Supporting Information

Protonation and reduction of the FeMo cluster in nitrogenase studied by QM/MM calculations

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2018-10-15

Figure S1. BS state ordering of the quintet E_1 state protonated on S2B(3), obtained from single-point TPSS-D3 or B3LYP-D3 calculations with the def2-SV(P) basis set.

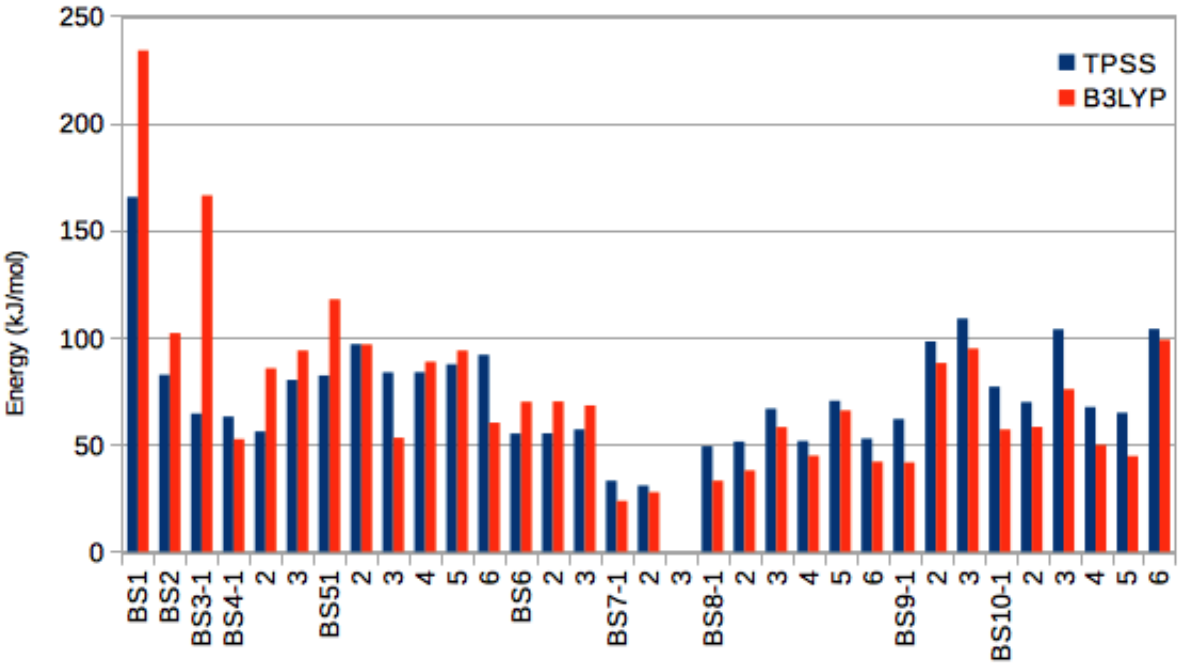

Table S1. Definition of the 35 BS states, indicated by which three Fe ions (numbering shown in Figure 1) have a negative net spin. The states are the same as in our previous study.[37]

BS1	(5,6,7)	BS5-1	(2,5,6)	BS7-1	(2,3,5)	BS9-1	(1,2,6)
BS2	(2,3,4)	BS5-2	(2,6,7)	BS7-2	(2,4,7)	BS9-2	(1,3,7)
BS3-1	(1,2,3)	BS5-3	(3,5,7)	BS7-3	(3,4,6)	BS9-3	(1,4,5)
BS3-2	(1,2,4)	BS5-4	(3,6,7)	BS8-1	(2,3,6)	BS10-1	(1,2,5)
BS3-3	(1,3,4)	BS5-5	(4,5,6)	BS8-2	(2,4,6)	BS10-2	(1,2,7)
BS4-1	(2,5,7)	BS5-6	(4,5,7)	BS8-3	(2,3,7)	BS10-3	(1,3,5)
BS4-2	(3,5,6)	BS6-1	(1,5,6)	BS8-4	(3,4,7)	BS10-4	(1,3,6)
BS4-3	(4,6,7)	BS6-2	(1,5,7)	BS8-5	(2,4,5)	BS10-5	(1,4,6)
		BS6-3	(1,6,7)	BS8-6	(3,4,5)	BS10-6	(1,4,7)

Table S2. Relative energy of the various BS states for the best E_2 states protonated on S2B(3) + Fe2/6(5), C(2367) + C(3457), S2B(3) + C(3457) or S2B(3) + S2A(Fe1), obtained from single-point TPSS-D3 or B3LYP-D3 calculations (Fe2/6(5)) or from B3LYP-D3/def2-SV(P) geometry optimisations (the other three), all with the def2-SV(P) basis set.

BS state	Fe2/6(5)		C(2367)+C(3457)	C(3457)	S2A(Fe1)
	TPSS	B3LYP	B3LYP	B3LYP	B3LYP
BS1	118		188	93	133
BS2	30	53	72	73	
BS3-1			73	68	42
BS3-2	73	63	91	39	87
BS3-3			68	42	80
BS4-1	73	116	90	79	67
BS4-2	32	38	118	36	60
BS4-3	48	60	119	83	43
BS5-1	79	144	103	62	31
BS5-2	98	115	53	48	56
BS5-3	51	34		69	48
BS5-4	66	55	83	88	62
BS5-5	75	78	88	87	23
BS5-6	69	53	55	54	39
BS6-1	56	55	46	68	34
BS6-2	61	57	100	48	43
BS6-3	59	72	63	78	39
BS7-1	41	23	68	47	13
BS7-2	34	27	50	50	
BS7-3	**0**	**0**	58	43	**0**
BS8-1	59	50	2	31	25
BS8-2	48	43	51	49	20
BS8-3	69	53	42	51	24
BS8-4	29	28	24	27	28
BS8-5	80	51	75	46	15
BS8-6	34	32	**0**	32	30
BS9-1	40	62	9	3	25
BS9-2	86	74	42	**0**	18
BS9-3	97	87	48	14	78
BS10-1	41	53	47	32	25
BS10-2	43	51	36	36	29
BS10-3	83	91	95	37	31
BS10-4	87	47	16	45	34
BS10-5	84	53	18	50	47
BS10-6	70	102	37	36	56

Table S3. Relative energies (kJ/mol) for the doublet, quartet and sextet spin states for the six best protonation states of the E_2 state, calculated either with TPSS geometry optimisations or B3LYP single-point (B3LYP) or geometry optimisations (B3Opt), all with the def2-SV(P) basis set. The calculations were performed with the BS7-3 state, except for the C(2367) + C(3457) and S2B(3) + C(3457) states, for which BS8-6 or BS9-2 was used, respectively.

	Fe2/6(5)			Fe2/6(3)	Fe5	C(2367)+C(3457)	C(3457)	S2A(Fe1)
S	TPSS	B3LYP	B3Opt	TPSS	TPSS	B3Opt	B3Opt	B3Opt
2	10	4	19	11	19	7	-3	-6
4	0	0	0	0	0	0	0	0
6	-5	-9	-2	5	19	42	25	66

Table S4. Relative energy of the various BS states for the best E_3 states, obtained from single-point TPSS or B3LYP calculations or from B3LYP-D3/def2-SV(P) geometry optimisations (B3Opt).

1st	S2B(3)	S2B(3)		C(2367)	S2B(3)	S2B(3)	S2B(3)		S2B(3)	
2nd	Fe2/6(5)	Fe2/6(3)		C(3457)	C(2367)	S2A(Fe1)	S2A(Mo)		S2A(Mo)	
3rd	Fe5	Fe5		C(2456)	C(3457)	C(3457)	C(3457)		Fe2/6(5)	
Method	TPSS	TPSS	B3LYP	B3Opt	B3Opt	B3Opt	TPSS	B3LYP	TPSS	B3LYP
BS1		76			148	88		169	78	131
BS2	36	24	38	88	47	55	**0**	**0**	22	
BS3-1		32	24	76		36	42	17		
BS3-2	50	50	62	76			62	60	80	96
BS3-3		96	135		47	40	66	124		
BS4-1	87	88	194	77	38		54	98	79	142
BS4-2	32	31	73	71	83	35	51	35	51	69
BS4-3	62	42	23		66	30	26	54	38	40
BS5-1				94		28	113	111	94	148
BS5-2	93	91	142	87			69	134		
BS5-3	45	46		106	43	56	63	123	64	61
BS5-4	64	59	73	71		67	93	126	89	93
BS5-5	61	44	76		85	69	81	64	69	102
BS5-6	30	23	50	83	48	41	27	83	42	31
BS6-1	47	55	81	71	86	33	26	65	32	49
BS6-2		28	59				26	76	37	50
BS6-3	55	39	44	60	91	25	13	35	42	63
BS7-1		71	108	22	20	**0**	28	13	64	47
BS7-2	37	40	40			66	34	35	41	43
BS7-3	**0**	**0**	**0**	44	36	21	5	35	**0**	**0**
BS8-1	66	63	63	31		12	58	51	68	130
BS8-2	82	66	67	54		19	76	35	59	76
BS8-3	61	45	48	32		29	70	53	93	83
BS8-4	34	28	44	57	37	25	32	24	36	26
BS8-5	69	69	114	38	27		73	65	71	72
BS8-6	22	11	18	57	**0**	11	27	60	38	29
BS9-1	24	18	49	28	35	24	52	59	95	134
BS9-2	57	58	64	17	34	23	57	73	58	48
BS9-3	53	40	56	14	30	38	59	105	79	79
BS10-1	52	25	78	3	13		35	36	38	72
BS10-2	18	11	25	19		24	40	65	38	67
BS10-3	42	40	44			22	25	34	43	31
BS10-4		54	39	**0**	14	33	55	70	50	134
BS10-5	70	57	53	18	34	54	51	75	74	88
BS10-6	76	65	58	24	25	45	45	35	55	42

Table S5. Relative energies (kJ/mol) for the open-shell singlet, triplet and quintet spin states for six low-energy protonation states of the E_3 state, calculated either with TPSS or B3LYP geometry optimisations, all with the def2-SV(P) basis set. The calculations were performed with the BS7-3 state, except for the C(2367) + C(3457) + C(2456) state which was studied in the BS9-1 state.

1st	S2B	S2B	S2B	S2B	S2B	C(2367)
2nd	Fe2/6(5)	Fe2/6(3)	Fe4	Fe2/6(5)	S2A(Mo)	C(3457)
3rd	Fe5(Mo)	Fe5	Fe5	Fe5	S4A(Fe1)	C(2456)
Method	TPSS	TPSS	TPSS	TPSS	TPSS	B3LYP
S=1	-5	21	-15	20	12	-11
S=3	0	0	0	0	0	0
S=5	22	31	-9	20	45	29

Table S6. Relative energy of the various BS states for the best E_4 states, obtained from TPSS or B3LYP geometry optimisations with the def2-SV(P) basis set.

1st	S2B(3)	S2B(3)	S2B(3)	S2B(5)	S2B(3)	S2B(3)	S2B(3)	S2B(3)
2nd	Fe2/6(3)	Fe2/6(3)	Fe2/6(3)	S5A(2)	C(2367)	S2A(Fe1)	S2A(Mo)	S2A(Mo)
3rd	Fe5	Fe4	Fe4	Fe2/6(5)	C(3457)	C(2367)	C(2367)	C(3457)
4th	Fe6	Fe5	Fe6	Fe3/7(2)	C(2456)	C(3457)	C(3457)	Fe2/6(5)
Method	TPSS	TPSS	TPSS	TPSS	B3LYP	B3LYP	B3LYP	B3LYP
BS1					128	106	188	
BS2	**0**	31	4	28	**0**	1	5	9
BS3-1	23	13	45		13	1	137	20
BS3-2	50	55	45	29	7	10	36	193
BS3-3	45	49		34		1	29	14
BS4-1	68	41	43		41	47	52	
BS4-2	11	46		25	80	62	154	251
BS4-3					80	21	130	82
BS5-1				29	107		186	
BS5-2	60	58			99	35	185	180
BS5-3	50	43	59		97	54	82	80
BS5-4		57			85	60	169	98
BS5-5				43	80	53	143	92
BS5-6	19		50	37	52	27	34	96
BS6-1	41	38	36	18	75	63	153	83
BS6-2	8	**0**	**0**	4		31	19	49
BS6-3	24	18	27	63	74	31	144	95
BS7-1	12		25	19	60	22	133	37
BS7-2	26	19	19		4	11	136	137
BS7-3		11	4	11	18	6	157	65
BS8-1			4		39	7	143	137
BS8-2	47	44	4	19	66	17	146	177
BS8-3	25		34		63	16	136	47
BS8-4	23	29	38	12	41	15	22	36
BS8-5	28	22	29	28	91	27	16	
BS8-6	19	13	8	31	43	6	13	33
BS9-1	24	9	47	8	20	48	25	133
BS9-2	20	19	19	**0**	39		**0**	75
BS9-3	16	22	27	26	17	28	55	52
BS10-1	22	34	42	14	36		30	**0**
BS10-2	34	13	15	11	36	29	22	79
BS10-3	7	15			28	8	30	42
BS10-4	15	35		41	11	25	90	71
BS10-5		44	51		39	**0**	187	125
BS10-6	42	28	24		16	11	38	69

Table S7. Relative energies (kJ/mol) for the doublet and quartet spin states for three low-energy protonation states of the E_4 state, calculated either with TPSS or B3LYP geometry optimisations, all with the def2-SV(P) basis set. All structures have the first proton on S2B(3).

2^{nd}	Fe2/6(3)	Fe2/6(3)	C(2367)
3^{rd}	Fe4	Fe5	C(3457)
4^{th}	Fe5	Fe6	C(2456)
Method	TPSS	TPSS	B3LYP
BS state	BS6-2	BS6-2/9-1	BS2
$S = 2$	0	0	0
$S = 4$	14	-3	65

Table S8. Relative energies (ΔE in kJ/mol) and bond lengths between the added H atoms and other atoms (Å) for the best E_n states optimised with either the def2-SV(P) or def2-SVP basis sets (called A and B in the table, respectively). Some structures were optimised with TPSS, others with B3LYP, as indicated. C1=C(2367), C2=C(3457), C3=C(2456).

State		DFT	basis	ΔE	S2B	S2A	C1	C2	C3	Fe2	Fe6	Fe4	Fe5	Fe6
E_1			A		1.37									
			B		1.37									
E_2	C1 C2	B3LYP	A	0			1.13	1.15						
			B	0			1.13	1.15						
	S2B S2A		A	53	1.36	1.37								
			B	46	1.36	1.36								
	S2B Fe2/6(3)	TPSS	A	0	1.37					1.53	2.28			
			B	0	1.36					1.52	2.30			
	S2B Fe2/6(5)		A	-2	1.38					1.57	2.01			
			B	-3	1.37					1.56	1.99			
	S2B Fe5		A	1	1.37								1.54	
			B	2	1.37								1.53	
E_3	C1 C2 C3	B3LYP	A	0			1.11	1.14	1.10					
			B	0			1.10	1.14	1.10					
	S2B Fe2/6 Fe5	TPSS	A	0	1.38					1.55	2.13		1.54	
			B	0	1.37					1.54	2.14		1.52	
	S2B Fe4 Fe5		A	5	1.38							1.55	1.56	
			B	7	1.37							1.54	1.55	
E_4	S2B C1 C2 C3	B3LYP	A	0	1.36		1.10	1.10	1.10					
			B	0	1.35		1.09	1.10	1.10					
	S2B S2A C1 C2		A	38	1.36	1.36	1.11	1.11						
			B	37	1.35	1.36	1.11	1.11						
	S2B Fe2/6 Fe5 Fe6	TPSS	A	0	1.37					1.70	1.65		1.51	1.52
			B	0	1.36					1.70	1.63		1.50	1.51
	S2B Fe2/6 Fe4 Fe5		A	-2	1.37					1.70	1.65	1.55	1.55	
			B	-2	1.36					1.70	1.63	1.53	1.53	

Table S9. Relative energies (ΔE in kJ/mol) and bond lengths between the added H atoms and other atoms (Å) for the best E_n states optimised with either system 2 fixed or optimised for each state by MM (called fix and free in the table, respectively). Some structures were optimised with TPSS, others with B3LYP, as indicated. C1=C(2367), C2=C(3457), C3=C(2456).

State		DFT	Opt	ΔE	S2B	S2A	C1	C2	C3	Fe2	Fe6	Fe4	Fe5	Fe6
E_1			fix		1.37									
			free		1.37									
E_2	C1 C2	B3LYP	fix	0			1.13	1.15						
			free	0			1.13	1.15						
	S2B S2A		fix	53	1.36	1.37								
			free	56	1.36	1.37								
	S2B Fe2/6(3)	TPSS	fix	0	1.37					1.53	2.28			
			free	0	1.37					1.52	2.27			
	S2B Fe2/6(5)		fix	-2	1.38					1.57	2.01			
			free	-15	1.37					1.57	2.03			
	S2B Fe5		fix	1	1.37								1.54	
			free	-9	1.37								1.54	
E_3	C1 C2 C3	B3LYP	fix	0			1.11	1.14	1.10					
			free	0			1.11	1.14	1.10					
	S2B C1 C2		fix	30	1.36		1.12	1.12						
			free	25	1.36		1.12	1.12						
	S2B Fe2/6 Fe5	TPSS	fix	0	1.38					1.55	2.13		1.54	
			free	0	1.37					1.55	2.20		1.53	
	S2B Fe4 Fe5		fix	5	1.38							1.55	1.56	
			free	-6	1.37							1.57	1.55	
E_4	S2B C1 C2 C3	B3LYP	fix	0	1.36		1.10	1.10	1.10					
			free	0	1.36		1.10	1.10	1.10					
	S2B S2A C1 C2		fix	38	1.36	1.36	1.11	1.11						
			free	44	1.36	1.37	1.11	1.11						
	S2B Fe2/6 Fe5 Fe6	TPSS	fix	0	1.37					1.91	1.56		1.51	1.52
			free	0	1.37					1.84	1.56		1.52	1.52
	S2B Fe2/6 Fe4 Fe5		fix	-2	1.37					1.70	1.65	1.55	1.55	
			free	-2	1.37					1.70	1.63	1.57	1.54	

Table S10. Coordinates of the best structures of each E_n state in PDB format.

Resting E_0 state optimised with the TPSS fucntional.

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REMARK Energies (QM/MM, QM+ptch) = -16163.019178 -15323.450724
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E0/Tpss
ATOM      1  H   ???     1       3.503   2.240 -29.686
ATOM      2  C   ???     1       3.916   2.092 -30.704
ATOM      3  H   ???     1       5.020   2.132 -30.633
ATOM      4  H   ???     1       3.623   1.099 -31.081
ATOM      5  N   ???     1       3.485   3.122 -31.637
ATOM      6  H   ???     1       4.007   4.012 -31.602
ATOM      7  C   ???     1       2.826   2.872 -32.782
ATOM      8  N   ???     1       1.959   1.827 -32.864
ATOM      9  H   ???     1       1.813   1.228 -32.049
ATOM     10  H   ???     1       1.754   1.419 -33.787
ATOM     11  N   ???     1       3.025   3.660 -33.838
ATOM     12  H   ???     1       3.573   4.545 -33.717
ATOM     13  H   ???     1       2.363   3.660 -34.619
ATOM     14  H   ???     1       7.271   1.572 -41.612
ATOM     15  C   ???     1       7.566   2.059 -40.675
ATOM     16  N   ???     1       8.383   3.175 -40.723
ATOM     17  C   ???     1       8.463   3.603 -39.467
ATOM     18  H   ???     1       9.004   4.477 -39.104
ATOM     19  N   ???     1       7.734   2.821 -38.627
ATOM     20  H   ???     1       7.634   3.011 -37.608
ATOM     21  C   ???     1       7.141   1.829 -39.377
ATOM     22  H   ???     1       6.492   1.076 -38.929
ATOM     23  H   ???     1       2.973   9.552 -40.109
ATOM     24  C   ???     1       3.081   8.696 -39.401
ATOM     25  H   ???     1       2.357   7.910 -39.680
ATOM     26  H   ???     1       2.852   9.065 -38.386
ATOM     27  S   ???     1       4.826   8.062 -39.472
ATOM     28  H   ???     1      13.631  11.344 -31.928
ATOM     29  C   ???     1      12.717  10.655 -31.974
ATOM     30  H   ???     1      12.873   9.949 -31.134
ATOM     31  H   ???     1      11.736  11.192 -31.789
ATOM     32  C   ???     1      12.890   9.819 -33.263
ATOM     33  O   ???     1      14.028   9.612 -33.687
ATOM     34  N   ???     1      11.791   9.235 -33.800
ATOM     35  H   ???     1      10.832   9.464 -33.496
ATOM     36  C   ???     1      11.928   8.138 -34.758
ATOM     37  H   ???     1      12.856   7.598 -34.521
ATOM     38  H   ???     1      11.062   7.475 -34.592
ATOM     39  C   ???     1      12.007   8.521 -36.253
ATOM     40  O   ???     1      13.056   8.366 -36.891
ATOM     41  N   ???     1      10.841   8.980 -36.776
ATOM     42  H   ???     1      10.005   8.919 -36.180
ATOM     43  C   ???     1      10.639   9.222 -38.212
ATOM     44  H   ???     1      11.639   9.370 -38.656
ATOM     45  H   ???     1      10.197   8.313 -38.665
ATOM     46  H   ???     1       9.970  10.066 -38.478
ATOM     47  H   ???     1       6.094  12.252 -32.940
ATOM     48  C   ???     1       5.946  11.599 -32.054
ATOM     49  H   ???     1       6.678  10.768 -32.122
ATOM     50  H   ???     1       6.136  12.196 -31.139
ATOM     51  N   ???     1       4.571  11.109 -32.064
ATOM     52  H   ???     1       3.975  11.247 -32.892
ATOM     53  C   ???     1       4.025  10.369 -31.084
ATOM     54  N   ???     1       4.710  10.131 -29.957
ATOM     55  H   ???     1       5.653  10.512 -29.833
ATOM     56  H   ???     1       4.398   9.437 -29.269
ATOM     57  N   ???     1       2.776   9.892 -31.253
ATOM     58  H   ???     1       2.284  10.154 -32.118
ATOM     59  H   ???     1       2.188   9.704 -30.441
ATOM     60  H   ???     1       8.407   7.461 -28.183
ATOM     61  C   ???     1       9.355   7.502 -28.739
ATOM     62  N   ???     1       9.569   6.749 -29.884
ATOM     63  C   ???     1      10.870   6.851 -30.165
ATOM     64  H   ???     1      11.382   6.382 -31.008
ATOM     65  N   ???     1      11.493   7.644 -29.259
ATOM     66  H   ???     1      12.500   7.886 -29.277
ATOM     67  C   ???     1      10.553   8.063 -28.339
ATOM     68  H   ???     1      10.817   8.744 -27.530
ATOM     69  O   ???     1      10.674   5.261 -25.618
ATOM     70  C   ???     1      10.954   4.623 -26.695
ATOM     71  O   ???     1      12.099   4.355 -27.136
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ATOM     72  C   ???     1       9.738   4.229 -27.556
ATOM     73  H   ???     1       8.848   4.129 -26.909
ATOM     74  H   ???     1       9.554   5.103 -28.206
ATOM     75  C   ???     1       9.866   3.023 -28.487
ATOM     76  H   ???     1      10.857   3.042 -28.971
ATOM     77  H   ???     1       9.804   2.070 -27.924
ATOM     78  C   ???     1       8.807   3.090 -29.626
ATOM     79  O   ???     1       9.298   3.982 -30.615
ATOM     80  H   ???     1      10.002   3.062 -31.400
ATOM     81  C   ???     1       7.483   3.613 -29.049
ATOM     82  O   ???     1       7.113   4.758 -29.494
ATOM     83  O   ???     1       6.844   2.957 -28.193
ATOM     84  C   ???     1       8.516   1.727 -30.309
ATOM     85  H   ???     1       8.141   0.979 -29.591
ATOM     86  H   ???     1       7.724   1.915 -31.066
ATOM     87  C   ???     1       9.727   1.173 -31.044
ATOM     88  O   ???     1      10.434   2.091 -31.696
ATOM     89  O   ???     1       9.998  -0.028 -31.045
ATOM     90 FE   ???     1       7.017   8.344 -35.388
ATOM     91 MO   ???     1       8.091   5.602 -31.267
ATOM     92 FE   ???     1       5.376   7.555 -37.297
ATOM     93 FE   ???     1       5.922   6.235 -32.603
ATOM     94 FE   ???     1       6.868   5.860 -36.054
ATOM     95 FE   ???     1       8.043   7.614 -33.134
ATOM     96 FE   ???     1       7.827   5.142 -33.816
ATOM     97 FE   ???     1       4.890   6.995 -34.816
ATOM     98  C   ???     1       6.758   6.712 -34.307
ATOM     99  S   ???     1       7.688   7.421 -37.401
ATOM    100  S   ???     1       9.689   6.038 -32.973
ATOM    101  S   ???     1       4.686   5.531 -36.570
ATOM    102  S   ???     1       8.033   4.031 -35.678
ATOM    103  S   ???     1       8.469   9.568 -34.158
ATOM    104  S   ???     1       6.564   4.071 -32.298
ATOM    105  S   ???     1       4.821   9.080 -35.628
ATOM    106  S   ???     1       6.873   7.660 -31.182
ATOM    107  S   ???     1       3.748   6.577 -32.921
ATOM    108  O   ???     1       4.511   5.539 -29.468
ATOM    109  H   ???     1       5.461   5.247 -29.519
ATOM    110  H   ???     1       4.394   6.128 -30.249
ATOM    111  O   ???     1       1.102   8.384 -34.233
ATOM    112  H   ???     1       1.955   8.023 -33.885
ATOM    113  H   ???     1       0.588   8.665 -33.420
END
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Resting E_0 state optimised with the B3LYP fucntional.

```
REMARK Energies (QM/MM, QM+ptch) = -16159.5100271987 15227.5880376700
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E0/B3lyp/SVP
ATOM      1  H   ???     1       3.502   2.238 -29.684
ATOM      2  C   ???     1       3.914   2.088 -30.696
ATOM      3  H   ???     1       5.012   2.146 -30.617
ATOM      4  H   ???     1       3.649   1.083 -31.050
ATOM      5  N   ???     1       3.468   3.087 -31.645
ATOM      6  H   ???     1       3.969   3.980 -31.628
ATOM      7  C   ???     1       2.800   2.813 -32.772
ATOM      8  N   ???     1       1.965   1.753 -32.835
ATOM      9  H   ???     1       1.823   1.167 -32.019
ATOM     10  H   ???     1       1.734   1.356 -33.749
ATOM     11  N   ???     1       2.968   3.589 -33.833
ATOM     12  H   ???     1       3.468   4.492 -33.715
ATOM     13  H   ???     1       2.319   3.545 -34.615
ATOM     14  H   ???     1       7.270   1.571 -41.615
ATOM     15  C   ???     1       7.564   2.054 -40.683
ATOM     16  N   ???     1       8.371   3.171 -40.715
ATOM     17  C   ???     1       8.449   3.585 -39.461
ATOM     18  H   ???     1       8.986   4.454 -39.086
ATOM     19  N   ???     1       7.730   2.788 -38.635
ATOM     20  H   ???     1       7.645   2.956 -37.619
ATOM     21  C   ???     1       7.147   1.806 -39.392
ATOM     22  H   ???     1       6.505   1.044 -38.959
ATOM     23  H   ???     1       2.975   9.556 -40.123
ATOM     24  C   ???     1       3.095   8.700 -39.438
ATOM     25  H   ???     1       2.364   7.922 -39.696
ATOM     26  H   ???     1       2.912   9.053 -38.414
ATOM     27  S   ???     1       4.839   8.097 -39.634
ATOM     28  H   ???     1      13.630  11.345 -31.930
ATOM     29  C   ???     1      12.721  10.661 -31.981
ATOM     30  H   ???     1      12.876   9.956 -31.147
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ATOM     31  H   ???     1      11.739  11.193 -31.792
ATOM     32  C   ???     1      12.900   9.824 -33.264
ATOM     33  O   ???     1      14.033   9.621 -33.681
ATOM     34  N   ???     1      11.809   9.246 -33.805
ATOM     35  H   ???     1      10.859   9.491 -33.516
ATOM     36  C   ???     1      11.940   8.157 -34.763
ATOM     37  H   ???     1      12.852   7.599 -34.529
ATOM     38  H   ???     1      11.072   7.501 -34.615
ATOM     39  C   ???     1      12.029   8.534 -36.254
ATOM     40  O   ???     1      13.072   8.358 -36.880
ATOM     41  N   ???     1      10.882   9.010 -36.783
ATOM     42  H   ???     1      10.054   8.974 -36.190
ATOM     43  C   ???     1      10.677   9.251 -38.213
ATOM     44  H   ???     1      11.662   9.430 -38.667
ATOM     45  H   ???     1      10.264   8.341 -38.677
ATOM     46  H   ???     1       9.988  10.078 -38.477
ATOM     47  H   ???     1       6.091  12.253 -32.940
ATOM     48  C   ???     1       5.937  11.607 -32.055
ATOM     49  H   ???     1       6.691  10.802 -32.106
ATOM     50  H   ???     1       6.105  12.213 -31.148
ATOM     51  N   ???     1       4.583  11.083 -32.087
ATOM     52  H   ???     1       3.991  11.223 -32.910
ATOM     53  C   ???     1       4.038  10.344 -31.114
ATOM     54  N   ???     1       4.721  10.104 -29.993
ATOM     55  H   ???     1       5.659  10.477 -29.871
ATOM     56  H   ???     1       4.396   9.442 -29.289
ATOM     57  N   ???     1       2.796   9.876 -31.284
ATOM     58  H   ???     1       2.301  10.132 -32.141
ATOM     59  H   ???     1       2.235   9.586 -30.493
ATOM     60  H   ???     1       8.413   7.466 -28.169
ATOM     61  C   ???     1       9.372   7.516 -28.697
ATOM     62  N   ???     1       9.635   6.742 -29.809
ATOM     63  C   ???     1      10.934   6.870 -30.063
ATOM     64  H   ???     1      11.478   6.397 -30.878
ATOM     65  N   ???     1      11.510   7.700 -29.169
ATOM     66  H   ???     1      12.509   7.952 -29.176
ATOM     67  C   ???     1      10.541   8.117 -28.285
ATOM     68  H   ???     1      10.763   8.823 -27.490
ATOM     69  O   ???     1      10.686   5.263 -25.603
ATOM     70  C   ???     1      10.959   4.623 -26.668
ATOM     71  O   ???     1      12.093   4.366 -27.122
ATOM     72  C   ???     1       9.746   4.212 -27.508
ATOM     73  H   ???     1       8.863   4.129 -26.861
ATOM     74  H   ???     1       9.564   5.073 -28.161
ATOM     75  C   ???     1       9.871   2.997 -28.415
ATOM     76  H   ???     1      10.859   3.008 -28.890
ATOM     77  H   ???     1       9.813   2.056 -27.842
ATOM     78  C   ???     1       8.829   3.053 -29.562
ATOM     79  O   ???     1       9.325   3.942 -30.531
ATOM     80  H   ???     1      10.046   2.998 -31.357
ATOM     81  C   ???     1       7.500   3.584 -29.004
ATOM     82  O   ???     1       7.171   4.738 -29.426
ATOM     83  O   ???     1       6.835   2.928 -28.183
ATOM     84  C   ???     1       8.558   1.687 -30.229
ATOM     85  H   ???     1       8.224   0.932 -29.508
ATOM     86  H   ???     1       7.748   1.840 -30.965
ATOM     87  C   ???     1       9.746   1.149 -30.999
ATOM     88  O   ???     1      10.443   2.064 -31.649
ATOM     89  O   ???     1      10.004  -0.044 -31.034
ATOM     90 FE   ???     1       7.058   8.412 -35.435
ATOM     91 MO   ???     1       8.179   5.566 -31.176
ATOM     92 FE   ???     1       5.405   7.638 -37.475
ATOM     93 FE   ???     1       5.919   6.168 -32.587
ATOM     94 FE   ???     1       6.927   5.761 -36.112
ATOM     95 FE   ???     1       8.137   7.651 -33.129
ATOM     96 FE   ???     1       7.906   5.024 -33.825
ATOM     97 FE   ???     1       4.817   6.959 -34.831
ATOM     98  C   ???     1       6.823   6.704 -34.326
ATOM     99  S   ???     1       7.771   7.451 -37.436
ATOM    100  S   ???     1       9.773   5.975 -32.876
ATOM    101  S   ???     1       4.715   5.542 -36.739
ATOM    102  S   ???     1       8.156   3.921 -35.731
ATOM    103  S   ???     1       8.506   9.659 -34.160
ATOM    104  S   ???     1       6.655   3.996 -32.188
ATOM    105  S   ???     1       4.831   9.114 -35.682
ATOM    106  S   ???     1       6.929   7.598 -31.127
ATOM    107  S   ???     1       3.691   6.492 -32.877
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ATOM    108  O   ???     1       4.534   5.527 -29.424
ATOM    109  H   ???     1       5.471   5.251 -29.496
ATOM    110  H   ???     1       4.378   6.104 -30.188
ATOM    111  O   ???     1       1.120   8.397 -34.218
ATOM    112  H   ???     1       1.942   8.015 -33.855
ATOM    113  H   ???     1       0.595   8.661 -33.423
END
```

Best E_1 structure optimised with the TPSS functional. The proton is on the S2B atom.

```
REMARK Energies (QM/MM, QM+ptch) = -16163.590296 -15324.025207
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E1
ATOM      1  H   ???     1       3.503   2.240 -29.686
ATOM      2  C   ???     1       3.915   2.093 -30.704
ATOM      3  H   ???     1       5.019   2.108 -30.632
ATOM      4  H   ???     1       3.602   1.110 -31.092
ATOM      5  N   ???     1       3.501   3.144 -31.623
ATOM      6  H   ???     1       4.013   4.037 -31.548
ATOM      7  C   ???     1       2.856   2.922 -32.781
ATOM      8  N   ???     1       1.985   1.882 -32.893
ATOM      9  H   ???     1       1.829   1.268 -32.091
ATOM     10  H   ???     1       1.783   1.490 -33.824
ATOM     11  N   ???     1       3.070   3.733 -33.817
ATOM     12  H   ???     1       3.627   4.609 -33.674
ATOM     13  H   ???     1       2.420   3.754 -34.608
ATOM     14  H   ???     1       7.272   1.572 -41.612
ATOM     15  C   ???     1       7.566   2.057 -40.674
ATOM     16  N   ???     1       8.361   3.188 -40.721
ATOM     17  C   ???     1       8.440   3.613 -39.465
ATOM     18  H   ???     1       8.958   4.503 -39.108
ATOM     19  N   ???     1       7.732   2.810 -38.624
ATOM     20  H   ???     1       7.636   2.978 -37.603
ATOM     21  C   ???     1       7.156   1.810 -39.376
ATOM     22  H   ???     1       6.525   1.042 -38.929
ATOM     23  H   ???     1       2.972   9.554 -40.117
ATOM     24  C   ???     1       3.080   8.695 -39.421
ATOM     25  H   ???     1       2.344   7.918 -39.689
ATOM     26  H   ???     1       2.891   9.055 -38.395
ATOM     27  S   ???     1       4.813   8.037 -39.563
ATOM     28  H   ???     1      13.631  11.343 -31.928
ATOM     29  C   ???     1      12.717  10.654 -31.974
ATOM     30  H   ???     1      12.873   9.948 -31.133
ATOM     31  H   ???     1      11.736  11.192 -31.789
ATOM     32  C   ???     1      12.887   9.818 -33.262
ATOM     33  O   ???     1      14.025   9.617 -33.693
ATOM     34  N   ???     1      11.790   9.229 -33.795
ATOM     35  H   ???     1      10.829   9.443 -33.484
ATOM     36  C   ???     1      11.933   8.135 -34.755
ATOM     37  H   ???     1      12.861   7.595 -34.519
ATOM     38  H   ???     1      11.067   7.471 -34.589
ATOM     39  C   ???     1      12.014   8.519 -36.249
ATOM     40  O   ???     1      13.060   8.351 -36.891
ATOM     41  N   ???     1      10.853   8.991 -36.772
ATOM     42  H   ???     1      10.015   8.935 -36.177
ATOM     43  C   ???     1      10.653   9.232 -38.209
ATOM     44  H   ???     1      11.652   9.388 -38.651
ATOM     45  H   ???     1      10.221   8.318 -38.665
ATOM     46  H   ???     1       9.976  10.071 -38.476
ATOM     47  H   ???     1       6.094  12.252 -32.940
ATOM     48  C   ???     1       5.944  11.599 -32.052
ATOM     49  H   ???     1       6.676  10.768 -32.121
ATOM     50  H   ???     1       6.132  12.195 -31.137
ATOM     51  N   ???     1       4.568  11.109 -32.065
ATOM     52  H   ???     1       3.972  11.253 -32.892
ATOM     53  C   ???     1       4.018  10.370 -31.087
ATOM     54  N   ???     1       4.705  10.123 -29.962
ATOM     55  H   ???     1       5.662  10.470 -29.856
ATOM     56  H   ???     1       4.392   9.425 -29.278
ATOM     57  N   ???     1       2.764   9.909 -31.253
ATOM     58  H   ???     1       2.269  10.180 -32.114
ATOM     59  H   ???     1       2.181   9.699 -30.443
ATOM     60  H   ???     1       8.409   7.460 -28.182
ATOM     61  C   ???     1       9.360   7.498 -28.737
ATOM     62  N   ???     1       9.578   6.745 -29.881
ATOM     63  C   ???     1      10.878   6.856 -30.165
ATOM     64  H   ???     1      11.389   6.390 -31.010
ATOM     65  N   ???     1      11.497   7.653 -29.260
ATOM     66  H   ???     1      12.503   7.898 -29.277
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ATOM     67  C   ???     1      10.554   8.066 -28.339
ATOM     68  H   ???     1      10.815   8.752 -27.532
ATOM     69  O   ???     1      10.671   5.261 -25.612
ATOM     70  C   ???     1      10.953   4.626 -26.690
ATOM     71  O   ???     1      12.099   4.365 -27.133
ATOM     72  C   ???     1       9.740   4.226 -27.552
ATOM     73  H   ???     1       8.846   4.136 -26.909
ATOM     74  H   ???     1       9.563   5.092 -28.214
ATOM     75  C   ???     1       9.873   3.005 -28.463
ATOM     76  H   ???     1      10.862   3.015 -28.950
ATOM     77  H   ???     1       9.814   2.060 -27.888
ATOM     78  C   ???     1       8.814   3.043 -29.600
ATOM     79  O   ???     1       9.319   3.949 -30.603
ATOM     80  H   ???     1       9.902   3.255 -31.260
ATOM     81  C   ???     1       7.494   3.595 -29.049
ATOM     82  O   ???     1       7.134   4.741 -29.499
ATOM     83  O   ???     1       6.845   2.950 -28.192
ATOM     84  C   ???     1       8.552   1.687 -30.288
ATOM     85  H   ???     1       8.205   0.937 -29.557
ATOM     86  H   ???     1       7.743   1.847 -31.030
ATOM     87  C   ???     1       9.780   1.157 -31.051
ATOM     88  O   ???     1      10.462   2.066 -31.678
ATOM     89  O   ???     1      10.005  -0.067 -31.040
ATOM     90 FE   ???     1       5.385   7.638 -37.399
ATOM     91 MO   ???     1       8.100   5.624 -31.258
ATOM     92 FE   ???     1       7.089   8.346 -35.323
ATOM     93 FE   ???     1       5.936   6.237 -32.576
ATOM     94 FE   ???     1       6.934   5.839 -36.004
ATOM     95 FE   ???     1       8.072   7.572 -33.066
ATOM     96 FE   ???     1       7.827   5.179 -33.816
ATOM     97 FE   ???     1       4.916   6.966 -34.776
ATOM     98  C   ???     1       6.791   6.715 -34.270
ATOM     99  S   ???     1       7.763   7.497 -37.324
ATOM    100  S   ???     1       9.713   5.981 -32.974
ATOM    101  S   ???     1       4.733   5.511 -36.506
ATOM    102  S   ???     1       8.208   3.889 -35.609
ATOM    103  S   ???     1       8.475   9.564 -34.066
ATOM    104  S   ???     1       6.595   4.083 -32.333
ATOM    105  S   ???     1       4.885   9.076 -35.691
ATOM    106  S   ???     1       6.880   7.660 -31.129
ATOM    107  S   ???     1       3.775   6.664 -32.861
ATOM    108  H   ???     1       9.448   4.207 -36.108
ATOM    109  O   ???     1       4.531   5.530 -29.475
ATOM    110  H   ???     1       5.484   5.243 -29.510
ATOM    111  H   ???     1       4.442   6.161 -30.226
ATOM    112  O   ???     1       1.108   8.386 -34.230
ATOM    113  H   ???     1       1.964   8.037 -33.874
ATOM    114  H   ???     1       0.590   8.668 -33.420
END
```

Best E_2 structure optimised with the B3LPY functional. Both protons are on the carbide ion.

```
REMARK Energies (QM/MM, QM+ptch) = -16160.683272 -15321.126692
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E2/C12
ATOM      1  H   ???     1       3.498   2.233 -29.683
ATOM      2  C   ???     1       3.902   2.071 -30.699
ATOM      3  H   ???     1       5.002   2.147 -30.640
ATOM      4  H   ???     1       3.644   1.057 -31.035
ATOM      5  N   ???     1       3.425   3.050 -31.655
ATOM      6  H   ???     1       3.948   3.930 -31.688
ATOM      7  C   ???     1       2.749   2.745 -32.769
ATOM      8  N   ???     1       1.917   1.683 -32.803
ATOM      9  H   ???     1       1.769   1.119 -31.969
ATOM     10  H   ???     1       1.676   1.272 -33.710
ATOM     11  N   ???     1       2.913   3.496 -33.853
ATOM     12  H   ???     1       3.392   4.411 -33.758
ATOM     13  H   ???     1       2.259   3.429 -34.632
ATOM     14  H   ???     1       7.270   1.566 -41.621
ATOM     15  C   ???     1       7.567   2.043 -40.691
ATOM     16  N   ???     1       8.400   3.139 -40.711
ATOM     17  C   ???     1       8.501   3.520 -39.447
ATOM     18  H   ???     1       9.069   4.362 -39.055
ATOM     19  N   ???     1       7.767   2.725 -38.632
ATOM     20  H   ???     1       7.699   2.876 -37.609
ATOM     21  C   ???     1       7.152   1.777 -39.403
ATOM     22  H   ???     1       6.490   1.024 -38.981
ATOM     23  H   ???     1       2.975   9.554 -40.123
ATOM     24  C   ???     1       3.093   8.694 -39.438
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ATOM     25  H   ???     1       2.346   7.927 -39.698
ATOM     26  H   ???     1       2.916   9.050 -38.411
ATOM     27  S   ???     1       4.822   8.053 -39.632
ATOM     28  H   ???     1      13.630  11.347 -31.930
ATOM     29  C   ???     1      12.720  10.660 -31.981
ATOM     30  H   ???     1      12.873   9.953 -31.144
ATOM     31  H   ???     1      11.738  11.193 -31.792
ATOM     32  C   ???     1      12.903   9.825 -33.266
ATOM     33  O   ???     1      14.038   9.619 -33.673
ATOM     34  N   ???     1      11.813   9.250 -33.811
ATOM     35  H   ???     1      10.858   9.515 -33.547
ATOM     36  C   ???     1      11.948   8.158 -34.766
ATOM     37  H   ???     1      12.861   7.602 -34.525
ATOM     38  H   ???     1      11.080   7.500 -34.615
ATOM     39  C   ???     1      12.041   8.533 -36.257
ATOM     40  O   ???     1      13.079   8.345 -36.887
ATOM     41  N   ???     1      10.896   9.021 -36.783
ATOM     42  H   ???     1      10.072   9.008 -36.182
ATOM     43  C   ???     1      10.687   9.256 -38.212
ATOM     44  H   ???     1      11.673   9.440 -38.669
ATOM     45  H   ???     1      10.276   8.341 -38.674
ATOM     46  H   ???     1       9.992  10.081 -38.477
ATOM     47  H   ???     1       6.091  12.251 -32.941
ATOM     48  C   ???     1       5.938  11.599 -32.059
ATOM     49  H   ???     1       6.701  10.799 -32.113
ATOM     50  H   ???     1       6.090  12.201 -31.143
ATOM     51  N   ???     1       4.587  11.062 -32.103
ATOM     52  H   ???     1       4.007  11.188 -32.938
ATOM     53  C   ???     1       4.026  10.355 -31.115
ATOM     54  N   ???     1       4.705  10.132 -29.984
ATOM     55  H   ???     1       5.657  10.475 -29.874
ATOM     56  H   ???     1       4.339   9.535 -29.244
ATOM     57  N   ???     1       2.779   9.896 -31.279
ATOM     58  H   ???     1       2.280  10.138 -32.140
ATOM     59  H   ???     1       2.222   9.587 -30.491
ATOM     60  H   ???     1       8.414   7.467 -28.165
ATOM     61  C   ???     1       9.377   7.520 -28.685
ATOM     62  N   ???     1       9.647   6.735 -29.786
ATOM     63  C   ???     1      10.946   6.864 -30.038
ATOM     64  H   ???     1      11.493   6.384 -30.849
ATOM     65  N   ???     1      11.516   7.707 -29.152
ATOM     66  H   ???     1      12.513   7.971 -29.165
ATOM     67  C   ???     1      10.542   8.131 -28.276
ATOM     68  H   ???     1      10.757   8.855 -27.493
ATOM     69  O   ???     1      10.683   5.262 -25.597
ATOM     70  C   ???     1      10.958   4.623 -26.662
ATOM     71  O   ???     1      12.091   4.373 -27.119
ATOM     72  C   ???     1       9.742   4.203 -27.497
ATOM     73  H   ???     1       8.860   4.117 -26.844
ATOM     74  H   ???     1       9.556   5.061 -28.158
ATOM     75  C   ???     1       9.870   2.980 -28.395
ATOM     76  H   ???     1      10.856   2.991 -28.880
ATOM     77  H   ???     1       9.819   2.043 -27.811
ATOM     78  C   ???     1       8.824   3.028 -29.539
ATOM     79  O   ???     1       9.323   3.911 -30.511
ATOM     80  H   ???     1      10.039   3.004 -31.318
ATOM     81  C   ???     1       7.492   3.555 -28.981
ATOM     82  O   ???     1       7.165   4.719 -29.380
ATOM     83  O   ???     1       6.811   2.896 -28.177
ATOM     84  C   ???     1       8.554   1.663 -30.210
ATOM     85  H   ???     1       8.225   0.902 -29.487
ATOM     86  H   ???     1       7.739   1.818 -30.942
ATOM     87  C   ???     1       9.746   1.133 -30.987
ATOM     88  O   ???     1      10.438   2.054 -31.633
ATOM     89  O   ???     1      10.002  -0.060 -31.027
ATOM     90 FE   ???     1       7.132   8.512 -35.465
ATOM     91 MO   ???     1       8.182   5.567 -31.130
ATOM     92 FE   ???     1       5.383   7.677 -37.449
ATOM     93 FE   ???     1       5.453   6.078 -32.077
ATOM     94 FE   ???     1       6.984   5.793 -36.198
ATOM     95 FE   ???     1       8.040   4.870 -33.811
ATOM     96 FE   ???     1       8.243   7.711 -33.066
ATOM     97 FE   ???     1       4.136   7.034 -35.037
ATOM     98  C   ???     1       6.820   6.745 -34.280
ATOM     99  S   ???     1       7.781   7.562 -37.457
ATOM    100  S   ???     1       9.826   5.971 -32.840
ATOM    101  S   ???     1       4.697   5.501 -36.658
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ATOM    102  S   ???     1       8.194   3.903 -35.834
ATOM    103  S   ???     1       8.554   9.752 -34.125
ATOM    104  S   ???     1       6.592   4.018 -32.191
ATOM    105  S   ???     1       4.804   9.165 -35.727
ATOM    106  S   ???     1       6.894   7.623 -31.094
ATOM    107  S   ???     1       3.393   6.504 -32.931
ATOM    108  H   ???     1       6.150   7.542 -33.845
ATOM    109  H   ???     1       6.123   5.830 -34.178
ATOM    110  O   ???     1       4.684   5.687 -29.348
ATOM    111  H   ???     1       5.589   5.277 -29.316
ATOM    112  H   ???     1       4.845   6.640 -29.470
ATOM    113  O   ???     1       1.019   8.396 -34.237
ATOM    114  H   ???     1       1.805   7.966 -33.838
ATOM    115  H   ???     1       0.484   8.700 -33.452
END
```

Second best E_2 structure optimised with the B3LYP functional. One proton binds to the S2B atom and the other one binds to the carbide ion.

```
REMARK Energy = -16160.671367 -15321.115802
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E2/S2bC2
ATOM      1  H   ???     1       3.501   2.238 -29.683
ATOM      2  C   ???     1       3.910   2.088 -30.698
ATOM      3  H   ???     1       5.010   2.163 -30.630
ATOM      4  H   ???     1       3.658   1.075 -31.046
ATOM      5  N   ???     1       3.435   3.074 -31.648
ATOM      6  H   ???     1       3.930   3.970 -31.656
ATOM      7  C   ???     1       2.763   2.773 -32.768
ATOM      8  N   ???     1       1.941   1.702 -32.809
ATOM      9  H   ???     1       1.796   1.131 -31.981
ATOM     10  H   ???     1       1.698   1.298 -33.718
ATOM     11  N   ???     1       2.923   3.532 -33.845
ATOM     12  H   ???     1       3.366   4.471 -33.733
ATOM     13  H   ???     1       2.262   3.465 -34.619
ATOM     14  H   ???     1       7.269   1.572 -41.617
ATOM     15  C   ???     1       7.559   2.061 -40.686
ATOM     16  N   ???     1       8.359   3.183 -40.730
ATOM     17  C   ???     1       8.416   3.624 -39.486
ATOM     18  H   ???     1       8.931   4.516 -39.132
ATOM     19  N   ???     1       7.687   2.842 -38.653
ATOM     20  H   ???     1       7.596   3.016 -37.643
ATOM     21  C   ???     1       7.123   1.837 -39.397
ATOM     22  H   ???     1       6.477   1.080 -38.956
ATOM     23  H   ???     1       2.968   9.556 -40.123
ATOM     24  C   ???     1       3.074   8.698 -39.438
ATOM     25  H   ???     1       2.321   7.937 -39.695
ATOM     26  H   ???     1       2.915   9.052 -38.408
ATOM     27  S   ???     1       4.789   8.048 -39.644
ATOM     28  H   ???     1      13.630  11.348 -31.929
ATOM     29  C   ???     1      12.722  10.661 -31.981
ATOM     30  H   ???     1      12.875   9.953 -31.145
ATOM     31  H   ???     1      11.738  11.193 -31.792
ATOM     32  C   ???     1      12.911   9.829 -33.266
ATOM     33  O   ???     1      14.049   9.623 -33.668
ATOM     34  N   ???     1      11.825   9.254 -33.818
ATOM     35  H   ???     1      10.868   9.521 -33.568
ATOM     36  C   ???     1      11.968   8.164 -34.773
ATOM     37  H   ???     1      12.885   7.615 -34.532
ATOM     38  H   ???     1      11.103   7.503 -34.619
ATOM     39  C   ???     1      12.054   8.533 -36.267
ATOM     40  O   ???     1      13.083   8.322 -36.906
ATOM     41  N   ???     1      10.910   9.028 -36.786
ATOM     42  H   ???     1      10.100   9.060 -36.165
ATOM     43  C   ???     1      10.691   9.259 -38.214
ATOM     44  H   ???     1      11.672   9.443 -38.681
ATOM     45  H   ???     1      10.276   8.343 -38.671
ATOM     46  H   ???     1       9.994  10.082 -38.478
ATOM     47  H   ???     1       6.093  12.252 -32.941
ATOM     48  C   ???     1       5.941  11.601 -32.058
ATOM     49  H   ???     1       6.705  10.803 -32.108
ATOM     50  H   ???     1       6.093  12.206 -31.144
ATOM     51  N   ???     1       4.592  11.060 -32.102
ATOM     52  H   ???     1       4.005  11.198 -32.931
ATOM     53  C   ???     1       4.035  10.342 -31.119
ATOM     54  N   ???     1       4.709  10.126 -29.985
ATOM     55  H   ???     1       5.657  10.479 -29.868
ATOM     56  H   ???     1       4.362   9.495 -29.262
ATOM     57  N   ???     1       2.795   9.872 -31.291
ATOM     58  H   ???     1       2.301  10.098 -32.159
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ATOM     59  H   ???     1       2.238   9.554 -30.507
ATOM     60  H   ???     1       8.413   7.466 -28.168
ATOM     61  C   ???     1       9.373   7.517 -28.693
ATOM     62  N   ???     1       9.636   6.739 -29.802
ATOM     63  C   ???     1      10.936   6.862 -30.054
ATOM     64  H   ???     1      11.479   6.385 -30.869
ATOM     65  N   ???     1      11.512   7.696 -29.164
ATOM     66  H   ???     1      12.511   7.953 -29.175
ATOM     67  C   ???     1      10.542   8.119 -28.283
ATOM     68  H   ???     1      10.763   8.834 -27.494
ATOM     69  O   ???     1      10.682   5.265 -25.602
ATOM     70  C   ???     1      10.962   4.630 -26.668
ATOM     71  O   ???     1      12.096   4.386 -27.123
ATOM     72  C   ???     1       9.750   4.206 -27.509
ATOM     73  H   ???     1       8.867   4.115 -26.859
ATOM     74  H   ???     1       9.562   5.065 -28.167
ATOM     75  C   ???     1       9.889   2.982 -28.405
ATOM     76  H   ???     1      10.876   2.992 -28.888
ATOM     77  H   ???     1       9.839   2.045 -27.822
ATOM     78  C   ???     1       8.846   3.006 -29.548
ATOM     79  O   ???     1       9.355   3.899 -30.543
ATOM     80  H   ???     1       9.928   3.235 -31.195
ATOM     81  C   ???     1       7.521   3.563 -29.011
ATOM     82  O   ???     1       7.191   4.720 -29.431
ATOM     83  O   ???     1       6.848   2.920 -28.190
ATOM     84  C   ???     1       8.595   1.646 -30.218
ATOM     85  H   ???     1       8.286   0.892 -29.479
ATOM     86  H   ???     1       7.765   1.773 -30.938
ATOM     87  C   ???     1       9.803   1.129 -31.017
ATOM     88  O   ???     1      10.474   2.034 -31.638
ATOM     89  O   ???     1      10.009  -0.089 -31.030
ATOM     90 FE   ???     1       5.522   7.493 -37.586
ATOM     91 MO   ???     1       8.166   5.605 -31.166
ATOM     92 FE   ???     1       7.121   8.600 -35.605
ATOM     93 FE   ???     1       7.884   5.265 -33.803
ATOM     94 FE   ???     1       7.003   5.870 -36.042
ATOM     95 FE   ???     1       8.257   7.791 -32.988
ATOM     96 FE   ???     1       5.577   6.074 -32.387
ATOM     97 FE   ???     1       4.651   6.885 -34.944
ATOM     98  C   ???     1       6.561   6.743 -34.240
ATOM     99  S   ???     1       7.850   7.371 -37.537
ATOM    100  S   ???     1       9.820   6.023 -32.866
ATOM    101  S   ???     1       4.849   5.357 -36.692
ATOM    102  S   ???     1       8.273   3.804 -35.664
ATOM    103  S   ???     1       8.602   9.740 -34.223
ATOM    104  S   ???     1       6.644   4.036 -32.273
ATOM    105  S   ???     1       4.834   9.061 -35.860
ATOM    106  S   ???     1       6.844   7.639 -31.116
ATOM    107  S   ???     1       3.412   6.538 -33.015
ATOM    108  H   ???     1       6.342   7.751 -33.821
ATOM    109  H   ???     1       9.517   4.187 -36.058
ATOM    110  O   ???     1       4.639   5.612 -29.321
ATOM    111  H   ???     1       5.559   5.253 -29.359
ATOM    112  H   ???     1       4.709   6.515 -29.675
ATOM    113  O   ???     1       1.035   8.400 -34.259
ATOM    114  H   ???     1       1.847   7.973 -33.904
ATOM    115  H   ???     1       0.523   8.685 -33.456
END
```

Third best E_2 structure optimised with the B3LYP functional. The two protons are on the S2B and S2A atoms, respectively.

```
REMARK Energy = -16160.663018 -15321.108364
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E2/S2bS2a
ATOM      1  H   ???     1       3.501   2.241 -29.682
ATOM      2  C   ???     1       3.913   2.098 -30.696
ATOM      3  H   ???     1       5.014   2.140 -30.619
ATOM      4  H   ???     1       3.631   1.104 -31.071
ATOM      5  N   ???     1       3.479   3.130 -31.617
ATOM      6  H   ???     1       3.978   4.021 -31.543
ATOM      7  C   ???     1       2.835   2.896 -32.765
ATOM      8  N   ???     1       2.003   1.835 -32.879
ATOM      9  H   ???     1       1.855   1.220 -32.084
ATOM     10  H   ???     1       1.776   1.466 -33.807
ATOM     11  N   ???     1       3.020   3.715 -33.796
ATOM     12  H   ???     1       3.497   4.629 -33.633
ATOM     13  H   ???     1       2.383   3.694 -34.592
ATOM     14  H   ???     1       7.269   1.568 -41.625
ATOM     15  C   ???     1       7.563   2.050 -40.701
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ATOM     16  N   ???     1       8.364   3.169 -40.733
ATOM     17  C   ???     1       8.436   3.581 -39.480
ATOM     18  H   ???     1       8.971   4.455 -39.110
ATOM     19  N   ???     1       7.715   2.782 -38.658
ATOM     20  H   ???     1       7.646   2.930 -37.640
ATOM     21  C   ???     1       7.140   1.796 -39.414
ATOM     22  H   ???     1       6.499   1.031 -38.982
ATOM     23  H   ???     1       2.962   9.557 -40.122
ATOM     24  C   ???     1       3.053   8.699 -39.437
ATOM     25  H   ???     1       2.307   7.940 -39.716
ATOM     26  H   ???     1       2.864   9.043 -38.409
ATOM     27  S   ???     1       4.753   7.998 -39.600
ATOM     28  H   ???     1      13.630  11.346 -31.929
ATOM     29  C   ???     1      12.721  10.659 -31.978
ATOM     30  H   ???     1      12.873   9.953 -31.141
ATOM     31  H   ???     1      11.738  11.193 -31.791
ATOM     32  C   ???     1      12.900   9.826 -33.264
ATOM     33  O   ???     1      14.033   9.629 -33.685
ATOM     34  N   ???     1      11.810   9.244 -33.803
ATOM     35  H   ???     1      10.857   9.473 -33.503
ATOM     36  C   ???     1      11.952   8.157 -34.760
ATOM     37  H   ???     1      12.865   7.599 -34.518
ATOM     38  H   ???     1      11.082   7.499 -34.613
ATOM     39  C   ???     1      12.053   8.535 -36.250
ATOM     40  O   ???     1      13.087   8.329 -36.881
ATOM     41  N   ???     1      10.918   9.044 -36.779
ATOM     42  H   ???     1      10.085   9.028 -36.190
ATOM     43  C   ???     1      10.722   9.283 -38.211
ATOM     44  H   ???     1      11.708   9.488 -38.659
ATOM     45  H   ???     1      10.341   8.361 -38.687
ATOM     46  H   ???     1      10.010  10.095 -38.476
ATOM     47  H   ???     1       6.092  12.253 -32.940
ATOM     48  C   ???     1       5.938  11.605 -32.055
ATOM     49  H   ???     1       6.693  10.798 -32.111
ATOM     50  H   ???     1       6.102  12.207 -31.142
ATOM     51  N   ???     1       4.582  11.082 -32.090
ATOM     52  H   ???     1       4.001  11.209 -32.924
ATOM     53  C   ???     1       4.034  10.351 -31.113
ATOM     54  N   ???     1       4.720  10.107 -29.992
ATOM     55  H   ???     1       5.682  10.429 -29.897
ATOM     56  H   ???     1       4.390   9.444 -29.290
ATOM     57  N   ???     1       2.783   9.899 -31.274
ATOM     58  H   ???     1       2.280  10.160 -32.126
ATOM     59  H   ???     1       2.234   9.585 -30.483
ATOM     60  H   ???     1       8.413   7.464 -28.169
ATOM     61  C   ???     1       9.372   7.511 -28.699
ATOM     62  N   ???     1       9.626   6.730 -29.808
ATOM     63  C   ???     1      10.923   6.851 -30.070
ATOM     64  H   ???     1      11.456   6.372 -30.891
ATOM     65  N   ???     1      11.508   7.685 -29.185
ATOM     66  H   ???     1      12.507   7.940 -29.199
ATOM     67  C   ???     1      10.544   8.111 -28.298
ATOM     68  H   ???     1      10.773   8.827 -27.512
ATOM     69  O   ???     1      10.681   5.262 -25.603
ATOM     70  C   ???     1      10.956   4.629 -26.672
ATOM     71  O   ???     1      12.090   4.385 -27.130
ATOM     72  C   ???     1       9.741   4.207 -27.510
ATOM     73  H   ???     1       8.860   4.114 -26.858
ATOM     74  H   ???     1       9.549   5.068 -28.165
ATOM     75  C   ???     1       9.874   2.986 -28.412
ATOM     76  H   ???     1      10.859   2.996 -28.897
ATOM     77  H   ???     1       9.826   2.047 -27.832
ATOM     78  C   ???     1       8.824   3.011 -29.550
ATOM     79  O   ???     1       9.327   3.906 -30.547
ATOM     80  H   ???     1       9.905   3.258 -31.190
ATOM     81  C   ???     1       7.497   3.568 -29.011
ATOM     82  O   ???     1       7.157   4.717 -29.433
ATOM     83  O   ???     1       6.837   2.917 -28.182
ATOM     84  C   ???     1       8.578   1.652 -30.224
ATOM     85  H   ???     1       8.262   0.898 -29.489
ATOM     86  H   ???     1       7.753   1.783 -30.950
ATOM     87  C   ???     1       9.793   1.134 -31.016
ATOM     88  O   ???     1      10.466   2.036 -31.637
ATOM     89  O   ???     1       9.999  -0.086 -31.025
ATOM     90 FE   ???     1       7.074   8.519 -35.300
ATOM     91 MO   ???     1       8.142   5.610 -31.181
ATOM     92 FE   ???     1       5.754   8.521 -37.619
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ATOM     93 FE   ???     1       5.919   6.286 -32.628
ATOM     94 FE   ???     1       7.109   5.944 -36.245
ATOM     95 FE   ???     1       8.113   7.628 -33.065
ATOM     96 FE   ???     1       7.899   5.055 -33.868
ATOM     97 FE   ???     1       4.791   7.084 -34.910
ATOM     98  C   ???     1       6.811   6.759 -34.393
ATOM     99  S   ???     1       7.898   7.801 -37.414
ATOM    100  S   ???     1       9.780   5.995 -32.899
ATOM    101  S   ???     1       4.790   5.282 -36.611
ATOM    102  S   ???     1       8.264   3.810 -35.802
ATOM    103  S   ???     1       8.528   9.693 -34.031
ATOM    104  S   ???     1       6.577   4.083 -32.259
ATOM    105  S   ???     1       4.832   9.323 -35.701
ATOM    106  S   ???     1       6.903   7.655 -31.072
ATOM    107  S   ???     1       3.690   6.686 -32.923
ATOM    108  H   ???     1       4.492   6.080 -37.679
ATOM    109  H   ???     1       9.562   4.097 -36.109
ATOM    110  O   ???     1       4.541   5.514 -29.434
ATOM    111  H   ???     1       5.485   5.230 -29.465
ATOM    112  H   ???     1       4.458   6.216 -30.104
ATOM    113  O   ???     1       1.093   8.391 -34.235
ATOM    114  H   ???     1       1.934   8.032 -33.875
ATOM    115  H   ???     1       0.572   8.679 -33.440
END
```

Best E_2 structure optimised with TPSS functional. One proton is on S2B and the other one is bridging Fe2 and Fe6 on the 3 side.

```
REMARK Energy = -16164.154634 -15324.587754
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E2/S2bF26b
ATOM      1  H   ???     1       3.506   2.240 -29.685
ATOM      2  C   ???     1       3.926   2.094 -30.701
ATOM      3  H   ???     1       5.029   2.118 -30.620
ATOM      4  H   ???     1       3.625   1.106 -31.087
ATOM      5  N   ???     1       3.511   3.136 -31.629
ATOM      6  H   ???     1       4.021   4.030 -31.564
ATOM      7  C   ???     1       2.854   2.901 -32.777
ATOM      8  N   ???     1       1.985   1.858 -32.872
ATOM      9  H   ???     1       1.831   1.254 -32.063
ATOM     10  H   ???     1       1.778   1.458 -33.798
ATOM     11  N   ???     1       3.055   3.701 -33.825
ATOM     12  H   ???     1       3.601   4.588 -33.695
ATOM     13  H   ???     1       2.387   3.713 -34.601
ATOM     14  H   ???     1       7.267   1.572 -41.617
ATOM     15  C   ???     1       7.554   2.061 -40.685
ATOM     16  N   ???     1       8.363   3.182 -40.722
ATOM     17  C   ???     1       8.396   3.629 -39.472
ATOM     18  H   ???     1       8.917   4.515 -39.108
ATOM     19  N   ???     1       7.643   2.851 -38.647
ATOM     20  H   ???     1       7.500   3.042 -37.635
ATOM     21  C   ???     1       7.086   1.844 -39.401
ATOM     22  H   ???     1       6.429   1.091 -38.965
ATOM     23  H   ???     1       2.968   9.553 -40.111
ATOM     24  C   ???     1       3.067   8.696 -39.406
ATOM     25  H   ???     1       2.335   7.919 -39.686
ATOM     26  H   ???     1       2.848   9.063 -38.389
ATOM     27  S   ???     1       4.799   8.037 -39.481
ATOM     28  H   ???     1      13.631  11.343 -31.928
ATOM     29  C   ???     1      12.716  10.655 -31.975
ATOM     30  H   ???     1      12.872   9.948 -31.135
ATOM     31  H   ???     1      11.735  11.192 -31.789
ATOM     32  C   ???     1      12.883   9.821 -33.265
ATOM     33  O   ???     1      14.020   9.614 -33.694
ATOM     34  N   ???     1      11.784   9.239 -33.802
ATOM     35  H   ???     1      10.825   9.459 -33.493
ATOM     36  C   ???     1      11.929   8.143 -34.760
ATOM     37  H   ???     1      12.858   7.606 -34.521
ATOM     38  H   ???     1      11.065   7.476 -34.595
ATOM     39  C   ???     1      12.008   8.521 -36.254
ATOM     40  O   ???     1      13.054   8.353 -36.896
ATOM     41  N   ???     1      10.846   8.986 -36.780
ATOM     42  H   ???     1      10.008   8.948 -36.184
ATOM     43  C   ???     1      10.654   9.234 -38.215
ATOM     44  H   ???     1      11.655   9.396 -38.651
ATOM     45  H   ???     1      10.229   8.322 -38.681
ATOM     46  H   ???     1       9.977  10.072 -38.479
ATOM     47  H   ???     1       6.092  12.253 -32.939
ATOM     48  C   ???     1       5.940  11.603 -32.050
ATOM     49  H   ???     1       6.675  10.774 -32.114
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ATOM     50  H   ???     1       6.123  12.203 -31.136
ATOM     51  N   ???     1       4.567  11.108 -32.066
ATOM     52  H   ???     1       3.970  11.252 -32.893
ATOM     53  C   ???     1       4.015  10.372 -31.087
ATOM     54  N   ???     1       4.696  10.134 -29.957
ATOM     55  H   ???     1       5.652  10.483 -29.848
ATOM     56  H   ???     1       4.385   9.432 -29.276
ATOM     57  N   ???     1       2.762   9.901 -31.257
ATOM     58  H   ???     1       2.273  10.171 -32.121
ATOM     59  H   ???     1       2.171   9.723 -30.446
ATOM     60  H   ???     1       8.406   7.462 -28.183
ATOM     61  C   ???     1       9.353   7.504 -28.741
ATOM     62  N   ???     1       9.561   6.768 -29.897
ATOM     63  C   ???     1      10.863   6.868 -30.178
ATOM     64  H   ???     1      11.370   6.410 -31.030
ATOM     65  N   ???     1      11.491   7.645 -29.262
ATOM     66  H   ???     1      12.499   7.882 -29.278
ATOM     67  C   ???     1      10.553   8.055 -28.335
ATOM     68  H   ???     1      10.820   8.728 -27.520
ATOM     69  O   ???     1      10.668   5.259 -25.621
ATOM     70  C   ???     1      10.950   4.628 -26.702
ATOM     71  O   ???     1      12.097   4.362 -27.140
ATOM     72  C   ???     1       9.737   4.241 -27.572
ATOM     73  H   ???     1       8.844   4.139 -26.930
ATOM     74  H   ???     1       9.558   5.118 -28.218
ATOM     75  C   ???     1       9.871   3.036 -28.505
ATOM     76  H   ???     1      10.859   3.053 -28.992
ATOM     77  H   ???     1       9.812   2.082 -27.944
ATOM     78  C   ???     1       8.807   3.080 -29.638
ATOM     79  O   ???     1       9.298   3.988 -30.648
ATOM     80  H   ???     1       9.880   3.309 -31.294
ATOM     81  C   ???     1       7.488   3.624 -29.081
ATOM     82  O   ???     1       7.110   4.759 -29.546
ATOM     83  O   ???     1       6.859   2.980 -28.208
ATOM     84  C   ???     1       8.545   1.721 -30.322
ATOM     85  H   ???     1       8.190   0.978 -29.587
ATOM     86  H   ???     1       7.740   1.879 -31.071
ATOM     87  C   ???     1       9.779   1.182 -31.072
ATOM     88  O   ???     1      10.462   2.087 -31.701
ATOM     89  O   ???     1      10.004  -0.042 -31.046
ATOM     90 FE   ???     1       6.968   8.500 -35.348
ATOM     91 MO   ???     1       8.071   5.680 -31.301
ATOM     92 FE   ???     1       5.381   7.660 -37.303
ATOM     93 FE   ???     1       5.901   6.317 -32.630
ATOM     94 FE   ???     1       7.117   6.108 -36.055
ATOM     95 FE   ???     1       8.041   7.687 -33.084
ATOM     96 FE   ???     1       7.820   5.299 -33.876
ATOM     97 FE   ???     1       4.924   6.954 -34.882
ATOM     98  C   ???     1       6.771   6.850 -34.309
ATOM     99  S   ???     1       7.647   7.829 -37.390
ATOM    100  S   ???     1       9.697   6.102 -32.984
ATOM    101  S   ???     1       4.929   5.516 -36.615
ATOM    102  S   ???     1       7.962   3.963 -35.706
ATOM    103  S   ???     1       8.436   9.669 -34.121
ATOM    104  S   ???     1       6.576   4.166 -32.416
ATOM    105  S   ???     1       4.734   9.085 -35.678
ATOM    106  S   ???     1       6.837   7.709 -31.142
ATOM    107  S   ???     1       3.741   6.652 -32.988
ATOM    108  H   ???     1       8.607   6.301 -35.766
ATOM    109  H   ???     1       9.275   4.089 -36.079
ATOM    110  O   ???     1       4.515   5.530 -29.478
ATOM    111  H   ???     1       5.470   5.249 -29.519
ATOM    112  H   ???     1       4.428   6.187 -30.206
ATOM    113  O   ???     1       1.095   8.388 -34.244
ATOM    114  H   ???     1       1.957   8.040 -33.901
ATOM    115  H   ???     1       0.586   8.668 -33.428
END
```

Second best E_2 structure optimised with theTPSS functional. One proton is on S2B and the other one is bridging Fe2 and Fe6 in the 5 side.

```
REMARK Energy = -16164.155446 -15324.595534
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E2/S2bF26f
ATOM      1  H   ???     1       3.499   2.240 -29.686
ATOM      2  C   ???     1       3.906   2.094 -30.705
ATOM      3  H   ???     1       5.011   2.115 -30.640
ATOM      4  H   ???     1       3.594   1.110 -31.092
ATOM      5  N   ???     1       3.483   3.147 -31.617
ATOM      6  H   ???     1       4.008   4.033 -31.544
```

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ATOM      7  C   ???     1       2.852   2.928 -32.784
ATOM      8  N   ???     1       1.985   1.886 -32.907
ATOM      9  H   ???     1       1.831   1.267 -32.110
ATOM     10  H   ???     1       1.788   1.498 -33.840
ATOM     11  N   ???     1       3.072   3.746 -33.814
ATOM     12  H   ???     1       3.617   4.627 -33.662
ATOM     13  H   ???     1       2.429   3.767 -34.610
ATOM     14  H   ???     1       7.273   1.571 -41.613
ATOM     15  C   ???     1       7.573   2.056 -40.678
ATOM     16  N   ???     1       8.362   3.190 -40.734
ATOM     17  C   ???     1       8.456   3.614 -39.479
ATOM     18  H   ???     1       8.975   4.506 -39.128
ATOM     19  N   ???     1       7.765   2.807 -38.630
ATOM     20  H   ???     1       7.695   2.974 -37.607
ATOM     21  C   ???     1       7.184   1.804 -39.374
ATOM     22  H   ???     1       6.567   1.031 -38.916
ATOM     23  H   ???     1       2.976   9.552 -40.106
ATOM     24  C   ???     1       3.090   8.697 -39.394
ATOM     25  H   ???     1       2.352   7.919 -39.659
ATOM     26  H   ???     1       2.882   9.072 -38.377
ATOM     27  S   ???     1       4.817   8.015 -39.478
ATOM     28  H   ???     1      13.631  11.343 -31.928
ATOM     29  C   ???     1      12.717  10.653 -31.974
ATOM     30  H   ???     1      12.873   9.949 -31.133
ATOM     31  H   ???     1      11.736  11.191 -31.789
ATOM     32  C   ???     1      12.886   9.817 -33.263
ATOM     33  O   ???     1      14.022   9.616 -33.696
ATOM     34  N   ???     1      11.786   9.227 -33.793
ATOM     35  H   ???     1      10.828   9.439 -33.478
ATOM     36  C   ???     1      11.922   8.131 -34.753
ATOM     37  H   ???     1      12.849   7.589 -34.519
ATOM     38  H   ???     1      11.052   7.471 -34.583
ATOM     39  C   ???     1      12.000   8.515 -36.249
ATOM     40  O   ???     1      13.049   8.359 -36.887
ATOM     41  N   ???     1      10.833   8.972 -36.772
ATOM     42  H   ???     1      10.000   8.917 -36.168
ATOM     43  C   ???     1      10.624   9.210 -38.208
ATOM     44  H   ???     1      11.622   9.345 -38.661
ATOM     45  H   ???     1      10.166   8.303 -38.652
ATOM     46  H   ???     1       9.963  10.060 -38.476
ATOM     47  H   ???     1       6.094  12.249 -32.941
ATOM     48  C   ???     1       5.944  11.593 -32.056
ATOM     49  H   ???     1       6.669  10.755 -32.130
ATOM     50  H   ???     1       6.144  12.184 -31.140
ATOM     51  N   ???     1       4.566  11.112 -32.062
ATOM     52  H   ???     1       3.964  11.263 -32.883
ATOM     53  C   ???     1       4.018  10.371 -31.082
ATOM     54  N   ???     1       4.711  10.118 -29.963
ATOM     55  H   ???     1       5.670  10.461 -29.860
ATOM     56  H   ???     1       4.399   9.418 -29.280
ATOM     57  N   ???     1       2.761   9.917 -31.242
ATOM     58  H   ???     1       2.263  10.182 -32.102
ATOM     59  H   ???     1       2.183   9.701 -30.431
ATOM     60  H   ???     1       8.408   7.456 -28.188
ATOM     61  C   ???     1       9.355   7.487 -28.752
ATOM     62  N   ???     1       9.557   6.733 -29.900
ATOM     63  C   ???     1      10.854   6.836 -30.197
ATOM     64  H   ???     1      11.353   6.366 -31.047
ATOM     65  N   ???     1      11.488   7.628 -29.297
ATOM     66  H   ???     1      12.496   7.866 -29.319
ATOM     67  C   ???     1      10.558   8.045 -28.366
ATOM     68  H   ???     1      10.833   8.724 -27.559
ATOM     69  O   ???     1      10.671   5.262 -25.617
ATOM     70  C   ???     1      10.953   4.625 -26.694
ATOM     71  O   ???     1      12.098   4.362 -27.137
ATOM     72  C   ???     1       9.738   4.225 -27.555
ATOM     73  H   ???     1       8.846   4.136 -26.911
ATOM     74  H   ???     1       9.559   5.090 -28.217
ATOM     75  C   ???     1       9.868   3.004 -28.468
ATOM     76  H   ???     1      10.852   3.017 -28.964
ATOM     77  H   ???     1       9.818   2.060 -27.891
ATOM     78  C   ???     1       8.798   3.035 -29.596
ATOM     79  O   ???     1       9.289   3.938 -30.607
ATOM     80  H   ???     1       9.881   3.243 -31.262
ATOM     81  C   ???     1       7.484   3.589 -29.035
ATOM     82  O   ???     1       7.134   4.746 -29.464
ATOM     83  O   ???     1       6.833   2.940 -28.184
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ATOM     84  C   ???     1       8.541   1.675 -30.278
ATOM     85  H   ???     1       8.201   0.924 -29.545
ATOM     86  H   ???     1       7.728   1.828 -31.019
ATOM     87  C   ???     1       9.770   1.150 -31.044
ATOM     88  O   ???     1      10.450   2.062 -31.672
ATOM     89  O   ???     1      10.002  -0.072 -31.034
ATOM     90 FE   ???     1       7.117   8.161 -35.440
ATOM     91 MO   ???     1       8.060   5.605 -31.257
ATOM     92 FE   ???     1       5.442   7.528 -37.317
ATOM     93 FE   ???     1       5.882   6.240 -32.564
ATOM     94 FE   ???     1       6.739   5.623 -35.903
ATOM     95 FE   ???     1       8.045   7.514 -33.119
ATOM     96 FE   ???     1       7.726   5.061 -33.804
ATOM     97 FE   ???     1       4.895   6.979 -34.814
ATOM     98  C   ???     1       6.734   6.646 -34.277
ATOM     99  S   ???     1       7.690   7.115 -37.373
ATOM    100  S   ???     1       9.640   5.893 -33.008
ATOM    101  S   ???     1       4.601   5.549 -36.517
ATOM    102  S   ???     1       8.302   3.891 -35.657
ATOM    103  S   ???     1       8.478   9.447 -34.206
ATOM    104  S   ???     1       6.495   4.072 -32.233
ATOM    105  S   ???     1       4.999   9.057 -35.730
ATOM    106  S   ???     1       6.887   7.673 -31.156
ATOM    107  S   ???     1       3.734   6.708 -32.900
ATOM    108  H   ???     1       6.246   4.435 -35.004
ATOM    109  H   ???     1       9.570   4.237 -36.063
ATOM    110  O   ???     1       4.527   5.545 -29.461
ATOM    111  H   ???     1       5.479   5.255 -29.497
ATOM    112  H   ???     1       4.434   6.169 -30.218
ATOM    113  O   ???     1       1.100   8.389 -34.237
ATOM    114  H   ???     1       1.950   8.025 -33.882
ATOM    115  H   ???     1       0.584   8.672 -33.426
END
```

The third best E_2 structure optimised with theTPSS functional. One proton is on the S2B atom and the other one is on the Fe5 ion.

```
REMARK Energy = -16164.154302 -15324.589045
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E2/S2bF5
ATOM      1  H   ???     1       3.503   2.240 -29.686
ATOM      2  C   ???     1       3.916   2.095 -30.705
ATOM      3  H   ???     1       5.020   2.107 -30.630
ATOM      4  H   ???     1       3.602   1.113 -31.094
ATOM      5  N   ???     1       3.506   3.149 -31.622
ATOM      6  H   ???     1       4.015   4.042 -31.539
ATOM      7  C   ???     1       2.862   2.932 -32.782
ATOM      8  N   ???     1       1.993   1.892 -32.902
ATOM      9  H   ???     1       1.838   1.272 -32.105
ATOM     10  H   ???     1       1.791   1.506 -33.835
ATOM     11  N   ???     1       3.074   3.751 -33.813
ATOM     12  H   ???     1       3.626   4.628 -33.667
ATOM     13  H   ???     1       2.424   3.773 -34.604
ATOM     14  H   ???     1       7.270   1.572 -41.613
ATOM     15  C   ???     1       7.563   2.058 -40.676
ATOM     16  N   ???     1       8.359   3.188 -40.722
ATOM     17  C   ???     1       8.423   3.621 -39.468
ATOM     18  H   ???     1       8.938   4.514 -39.112
ATOM     19  N   ???     1       7.705   2.824 -38.630
ATOM     20  H   ???     1       7.594   3.002 -37.612
ATOM     21  C   ???     1       7.137   1.819 -39.381
ATOM     22  H   ???     1       6.503   1.054 -38.935
ATOM     23  H   ???     1       2.972   9.552 -40.108
ATOM     24  C   ???     1       3.079   8.694 -39.399
ATOM     25  H   ???     1       2.344   7.918 -39.674
ATOM     26  H   ???     1       2.860   9.066 -38.383
ATOM     27  S   ???     1       4.809   8.021 -39.466
ATOM     28  H   ???     1      13.631  11.343 -31.928
ATOM     29  C   ???     1      12.716  10.654 -31.973
ATOM     30  H   ???     1      12.871   9.949 -31.132
ATOM     31  H   ???     1      11.735  11.192 -31.789
ATOM     32  C   ???     1      12.881   9.819 -33.262
ATOM     33  O   ???     1      14.015   9.621 -33.702
ATOM     34  N   ???     1      11.780   9.231 -33.791
ATOM     35  H   ???     1      10.828   9.420 -33.448
ATOM     36  C   ???     1      11.921   8.138 -34.753
ATOM     37  H   ???     1      12.844   7.591 -34.515
ATOM     38  H   ???     1      11.049   7.481 -34.591
ATOM     39  C   ???     1      12.010   8.521 -36.248
ATOM     40  O   ???     1      13.060   8.353 -36.882
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ATOM     41  N   ???     1      10.850   8.985 -36.779
ATOM     42  H   ???     1      10.011   8.948 -36.183
ATOM     43  C   ???     1      10.655   9.232 -38.214
ATOM     44  H   ???     1      11.655   9.390 -38.656
ATOM     45  H   ???     1      10.223   8.321 -38.676
ATOM     46  H   ???     1       9.978  10.071 -38.478
ATOM     47  H   ???     1       6.095  12.251 -32.940
ATOM     48  C   ???     1       5.948  11.599 -32.053
ATOM     49  H   ???     1       6.682  10.770 -32.119
ATOM     50  H   ???     1       6.135  12.196 -31.138
ATOM     51  N   ???     1       4.574  11.106 -32.066
ATOM     52  H   ???     1       3.977  11.251 -32.892
ATOM     53  C   ???     1       4.023  10.370 -31.086
ATOM     54  N   ???     1       4.709  10.125 -29.960
ATOM     55  H   ???     1       5.664  10.478 -29.849
ATOM     56  H   ???     1       4.392   9.433 -29.273
ATOM     57  N   ???     1       2.767   9.910 -31.251
ATOM     58  H   ???     1       2.275  10.178 -32.114
ATOM     59  H   ???     1       2.183   9.710 -30.440
ATOM     60  H   ???     1       8.408   7.459 -28.185
ATOM     61  C   ???     1       9.355   7.497 -28.745
ATOM     62  N   ???     1       9.566   6.742 -29.889
ATOM     63  C   ???     1      10.864   6.856 -30.182
ATOM     64  H   ???     1      11.369   6.394 -31.033
ATOM     65  N   ???     1      11.489   7.652 -29.281
ATOM     66  H   ???     1      12.495   7.896 -29.302
ATOM     67  C   ???     1      10.552   8.065 -28.354
ATOM     68  H   ???     1      10.818   8.749 -27.548
ATOM     69  O   ???     1      10.669   5.259 -25.616
ATOM     70  C   ???     1      10.949   4.625 -26.695
ATOM     71  O   ???     1      12.095   4.362 -27.138
ATOM     72  C   ???     1       9.734   4.229 -27.558
ATOM     73  H   ???     1       8.844   4.127 -26.912
ATOM     74  H   ???     1       9.550   5.102 -28.208
ATOM     75  C   ???     1       9.870   3.020 -28.485
ATOM     76  H   ???     1      10.859   3.039 -28.972
ATOM     77  H   ???     1       9.815   2.068 -27.921
ATOM     78  C   ???     1       8.809   3.061 -29.621
ATOM     79  O   ???     1       9.306   3.962 -30.632
ATOM     80  H   ???     1       9.892   3.269 -31.281
ATOM     81  C   ???     1       7.490   3.611 -29.069
ATOM     82  O   ???     1       7.120   4.750 -29.532
ATOM     83  O   ???     1       6.852   2.970 -28.201
ATOM     84  C   ???     1       8.546   1.701 -30.304
ATOM     85  H   ???     1       8.197   0.955 -29.570
ATOM     86  H   ???     1       7.738   1.857 -31.049
ATOM     87  C   ???     1       9.777   1.166 -31.060
ATOM     88  O   ???     1      10.460   2.073 -31.689
ATOM     89  O   ???     1      10.003  -0.057 -31.041
ATOM     90 FE   ???     1       7.067   8.362 -35.394
ATOM     91 MO   ???     1       8.092   5.646 -31.287
ATOM     92 FE   ???     1       5.385   7.607 -37.280
ATOM     93 FE   ???     1       5.931   6.308 -32.622
ATOM     94 FE   ???     1       6.873   5.910 -36.027
ATOM     95 FE   ???     1       8.152   7.646 -33.047
ATOM     96 FE   ???     1       7.813   5.266 -33.856
ATOM     97 FE   ???     1       4.873   7.002 -34.816
ATOM     98  C   ???     1       6.753   6.783 -34.313
ATOM     99  S   ???     1       7.718   7.534 -37.385
ATOM    100  S   ???     1       9.704   6.000 -32.999
ATOM    101  S   ???     1       4.688   5.521 -36.503
ATOM    102  S   ???     1       8.147   3.947 -35.645
ATOM    103  S   ???     1       8.458   9.610 -34.242
ATOM    104  S   ???     1       6.582   4.142 -32.389
ATOM    105  S   ???     1       4.860   9.110 -35.684
ATOM    106  S   ???     1       6.882   7.684 -31.166
ATOM    107  S   ???     1       3.764   6.696 -32.882
ATOM    108  H   ???     1       9.122   8.452 -32.162
ATOM    109  H   ???     1       9.386   4.232 -36.166
ATOM    110  O   ???     1       4.524   5.532 -29.483
ATOM    111  H   ???     1       5.477   5.244 -29.521
ATOM    112  H   ???     1       4.432   6.157 -30.238
ATOM    113  O   ???     1       1.099   8.388 -34.236
ATOM    114  H   ???     1       1.957   8.045 -33.881
ATOM    115  H   ???     1       0.582   8.672 -33.425
END
```

Best E_3 structure optimised with theB3LYP functional. All three protons are on the carbide ion.

```
REMARK Energies (QM/MM, QM+ptch) = -16161.272854 -15321.713448
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E3/C123
ATOM      1  H   ???     1       3.494   2.228 -29.684
ATOM      2  C   ???     1       3.892   2.056 -30.702
ATOM      3  H   ???     1       4.994   2.112 -30.651
ATOM      4  H   ???     1       3.613   1.045 -31.033
ATOM      5  N   ???     1       3.424   3.044 -31.653
ATOM      6  H   ???     1       3.979   3.904 -31.691
ATOM      7  C   ???     1       2.755   2.759 -32.779
ATOM      8  N   ???     1       1.914   1.704 -32.830
ATOM      9  H   ???     1       1.777   1.118 -32.010
ATOM     10  H   ???     1       1.675   1.307 -33.745
ATOM     11  N   ???     1       2.930   3.526 -33.848
ATOM     12  H   ???     1       3.406   4.448 -33.743
ATOM     13  H   ???     1       2.284   3.466 -34.635
ATOM     14  H   ???     1       7.275   1.561 -41.620
ATOM     15  C   ???     1       7.583   2.024 -40.688
ATOM     16  N   ???     1       8.426   3.113 -40.694
ATOM     17  C   ???     1       8.589   3.431 -39.420
ATOM     18  H   ???     1       9.190   4.245 -39.019
ATOM     19  N   ???     1       7.887   2.602 -38.610
ATOM     20  H   ???     1       7.863   2.698 -37.581
ATOM     21  C   ???     1       7.225   1.699 -39.397
ATOM     22  H   ???     1       6.570   0.938 -38.982
ATOM     23  H   ???     1       2.968   9.555 -40.125
ATOM     24  C   ???     1       3.073   8.695 -39.443
ATOM     25  H   ???     1       2.324   7.932 -39.705
ATOM     26  H   ???     1       2.909   9.045 -38.413
ATOM     27  S   ???     1       4.793   8.053 -39.649
ATOM     28  H   ???     1      13.630  11.346 -31.930
ATOM     29  C   ???     1      12.720  10.660 -31.981
ATOM     30  H   ???     1      12.874   9.952 -31.145
ATOM     31  H   ???     1      11.738  11.193 -31.792
ATOM     32  C   ???     1      12.898   9.825 -33.267
ATOM     33  O   ???     1      14.032   9.615 -33.676
ATOM     34  N   ???     1      11.805   9.251 -33.811
ATOM     35  H   ???     1      10.852   9.532 -33.561
ATOM     36  C   ???     1      11.937   8.157 -34.764
ATOM     37  H   ???     1      12.848   7.599 -34.522
ATOM     38  H   ???     1      11.066   7.503 -34.612
ATOM     39  C   ???     1      12.030   8.532 -36.256
ATOM     40  O   ???     1      13.070   8.349 -36.884
ATOM     41  N   ???     1      10.883   9.013 -36.783
ATOM     42  H   ???     1      10.061   9.010 -36.178
ATOM     43  C   ???     1      10.676   9.249 -38.212
ATOM     44  H   ???     1      11.662   9.428 -38.669
ATOM     45  H   ???     1      10.257   8.337 -38.673
ATOM     46  H   ???     1       9.987  10.078 -38.477
ATOM     47  H   ???     1       6.091  12.253 -32.940
ATOM     48  C   ???     1       5.937  11.605 -32.056
ATOM     49  H   ???     1       6.707  10.811 -32.099
ATOM     50  H   ???     1       6.074  12.212 -31.142
ATOM     51  N   ???     1       4.593  11.052 -32.111
ATOM     52  H   ???     1       4.010  11.187 -32.943
ATOM     53  C   ???     1       4.027  10.348 -31.124
ATOM     54  N   ???     1       4.694  10.141 -29.984
ATOM     55  H   ???     1       5.656  10.461 -29.879
ATOM     56  H   ???     1       4.332   9.531 -29.253
ATOM     57  N   ???     1       2.784   9.881 -31.297
ATOM     58  H   ???     1       2.293  10.119 -32.164
ATOM     59  H   ???     1       2.214   9.600 -30.507
ATOM     60  H   ???     1       8.414   7.465 -28.166
ATOM     61  C   ???     1       9.374   7.513 -28.690
ATOM     62  N   ???     1       9.629   6.721 -29.790
ATOM     63  C   ???     1      10.928   6.836 -30.051
ATOM     64  H   ???     1      11.462   6.349 -30.867
ATOM     65  N   ???     1      11.512   7.680 -29.174
ATOM     66  H   ???     1      12.510   7.936 -29.191
ATOM     67  C   ???     1      10.547   8.117 -28.293
ATOM     68  H   ???     1      10.775   8.842 -27.514
ATOM     69  O   ???     1      10.674   5.260 -25.603
ATOM     70  C   ???     1      10.949   4.624 -26.670
ATOM     71  O   ???     1      12.081   4.384 -27.133
ATOM     72  C   ???     1       9.732   4.196 -27.503
ATOM     73  H   ???     1       8.854   4.101 -26.845
ATOM     74  H   ???     1       9.535   5.056 -28.157
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ATOM     75  C   ???     1       9.864   2.975 -28.403
ATOM     76  H   ???     1      10.846   2.989 -28.897
ATOM     77  H   ???     1       9.827   2.036 -27.822
ATOM     78  C   ???     1       8.808   2.996 -29.538
ATOM     79  O   ???     1       9.308   3.889 -30.535
ATOM     80  H   ???     1       9.900   3.218 -31.182
ATOM     81  C   ???     1       7.485   3.543 -28.985
ATOM     82  O   ???     1       7.161   4.715 -29.365
ATOM     83  O   ???     1       6.805   2.887 -28.179
ATOM     84  C   ???     1       8.564   1.635 -30.210
ATOM     85  H   ???     1       8.261   0.877 -29.473
ATOM     86  H   ???     1       7.732   1.762 -30.928
ATOM     87  C   ???     1       9.778   1.130 -31.009
ATOM     88  O   ???     1      10.443   2.045 -31.626
ATOM     89  O   ???     1       9.999  -0.084 -31.026
ATOM     90 FE   ???     1       5.480   7.510 -37.556
ATOM     91 MO   ???     1       8.126   5.602 -31.137
ATOM     92 FE   ???     1       6.979   8.648 -35.532
ATOM     93 FE   ???     1       5.322   6.040 -31.830
ATOM     94 FE   ???     1       7.110   5.341 -36.705
ATOM     95 FE   ???     1       8.382   7.931 -32.811
ATOM     96 FE   ???     1       8.111   4.677 -33.767
ATOM     97 FE   ???     1       4.653   7.000 -35.049
ATOM     98  C   ???     1       6.595   6.842 -34.289
ATOM     99  S   ???     1       7.772   7.432 -37.498
ATOM    100  S   ???     1       9.743   6.042 -32.868
ATOM    101  S   ???     1       4.781   5.386 -36.742
ATOM    102  S   ???     1       8.383   3.740 -35.767
ATOM    103  S   ???     1       8.516   9.788 -34.181
ATOM    104  S   ???     1       6.532   4.060 -32.166
ATOM    105  S   ???     1       4.722   9.126 -35.938
ATOM    106  S   ???     1       6.831   7.661 -31.031
ATOM    107  S   ???     1       3.489   6.549 -33.080
ATOM    108  H   ???     1       6.346   5.771 -34.178
ATOM    109  H   ???     1       7.665   6.872 -34.695
ATOM    110  H   ???     1       6.495   7.329 -33.312
ATOM    111  O   ???     1       4.747   5.743 -29.466
ATOM    112  H   ???     1       5.626   5.279 -29.331
ATOM    113  H   ???     1       4.961   6.693 -29.374
ATOM    114  O   ???     1       1.044   8.399 -34.247
ATOM    115  H   ???     1       1.848   7.971 -33.878
ATOM    116  H   ???     1       0.522   8.688 -33.451
END
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Second best E_2 structure optimised with theB3LYP functional. One proton is on the S2B atom and the other two are on the carbide ion.

```
REMARK Energies (QM/MM, QM+ptch) = -16161.261241 -15321. 702785
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E3/S2bC12
ATOM      1  H   ???     1       3.498   2.228 -29.683
ATOM      2  C   ???     1       3.904   2.056 -30.698
ATOM      3  H   ???     1       5.005   2.118 -30.638
ATOM      4  H   ???     1       3.635   1.042 -31.027
ATOM      5  N   ???     1       3.441   3.036 -31.658
ATOM      6  H   ???     1       3.999   3.894 -31.711
ATOM      7  C   ???     1       2.756   2.744 -32.771
ATOM      8  N   ???     1       1.916   1.688 -32.810
ATOM      9  H   ???     1       1.785   1.106 -31.986
ATOM     10  H   ???     1       1.667   1.290 -33.720
ATOM     11  N   ???     1       2.920   3.507 -33.846
ATOM     12  H   ???     1       3.375   4.436 -33.729
ATOM     13  H   ???     1       2.263   3.447 -34.623
ATOM     14  H   ???     1       7.270   1.570 -41.620
ATOM     15  C   ???     1       7.564   2.056 -40.691
ATOM     16  N   ???     1       8.359   3.179 -40.733
ATOM     17  C   ???     1       8.431   3.607 -39.486
ATOM     18  H   ???     1       8.950   4.495 -39.128
ATOM     19  N   ???     1       7.716   2.812 -38.653
ATOM     20  H   ???     1       7.644   2.970 -37.639
ATOM     21  C   ???     1       7.145   1.814 -39.400
ATOM     22  H   ???     1       6.508   1.051 -38.960
ATOM     23  H   ???     1       2.974   9.554 -40.124
ATOM     24  C   ???     1       3.090   8.694 -39.442
ATOM     25  H   ???     1       2.338   7.931 -39.698
ATOM     26  H   ???     1       2.929   9.049 -38.412
ATOM     27  S   ???     1       4.815   8.049 -39.655
ATOM     28  H   ???     1      13.629  11.349 -31.930
ATOM     29  C   ???     1      12.721  10.662 -31.982
ATOM     30  H   ???     1      12.875   9.952 -31.149
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ATOM     31  H   ???     1      11.738  11.194 -31.792
ATOM     32  C   ???     1      12.908   9.834 -33.270
ATOM     33  O   ???     1      14.046   9.621 -33.666
ATOM     34  N   ???     1      11.821   9.268 -33.830
ATOM     35  H   ???     1      10.866   9.541 -33.581
ATOM     36  C   ???     1      11.971   8.173 -34.779
ATOM     37  H   ???     1      12.892   7.634 -34.534
ATOM     38  H   ???     1      11.113   7.503 -34.620
ATOM     39  C   ???     1      12.056   8.533 -36.275
ATOM     40  O   ???     1      13.082   8.310 -36.915
ATOM     41  N   ???     1      10.915   9.031 -36.793
ATOM     42  H   ???     1      10.109   9.097 -36.169
ATOM     43  C   ???     1      10.696   9.263 -38.220
ATOM     44  H   ???     1      11.676   9.450 -38.688
ATOM     45  H   ???     1      10.284   8.347 -38.679
ATOM     46  H   ???     1       9.996  10.085 -38.480
ATOM     47  H   ???     1       6.093  12.251 -32.942
ATOM     48  C   ???     1       5.943  11.596 -32.061
ATOM     49  H   ???     1       6.715  10.805 -32.107
ATOM     50  H   ???     1       6.078  12.197 -31.142
ATOM     51  N   ???     1       4.601  11.039 -32.119
ATOM     52  H   ???     1       4.025  11.163 -32.957
ATOM     53  C   ???     1       4.033  10.339 -31.131
ATOM     54  N   ???     1       4.703  10.126 -29.993
ATOM     55  H   ???     1       5.681  10.400 -29.913
ATOM     56  H   ???     1       4.332   9.531 -29.255
ATOM     57  N   ???     1       2.785   9.887 -31.298
ATOM     58  H   ???     1       2.284  10.143 -32.154
ATOM     59  H   ???     1       2.234   9.549 -30.518
ATOM     60  H   ???     1       8.416   7.468 -28.158
ATOM     61  C   ???     1       9.383   7.521 -28.667
ATOM     62  N   ???     1       9.661   6.715 -29.749
ATOM     63  C   ???     1      10.959   6.845 -30.004
ATOM     64  H   ???     1      11.507   6.357 -30.809
ATOM     65  N   ???     1      11.522   7.710 -29.134
ATOM     66  H   ???     1      12.517   7.978 -29.152
ATOM     67  C   ???     1      10.544   8.146 -28.267
ATOM     68  H   ???     1      10.754   8.889 -27.501
ATOM     69  O   ???     1      10.678   5.259 -25.596
ATOM     70  C   ???     1      10.954   4.617 -26.659
ATOM     71  O   ???     1      12.086   4.382 -27.125
ATOM     72  C   ???     1       9.738   4.174 -27.483
ATOM     73  H   ???     1       8.862   4.077 -26.824
ATOM     74  H   ???     1       9.534   5.030 -28.142
ATOM     75  C   ???     1       9.875   2.948 -28.377
ATOM     76  H   ???     1      10.857   2.963 -28.869
ATOM     77  H   ???     1       9.839   2.011 -27.793
ATOM     78  C   ???     1       8.825   2.970 -29.517
ATOM     79  O   ???     1       9.338   3.862 -30.509
ATOM     80  H   ???     1       9.913   3.213 -31.156
ATOM     81  C   ???     1       7.498   3.527 -28.971
ATOM     82  O   ???     1       7.183   4.705 -29.337
ATOM     83  O   ???     1       6.803   2.869 -28.180
ATOM     84  C   ???     1       8.577   1.613 -30.194
ATOM     85  H   ???     1       8.268   0.853 -29.463
ATOM     86  H   ???     1       7.748   1.749 -30.915
ATOM     87  C   ???     1       9.789   1.100 -30.996
ATOM     88  O   ???     1      10.463   2.001 -31.616
ATOM     89  O   ???     1       9.992  -0.119 -31.010
ATOM     90 FE   ???     1       7.124   8.659 -35.637
ATOM     91 MO   ???     1       8.182   5.598 -31.078
ATOM     92 FE   ???     1       5.377   7.598 -37.497
ATOM     93 FE   ???     1       5.336   6.119 -31.795
ATOM     94 FE   ???     1       6.987   5.852 -36.216
ATOM     95 FE   ???     1       7.975   5.106 -33.724
ATOM     96 FE   ???     1       8.185   7.865 -33.266
ATOM     97 FE   ???     1       4.348   6.922 -34.956
ATOM     98  C   ???     1       6.754   6.777 -34.352
ATOM     99  S   ???     1       7.785   7.503 -37.571
ATOM    100  S   ???     1       9.792   6.114 -32.848
ATOM    101  S   ???     1       4.748   5.406 -36.696
ATOM    102  S   ???     1       8.289   3.776 -35.702
ATOM    103  S   ???     1       8.573   9.899 -34.344
ATOM    104  S   ???     1       6.544   4.096 -32.186
ATOM    105  S   ???     1       4.774   9.098 -35.831
ATOM    106  S   ???     1       6.925   7.718 -31.147
ATOM    107  S   ???     1       3.385   6.512 -32.919
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ATOM    108  H   ???     1       6.125   5.893 -34.075
ATOM    109  H   ???     1       9.558   4.136 -36.039
ATOM    110  H   ???     1       6.207   7.593 -33.824
ATOM    111  O   ???     1       4.797   5.802 -29.449
ATOM    112  H   ???     1       5.665   5.317 -29.311
ATOM    113  H   ???     1       5.026   6.748 -29.350
ATOM    114  O   ???     1       1.039   8.399 -34.241
ATOM    115  H   ???     1       1.839   7.988 -33.846
ATOM    116  H   ???     1       0.504   8.694 -33.454
END
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Best E_3 structure optimised with theTPSS functional. The protons bind to S2B, terminally to Fe5 and bridging between Fe2 and Fe6.

```
REMARK Energy =  -16164.723275 15325.160075
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E3/S2bF26F5
ATOM      1  H   ???     1       3.500   2.240 -29.686
ATOM      2  C   ???     1       3.907   2.093 -30.705
ATOM      3  H   ???     1       5.012   2.111 -30.640
ATOM      4  H   ???     1       3.593   1.109 -31.091
ATOM      5  N   ???     1       3.486   3.146 -31.619
ATOM      6  H   ???     1       4.009   4.033 -31.545
ATOM      7  C   ???     1       2.851   2.926 -32.782
ATOM      8  N   ???     1       1.985   1.884 -32.904
ATOM      9  H   ???     1       1.829   1.265 -32.106
ATOM     10  H   ???     1       1.785   1.496 -33.837
ATOM     11  N   ???     1       3.069   3.743 -33.813
ATOM     12  H   ???     1       3.618   4.622 -33.664
ATOM     13  H   ???     1       2.426   3.764 -34.610
ATOM     14  H   ???     1       7.272   1.571 -41.613
ATOM     15  C   ???     1       7.569   2.056 -40.677
ATOM     16  N   ???     1       8.364   3.186 -40.729
ATOM     17  C   ???     1       8.448   3.614 -39.475
ATOM     18  H   ???     1       8.969   4.505 -39.122
ATOM     19  N   ???     1       7.743   2.814 -38.629
ATOM     20  H   ???     1       7.661   2.987 -37.609
ATOM     21  C   ???     1       7.163   1.811 -39.376
ATOM     22  H   ???     1       6.535   1.045 -38.923
ATOM     23  H   ???     1       2.976   9.551 -40.106
ATOM     24  C   ???     1       3.089   8.696 -39.393
ATOM     25  H   ???     1       2.351   7.919 -39.658
ATOM     26  H   ???     1       2.880   9.073 -38.377
ATOM     27  S   ???     1       4.817   8.015 -39.474
ATOM     28  H   ???     1      13.631  11.342 -31.928
ATOM     29  C   ???     1      12.716  10.652 -31.972
ATOM     30  H   ???     1      12.871   9.949 -31.130
ATOM     31  H   ???     1      11.735  11.191 -31.788
ATOM     32  C   ???     1      12.881   9.817 -33.262
ATOM     33  O   ???     1      14.015   9.621 -33.704
ATOM     34  N   ???     1      11.781   9.228 -33.790
ATOM     35  H   ???     1      10.830   9.408 -33.438
ATOM     36  C   ???     1      11.916   8.133 -34.751
ATOM     37  H   ???     1      12.842   7.587 -34.517
ATOM     38  H   ???     1      11.044   7.477 -34.583
ATOM     39  C   ???     1      12.000   8.516 -36.248
ATOM     40  O   ???     1      13.053   8.360 -36.882
ATOM     41  N   ???     1      10.836   8.971 -36.777
ATOM     42  H   ???     1      10.000   8.914 -36.178
ATOM     43  C   ???     1      10.629   9.212 -38.212
ATOM     44  H   ???     1      11.627   9.350 -38.663
ATOM     45  H   ???     1      10.174   8.305 -38.659
ATOM     46  H   ???     1       9.965  10.061 -38.478
ATOM     47  H   ???     1       6.094  12.249 -32.941
ATOM     48  C   ???     1       5.945  11.594 -32.055
ATOM     49  H   ???     1       6.671  10.757 -32.125
ATOM     50  H   ???     1       6.143  12.186 -31.139
ATOM     51  N   ???     1       4.567  11.112 -32.062
ATOM     52  H   ???     1       3.967  11.262 -32.884
ATOM     53  C   ???     1       4.018  10.371 -31.083
ATOM     54  N   ???     1       4.709  10.118 -29.962
ATOM     55  H   ???     1       5.663  10.473 -29.851
ATOM     56  H   ???     1       4.393   9.424 -29.275
ATOM     57  N   ???     1       2.762   9.916 -31.245
ATOM     58  H   ???     1       2.266  10.181 -32.107
ATOM     59  H   ???     1       2.182   9.702 -30.435
ATOM     60  H   ???     1       8.408   7.456 -28.186
ATOM     61  C   ???     1       9.355   7.487 -28.748
ATOM     62  N   ???     1       9.558   6.727 -29.891
ATOM     63  C   ???     1      10.854   6.837 -30.194
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ATOM     64  H   ???     1      11.350   6.370 -31.046
ATOM     65  N   ???     1      11.486   7.634 -29.297
ATOM     66  H   ???     1      12.493   7.875 -29.321
ATOM     67  C   ???     1      10.556   8.050 -28.365
ATOM     68  H   ???     1      10.831   8.729 -27.558
ATOM     69  O   ???     1      10.673   5.261 -25.615
ATOM     70  C   ???     1      10.953   4.624 -26.692
ATOM     71  O   ???     1      12.098   4.361 -27.135
ATOM     72  C   ???     1       9.738   4.223 -27.552
ATOM     73  H   ???     1       8.845   4.134 -26.907
ATOM     74  H   ???     1       9.560   5.088 -28.214
ATOM     75  C   ???     1       9.868   3.002 -28.463
ATOM     76  H   ???     1      10.854   3.015 -28.957
ATOM     77  H   ???     1       9.816   2.057 -27.887
ATOM     78  C   ???     1       8.803   3.037 -29.595
ATOM     79  O   ???     1       9.297   3.938 -30.603
ATOM     80  H   ???     1       9.889   3.236 -31.262
ATOM     81  C   ???     1       7.486   3.590 -29.037
ATOM     82  O   ???     1       7.134   4.744 -29.473
ATOM     83  O   ???     1       6.833   2.942 -28.186
ATOM     84  C   ???     1       8.542   1.678 -30.279
ATOM     85  H   ???     1       8.200   0.926 -29.547
ATOM     86  H   ???     1       7.729   1.835 -31.019
ATOM     87  C   ???     1       9.770   1.153 -31.044
ATOM     88  O   ???     1      10.450   2.066 -31.672
ATOM     89  O   ???     1      10.002  -0.069 -31.036
ATOM     90 FE   ???     1       7.131   8.128 -35.425
ATOM     91 MO   ???     1       8.078   5.608 -31.254
ATOM     92 FE   ???     1       5.438   7.529 -37.309
ATOM     93 FE   ???     1       5.898   6.263 -32.575
ATOM     94 FE   ???     1       6.709   5.636 -35.905
ATOM     95 FE   ???     1       8.148   7.560 -33.066
ATOM     96 FE   ???     1       7.766   5.121 -33.803
ATOM     97 FE   ???     1       4.858   6.985 -34.810
ATOM     98  C   ???     1       6.701   6.649 -34.296
ATOM     99  S   ???     1       7.703   7.142 -37.364
ATOM    100  S   ???     1       9.672   5.903 -32.992
ATOM    101  S   ???     1       4.588   5.554 -36.531
ATOM    102  S   ???     1       8.277   3.919 -35.655
ATOM    103  S   ???     1       8.464   9.465 -34.301
ATOM    104  S   ???     1       6.521   4.090 -32.257
ATOM    105  S   ???     1       5.008   9.060 -35.720
ATOM    106  S   ???     1       6.892   7.666 -31.169
ATOM    107  S   ???     1       3.737   6.701 -32.876
ATOM    108  H   ???     1       6.175   4.454 -35.053
ATOM    109  H   ???     1       9.541   4.248 -36.087
ATOM    110  H   ???     1       9.123   8.365 -32.191
ATOM    111  O   ???     1       4.530   5.548 -29.460
ATOM    112  H   ???     1       5.480   5.251 -29.502
ATOM    113  H   ???     1       4.436   6.167 -30.221
ATOM    114  O   ???     1       1.097   8.388 -34.237
ATOM    115  H   ???     1       1.947   8.026 -33.880
ATOM    116  H   ???     1       0.580   8.672 -33.427
END
```

Second best E_3 structure with theTPSS functional. The protons bind to S2B and terminally to Fe4 and Fe5.

```
REMARK Energies (QM/MM, QM+ptch) =  -16164.721512 -15325.151337
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E3/S2bF4F5
ATOM      1  H   ???     1       3.504   2.242 -29.686
ATOM      2  C   ???     1       3.918   2.100 -30.705
ATOM      3  H   ???     1       5.022   2.115 -30.628
ATOM      4  H   ???     1       3.608   1.118 -31.096
ATOM      5  N   ???     1       3.508   3.154 -31.622
ATOM      6  H   ???     1       4.024   4.045 -31.546
ATOM      7  C   ???     1       2.863   2.935 -32.780
ATOM      8  N   ???     1       1.996   1.893 -32.898
ATOM      9  H   ???     1       1.841   1.274 -32.100
ATOM     10  H   ???     1       1.793   1.506 -33.831
ATOM     11  N   ???     1       3.073   3.753 -33.812
ATOM     12  H   ???     1       3.607   4.642 -33.658
ATOM     13  H   ???     1       2.413   3.777 -34.595
ATOM     14  H   ???     1       7.269   1.572 -41.613
ATOM     15  C   ???     1       7.557   2.060 -40.676
ATOM     16  N   ???     1       8.365   3.181 -40.721
ATOM     17  C   ???     1       8.419   3.624 -39.470
ATOM     18  H   ???     1       8.943   4.511 -39.114
ATOM     19  N   ???     1       7.682   2.842 -38.634
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ATOM     20  H   ???     1       7.555   3.036 -37.619
ATOM     21  C   ???     1       7.113   1.837 -39.384
ATOM     22  H   ???     1       6.463   1.083 -38.939
ATOM     23  H   ???     1       2.971   9.553 -40.105
ATOM     24  C   ???     1       3.073   8.698 -39.391
ATOM     25  H   ???     1       2.337   7.923 -39.665
ATOM     26  H   ???     1       2.849   9.077 -38.379
ATOM     27  S   ???     1       4.796   8.012 -39.438
ATOM     28  H   ???     1      13.632  11.340 -31.927
ATOM     29  C   ???     1      12.717  10.649 -31.969
ATOM     30  H   ???     1      12.870   9.949 -31.124
ATOM     31  H   ???     1      11.736  11.190 -31.787
ATOM     32  C   ???     1      12.877   9.811 -33.256
ATOM     33  O   ???     1      14.005   9.636 -33.722
ATOM     34  N   ???     1      11.778   9.203 -33.766
ATOM     35  H   ???     1      10.844   9.322 -33.353
ATOM     36  C   ???     1      11.919   8.122 -34.743
ATOM     37  H   ???     1      12.850   7.580 -34.523
ATOM     38  H   ???     1      11.056   7.455 -34.578
ATOM     39  C   ???     1      11.992   8.520 -36.237
ATOM     40  O   ???     1      13.041   8.364 -36.877
ATOM     41  N   ???     1      10.826   8.974 -36.765
ATOM     42  H   ???     1       9.990   8.933 -36.168
ATOM     43  C   ???     1      10.627   9.214 -38.203
ATOM     44  H   ???     1      11.628   9.350 -38.648
ATOM     45  H   ???     1      10.175   8.306 -38.652
ATOM     46  H   ???     1       9.964  10.062 -38.475
ATOM     47  H   ???     1       6.094  12.252 -32.939
ATOM     48  C   ???     1       5.944  11.601 -32.050
ATOM     49  H   ???     1       6.678  10.771 -32.109
ATOM     50  H   ???     1       6.129  12.201 -31.136
ATOM     51  N   ???     1       4.570  11.107 -32.066
ATOM     52  H   ???     1       3.972  11.258 -32.890
ATOM     53  C   ???     1       4.020  10.365 -31.089
ATOM     54  N   ???     1       4.706  10.117 -29.964
ATOM     55  H   ???     1       5.667  10.456 -29.862
ATOM     56  H   ???     1       4.396   9.413 -29.285
ATOM     57  N   ???     1       2.766   9.907 -31.256
ATOM     58  H   ???     1       2.271  10.170 -32.119
ATOM     59  H   ???     1       2.188   9.673 -30.451
ATOM     60  H   ???     1       8.407   7.458 -28.189
ATOM     61  C   ???     1       9.351   7.495 -28.755
ATOM     62  N   ???     1       9.549   6.748 -29.907
ATOM     63  C   ???     1      10.843   6.859 -30.212
ATOM     64  H   ???     1      11.336   6.401 -31.072
ATOM     65  N   ???     1      11.481   7.645 -29.309
ATOM     66  H   ???     1      12.488   7.884 -29.333
ATOM     67  C   ???     1      10.554   8.055 -28.370
ATOM     68  H   ???     1      10.830   8.731 -27.561
ATOM     69  O   ???     1      10.667   5.255 -25.624
ATOM     70  C   ???     1      10.945   4.622 -26.705
ATOM     71  O   ???     1      12.091   4.348 -27.141
ATOM     72  C   ???     1       9.730   4.241 -27.575
ATOM     73  H   ???     1       8.836   4.144 -26.932
ATOM     74  H   ???     1       9.556   5.117 -28.223
ATOM     75  C   ???     1       9.853   3.036 -28.509
ATOM     76  H   ???     1      10.843   3.052 -28.995
ATOM     77  H   ???     1       9.791   2.082 -27.946
ATOM     78  C   ???     1       8.789   3.095 -29.645
ATOM     79  O   ???     1       9.272   3.980 -30.650
ATOM     80  H   ???     1       9.947   3.126 -31.381
ATOM     81  C   ???     1       7.464   3.618 -29.072
ATOM     82  O   ???     1       7.077   4.749 -29.537
ATOM     83  O   ???     1       6.841   2.965 -28.200
ATOM     84  C   ???     1       8.510   1.728 -30.321
ATOM     85  H   ???     1       8.151   0.977 -29.597
ATOM     86  H   ???     1       7.711   1.901 -31.074
ATOM     87  C   ???     1       9.730   1.190 -31.064
ATOM     88  O   ???     1      10.419   2.115 -31.708
ATOM     89  O   ???     1      10.004  -0.014 -31.062
ATOM     90 FE   ???     1       7.051   8.471 -35.420
ATOM     91 MO   ???     1       8.065   5.636 -31.291
ATOM     92 FE   ???     1       5.373   7.561 -37.267
ATOM     93 FE   ???     1       5.864   6.321 -32.572
ATOM     94 FE   ???     1       6.818   5.990 -35.869
ATOM     95 FE   ???     1       8.146   7.704 -33.069
ATOM     96 FE   ???     1       7.738   5.318 -33.866
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ATOM     97 FE   ???     1       4.870   7.068 -34.764
ATOM     98  C   ???     1       6.716   6.850 -34.228
ATOM     99  S   ???     1       7.646   7.378 -37.332
ATOM    100  S   ???     1       9.647   5.983 -33.040
ATOM    101  S   ???     1       4.741   5.535 -36.435
ATOM    102  S   ???     1       8.007   4.072 -35.697
ATOM    103  S   ???     1       8.475   9.589 -34.186
ATOM    104  S   ???     1       6.538   4.167 -32.420
ATOM    105  S   ???     1       4.814   9.095 -35.710
ATOM    106  S   ???     1       6.874   7.690 -31.153
ATOM    107  S   ???     1       3.690   6.700 -32.889
ATOM    108  H   ???     1       7.329   9.747 -36.262
ATOM    109  H   ???     1       9.271   4.312 -36.194
ATOM    110  H   ???     1       9.157   8.435 -32.132
ATOM    111  O   ???     1       4.495   5.546 -29.478
ATOM    112  H   ???     1       5.448   5.256 -29.520
ATOM    113  H   ???     1       4.403   6.167 -30.238
ATOM    114  O   ???     1       1.087   8.387 -34.247
ATOM    115  H   ???     1       1.940   8.023 -33.898
ATOM    116  H   ???     1       0.578   8.672 -33.433
END
```

Best E_4 structure optimised with theB3LYP functional. One of the protons is on S2B and the other three are all on the carbide ion.

```
REMARK Energies (QM/MM, QM+ptch) = -16161.846309 -15322.290188
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E4/S2bC123
ATOM      1  H   ???     1       3.492   2.230 -29.683
ATOM      2  C   ???     1       3.887   2.063 -30.701
ATOM      3  H   ???     1       4.987   2.150 -30.656
ATOM      4  H   ???     1       3.633   1.043 -31.024
ATOM      5  N   ???     1       3.382   3.026 -31.658
ATOM      6  H   ???     1       3.870   3.925 -31.698
ATOM      7  C   ???     1       2.715   2.702 -32.775
ATOM      8  N   ???     1       1.894   1.632 -32.796
ATOM      9  H   ???     1       1.741   1.082 -31.954
ATOM     10  H   ???     1       1.655   1.212 -33.700
ATOM     11  N   ???     1       2.881   3.440 -33.864
ATOM     12  H   ???     1       3.350   4.371 -33.768
ATOM     13  H   ???     1       2.227   3.363 -34.643
ATOM     14  H   ???     1       7.269   1.569 -41.622
ATOM     15  C   ???     1       7.560   2.054 -40.694
ATOM     16  N   ???     1       8.352   3.181 -40.728
ATOM     17  C   ???     1       8.408   3.610 -39.479
ATOM     18  H   ???     1       8.914   4.504 -39.118
ATOM     19  N   ???     1       7.686   2.809 -38.656
ATOM     20  H   ???     1       7.602   2.954 -37.643
ATOM     21  C   ???     1       7.128   1.810 -39.408
ATOM     22  H   ???     1       6.487   1.046 -38.975
ATOM     23  H   ???     1       2.970   9.556 -40.132
ATOM     24  C   ???     1       3.081   8.692 -39.460
ATOM     25  H   ???     1       2.330   7.930 -39.723
ATOM     26  H   ???     1       2.922   9.034 -38.425
ATOM     27  S   ???     1       4.811   8.073 -39.685
ATOM     28  H   ???     1      13.630  11.348 -31.930
ATOM     29  C   ???     1      12.721  10.661 -31.982
ATOM     30  H   ???     1      12.875   9.953 -31.147
ATOM     31  H   ???     1      11.738  11.193 -31.792
ATOM     32  C   ???     1      12.907   9.827 -33.267
ATOM     33  O   ???     1      14.044   9.615 -33.666
ATOM     34  N   ???     1      11.819   9.256 -33.820
ATOM     35  H   ???     1      10.864   9.540 -33.581
ATOM     36  C   ???     1      11.956   8.162 -34.771
ATOM     37  H   ???     1      12.866   7.604 -34.522
ATOM     38  H   ???     1      11.084   7.508 -34.620
ATOM     39  C   ???     1      12.058   8.531 -36.265
ATOM     40  O   ???     1      13.097   8.328 -36.889
ATOM     41  N   ???     1      10.921   9.028 -36.793
ATOM     42  H   ???     1      10.095   9.019 -36.194
ATOM     43  C   ???     1      10.711   9.271 -38.221
ATOM     44  H   ???     1      11.694   9.470 -38.677
ATOM     45  H   ???     1      10.308   8.357 -38.689
ATOM     46  H   ???     1      10.004  10.089 -38.480
ATOM     47  H   ???     1       6.092  12.251 -32.942
ATOM     48  C   ???     1       5.939  11.597 -32.061
ATOM     49  H   ???     1       6.704  10.799 -32.110
ATOM     50  H   ???     1       6.085  12.199 -31.145
ATOM     51  N   ???     1       4.592  11.055 -32.113
ATOM     52  H   ???     1       4.020  11.171 -32.955
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ATOM     53  C   ???     1       4.028  10.343 -31.131
ATOM     54  N   ???     1       4.695  10.133 -29.990
ATOM     55  H   ???     1       5.646  10.478 -29.872
ATOM     56  H   ???     1       4.331   9.524 -29.259
ATOM     57  N   ???     1       2.790   9.865 -31.310
ATOM     58  H   ???     1       2.301  10.104 -32.179
ATOM     59  H   ???     1       2.219   9.581 -30.523
ATOM     60  H   ???     1       8.417   7.472 -28.156
ATOM     61  C   ???     1       9.386   7.533 -28.660
ATOM     62  N   ???     1       9.673   6.738 -29.747
ATOM     63  C   ???     1      10.973   6.877 -29.996
ATOM     64  H   ???     1      11.524   6.395 -30.804
ATOM     65  N   ???     1      11.526   7.737 -29.118
ATOM     66  H   ???     1      12.521   8.007 -29.128
ATOM     67  C   ???     1      10.542   8.161 -28.251
ATOM     68  H   ???     1      10.744   8.899 -27.478
ATOM     69  O   ???     1      10.695   5.270 -25.575
ATOM     70  C   ???     1      10.973   4.628 -26.636
ATOM     71  O   ???     1      12.105   4.389 -27.101
ATOM     72  C   ???     1       9.761   4.188 -27.461
ATOM     73  H   ???     1       8.873   4.126 -26.812
ATOM     74  H   ???     1       9.583   5.026 -28.149
ATOM     75  C   ???     1       9.894   2.936 -28.313
ATOM     76  H   ???     1      10.878   2.931 -28.799
ATOM     77  H   ???     1       9.847   2.017 -27.702
ATOM     78  C   ???     1       8.855   2.951 -29.458
ATOM     79  O   ???     1       9.388   3.856 -30.428
ATOM     80  H   ???     1       9.940   3.198 -31.113
ATOM     81  C   ???     1       7.522   3.510 -28.931
ATOM     82  O   ???     1       7.237   4.703 -29.275
ATOM     83  O   ???     1       6.798   2.850 -28.171
ATOM     84  C   ???     1       8.619   1.595 -30.140
ATOM     85  H   ???     1       8.365   0.819 -29.404
ATOM     86  H   ???     1       7.754   1.709 -30.820
ATOM     87  C   ???     1       9.796   1.116 -31.003
ATOM     88  O   ???     1      10.422   2.041 -31.652
ATOM     89  O   ???     1      10.020  -0.095 -31.049
ATOM     90 FE   ???     1       7.185   8.902 -35.884
ATOM     91 MO   ???     1       8.214   5.558 -31.026
ATOM     92 FE   ???     1       4.733   6.801 -35.040
ATOM     93 FE   ???     1       5.400   5.974 -31.916
ATOM     94 FE   ???     1       8.333   4.411 -33.486
ATOM     95 FE   ???     1       8.349   7.866 -32.944
ATOM     96 FE   ???     1       6.983   5.734 -36.441
ATOM     97 FE   ???     1       5.387   7.549 -37.593
ATOM     98  C   ???     1       6.838   6.450 -34.382
ATOM     99  S   ???     1       7.848   7.522 -37.635
ATOM    100  S   ???     1       9.846   5.991 -32.799
ATOM    101  S   ???     1       4.774   5.333 -36.911
ATOM    102  S   ???     1       8.360   3.739 -35.737
ATOM    103  S   ???     1       8.558   9.757 -34.227
ATOM    104  S   ???     1       6.629   3.902 -32.024
ATOM    105  S   ???     1       4.862   9.065 -35.791
ATOM    106  S   ???     1       6.870   7.618 -31.104
ATOM    107  S   ???     1       3.517   6.404 -33.042
ATOM    108  H   ???     1       6.687   5.576 -33.740
ATOM    109  H   ???     1       9.640   3.977 -36.138
ATOM    110  H   ???     1       7.889   6.572 -34.693
ATOM    111  H   ???     1       6.514   7.357 -33.845
ATOM    112  O   ???     1       4.769   5.686 -29.425
ATOM    113  H   ???     1       5.658   5.257 -29.291
ATOM    114  H   ???     1       4.960   6.644 -29.457
ATOM    115  O   ???     1       1.083   8.389 -34.226
ATOM    116  H   ???     1       1.885   7.951 -33.866
ATOM    117  H   ???     1       0.558   8.670 -33.429
END
```

Second best E_4 structure optimised with theB3LYP functional. Two protons bind to S2B and S2A and the other two bind to the carbide ion.
Bs30

```
REMARK Energies (QM/MM, QM+ptch) = -16161.838658 -15322.281763
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E4/S2bS2aC12/Bs30
ATOM      1  H   ???     1       3.496   2.227 -29.682
ATOM      2  C   ???     1       3.897   2.052 -30.697
ATOM      3  H   ???     1       4.998   2.120 -30.643
ATOM      4  H   ???     1       3.630   1.036 -31.023
ATOM      5  N   ???     1       3.426   3.030 -31.656
ATOM      6  H   ???     1       3.994   3.880 -31.715
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ATOM      7  C   ???     1       2.746   2.733 -32.771
ATOM      8  N   ???     1       1.915   1.669 -32.808
ATOM      9  H   ???     1       1.800   1.079 -31.989
ATOM     10  H   ???     1       1.664   1.274 -33.719
ATOM     11  N   ???     1       2.903   3.500 -33.845
ATOM     12  H   ???     1       3.296   4.465 -33.712
ATOM     13  H   ???     1       2.246   3.419 -34.621
ATOM     14  H   ???     1       7.270   1.567 -41.626
ATOM     15  C   ???     1       7.566   2.049 -40.702
ATOM     16  N   ???     1       8.367   3.168 -40.739
ATOM     17  C   ???     1       8.452   3.576 -39.485
ATOM     18  H   ???     1       8.987   4.451 -39.117
ATOM     19  N   ???     1       7.739   2.774 -38.659
ATOM     20  H   ???     1       7.688   2.916 -37.640
ATOM     21  C   ???     1       7.156   1.791 -39.412
ATOM     22  H   ???     1       6.518   1.026 -38.976
ATOM     23  H   ???     1       2.970   9.557 -40.119
ATOM     24  C   ???     1       3.078   8.702 -39.428
ATOM     25  H   ???     1       2.340   7.932 -39.701
ATOM     26  H   ???     1       2.887   9.047 -38.400
ATOM     27  S   ???     1       4.791   8.023 -39.591
ATOM     28  H   ???     1      13.630  11.348 -31.929
ATOM     29  C   ???     1      12.723  10.661 -31.982
ATOM     30  H   ???     1      12.876   9.953 -31.146
ATOM     31  H   ???     1      11.739  11.193 -31.792
ATOM     32  C   ???     1      12.914   9.830 -33.267
ATOM     33  O   ???     1      14.053   9.621 -33.665
ATOM     34  N   ???     1      11.827   9.262 -33.824
ATOM     35  H   ???     1      10.874   9.531 -33.561
ATOM     36  C   ???     1      11.960   8.165 -34.772
ATOM     37  H   ???     1      12.870   7.606 -34.525
ATOM     38  H   ???     1      11.088   7.513 -34.618
ATOM     39  C   ???     1      12.056   8.535 -36.263
ATOM     40  O   ???     1      13.091   8.333 -36.895
ATOM     41  N   ???     1      10.918   9.037 -36.789
ATOM     42  H   ???     1      10.087   9.009 -36.200
ATOM     43  C   ???     1      10.717   9.278 -38.218
ATOM     44  H   ???     1      11.701   9.484 -38.668
ATOM     45  H   ???     1      10.330   8.359 -38.693
ATOM     46  H   ???     1      10.007  10.092 -38.479
ATOM     47  H   ???     1       6.092  12.252 -32.941
ATOM     48  C   ???     1       5.939  11.600 -32.059
ATOM     49  H   ???     1       6.707  10.806 -32.105
ATOM     50  H   ???     1       6.079  12.203 -31.143
ATOM     51  N   ???     1       4.594  11.050 -32.113
ATOM     52  H   ???     1       4.034  11.143 -32.965
ATOM     53  C   ???     1       4.027  10.350 -31.125
ATOM     54  N   ???     1       4.688  10.156 -29.978
ATOM     55  H   ???     1       5.655  10.461 -29.879
ATOM     56  H   ???     1       4.322   9.550 -29.245
ATOM     57  N   ???     1       2.788   9.876 -31.301
ATOM     58  H   ???     1       2.297  10.110 -32.169
ATOM     59  H   ???     1       2.225   9.565 -30.518
ATOM     60  H   ???     1       8.416   7.471 -28.160
ATOM     61  C   ???     1       9.382   7.531 -28.673
ATOM     62  N   ???     1       9.645   6.749 -29.777
ATOM     63  C   ???     1      10.944   6.873 -30.038
ATOM     64  H   ???     1      11.478   6.397 -30.859
ATOM     65  N   ???     1      11.519   7.714 -29.152
ATOM     66  H   ???     1      12.517   7.971 -29.165
ATOM     67  C   ???     1      10.549   8.140 -28.270
ATOM     68  H   ???     1      10.771   8.863 -27.489
ATOM     69  O   ???     1      10.677   5.261 -25.599
ATOM     70  C   ???     1      10.951   4.626 -26.668
ATOM     71  O   ???     1      12.084   4.382 -27.127
ATOM     72  C   ???     1       9.735   4.203 -27.503
ATOM     73  H   ???     1       8.852   4.124 -26.851
ATOM     74  H   ???     1       9.551   5.058 -28.169
ATOM     75  C   ???     1       9.862   2.972 -28.391
ATOM     76  H   ???     1      10.843   2.976 -28.884
ATOM     77  H   ???     1       9.819   2.040 -27.800
ATOM     78  C   ???     1       8.807   2.990 -29.526
ATOM     79  O   ???     1       9.307   3.893 -30.516
ATOM     80  H   ???     1       9.883   3.250 -31.170
ATOM     81  C   ???     1       7.477   3.534 -28.976
ATOM     82  O   ???     1       7.149   4.705 -29.349
ATOM     83  O   ???     1       6.797   2.871 -28.174
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ATOM     84  C   ???     1       8.571   1.633 -30.206
ATOM     85  H   ???     1       8.268   0.871 -29.474
ATOM     86  H   ???     1       7.740   1.762 -30.925
ATOM     87  C   ???     1       9.786   1.130 -31.009
ATOM     88  O   ???     1      10.449   2.041 -31.629
ATOM     89  O   ???     1      10.001  -0.087 -31.025
ATOM     90 FE   ???     1       5.841   8.528 -37.593
ATOM     91 MO   ???     1       8.147   5.634 -31.063
ATOM     92 FE   ???     1       7.125   8.403 -35.265
ATOM     93 FE   ???     1       5.291   6.067 -31.904
ATOM     94 FE   ???     1       7.043   5.866 -36.289
ATOM     95 FE   ???     1       8.508   8.041 -32.660
ATOM     96 FE   ???     1       7.875   5.062 -33.808
ATOM     97 FE   ???     1       4.474   7.071 -35.104
ATOM     98  C   ???     1       6.528   6.485 -34.415
ATOM     99  S   ???     1       7.949   7.609 -37.441
ATOM    100  S   ???     1       9.753   6.106 -32.881
ATOM    101  S   ???     1       4.761   5.223 -36.824
ATOM    102  S   ???     1       8.306   3.764 -35.793
ATOM    103  S   ???     1       8.570   9.792 -34.106
ATOM    104  S   ???     1       6.516   4.067 -32.159
ATOM    105  S   ???     1       4.834   9.289 -35.653
ATOM    106  S   ???     1       6.808   7.705 -31.087
ATOM    107  S   ???     1       3.364   6.517 -33.081
ATOM    108  H   ???     1       5.700   5.769 -34.225
ATOM    109  H   ???     1       9.606   4.106 -36.007
ATOM    110  H   ???     1       4.587   6.035 -37.908
ATOM    111  H   ???     1       6.597   7.129 -33.524
ATOM    112  O   ???     1       4.735   5.764 -29.466
ATOM    113  H   ???     1       5.610   5.293 -29.347
ATOM    114  H   ???     1       4.956   6.713 -29.389
ATOM    115  O   ???     1       1.025   8.403 -34.261
ATOM    116  H   ???     1       1.822   7.964 -33.885
ATOM    117  H   ???     1       0.506   8.696 -33.465
END
```

Best E_4 structure optimised with theTPSS functional. The protons are on S2B, bridging Fe2 and Fe6, and terminally on Fe5 and Fe4.

```
REMARK Energies (QM/MM, QM+ptch, MM3) = -16165.297723 -15325.728172
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E4/S2bF26F4F5
ATOM      1  H   ???     1       3.507   2.242 -29.687
ATOM      2  C   ???     1       3.928   2.098 -30.704
ATOM      3  H   ???     1       5.031   2.100 -30.616
ATOM      4  H   ???     1       3.613   1.119 -31.098
ATOM      5  N   ???     1       3.537   3.155 -31.626
ATOM      6  H   ???     1       4.038   4.052 -31.529
ATOM      7  C   ???     1       2.883   2.945 -32.782
ATOM      8  N   ???     1       2.012   1.906 -32.900
ATOM      9  H   ???     1       1.858   1.285 -32.104
ATOM     10  H   ???     1       1.804   1.522 -33.832
ATOM     11  N   ???     1       3.089   3.766 -33.813
ATOM     12  H   ???     1       3.634   4.650 -33.666
ATOM     13  H   ???     1       2.427   3.790 -34.594
ATOM     14  H   ???     1       7.267   1.574 -41.616
ATOM     15  C   ???     1       7.552   2.068 -40.682
ATOM     16  N   ???     1       8.358   3.190 -40.732
ATOM     17  C   ???     1       8.383   3.657 -39.489
ATOM     18  H   ???     1       8.899   4.551 -39.138
ATOM     19  N   ???     1       7.628   2.892 -38.655
ATOM     20  H   ???     1       7.485   3.102 -37.644
ATOM     21  C   ???     1       7.078   1.870 -39.396
ATOM     22  H   ???     1       6.424   1.121 -38.950
ATOM     23  H   ???     1       2.970   9.553 -40.109
ATOM     24  C   ???     1       3.073   8.697 -39.399
ATOM     25  H   ???     1       2.341   7.918 -39.675
ATOM     26  H   ???     1       2.855   9.067 -38.383
ATOM     27  S   ???     1       4.803   8.032 -39.473
ATOM     28  H   ???     1      13.631  11.341 -31.927
ATOM     29  C   ???     1      12.718  10.650 -31.970
ATOM     30  H   ???     1      12.872   9.948 -31.127
ATOM     31  H   ???     1      11.736  11.190 -31.788
ATOM     32  C   ???     1      12.888   9.815 -33.258
ATOM     33  O   ???     1      14.022   9.639 -33.710
ATOM     34  N   ???     1      11.796   9.209 -33.783
ATOM     35  H   ???     1      10.853   9.346 -33.394
ATOM     36  C   ???     1      11.950   8.132 -34.760
ATOM     37  H   ???     1      12.885   7.600 -34.536
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ATOM     38  H   ???     1      11.095   7.453 -34.599
ATOM     39  C   ???     1      12.017   8.525 -36.252
ATOM     40  O   ???     1      13.058   8.354 -36.901
ATOM     41  N   ???     1      10.853   8.992 -36.774
ATOM     42  H   ???     1      10.017   8.953 -36.176
ATOM     43  C   ???     1      10.653   9.233 -38.210
ATOM     44  H   ???     1      11.652   9.390 -38.652
ATOM     45  H   ???     1      10.223   8.319 -38.668
ATOM     46  H   ???     1       9.976  10.072 -38.477
ATOM     47  H   ???     1       6.093  12.253 -32.939
ATOM     48  C   ???     1       5.943  11.604 -32.050
ATOM     49  H   ???     1       6.678  10.774 -32.107
ATOM     50  H   ???     1       6.127  12.205 -31.136
ATOM     51  N   ???     1       4.570  11.109 -32.065
ATOM     52  H   ???     1       3.971  11.260 -32.889
ATOM     53  C   ???     1       4.019  10.370 -31.087
ATOM     54  N   ???     1       4.705  10.125 -29.961
ATOM     55  H   ???     1       5.659  10.481 -29.849
ATOM     56  H   ???     1       4.392   9.428 -29.277
ATOM     57  N   ???     1       2.765   9.907 -31.254
ATOM     58  H   ???     1       2.273  10.174 -32.118
ATOM     59  H   ???     1       2.179   9.707 -30.444
ATOM     60  H   ???     1       8.406   7.463 -28.177
ATOM     61  C   ???     1       9.356   7.509 -28.724
ATOM     62  N   ???     1       9.588   6.745 -29.856
ATOM     63  C   ???     1      10.892   6.859 -30.124
ATOM     64  H   ???     1      11.417   6.394 -30.960
ATOM     65  N   ???     1      11.497   7.668 -29.221
ATOM     66  H   ???     1      12.502   7.916 -29.236
ATOM     67  C   ???     1      10.542   8.087 -28.315
ATOM     68  H   ???     1      10.788   8.785 -27.515
ATOM     69  O   ???     1      10.670   5.258 -25.614
ATOM     70  C   ???     1      10.952   4.623 -26.692
ATOM     71  O   ???     1      12.098   4.364 -27.135
ATOM     72  C   ???     1       9.738   4.220 -27.553
ATOM     73  H   ???     1       8.851   4.105 -26.906
ATOM     74  H   ???     1       9.544   5.098 -28.195
ATOM     75  C   ???     1       9.881   3.020 -28.491
ATOM     76  H   ???     1      10.873   3.044 -28.971
ATOM     77  H   ???     1       9.822   2.063 -27.936
ATOM     78  C   ???     1       8.828   3.072 -29.633
ATOM     79  O   ???     1       9.338   3.976 -30.636
ATOM     80  H   ???     1       9.916   3.280 -31.286
ATOM     81  C   ???     1       7.506   3.621 -29.088
ATOM     82  O   ???     1       7.126   4.749 -29.570
ATOM     83  O   ???     1       6.870   2.984 -28.214
ATOM     84  C   ???     1       8.557   1.716 -30.320
ATOM     85  H   ???     1       8.195   0.974 -29.589
ATOM     86  H   ???     1       7.757   1.881 -31.072
ATOM     87  C   ???     1       9.788   1.172 -31.067
ATOM     88  O   ???     1      10.479   2.076 -31.692
ATOM     89  O   ???     1      10.009  -0.052 -31.044
ATOM     90 FE   ???     1       5.931   6.293 -32.618
ATOM     91 MO   ???     1       8.131   5.671 -31.295
ATOM     92 FE   ???     1       5.447   7.634 -37.320
ATOM     93 FE   ???     1       7.020   8.638 -35.354
ATOM     94 FE   ???     1       6.999   6.128 -35.901
ATOM     95 FE   ???     1       7.969   5.404 -33.893
ATOM     96 FE   ???     1       8.145   7.751 -33.010
ATOM     97 FE   ???     1       4.951   7.107 -34.825
ATOM     98  C   ???     1       6.746   6.923 -34.224
ATOM     99  S   ???     1       7.692   7.667 -37.350
ATOM    100  S   ???     1       9.789   6.169 -32.921
ATOM    101  S   ???     1       4.874   5.581 -36.521
ATOM    102  S   ???     1       8.011   3.913 -35.684
ATOM    103  S   ???     1       8.509   9.640 -34.111
ATOM    104  S   ???     1       6.695   4.175 -32.492
ATOM    105  S   ???     1       4.784   9.139 -35.733
ATOM    106  S   ???     1       6.853   7.657 -31.135
ATOM    107  S   ???     1       3.773   6.706 -32.931
ATOM    108  H   ???     1       9.024   8.541 -32.013
ATOM    109  H   ???     1       9.271   4.117 -36.176
ATOM    110  H   ???     1       8.563   6.161 -35.234
ATOM    111  H   ???     1       7.286   9.953 -36.124
ATOM    112  O   ???     1       4.526   5.520 -29.508
ATOM    113  H   ???     1       5.482   5.240 -29.542
ATOM    114  H   ???     1       4.444   6.160 -30.255
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ATOM    115  O   ???     1       1.096   8.385 -34.238
ATOM    116  H   ???     1       1.951   8.029 -33.886
ATOM    117  H   ???     1       0.583   8.671 -33.426
END
```

Second best E_4 structure optimised with theTPSS functional. The protons are on S2B, bridging Fe2 and Fe6, and terminally on Fe5 and Fe6.

```
REMARK Energies (QM/MM, QM+ptch) = -16165.296978 -15325.726903
REMARK /pfs/nobackup/home/l/lili/DFT/Def2-SVP/E4/S2bF26F5F6
ATOM      1  H   ???     1       3.508   2.241 -29.686
ATOM      2  C   ???     1       3.933   2.096 -30.702
ATOM      3  H   ???     1       5.036   2.123 -30.614
ATOM      4  H   ???     1       3.639   1.106 -31.085
ATOM      5  N   ???     1       3.522   3.130 -31.640
ATOM      6  H   ???     1       4.029   4.028 -31.585
ATOM      7  C   ???     1       2.851   2.887 -32.778
ATOM      8  N   ???     1       1.981   1.843 -32.857
ATOM      9  H   ???     1       1.837   1.241 -32.045
ATOM     10  H   ???     1       1.768   1.438 -33.780
ATOM     11  N   ???     1       3.039   3.679 -33.834
ATOM     12  H   ???     1       3.573   4.576 -33.712
ATOM     13  H   ???     1       2.362   3.681 -34.602
ATOM     14  H   ???     1       7.264   1.575 -41.619
ATOM     15  C   ???     1       7.543   2.071 -40.688
ATOM     16  N   ???     1       8.347   3.196 -40.734
ATOM     17  C   ???     1       8.332   3.685 -39.499
ATOM     18  H   ???     1       8.830   4.589 -39.146
ATOM     19  N   ???     1       7.553   2.930 -38.678
ATOM     20  H   ???     1       7.361   3.157 -37.683
ATOM     21  C   ???     1       7.030   1.893 -39.416
ATOM     22  H   ???     1       6.366   1.148 -38.976
ATOM     23  H   ???     1       2.972   9.552 -40.111
ATOM     24  C   ???     1       3.080   8.694 -39.407
ATOM     25  H   ???     1       2.342   7.918 -39.674
ATOM     26  H   ???     1       2.886   9.058 -38.383
ATOM     27  S   ???     1       4.810   8.031 -39.521
ATOM     28  H   ???     1      13.630  11.341 -31.928
ATOM     29  C   ???     1      12.714  10.651 -31.973
ATOM     30  H   ???     1      12.870   9.946 -31.132
ATOM     31  H   ???     1      11.734  11.191 -31.788
ATOM     32  C   ???     1      12.873   9.820 -33.264
ATOM     33  O   ???     1      14.005   9.629 -33.713
ATOM     34  N   ???     1      11.774   9.226 -33.797
ATOM     35  H   ???     1      10.827   9.380 -33.429
ATOM     36  C   ???     1      11.941   8.141 -34.766
ATOM     37  H   ???     1      12.879   7.619 -34.532
ATOM     38  H   ???     1      11.091   7.456 -34.609
ATOM     39  C   ???     1      12.012   8.525 -36.260
ATOM     40  O   ???     1      13.055   8.352 -36.906
ATOM     41  N   ???     1      10.848   8.987 -36.781
ATOM     42  H   ???     1      10.014   8.965 -36.176
ATOM     43  C   ???     1      10.647   9.230 -38.215
ATOM     44  H   ???     1      11.646   9.384 -38.660
ATOM     45  H   ???     1      10.212   8.318 -38.673
ATOM     46  H   ???     1       9.973  10.070 -38.479
ATOM     47  H   ???     1       6.093  12.253 -32.938
ATOM     48  C   ???     1       5.943  11.603 -32.049
ATOM     49  H   ???     1       6.678  10.774 -32.106
ATOM     50  H   ???     1       6.122  12.205 -31.135
ATOM     51  N   ???     1       4.571  11.103 -32.068
ATOM     52  H   ???     1       3.969  11.261 -32.888
ATOM     53  C   ???     1       4.020  10.364 -31.090
ATOM     54  N   ???     1       4.699  10.129 -29.958
ATOM     55  H   ???     1       5.651  10.489 -29.843
ATOM     56  H   ???     1       4.392   9.422 -29.280
ATOM     57  N   ???     1       2.771   9.888 -31.264
ATOM     58  H   ???     1       2.282  10.148 -32.131
ATOM     59  H   ???     1       2.181   9.692 -30.456
ATOM     60  H   ???     1       8.402   7.465 -28.182
ATOM     61  C   ???     1       9.346   7.512 -28.737
ATOM     62  N   ???     1       9.555   6.773 -29.890
ATOM     63  C   ???     1      10.861   6.867 -30.161
ATOM     64  H   ???     1      11.378   6.402 -31.001
ATOM     65  N   ???     1      11.486   7.646 -29.245
ATOM     66  H   ???     1      12.495   7.881 -29.259
ATOM     67  C   ???     1      10.544   8.062 -28.325
ATOM     68  H   ???     1      10.807   8.736 -27.511
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ATOM     69  O   ???     1      10.667   5.259 -25.623
ATOM     70  C   ???     1      10.952   4.628 -26.703
ATOM     71  O   ???     1      12.100   4.363 -27.138
ATOM     72  C   ???     1       9.742   4.241 -27.576
ATOM     73  H   ???     1       8.849   4.130 -26.935
ATOM     74  H   ???     1       9.558   5.122 -28.215
ATOM     75  C   ???     1       9.880   3.044 -28.520
ATOM     76  H   ???     1      10.873   3.064 -28.999
ATOM     77  H   ???     1       9.815   2.085 -27.968
ATOM     78  C   ???     1       8.826   3.098 -29.661
ATOM     79  O   ???     1       9.327   4.009 -30.665
ATOM     80  H   ???     1       9.897   3.322 -31.315
ATOM     81  C   ???     1       7.505   3.640 -29.107
ATOM     82  O   ???     1       7.115   4.765 -29.590
ATOM     83  O   ???     1       6.883   3.002 -28.225
ATOM     84  C   ???     1       8.555   1.743 -30.351
ATOM     85  H   ???     1       8.181   1.004 -29.622
ATOM     86  H   ???     1       7.765   1.918 -31.111
ATOM     87  C   ???     1       9.793   1.195 -31.085
ATOM     88  O   ???     1      10.485   2.097 -31.708
ATOM     89  O   ???     1      10.014  -0.030 -31.052
ATOM     90 FE   ???     1       6.918   8.363 -35.428
ATOM     91 MO   ???     1       8.084   5.693 -31.328
ATOM     92 FE   ???     1       4.873   6.961 -34.936
ATOM     93 FE   ???     1       5.899   6.242 -32.692
ATOM     94 FE   ???     1       6.982   5.994 -35.951
ATOM     95 FE   ???     1       7.997   7.776 -33.106
ATOM     96 FE   ???     1       8.084   5.294 -33.918
ATOM     97 FE   ???     1       5.456   7.516 -37.406
ATOM     98  C   ???     1       6.666   6.840 -34.322
ATOM     99  S   ???     1       7.701   7.547 -37.426
ATOM    100  S   ???     1       9.700   6.332 -32.932
ATOM    101  S   ???     1       4.868   5.456 -36.644
ATOM    102  S   ???     1       7.936   3.902 -35.729
ATOM    103  S   ???     1       8.326   9.665 -34.363
ATOM    104  S   ???     1       6.695   4.155 -32.511
ATOM    105  S   ???     1       4.752   9.014 -35.868
ATOM    106  S   ???     1       6.741   7.647 -31.183
ATOM    107  S   ???     1       3.718   6.626 -33.025
ATOM    108  H   ???     1       9.070   4.177 -33.619
ATOM    109  H   ???     1       9.204   4.031 -36.225
ATOM    110  H   ???     1       8.710   6.045 -35.134
ATOM    111  H   ???     1       8.832   8.622 -32.179
ATOM    112  O   ???     1       4.516   5.525 -29.497
ATOM    113  H   ???     1       5.470   5.239 -29.540
ATOM    114  H   ???     1       4.437   6.161 -30.246
ATOM    115  O   ???     1       1.086   8.385 -34.249
ATOM    116  H   ???     1       1.937   8.004 -33.911
ATOM    117  H   ???     1       0.583   8.665 -33.430
END
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