	-36.730
ATOM	58	H	???	1	10.008	8.880	-36.113
ATOM	59	C	???	1	10.625	9.159	-38.153
ATOM	60	H	???	1	11.609	9.301	-38.634
ATOM	61	H	???	1	10.169	8.255	-38.597
ATOM	62	C	???	1	9.697	10.295	-38.579
ATOM	63	O	???	1	9.556	10.538	-39.784
ATOM	64	N	???	1	9.054	10.984	-37.597
ATOM	65	H	???	1	9.092	10.623	-36.633
ATOM	66	C	???	1	8.105	12.045	-37.918
ATOM	67	H	???	1	8.343	12.399	-38.931
ATOM	68	H	???	1	7.045	11.653	-37.926
ATOM	69	C	???	1	8.205	13.232	-36.945
ATOM	70	O	???	1	8.459	14.374	-37.351
ATOM	71	N	???	1	7.915	12.918	-35.659
ATOM	72	H	???	1	7.792	11.930	-35.401
ATOM	73	C	???	1	7.847	13.913	-34.580
ATOM	74	H	???	1	7.005	14.598	-34.820
ATOM	75	C	???	1	7.524	13.195	-33.264
ATOM	76	H	???	1	8.257	12.379	-33.089
ATOM	77	H	???	1	7.640	13.923	-32.437
ATOM	78	C	???	1	6.101	12.617	-33.211
ATOM	79	H	???	1	5.370	13.443	-33.333
ATOM	80	H	???	1	5.928	11.909	-34.047
ATOM	81	C	???	1	5.826	11.899	-31.890
ATOM	82	H	???	1	6.469	11.001	-31.789
ATOM	83	H	???	1	6.096	12.565	-31.045
ATOM	84	N	???	1	4.414	11.523	-31.790
ATOM	85	H	???	1	3.833	11.626	-32.634
ATOM	86	C	???	1	3.957	10.577	-30.947
ATOM	87	N	???	1	4.709	10.196	-29.906
ATOM	88	H	???	1	5.579	10.691	-29.686
ATOM	89	H	???	1	4.424	9.437	-29.279
ATOM	90	N	???	1	2.733	10.045	-31.149
ATOM	91	H	???	1	2.241	10.331	-32.006
ATOM	92	H	???	1	2.140	9.825	-30.348
ATOM	93	H	???	1	8.733	14.571	-34.486
ATOM	94	H	???	1	8.403	7.457	-28.193
ATOM	95	C	???	1	9.342	7.492	-28.768
ATOM	96	N	???	1	9.534	6.757	-29.931
ATOM	97	C	???	1	10.834	6.853	-30.222
ATOM	98	H	???	1	11.334	6.391	-31.074
ATOM	99	N	???	1	11.476	7.623	-29.308
ATOM	100	H	???	1	12.486	7.855	-29.326
ATOM	101	C	???	1	10.549	8.034	-28.372
ATOM	102	H	???	1	10.829	8.696	-27.553
ATOM	103	O	???	1	10.670	5.260	-25.626
ATOM	104	C	???	1	10.948	4.627	-26.705
ATOM	105	O	???	1	12.093	4.356	-27.146
ATOM	106	C	???	1	9.732	4.242	-27.572
ATOM	107	H	???	1	8.840	4.144	-26.927
ATOM	108	H	???	1	9.555	5.117	-28.221
ATOM	109	C	???	1	9.859	3.036	-28.505
ATOM	110	H	???	1	10.851	3.054	-28.987
ATOM	111	H	???	1	9.794	2.083	-27.943
ATOM	112	C	???	1	8.800	3.099	-29.645
ATOM	113	O	???	1	9.287	3.988	-30.638
ATOM	114	H	???	1	10.003	3.057	-31.419



ATOM	115	C	???	1	7.475	3.621	-29.071
ATOM	116	O	???	1	7.094	4.757	-29.537
ATOM	117	O	???	1	6.847	2.974	-28.201
ATOM	118	C	???	1	8.514	1.732	-30.321
ATOM	119	H	???	1	8.138	0.988	-29.599
ATOM	120	H	???	1	7.725	1.914	-31.082
ATOM	121	C	???	1	9.728	1.174	-31.047
ATOM	122	O	???	1	10.437	2.090	-31.702
ATOM	123	O	???	1	10.000	-0.026	-31.042
ATOM	124	FE	???	1	8.025	7.526	-33.252
ATOM	125	MO	???	1	8.058	5.573	-31.326
ATOM	126	FE	???	1	7.817	5.076	-33.873
ATOM	127	FE	???	1	5.866	6.152	-32.723
ATOM	128	FE	???	1	6.652	8.422	-35.229
ATOM	129	FE	???	1	5.604	7.362	-37.557
ATOM	130	FE	???	1	7.031	5.827	-36.144
ATOM	131	FE	???	1	4.863	6.655	-35.114
ATOM	132	C	???	1	6.698	6.628	-34.409
ATOM	133	S	???	1	7.801	7.684	-37.155
ATOM	134	S	???	1	9.662	5.985	-33.035
ATOM	135	S	???	1	4.992	5.296	-36.970
ATOM	136	S	???	1	8.153	3.985	-35.709
ATOM	137	S	???	1	8.572	9.407	-34.383
ATOM	138	S	???	1	6.557	4.017	-32.347
ATOM	139	S	???	1	4.528	8.681	-36.115
ATOM	140	S	???	1	6.814	7.603	-31.281
ATOM	141	S	???	1	3.678	6.301	-33.213
ATOM	142	N	???	1	5.850	9.231	-33.735
ATOM	143	H	???	1	6.561	9.684	-33.128
ATOM	144	N	???	1	4.699	9.282	-33.229
ATOM	145	H	???	1	4.039	8.783	-33.862
ATOM	146	O	???	1	4.518	5.571	-29.410
ATOM	147	H	???	1	5.459	5.257	-29.493
ATOM	148	H	???	1	4.424	6.249	-30.112
ATOM	149	O	???	1	1.099	8.363	-34.222
ATOM	150	H	???	1	1.882	7.863	-33.881
ATOM	151	H	???	1	0.602	8.665	-33.405
END							

Fe2(cis)

REMARK Energies (QM/MM, QM+ptch) = -17129.760697 -16290.131410

ATOM	1	H	???	1	3.501	2.242	-29.688
ATOM	2	C	???	1	3.910	2.100	-30.708
ATOM	3	H	???	1	5.014	2.104	-30.636
ATOM	4	H	???	1	3.588	1.123	-31.102
ATOM	5	N	???	1	3.502	3.162	-31.616
ATOM	6	H	???	1	3.992	4.063	-31.504
ATOM	7	C	???	1	2.871	2.958	-32.785
ATOM	8	N	???	1	2.007	1.916	-32.923
ATOM	9	H	???	1	1.832	1.300	-32.128
ATOM	10	H	???	1	1.806	1.537	-33.859
ATOM	11	N	???	1	3.092	3.786	-33.808
ATOM	12	H	???	1	3.648	4.656	-33.647
ATOM	13	H	???	1	2.436	3.826	-34.594
ATOM	14	H	???	1	7.281	1.556	-41.605
ATOM	15	C	???	1	7.604	2.004	-40.655
ATOM	16	N	???	1	8.573	2.988	-40.665
ATOM	17	C	???	1	8.805	3.266	-39.386
ATOM	18	H	???	1	9.506	4.003	-38.995
ATOM	19	N	???	1	8.013	2.527	-38.562
ATOM	20	H	???	1	7.928	2.719	-37.542
ATOM	21	C	???	1	7.224	1.718	-39.355
ATOM	22	H	???	1	6.488	1.035	-38.932
ATOM	23	H	???	1	2.981	9.553	-40.116
ATOM	24	C	???	1	3.112	8.696	-39.419
ATOM	25	H	???	1	2.527	7.828	-39.770
ATOM	26	H	???	1	2.768	9.012	-38.420
ATOM	27	S	???	1	4.934	8.295	-39.364
ATOM	28	H	???	1	6.632	8.637	-42.917
ATOM	29	C	???	1	7.424	7.830	-42.945
ATOM	30	H	???	1	7.989	7.993	-43.875
ATOM	31	H	???	1	8.089	7.977	-42.076
ATOM	32	C	???	1	6.823	6.410	-42.977
ATOM	33	O	???	1	7.229	5.623	-43.840
ATOM	34	N	???	1	5.925	6.104	-42.010
ATOM	35	H	???	1	5.570	6.832	-41.368
ATOM	36	C	???	1	5.374	4.747	-41.926
ATOM	37	H	???	1	6.224	4.070	-42.127
ATOM	38	C	???	1	4.836	4.442	-40.525
ATOM	39	H	???	1	4.386	3.434	-40.554
ATOM	40	H	???	1	5.667	4.379	-39.784
ATOM	41	O	???	1	3.823	5.331	-40.066
ATOM	42	H	???	1	4.239	6.174	-39.733
ATOM	43	H	???	1	4.602	4.490	-42.660
ATOM	44	H	???	1	13.632	11.343	-31.927
ATOM	45	C	???	1	12.721	10.656	-31.970
ATOM	46	H	???	1	12.875	9.951	-31.128
ATOM	47	H	???	1	11.737	11.192	-31.788
ATOM	48	C	???	1	12.898	9.819	-33.251
ATOM	49	O	???	1	14.031	9.622	-33.694
ATOM	50	N	???	1	11.802	9.215	-33.774
ATOM	51	H	???	1	10.840	9.435	-33.468
ATOM	52	C	???	1	11.955	8.132	-34.737
ATOM	53	H	???	1	12.912	7.632	-34.537
ATOM	54	H	???	1	11.125	7.426	-34.556
ATOM	55	C	???	1	11.969	8.532	-36.221
ATOM	56	O	???	1	12.979	8.418	-36.920
ATOM	57	N	???	1	10.760	8.969	-36.708
ATOM	58	H	???	1	9.923	8.806	-36.123
ATOM	59	C	???	1	10.559	9.135	-38.137
ATOM	60	H	???	1	11.554	9.236	-38.603
ATOM	61	H	???	1	10.066	8.246	-38.571
ATOM	62	C	???	1	9.678	10.299	-38.581
ATOM	63	O	???	1	9.540	10.525	-39.789
ATOM	64	N	???	1	9.068	11.028	-37.607

ATOM	65	H	???	1	9.110	10.678	-36.643
ATOM	66	C	???	1	8.103	12.071	-37.930
ATOM	67	H	???	1	8.332	12.424	-38.946
ATOM	68	H	???	1	7.045	11.662	-37.930
ATOM	69	C	???	1	8.206	13.259	-36.958
ATOM	70	O	???	1	8.476	14.399	-37.360
ATOM	71	N	???	1	7.916	12.936	-35.677
ATOM	72	H	???	1	7.735	11.951	-35.445
ATOM	73	C	???	1	7.845	13.902	-34.572
ATOM	74	H	???	1	6.992	14.582	-34.786
ATOM	75	C	???	1	7.535	13.124	-33.286
ATOM	76	H	???	1	8.317	12.356	-33.115
ATOM	77	H	???	1	7.572	13.827	-32.432
ATOM	78	C	???	1	6.158	12.433	-33.313
ATOM	79	H	???	1	5.361	13.206	-33.300
ATOM	80	H	???	1	6.024	11.847	-34.244
ATOM	81	C	???	1	5.964	11.472	-32.139
ATOM	82	H	???	1	6.648	10.606	-32.244
ATOM	83	H	???	1	6.201	11.993	-31.188
ATOM	84	N	???	1	4.569	11.022	-32.097
ATOM	85	H	???	1	3.965	11.191	-32.916
ATOM	86	C	???	1	3.997	10.360	-31.086
ATOM	87	N	???	1	4.683	10.129	-29.956
ATOM	88	H	???	1	5.629	10.505	-29.842
ATOM	89	H	???	1	4.347	9.477	-29.240
ATOM	90	N	???	1	2.718	9.933	-31.218
ATOM	91	H	???	1	2.246	10.199	-32.093
ATOM	92	H	???	1	2.113	9.912	-30.395
ATOM	93	H	???	1	8.731	14.566	-34.480
ATOM	94	H	???	1	8.407	7.458	-28.188
ATOM	95	C	???	1	9.353	7.495	-28.752
ATOM	96	N	???	1	9.565	6.746	-29.901
ATOM	97	C	???	1	10.865	6.851	-30.186
ATOM	98	H	???	1	11.371	6.387	-31.035
ATOM	99	N	???	1	11.490	7.642	-29.279
ATOM	100	H	???	1	12.496	7.886	-29.297
ATOM	101	C	???	1	10.551	8.056	-28.355
ATOM	102	H	???	1	10.816	8.736	-27.546
ATOM	103	O	???	1	10.666	5.254	-25.629
ATOM	104	C	???	1	10.946	4.621	-26.708
ATOM	105	O	???	1	12.091	4.350	-27.148
ATOM	106	C	???	1	9.729	4.236	-27.576
ATOM	107	H	???	1	8.840	4.126	-26.931
ATOM	108	H	???	1	9.546	5.117	-28.215
ATOM	109	C	???	1	9.860	3.041	-28.523
ATOM	110	H	???	1	10.853	3.066	-29.004
ATOM	111	H	???	1	9.798	2.081	-27.971
ATOM	112	C	???	1	8.800	3.108	-29.663
ATOM	113	O	???	1	9.287	3.988	-30.668
ATOM	114	H	???	1	9.991	3.077	-31.424
ATOM	115	C	???	1	7.477	3.633	-29.087
ATOM	116	O	???	1	7.093	4.764	-29.558
ATOM	117	O	???	1	6.854	2.984	-28.213
ATOM	118	C	???	1	8.510	1.739	-30.335
ATOM	119	H	???	1	8.136	0.997	-29.609
ATOM	120	H	???	1	7.718	1.915	-31.094
ATOM	121	C	???	1	9.725	1.180	-31.062
ATOM	122	O	???	1	10.430	2.094	-31.717
ATOM	123	O	???	1	9.996	-0.021	-31.051
ATOM	124	FE	???	1	5.908	6.327	-32.613
ATOM	125	MO	???	1	8.096	5.628	-31.318
ATOM	126	FE	???	1	7.771	5.250	-33.935
ATOM	127	FE	???	1	8.072	7.644	-33.074
ATOM	128	FE	???	1	4.853	7.274	-34.664
ATOM	129	FE	???	1	6.935	6.149	-36.227
ATOM	130	FE	???	1	5.313	7.985	-37.100
ATOM	131	FE	???	1	6.933	8.629	-35.128
ATOM	132	C	???	1	6.749	6.880	-34.297
ATOM	133	S	???	1	7.639	8.104	-37.173
ATOM	134	S	???	1	9.691	6.037	-33.024
ATOM	135	S	???	1	4.606	5.946	-36.456
ATOM	136	S	???	1	7.964	4.147	-35.785
ATOM	137	S	???	1	8.574	9.622	-33.989
ATOM	138	S	???	1	6.537	4.165	-32.424
ATOM	139	S	???	1	4.766	9.399	-35.349
ATOM	140	S	???	1	6.893	7.676	-31.155
ATOM	141	S	???	1	3.734	6.717	-32.813
ATOM	142	N	???	1	6.938	5.531	-38.048
ATOM	143	H	???	1	6.124	4.905	-38.241
ATOM	144	N	???	1	7.667	5.823	-39.033
ATOM	145	H	???	1	7.290	5.366	-39.894
ATOM	146	O	???	1	4.497	5.524	-29.484
ATOM	147	H	???	1	5.457	5.261	-29.533
ATOM	148	H	???	1	4.389	6.205	-30.186
ATOM	149	O	???	1	1.092	8.387	-34.237
ATOM	150	H	???	1	1.961	8.078	-33.879
ATOM	151	H	???	1	0.578	8.681	-33.428

END

Fe6-cis  
REMARK Energies (QM/MM, QM+ptch) = -17129.748904 -16290.123550

ATOM	1	H	???	1	3.503	2.240	-29.688
ATOM	2	C	???	1	3.916	2.095	-30.708
ATOM	3	H	???	1	5.020	2.099	-30.633
ATOM	4	H	???	1	3.597	1.115	-31.098
ATOM	5	N	???	1	3.511	3.150	-31.625
ATOM	6	H	???	1	4.011	4.047	-31.529
ATOM	7	C	???	1	2.870	2.937	-32.789
ATOM	8	N	???	1	2.001	1.900	-32.913
ATOM	9	H	???	1	1.833	1.286	-32.114
ATOM	10	H	???	1	1.798	1.513	-33.846
ATOM	11	N	???	1	3.085	3.757	-33.819
ATOM	12	H	???	1	3.659	4.618	-33.682
ATOM	13	H	???	1	2.437	3.782	-34.612
ATOM	14	H	???	1	7.279	1.559	-41.618

ATOM	15	C	???	1	7.594	2.018	-40.682
ATOM	16	N	???	1	8.453	3.100	-40.691
ATOM	17	C	???	1	8.573	3.456	-39.417
ATOM	18	H	???	1	9.154	4.287	-39.017
ATOM	19	N	???	1	7.838	2.650	-38.604
ATOM	20	H	???	1	7.726	2.814	-37.588
ATOM	21	C	???	1	7.187	1.731	-39.393
ATOM	22	H	???	1	6.504	0.993	-38.976
ATOM	23	H	???	1	2.977	9.557	-40.117
ATOM	24	C	???	1	3.102	8.705	-39.420
ATOM	25	H	???	1	2.513	7.838	-39.764
ATOM	26	H	???	1	2.782	9.024	-38.414
ATOM	27	S	???	1	4.917	8.308	-39.408
ATOM	28	H	???	1	6.637	8.643	-42.923
ATOM	29	C	???	1	7.435	7.841	-42.957
ATOM	30	H	???	1	8.005	8.021	-43.881
ATOM	31	H	???	1	8.092	7.980	-42.081
ATOM	32	C	???	1	6.836	6.419	-43.008
ATOM	33	O	???	1	7.260	5.639	-43.871
ATOM	34	N	???	1	5.922	6.124	-42.063
ATOM	35	H	???	1	5.592	6.845	-41.403
ATOM	36	C	???	1	5.391	4.763	-41.926
ATOM	37	H	???	1	6.247	4.094	-42.127
ATOM	38	C	???	1	4.926	4.520	-40.486
ATOM	39	H	???	1	4.593	3.469	-40.414
ATOM	40	H	???	1	5.764	4.661	-39.770
ATOM	41	O	???	1	3.814	5.337	-40.092
ATOM	42	H	???	1	4.183	6.175	-39.711
ATOM	43	H	???	1	4.607	4.494	-42.655
ATOM	44	H	???	1	13.631	11.344	-31.927
ATOM	45	C	???	1	12.720	10.656	-31.972
ATOM	46	H	???	1	12.875	9.949	-31.132
ATOM	47	H	???	1	11.737	11.192	-31.789
ATOM	48	C	???	1	12.899	9.823	-33.255
ATOM	49	O	???	1	14.036	9.628	-33.692
ATOM	50	N	???	1	11.810	9.218	-33.794
ATOM	51	H	???	1	10.844	9.421	-33.493
ATOM	52	C	???	1	11.992	8.141	-34.757
ATOM	53	H	???	1	12.962	7.666	-34.553
ATOM	54	H	???	1	11.182	7.411	-34.582
ATOM	55	C	???	1	11.999	8.531	-36.243
ATOM	56	O	???	1	13.001	8.398	-36.949
ATOM	57	N	???	1	10.793	8.975	-36.724
ATOM	58	H	???	1	9.959	8.833	-36.128
ATOM	59	C	???	1	10.592	9.154	-38.150
ATOM	60	H	???	1	11.585	9.292	-38.613
ATOM	61	H	???	1	10.138	8.254	-38.602
ATOM	62	C	???	1	9.678	10.296	-38.582
ATOM	63	O	???	1	9.535	10.524	-39.790
ATOM	64	N	???	1	9.052	11.005	-37.605
ATOM	65	H	???	1	9.110	10.670	-36.635
ATOM	66	C	???	1	8.100	12.061	-37.929
ATOM	67	H	???	1	8.333	12.410	-38.946
ATOM	68	H	???	1	7.043	11.659	-37.930
ATOM	69	C	???	1	8.208	13.251	-36.959
ATOM	70	O	???	1	8.477	14.390	-37.365
ATOM	71	N	???	1	7.919	12.931	-35.678
ATOM	72	H	???	1	7.749	11.945	-35.442
ATOM	73	C	???	1	7.845	13.898	-34.573
ATOM	74	H	???	1	6.991	14.577	-34.787
ATOM	75	C	???	1	7.534	13.113	-33.290
ATOM	76	H	???	1	8.322	12.351	-33.119
ATOM	77	H	???	1	7.563	13.814	-32.433
ATOM	78	C	???	1	6.163	12.412	-33.327
ATOM	79	H	???	1	5.360	13.180	-33.309
ATOM	80	H	???	1	6.034	11.832	-34.262
ATOM	81	C	???	1	5.972	11.443	-32.159
ATOM	82	H	???	1	6.655	10.577	-32.271
ATOM	83	H	???	1	6.212	11.957	-31.206
ATOM	84	N	???	1	4.577	10.990	-32.115
ATOM	85	H	???	1	3.967	11.173	-32.925
ATOM	86	C	???	1	3.998	10.352	-31.092
ATOM	87	N	???	1	4.681	10.132	-29.957
ATOM	88	H	???	1	5.625	10.512	-29.842
ATOM	89	H	???	1	4.338	9.494	-29.232
ATOM	90	N	???	1	2.716	9.931	-31.218
ATOM	91	H	???	1	2.245	10.189	-32.097
ATOM	92	H	???	1	2.110	9.934	-30.395
ATOM	93	H	???	1	8.732	14.564	-34.480
ATOM	94	H	???	1	8.406	7.466	-28.179
ATOM	95	C	???	1	9.355	7.516	-28.727
ATOM	96	N	???	1	9.581	6.778	-29.878
ATOM	97	C	???	1	10.887	6.887	-30.144
ATOM	98	H	???	1	11.411	6.435	-30.986
ATOM	99	N	???	1	11.496	7.673	-29.224
ATOM	100	H	???	1	12.503	7.917	-29.233
ATOM	101	C	???	1	10.545	8.079	-28.310
ATOM	102	H	???	1	10.795	8.762	-27.498
ATOM	103	O	???	1	10.682	5.267	-25.600
ATOM	104	C	???	1	10.959	4.644	-26.683
ATOM	105	O	???	1	12.100	4.376	-27.134
ATOM	106	C	???	1	9.741	4.262	-27.546
ATOM	107	H	???	1	8.845	4.175	-26.907
ATOM	108	H	???	1	9.573	5.131	-28.205
ATOM	109	C	???	1	9.877	3.046	-28.458
ATOM	110	H	???	1	10.873	3.049	-28.930
ATOM	111	H	???	1	9.804	2.099	-27.889
ATOM	112	C	???	1	8.834	3.087	-29.603
ATOM	113	O	???	1	9.345	4.009	-30.600
ATOM	114	H	???	1	10.132	3.943	-33.143
ATOM	115	C	???	1	7.507	3.639	-29.079
ATOM	116	O	???	1	7.142	4.773	-29.557
ATOM	117	O	???	1	6.866	2.996	-28.216
ATOM	118	C	???	1	8.598	1.732	-30.294
ATOM	119	H	???	1	8.177	1.002	-29.581

ATOM	120	H	???	1	7.851	1.892	-31.101
ATOM	121	C	???	1	9.860	1.158	-30.959
ATOM	122	O	???	1	10.637	2.043	-31.515
ATOM	123	O	???	1	10.013	-0.074	-30.983
ATOM	124	FE	???	1	8.002	7.718	-33.112
ATOM	125	MO	???	1	8.106	5.707	-31.307
ATOM	126	FE	???	1	7.038	8.484	-35.324
ATOM	127	FE	???	1	5.918	6.338	-32.636
ATOM	128	FE	???	1	8.043	5.115	-33.900
ATOM	129	FE	???	1	6.842	6.012	-36.058
ATOM	130	FE	???	1	5.506	7.810	-37.271
ATOM	131	FE	???	1	4.931	7.143	-34.802
ATOM	132	C	???	1	6.814	6.811	-34.303
ATOM	133	S	???	1	7.727	7.676	-37.364
ATOM	134	S	???	1	9.730	6.319	-32.955
ATOM	135	S	???	1	4.729	5.731	-36.605
ATOM	136	S	???	1	7.970	4.203	-35.955
ATOM	137	S	???	1	8.551	9.629	-34.175
ATOM	138	S	???	1	6.589	4.211	-32.397
ATOM	139	S	???	1	4.952	9.291	-35.569
ATOM	140	S	???	1	6.856	7.715	-31.164
ATOM	141	S	???	1	3.764	6.713	-32.919
ATOM	142	N	???	1	9.209	3.656	-33.551
ATOM	143	H	???	1	9.852	1.927	-33.307
ATOM	144	N	???	1	9.022	2.424	-33.691
ATOM	145	H	???	1	9.992	3.379	-31.137
ATOM	146	O	???	1	4.526	5.525	-29.486
ATOM	147	H	???	1	5.483	5.254	-29.540
ATOM	148	H	???	1	4.426	6.208	-30.188
ATOM	149	O	???	1	1.092	8.389	-34.233
ATOM	150	H	???	1	1.947	8.051	-33.868
ATOM	151	H	???	1	0.573	8.683	-33.426
END							