Electronic Supplementary Information for

Synthesis, characterization and computational study of heterobimetallic CoFe complexes for hydrogen generation

Hui Gao,[a] Jing Huang,[a] Limin Chen,[b] Ruliang Liu[a] and Jinzhu Chen*[a,c]

[a] *Key Laboratory of Renewable Energy and Natural Gas Hydrate, Guangzhou Institute of Energy Conversion, Chinese Academy of Sciences, Guangzhou 510640, P. R. China.*
[b]*College of Environmental Science and Engineering, South China University of Technology, Guangzhou 510006, P. R. China*
[c]*State Key Laboratory of Elemento-organic Chemistry, Nankai University, Tianjin 300071, P. R. China.*

Fax/Tel.: +86 20 3722 3380
E-mail: chenjz@ms.giec.ac.cn

Contents of the Electronic Supplementary Information

Complete list of authors for references with more than 10 authors:

(29) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2009.

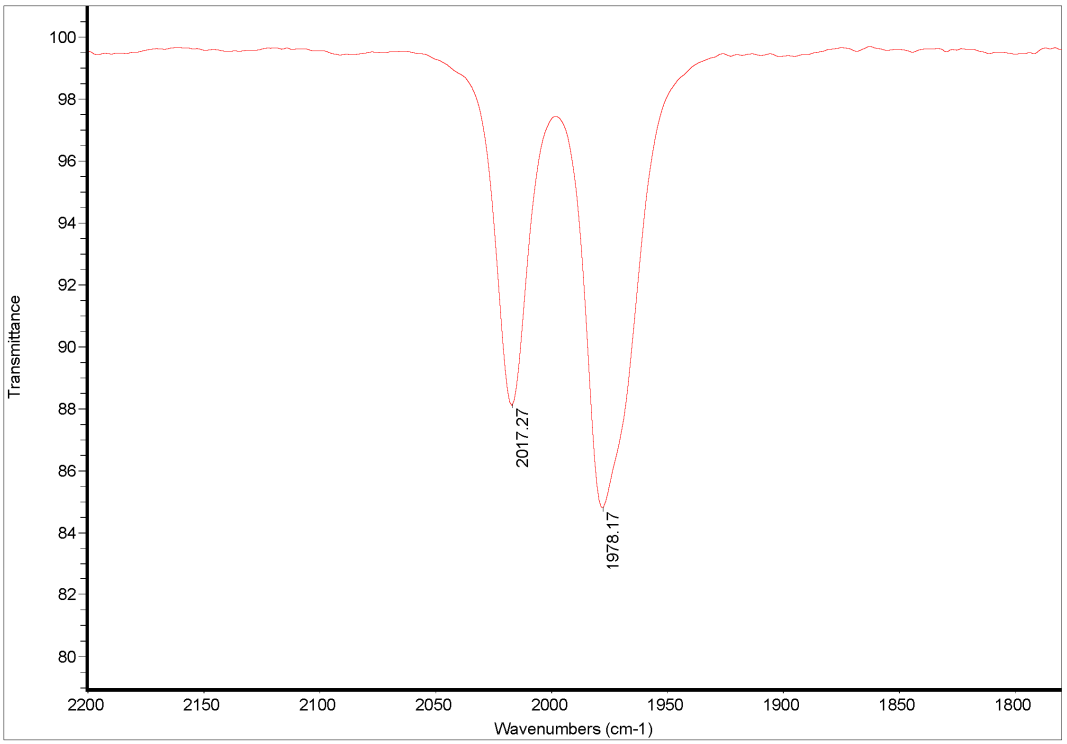

Fig. S1 IR spectra (CH_2Cl_2) of the complex $Fe(S_2C_2H_4)(CO)_2(dppv)$

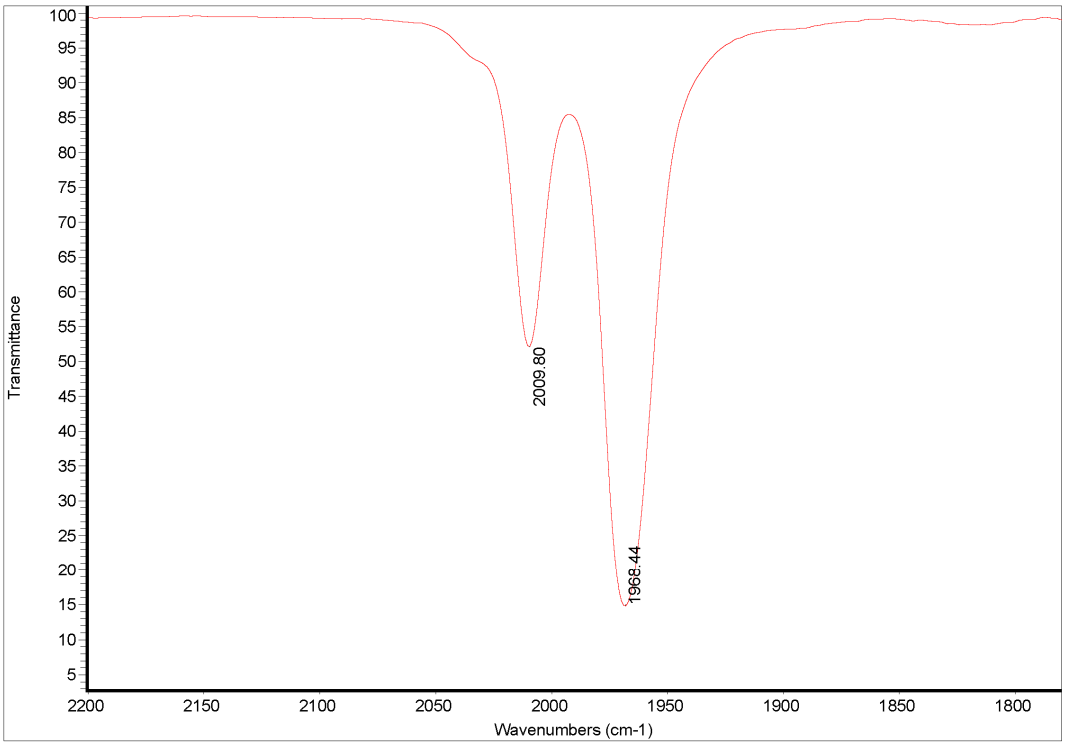

Fig. S2 IR spectra (CH_2Cl_2) of the complex $Fe(S_2C_3H_6)(CO)_2(dppe)$

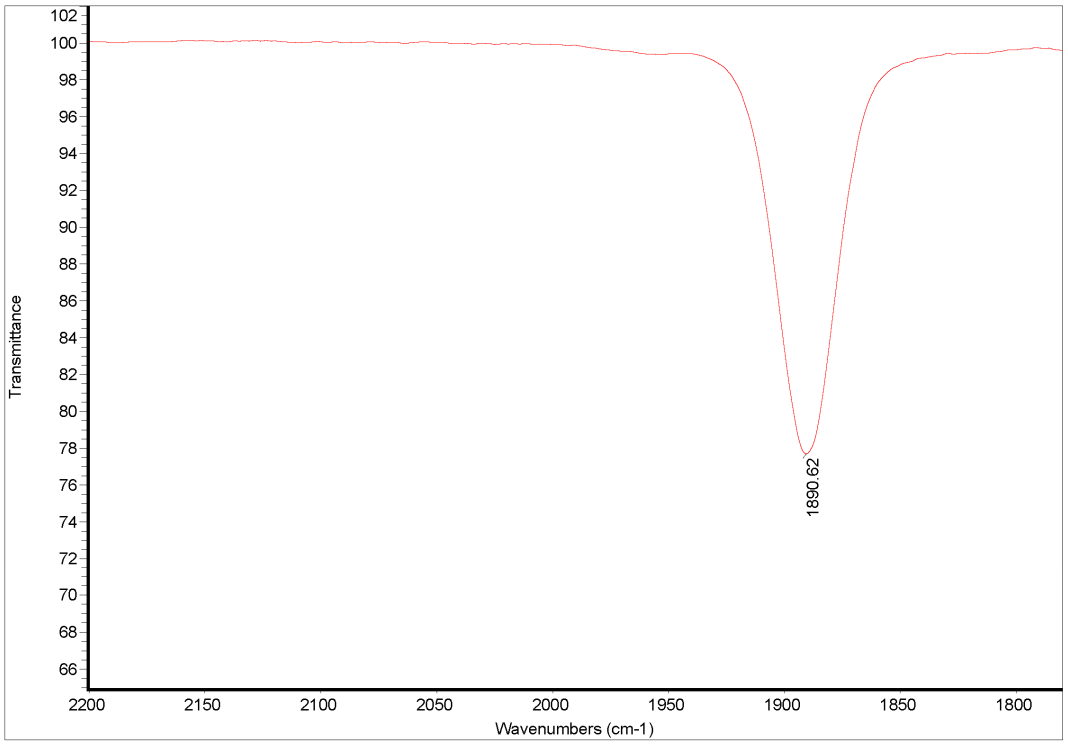

Fig. S3 IR spectra (CH_2Cl_2)of the complex $CpCo(\mu\text{-}S_2C_2H_4)Fe(CO)(dppv)$ (**1**)

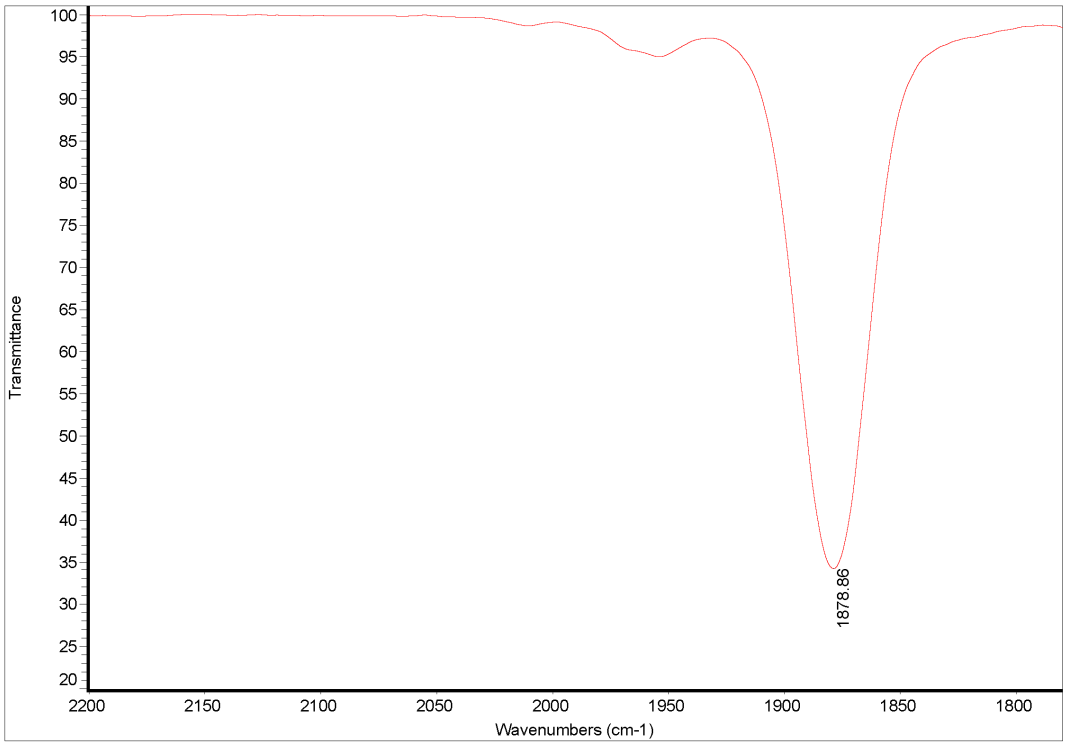

Fig. S4 IR spectra (CH_2Cl_2) of the complex $CpCo(\mu\text{-}S_2C_3H_6)Fe(CO)(dppe)$ (**2**)

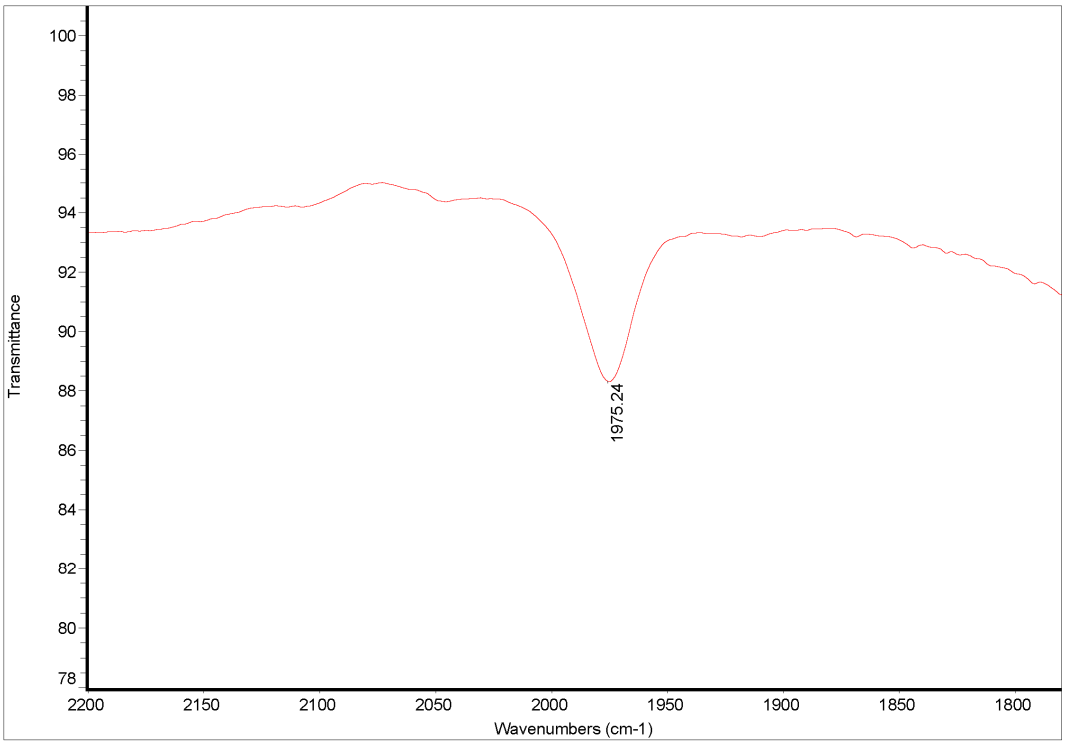

Fig. S5 IR spectra (CH_2Cl_2) of the complex $[CpCo(\mu\text{-}S_2C_2H_4)(\mu\text{-}H)Fe(CO)(dppv)]^+$ ($[\mathbf{1}\mu H]^+$)

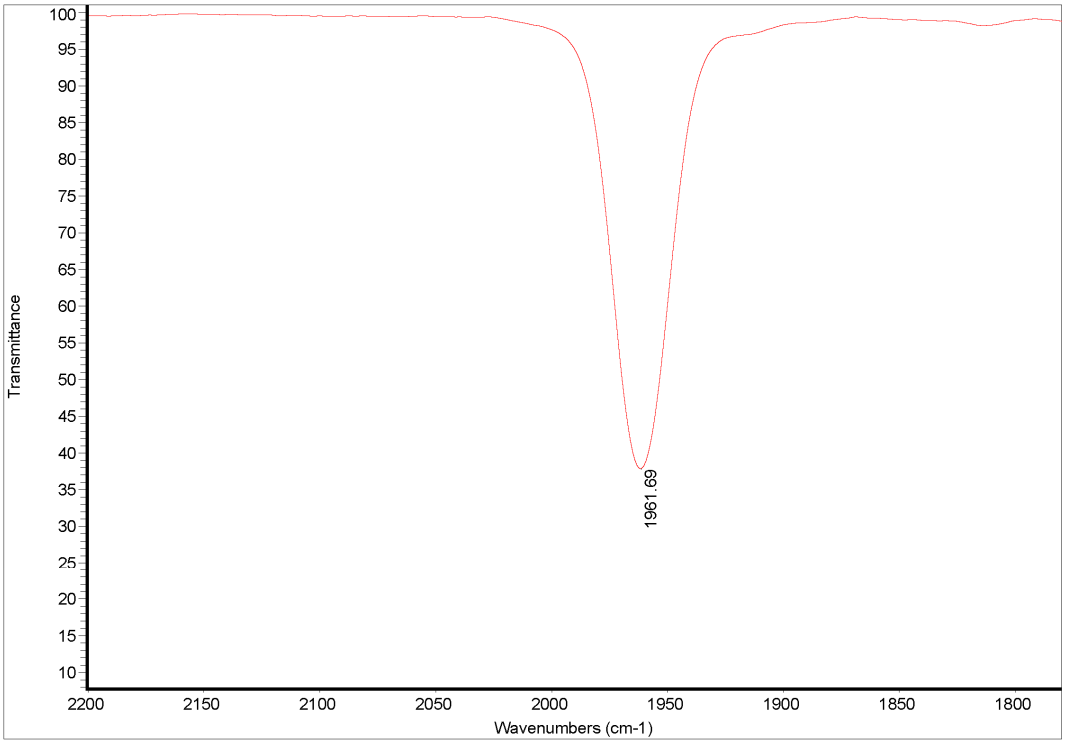

Fig. S6 IR spectra (CH_2Cl_2) of the complex $[CpCo(\mu\text{-}S_2C_3H_6)(\mu\text{-}H)Fe(CO)(dppe)]^+$ ($[\mathbf{2}\mu H]^+$)

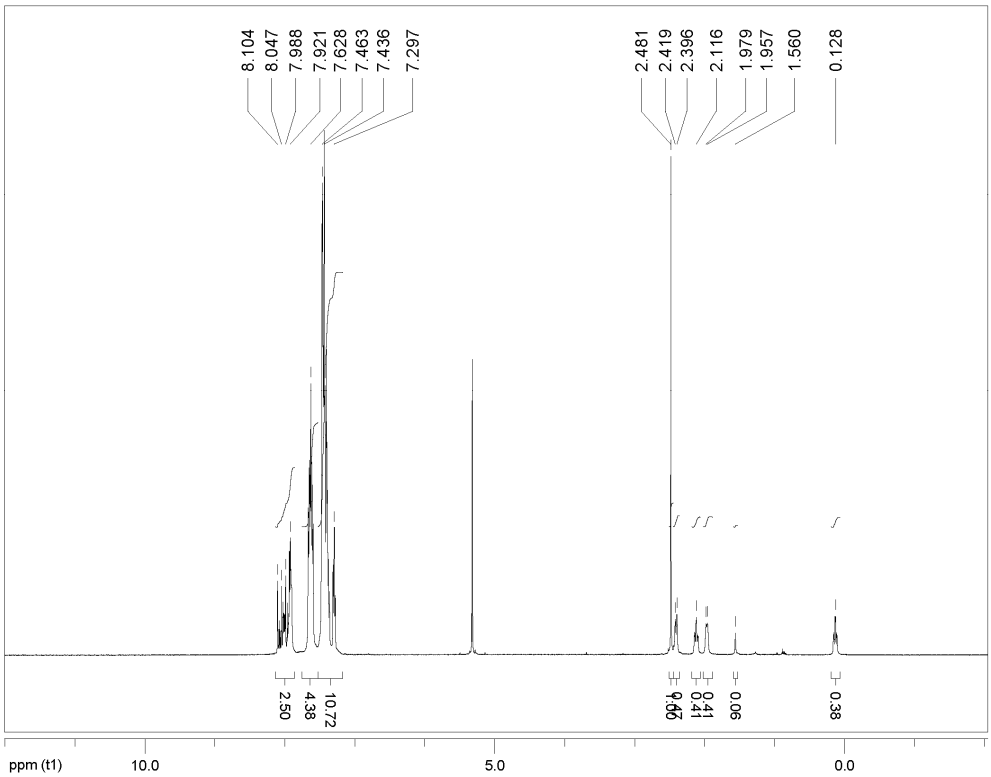

Fig. S7 ^{1}H NMR spectrum of the complex $Fe(S_2C_2H_4)(CO)_2(dppv)$ in CD_2Cl_2.

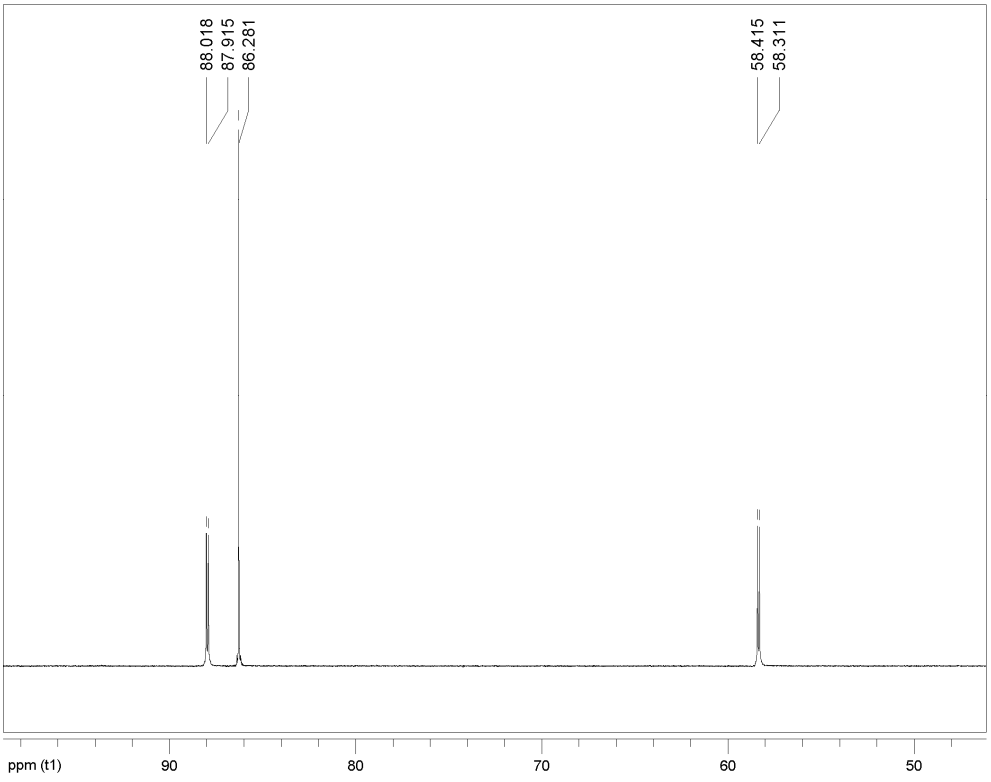

Fig. S8 $^{31}P\{^{1}H\}$ NMR spectrum of the complex $Fe(S_2C_2H_4)(CO)_2(dppv)$ in CD_2Cl_2.

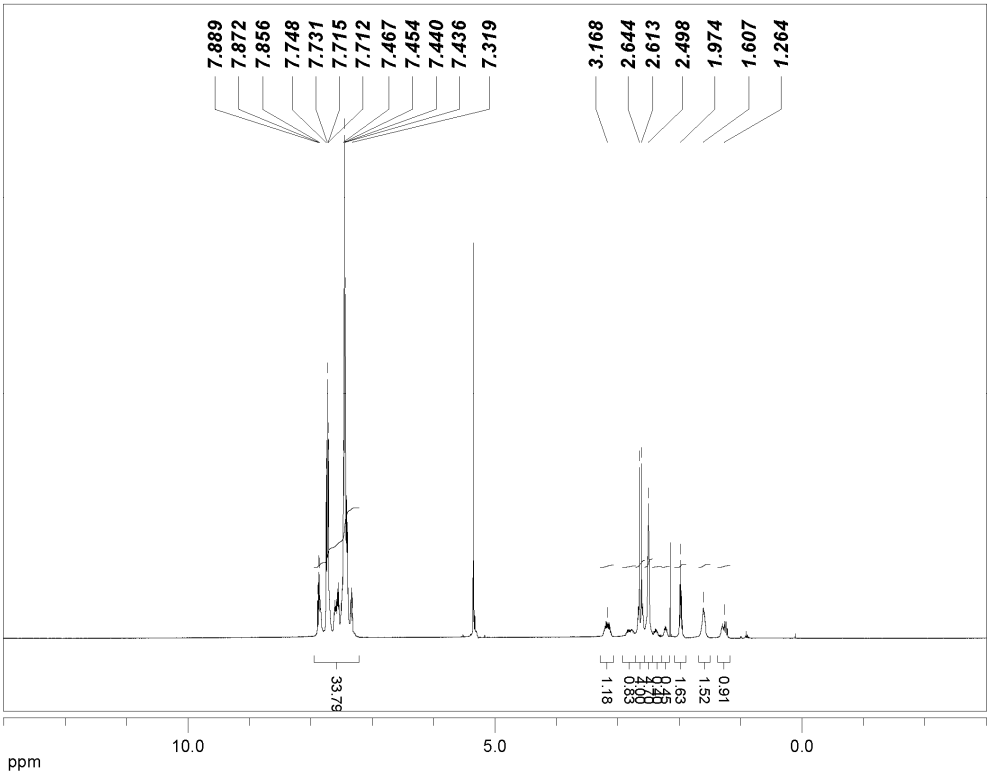

Fig. S9 ^{1}H NMR spectrum of the complex $Fe(S_2C_3H_6)(CO)_2(dppe)$ in CD_2Cl_2.

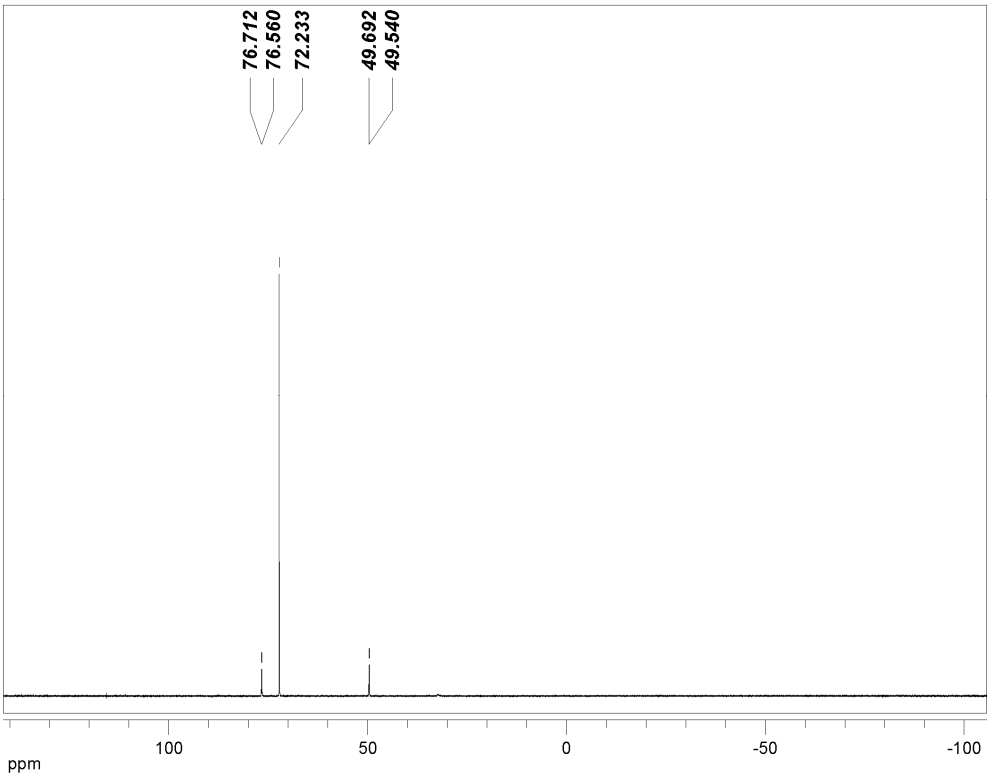

Fig. S10 $^{31}P\{^{1}H\}$ NMR spectrum of the complex $Fe(S_2C_3H_6)(CO)_2(dppe)$ in CD_2Cl_2.

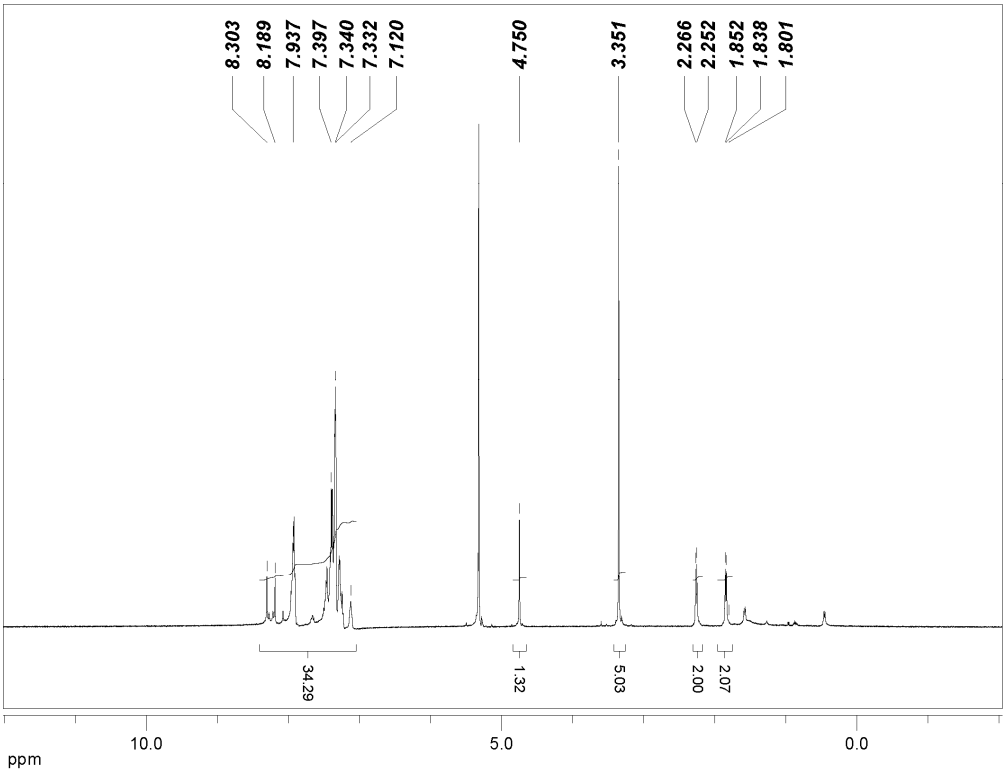

Fig. S11 ^{1}H NMR spectrum of the complex $CpCo(\mu\text{-}S_2C_2H_4)Fe(CO)(dppv)$ (**1**) in CD_2Cl_2.

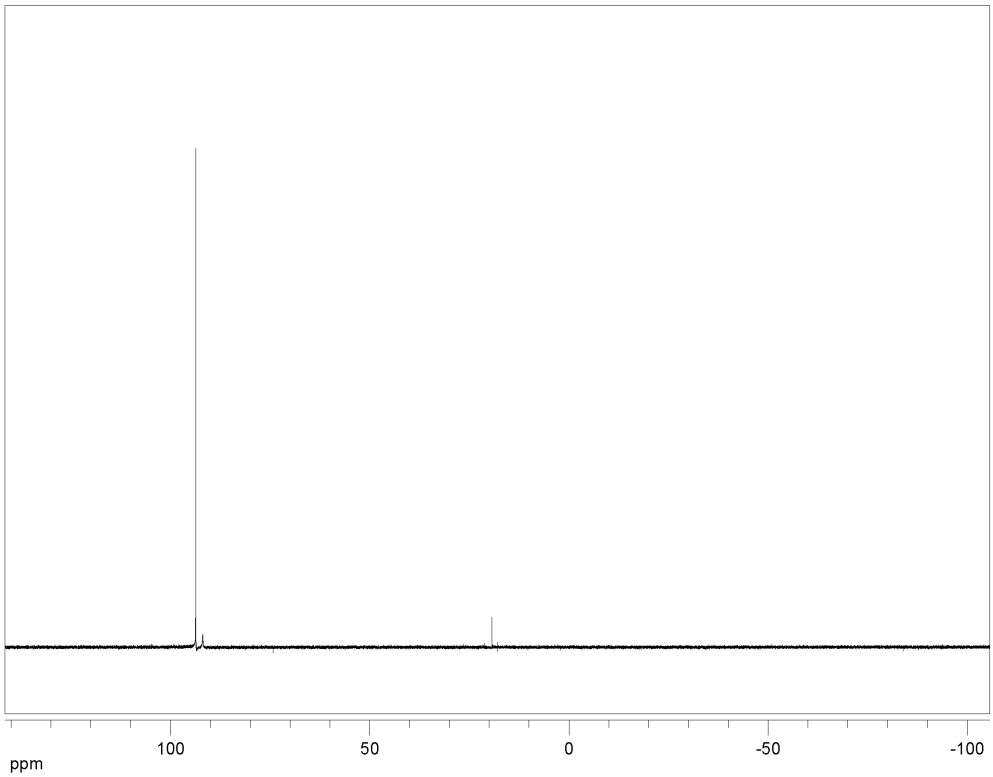

Fig. S12 $^{31}P\{^{1}H\}$ NMR spectrum of the complex $CpCo(\mu\text{-}S_2C_2H_4)Fe(CO)(dppv)$ (**1**) in CD_2Cl_2.

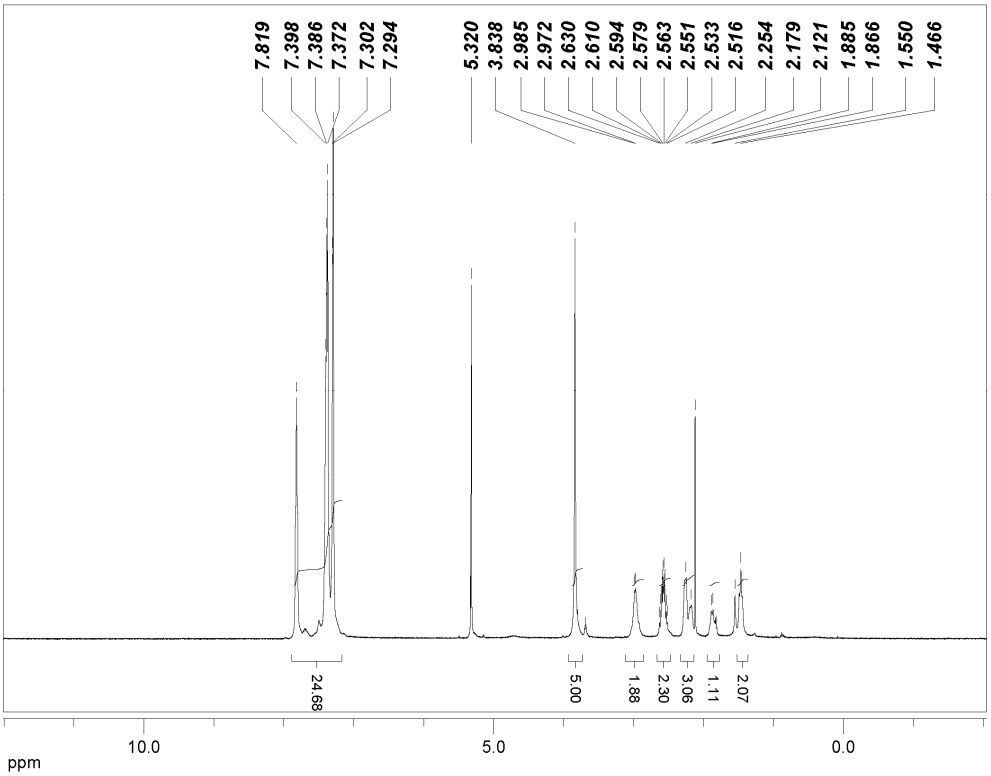

Fig. S13 ^{1}H NMR spectrum of the complex $CpCo(\mu\text{-}S_2C_3H_6)Fe(CO)(dppe)$ (**2**) in CD_2Cl_2.

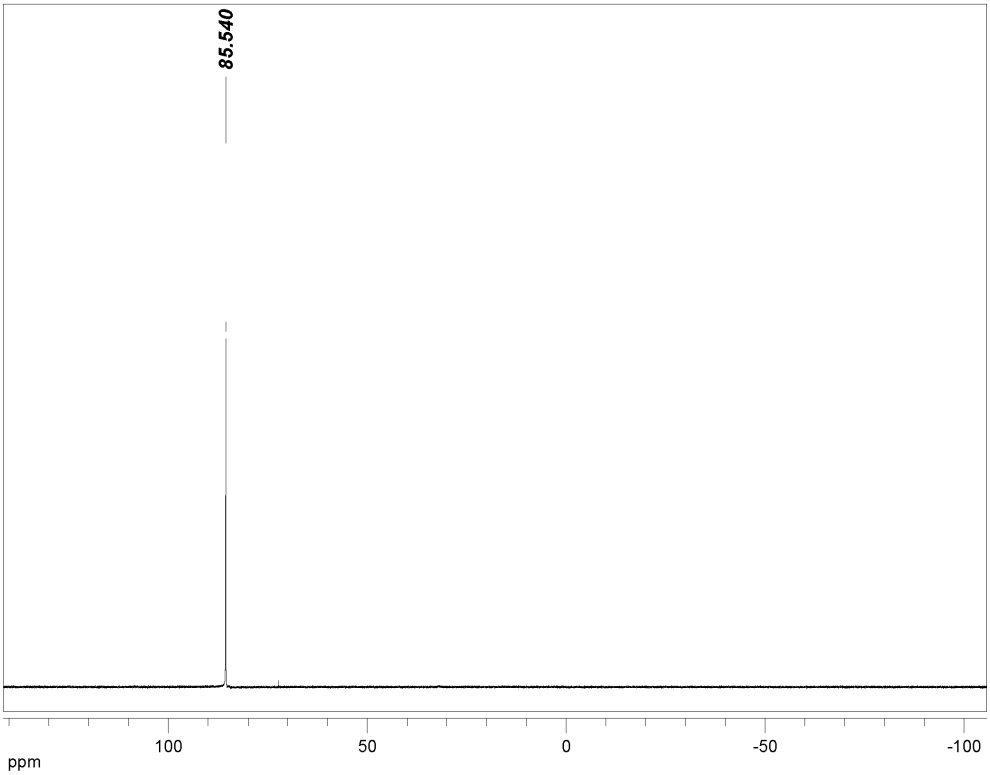

Fig. S14 $^{31}P\{^{1}H\}$ NMR spectrum of the complex $CpCo(\mu\text{-}S_2C_3H_6)Fe(CO)(dppe)$ (**2**) in CD_2Cl_2.

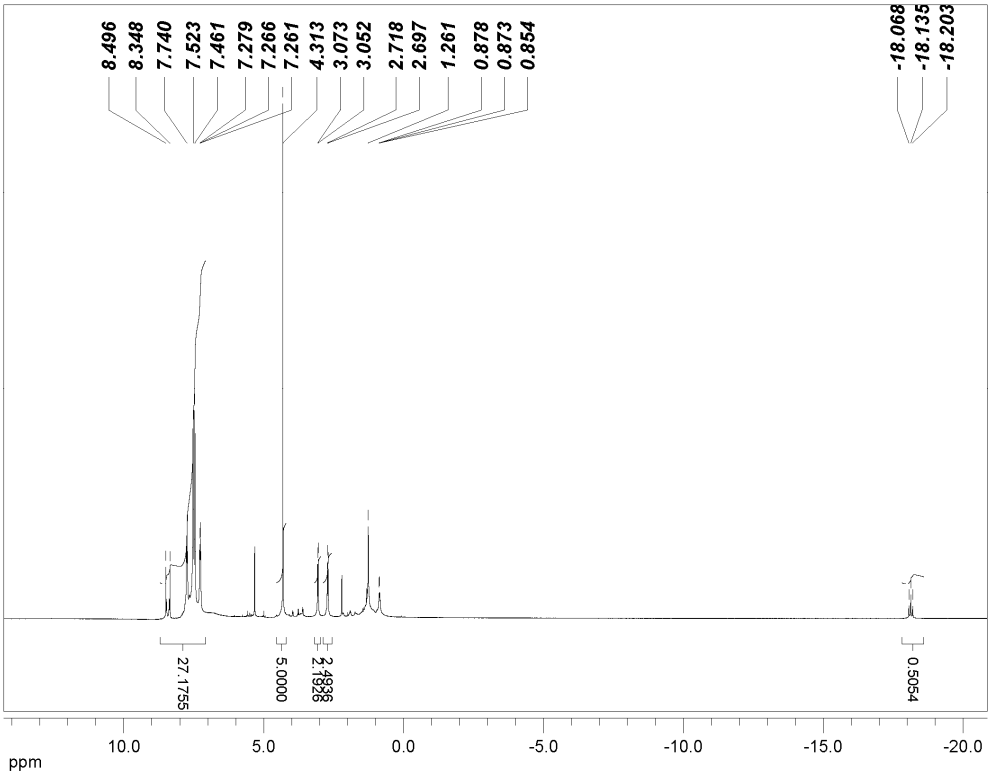

Fig. S15 ^{1}H NMR spectrum of the complex $[CpCo(\mu\text{-}S_2C_2H_4)(\mu\text{-}H)Fe(CO)(dppv)]^+$ ($[\mathbf{1}\mu H]^+$) in CD_2Cl_2.

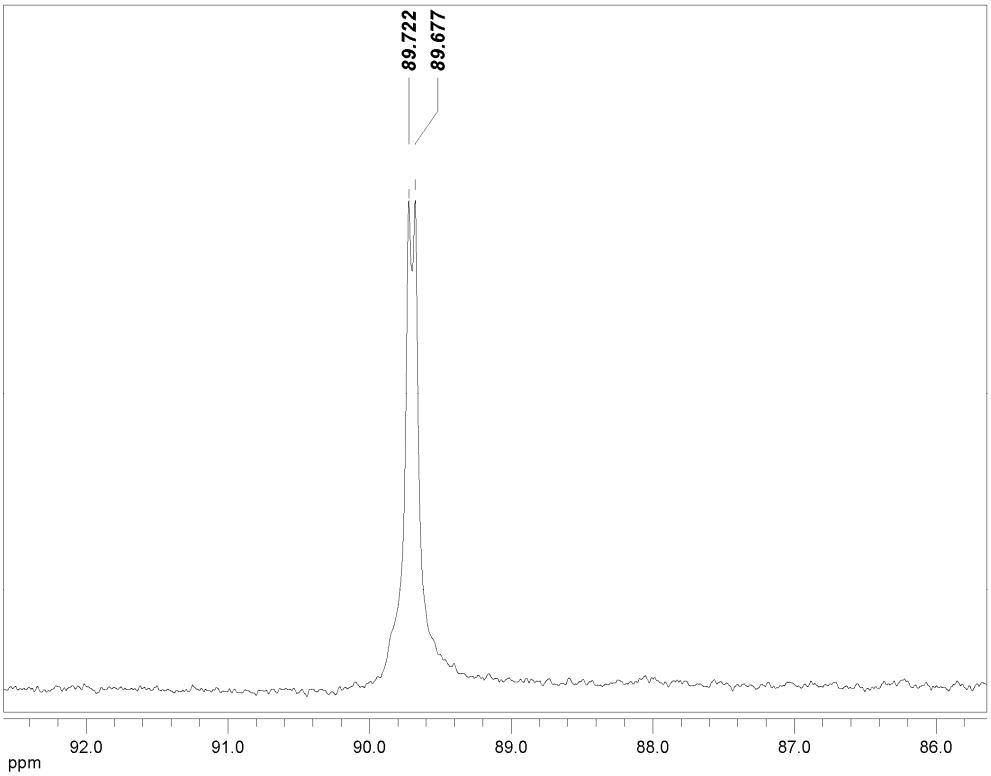

Fig. S16 $^{31}P\{^{1}H\}$ NMR spectrum of the complex $[CpCo(\mu\text{-}S_2C_2H_4)(\mu\text{-}H)Fe(CO)(dppv)]^+$ ($[\mathbf{1}\mu H]^+$) in CD_2Cl_2.

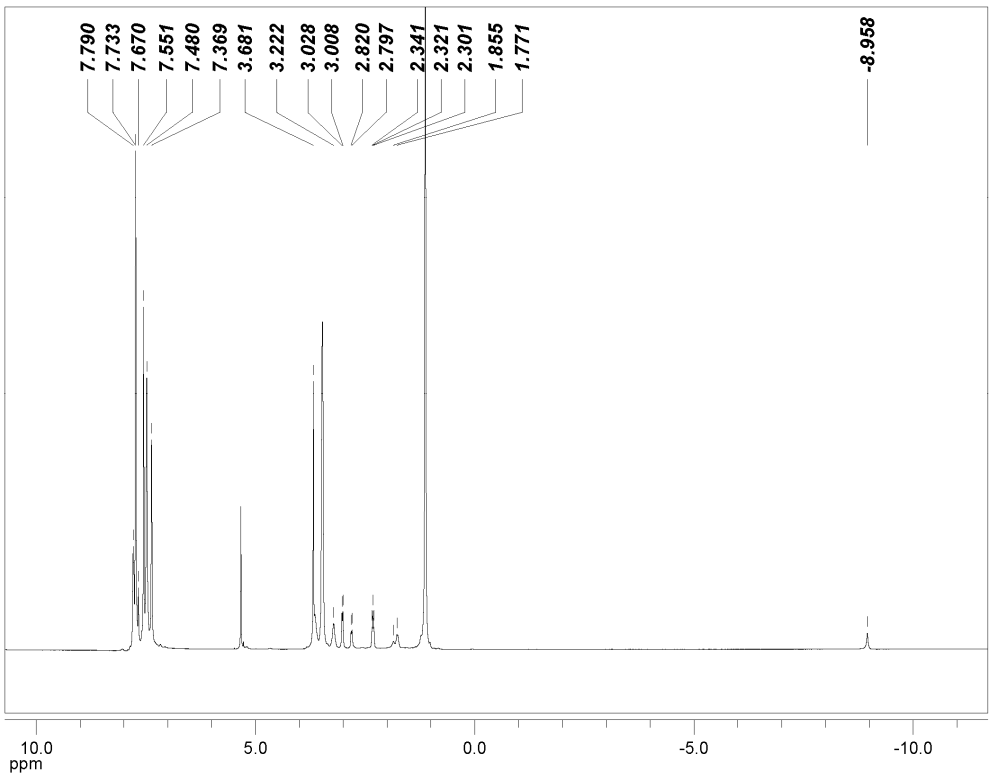

Fig. S17 ^{1}H NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 213K.

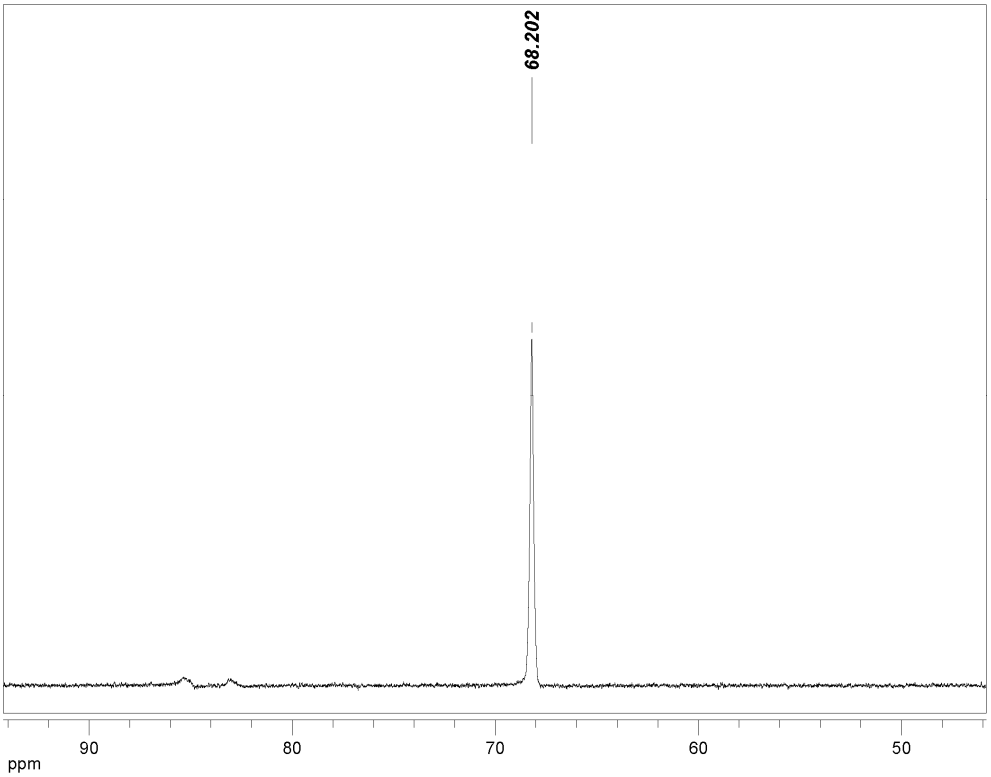

Fig. S18 $^{31}P\{^{1}H\}$ NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 213K.

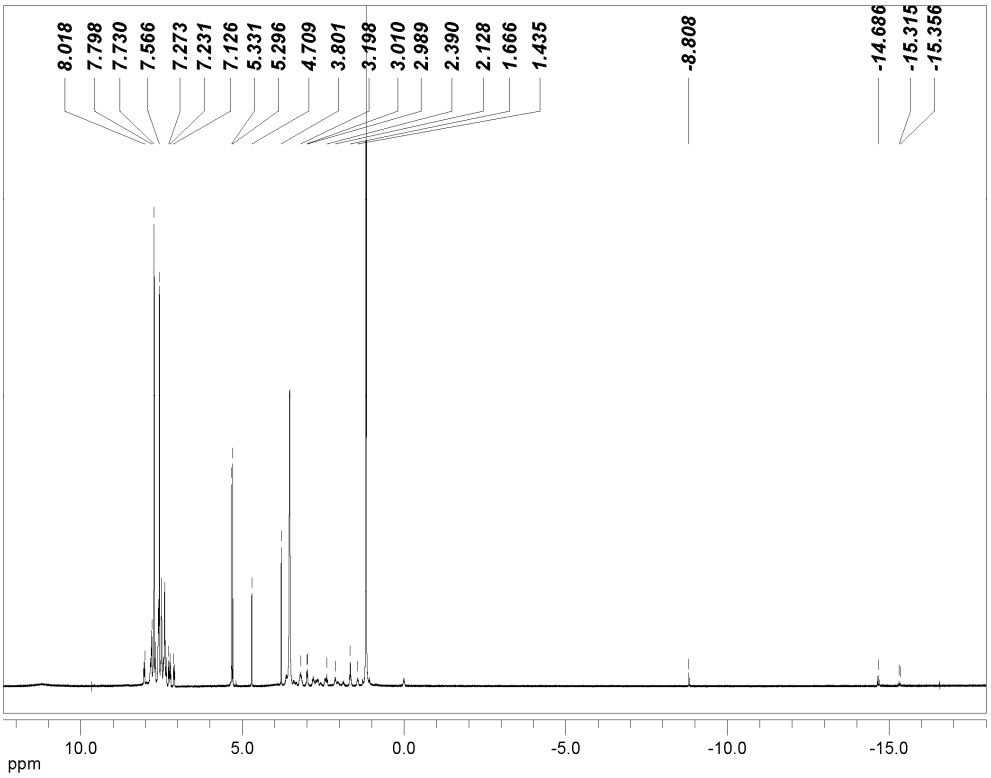

Fig. S19 ^{1}H NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 263K.

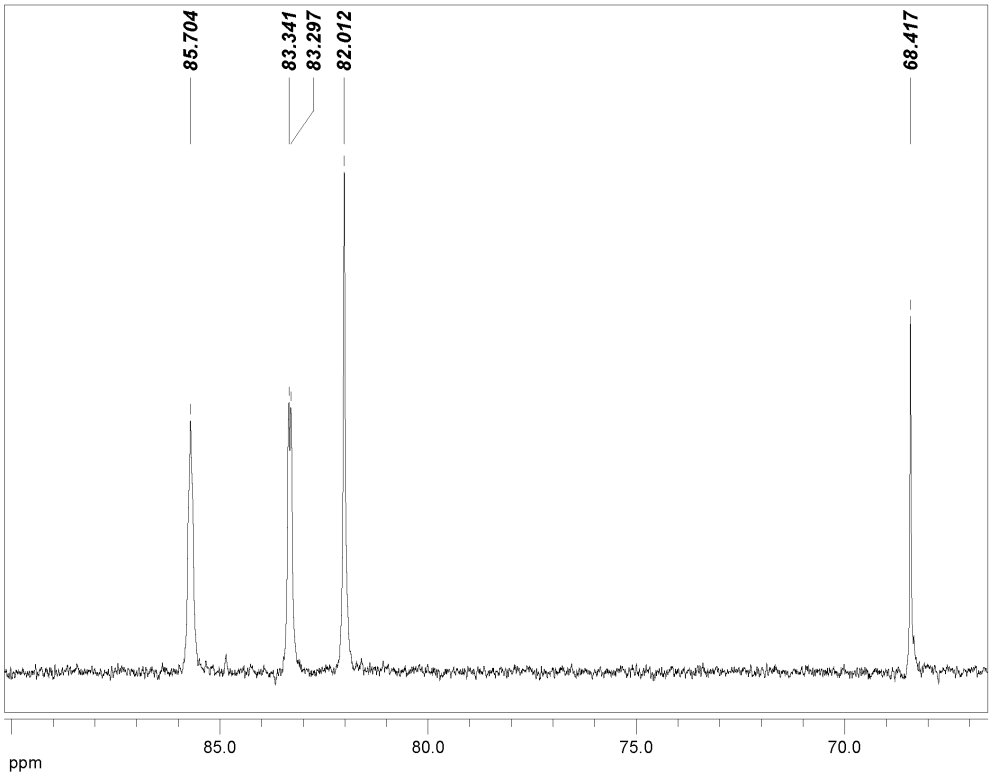

Fig. S20 $^{31}P\{^{1}H\}$ NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 263K.

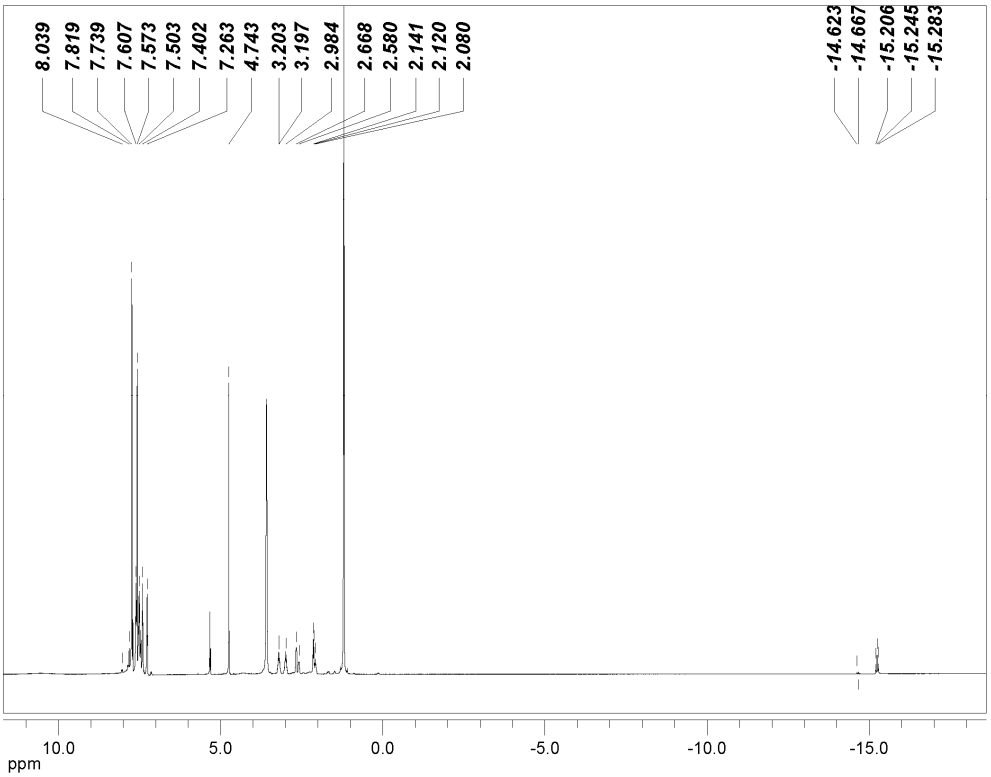

Fig. S21 ^{1}H NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 293K.

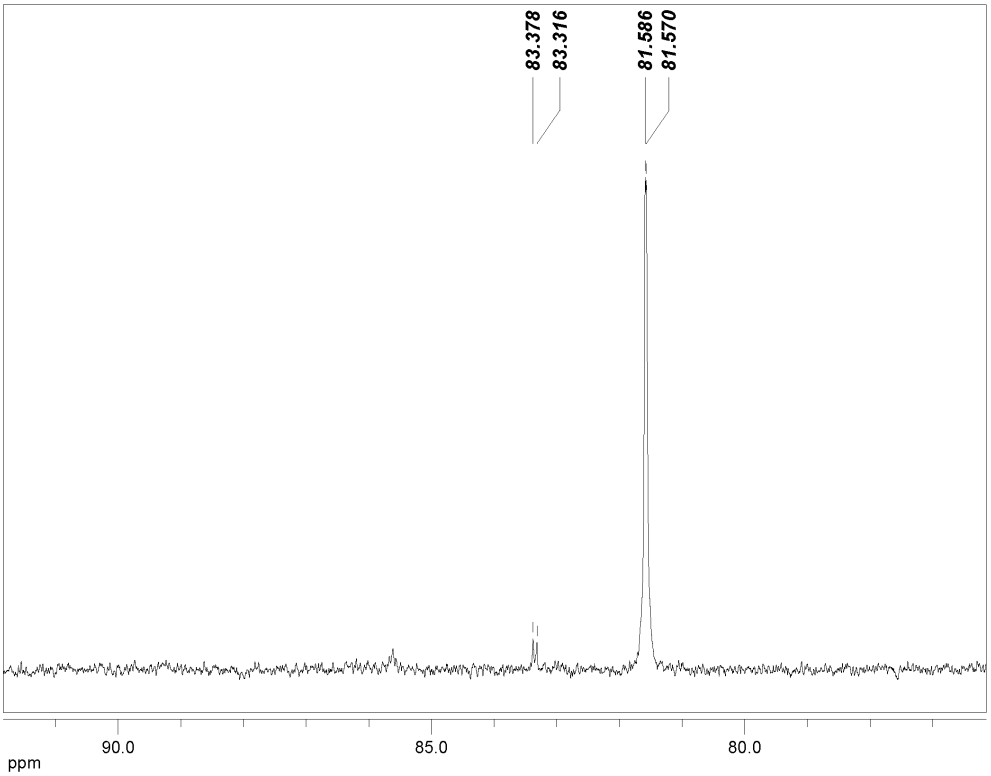

Fig. S22 $^{31}P\{^{1}H\}$ NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 293K.

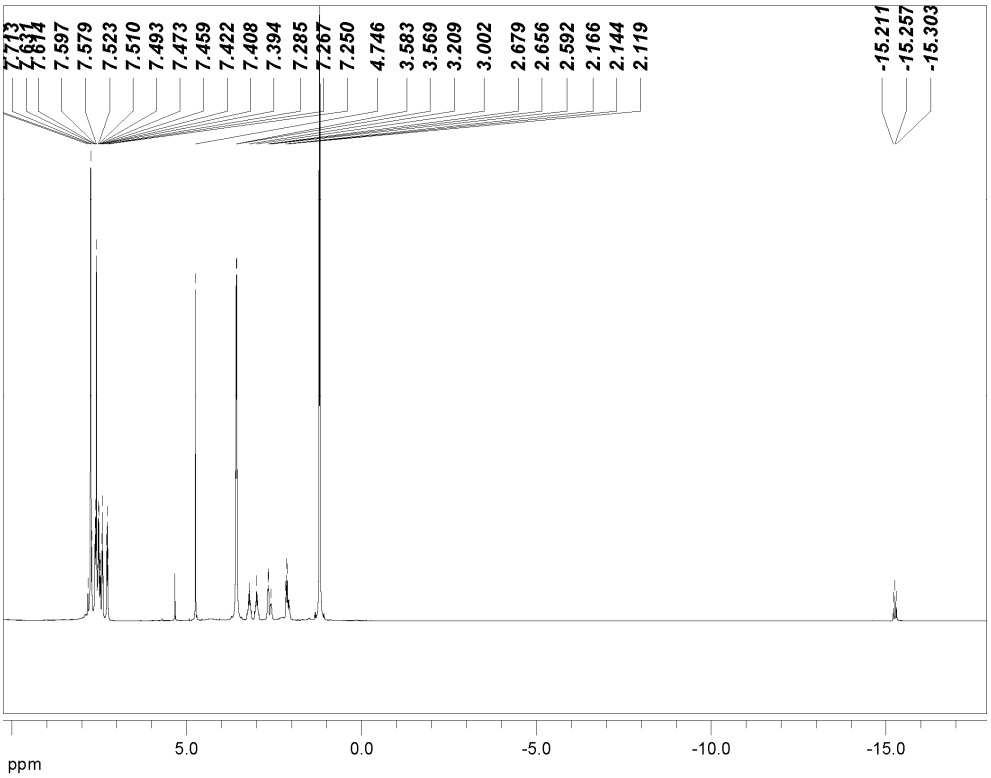

Fig. S23 ^{1}H NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 298K.

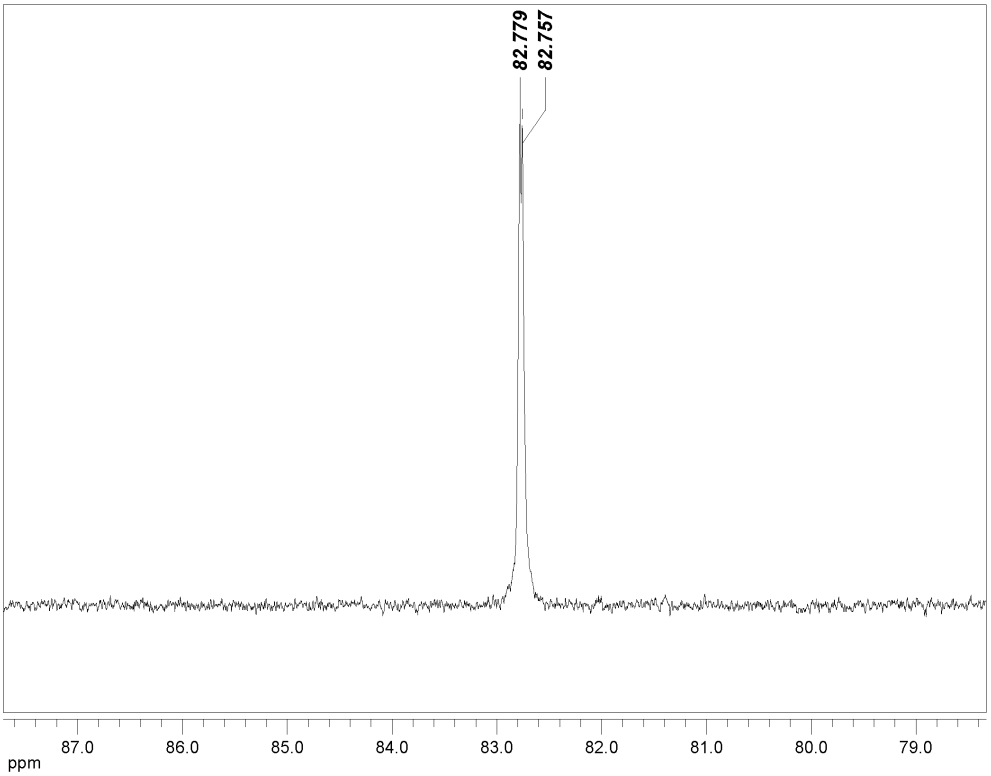

Fig. S24 $^{31}P\{^{1}H\}$ NMR spectrum of the protonated isomers of **2** in CD_2Cl_2 at 298K.

Table S1. Crystal data and structure refinement for **1**.

Empirical formula	C34 H31 Co Fe O P2 S2	
Formula weight	696.43	
Temperature	393(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 16.0226(10) Å	α= 90°.
	b = 21.7926(11) Å	β= 90°.
	c = 8.8475(6) Å	γ = 90°.
Volume	3089.3(3) $Å^3$	
Z	4	
Density (calculated)	1.497 Mg/m^3	
Absorption coefficient	1.272 mm^{-1}	
F(000)	1432	
Crystal size	0.40 x 0.14 x 0.14 mm^3	
Theta range for data collection	1.87 to 28.31°.	
Index ranges	-21<=h<=20, -28<=k<=29, -8<=l<=11	
Reflections collected	19007	
Independent reflections	3903 [R(int) = 0.0882]	
Completeness to theta = 28.31°	99.0 %	
Max. and min. transmission	0.8420 and 0.6301	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3903 / 0 / 194	
Goodness-of-fit on F^2	0.980	
Final R indices [I>2sigma(I)]	R1 = 0.0351, wR2 = 0.0862	
R indices (all data)	R1 = 0.0469, wR2 = 0.0904	
Extinction coefficient	0.00023(13)	
Largest diff. peak and hole	0.464 and -0.380 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	1601(1)	2500	9706(1)	21(1)
Fe(1)	2996(1)	2500	8430(1)	17(1)
P(1)	3727(1)	3191(1)	9678(1)	20(1)
S(4)	1963(1)	3163(1)	7990(1)	23(1)
O(1)	3689(2)	2500	5394(3)	38(1)
C(2)	4503(1)	2804(1)	10836(3)	27(1)
C(17)	1247(1)	3025(1)	11528(3)	29(1)
C(9)	3214(1)	3698(1)	11049(3)	25(1)
C(1)	3477(2)	2500	6649(4)	23(1)
C(3)	4371(1)	3761(1)	8678(3)	26(1)
C(15)	1470(1)	2848(1)	6282(3)	34(1)
C(18)	531(1)	2823(1)	10715(3)	30(1)
C(10)	2747(1)	4196(1)	10498(3)	30(1)
C(8)	4981(2)	4093(1)	9432(3)	48(1)
C(14)	3226(1)	3587(1)	12597(3)	32(1)
C(16)	1674(2)	2500	12050(4)	30(1)
C(13)	2777(2)	3963(1)	13581(3)	44(1)
C(11)	2306(2)	4568(1)	11490(3)	40(1)
C(6)	5389(2)	4588(1)	7142(4)	57(1)
C(5)	4771(2)	4278(1)	6370(4)	59(1)
C(12)	2316(2)	4451(1)	13019(3)	46(1)
C(4)	4270(2)	3863(1)	7146(3)	43(1)
C(7)	5492(2)	4505(1)	8653(4)	60(1)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Co(1)-C(17)#1	2.057(2)
Co(1)-C(17)	2.057(2)
Co(1)-C(18)#1	2.058(2)
Co(1)-C(18)	2.058(2)
Co(1)-C(16)	2.077(3)
Co(1)-S(4)	2.1748(6)
Co(1)-S(4)#1	2.1748(6)
Co(1)-Fe(1)	2.5038(5)
Fe(1)-C(1)	1.754(3)
Fe(1)-P(1)	2.2038(5)
Fe(1)-P(1)#1	2.2038(5)
Fe(1)-S(4)#1	2.2318(5)
Fe(1)-S(4)	2.2318(5)
P(1)-C(2)	1.819(2)
P(1)-C(9)	1.836(2)
P(1)-C(3)	1.842(2)
S(4)-C(15)	1.838(2)
O(1)-C(1)	1.161(4)
C(2)-C(2)#1	1.323(4)
C(17)-C(16)	1.411(3)
C(17)-C(18)	1.424(3)
C(9)-C(14)	1.392(3)
C(9)-C(10)	1.405(3)
C(3)-C(4)	1.383(3)
C(3)-C(8)	1.387(3)
C(15)-C(15)#1	1.515(4)
C(18)-C(18)#1	1.409(4)
C(10)-C(11)	1.389(3)
C(8)-C(7)	1.396(4)
C(14)-C(13)	1.395(3)
C(16)-C(17)#1	1.411(3)
C(13)-C(12)	1.387(4)
C(11)-C(12)	1.377(4)
C(6)-C(7)	1.359(4)
C(6)-C(5)	1.380(4)
C(5)-C(4)	1.391(4)
C(17)#1-Co(1)-C(17)	67.61(12)
C(17)#1-Co(1)-C(18)#1	40.50(9)
C(17)-Co(1)-C(18)#1	67.70(9)
C(17)#1-Co(1)-C(18)	67.70(9)
C(17)-Co(1)-C(18)	40.50(9)

C(18)#1-Co(1)-C(18)	40.05(11)
C(17)#1-Co(1)-C(16)	39.92(8)
C(17)-Co(1)-C(16)	39.92(7)
C(18)#1-Co(1)-C(16)	67.29(10)
C(18)-Co(1)-C(16)	67.29(10)
C(17)#1-Co(1)-S(4)	172.08(6)
C(17)-Co(1)-S(4)	104.54(6)
C(18)#1-Co(1)-S(4)	138.80(6)
C(18)-Co(1)-S(4)	107.30(6)
C(16)-Co(1)-S(4)	133.01(4)
C(17)#1-Co(1)-S(4)#1	104.54(6)
C(17)-Co(1)-S(4)#1	172.08(6)
C(18)#1-Co(1)-S(4)#1	107.30(6)
C(18)-Co(1)-S(4)#1	138.80(7)
C(16)-Co(1)-S(4)#1	133.01(4)
S(4)-Co(1)-S(4)#1	83.28(3)
C(17)#1-Co(1)-Fe(1)	126.85(6)
C(17)-Co(1)-Fe(1)	126.85(6)
C(18)#1-Co(1)-Fe(1)	159.96(6)
C(18)-Co(1)-Fe(1)	159.96(6)
C(16)-Co(1)-Fe(1)	113.56(8)
S(4)-Co(1)-Fe(1)	56.456(16)
S(4)#1-Co(1)-Fe(1)	56.456(16)
C(1)-Fe(1)-P(1)	102.51(7)
C(1)-Fe(1)-P(1)#1	102.51(7)
P(1)-Fe(1)-P(1)#1	86.14(3)
C(1)-Fe(1)-S(4)#1	99.74(7)
P(1)-Fe(1)-S(4)#1	157.51(3)
P(1)#1-Fe(1)-S(4)#1	92.267(19)
C(1)-Fe(1)-S(4)	99.74(7)
P(1)-Fe(1)-S(4)	92.267(19)
P(1)#1-Fe(1)-S(4)	157.51(3)
S(4)#1-Fe(1)-S(4)	80.71(3)
C(1)-Fe(1)-Co(1)	142.87(9)
P(1)-Fe(1)-Co(1)	104.39(2)
P(1)#1-Fe(1)-Co(1)	104.39(2)
S(4)#1-Fe(1)-Co(1)	54.310(16)
S(4)-Fe(1)-Co(1)	54.310(16)
C(2)-P(1)-C(9)	102.32(10)
C(2)-P(1)-C(3)	101.57(9)
C(9)-P(1)-C(3)	99.31(9)
C(2)-P(1)-Fe(1)	109.20(6)
C(9)-P(1)-Fe(1)	120.31(7)
C(3)-P(1)-Fe(1)	121.19(8)

C(15)-S(4)-Co(1)	102.19(7)
C(15)-S(4)-Fe(1)	102.68(7)
Co(1)-S(4)-Fe(1)	69.235(19)
C(2)#1-C(2)-P(1)	117.64(6)
C(16)-C(17)-C(18)	107.82(19)
C(16)-C(17)-Co(1)	70.81(15)
C(18)-C(17)-Co(1)	69.80(12)
C(14)-C(9)-C(10)	119.0(2)
C(14)-C(9)-P(1)	122.59(16)
C(10)-C(9)-P(1)	118.32(17)
O(1)-C(1)-Fe(1)	171.0(3)
C(4)-C(3)-C(8)	118.1(2)
C(4)-C(3)-P(1)	120.89(16)
C(8)-C(3)-P(1)	121.04(19)
C(15)#1-C(15)-S(4)	111.98(7)
C(18)#1-C(18)-C(17)	107.98(12)
C(18)#1-C(18)-Co(1)	69.98(6)
C(17)-C(18)-Co(1)	69.70(12)
C(11)-C(10)-C(9)	120.2(2)
C(3)-C(8)-C(7)	120.7(3)
C(9)-C(14)-C(13)	120.3(2)
C(17)#1-C(16)-C(17)	108.4(3)
C(17)#1-C(16)-Co(1)	69.27(16)
C(17)-C(16)-Co(1)	69.27(16)
C(12)-C(13)-C(14)	120.1(2)
C(12)-C(11)-C(10)	120.4(2)
C(7)-C(6)-C(5)	120.5(2)
C(6)-C(5)-C(4)	119.3(3)
C(11)-C(12)-C(13)	120.0(2)
C(3)-C(4)-C(5)	121.4(2)
C(6)-C(7)-C(8)	120.1(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	19(1)	24(1)	20(1)	0	3(1)	0
Fe(1)	16(1)	19(1)	17(1)	0	-2(1)	0
P(1)	21(1)	18(1)	22(1)	0(1)	-4(1)	-1(1)
S(4)	21(1)	24(1)	23(1)	3(1)	-1(1)	3(1)
O(1)	38(1)	45(1)	30(1)	0	10(1)	0
C(2)	24(1)	28(1)	28(1)	-2(1)	-10(1)	-4(1)
C(17)	29(1)	32(1)	27(1)	-5(1)	8(1)	-1(1)
C(9)	30(1)	20(1)	25(1)	-4(1)	-2(1)	-7(1)
C(1)	20(1)	23(1)	26(2)	0	1(1)	0
C(3)	23(1)	20(1)	34(1)	2(1)	3(1)	0(1)
C(15)	32(1)	41(1)	27(1)	1(1)	-12(1)	3(1)
C(18)	23(1)	38(1)	31(1)	0(1)	7(1)	7(1)
C(10)	39(1)	20(1)	31(1)	0(1)	5(1)	-1(1)
C(8)	42(1)	45(1)	55(2)	13(1)	-14(1)	-18(1)
C(14)	41(1)	32(1)	24(1)	-2(1)	-3(1)	-9(1)
C(16)	26(2)	42(2)	22(2)	0	4(1)	0
C(13)	58(2)	48(1)	25(1)	-10(1)	6(1)	-18(1)
C(11)	50(2)	21(1)	50(2)	-5(1)	11(1)	1(1)
C(6)	50(2)	40(1)	81(2)	20(2)	22(2)	-7(1)
C(5)	96(2)	36(1)	44(2)	10(1)	20(2)	-12(1)
C(12)	58(2)	34(1)	47(2)	-21(1)	17(1)	-10(1)
C(4)	60(2)	32(1)	37(2)	5(1)	-2(1)	-10(1)
C(7)	39(2)	48(1)	93(3)	21(2)	-12(2)	-22(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **1**.

	x	y	z	U(eq)
H(2)	4886	3024	11408	32
H(17)	1405	3431	11687	35
H(15A)	900	2994	6218	40
H(15B)	1768	2994	5398	40
H(18)	133	3074	10264	36
H(10)	2732	4275	9465	36
H(8)	5051	4041	10468	57
H(14)	3535	3260	12978	39
H(16)	2156	2500	12637	36
H(13)	2788	3886	14615	52
H(11)	2002	4899	11119	48
H(6)	5737	4857	6624	68
H(5)	4691	4345	5342	70
H(12)	2013	4698	13676	55
H(4)	3858	3649	6624	51
H(7)	5903	4722	9168	72

Cartesian coordinates for all of the species (in Å). ($CF_3SO_3^-$ is included in all of the below protonated sturcures, except for special annotations)

$\mathbf{1}_{\text{ba-ba}}$

Fe	0.027143	0.275886	0.882721
C	0.030664	1.742514	1.836259
O	0.063074	2.640847	2.595215
P	1.534524	0.866552	-0.657758
P	-1.520158	0.718058	-0.664308
C	0.649220	1.388487	-2.203965
H	1.222236	1.790520	-3.046562
C	-0.688400	1.357352	-2.194755
H	-1.283752	1.715247	-3.041068
C	-0.999210	-3.583571	-0.095057
C	0.157512	-3.164435	-0.825344
C	1.313632	-3.521012	-0.062703
C	0.870111	-4.191810	1.137317
C	-0.553682	-4.231178	1.116549
H	-2.032867	-3.431493	-0.393514
H	0.156689	-2.642513	-1.777425
H	2.345580	-3.314237	-0.333930
H	1.512266	-4.574631	1.926967
H	-1.196184	-4.649266	1.887777
C	0.791243	-0.802889	3.822628
C	-0.730305	-0.864974	3.808963
H	1.234271	-1.630956	4.393545
H	1.163342	0.146231	4.232808
H	-1.184798	0.043119	4.229631
H	-1.114414	-1.735816	4.358538
S	-1.397548	-1.026382	2.054402
S	1.501330	-0.936014	2.082918
Co	0.103911	-2.255499	1.055381
C	-2.618463	-0.613231	-1.382408
C	-3.776585	-0.999905	-0.684121
C	-2.303178	-1.261844	-2.587717
C	-4.600286	-2.012267	-1.184872
H	-4.039195	-0.504626	0.252860
C	-3.133348	-2.270253	-3.091469
H	-1.404331	-0.977557	-3.140314
C	-4.283807	-2.648832	-2.391263
H	-5.496234	-2.302541	-0.631278
H	-2.878750	-2.760526	-4.034034
H	-4.931404	-3.435689	-2.783998
C	-2.828386	2.034203	-0.391666
C	-3.017781	2.592983	0.879257
C	-3.652207	2.455214	-1.452206
C	-4.003901	3.566308	1.086526
H	-2.394367	2.263855	1.710574
C	-4.628685	3.433073	-1.247355
H	-3.548262	2.004229	-2.441929
C	-4.805481	3.993049	0.024402
H	-4.141388	3.990544	2.083671
H	-5.258106	3.754028	-2.080717
H	-5.571644	4.754776	0.185688
C	2.558041	2.426944	-0.430986
C	3.946058	2.491526	-0.633817
C	1.869562	3.602542	-0.081215
C	4.631554	3.701682	-0.469490
H	4.501548	1.599398	-0.925271
C	2.553874	4.810710	0.072574
H	0.789953	3.575970	0.076622
C	3.939862	4.863219	-0.114617
H	5.712859	3.732114	-0.623312
H	2.001174	5.711791	0.347536
H	4.476759	5.805764	0.013730
C	2.799569	-0.339216	-1.300388
C	2.725651	-0.863411	-2.601974
C	3.830834	-0.782569	-0.449665
C	3.665550	-1.799102	-3.049424
H	1.926003	-0.545982	-3.274735
C	4.772499	-1.712425	-0.901087
H	3.889298	-0.412157	0.575800
C	4.695064	-2.222408	-2.202730
H	3.592925	-2.195181	-4.064979
H	5.567490	-2.043489	-0.228908
H	5.430616	-2.949897	-2.552719

$[\mathbf{1}\mu\text{H}]^+_{\text{ba-ba}}$ ($CF_3SO_3^-$ is not included)

Fe	0.012524	0.315859	0.762554
C	0.035891	1.873503	1.571639
O	0.076366	2.859900	2.189850
P	1.571132	0.923461	-0.765747
P	-1.541211	0.834380	-0.786288
C	0.671145	1.634188	-2.214829

H	1.247472	2.108379	-3.016019
C	-0.666807	1.607111	-2.220150
H	-1.250417	2.037227	-3.040090
C	-0.962887	-3.717623	0.196309
C	0.397757	-3.634938	-0.258643
C	1.260447	-3.825769	0.859678
C	0.438516	-4.030516	2.025938
C	-0.929233	-3.971595	1.607376
H	-1.853046	-3.601990	-0.416408
H	0.718370	-3.425376	-1.275827
H	2.346019	-3.792183	0.840842
H	0.794003	-4.206982	3.037756
H	-1.797122	-4.065327	2.255544
C	0.682814	-0.450128	3.839776
C	-0.840436	-0.522135	3.796519
H	1.112950	-1.197679	4.520003
H	1.042569	0.541519	4.147265
H	-1.308869	0.407740	4.148807
H	-1.231990	-1.350908	4.401713
S	-1.481621	-0.800534	2.060332
S	1.442736	-0.765911	2.160020
Co	0.023887	-2.175841	1.205142
C	-2.461726	-0.569157	-1.581160
C	-3.704460	-0.976953	-1.066851
C	-1.895283	-1.270591	-2.658790
C	-4.371805	-2.069902	-1.630699
H	-4.161471	-0.433527	-0.237313
C	-2.571352	-2.356110	-3.225794
H	-0.929948	-0.963832	-3.067699
C	-3.809521	-2.759150	-2.711610
H	-5.340652	-2.375603	-1.230357
H	-2.134207	-2.882701	-4.076827
H	-4.339393	-3.602835	-3.158160
C	-2.900031	2.045518	-0.428820
C	-3.150515	2.487420	0.878283
C	-3.708062	2.515037	-1.482401
C	-4.184890	3.396740	1.129504
H	-2.544484	2.119591	1.705951
C	-4.734687	3.426993	-1.228628
H	-3.552985	2.158658	-2.503074
C	-4.973099	3.871397	0.077896
H	-4.371224	3.734556	2.150765
H	-5.353094	3.788243	-2.052722
H	-5.776886	4.583563	0.274336
C	2.749170	2.309818	-0.384553
C	4.132260	2.119247	-0.236871
C	2.211464	3.603007	-0.246311
C	4.962431	3.207806	0.052677
H	4.572638	1.129864	-0.363852
C	3.046723	4.686723	0.035526
H	1.139405	3.772837	-0.367624
C	4.423574	4.490534	0.189835
H	6.037201	3.049831	0.162599
H	2.619220	5.686350	0.134506
H	5.075625	5.337590	0.411392
C	2.634800	-0.398566	-1.516347
C	2.591425	-0.683076	-2.891947
C	3.495845	-1.146284	-0.691110
C	3.399416	-1.690090	-3.432545
H	1.930925	-0.120213	-3.553813
C	4.309125	-2.144142	-1.237616
H	3.535826	-0.951136	0.383092
C	4.262244	-2.419710	-2.609124
H	3.358753	-1.896826	-4.504009
H	4.986167	-2.704765	-0.589300
H	4.898733	-3.197831	-3.034806
H	0.080234	-1.166192	-0.052732

2$_{ba\text{-}ba}$

Fe	-0.010049	0.080514	0.846852
C	-0.195615	1.354864	2.030771
O	-0.280923	2.151108	2.893889
P	1.455876	1.043545	-0.562434
P	-1.588162	0.674784	-0.651796
C	0.637825	1.191604	-2.256057
H	0.639460	0.187176	-2.705250
C	-0.794446	1.680790	-2.039079
H	-1.390770	1.629377	-2.961952
C	-0.459586	-3.647896	-0.965818
C	0.660838	-2.965037	-1.531992
C	1.817177	-3.291049	-0.757084
C	1.414165	-4.210413	0.281370
C	0.012476	-4.429483	0.153198
H	-1.488649	-3.581992	-1.309126
H	0.634968	-2.310296	-2.398586
H	2.821430	-2.904778	-0.911394

H	2.066741	-4.641603	1.036914
H	-0.601304	-5.060101	0.792072
S	-1.360782	-1.620613	1.522202
S	1.631654	-1.175950	1.787020
Co	0.391099	-2.406725	0.484875
H	-0.795012	2.727776	-1.698834
H	1.211706	1.872140	-2.903666
C	-1.231702	-1.963468	3.359144
C	-0.107529	-1.250991	4.098129
H	-1.142286	-3.057640	3.446027
H	-2.208067	-1.669335	3.774756
C	1.290272	-1.570816	3.584995
H	-0.271717	-0.164614	4.058075
H	-0.158727	-1.533598	5.167560
H	2.041799	-0.998204	4.150323
H	1.524294	-2.641323	3.695838
C	-3.003270	1.775471	-0.122813
C	-3.752023	2.497639	-1.070200
C	-3.352837	1.865651	1.232047
C	-4.814212	3.310096	-0.664129
H	-3.514494	2.421203	-2.133664
C	-4.424642	2.670589	1.637212
H	-2.777465	1.305907	1.970410
C	-5.152940	3.398452	0.691922
H	-5.383295	3.871245	-1.409089
H	-4.683927	2.732216	2.696531
H	-5.984996	4.031616	1.008185
C	-2.563188	-0.619340	-1.590973
C	-2.205138	-1.028725	-2.886731
C	-3.669785	-1.231448	-0.974314
C	-2.935336	-2.018539	-3.553915
H	-1.352488	-0.574823	-3.395526
C	-4.395301	-2.225418	-1.638515
H	-3.970393	-0.924885	0.028389
C	-4.032005	-2.622978	-2.929997
H	-2.644858	-2.316769	-4.563969
H	-5.252357	-2.688171	-1.143786
H	-4.602368	-3.396244	-3.449200
C	1.946049	2.846875	-0.339647
C	3.171512	3.350532	-0.813092
C	1.024729	3.743932	0.226064
C	3.468629	4.713765	-0.711685
H	3.903109	2.675016	-1.259284
C	1.319035	5.108816	0.319306
H	0.073733	3.374953	0.611207
C	2.543809	5.597624	-0.144923
H	4.429027	5.084724	-1.077746
H	0.589843	5.787109	0.768030
H	2.778110	6.661488	-0.064088
C	3.110553	0.282377	-0.944396
C	3.426805	-0.276065	-2.194357
C	4.082205	0.247052	0.074611
C	4.681105	-0.855489	-2.421890
H	2.701923	-0.260247	-3.009441
C	5.334855	-0.328865	-0.154594
H	3.859541	0.680251	1.050817
C	5.638333	-0.884527	-1.402647
H	4.909290	-1.280614	-3.402033
H	6.075432	-0.345956	0.648119
H	6.617160	-1.335069	-1.581144

2′$_{\text{ba-ba}}$

Fe	-0.008558	0.071400	0.821333
C	-0.180582	1.227595	2.119964
O	-0.258088	1.872208	3.103301
P	1.449388	1.083079	-0.563885
P	-1.595761	0.734119	-0.639180
C	0.617431	1.323915	-2.241115
H	0.611226	0.347811	-2.748730
C	-0.809783	1.806218	-1.980670
H	-1.418026	1.813192	-2.897326
C	-0.502067	-3.608609	-0.996978
C	0.621204	-2.915716	-1.547662
C	1.779800	-3.281943	-0.792412
C	1.375420	-4.234403	0.214850
C	-0.029642	-4.434461	0.089429
H	-1.533057	-3.518483	-1.328890
H	0.594461	-2.227060	-2.387744
H	2.786304	-2.898136	-0.938723
H	2.028699	-4.697903	0.950179
H	-0.645665	-5.078771	0.712158
S	-1.372718	-1.600521	1.510787
S	1.638196	-1.176967	1.749414
Co	0.372495	-2.425781	0.476797
H	-0.799302	2.831544	-1.579083
H	1.188088	2.037389	-2.855263

C	-1.235752	-1.831046	3.365140
C	0.098049	-2.390330	3.842295
H	-2.056245	-2.517824	3.623510
H	-1.447136	-0.853599	3.825276
C	1.282686	-1.474302	3.563728
H	0.037349	-2.571648	4.932625
H	0.274165	-3.366802	3.360534
H	1.147556	-0.486423	4.029814
H	2.210420	-1.916239	3.958250
C	-3.016908	1.809816	-0.074058
C	-3.814550	2.493452	-1.010513
C	-3.318370	1.928102	1.289642
C	-4.877032	3.295657	-0.586109
H	-3.615234	2.392621	-2.079869
C	-4.390083	2.723680	1.714279
H	-2.708640	1.396764	2.020824
C	-5.166987	3.413146	0.779175
H	-5.484277	3.826041	-1.323463
H	-4.612218	2.806030	2.780621
H	-5.999813	4.037721	1.110196
C	-2.566797	-0.526238	-1.626253
C	-2.210616	-0.887897	-2.936804
C	-3.662934	-1.172235	-1.024874
C	-2.932497	-1.863986	-3.632983
H	-1.367173	-0.404765	-3.434202
C	-4.380259	-2.151888	-1.718522
H	-3.960277	-0.904106	-0.010178
C	-4.018765	-2.501961	-3.024363
H	-2.644419	-2.124568	-4.654127
H	-5.229289	-2.641210	-1.235561
H	-4.582488	-3.264406	-3.566340
C	1.975968	2.864386	-0.265275
C	3.132995	3.398246	-0.863142
C	1.150524	3.718215	0.482117
C	3.455735	4.750022	-0.708061
H	3.792865	2.754160	-1.447535
C	1.470482	5.072932	0.632272
H	0.255799	3.319807	0.961139
C	2.625140	5.592425	0.040155
H	4.361893	5.145283	-1.173539
H	0.816130	5.718450	1.222507
H	2.879559	6.647687	0.162506
C	3.090695	0.317978	-0.993722
C	3.369284	-0.252005	-2.247410
C	4.086971	0.276919	0.001188
C	4.612171	-0.843958	-2.503733
H	2.623395	-0.235321	-3.043408
C	5.327391	-0.313211	-0.255949
H	3.893067	0.717256	0.980498
C	5.594430	-0.877303	-1.508658
H	4.811782	-1.275913	-3.487154
H	6.087522	-0.334128	0.528230
H	6.564266	-1.337843	-1.709360

2$_{\text{ba-ap}}$

Fe	-0.013839	-0.340747	-0.364748
C	-0.185639	0.470176	-1.903523
O	-0.357404	0.961031	-2.957671
P	-0.998004	1.301819	0.787325
P	1.911320	0.429789	0.470722
C	0.122028	1.646339	2.268496
H	0.053725	0.768067	2.929243
C	1.544908	1.814575	1.728384
H	2.291943	1.815136	2.535173
C	-3.705490	-1.946268	-1.238970
C	-3.195340	-1.140849	-2.304953
C	-2.405803	-1.975899	-3.153747
C	-2.447790	-3.316218	-2.617589
C	-3.252773	-3.301752	-1.441168
H	-4.306639	-1.596686	-0.403570
H	-3.349159	-0.072968	-2.435884
H	-1.855783	-1.656024	-4.035048
H	-1.933350	-4.180360	-3.031870
H	-3.479499	-4.153249	-0.804109
S	-1.194801	-1.831016	0.932291
S	0.544275	-2.217842	-1.579298
Co	-1.617782	-2.024727	-1.219615
H	1.634050	2.768343	1.186238
H	-0.218133	2.537049	2.818918
C	-0.278697	-3.362038	1.488587
C	1.125322	-3.542226	0.930382
H	-0.932470	-4.208977	1.227724
H	-0.240573	-3.291477	2.587030
C	1.211969	-3.653855	-0.585054
H	1.755856	-2.709215	1.268340
H	1.561391	-4.460820	1.368611

H	2.263581	-3.753133	-0.895601
H	0.665052	-4.535869	-0.954608
C	3.130030	1.243335	-0.687068
C	4.062667	2.194863	-0.235912
C	3.134704	0.872280	-2.040574
C	4.968106	2.777025	-1.127999
H	4.090730	2.482454	0.817582
C	4.051583	1.445407	-2.930336
H	2.412241	0.133132	-2.393040
C	4.964978	2.402485	-2.477560
H	5.682108	3.521389	-0.767437
H	4.043405	1.147037	-3.981074
H	5.674494	2.856853	-3.172888
C	3.101497	-0.630858	1.460076
C	2.893399	-0.853347	2.833386
C	4.177326	-1.280877	0.830252
C	3.742513	-1.694332	3.559765
H	2.056069	-0.374910	3.347130
C	5.023129	-2.126700	1.555714
H	4.363979	-1.116930	-0.233206
C	4.810588	-2.336176	2.922735
H	3.567862	-1.848526	4.627295
H	5.857197	-2.618697	1.049609
H	5.473507	-2.994042	3.488800
C	-1.126507	3.049539	0.117957
C	-2.059102	3.963934	0.643112
C	-0.210366	3.504112	-0.845208
C	-2.082381	5.291252	0.203953
H	-2.779992	3.637540	1.394663
C	-0.231616	4.834207	-1.280668
H	0.521564	2.817012	-1.270379
C	-1.169748	5.730804	-0.761348
H	-2.819548	5.983109	0.618410
H	0.485301	5.163131	-2.036086
H	-1.191195	6.766826	-1.106906
C	-2.688806	1.076398	1.531600
C	-2.891371	0.787895	2.890226
C	-3.806216	1.148348	0.680860
C	-4.184057	0.587715	3.389856
H	-2.043330	0.714365	3.572664
C	-5.096661	0.955160	1.180388
H	-3.664362	1.368221	-0.379715
C	-5.289132	0.671613	2.538283
H	-4.324530	0.362813	4.449641
H	-5.954098	1.023403	0.506906
H	-6.297047	0.516047	2.929245

$\mathbf{2'}_{\text{ba-ap}}$

Fe	-0.016238	-0.286412	-0.432166
C	-0.176722	0.557184	-1.957072
O	-0.352115	1.056094	-3.007069
P	-0.978091	1.348232	0.748756
P	1.901907	0.389460	0.472528
C	0.098263	1.571214	2.284278
H	-0.029511	0.665600	2.897233
C	1.546961	1.707629	1.803305
H	2.263693	1.629599	2.633653
C	-3.715212	-1.811863	-1.064760
C	-3.214640	-1.087570	-2.192308
C	-2.522963	-2.009455	-3.038087
C	-2.619076	-3.321506	-2.441323
C	-3.354181	-3.200252	-1.226493
H	-4.253363	-1.386663	-0.221697
H	-3.312777	-0.019682	-2.366530
H	-1.998895	-1.763244	-3.958110
H	-2.184080	-4.234301	-2.841540
H	-3.589382	-4.004249	-0.533304
S	-1.061253	-1.784601	0.961715
S	0.499980	-2.149749	-1.666920
Co	-1.643009	-2.009996	-1.153756
H	1.693785	2.685569	1.320247
H	-0.227151	2.446616	2.866721
C	-0.013265	-3.244274	1.490707
C	0.418904	-4.169060	0.359947
H	-0.643219	-3.788440	2.210889
H	0.859633	-2.847636	2.030863
C	1.322604	-3.499158	-0.666217
H	0.954523	-5.033933	0.796230
H	-0.476875	-4.563234	-0.149037
H	2.209819	-3.058303	-0.188719
H	1.661929	-4.228905	-1.417129
C	3.194433	1.219513	-0.588003
C	4.184153	2.054223	-0.037194
C	3.193888	0.983123	-1.971212
C	5.142959	2.652952	-0.859613
H	4.215501	2.235540	1.039803

C	4.162611	1.573441	-2.792480
H	2.427257	0.334803	-2.400667
C	5.134790	2.412540	-2.239532
H	5.902171	3.305382	-0.421646
H	4.150462	1.379633	-3.867405
H	5.886483	2.879088	-2.880330
C	2.995762	-0.798357	1.423467
C	2.718686	-1.113453	2.765976
C	4.071239	-1.447814	0.791553
C	3.503574	-2.038649	3.462810
H	1.883408	-0.633956	3.282002
C	4.852974	-2.377280	1.486510
H	4.311934	-1.212352	-0.247507
C	4.573299	-2.676099	2.824392
H	3.276428	-2.261874	4.508004
H	5.688329	-2.865612	0.979118
H	5.186343	-3.398631	3.367329
C	-0.998541	3.129368	0.162463
C	-1.835886	4.081568	0.774971
C	-0.090636	3.565104	-0.816237
C	-1.775840	5.428281	0.404868
H	-2.548928	3.769506	1.540541
C	-0.029338	4.914632	-1.184367
H	0.572429	2.849667	-1.302938
C	-0.873326	5.849305	-0.578685
H	-2.439027	6.150345	0.887181
H	0.679468	5.229637	-1.953270
H	-0.829258	6.901096	-0.870291
C	-2.706731	1.164704	1.410979
C	-2.974033	0.664437	2.695508
C	-3.788474	1.459506	0.560300
C	-4.294089	0.481464	3.126608
H	-2.155279	0.412949	3.370719
C	-5.104828	1.280459	0.991972
H	-3.597976	1.845047	-0.444076
C	-5.361677	0.789096	2.278659
H	-4.485187	0.093961	4.129981
H	-5.932488	1.522318	0.321278
H	-6.390551	0.647026	2.616558

2$^{+}_{\text{ba-ba}}$

Fe	-0.012124	0.061524	0.777319
C	-0.214903	1.346881	1.923875
O	-0.329954	2.139318	2.775604
P	1.477401	1.113936	-0.618891
P	-1.615053	0.725074	-0.725702
C	0.634793	1.292532	-2.291208
H	0.647394	0.308194	-2.782606
C	-0.801563	1.765989	-2.065091
H	-1.390082	1.730998	-2.993208
C	-0.476960	-3.714658	-0.853031
C	0.605496	-2.967835	-1.411128
C	1.788867	-3.309884	-0.689797
C	1.446080	-4.294379	0.299916
C	0.041308	-4.545740	0.197020
H	-1.518066	-3.650200	-1.160300
H	0.531009	-2.260055	-2.230340
H	2.776628	-2.883134	-0.846324
H	2.136838	-4.757652	1.000490
H	-0.538630	-5.235117	0.806292
S	-1.418886	-1.544413	1.509229
S	1.646514	-1.090141	1.780052
Co	0.381569	-2.536565	0.697356
H	-0.812463	2.804665	-1.701785
H	1.202592	1.997543	-2.916579
C	-1.242805	-1.942615	3.339352
C	-0.118327	-1.225163	4.070383
H	-1.145601	-3.036948	3.407553
H	-2.219705	-1.669754	3.764657
C	1.282836	-1.539505	3.567241
H	-0.288756	-0.139914	4.048338
H	-0.166125	-1.524199	5.134013
H	2.034322	-0.975646	4.139070
H	1.522482	-2.609440	3.665371
C	-3.015742	1.781061	-0.122527
C	-3.718078	2.603887	-1.023066
C	-3.417889	1.735005	1.221315
C	-4.792280	3.378152	-0.577346
H	-3.439047	2.640151	-2.078035
C	-4.500580	2.504861	1.661749
H	-2.885333	1.097031	1.927412
C	-5.185444	3.330067	0.765501
H	-5.327134	4.017249	-1.282785
H	-4.803149	2.463003	2.709953
H	-6.026369	3.934682	1.110669
C	-2.526508	-0.590553	-1.679843

C	-2.098872	-1.016300	-2.949884
C	-3.660666	-1.194215	-1.106807
C	-2.791412	-2.021337	-3.634308
H	-1.234797	-0.554763	-3.432199
C	-4.348316	-2.201304	-1.791023
H	-4.024255	-0.861343	-0.133502
C	-3.914803	-2.620232	-3.054058
H	-2.456884	-2.328985	-4.627246
H	-5.234519	-2.651450	-1.338960
H	-4.458590	-3.400041	-3.590702
C	1.963620	2.886069	-0.298281
C	3.223785	3.376470	-0.687206
C	1.020967	3.781657	0.236286
C	3.534249	4.730710	-0.528801
H	3.968731	2.703804	-1.113559
C	1.333269	5.136741	0.386240
H	0.038135	3.430070	0.549499
C	2.592218	5.613478	0.009286
H	4.518886	5.094954	-0.829069
H	0.591089	5.816645	0.809098
H	2.838968	6.669537	0.134595
C	3.099088	0.300912	-1.001238
C	3.374454	-0.289275	-2.247289
C	4.086801	0.259104	0.002981
C	4.608272	-0.907794	-2.483508
H	2.643382	-0.259722	-3.056145
C	5.317955	-0.356401	-0.237341
H	3.903174	0.727510	0.971331
C	5.581016	-0.945167	-1.479650
H	4.810856	-1.350495	-3.460927
H	6.075841	-0.371649	0.548398
H	6.544837	-1.422036	-1.668055

CF_3SO_3H

S	0.885477	-0.156867	-0.000109
C	-1.045146	-0.001837	0.000000
F	-1.532591	-1.250629	0.000255
F	-1.452104	0.646046	1.096285
F	-1.452257	0.645665	-1.096453
O	1.119791	1.499463	-0.000419
H	2.088612	1.656006	0.000191
O	1.315663	-0.728799	-1.291108
O	1.315891	-0.728292	1.291047

$[\mathbf{2}\mu\mathrm{H}]^+_{\text{ba-ba}}$ ($CF_3SO_3^-$ is included)

Fe	0.007642	0.035232	0.714742
C	-0.164412	1.300115	1.916224
O	-0.248561	2.097600	2.762870
P	1.493112	1.142723	-0.618622
P	-1.607249	0.761463	-0.723114
C	0.657623	1.302099	-2.293750
H	0.680403	0.309881	-2.768345
C	-0.784694	1.769918	-2.085091
H	-1.367652	1.703284	-3.015044
C	-0.534295	-3.919387	-0.806938
C	0.652695	-3.423964	-1.430978
C	1.762056	-3.653643	-0.560495
C	1.258833	-4.309099	0.618320
C	-0.153592	-4.473223	0.465130
H	-1.541354	-3.867698	-1.211843
H	0.697464	-2.926873	-2.396348
H	2.793309	-3.364428	-0.743353
H	1.850131	-4.620524	1.475644
H	-0.826356	-4.929082	1.187265
S	-1.400928	-1.601334	1.483162
S	1.633386	-1.220533	1.725224
Co	0.342872	-2.461797	0.427097
H	-0.803772	2.818501	-1.751666
H	1.222229	2.002745	-2.926642
C	-1.250100	-1.923314	3.315152
C	-0.105853	-1.230428	4.040343
H	-1.194440	-3.017844	3.417660
H	-2.217844	-1.601370	3.728190
C	1.282364	-1.578268	3.521322
H	-0.251783	-0.141776	4.015663
H	-0.152421	-1.519995	5.106206
H	2.048478	-1.005199	4.064868
H	1.509463	-2.646915	3.655541
C	-2.961569	1.860174	-0.097496
C	-3.629314	2.735650	-0.974189
C	-3.367624	1.791133	1.244540
C	-4.673365	3.538226	-0.506736
H	-3.346441	2.792488	-2.027212
C	-4.419531	2.590157	1.706703

H	-2.862223	1.111023	1.931566
C	-5.070177	3.466931	0.833902
H	-5.181500	4.218012	-1.193630
H	-4.725386	2.530162	2.753063
H	-5.887123	4.094022	1.196093
C	-2.559513	-0.543229	-1.647609
C	-2.096662	-1.053720	-2.872995
C	-3.746335	-1.059436	-1.099637
C	-2.811370	-2.053051	-3.541801
H	-1.183976	-0.666312	-3.330556
C	-4.455386	-2.063813	-1.766642
H	-4.132021	-0.662284	-0.159278
C	-3.990526	-2.564155	-2.987636
H	-2.450937	-2.425718	-4.503071
H	-5.381445	-2.447735	-1.333869
H	-4.551327	-3.339929	-3.512594
C	1.959040	2.915399	-0.289298
C	3.219080	3.416616	-0.665357
C	1.003689	3.802292	0.237456
C	3.515997	4.773406	-0.503860
H	3.973807	2.749860	-1.083906
C	1.303014	5.159827	0.391418
H	0.020763	3.442574	0.541513
C	2.561120	5.647560	0.025672
H	4.500192	5.146476	-0.794534
H	0.551419	5.833209	0.807980
H	2.797442	6.705694	0.153542
C	3.118695	0.331683	-0.975381
C	3.411290	-0.263953	-2.214374
C	4.088263	0.291140	0.045395
C	4.648727	-0.882854	-2.428913
H	2.691696	-0.236477	-3.033754
C	5.324009	-0.322701	-0.174068
H	3.885921	0.757445	1.011384
C	5.606376	-0.914532	-1.410520
H	4.866987	-1.329349	-3.401302
H	6.069044	-0.336820	0.623869
H	6.573635	-1.390677	-1.582757
H	0.259264	-1.136939	-0.493248

$[\mathbf{2}\mu\mathrm{H}]^{+}_{\text{ba-ba}}$

Fe	-1.597940	0.325846	0.566607
C	-3.169142	0.873346	0.034463
O	-4.230258	1.280230	-0.244281
P	-0.361942	1.732945	-0.732149
P	-1.178496	-1.244152	-1.048139
C	0.815758	0.643677	-1.684447
H	1.586954	0.274158	-0.991676
C	0.026772	-0.511829	-2.300759
H	0.717181	-1.280892	-2.675572
C	1.149135	-1.761785	3.050926
C	1.867133	-0.610569	2.592891
C	1.558157	0.481469	3.459275
C	0.652075	0.005545	4.474429
C	0.404935	-1.381350	4.221941
H	1.154981	-2.741864	2.581398
H	2.512294	-0.555375	1.710328
H	1.922196	1.499673	3.350551
H	0.229818	0.595401	5.284343
H	-0.248109	-2.029920	4.801246
S	-2.074695	-1.329728	2.085050
S	-1.377553	1.645772	2.425881
Co	-0.227187	-0.235108	2.625216
H	-0.588696	-0.158387	-3.141885
H	1.328237	1.228978	-2.461504
C	-3.428859	-0.883048	3.287334
C	-3.937881	0.550708	3.242725
H	-3.037437	-1.141443	4.283313
H	-4.244460	-1.585349	3.057158
C	-2.882284	1.609957	3.530639
H	-4.409304	0.748640	2.270079
H	-4.739511	0.655110	3.998082
H	-3.316103	2.616441	3.429452
H	-2.491965	1.517720	4.556104
C	-2.586301	-1.867546	-2.090322
C	-2.340462	-2.372342	-3.380629
C	-3.894514	-1.899448	-1.583420
C	-3.389490	-2.879246	-4.152337
H	-1.326731	-2.380492	-3.786192
C	-4.942513	-2.414930	-2.355475
H	-4.098904	-1.518062	-0.581868
C	-4.693065	-2.901000	-3.641988
H	-3.185645	-3.263084	-5.154343
H	-5.956414	-2.429500	-1.949713
H	-5.511137	-3.298103	-4.246757
C	-0.395374	-2.837353	-0.503370

C	1.000111	-2.986285	-0.522646
C	-1.196367	-3.890351	-0.025232
C	1.591826	-4.171539	-0.071058
H	1.650143	-2.201296	-0.913516
C	-0.602686	-5.074460	0.421403
H	-2.283688	-3.796146	-0.017673
C	0.790972	-5.215088	0.405225
H	2.681038	-4.250490	-0.098581
H	-1.233201	-5.891071	0.780853
H	1.251015	-6.142588	0.753878
C	-1.163297	2.697631	-2.114539
C	-0.580884	3.884525	-2.598094
C	-2.283997	2.174892	-2.781266
C	-1.120237	4.536208	-3.711392
H	0.298197	4.302248	-2.104973
C	-2.818558	2.826443	-3.898100
H	-2.754384	1.254779	-2.434161
C	-2.241437	4.011256	-4.363284
H	-0.656973	5.457598	-4.071306
H	-3.692453	2.405251	-4.399487
H	-2.660827	4.522859	-5.232252
C	0.688775	2.994183	0.118529
C	2.065790	2.792112	0.315051
C	0.080474	4.159969	0.623034
C	2.820739	3.759617	0.991577
H	2.572175	1.889410	-0.038123
C	0.841751	5.120911	1.291943
H	-0.990150	4.324314	0.481345
C	2.215709	4.922543	1.477268
H	3.891301	3.593666	1.129367
H	0.360156	6.024782	1.671683
H	2.811920	5.674715	1.998906
H	-0.011892	-0.093782	1.034618
O	3.661109	-0.038768	0.052809
S	4.207152	-1.111059	-0.878349
O	4.545730	-2.404402	-0.203698
O	3.443821	-1.219304	-2.171868
C	5.908451	-0.386958	-1.405202
F	5.750190	0.814924	-2.014861
F	6.534676	-1.218357	-2.267318
F	6.709411	-0.208217	-0.328597

$\mathbf{TS1}_{\text{ba-ba}}$

Fe	0.850318	0.006410	-0.590349
C	1.544560	-0.150210	-2.179830
O	1.949074	-0.236632	-3.278690
P	2.319679	1.540457	0.230332
P	2.147586	-1.546485	0.443793
C	3.315588	0.717148	1.606661
H	2.679515	0.693927	2.504680
C	3.672495	-0.702914	1.167537
H	4.092535	-1.290363	1.997032
C	-1.430852	-0.637608	2.602425
C	-0.530556	0.471530	2.647760
C	-1.259670	1.644487	2.277943
C	-2.619602	1.266328	2.030086
C	-2.727320	-0.152632	2.232327
H	-1.171806	-1.675378	2.794233
H	0.518042	0.426943	2.922891
H	-0.846825	2.644408	2.175674
H	-3.426589	1.927430	1.726977
H	-3.636835	-0.739123	2.116699
S	-0.893757	-1.446369	-0.597716
S	-0.761626	1.554257	-0.968401
Co	-1.388829	0.264349	0.688501
H	4.424354	-0.680453	0.364728
H	4.213575	1.312029	1.832603
C	-1.830487	-1.389045	-2.213083
C	-1.550069	-0.200497	-3.124857
H	-2.894332	-1.468969	-1.953096
H	-1.542058	-2.324372	-2.717067
C	-1.752485	1.177616	-2.506935
H	-0.532875	-0.273617	-3.532175
H	-2.236164	-0.280725	-3.988690
H	-1.446380	1.957790	-3.220459
H	-2.799821	1.345312	-2.224129
C	2.887249	-2.915217	-0.583134
C	4.049651	-3.585807	-0.158887
C	2.268788	-3.313995	-1.777400
C	4.590127	-4.620568	-0.927171
H	4.536138	-3.310262	0.779281
C	2.805144	-4.358191	-2.539964
H	1.366223	-2.802132	-2.113275
C	3.968678	-5.008863	-2.120301
H	5.496255	-5.128858	-0.589734

H	2.313161	-4.656909	-3.468044
H	4.390495	-5.819418	-2.718494
C	1.499392	-2.548760	1.880625
C	1.776788	-2.208034	3.215952
C	0.678173	-3.662615	1.624296
C	1.249299	-2.961835	4.270557
H	2.414716	-1.353731	3.452148
C	0.149115	-4.412383	2.679016
H	0.454466	-3.949659	0.595876
C	0.431780	-4.065183	4.005177
H	1.480247	-2.684441	5.301500
H	-0.486425	-5.273425	2.461384
H	0.018772	-4.653072	4.827406
C	3.739387	2.139238	-0.842638
C	4.238748	3.451213	-0.753721
C	4.387736	1.230097	-1.697280
C	5.350578	3.842790	-1.507255
H	3.759512	4.176162	-0.094765
C	5.505258	1.620790	-2.442241
H	4.014444	0.211474	-1.802465
C	5.987755	2.929987	-2.353571
H	5.717954	4.868717	-1.429942
H	5.988741	0.899212	-3.104267
H	6.854053	3.238132	-2.942966
C	1.747799	3.134280	0.999491
C	1.926904	3.433314	2.361404
C	1.086812	4.073371	0.183102
C	1.448312	4.635125	2.897162
H	2.446568	2.737677	3.021464
C	0.612850	5.273862	0.719622
H	0.942349	3.864793	-0.877603
C	0.787717	5.556937	2.079093
H	1.597307	4.849916	3.957653
H	0.100259	5.988199	0.071852
H	0.413617	6.493464	2.497995
H	-2.893875	0.229455	-0.045892
O	-4.103076	0.423577	-0.600488
S	-5.260498	-0.632631	-0.497974
O	-5.189646	-1.665243	-1.569913
O	-5.524921	-1.074741	0.901075
C	-6.745661	0.503801	-0.969204
F	-6.864923	1.517940	-0.087341
F	-6.574117	1.019997	-2.203793
F	-7.882673	-0.220041	-0.955348

$[\mathbf{2}H]^+$

Fe	0.895238	0.000145	-0.582667
C	1.543410	-0.181784	-2.186025
O	1.911241	-0.280557	-3.295009
P	2.423533	1.506714	0.198761
P	2.178359	-1.579252	0.442372
C	3.404868	0.669152	1.574413
H	2.772331	0.667958	2.475028
C	3.726715	-0.762062	1.143928
H	4.140968	-1.351682	1.974825
C	-1.456083	-0.566142	2.629757
C	-0.509333	0.505390	2.691826
C	-1.183615	1.708129	2.308826
C	-2.547573	1.383626	2.020931
C	-2.719959	-0.033207	2.221918
H	-1.243687	-1.613747	2.827274
H	0.526856	0.419004	3.002586
H	-0.728415	2.690845	2.217664
H	-3.320794	2.061734	1.670573
H	-3.652240	-0.574608	2.053940
S	-0.866262	-1.412759	-0.542041
S	-0.660540	1.591118	-0.952543
Co	-1.340837	0.332844	0.713662
H	4.471768	-0.762215	0.334436
H	4.317182	1.244992	1.791788
C	-1.889199	-1.337929	-2.100179
C	-1.619356	-0.162712	-3.031869
H	-2.941135	-1.380524	-1.776671
H	-1.657946	-2.285885	-2.610336
C	-1.765021	1.221638	-2.412105
H	-0.626295	-0.263163	-3.492092
H	-2.354056	-0.230130	-3.855202
H	-1.503100	1.996351	-3.148674
H	-2.789403	1.393420	-2.049787
C	2.870890	-2.967989	-0.587036
C	4.018749	-3.666978	-0.168790
C	2.231741	-3.355203	-1.774217
C	4.524964	-4.718899	-0.936916
H	4.519642	-3.400171	0.764288
C	2.734109	-4.416371	-2.536398
H	1.339454	-2.823663	-2.106393

C	3.883359	-5.095637	-2.123151
H	5.419858	-5.249695	-0.604453
H	2.226323	-4.706188	-3.458658
H	4.278452	-5.919796	-2.720861
C	1.511440	-2.546264	1.892320
C	1.793426	-2.186643	3.221841
C	0.669985	-3.648712	1.653671
C	1.249605	-2.911123	4.288515
H	2.449835	-1.342535	3.443818
C	0.124353	-4.368757	2.720721
H	0.444494	-3.952195	0.630479
C	0.410648	-4.002537	4.040810
H	1.484862	-2.620771	5.314848
H	-0.527263	-5.221037	2.517174
H	-0.015549	-4.567224	4.872429
C	3.840464	2.056351	-0.898277
C	4.386252	3.349912	-0.812256
C	4.441464	1.127536	-1.766001
C	5.498431	3.704822	-1.582849
H	3.942746	4.088557	-0.143491
C	5.559048	1.482149	-2.528726
H	4.032081	0.122315	-1.865623
C	6.088206	2.773381	-2.443269
H	5.903325	4.716631	-1.508221
H	6.006177	0.747053	-3.201230
H	6.954595	3.053404	-3.046280
C	1.886991	3.116688	0.955699
C	2.050923	3.410487	2.320693
C	1.264039	4.072230	0.128573
C	1.594340	4.624276	2.848562
H	2.542341	2.702588	2.989307
C	0.810879	5.283894	0.657720
H	1.136640	3.870613	-0.935687
C	0.969912	5.561939	2.020066
H	1.731803	4.835785	3.911203
H	0.327022	6.010691	0.001952
H	0.611916	6.507181	2.433205
H	-2.613943	0.352252	-0.043336
O	-4.416541	0.774681	-0.649739
S	-5.365792	-0.406566	-0.462239
O	-5.135379	-1.527138	-1.433373
O	-5.575162	-0.796257	0.971896
C	-7.054112	0.345286	-0.998161
F	-7.377862	1.405241	-0.220152
F	-7.003551	0.765890	-2.284706
F	-8.037518	-0.575663	-0.891227

$\mathbf{TS2}_{\text{ba-ba}}$

Fe	-0.915834	0.095435	0.913526
C	-2.301601	0.849639	1.633671
O	-3.227996	1.311013	2.188768
P	-0.399563	1.976561	-0.273155
P	-1.781934	-0.663619	-1.046304
C	-0.292966	1.521738	-2.091078
H	0.679618	1.042108	-2.255233
C	-1.452356	0.584168	-2.436234
H	-1.268735	0.052488	-3.381238
C	1.417595	-3.710383	1.206665
C	2.395721	-2.884205	0.592478
C	3.036698	-2.118468	1.629450
C	2.473162	-2.518189	2.890526
C	1.475969	-3.493276	2.634921
H	0.736341	-4.382843	0.691924
H	2.630771	-2.847792	-0.467725
H	3.826346	-1.387063	1.489968
H	2.749018	-2.119618	3.863973
H	0.849456	-3.982718	3.376692
S	-1.189283	-1.936615	1.829839
S	0.737626	0.333512	2.451026
Co	0.989999	-1.682195	1.624212
H	-2.386297	1.154076	-2.550212
H	-0.334549	2.434129	-2.705247
C	-1.548263	-1.824570	3.669542
C	-1.289856	-0.487226	4.355750
H	-0.952701	-2.629688	4.125343
H	-2.610665	-2.097322	3.766100
C	0.117523	0.077231	4.202662
H	-2.018773	0.254157	4.005077
H	-1.489837	-0.620285	5.436398
H	0.173863	1.071307	4.672713
H	0.867694	-0.566284	4.686310
C	-3.625414	-0.926385	-1.186749
C	-4.243956	-0.968960	-2.450265
C	-4.407785	-1.127033	-0.040000
C	-5.619697	-1.188126	-2.558743
H	-3.650476	-0.841729	-3.358041

C	-5.785055	-1.355330	-0.150313
H	-3.936427	-1.106671	0.943049
C	-6.394059	-1.381390	-1.407943
H	-6.087509	-1.214611	-3.545536
H	-6.381251	-1.507748	0.752059
H	-7.469010	-1.554668	-1.494174
C	-1.175247	-2.286191	-1.730223
C	-0.041409	-2.342724	-2.556157
C	-1.823499	-3.483090	-1.375402
C	0.430132	-3.570317	-3.031738
H	0.491350	-1.432974	-2.837365
C	-1.350001	-4.709350	-1.852450
H	-2.707894	-3.458245	-0.736538
C	-0.224015	-4.756499	-2.682576
H	1.319407	-3.590592	-3.664095
H	-1.868441	-5.631016	-1.577612
H	0.143111	-5.715081	-3.055926
C	-1.721211	3.312816	-0.382580
C	-1.380705	4.676717	-0.438772
C	-3.075523	2.959215	-0.521544
C	-2.365598	5.653952	-0.619176
H	-0.339244	4.984482	-0.341195
C	-4.058604	3.936244	-0.709835
H	-3.383917	1.914515	-0.468491
C	-3.708237	5.288763	-0.754552
H	-2.076468	6.707022	-0.652426
H	-5.103449	3.633888	-0.808561
H	-4.476367	6.052823	-0.893226
C	1.093747	3.011559	0.087317
C	2.060718	3.310944	-0.884280
C	1.222734	3.559640	1.376702
C	3.130606	4.158210	-0.573206
H	2.000112	2.877966	-1.883247
C	2.292659	4.404532	1.683148
H	0.475005	3.336456	2.140305
C	3.248889	4.707164	0.707050
H	3.876952	4.382211	-1.338145
H	2.380921	4.823751	2.687931
H	4.085902	5.367298	0.945334
H	1.643825	-0.784469	0.141243
O	2.311354	-0.016577	-0.604869
S	3.178277	-0.327605	-1.889545
O	3.287977	-1.776516	-2.213685
O	2.838178	0.621138	-2.987664
C	4.953780	0.183044	-1.325594
F	4.990991	1.478485	-0.970012
F	5.809150	-0.017667	-2.345577
F	5.347102	-0.569456	-0.274196

TS_{iso}

Fe	1.028617	0.097009	-0.680975
C	1.634389	0.919067	-2.102477
O	1.955496	1.419817	-3.112717
P	0.769334	1.858368	0.745956
P	3.013325	-0.245689	0.343557
C	1.980472	1.595854	2.163491
H	1.549051	0.816026	2.809088
C	3.318164	1.137520	1.584946
H	4.014893	0.813168	2.372130
C	-0.200328	-3.055906	1.648622
C	-0.742252	-1.917282	2.305460
C	-2.060806	-1.697898	1.765740
C	-2.353374	-2.769157	0.819057
C	-1.210103	-3.587049	0.743923
H	0.796815	-3.462634	1.796332
H	-0.252234	-1.309216	3.060104
H	-2.791448	-0.942638	2.056644
H	-3.267571	-2.825912	0.227500
H	-1.079233	-4.451680	0.097612
S	0.926914	-2.089179	-1.219629
S	-1.177287	0.124404	-1.148369
Co	-0.671838	-1.600440	0.231551
H	3.799544	1.956428	1.028572
H	2.083064	2.521559	2.749551
C	0.098084	-2.455023	-2.857261
C	-0.583130	-1.286045	-3.553917
H	-0.612059	-3.269430	-2.649390
H	0.906475	-2.860468	-3.484885
C	-1.714529	-0.649907	-2.763757
H	0.166270	-0.525149	-3.820199
H	-1.005602	-1.652952	-4.507927
H	-2.161873	0.199036	-3.301129
H	-2.533517	-1.335245	-2.494810
C	4.565566	-0.252755	-0.686658
C	5.811032	0.068946	-0.116754
C	4.511033	-0.627834	-2.037652

C	6.974053	0.031597	-0.891071
H	5.882789	0.343418	0.937698
C	5.678491	-0.676822	-2.808290
H	3.550373	-0.877306	-2.489863
C	6.910343	-0.342429	-2.238645
H	7.933832	0.290767	-0.438605
H	5.620400	-0.969160	-3.858924
H	7.820287	-0.373266	-2.841732
C	3.295014	-1.793273	1.352648
C	3.074302	-1.822784	2.740862
C	3.703592	-2.975294	0.708771
C	3.263472	-3.002291	3.469533
H	2.758970	-0.923128	3.272787
C	3.884549	-4.155497	1.437122
H	3.897948	-2.972305	-0.364732
C	3.665203	-4.174018	2.818766
H	3.097069	-3.003271	4.549047
H	4.205813	-5.062985	0.921168
H	3.812070	-5.094733	3.387112
C	1.268580	3.581538	0.210226
C	0.646546	4.720926	0.752266
C	2.343212	3.755562	-0.678408
C	1.088897	6.001977	0.406805
H	-0.192937	4.609582	1.440151
C	2.789454	5.038090	-1.015309
H	2.830319	2.890196	-1.128523
C	2.161634	6.164909	-0.476089
H	0.588030	6.875823	0.829495
H	3.622534	5.152468	-1.712211
H	2.502738	7.166346	-0.747266
C	-0.850927	2.159261	1.596448
C	-1.021538	1.953002	2.977585
C	-1.958430	2.571857	0.829420
C	-2.272996	2.147661	3.573059
H	-0.183600	1.648984	3.606571
C	-3.210633	2.744271	1.424519
H	-1.856197	2.747223	-0.241858
C	-3.370373	2.532885	2.797083
H	-2.388468	1.988105	4.647662
H	-4.065275	3.005536	0.799732
H	-4.353352	2.652047	3.256122
H	-1.710304	-0.488709	0.366791
O	-4.914161	-0.292136	-0.637469
S	-6.832900	-0.416920	-0.673104
O	-7.288818	-0.518642	-1.943883
O	-7.260461	-1.503408	0.015475
C	-7.393951	0.682641	-0.111455
F	-4.603937	-0.203652	0.836441
F	-4.618225	0.945673	-1.434582
F	-4.472193	-1.588367	-1.280961

$TS3_{ba\text{-}ap}$

Fe	0.651287	-0.082550	-0.331541
C	0.208156	1.404105	-1.158501
O	-0.001011	2.360579	-1.792395
P	-0.081651	0.558575	1.739541
P	2.639785	0.806617	0.193809
C	1.470855	1.004871	2.719177
H	1.955184	0.079671	3.061700
C	2.402944	1.788750	1.793844
H	3.373081	1.985492	2.273451
C	-1.991057	-3.578968	-0.129476
C	-2.820338	-2.548977	-0.649824
C	-2.593542	-2.460232	-2.064846
C	-1.635450	-3.472875	-2.412176
C	-1.258604	-4.165073	-1.227227
H	-1.901139	-3.856413	0.917670
H	-3.484655	-1.916763	-0.071768
H	-3.050418	-1.747888	-2.747089
H	-1.243515	-3.651181	-3.410986
H	-0.544295	-4.981551	-1.155775
S	0.856418	-2.233440	0.418225
S	0.588819	-1.061378	-2.407139
Co	-0.783927	-2.115051	-1.053928
H	1.947884	2.752696	1.514538
H	1.199950	1.592468	3.607759
C	2.246845	-3.185393	-0.400785
C	2.918277	-2.545720	-1.607892
H	1.810481	-4.162526	-0.657902
H	2.987579	-3.346464	0.395886
C	1.992543	-2.242048	-2.773764
H	3.424148	-1.621265	-1.294269
H	3.714717	-3.229887	-1.958022
H	2.553845	-1.771231	-3.595738
H	1.523042	-3.156048	-3.169386
C	3.384185	2.055880	-0.964923

C	4.115653	3.162653	-0.497362
C	3.218526	1.885553	-2.348939
C	4.670502	4.076889	-1.398595
H	4.262482	3.317849	0.573157
C	3.781926	2.795622	-3.249293
H	2.621973	1.049658	-2.721631
C	4.507537	3.893400	-2.776297
H	5.229480	4.936305	-1.021632
H	3.636948	2.653852	-4.322308
H	4.938432	4.610048	-3.478804
C	4.153341	-0.204382	0.672561
C	4.053283	-1.189872	1.672822
C	5.410867	0.030886	0.088946
C	5.182543	-1.897194	2.097397
H	3.082359	-1.428738	2.110827
C	6.537105	-0.689950	0.503108
H	5.515278	0.784509	-0.692843
C	6.429722	-1.650515	1.512990
H	5.083657	-2.651422	2.881657
H	7.503565	-0.493116	0.033368
H	7.310437	-2.207284	1.840093
C	-1.103448	2.081932	2.114678
C	-1.340502	2.398613	3.468538
C	-1.614259	2.927270	1.122901
C	-2.056847	3.545105	3.816030
H	-0.984311	1.734181	4.259724
C	-2.334758	4.077094	1.474158
H	-1.494965	2.693004	0.069800
C	-2.552798	4.392331	2.816210
H	-2.235412	3.772521	4.869634
H	-2.737425	4.708979	0.680494
H	-3.118484	5.286801	3.086818
C	-0.959605	-0.691565	2.802803
C	-0.287375	-1.555867	3.681116
C	-2.357163	-0.798354	2.676958
C	-1.000117	-2.494469	4.437480
H	0.796785	-1.504339	3.790570
C	-3.065559	-1.738012	3.430037
H	-2.889352	-0.134625	1.992112
C	-2.389162	-2.588500	4.313782
H	-0.464307	-3.153599	5.124392
H	-4.151191	-1.802973	3.328495
H	-2.944496	-3.319141	4.906059
H	-1.582136	-0.442329	-0.839071
O	-2.560033	0.427754	-0.678439
S	-3.404934	1.146781	-1.802389
O	-5.191211	0.793301	-1.159690
O	-5.356578	1.274241	0.091004
C	-6.089610	1.380790	-1.972571
F	-5.435757	-0.539876	-1.139195
F	-3.324075	0.465629	-3.123159
F	-3.276141	2.624791	-1.735140

$[\mathbf{2}\mu\mathrm{H}]^{+}_{\text{ba-ap}}$

Fe	1.008839	-0.095521	-0.357079
C	0.552625	1.349601	-1.257790
O	0.265007	2.270098	-1.904885
P	0.294854	0.803770	1.623817
P	3.026784	0.798625	0.097390
C	1.834485	1.308628	2.563999
H	2.268086	0.397728	2.998767
C	2.812065	1.951916	1.578357
H	3.787195	2.149599	2.046799
C	-1.930176	-3.244784	-0.082563
C	-2.571777	-2.087771	-0.607613
C	-2.313497	-2.030076	-2.018143
C	-1.523880	-3.175593	-2.363753
C	-1.271160	-3.928637	-1.170839
H	-1.908634	-3.542726	0.962744
H	-3.154287	-1.340315	-0.060934
H	-2.690599	-1.247132	-2.672373
H	-1.147235	-3.411603	-3.356497
H	-0.704357	-4.853906	-1.100542
S	1.120683	-2.241486	0.545305
S	1.040470	-1.227167	-2.379815
Co	-0.476673	-2.038737	-0.987864
H	2.409302	2.900703	1.190217
H	1.586704	1.973910	3.402727
C	2.481784	-3.310527	-0.158096
C	3.237900	-2.778893	-1.367070
H	1.998404	-4.274023	-0.380356
H	3.177071	-3.469234	0.678841
C	2.381447	-2.503842	-2.590810
H	3.779572	-1.864618	-1.086774
H	4.008566	-3.523911	-1.640643
H	3.003900	-2.125109	-3.415894
H	1.874360	-3.414200	-2.945946

C	3.800086	1.890244	-1.189469
C	4.596631	2.995849	-0.837693
C	3.587376	1.608177	-2.548410
C	5.167383	3.799967	-1.828917
H	4.780008	3.236706	0.211212
C	4.166189	2.409294	-3.538049
H	2.944331	0.772054	-2.832374
C	4.955047	3.507007	-3.180799
H	5.776585	4.660006	-1.542569
H	3.984653	2.182801	-4.590697
H	5.397754	4.138769	-3.953669
C	4.482998	-0.224526	0.689976
C	4.314658	-1.123594	1.759989
C	5.763590	-0.079650	0.128308
C	5.403609	-1.834551	2.273860
H	3.322607	-1.294121	2.182973
C	6.848917	-0.804557	0.634430
H	5.920282	0.603595	-0.707310
C	6.675579	-1.677565	1.712133
H	5.253922	-2.520203	3.110972
H	7.835400	-0.679979	0.182250
H	7.524943	-2.236808	2.109844
C	-0.693872	2.368364	1.506804
C	-0.387366	3.507015	2.275101
C	-1.810316	2.401697	0.654615
C	-1.182412	4.653153	2.182958
H	0.464508	3.519475	2.956321
C	-2.622351	3.538200	0.585696
H	-2.083343	1.531201	0.055595
C	-2.301499	4.668146	1.343310
H	-0.928973	5.532185	2.780279
H	-3.511288	3.506350	-0.050411
H	-2.930108	5.559452	1.285119
C	-0.673954	-0.252580	2.803958
C	-0.027174	-1.072110	3.746221
C	-2.078292	-0.277619	2.720251
C	-0.771883	-1.883005	4.608565
H	1.061273	-1.086707	3.822004
C	-2.815980	-1.099112	3.578775
H	-2.620307	0.329297	1.990982
C	-2.168213	-1.897826	4.527285
H	-0.256544	-2.504714	5.344214
H	-3.904626	-1.102512	3.497077
H	-2.749492	-2.531106	5.201202
H	-0.606133	-0.516090	-0.439641
O	-4.363750	0.294325	0.344621
S	-5.002560	0.833402	-0.923904
O	-6.788920	0.128124	-0.818691
O	-7.423922	0.574355	0.292069
C	-7.519073	0.494511	-1.897257
F	-6.767005	-1.229914	-0.768694
F	-4.454959	0.224737	-2.185125
F	-5.205430	2.318439	-0.940983

Electronic energies, zero-point energies, enthalpies and free energies (in Hartrees) for all of the relevant species

2$_{ba\text{-}ba}$

SCF Done: E(RB-P86) = -5556.88919982
Zero-point correction= 0.588801 (Hartree/Particle)
Thermal correction to Energy= 0.630852
Thermal correction to Enthalpy= 0.631796
Thermal correction to Gibbs Free Energy= 0.512900
Sum of electronic and zero-point Energies= -5556.300399
Sum of electronic and thermal Energies= -5556.258348
Sum of electronic and thermal Enthalpies= -5556.257404
Sum of electronic and thermal Free Energies= -5556.376300
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -5556.93533229

2′$_{ba\text{-}ba}$

SCF Done: E(RB-P86) = -5556.89152408
Zero-point correction= 0.589171 (Hartree/Particle)
Thermal correction to Energy= 0.631098
Thermal correction to Enthalpy= 0.632042
Thermal correction to Gibbs Free Energy= 0.513842
Sum of electronic and zero-point Energies= -5556.302353
Sum of electronic and thermal Energies= -5556.260427
Sum of electronic and thermal Enthalpies= -5556.259482
Sum of electronic and thermal Free Energies= -5556.377682
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -5556.93714348

2$_{ba\text{-}ap}$

SCF Done: E(RB-P86) = -5556.88532303
Zero-point correction= 0.588905 (Hartree/Particle)
Thermal correction to Energy= 0.631003
Thermal correction to Enthalpy= 0.631947
Thermal correction to Gibbs Free Energy= 0.512569
Sum of electronic and zero-point Energies= -5556.296418
Sum of electronic and thermal Energies= -5556.254320
Sum of electronic and thermal Enthalpies= -5556.253376
Sum of electronic and thermal Free Energies= -5556.372754
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -5556.93247617

$\mathbf{2'}_{\text{ba-ap}}$

SCF Done: E(RB-P86) = -5556.88923269
Zero-point correction= 0.588949 (Hartree/Particle)
Thermal correction to Energy= 0.630937
Thermal correction to Enthalpy= 0.631881
Thermal correction to Gibbs Free Energy= 0.513122
Sum of electronic and zero-point Energies= -5556.300283
Sum of electronic and thermal Energies= -5556.258296
Sum of electronic and thermal Enthalpies= -5556.257352
Sum of electronic and thermal Free Energies= -5556.376111
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -5556.93507023

$\mathbf{2}^{+}_{\text{ba-ba}}$

SCF Done: E(UB-P86) = -5556.69401889
Zero-point correction= 0.590582 (Hartree/Particle)
Thermal correction to Energy= 0.632720
Thermal correction to Enthalpy= 0.633664
Thermal correction to Gibbs Free Energy= 0.514005
Sum of electronic and zero-point Energies= -5556.103437
Sum of electronic and thermal Energies= -5556.061299
Sum of electronic and thermal Enthalpies= -5556.060355
Sum of electronic and thermal Free Energies= -5556.180014
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(UB-P86) = -5556.78417090

CF_3SO_3H

SCF Done: E(RB-P86) = -962.305527977
Zero-point correction= 0.035472 (Hartree/Particle)
Thermal correction to Energy= 0.043236
Thermal correction to Enthalpy= 0.044180
Thermal correction to Gibbs Free Energy= 0.002112
Sum of electronic and zero-point Energies= -962.270056
Sum of electronic and thermal Energies= -962.262292
Sum of electronic and thermal Enthalpies= -962.261348
Sum of electronic and thermal Free Energies= -962.303416
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -962.312927503

$[\mathbf{2}\mu\mathrm{H}]^{+}_{\text{ba-ba}}$

SCF Done: E(RB-P86) = -6519.23347765
Zero-point correction= 0.625364 (Hartree/Particle)
Thermal correction to Energy= 0.676793
Thermal correction to Enthalpy= 0.677737
Thermal correction to Gibbs Free Energy= 0.535735
Sum of electronic and zero-point Energies= -6518.608113
Sum of electronic and thermal Energies= -6518.556685
Sum of electronic and thermal Enthalpies= -6518.555741
Sum of electronic and thermal Free Energies= -6518.697743
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -6519.23184836

$\mathbf{TS1}_{\text{ba-ba}}$

SCF Done: E(RB-P86) = -6519.20216269
Zero-point correction= 0.621713 (Hartree/Particle)
Thermal correction to Energy= 0.672860
Thermal correction to Enthalpy= 0.673804
Thermal correction to Gibbs Free Energy= 0.532793
Sum of electronic and zero-point Energies= -6518.580449
Sum of electronic and thermal Energies= -6518.529303
Sum of electronic and thermal Enthalpies= -6518.528359
Sum of electronic and thermal Free Energies= -6518.669370
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -6519.25460823

$[\mathbf{2}\mathrm{H}]^{+}$

SCF Done: E(RB-P86) = -6519.20427837
Zero-point correction= 0.625000 (Hartree/Particle)
Thermal correction to Energy= 0.676479
Thermal correction to Enthalpy= 0.677423
Thermal correction to Gibbs Free Energy= 0.534510
Sum of electronic and zero-point Energies= -6518.579278
Sum of electronic and thermal Energies= -6518.527799
Sum of electronic and thermal Enthalpies= -6518.526855
Sum of electronic and thermal Free Energies= -6518.669768
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -6519.26580960

$\mathbf{TS2}_{\text{ba-ba}}$

SCF Done: E(RB-P86) = -6519.18531036
Zero-point correction= 0.620853 (Hartree/Particle)

Thermal correction to Energy= 0.672136
Thermal correction to Enthalpy= 0.673081
Thermal correction to Gibbs Free Energy= 0.533409
Sum of electronic and zero-point Energies= -6518.564458
Sum of electronic and thermal Energies= -6518.513174
Sum of electronic and thermal Enthalpies= -6518.512230
Sum of electronic and thermal Free Energies= -6518.651901
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -6519.23184836

$\mathbf{TS}_{\mathrm{iso}}$

SCF Done: E(RB-P86) = -6519.16785311
Zero-point correction= 0.621837 (Hartree/Particle)
Thermal correction to Energy= 0.673556
Thermal correction to Enthalpy= 0.674500
Thermal correction to Gibbs Free Energy= 0.530776
Sum of electronic and zero-point Energies= -6518.546016
Sum of electronic and thermal Energies= -6518.494298
Sum of electronic and thermal Enthalpies= -6518.493353
Sum of electronic and thermal Free Energies= -6518.637077
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -6519.22869204

$\mathbf{TS3}_{\mathrm{ba\text{-}ap}}$

SCF Done: E(RB-P86) = -6519.18322380
Zero-point correction= 0.620279 (Hartree/Particle)
Thermal correction to Energy= 0.671741
Thermal correction to Enthalpy= 0.672685
Thermal correction to Gibbs Free Energy= 0.531334
Sum of electronic and zero-point Energies= -6518.562945
Sum of electronic and thermal Energies= -6518.511483
Sum of electronic and thermal Enthalpies= -6518.510539
Sum of electronic and thermal Free Energies= -6518.651890
PCM model with SMD (dichloromethane as solvent) :
SCF Done: E(RB-P86) = -6519.23579428

$[\mathbf{2}\mu\mathrm{H}]^{+}_{\mathrm{ba\text{-}ap}}$

SCF Done: E(RB-P86) = -6519.21634783
Zero-point correction= 0.625071 (Hartree/Particle)
Thermal correction to Energy= 0.676488

Thermal correction to Enthalpy= 0.677432

Thermal correction to Gibbs Free Energy= 0.535078

Sum of electronic and zero-point Energies= -6518.591277

Sum of electronic and thermal Energies= -6518.539860

Sum of electronic and thermal Enthalpies= -6518.538916

Sum of electronic and thermal Free Energies= -6518.681269

PCM model with SMD (dichloromethane as solvent) :

SCF Done: E(RB-P86) = -6519.28092178