Advanced Synthesis & Catalysis

Supporting Information

Coupling of CO_2 with Epoxides Efficiently Catalyzed by Thioether-Triphenolate Bimetallic Iron(III) Complexes: Catalyst Structure - Reactivity Relationship and Mechanistic DFT Study

Francesco Della Monica[a], Sai V.C. Vummaleti[b], Antonio Buonerba[ac], Assunta De Nisi[cd], Magda Monari[cd], Stefano Milione[ac], Alfonso Grassi[ac], Luigi Cavallo[b]*, Carmine Capacchione[ac]*

[a] Dipartimento di Chimica e Biologia "Adolfo Zambelli", Università degli Studi di Salerno, via Giovanni Paolo II, 84084 Fisciano(SA), Italy [e-mail: ccapacchione@unisa.it]

[b] KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia [e-mail: luigi.cavallo@kaust.edu.sa]

[c] Interuniversity Consortium Chemical Reactivity and Catalysis, CIRCC, via Celso Ulpiani 27, 70126 (BA), Italy

[d] Dipartimento di Chimica G. Ciamician, Alma Mater Studiorum, Università di Bologna, via Selmi 2, Bologna, Italy

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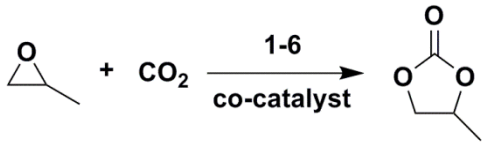
I. CATALYTIC TESTS

Table_S 1**. CO_2/propylene oxide coupling promoted by Iron(III) complexes 1-6.**



Entry[a]	**Catalyst**		**Co-Catalyst**		**PO/Co-cat/Cat**	**T**	**P_{CO2}**	**Conversion** [b,c]	**TOF** [d]
		(*mol*%)		(*mol*%)	(molar ratio)	(°C)	(MPa)	(*mol*%)	h^{-1}
S1	**6**	0.025	DMAP	0.05	4000/2/1	120	20	0.5	20
S2	**6**	0.025	PPNCl	0.05	4000/2/1	120	20	34.2	1368
S3	**6**	0.025	TBAC	0.05	4000/2/1	120	20	31.5	1260
S4	**6**	0.025	TBAI	0.05	4000/2/1	120	20	34.3	1372
S5	**6**	0.025	TBAB	0.05	4000/2/1	120	20	57.6	2304
S6	**6**	0.025	TBAB	0.10	4000/4/1	120	20	76.1	3044
S7	**6**	0.025	TBAB	0.25	4000/10/1	120	20	82.6	3304
S8	**6**	0.025	TBAB	0.05	4000/2/1	80	20	28.3	1132
S9	**6**	0.025	TBAB	0.05	4000/2/1	100	20	46	1840
S10	**6**	0.025	TBAB	0.05	4000/2/1	140	20	67.0	2680
S11	**-**	-	TBAB	0.25	4000/10/0	120	20	10.0	-
S12	**6**	0.025	TBAB	0.25	4000/10/1	120	5	80.6	3224
S13	**6**	0.025	TBAB	0.25	4000/10/1	120	40	>99	4000

[a] Reaction conditions: PO = 5 mL, 7.15×10^{-2} mol; reaction time = 1 h. [b] Determined by ^{1}H-NMR using mesitylene as internal standard. [c] The selectivity toward the formation of propylene carbonate was always found to be >99%. [d] Turnover Frequency ($mol_{PC} \times mol_{Catalyst}^{-1} \times$ reaction $time^{-1}$).

II. NMR CHARACTERIZATION

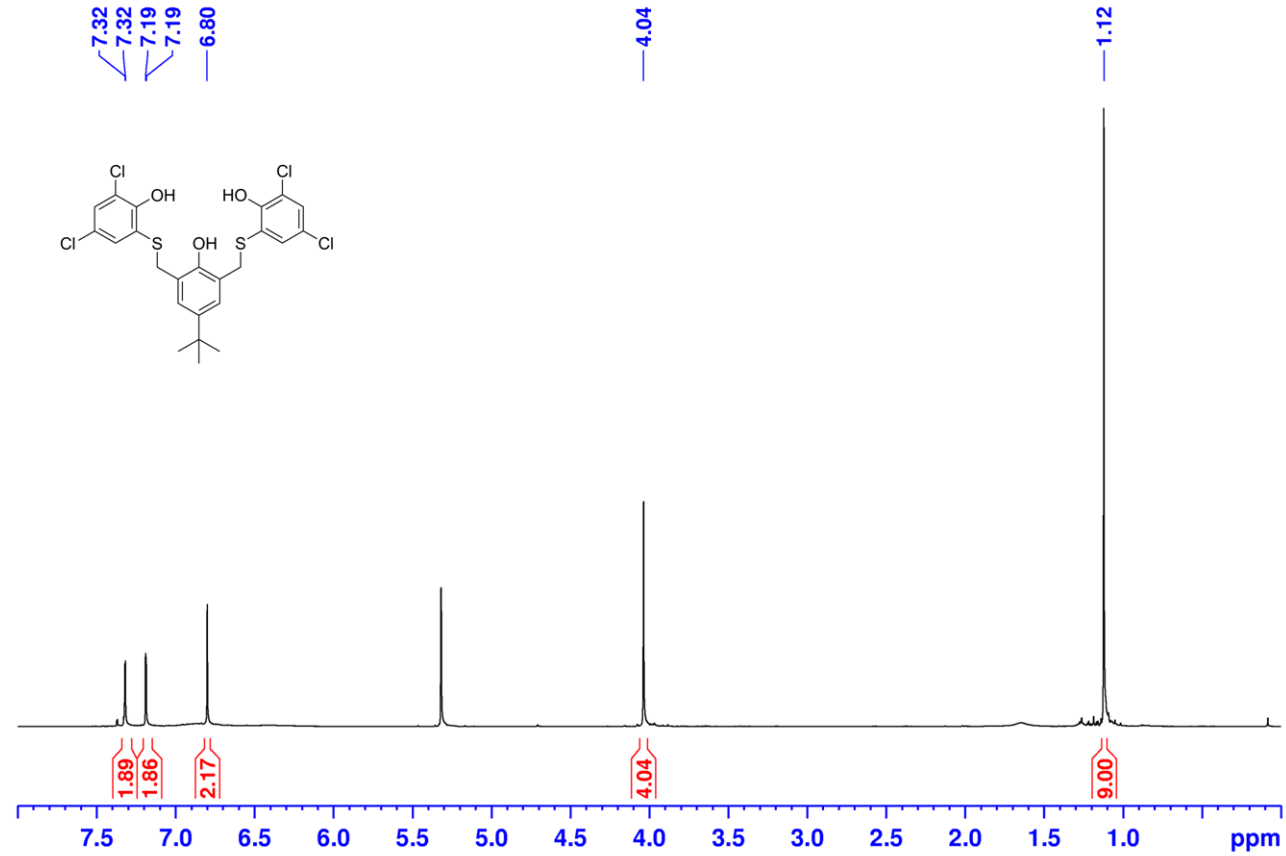


Figure S1. **^{1}H NMR spectrum of proligand L4 (CD_2Cl_2, 600MHz).**

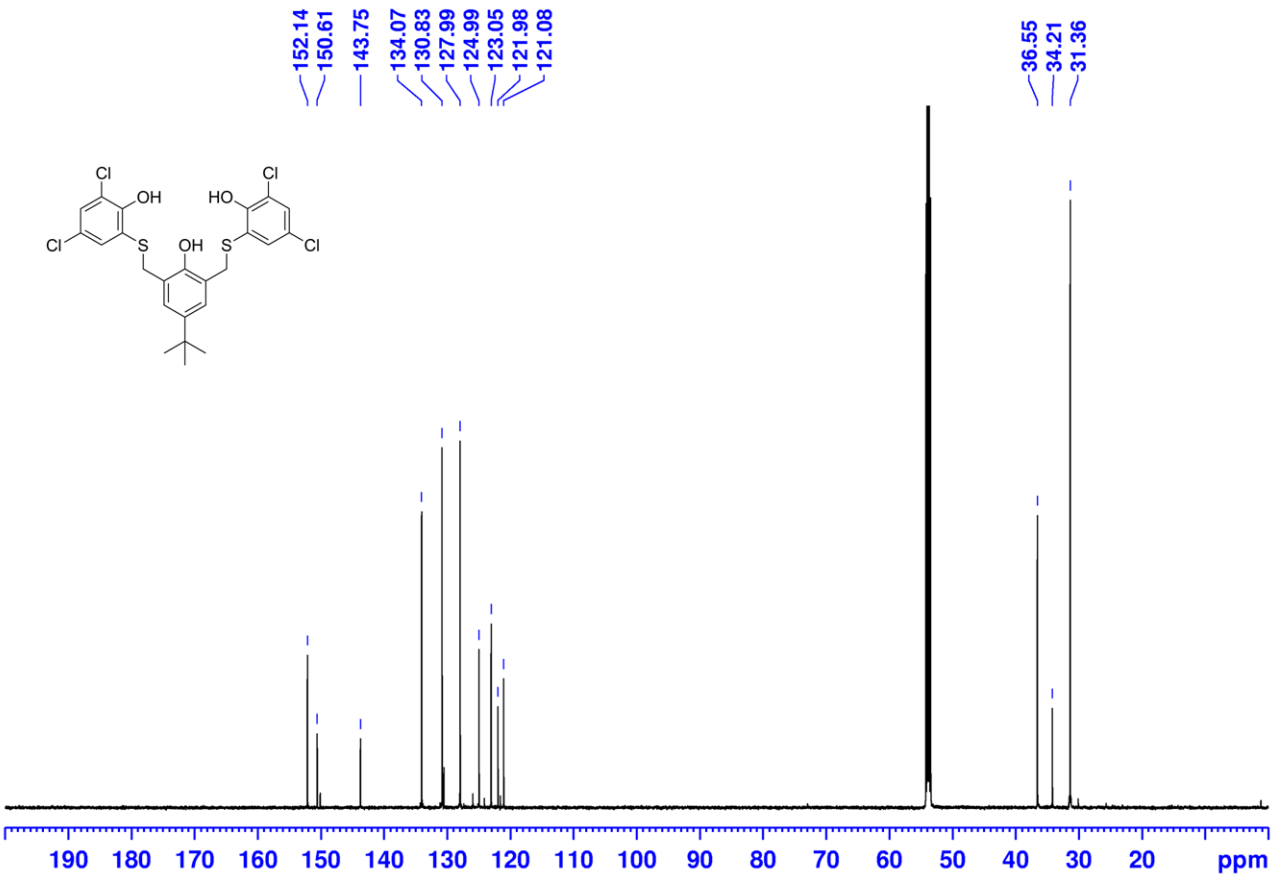


Figure S2. **^{13}C NMR spectrum of proligand L4 (CD_2Cl_2, 600MHz).**

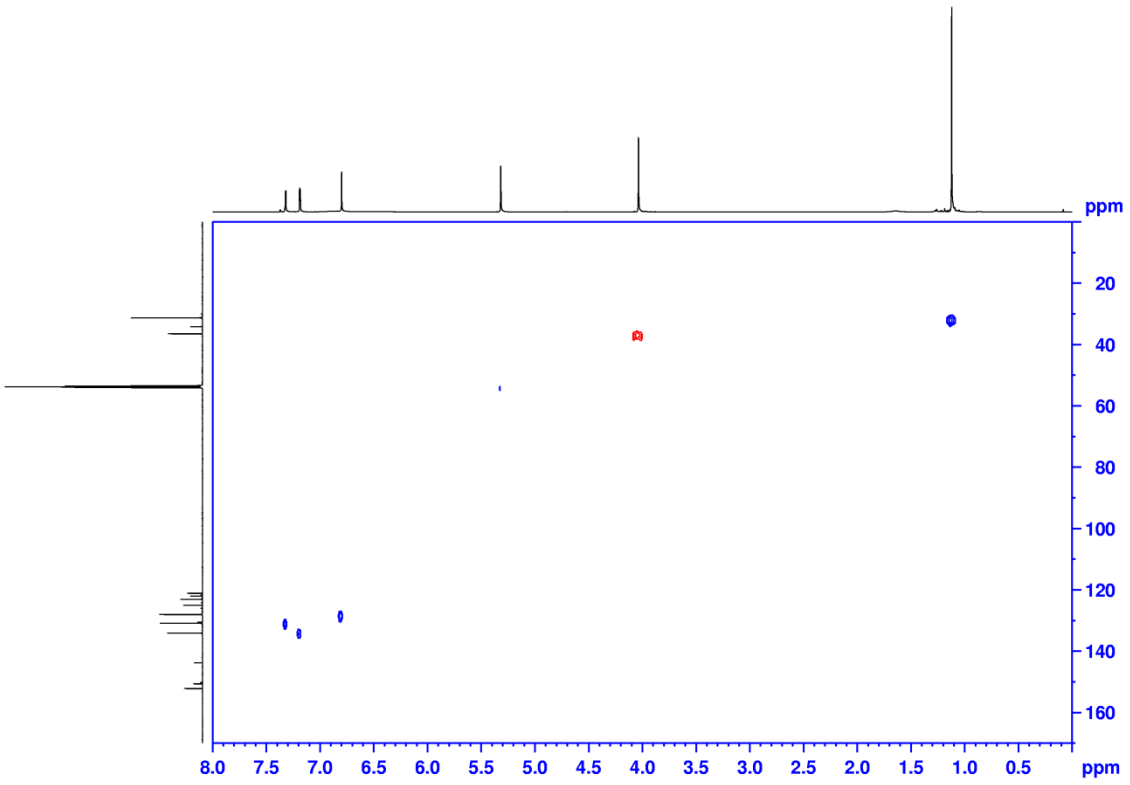


Figure S3. **^{1}H-^{13}C HSQC NMR spectrum of proligand L4 (CD_2Cl_2, 600MHz).**

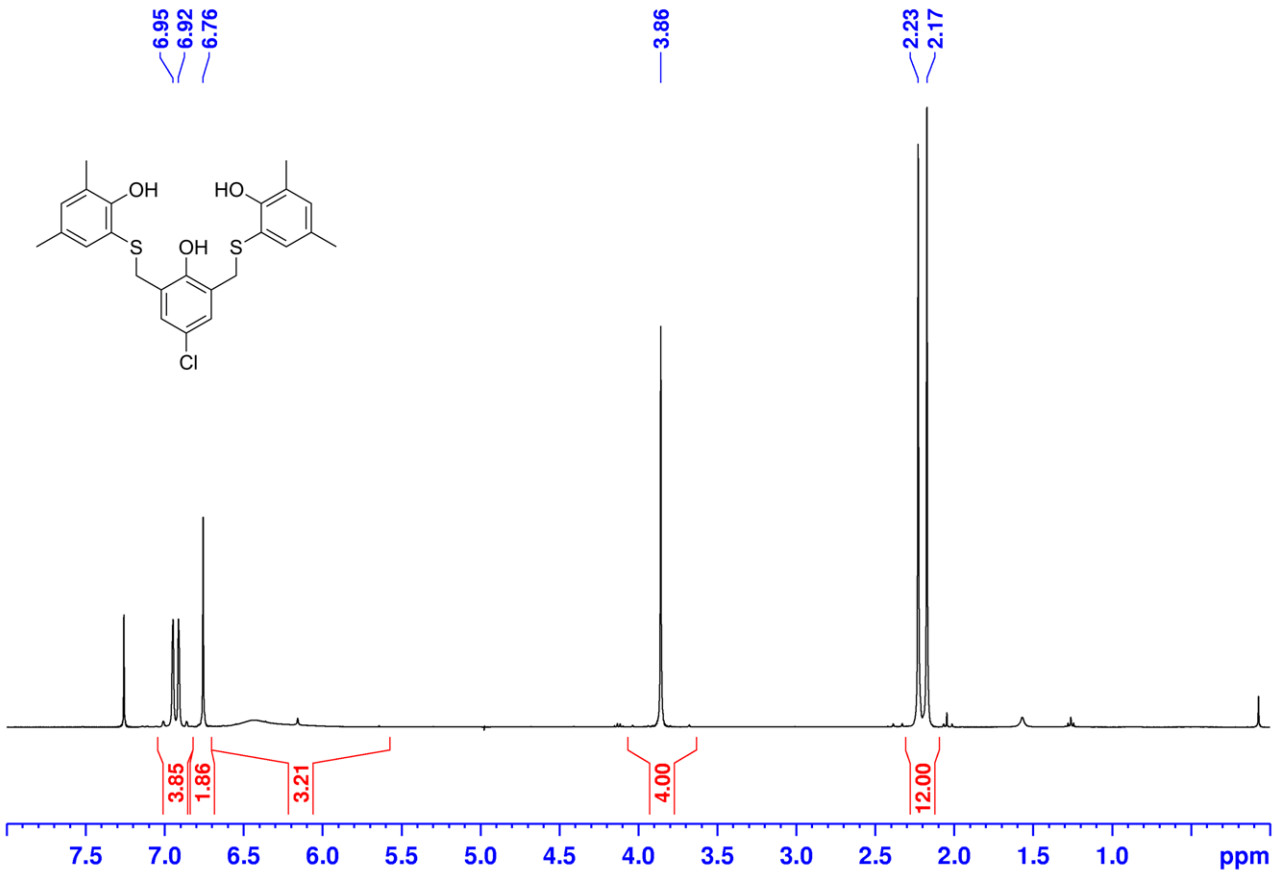


Figure S4. **^{1}H NMR spectrum of proligand L5 ($CDCl_3$, 400MHz).**

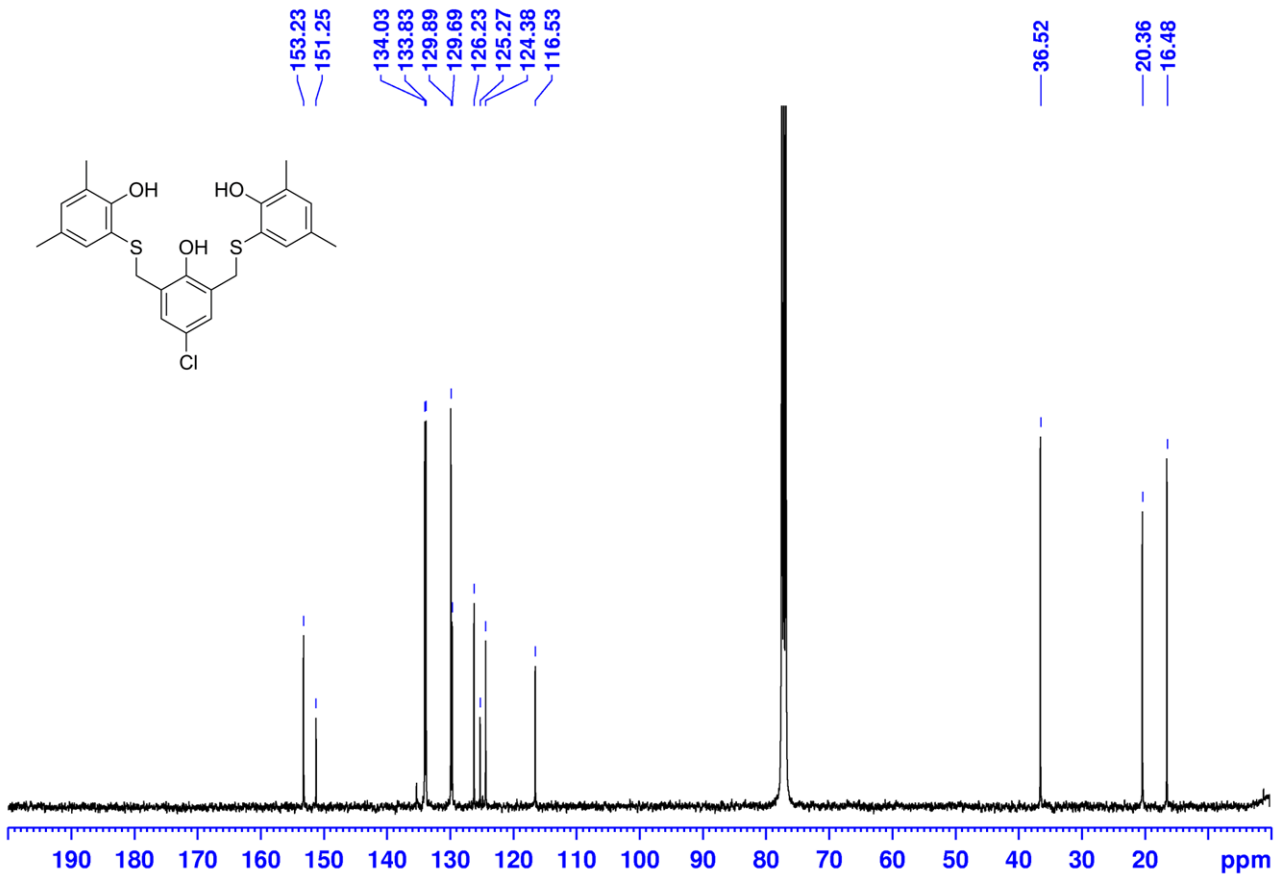


Figure S5. **^{13}C NMR spectrum of proligand L5 ($CDCl_3$, 400MHz).**

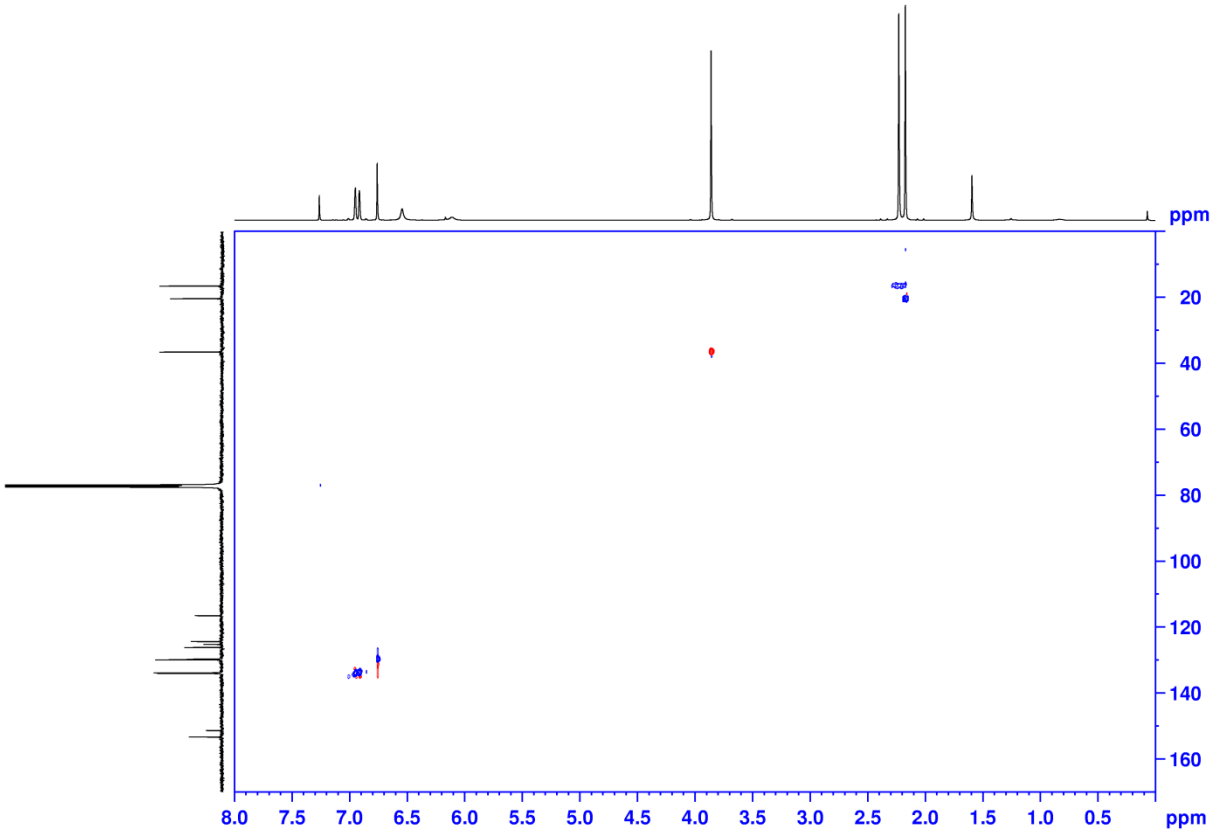


Figure S6. **^{1}H-^{13}C HSQC NMR spectrum of proligand L5 ($CDCl_3$, 400MHz).**

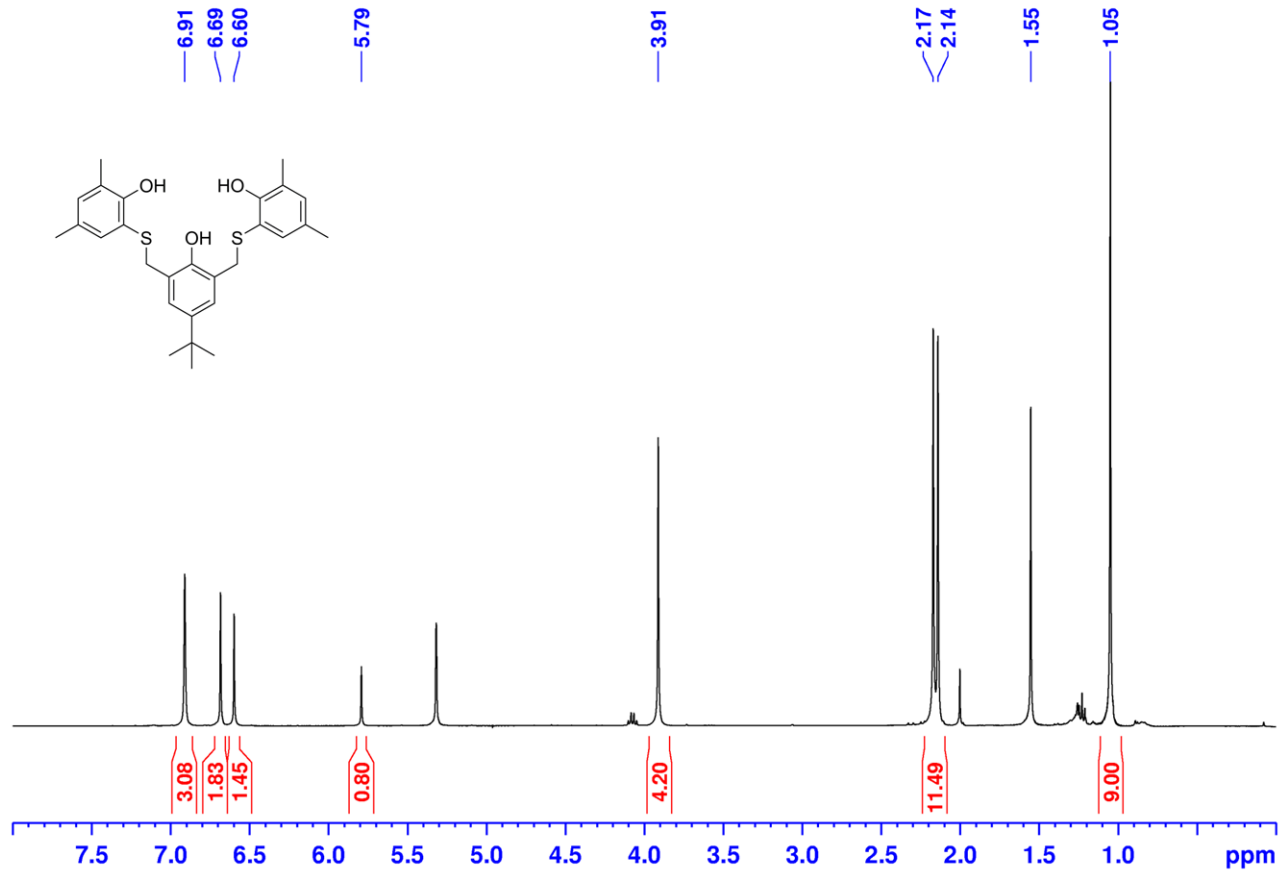


Figure S7. **^{1}H NMR spectrum of proligand L6 (CD_2Cl_2, 400MHz).**

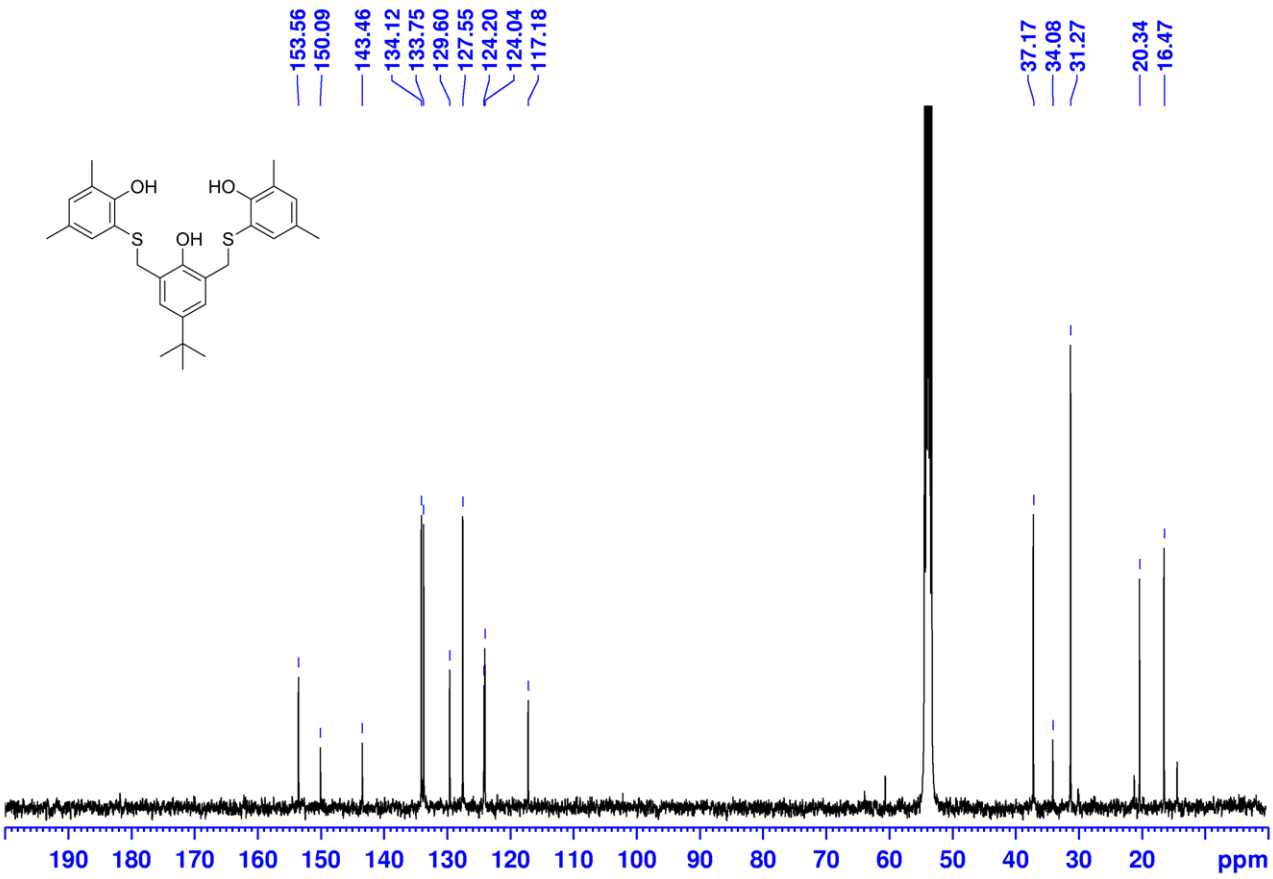


Figure S8. **^{13}C NMR spectrum of proligand L6 (CD_2Cl_2, 400MHz).**

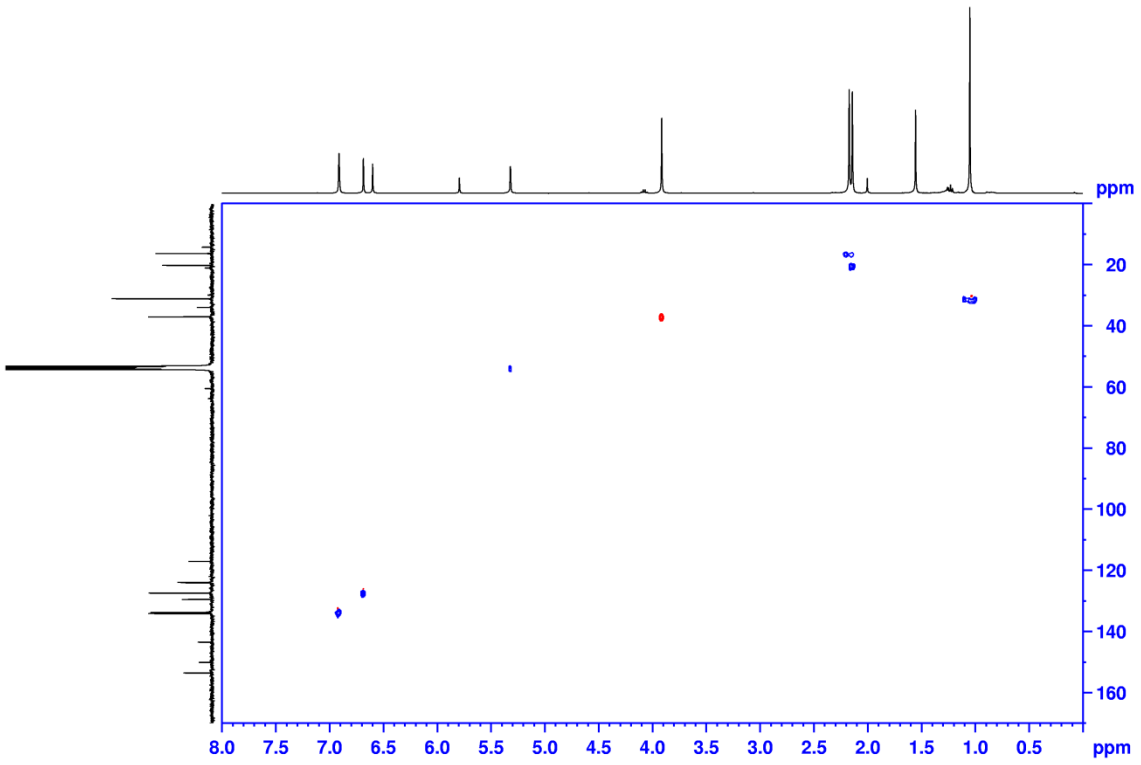


Figure S9. **^{1}H-^{13}C HSQC NMR spectrum of proligand L6 (CD_2Cl_2, 400MHz).**

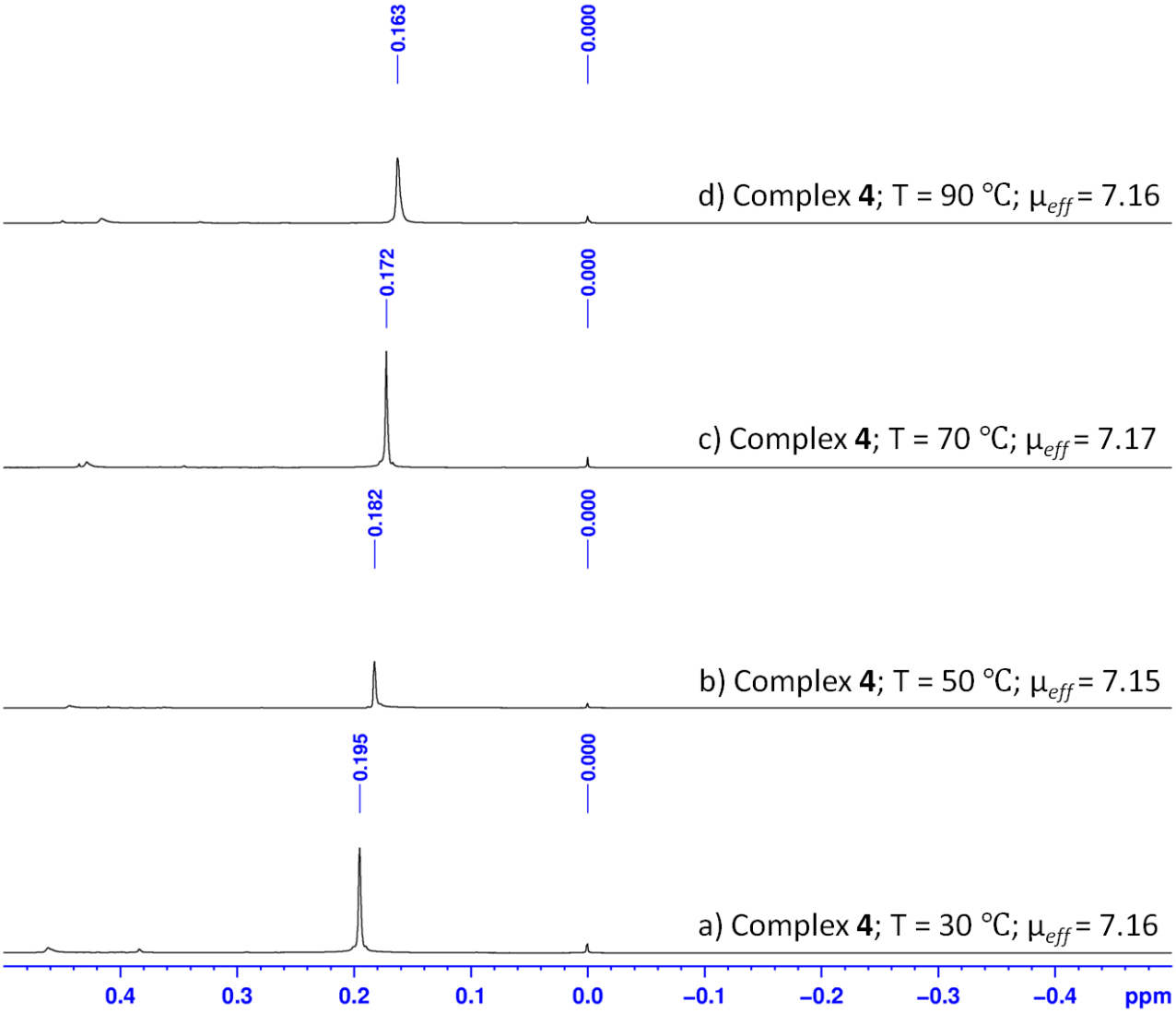


Figure S10. **Plot of the ^{1}H NMR spectra of the iron(III) complex 4 (2.22 mM in Tol$_{d8}$) at different temperatures, for the determination of the solution magnetic susceptibility (μ_{eff}) by means of the method of Evans.** a**) 30 °C;** b**) 50 °C;** c**) 70 °C;** d**) 90 °C.**

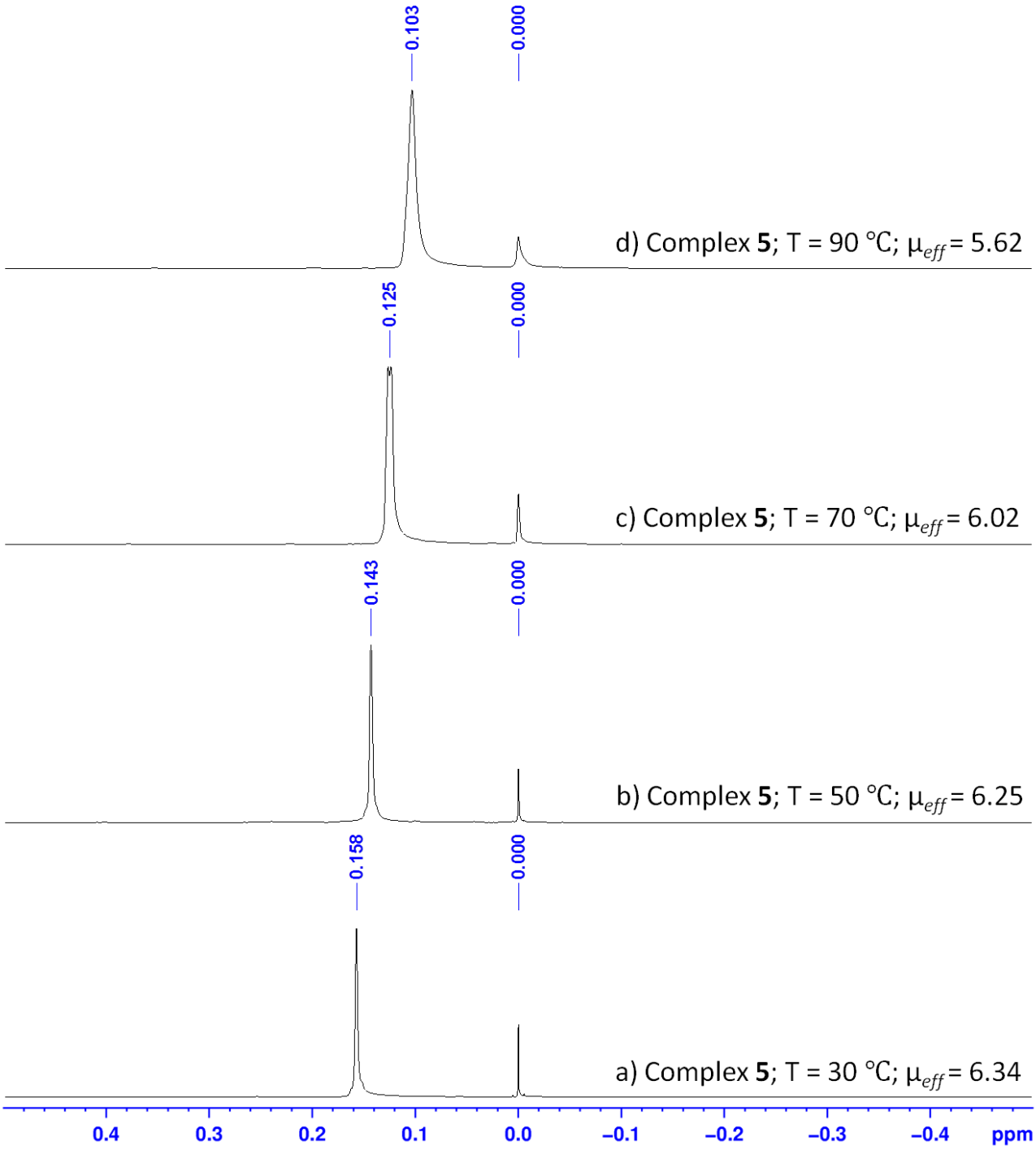


Figure S11. **Plot of the ^{1}H NMR spectra of the iron(III) complex 5 (2.29 mM in Tol$_{d8}$) at different temperatures, for the determination of the solution magnetic susceptibility (μ_{eff}) by means of the method of Evans.** a**) 30 °C;** b**) 50 °C;** c**) 70 °C;** d**) 90 °C.**

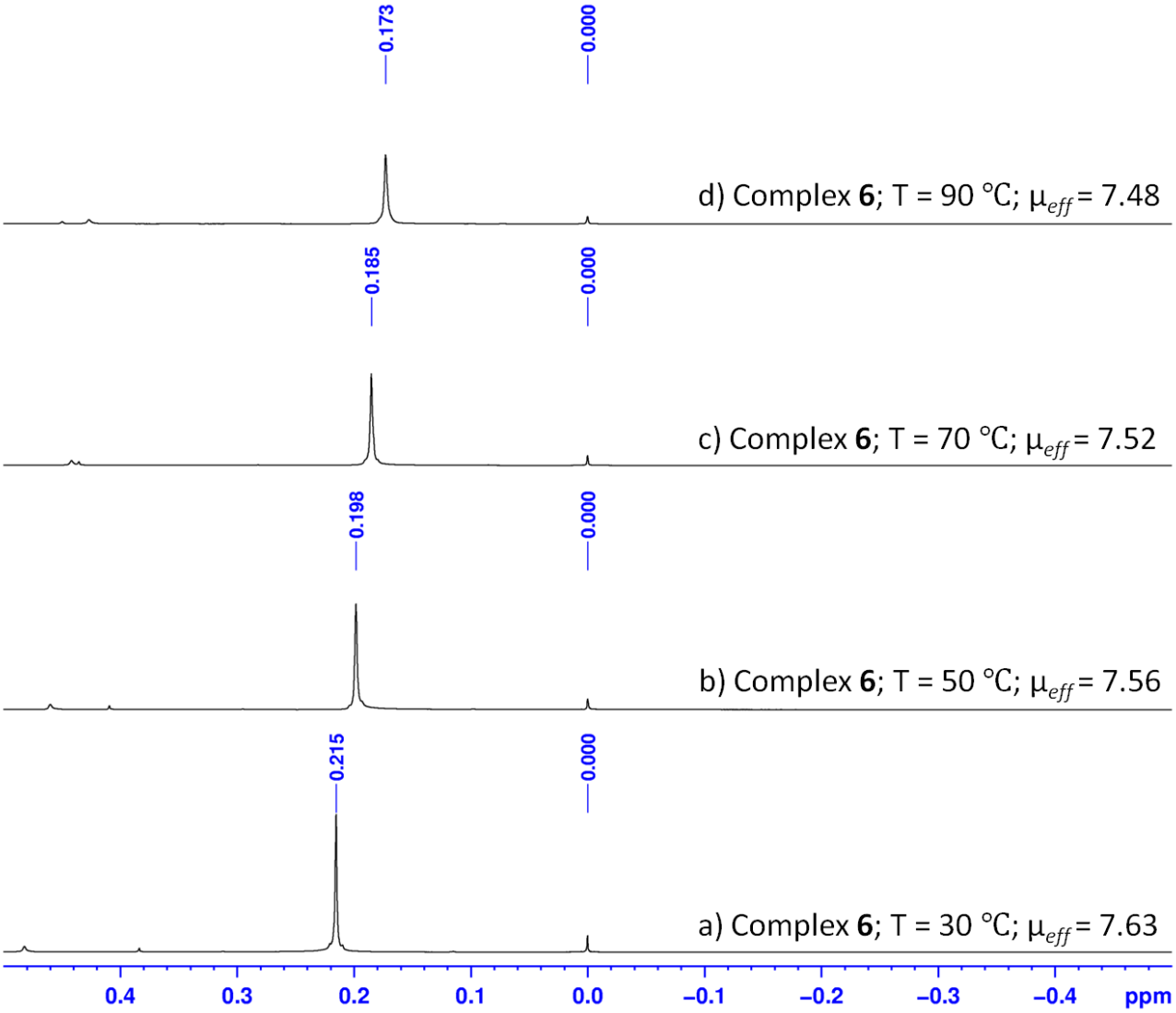


Figure S12. **Plot of the ^{1}H NMR spectra of the iron(III) complex 6 (2.16 mM in Tol$_{d8}$) at different temperatures, for the determination of the solution magnetic susceptibility (μ_{eff}) by means of the method of Evans.** a**) 30 °C;** b**) 50 °C;** c**) 70 °C;** d**) 90 °C.**

III. ESI-MS CHARACTERIZATION

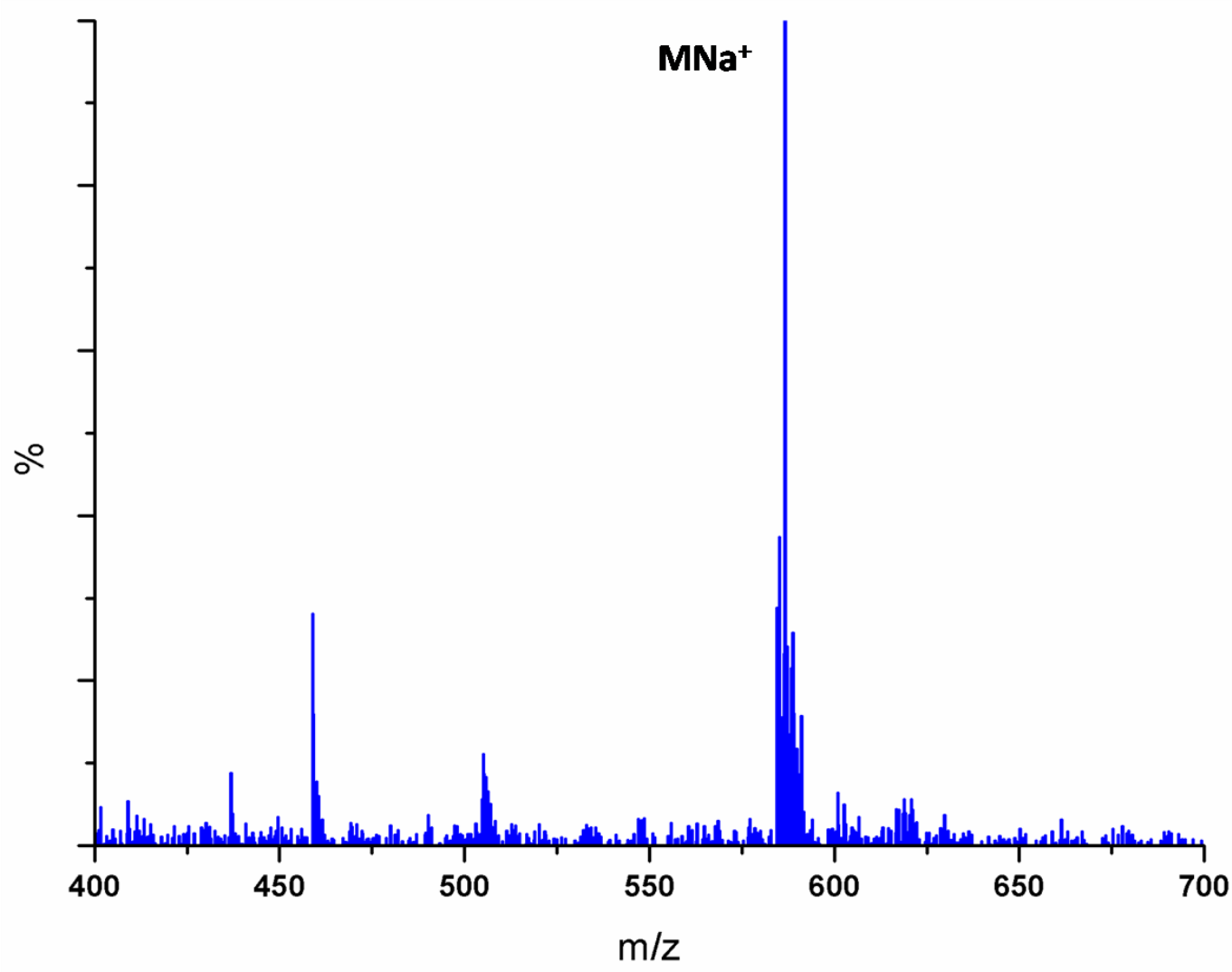


Figure S13. **Mass spectrum of proligand L4 (acetonitrile as solvent).**

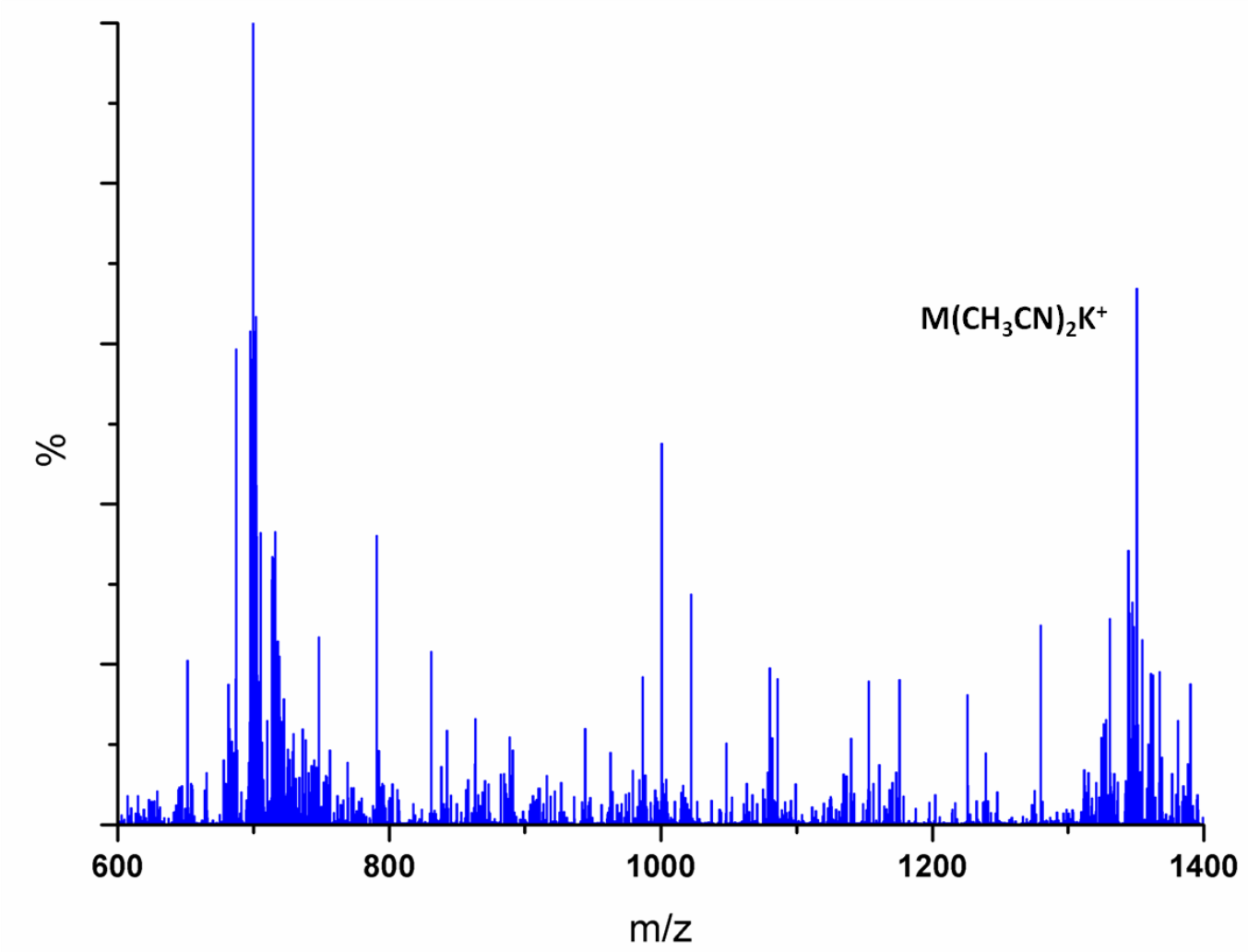


Figure S14. **Mass spectrum of complex 4 (acetonitrile as solvent).**

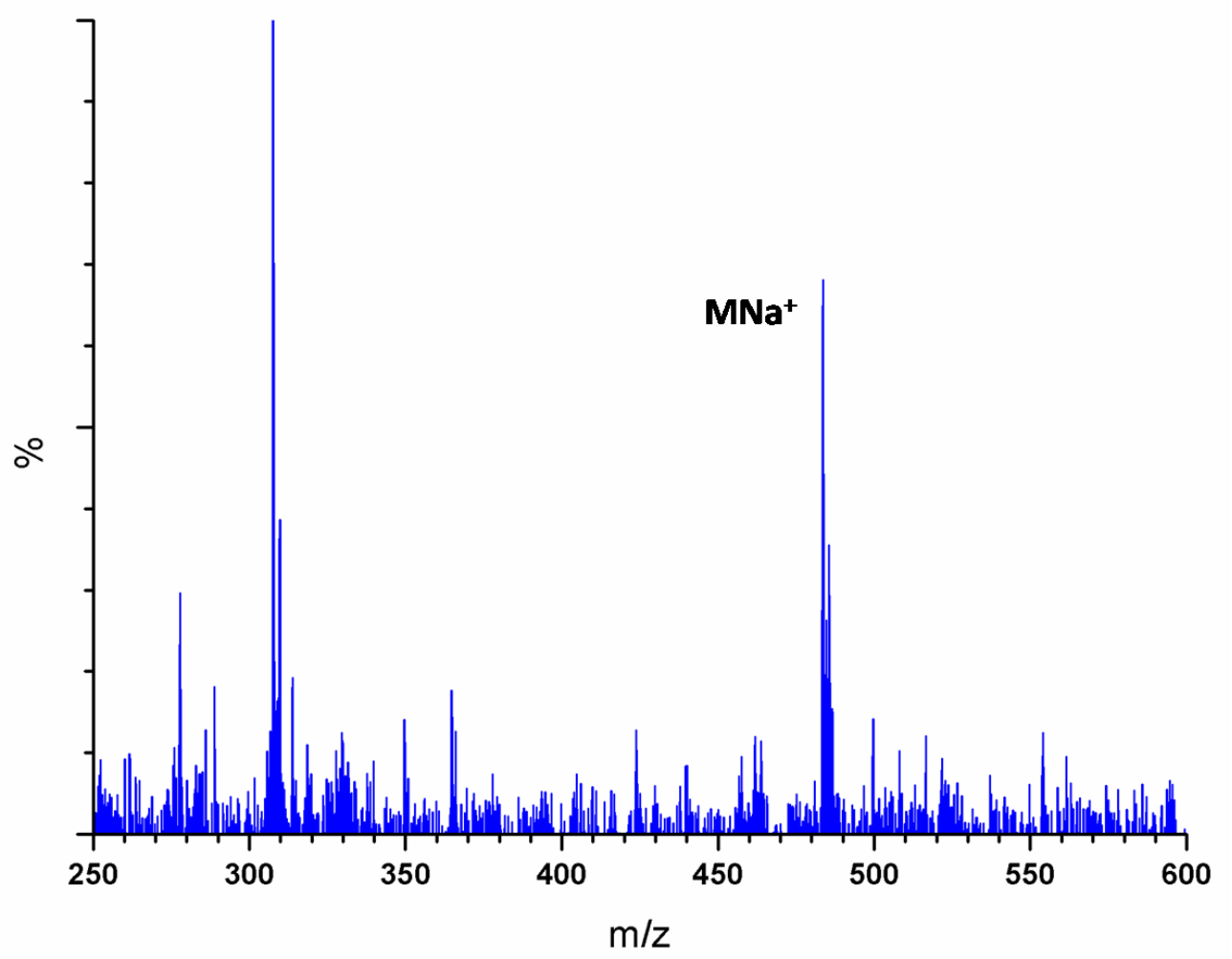


Figure S15. **Mass spectrum of proligand L5 (acetonitrile as solvent).**

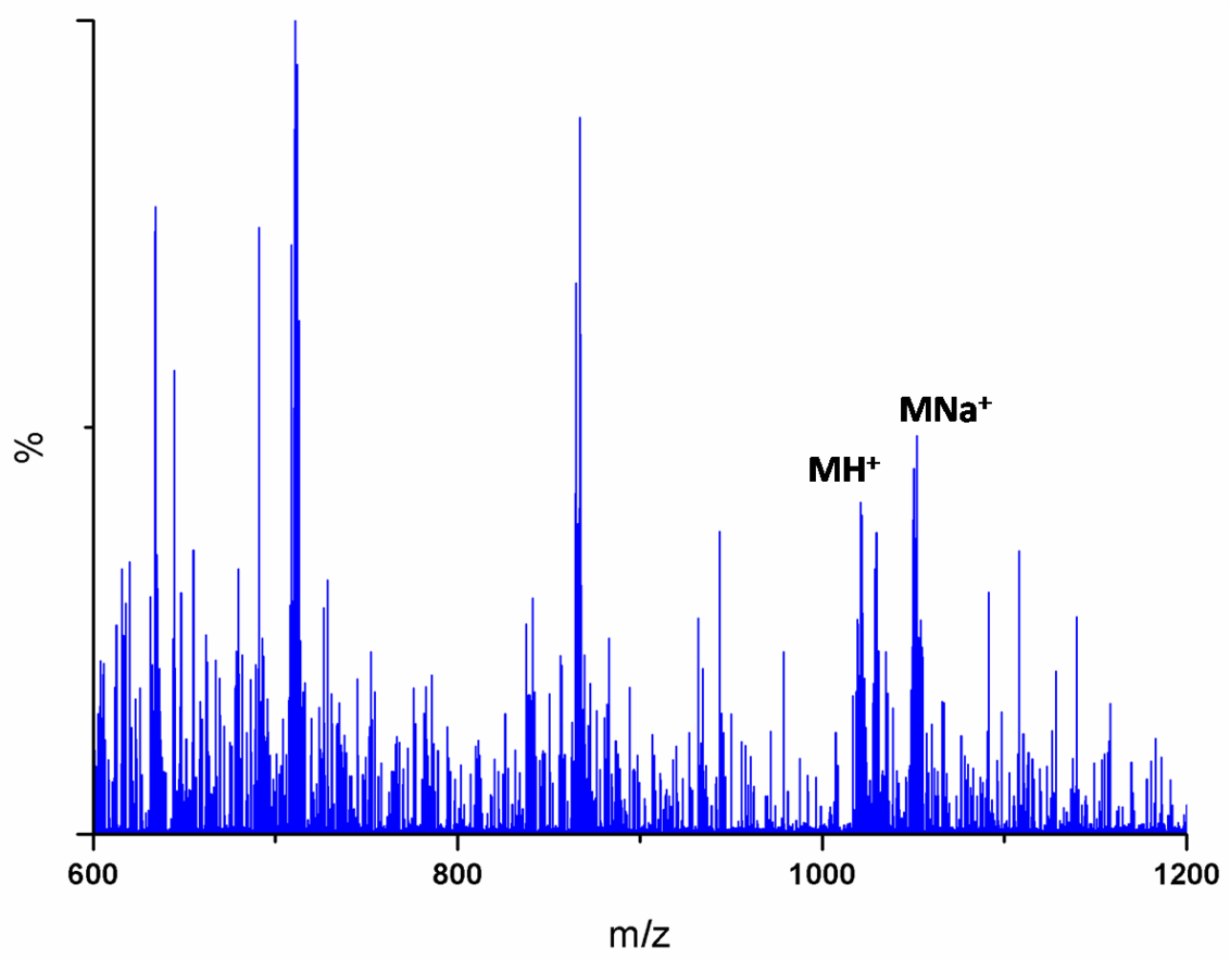


Figure S16. **Mass spectrum of complex 5 (acetonitrile as solvent).**

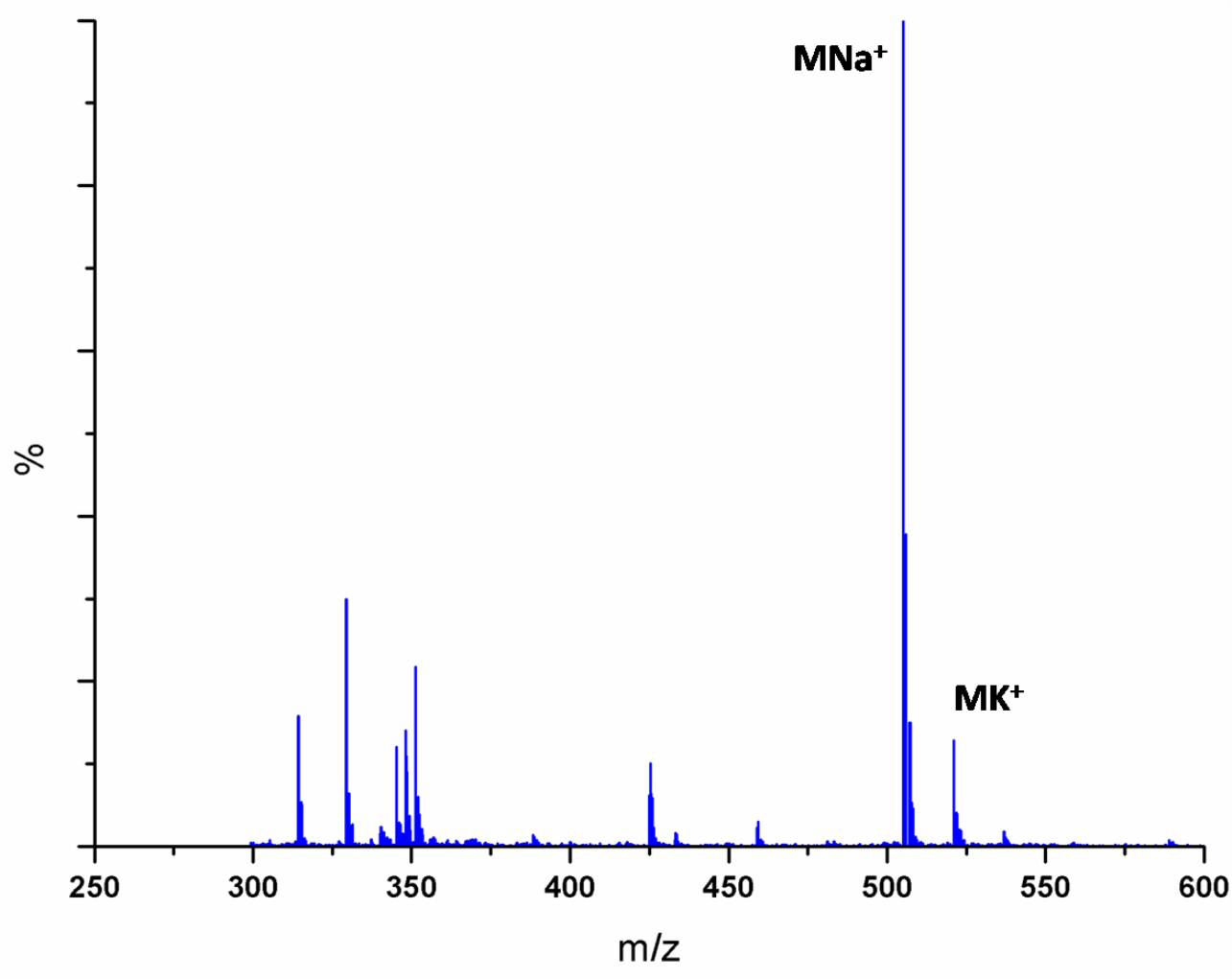


Figure S17. **Mass spectrum of proligand L6 (acetonitrile as solvent).**

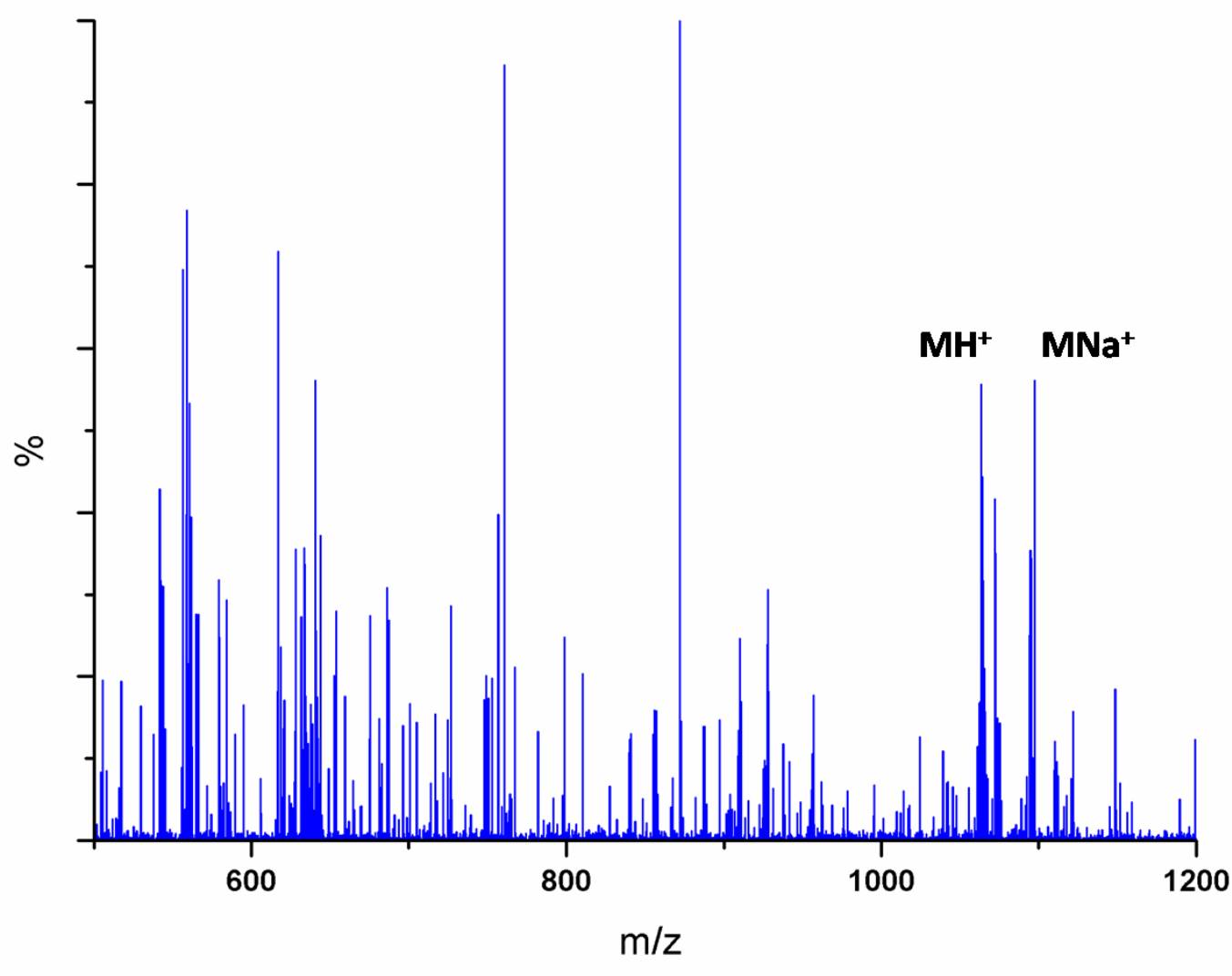


Figure S18. **Mass spectrum of complex 6 (acetonitrile as solvent).**

IV. UV-VIS CHARACTERIZATION.

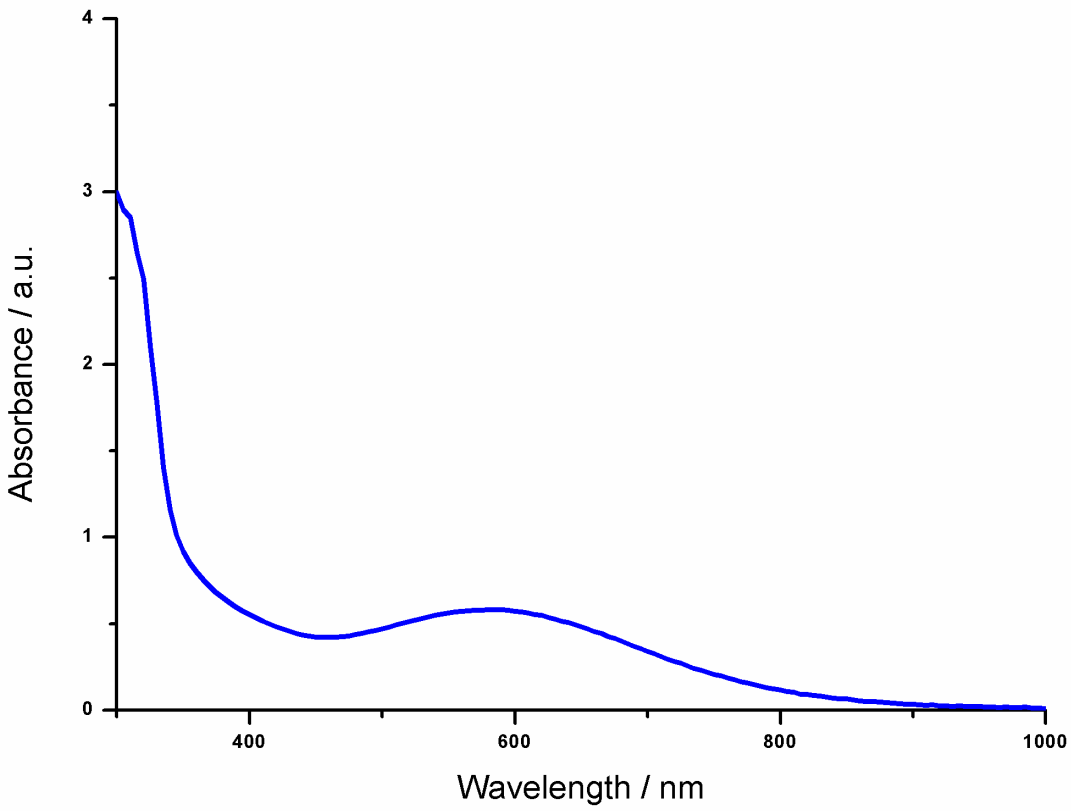


Figure S19. **UV-Vis spectrum of the complex 4 (1.07×10^{-4} M in toluene; ε_{585} = 5441 L mol^{-1} cm^{-1}).**

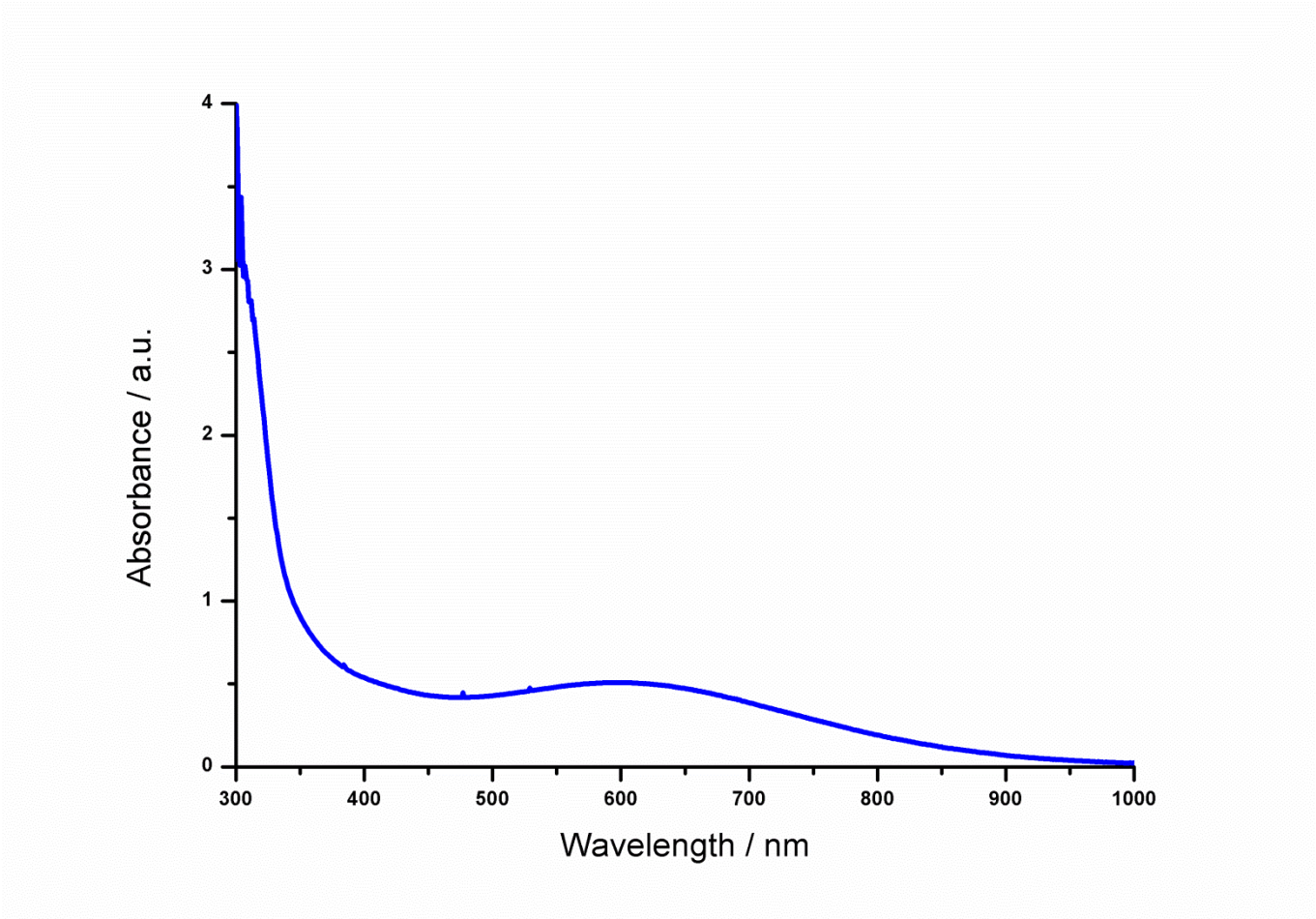


Figure S20. **UV-Vis spectrum of the complex 5 (1.07×10^{-4} M in toluene; ε_{596} = 4757 L mol^{-1} cm^{-1}).**

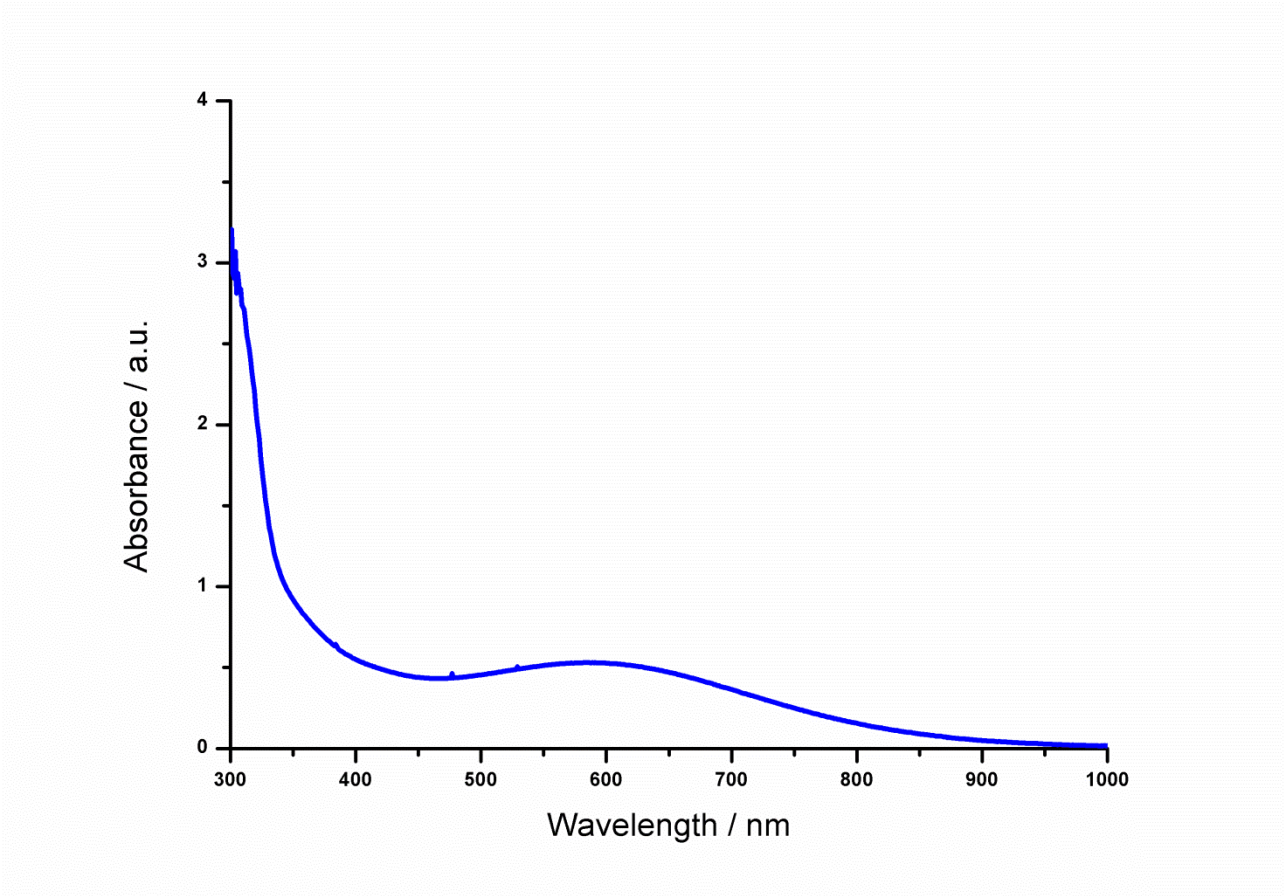


Figure S21. **UV-Vis spectrum of the complex 6 (1.07×10^{-4} M in toluene; ε_{586} = 4962 L mol^{-1} cm^{-1}).**

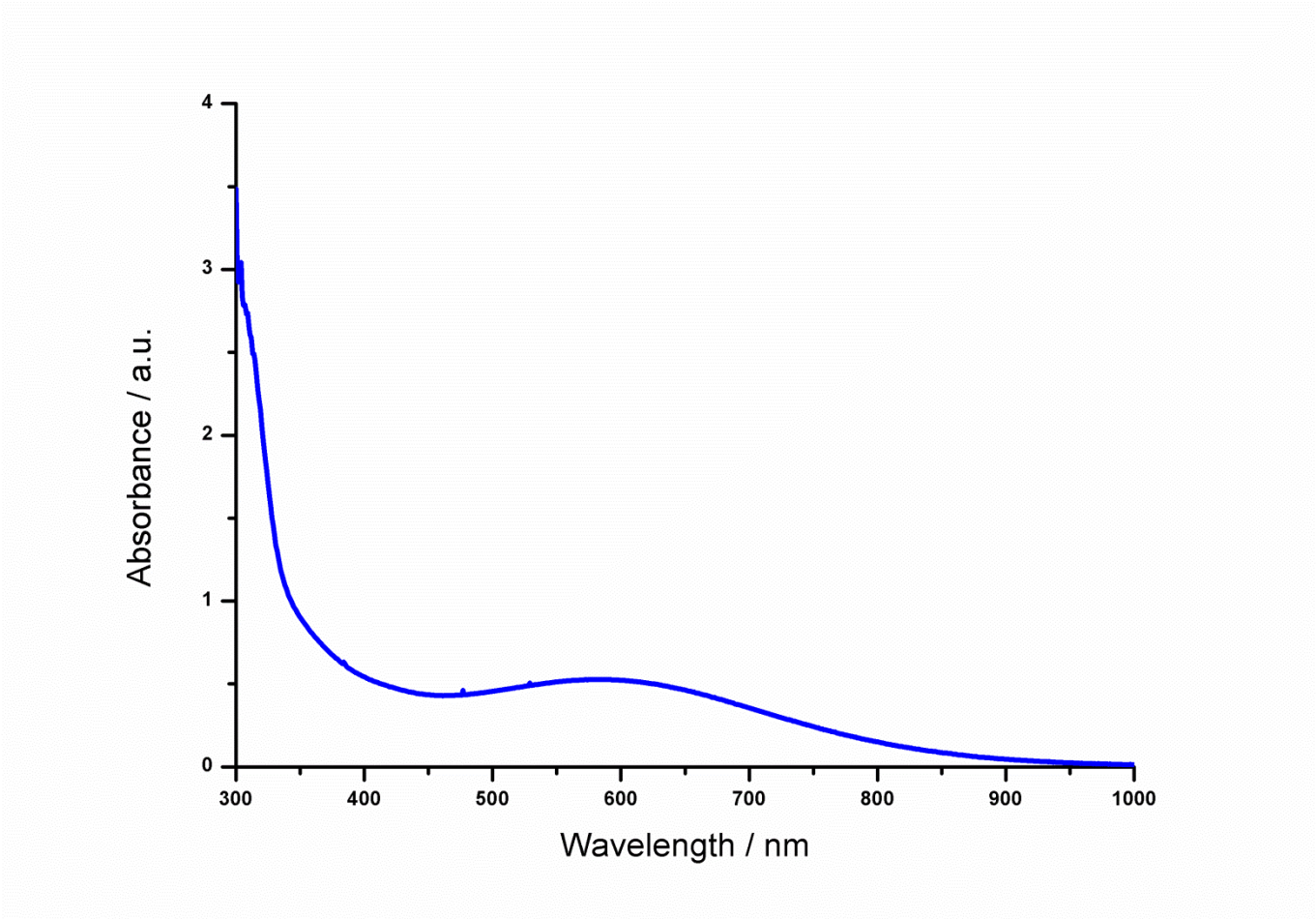


Figure S22. **UV-Vis spectrum of the complex 6 in the presence of 50 equivalents of Pyridine-d5 (1.07 × 10^{-4} M in toluene; ε_{586} = 4935 L mol^{-1} cm^{-1}).**

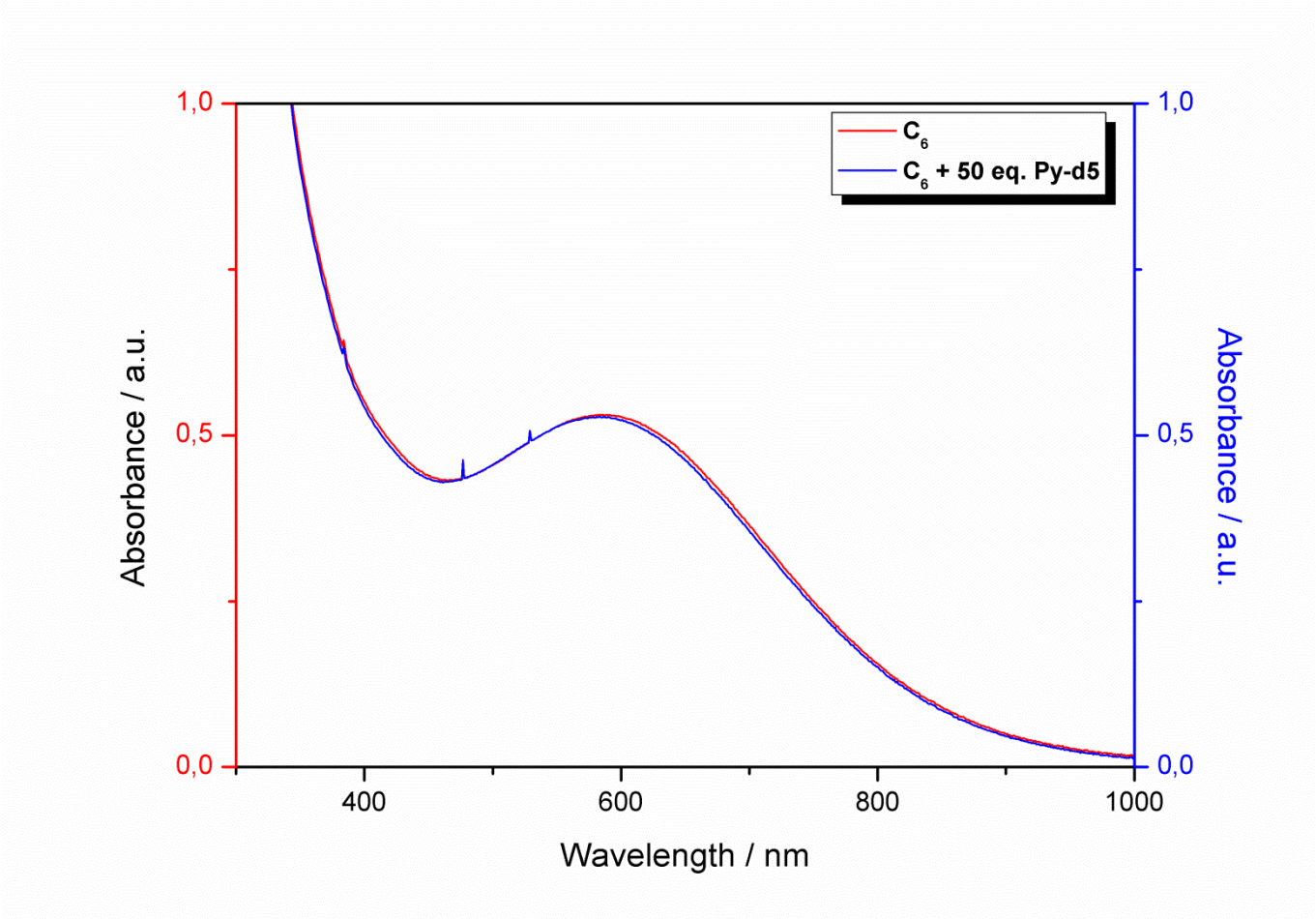


Figure S23. **Comparison of the UV-Vis spectra of the complex 6 before (red curve) and after the addition of 50 equivalents of Pyridine-d5 (blue curve).**

V. FT-IR CHARACTERIZATION.

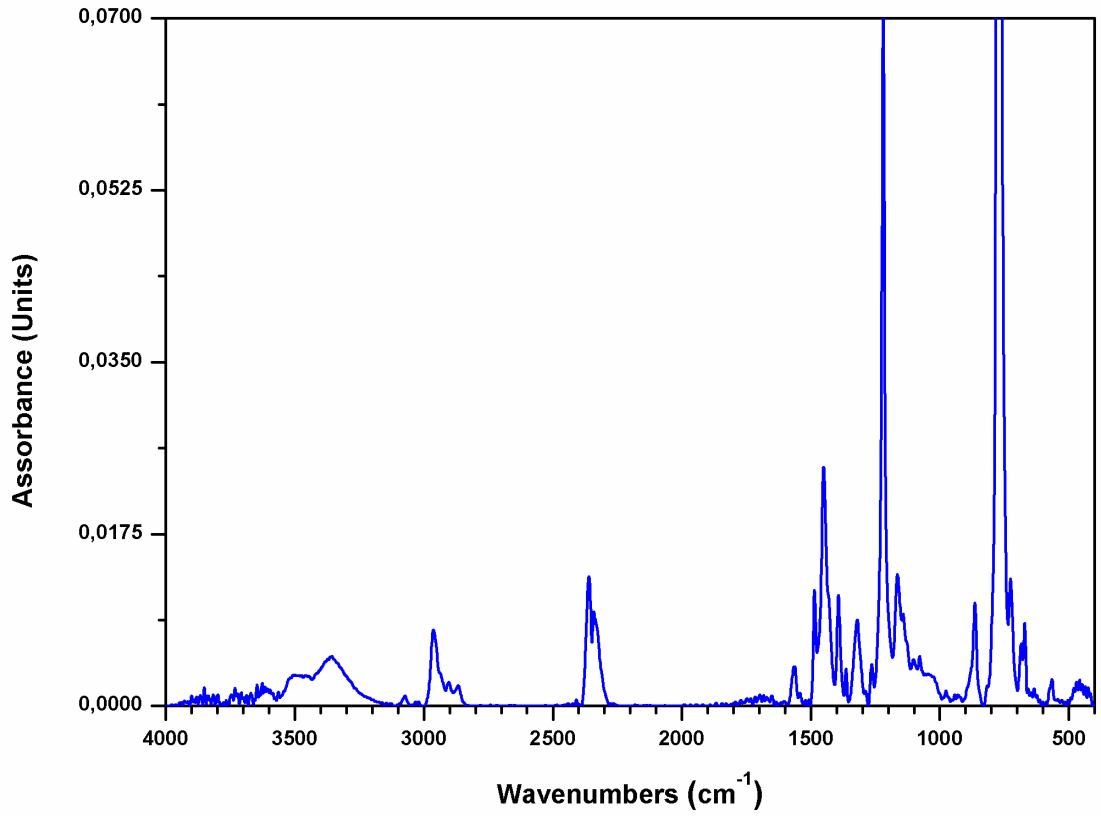


Figure S24. **FT-IR spectrum of the pro-ligand L4 (KBr disk).**

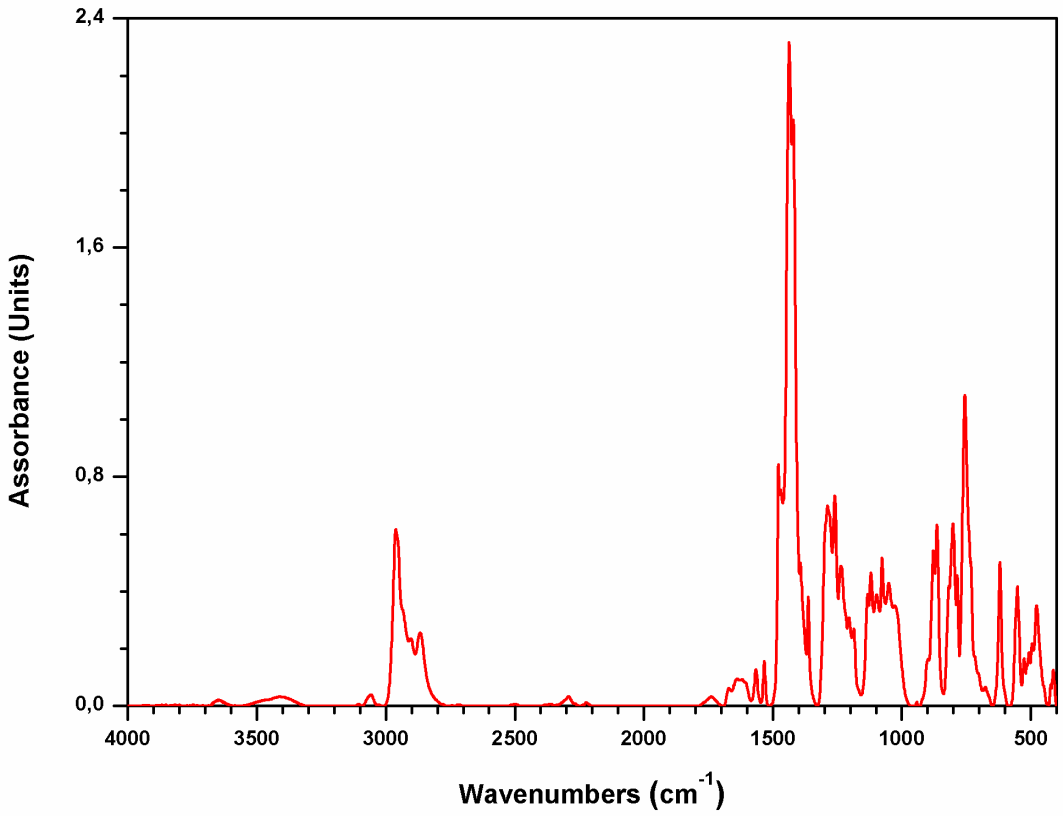


Figure S25. **FT-IR spectrum of the complex 4 (KBr disk).**

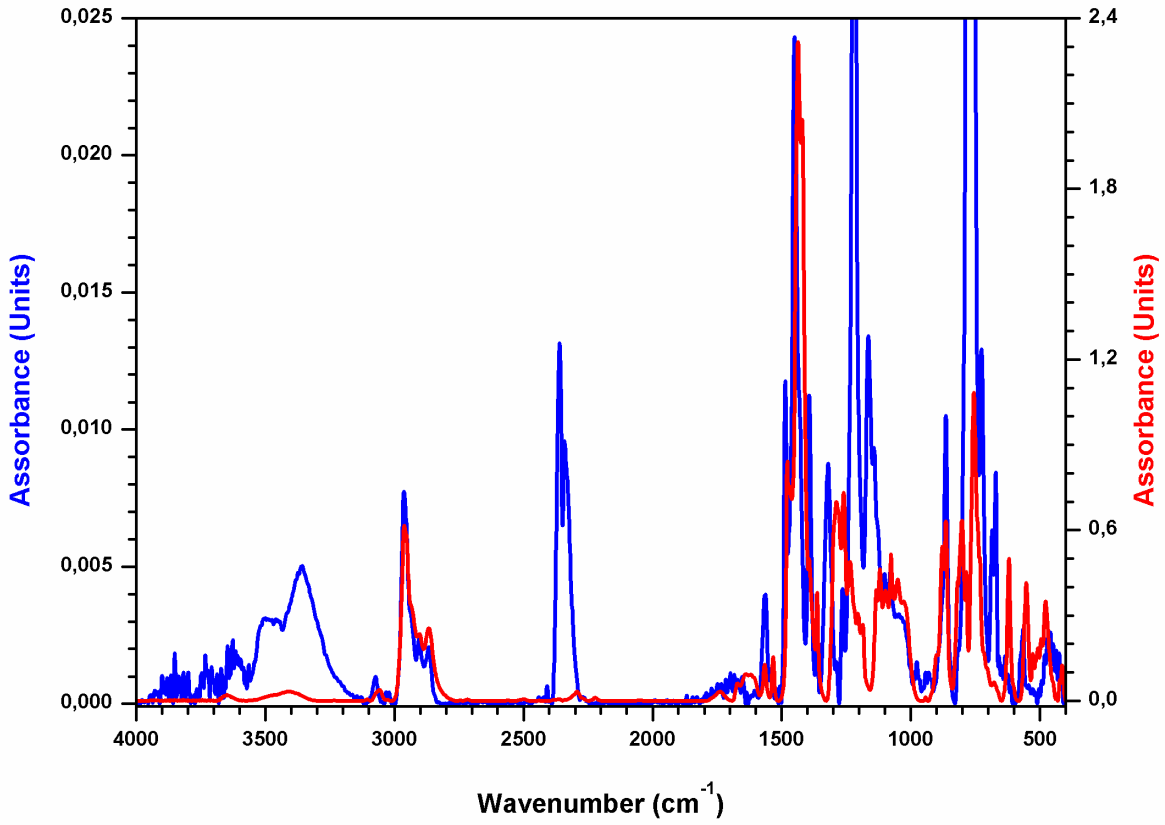


Figure S26. **Comparison of the FT-IR spectra of the pro-ligand L4 (blue curve) and of the iron(III) complex 4 (red curve).**

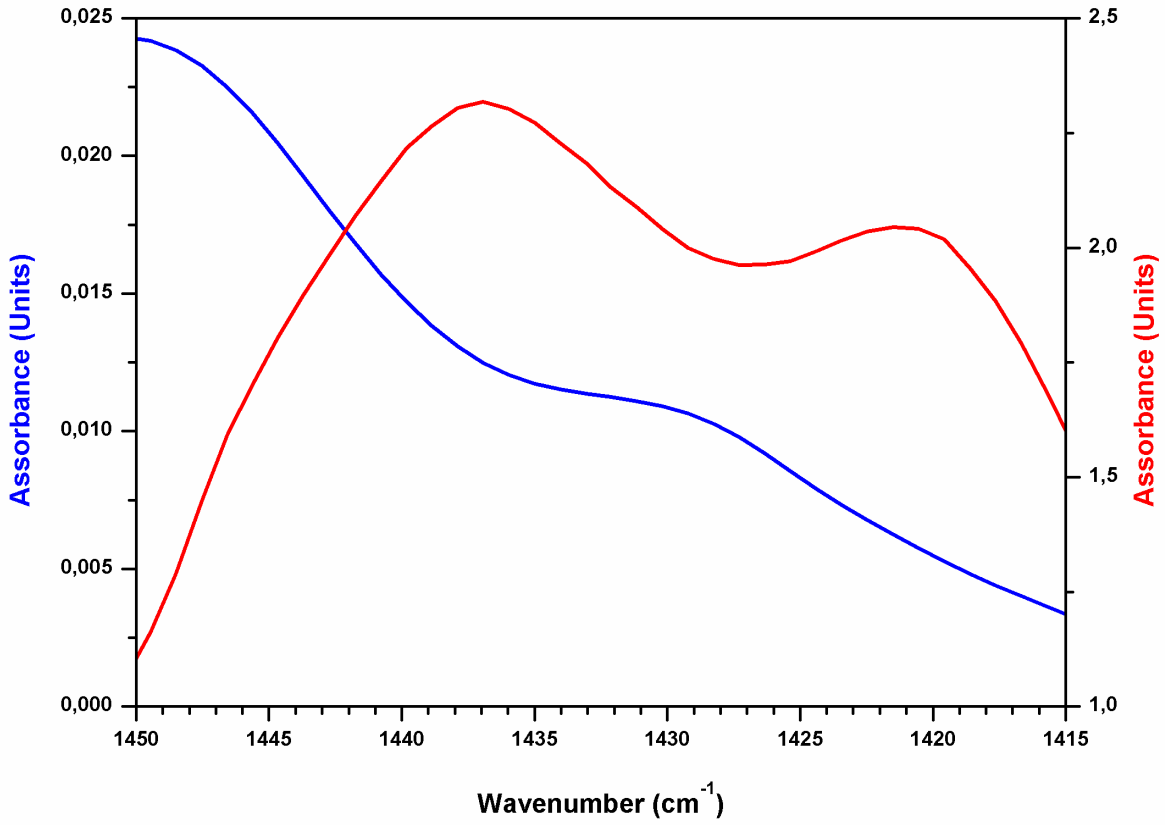


Figure S27. **Magnification of the region 1450-1415 cm^{-1} (for the CH_2-S-C deformation)[1,2] of the FT-IR spectra of the pro-ligand L4 (blue curve) and of the iron(III) complex 4 (red curve).**

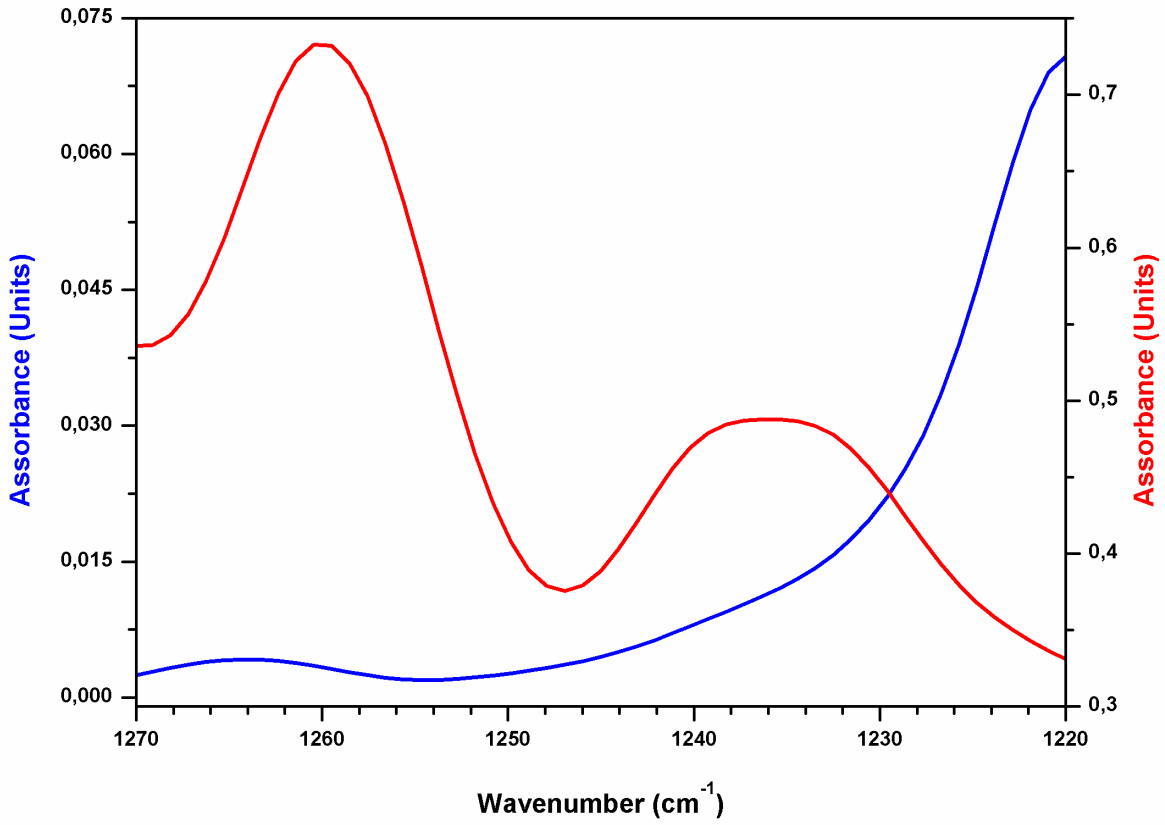


Figure S28. **Magnification of the region 1270-1220 cm^{-1} (for the CH_2-S-C wagging)[1,2] of the FT-IR spectra of the pro-ligand L4 (blue curve) and of the iron(III) complex 4 (red curve).**

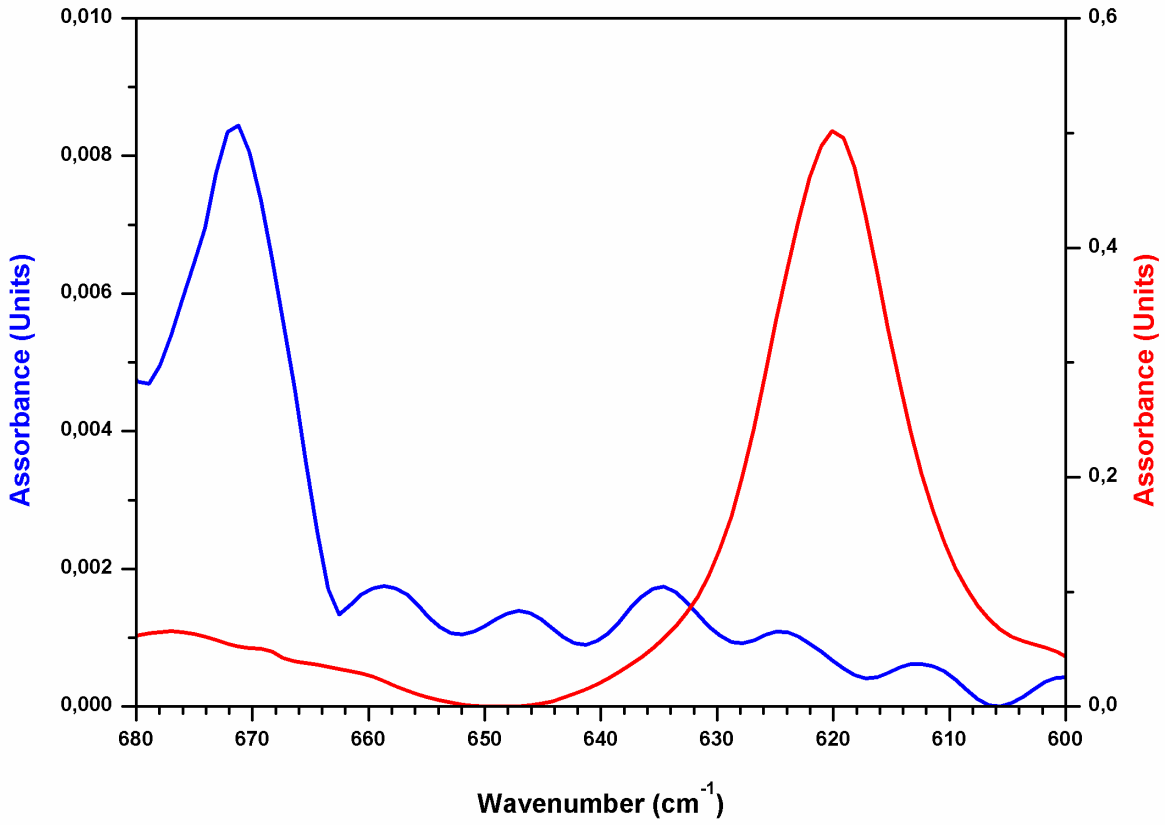


Figure S29. **Magnification of the region 680-600 cm^{-1} (for the C-S stretching vibration)[1,2] of the FT-IR spectra of the pro-ligand L4 (blue curve) and of the iron(III) complex 4 (red curve).**

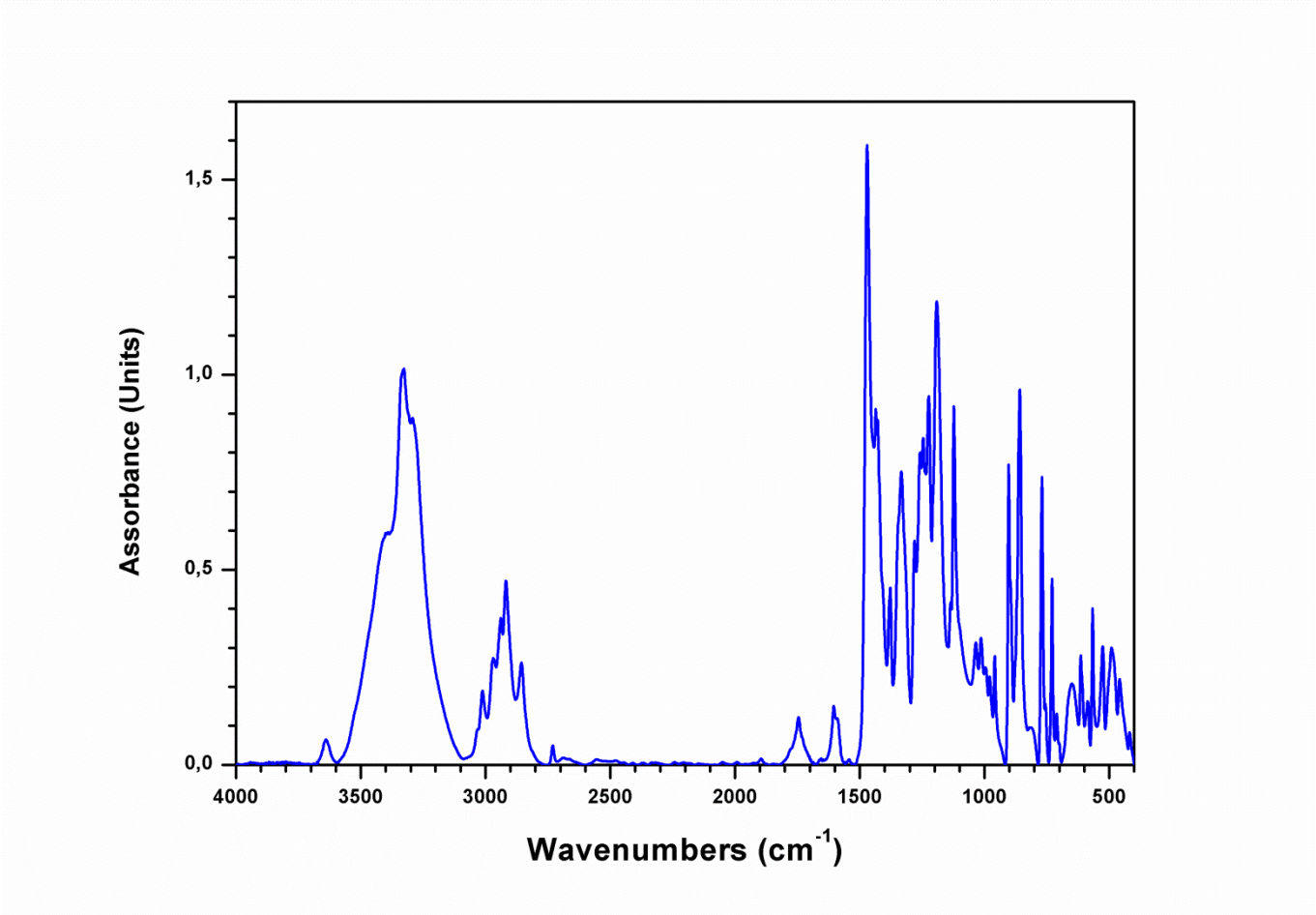


Figure S30. **FT-IR spectrum of the pro-ligand L5 (KBr disk).**

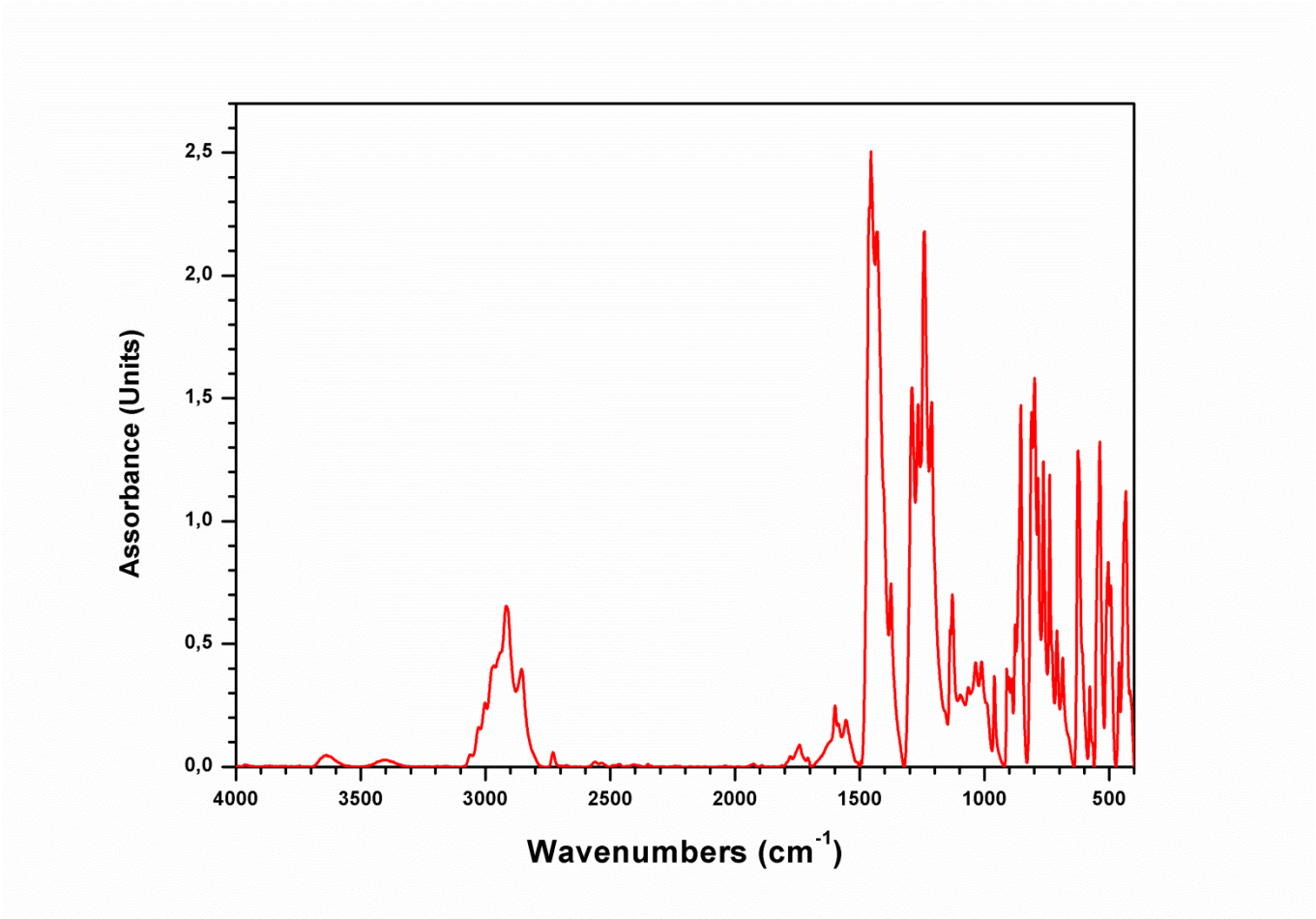


Figure S31. **FT-IR spectrum of the complex 5 (KBr disk).**

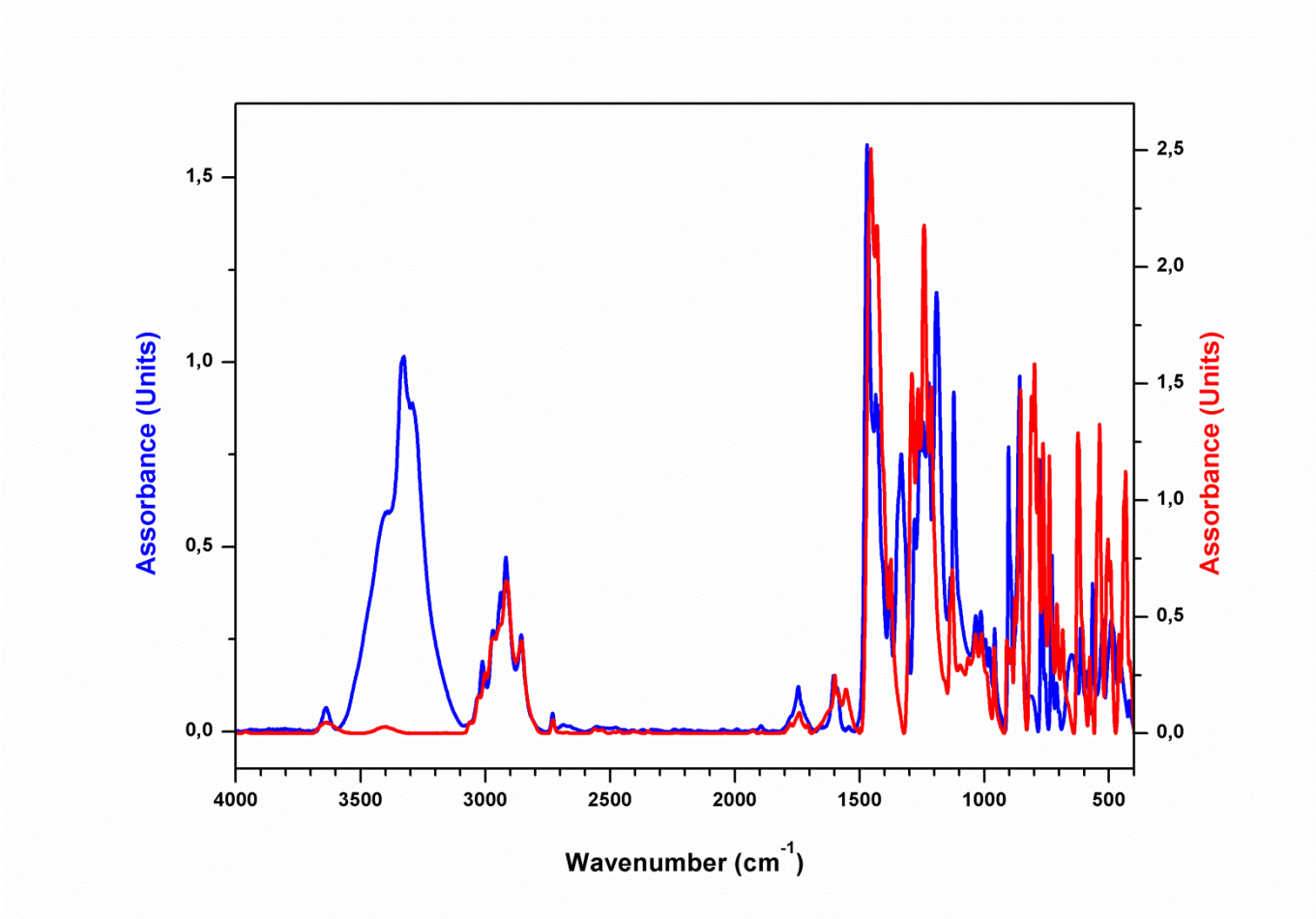


Figure S32. **Comparison of the FT-IR spectra of the pro-ligand L5 (blue curve) and of the iron(III) complex 5 (red curve).**

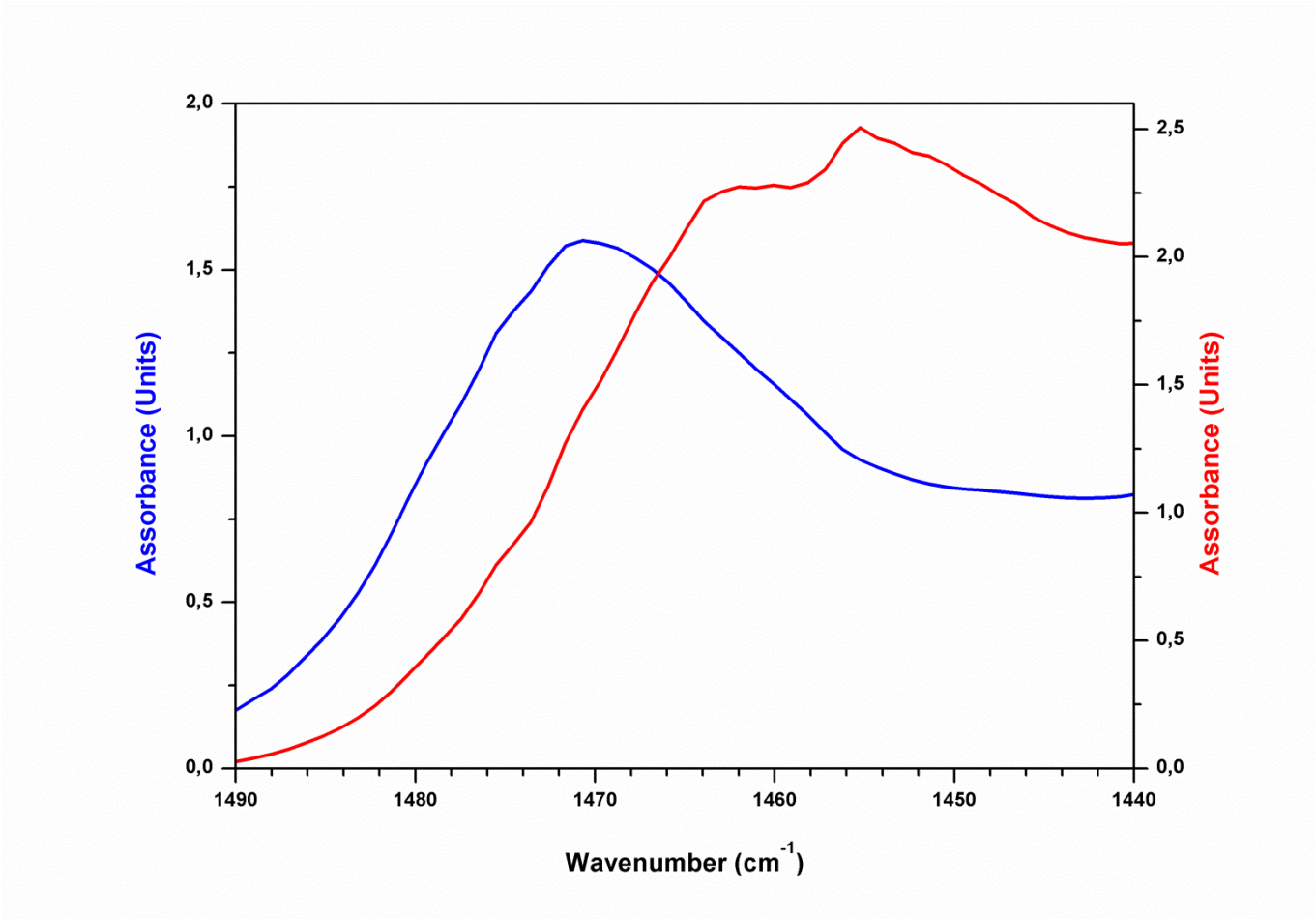


Figure S33. **Magnification of the region 1490-1440 cm^{-1} (for the CH_2-S-C deformation)[1,2] of the FT-IR spectra of the pro-ligand L5 (blue curve) and of the iron(III) complex 5 (red curve).**

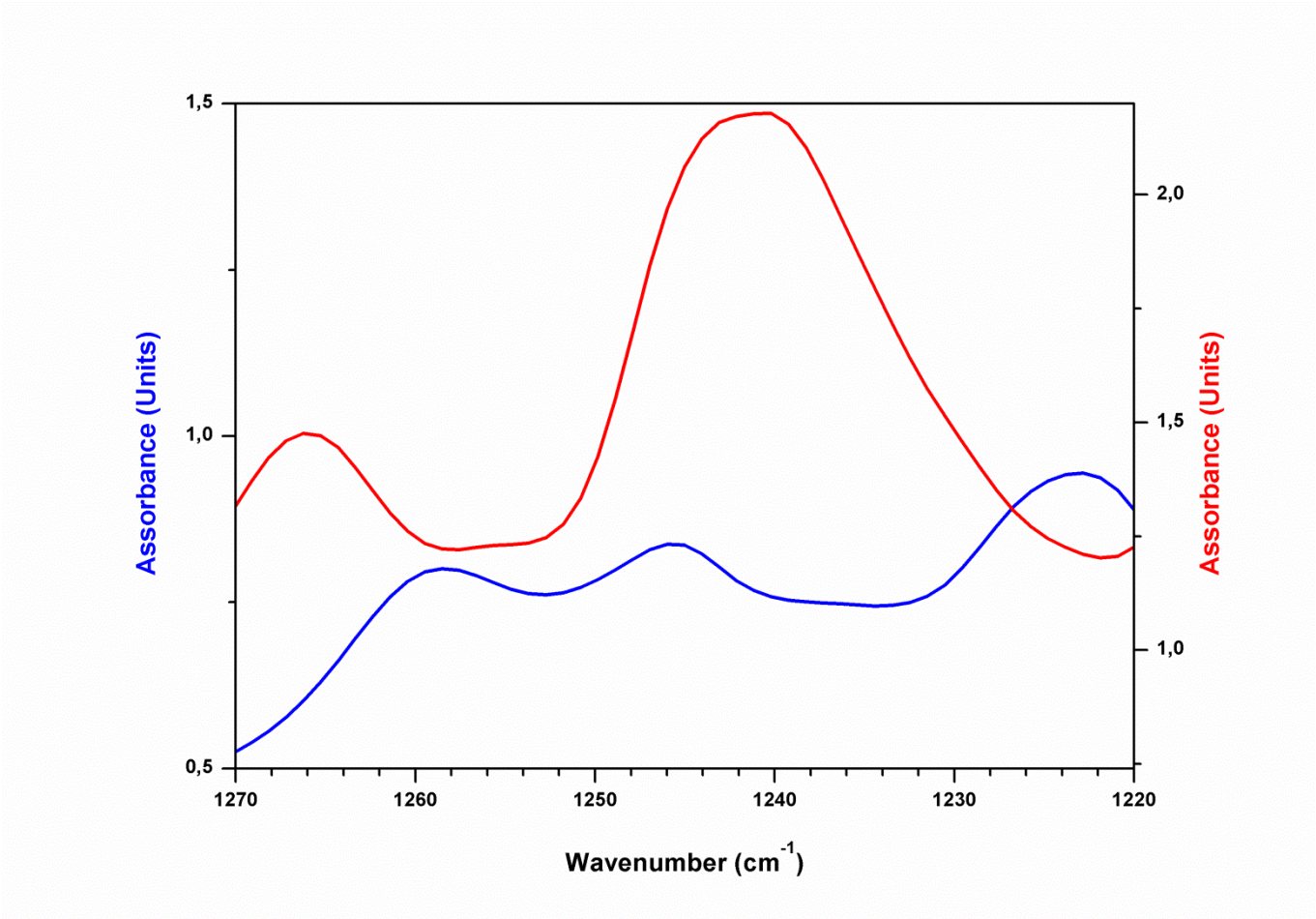


Figure S34. **Magnification of the region 1270-1220 cm^{-1} (for the CH_2-S-C wagging)[1,2] of the FT-IR spectra of the pro-ligand L5 (blue curve) and of the iron(III) complex 5 (red curve).**

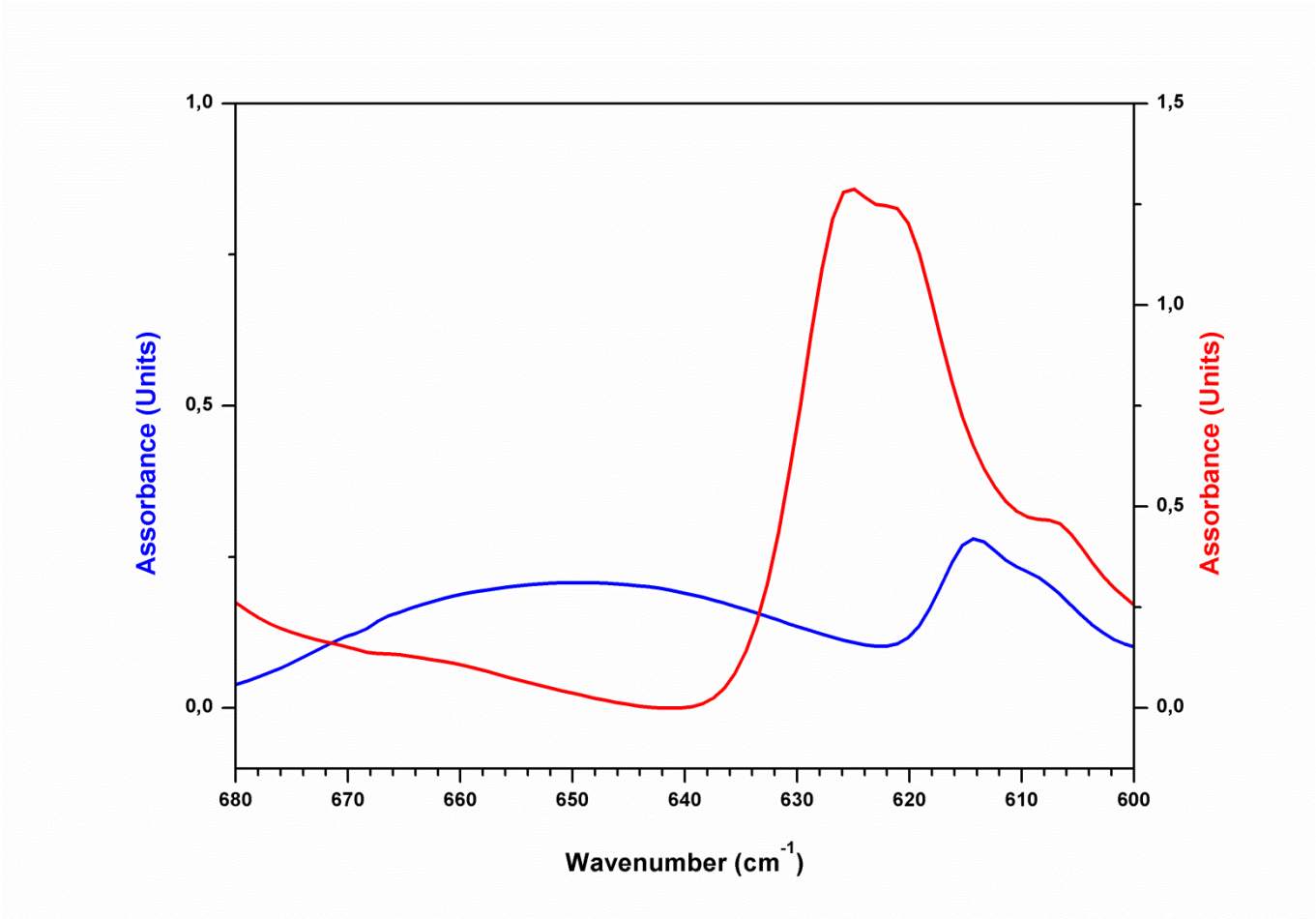


Figure S35. **Magnification of the region 680-600 cm^{-1} (for the C-S stretching vibration)[1,2] of the FT-IR spectra of the pro-ligand L5 (blue curve) and of the iron(III) complex 5 (red curve).**

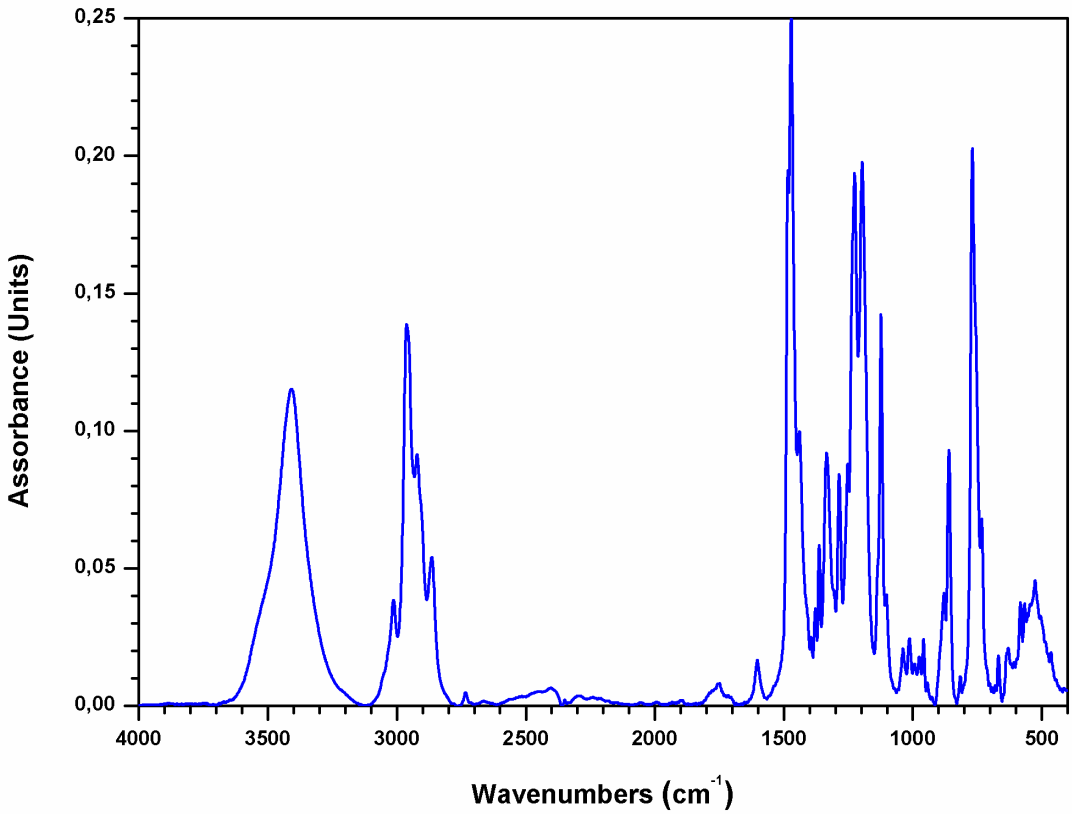


Figure S36. **FT-IR spectrum of the pro-ligand L6 (KBr disk).**

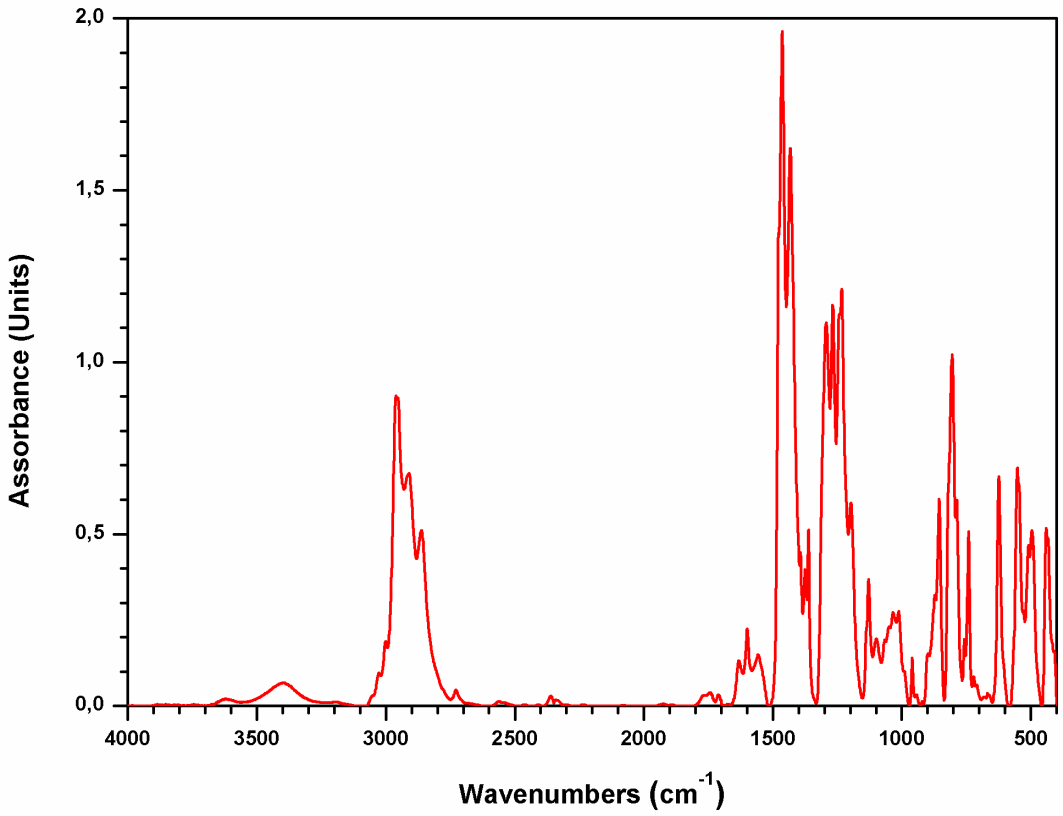


Figure S37. **FT-IR spectrum of the complex 6 (KBr disk).**

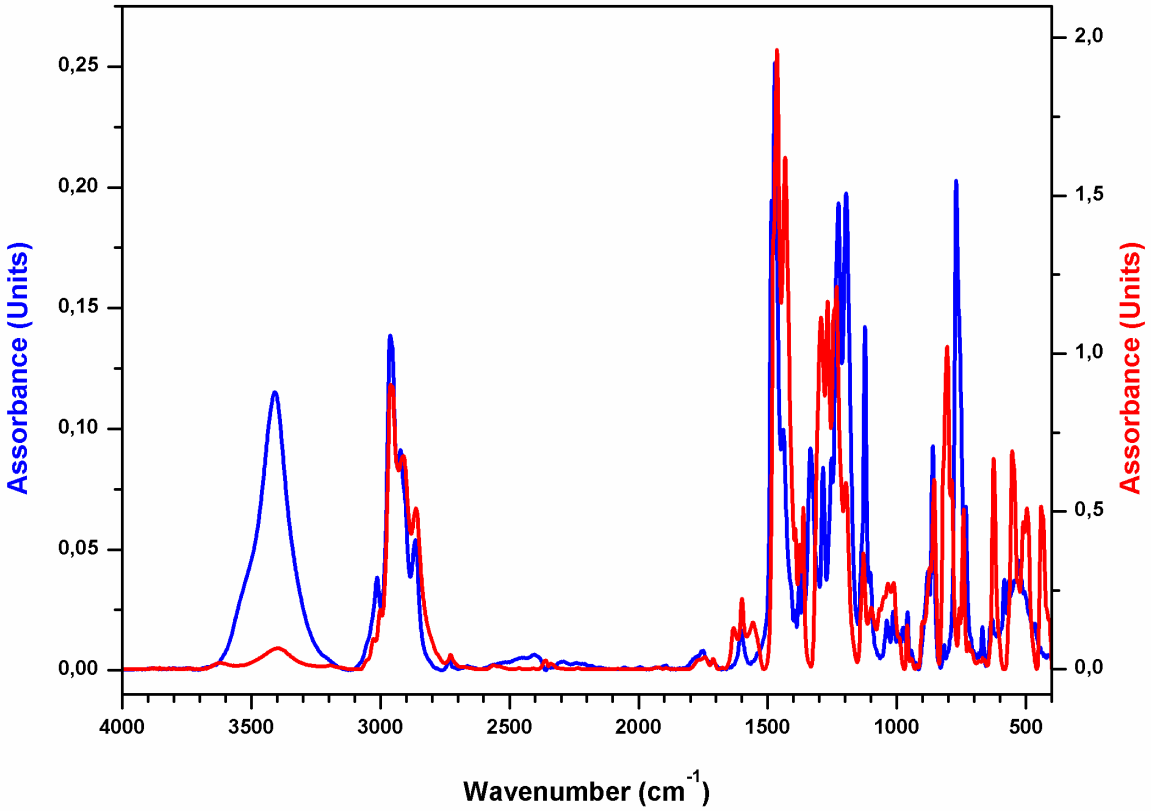


Figure S38. **Comparison of the FT-IR spectra of the pro-ligand L6 (blue curve) and of the iron(III) complex 6 (red curve).**

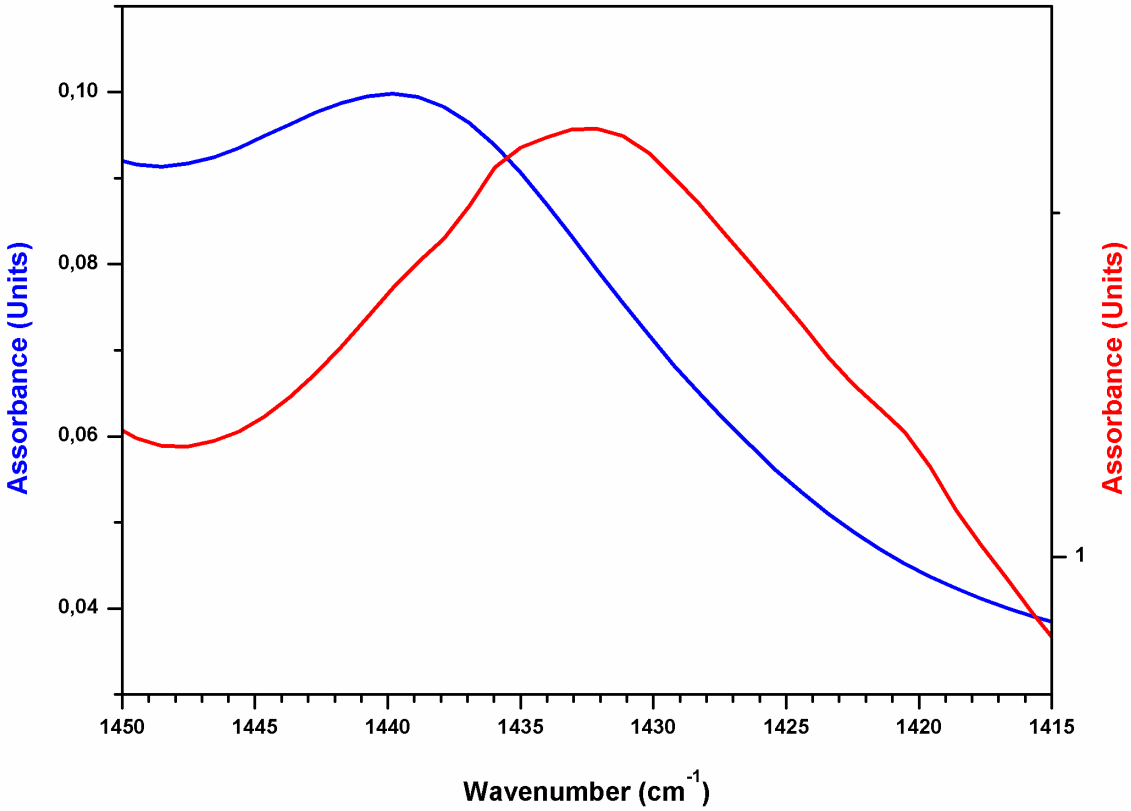


Figure S39. **Magnification of the region 1450-1415 cm^{-1} (for the CH_2-S-C deformation)[1,2] of the FT-IR spectra of the pro-ligand L6 (blue curve) and of the iron(III) complex 6 (red curve).**

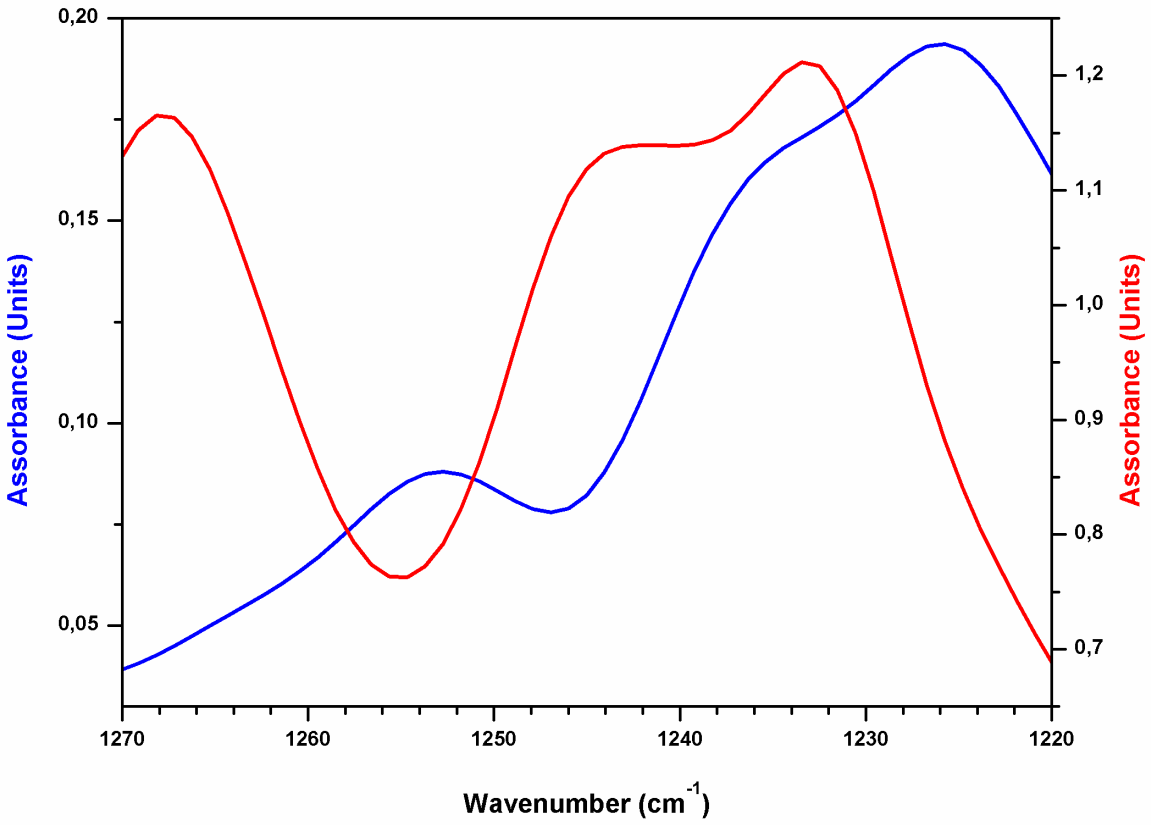


Figure S40. **Magnification of the region 1270-1220 cm^{-1} (for the CH_2-S-C wagging)[1,2] of the FT-IR spectra of the pro-ligand L6 (blue curve) and of the iron(III) complex 6 (red curve).**

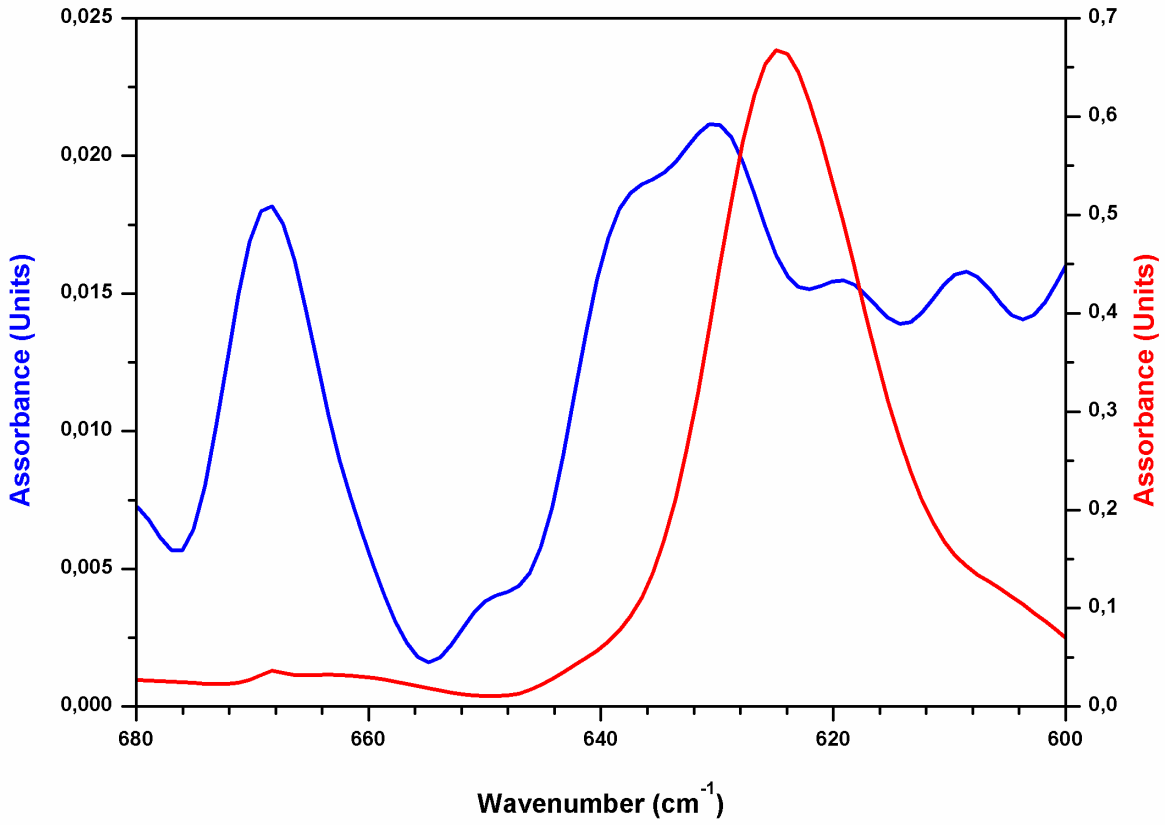


Figure S41. **Magnification of the region 680-600 cm^{-1} (for the C-S stretching vibration)[1,2] of the FT-IR spectra of the pro-ligand L6 (blue curve) and of the iron(III) complex 6 (red curve).**

VI. EFFECTIVE MAGNETIC MOMENTS

Table_S 2. List of effective magnetic μ_{eff} moments in solution and in solid state for Iron(III) complexes 1-6.

Complex	μ_{eff} (μB)	
	Solution[a]	Solid State[b]
1	8.10 ± 0.03	7.0 ± 0.7
2	7.34 ± 0.02	7.6 ± 0.8
3	7.20 ± 0.02	6.7 ± 0.7
4	7.16 ± 0.02	6.9 ± 0.7
5	6.34 ± 0.02	7.1 ± 0.7
6	7.63 ± 0.03	7.2 ± 0.7

a) Determined with the NMR Evans method at 30 °C in Tol-*d8*; b) Determined with the Faraday method at 25 °C using a magnetic susceptibility balance.

VII. CRYSTALLOGRAPHIC DATA

CCDC 1477580 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Table_S 3**. Crystal data and structure refinement for complex 6.**

	6
Empirical formula	$C_{56}\ H_{62}\ Fe_2\ O_6\ S_4$
Formula weight	1070.99
Temperature/K	100(2)
Crystal system	monoclinic
Space group	*C2*
a, Å	22.4656(6)
b, Å	15.5142(6)
c, Å	18.8242(6)
α, °	90
β, °	126.399(2)
γ, °	90
Cell volume, $Å^3$	2121(5)
Z	4
ρ_C, mg m^{-3}	1.347
μ(Mo-K_α), mm^{-1}	0.756
F(000)	2248
Crystal size mm	0.51 x 0.45 x 0.40
θ limits, °	1.344 to 27.993
Refl. collected, unique (R_{int})	47143 / 12667 [R(int) = 0.0229]
Goodness-of-fit-on F^2	1.042
$R_1(F)^a$, $wR_2(F^2)$ [$I > 2\sigma(I)$]^b	R1 = 0.0204, wR2 = 0.0537
Largest diff. peak and hole, e. $Å^{-3}$	0.302 and -0.236

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$ where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where $P = (F_o^2 + F_c^2)/3$.

Table_S 4**. Selected bond lengths [Å] for complex 6.**

Fe(1)-O(1)	1.8894(14)	**Fe(2)-O(6)**	1.8943(14)
Fe(1)-O(4)	1.9030(13)	**Fe(2)-O(3)**	1.8994(15)
Fe(1)-O(5)	2.0314(13)	**Fe(2)-O(5)**	2.0345(13)
Fe(1)-O(2)	2.0384(14)	**Fe(2)-O(2)**	2.0514(14)
Fe(1)-S(1)	2.6102(5)	**Fe(2)-S(2)**	2.5914(5)
Fe(1)-S(3)	2.6466(5)	**Fe(2)-S(4)**	2.6585(5)

VIII. COMPUTATIONAL DATA

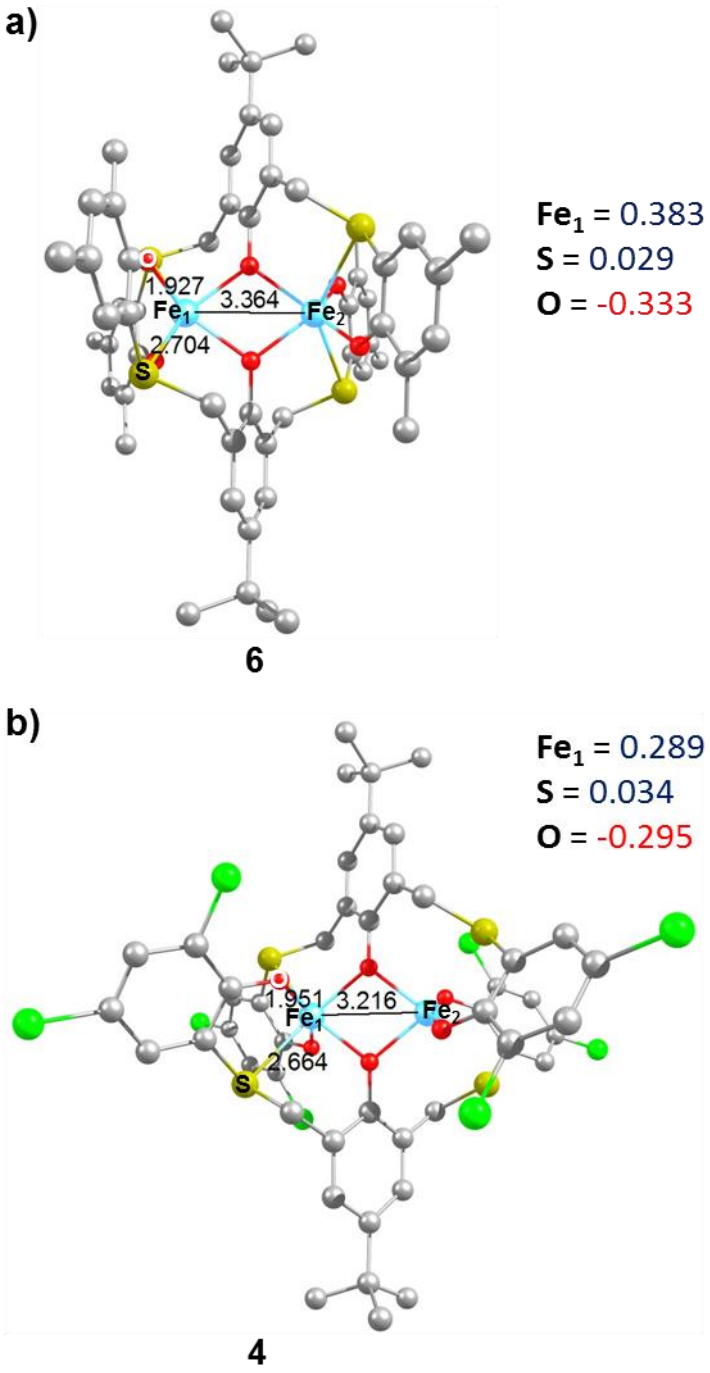


Figure S42. **Geometry of the starting catalyst species 6 (a) and 4 (b). Hydrogen atoms omitted for clarity, Mulliken charges (e^-) are presented, and the selected distances in Å.**

Table_S 5**. Cartesian coordinates and energies (in A.U.) of species: 6, 6 with Fe1-S bond dissociated, 6-A, 6-TS-AB, 6-B, 6-TS-BC, 6-TS- BC′, 6-TS-C, 6-TS-CD, 6-D**

Complex 6
E: -4462.47617135 A.U.

Fe	-0.026667	0.005105	-1.681799
Fe	0.026696	0.004929	1.681686
S	1.855980	1.769761	2.604281
S	1.797417	-1.730911	-2.708974
S	-1.855754	1.770198	-2.604159
S	-1.797633	-1.730930	2.708838
C	0.631092	3.025490	2.939479
C	-0.720265	2.568446	2.940975
C	0.962402	4.350520	3.279470
H	2.020404	4.660020	3.295094
C	-1.751295	3.493493	3.310988
C	-0.046401	5.273160	3.611993
C	-1.387215	4.811455	3.623911
H	-2.188254	5.519550	3.899992
C	0.278065	6.708863	3.961632
H	-0.151119	7.416765	3.218877
H	1.372065	6.884025	3.994944
H	-0.139327	6.993123	4.951541
C	-5.470913	-0.097078	0.037222
C	-2.601614	-0.019907	0.037451
C	-3.292883	-1.164747	0.514672
C	-4.759129	1.026888	-0.441119
H	-5.310764	1.899780	-0.828783
C	-3.354397	1.091072	-0.436639
C	-4.703176	-1.177329	0.518138
H	-5.201558	-2.077188	0.908958
O	-1.251376	0.019608	0.027972
C	0.720556	2.568668	-2.940807
C	1.751672	3.493652	-3.310735
C	-0.630751	3.025857	-2.939202
C	-0.961931	4.350970	-3.278995
H	-2.019901	4.660587	-3.294536
C	0.046961	5.273548	-3.611424
C	1.387723	4.811698	-3.623461
H	2.188829	5.519743	-3.899477
C	-0.277362	6.709343	-3.960820
H	0.151746	7.417065	-3.217848
H	-1.371346	6.884580	-3.994265
H	0.140203	6.993781	-4.950603
C	3.180579	3.014937	-3.350057
H	3.875387	3.837299	-3.612009
H	3.304885	2.198718	-4.093868
H	3.490815	2.582468	-2.375006
O	1.022542	1.318303	-2.624118
C	-2.613788	2.281935	-0.970651
H	-1.778584	2.589421	-0.310291
H	-3.284690	3.143169	-1.154082
C	-2.496394	-2.309888	1.068712
H	-1.637032	-2.579621	0.422968
H	-3.121138	-3.204434	1.255494
C	3.254120	-3.028209	3.298887
H	3.943899	-3.843514	3.594258
H	3.457299	-2.146468	3.944282
H	3.500608	-2.706636	2.264819
C	-0.575351	-2.959614	3.135900
C	1.813644	-3.458040	3.412862
C	0.784228	-2.554659	2.989848
C	-0.915856	-4.216755	3.670729
H	-1.978562	-4.484359	3.791191
C	0.088064	-5.121574	4.061020
C	1.437702	-4.709127	3.924077
H	2.237480	-5.401204	4.241597
O	1.098106	-1.374743	2.477170
O	-1.022381	1.318158	2.624106
C	4.703077	-1.177695	-0.518296
H	5.201361	-2.077576	-0.909192
C	3.292786	-1.164961	-0.514821
C	2.601641	-0.020079	-0.037526
C	4.759269	1.026436	0.441146
H	5.311001	1.899235	0.828882
C	5.470931	-0.097568	-0.037290
C	3.354544	1.090772	0.436674
C	-0.784538	-2.554264	-2.990133
C	0.574988	-2.959449	-3.136039
C	-1.814064	-3.457518	-3.413154
C	0.915339	-4.216683	-3.670747
H	1.978012	-4.484464	-3.791110
C	-1.438279	-4.708705	-3.924239
H	-2.238140	-5.400683	-4.241764
C	-0.088693	-5.121374	-4.061044
C	-3.254480	-3.027452	-3.299313
H	-3.944367	-3.842670	-3.594670
H	-3.457475	-2.145727	-3.944787
H	-3.500986	-2.705765	-2.265283
C	0.248673	-6.484275	-4.624497
H	1.344263	-6.635455	-4.698481
H	-0.179291	-6.624908	-5.640750
H	-0.159918	-7.301050	-3.990134
O	1.251408	0.019597	-0.028070
C	2.614057	2.281642	0.970834
H	1.778879	2.589296	0.310519
H	3.285044	3.142787	1.154377
C	2.496164	-2.309994	-1.068891
H	1.636791	-2.579649	-0.423128
H	3.120807	-3.204600	-1.255718
O	-1.098264	-1.374244	-2.477603
C	-3.180256	3.014929	3.350188
H	-3.874990	3.837345	3.612168
H	-3.304693	2.198664	4.093926
H	-3.490481	2.582572	2.375084
C	-0.249473	-6.484377	4.624609
H	-1.345081	-6.635395	4.698650
H	0.178512	-6.624979	5.640857
H	0.158978	-7.301266	3.990302
C	-7.016059	-0.105253	0.014408
C	7.016076	-0.105891	-0.014529
C	-7.507746	0.041458	-1.449443
H	-8.618187	0.047794	-1.490489
H	-7.150214	0.984023	-1.912149
H	-7.145480	-0.799346	-2.076907
C	-7.551570	1.079650	0.859818
H	-7.215343	1.000803	1.914653
H	-7.204448	2.057905	0.468259
H	-8.662603	1.092758	0.853218
C	-7.597827	-1.413278	0.591734
H	-7.277193	-2.302391	0.009740
H	-7.301552	-1.567718	1.650186
H	-8.706644	-1.378653	0.559009
C	7.551659	1.079083	-0.859792
H	7.204635	2.057312	-0.468079
H	8.662694	1.092094	-0.853237
H	7.215380	1.000417	-1.914624
C	7.507837	0.040565	1.449325
H	7.150428	0.983105	1.912176
H	7.145505	-0.800287	2.076686
H	8.618280	0.046775	1.490326
C	7.597703	-1.413888	-0.592062
H	7.277062	-2.303048	-0.010143
H	7.301323	-1.568184	-1.650505
H	8.706526	-1.379341	-0.559433

Complex 6 with Fe1-S bond dissociated

E: -4462.46742858 A.U.

Fe	0.691718	1.471963	0.802336
Fe	-0.061392	-1.376728	-0.567918
S	-0.880192	1.572302	3.053728
S	2.661632	3.051210	-0.186211
S	1.628766	-3.281918	-1.079794
C	5.253755	-0.247118	-2.537509
C	2.712996	-0.071159	-1.186657
C	3.515048	-1.242184	-1.088703
C	4.471996	0.928710	-2.569740
H	4.834333	1.810267	-3.124382
C	3.228074	1.036949	-1.923212
C	4.745886	-1.315832	-1.774616
H	5.320798	-2.249509	-1.681484
O	1.496147	0.002915	-0.600270
C	0.235853	4.290490	0.017816
C	-0.641377	5.421840	0.000400
C	1.617463	4.498494	-0.261076
C	2.129075	5.776265	-0.551780
H	3.206767	5.894127	-0.751111
C	1.273767	6.894284	-0.579796
C	-0.099127	6.681507	-0.300894
H	-0.782020	7.549172	-0.312463
C	1.794502	8.281889	-0.883860
H	1.275554	8.730376	-1.758624
H	2.880000	8.270262	-1.107561
H	1.635984	8.974549	-0.028719
C	-2.102894	5.225315	0.313434
H	-2.659543	6.181687	0.257721
H	-2.239150	4.796923	1.329090
H	-2.573827	4.501325	-0.384815
O	-0.225627	3.074309	0.271467
C	2.480534	2.336751	-1.914868
H	1.395392	2.217688	-2.107630
H	2.906158	3.070089	-2.626047
C	3.050262	-2.386175	-0.241577
H	2.657138	-2.046275	0.738146
H	3.847786	-3.136491	-0.080840
C	-1.255635	-3.827878	3.312535
H	-1.541463	-4.549275	4.103324
H	-2.181794	-3.466809	2.816294
H	-0.796494	-2.940851	3.799334
C	1.044197	-4.290025	0.284107
C	-0.309817	-4.452108	2.317992
C	0.143426	-3.677292	1.203304
C	1.475416	-5.620460	0.438831
H	2.164869	-6.053770	-0.304230
C	1.029976	-6.389838	1.529543
C	0.143992	-5.774845	2.447736
H	-0.215768	-6.362158	3.310834
O	-0.270922	-2.424572	1.033463
C	-4.255412	0.951867	1.467323
H	-4.783591	0.902238	2.434122
C	-2.894870	0.606505	1.439973
C	-2.188809	0.662812	0.207123
C	-4.216942	1.415281	-0.900487
H	-4.708388	1.722286	-1.836108
C	-4.953812	1.342802	0.299013
C	-2.843043	1.101155	-0.970033
C	1.653015	0.646501	3.466512
C	0.355628	0.756981	4.051151
C	2.713038	0.094658	4.257863
C	0.106025	0.323210	5.367255
H	-0.901174	0.450229	5.796913
C	2.423078	-0.343524	5.558023
H	3.244543	-0.774811	6.156580
C	1.133321	-0.250274	6.139192
C	4.095256	0.003474	3.662959
H	4.811030	-0.458684	4.371210
H	4.475566	1.008949	3.382072
H	4.092751	-0.590455	2.724372
C	0.886348	-0.736464	7.550209
H	-0.150979	-0.526339	7.879537
H	1.574643	-0.251905	8.275894
H	1.050031	-1.832910	7.638295
O	-0.878976	0.318093	0.200346
C	-2.038298	1.288782	-2.233278
H	-2.021858	2.362029	-2.522472
H	-0.992748	0.972479	-2.075315
S	-2.687584	0.510831	-3.783117
C	-2.122973	0.212299	2.667619
H	-1.525786	-0.707427	2.502668
H	-2.778931	0.092550	3.551485
O	1.894118	1.050465	2.226164
C	1.473031	-7.823623	1.721874
H	2.190606	-8.137336	0.937601
H	0.611689	-8.525733	1.687598
H	1.966135	-7.970255	2.707079
O	-1.297633	-1.615237	-1.941983
C	-2.418265	-2.025759	-2.512794
C	-2.909925	-3.361250	-2.298073
C	-4.057597	-3.787681	-2.977864
C	-4.781356	-2.944821	-3.855599
C	-4.325159	-1.625728	-4.021197
C	-3.163798	-1.152264	-3.374577
C	-2.168187	-4.284688	-1.369822
H	-4.408815	-4.821100	-2.814901
C	-6.010429	-3.450702	-4.574554
H	-4.887218	-0.927508	-4.663227
H	-2.642654	-5.284624	-1.337058
H	-1.111027	-4.419007	-1.683024
H	-2.137815	-3.883793	-0.334909
H	-6.531961	-2.637329	-5.117146
H	-5.747509	-4.235058	-5.318189
H	-6.735320	-3.911277	-3.869574
C	-6.462345	1.670937	0.376793
C	6.596774	-0.312932	-3.297648
C	7.288564	-1.682830	-3.132489
H	7.531167	-1.900419	-2.071388
H	6.662400	-2.512757	-3.521340
H	8.242967	-1.693601	-3.698794
C	6.342118	-0.075814	-4.809165
H	5.665703	-0.850821	-5.226057
H	5.877960	0.913497	-5.000750
H	7.297621	-0.112794	-5.375017
C	7.551606	0.783454	-2.756814
H	8.523259	0.753978	-3.294981
H	7.130021	1.801500	-2.885808
H	7.753316	0.638119	-1.675019
C	-7.033536	2.101543	-0.990760
H	-6.540557	3.018423	-1.375571
H	-6.922072	1.304702	-1.754807
H	-8.117245	2.321777	-0.894398
C	-6.692272	2.825382	1.386648
H	-6.336213	2.564115	2.404415
H	-6.157602	3.744898	1.069639
H	-7.774378	3.066003	1.463403
C	-7.234484	0.411546	0.850878
H	-7.095584	-0.430613	0.141383
H	-6.893288	0.069030	1.849506
H	-8.322656	0.625226	0.923213

6-A

E: -4654.46500760 A.U.

Fe	0.905657	1.488179	0.361033
Fe	-0.335928	-1.454917	-0.345550
S	-0.452321	2.793898	2.294055
S	3.179064	2.549289	-0.628206
S	1.026747	-3.675141	-0.091709
C	5.336902	-1.624290	-1.716838
C	2.721138	-0.741407	-0.865112
C	3.270455	-1.970793	-0.399414
C	4.797414	-0.384471	-2.127684
H	5.386139	0.276329	-2.785921
C	3.524946	0.064834	-1.730270
C	4.542067	-2.392266	-0.843208
H	4.916928	-3.352482	-0.457434
O	1.491259	-0.341293	-0.500375
C	0.920880	3.971812	-1.213395
C	0.206493	5.138223	-1.639027
C	2.346797	4.023941	-1.195987
C	3.053477	5.178686	-1.577469
H	4.155200	5.174782	-1.542348
C	2.357870	6.329142	-1.996142
C	0.942117	6.272832	-2.017897
H	0.382679	7.168118	-2.342025
C	3.087478	7.591165	-2.401072
H	2.811732	7.912217	-3.428900
H	4.186951	7.452744	-2.375642
H	2.841935	8.439304	-1.725102
C	-1.300193	5.111047	-1.654126
H	-1.719108	6.085239	-1.975260
H	-1.705806	4.863196	-0.650679
H	-1.682798	4.322260	-2.336324
O	0.282682	2.867001	-0.858681
C	3.038212	1.424938	-2.132093
H	1.970583	1.432375	-2.430496
H	3.657787	1.873828	-2.931663
C	2.523453	-2.773690	0.617712
H	2.107571	-2.122049	1.412647
H	3.159120	-3.558058	1.070977
C	-1.702877	-2.222198	4.157413
H	-2.108497	-2.579710	5.124634
H	-2.541101	-1.811014	3.555065
H	-1.019731	-1.369421	4.359262
C	0.259365	-4.111511	1.464916
C	-0.989329	-3.325666	3.418578
C	-0.432800	-3.052970	2.125799
C	0.378385	-5.395684	2.024965
H	0.922001	-6.179413	1.472239
C	-0.189606	-5.674877	3.282654
C	-0.854367	-4.617803	3.951813
H	-1.294142	-4.815501	4.945341
O	-0.556290	-1.860439	1.565610
C	-3.922084	2.126099	1.205754
H	-4.317610	2.497101	2.166107
C	-2.643657	1.545879	1.203956
C	-2.094569	1.054206	-0.015817
C	-4.126344	1.760726	-1.164311
H	-4.683171	1.821546	-2.111397
C	-4.703077	2.233572	0.030215
C	-2.838280	1.186679	-1.216017
C	1.777557	1.481955	3.188997
C	0.705564	2.341833	3.575480
C	2.762769	1.144537	4.175009
C	0.605540	2.855978	4.881849
H	-0.229004	3.531232	5.132720
C	2.625059	1.665297	5.470499
H	3.389963	1.398063	6.220968
C	1.562735	2.520098	5.857291
C	3.908810	0.246375	3.784734
H	4.618540	0.108842	4.624441
H	4.461484	0.659477	2.914691
H	3.544217	-0.754321	3.467711
C	1.479069	3.058558	7.268634
H	0.584878	3.698309	7.409008
H	2.371688	3.669210	7.526873
H	1.426394	2.238368	8.017291
O	-0.863833	0.497533	-0.000561
C	-2.218243	0.764888	-2.522301
H	-2.102168	1.637626	-3.200878
H	-1.215078	0.331264	-2.366047
S	-3.232996	-0.380335	-3.572522
C	-1.795378	1.476934	2.438935
H	-1.276903	0.501564	2.532678
H	-2.368303	1.702324	3.358830
O	1.866112	0.998186	1.961634
C	-0.097981	-7.050624	3.906096
H	0.520355	-7.736239	3.292478
H	-1.101466	-7.517106	4.017374
H	0.350233	-7.011831	4.922410
O	-1.994297	-1.953776	-1.109834
C	-3.241379	-2.252090	-1.409512
C	-3.942469	-3.272663	-0.669309
C	-5.246274	-3.624595	-1.037498
C	-5.934764	-2.996536	-2.103249
C	-5.264769	-1.976279	-2.799801
C	-3.941048	-1.601189	-2.485566
C	-3.244646	-3.958720	0.472385
H	-5.753430	-4.420832	-0.465458
C	-7.347888	-3.398801	-2.456813
H	-5.779276	-1.440839	-3.614881
H	-3.860749	-4.781799	0.883702
H	-2.263670	-4.375396	0.162765
H	-3.022111	-3.246145	1.293549
H	-7.742415	-2.805611	-3.305710
H	-7.405123	-4.472701	-2.739106
H	-8.038263	-3.259522	-1.596496
O	0.273683	-1.783237	-2.655547
C	-0.379807	-2.627626	-3.624366
C	0.987025	-2.117601	-3.878915
H	-1.257698	-2.163182	-4.109822
H	-0.500553	-3.680554	-3.306933
H	1.079580	-1.244201	-4.554334
C	2.209975	-2.991222	-3.772963
H	2.472209	-3.383443	-4.778834
H	3.079679	-2.418530	-3.391739
H	2.032114	-3.850385	-3.096027
C	6.742895	-2.057636	-2.187952
C	-6.119645	2.847311	0.095915
C	7.121545	-3.460176	-1.665881
H	7.156477	-3.495242	-0.557202
H	6.409294	-4.237394	-2.013483
H	8.129180	-3.741642	-2.036448
C	6.787656	-2.088157	-3.737790
H	6.055122	-2.816473	-4.144533
H	6.557261	-1.096760	-4.179128
H	7.797743	-2.384031	-4.093647
C	7.791764	-1.041793	-1.663144
H	7.589842	-0.014045	-2.028848
H	7.791861	-1.008534	-0.553736
H	8.812712	-1.323858	-1.999016
C	-6.790235	2.906470	-1.292985
H	-6.211184	3.529942	-2.005724
H	-6.909631	1.897075	-1.737852
H	-7.802158	3.354496	-1.204955
C	-7.007044	1.981937	1.029022
H	-7.090926	0.943501	0.646397
H	-6.593964	1.928454	2.057419
H	-8.031237	2.407602	1.099867
C	-6.036610	4.290410	0.658031
H	-5.597393	4.313934	1.676347
H	-5.411055	4.936261	0.007174
H	-7.049406	4.743506	0.720288

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E: -7228.68778360 A.U.

Fe	0.102563	2.057993	0.061529
Fe	-0.004352	-1.242870	0.445168
S	-2.278308	3.188750	0.843026
S	2.333710	3.379410	-0.833911
S	1.579734	-2.481550	2.172943
C	5.560755	-0.162741	0.313748
C	2.723340	0.366309	0.411131
C	3.362893	-0.409687	1.422226
C	4.924584	0.672771	-0.631042
H	5.515669	1.120723	-1.446905
C	3.542717	0.933113	-0.612731
C	4.745608	-0.677025	1.341019
H	5.183349	-1.309814	2.128439
O	1.392818	0.525313	0.422234
C	0.122624	3.733717	-2.397856
C	-0.632666	4.363452	-3.441313
C	1.456410	4.182813	-2.166014
C	2.032910	5.212716	-2.931724
H	3.066307	5.529707	-2.713643
C	1.299438	5.834034	-3.960317
C	-0.025216	5.385069	-4.188026
H	-0.616964	5.862825	-4.989531
C	1.892808	6.949730	-4.793703
H	1.882675	6.703982	-5.878418
H	2.944524	7.154480	-4.507969
H	1.324706	7.899232	-4.676556
C	-2.049461	3.910330	-3.685778
H	-2.520044	4.478273	-4.513367
H	-2.669196	4.033409	-2.772095
H	-2.090725	2.827349	-3.929217
O	-0.399929	2.755348	-1.681814
C	2.919847	1.802938	-1.662483
H	2.028578	1.333659	-2.128698
H	3.643768	2.084152	-2.450956
C	2.553177	-0.913492	2.574822
H	1.782210	-0.175872	2.873602
H	3.188777	-1.170962	3.444094
C	-2.730859	-0.412298	4.359783
H	-3.358266	-0.425971	5.274038
H	-3.378107	-0.652669	3.488740
H	-2.370814	0.626715	4.200318
C	0.420687	-2.422329	3.525777
C	-1.580020	-1.379353	4.468827
C	-0.669960	-1.510602	3.362384
C	0.599085	-3.187261	4.693109
H	1.459003	-3.874709	4.757866
C	-0.305510	-3.075060	5.764400
C	-1.374390	-2.156501	5.619430
H	-2.090806	-2.043456	6.453298
O	-0.830275	-0.823302	2.251546
C	-4.680899	0.872912	-0.757076
H	-5.511994	1.338426	-0.200229
C	-3.403321	0.909542	-0.175647
C	-2.294217	0.327859	-0.857992
C	-3.819624	-0.349233	-2.639961
H	-3.949377	-0.888529	-3.590526
C	-4.924656	0.244865	-2.000320
C	-2.516368	-0.322846	-2.100684
C	-0.268484	3.475370	2.662681
C	-1.669798	3.651784	2.455033
C	0.287390	3.904498	3.915405
C	-2.494665	4.225024	3.442124
H	-3.568783	4.362600	3.232840
C	-0.566614	4.458120	4.880014
H	-0.125823	4.778311	5.841213
C	-1.959639	4.628844	4.678812
C	1.767734	3.737315	4.145766
H	2.066831	4.109866	5.146144
H	2.355723	4.278259	3.373735
H	2.069083	2.671487	4.060192
C	-2.828880	5.235441	5.759334
H	-3.882784	5.330652	5.427463
H	-2.477196	6.249409	6.051747
H	-2.825846	4.618062	6.684920
O	-1.064526	0.396941	-0.308111
C	-1.368177	-0.991113	-2.812845
H	-1.173031	-0.514510	-3.798179
H	-0.434191	-0.939560	-2.224206
S	-1.664948	-2.756187	-3.298420
C	-3.153030	1.559097	1.152077
H	-2.469896	0.947954	1.776725
H	-4.092779	1.776272	1.696333
O	0.510030	2.944538	1.740007
C	-0.154049	-3.902355	7.023145
H	0.800239	-4.467799	7.024373
H	-0.976758	-4.644151	7.133980
H	-0.170127	-3.270237	7.937986
O	-1.294365	-2.516831	-0.132067
C	-2.237966	-3.328351	-0.550492
C	-3.013681	-4.072865	0.411887
C	-3.979726	-4.987824	-0.025064
C	-4.259098	-5.201187	-1.395609
C	-3.538453	-4.440366	-2.331885
C	-2.535522	-3.524029	-1.944789
C	-2.739174	-3.861925	1.876426
H	-4.544760	-5.556239	0.734898
C	-5.301816	-6.207460	-1.829821
H	-3.754043	-4.549743	-3.408191
H	-3.392829	-4.498569	2.505371
H	-1.681837	-4.086713	2.130636
H	-2.892639	-2.801000	2.163610
H	-5.518689	-6.128265	-2.914571
H	-4.968999	-7.251670	-1.634015
H	-6.259291	-6.070996	-1.281518
O	1.331853	-1.931685	-0.904268
C	2.112207	-3.114555	-1.073177
H	2.764812	-3.315812	-0.194361
C	2.725951	-2.206977	-2.052920
H	2.265416	-2.102446	-3.044446
H	3.479256	-1.481007	-1.728811
Br	4.816930	-3.599910	-3.177899
C	1.393068	-4.361146	-1.546396
H	0.696718	-4.116916	-2.374209
H	2.150268	-5.087408	-1.907615
H	0.809690	-4.818382	-0.721365
C	7.070542	-0.464751	0.195555
C	-6.355633	0.208918	-2.582727
C	-6.408079	-0.512210	-3.946594
H	-5.769579	-0.010724	-4.703380
H	-6.078108	-1.568343	-3.866983
H	-7.449207	-0.513698	-4.334114
C	-6.874573	1.656962	-2.778704
H	-7.908943	1.651375	-3.187158
H	-6.893175	2.220922	-1.823436
H	-6.228013	2.217868	-3.485474
C	-7.290874	-0.544469	-1.600843
H	-7.329939	-0.048826	-0.608906
H	-8.328711	-0.584935	-1.998604
H	-6.939682	-1.584999	-1.441291
C	7.872857	0.830206	0.490684
H	8.965186	0.647161	0.390268
H	7.601402	1.644902	-0.212657
H	7.677549	1.197579	1.520569
C	7.394829	-0.959841	-1.238442
H	8.469724	-1.233442	-1.315521
H	6.784301	-1.843985	-1.522932
H	7.202878	-0.174304	-1.998243
C	7.515321	-1.556300	1.192750
H	7.369807	-1.245508	2.248966
H	6.962878	-2.504610	1.029338
H	8.596619	-1.770059	1.058269

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E: -7229.76384855 A.U.

Fe	0.296307	2.049950	0.209706
Fe	-0.057216	-1.296730	0.302382
S	-1.980736	3.229993	1.239722
S	2.594847	3.256940	-0.760355
S	1.563183	-2.768719	1.867275
C	5.584514	-0.541014	0.087248
C	2.793050	0.169734	0.336360
C	3.415922	-0.723522	1.261334
C	4.962213	0.364266	-0.801247
H	5.548522	0.815132	-1.620142
C	3.603284	0.713449	-0.709559
C	4.774831	-1.067527	1.112733
H	5.198477	-1.769552	1.847504
O	1.497249	0.457024	0.456578
C	0.329587	3.893059	-2.147495
C	-0.422791	4.632807	-3.120155
C	1.717991	4.189256	-2.003876
C	2.347464	5.175454	-2.786109
H	3.421843	5.373559	-2.635362
C	1.617061	5.903364	-3.743983
C	0.238397	5.606038	-3.884939
H	-0.352272	6.168886	-4.630240
C	2.269832	6.973016	-4.593491
H	2.173531	6.753777	-5.679955
H	3.351640	7.066233	-4.367505
H	1.808000	7.971805	-4.428275
C	-1.892986	4.338366	-3.274849
H	-2.357147	4.983980	-4.047508
H	-2.431978	4.487009	-2.315026
H	-2.064820	3.275586	-3.548867
O	-0.249063	2.959072	-1.419115
C	2.994024	1.674609	-1.684229
H	2.039107	1.293846	-2.103671
H	3.687546	1.928295	-2.509095
C	2.603251	-1.278387	2.386834
H	1.866874	-0.536338	2.753458
H	3.237096	-1.632842	3.222763
C	-2.513894	-0.663998	4.439199
H	-3.096391	-0.726522	5.380926
H	-3.220286	-0.756396	3.585824
H	-2.075575	0.354697	4.367470
C	0.440770	-2.791791	3.250818
C	-1.444164	-1.724644	4.385047
C	-0.588212	-1.795132	3.229216
C	0.598341	-3.694357	4.319240
H	1.410925	-4.438996	4.275102
C	-0.263244	-3.646055	5.429647
C	-1.262751	-2.641384	5.431906
H	-1.939991	-2.570943	6.302761
O	-0.735813	-0.980638	2.210008
C	-4.603629	1.261414	-0.437909
H	-5.374253	1.722585	0.203518
C	-3.302459	1.150727	0.079134
C	-2.266028	0.572464	-0.712666
C	-3.915988	0.180461	-2.470953
H	-4.126181	-0.251624	-3.461077
C	-4.945404	0.785150	-1.724335
C	-2.592696	0.060375	-1.997522
C	0.165017	3.314485	2.911947
C	-1.246769	3.516648	2.839755
C	0.826113	3.608775	4.152782
C	-1.980675	3.987462	3.945539
H	-3.066195	4.152164	3.840460
C	0.060842	4.061543	5.236917
H	0.582127	4.276829	6.187115
C	-1.341956	4.257019	5.169541
C	2.317318	3.406656	4.241052
H	2.703743	3.667201	5.247149
H	2.849730	4.021672	3.484170
H	2.591433	2.353482	4.017679
C	-2.114882	4.742225	6.377222
H	-3.179745	4.929306	6.129754
H	-1.694458	5.687568	6.785427
H	-2.092748	3.999742	7.205992
O	-1.010505	0.508240	-0.223727
C	-1.537600	-0.631642	-2.820281
H	-1.364046	-0.101043	-3.781900
H	-0.571500	-0.691318	-2.285109
S	-1.994340	-2.336336	-3.405502
C	-2.948167	1.641090	1.451135
H	-2.281592	0.925245	1.975022
H	-3.845463	1.861688	2.061770
O	0.858721	2.880885	1.878336
C	-0.138427	-4.624643	6.578128
H	0.777677	-5.243483	6.485206
H	-1.003894	-5.323810	6.625503
H	-0.094141	-4.107051	7.561664
O	-1.520731	-2.409305	-0.243188
C	-2.556369	-3.074837	-0.695906
C	-3.381347	-3.815866	0.227566
C	-4.459771	-4.574465	-0.246115
C	-4.806532	-4.628627	-1.616385
C	-4.031449	-3.871135	-2.511667
C	-2.916881	-3.113307	-2.088161
C	-3.033416	-3.769418	1.691437
H	-5.061576	-5.143370	0.485232
C	-5.971272	-5.468322	-2.094020
H	-4.290242	-3.858267	-3.584145
H	-3.745301	-4.366366	2.296107
H	-2.006986	-4.149647	1.881026
H	-3.031705	-2.725272	2.067330
H	-6.218467	-5.256180	-3.154463
H	-5.752485	-6.557653	-2.017533
H	-6.887203	-5.285756	-1.490521
O	1.111312	-1.771815	-1.112930
C	1.855756	-2.891219	-1.502227
H	2.647210	-3.114114	-0.737440
C	2.581217	-2.441217	-2.784841
H	1.874512	-2.315815	-3.627982
H	3.137311	-1.504827	-2.598219
Br	3.961618	-3.741925	-3.426677
C	1.002870	-4.150928	-1.703829
H	0.193241	-3.948353	-2.435551
H	1.627278	-4.993541	-2.068168
H	0.530049	-4.448554	-0.746642
C	7.077481	-0.898159	-0.085695
C	7.535975	-1.971389	0.924746
H	8.608097	-2.211238	0.761317
H	7.429408	-1.626261	1.974425
H	6.960250	-2.913453	0.812366
C	7.320448	-1.446526	-1.515932
H	6.694243	-2.340647	-1.715302
H	7.074681	-0.693680	-2.292864
H	8.387855	-1.727933	-1.650684
C	7.938780	0.374124	0.129795
H	7.797696	0.781365	1.153066
H	9.019358	0.147954	-0.005977
H	7.668948	1.175952	-0.588278
C	-6.396653	0.913834	-2.239213
C	-6.809081	2.408697	-2.261609
H	-7.857321	2.523337	-2.615488
H	-6.742714	2.870796	-1.254917
H	-6.150568	2.990997	-2.939649
C	-6.558201	0.347459	-3.665949
H	-5.913054	0.879821	-4.395579
H	-6.306571	-0.732093	-3.711654
H	-7.610754	0.461820	-4.002256
C	-7.348284	0.131706	-1.296428
H	-7.307735	0.521133	-0.258252
H	-8.401518	0.210818	-1.645302
H	-7.073309	-0.942733	-1.261245

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E: -7417.16706692 A.U.

Fe	0.275833	2.128844	0.025448
Fe	-0.055660	-1.165751	0.007148
S	-1.582076	3.514512	1.466456
S	2.336499	3.505660	-1.080024
S	1.788929	-2.591248	1.402688
C	5.621590	-0.012414	-0.507964
C	2.770581	0.335610	-0.243635
C	3.501460	-0.472289	0.678744
C	4.897449	0.847186	-1.357149
H	5.415043	1.401284	-2.154911
C	3.504563	1.036334	-1.246409
C	4.886928	-0.647893	0.517063
H	5.406292	-1.293415	1.245708
O	1.437732	0.445379	-0.139070
C	-0.089819	4.040170	-2.219460
C	-0.977274	4.768027	-3.080585
C	1.282513	4.430647	-2.185589
C	1.766764	5.499575	-2.961730
H	2.833802	5.770346	-2.896620
C	0.902151	6.216562	-3.809921
C	-0.459047	5.823820	-3.845754
H	-1.153421	6.375666	-4.504766
C	1.399827	7.364605	-4.661863
H	1.299701	7.145658	-5.748378
H	2.469368	7.582328	-4.465122
H	0.827403	8.299035	-4.471180
C	-2.430144	4.370319	-3.127223
H	-3.007010	5.020738	-3.815281
H	-2.891397	4.419721	-2.118121
H	-2.545156	3.315644	-3.456614
O	-0.533456	3.037078	-1.489330
C	2.797123	2.015347	-2.133959
H	1.858789	1.597228	-2.555194
H	3.449176	2.385167	-2.948298
C	2.781764	-1.061856	1.850082
H	2.042994	-0.342575	2.257795
H	3.482986	-1.378969	2.646277
C	-2.240266	-0.891540	4.310979
H	-2.867596	-1.152658	5.187520
H	-2.875097	-0.900698	3.400209
H	-1.896894	0.158080	4.439207
C	0.821286	-2.707590	2.892992
C	-1.071910	-1.833695	4.171191
C	-0.281288	-1.800151	2.968807
C	1.130608	-3.611565	3.924411
H	1.992113	-4.289437	3.804490
C	0.349168	-3.652452	5.094228
C	-0.737086	-2.747717	5.182893
H	-1.364326	-2.761766	6.092771
O	-0.563969	-0.983441	1.978133
C	-4.579497	1.525303	0.735867
H	-5.098372	1.997655	1.587687
C	-3.184227	1.386072	0.818505
C	-2.462817	0.783031	-0.256268
C	-4.583883	0.498546	-1.436065
H	-5.097369	0.125365	-2.335301
C	-5.318430	1.072326	-0.381185
C	-3.180580	0.356942	-1.406288
C	0.817974	3.235676	2.747704
C	-0.472421	3.843137	2.824878
C	1.750825	3.503983	3.806329
C	-0.830311	4.686593	3.893692
H	-1.834595	5.142295	3.903623
C	1.356773	4.342372	4.859758
H	2.085932	4.539258	5.666367
C	0.078640	4.950285	4.934737
C	3.116642	2.869085	3.746991
H	3.752084	3.193351	4.595779
H	3.634126	3.118005	2.796578
H	3.042785	1.760425	3.767939
C	-0.283706	5.852604	6.094945
H	-1.315047	6.248053	5.994829
H	0.402081	6.725513	6.170185
H	-0.224991	5.317227	7.068509
O	-1.124583	0.645765	-0.166646
C	-2.430148	-0.193455	-2.588333
H	-2.570863	0.461697	-3.475878
H	-1.340801	-0.243908	-2.410968
S	-3.038682	-1.813612	-3.247021
C	-2.414406	1.910544	1.992531
H	-1.611100	1.208606	2.295440
H	-3.068335	2.151446	2.852698
O	1.149224	2.441457	1.749879
C	0.650895	-4.619360	6.219251
H	1.525429	-5.258477	5.980603
H	-0.208231	-5.295583	6.425693
H	0.875073	-4.090258	7.172256
O	-1.528935	-2.275130	-0.483168
C	-2.602744	-3.006606	-0.681957
C	-2.979852	-4.025459	0.269352
C	-4.107167	-4.822216	0.030565
C	-4.924405	-4.665816	-1.112849
C	-4.563408	-3.670363	-2.035504
C	-3.419987	-2.859363	-1.859265
C	-2.125089	-4.249641	1.486272
H	-4.360197	-5.602508	0.770072
C	-6.139936	-5.540382	-1.325575
H	-5.179261	-3.508324	-2.936244
H	-2.462083	-5.140204	2.053004
H	-1.058794	-4.394856	1.213168
H	-2.143876	-3.377586	2.171309
H	-6.690813	-5.256081	-2.245081
H	-5.860179	-6.613234	-1.421284
H	-6.850661	-5.472976	-0.472426
C	1.082129	-3.483099	-1.743563
H	0.606773	-3.900394	-0.827541
C	2.556162	-3.924960	-1.749961
H	3.057699	-3.664194	-2.697507
H	3.103064	-3.491344	-0.893712
Br	2.746219	-5.902215	-1.530453
C	0.286905	-3.967425	-2.959901
H	0.771193	-3.641300	-3.901780
H	0.228229	-5.075029	-2.957473
H	-0.739944	-3.553798	-2.930808
O	1.042627	-2.051550	-1.588406
C	1.426136	-1.138606	-2.995525
O	2.304624	-1.685365	-3.631400
O	0.707852	-0.153482	-2.989383
C	-6.856241	1.220155	-0.406520
C	-7.236839	2.718882	-0.287018
H	-8.341764	2.845747	-0.293196
H	-6.852321	3.168197	0.651595
H	-6.817911	3.302637	-1.133220
C	-7.469253	0.438366	0.784737
H	-7.089044	0.809746	1.758697
H	-8.576882	0.540199	0.793784
H	-7.221396	-0.641452	0.718952
C	-7.469490	0.669048	-1.711310
H	-7.090593	1.207878	-2.604580
H	-7.249990	-0.410123	-1.845464
H	-8.573668	0.788430	-1.691018
C	7.141667	-0.253775	-0.640846
C	7.857303	0.214780	0.653059
H	7.488179	-0.328598	1.547222
H	8.953384	0.039992	0.582326
H	7.691298	1.298494	0.828081
C	7.405711	-1.767031	-0.855488
H	7.026704	-2.375067	-0.008561
H	6.903736	-2.129808	-1.776193
H	8.495562	-1.965971	-0.952438
C	7.748796	0.514956	-1.834112
H	7.288871	0.209880	-2.796927
H	7.624302	1.612772	-1.726485
H	8.838029	0.308240	-1.902611

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E: -7417.13490038 A.U.

Fe	-1.261674	-0.533404	0.269634
S	1.382421	3.744595	-0.862193
S	0.011627	-2.328808	3.472227
C	3.808040	-3.597058	1.011596
C	1.789652	-1.628821	0.465156
C	2.164581	-1.922487	1.809525
C	3.399512	-3.309691	-0.304008
H	3.856560	-3.826405	-1.161556
C	2.405018	-2.353014	-0.590683
C	3.157479	-2.889393	2.047963
H	3.423105	-3.088831	3.100125
O	0.873410	-0.658846	0.198025
C	1.455731	-1.257476	2.952240
H	1.041689	-0.279958	2.641551
H	2.123697	-1.130343	3.828196
C	-2.668532	2.270975	3.257131
H	-3.164487	3.013603	3.915047
H	-3.345016	2.055153	2.403943
H	-1.762486	2.737476	2.815143
C	-1.082405	-1.107253	4.171888
C	-2.309511	1.020113	4.019780
C	-1.519968	0.004134	3.371559
C	-1.506083	-1.244849	5.508458
H	-1.139615	-2.110922	6.085253
C	-2.356448	-0.300268	6.113830
C	-2.718272	0.833669	5.349736
H	-3.339456	1.618438	5.818529
O	-1.162839	0.141465	2.113335
C	-2.280398	4.813872	-1.003676
H	-1.898471	5.842208	-0.882540
C	-1.454876	3.762861	-0.568151
C	-1.859930	2.393989	-0.707392
C	-3.996308	3.258132	-1.585407
H	-5.006285	3.019326	-1.952698
C	-3.566782	4.598157	-1.538938
C	-3.194231	2.164810	-1.195179
C	2.615144	2.987119	1.455043
C	2.512571	4.041319	0.497645
C	3.404348	3.224822	2.628879
C	3.175790	5.269323	0.664551
H	3.061757	6.052682	-0.103155
C	4.057831	4.460156	2.764469
H	4.668423	4.625790	3.670277
C	3.974586	5.496705	1.801967
C	3.509549	2.134965	3.664554
H	4.142861	2.447019	4.519240
H	3.935966	1.206724	3.226768
H	2.507093	1.851871	4.050289
C	4.723318	6.797872	1.996581
H	4.435479	7.550522	1.234551
H	5.824741	6.655813	1.920973
H	4.527076	7.240460	2.997333
O	-1.011310	1.420907	-0.367608
C	-3.776576	0.782116	-1.282119
H	-4.796044	0.796862	-1.713599
H	-3.108376	0.093170	-1.837280
S	-3.860203	0.135087	0.476744
C	-0.180341	4.063081	0.144884
H	-0.063796	3.415629	1.037142
H	-0.113900	5.127484	0.440883
O	1.999982	1.833878	1.271053
C	-2.856195	-0.480416	7.530939
H	-2.232957	-1.205846	8.094061
H	-3.902672	-0.862255	7.555074
H	-2.853556	0.477769	8.094221
O	-2.088945	-2.259754	0.573809
C	-3.368356	-2.564756	0.592648
C	-3.779674	-3.934454	0.743950
C	-5.147106	-4.237878	0.724955
C	-6.161159	-3.257611	0.573770
C	-5.757343	-1.917469	0.450330
C	-4.390479	-1.571038	0.449783
C	-2.714156	-4.989584	0.894769
H	-5.444573	-5.296363	0.833991
C	-7.622197	-3.652500	0.558579
H	-6.510523	-1.116679	0.361796
H	-3.153395	-5.975035	1.150580
H	-2.134130	-5.102761	-0.047004
H	-1.980143	-4.700132	1.675326
H	-8.281400	-2.766252	0.456880
H	-7.853763	-4.338856	-0.286031
H	-7.917192	-4.183178	1.490920
O	-1.299643	-0.890643	-1.854594
C	-1.453127	-2.096533	-2.580707
H	-1.004113	-2.946433	-2.007267
C	-2.959271	-2.398312	-2.732482
H	-3.486848	-2.386042	-1.764986
H	-3.444777	-1.699605	-3.441706
Br	-3.329042	-4.224273	-3.469823
O	3.064559	0.659571	-1.276171
C	4.244006	0.320166	-1.751293
C	4.418924	-0.769485	-2.677480
C	5.426879	1.049593	-1.354574
C	5.699352	-1.053605	-3.205888
C	6.667807	0.737306	-1.921818
C	6.834867	-0.304046	-2.864901
H	5.794494	-1.906863	-3.898470
H	7.547309	1.327060	-1.608756
S	3.133834	-1.805783	-3.329381
C	8.193629	-0.610355	-3.453175
H	8.156506	-1.486251	-4.132053
H	8.588726	0.250571	-4.036858
H	8.943994	-0.827981	-2.661538
C	5.308872	2.153546	-0.342443
H	4.597265	2.938968	-0.668343
H	4.916257	1.773971	0.623521
H	6.291266	2.630465	-0.155351
Fe	1.416571	1.145150	-0.468917
C	1.903785	-2.128173	-1.988014
H	1.135306	-1.336692	-1.993290
H	1.424412	-3.054692	-2.371776
O	0.566437	0.934924	-2.628922
C	-0.543365	0.846294	-3.068363
O	-1.478390	1.072382	-3.751806
C	-0.804309	-2.044382	-3.980170
H	-0.841901	-3.044757	-4.458368
H	-1.350763	-1.334932	-4.634976
H	0.253482	-1.721836	-3.938477
C	-4.429205	5.787110	-2.016145
C	-3.697835	6.518508	-3.172116
H	-4.294189	7.386016	-3.531180
H	-2.706143	6.899653	-2.852311
H	-3.531282	5.834347	-4.030175
C	-5.811196	5.330919	-2.531335
H	-5.721758	4.637203	-3.393020
H	-6.398904	4.820001	-1.740353
H	-6.399269	6.210229	-2.869964
C	-4.652834	6.777730	-0.843765
H	-5.265350	7.645523	-1.173199
H	-5.179538	6.283098	-0.001048
H	-3.694118	7.175311	-0.451459
C	4.900178	-4.636968	1.349068
C	5.490269	-5.290233	0.081215
H	4.716000	-5.829366	-0.502986
H	5.961732	-4.540032	-0.586751
H	6.270696	-6.028378	0.364507
C	6.054326	-3.943384	2.118433
H	5.698152	-3.478982	3.060823
H	6.847653	-4.677117	2.381602
H	6.514043	-3.142190	1.502838
C	4.291125	-5.755372	2.234723
H	3.874834	-5.350778	3.179964
H	3.466117	-6.275549	1.704542
H	5.062514	-6.511476	2.500219

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E: -7418.33735647 A.U.

Fe	1.819791	-1.713740	-0.237126
Fe	-0.546029	0.536325	0.531303
S	4.177624	-0.829262	0.897008
S	1.150079	-3.869513	-1.757291
S	-2.553033	-0.150511	2.165350
C	-3.436694	-4.331045	-0.153508
C	-1.184857	-2.540367	0.115436
C	-2.120954	-2.717709	1.177037
C	-2.506314	-4.137061	-1.198668
H	-2.635796	-4.675243	-2.152995
C	-1.414834	-3.258085	-1.098096
C	-3.216154	-3.591968	1.024827
H	-3.908400	-3.684010	1.875869
O	-0.155621	-1.697341	0.267485
C	2.963289	-2.222006	-2.956602
C	3.871929	-1.844501	-4.001743
C	2.229342	-3.435273	-3.110178
C	2.379243	-4.251698	-4.246913
H	1.798817	-5.186931	-4.316507
C	3.260407	-3.883445	-5.280090
C	3.988873	-2.677253	-5.124573
H	4.689594	-2.374561	-5.923618
C	3.433880	-4.738179	-6.517388
H	3.113142	-4.201813	-7.438174
H	2.837877	-5.671283	-6.453098
H	4.496068	-5.029740	-6.672531
C	4.667089	-0.573241	-3.847526
H	5.289136	-0.373151	-4.743247
H	5.333326	-0.625063	-2.959531
H	4.002555	0.298825	-3.670326
O	2.812420	-1.461426	-1.891415
C	-0.473824	-3.074254	-2.248345
H	-0.285472	-2.001028	-2.457422
H	-0.833402	-3.573986	-3.168059
C	-1.944079	-1.918412	2.427014
H	-0.877193	-1.821130	2.708740
H	-2.528825	-2.323859	3.275496
C	1.711890	1.661356	4.655890
H	2.062510	2.105895	5.609558
H	1.968342	2.357075	3.828234
H	2.295442	0.733447	4.471419
C	-1.813862	0.586099	3.612687
C	0.231643	1.378626	4.694063
C	-0.414448	0.867484	3.514934
C	-2.550866	0.823187	4.787261
H	-3.628592	0.588657	4.799384
C	-1.923314	1.348428	5.931703
C	-0.532201	1.603556	5.850269
H	-0.014517	2.004884	6.740595
O	0.247914	0.666449	2.395364
C	4.130761	2.748749	-0.067384
H	4.989066	2.968794	0.590243
C	3.296681	1.674439	0.282227
C	2.179254	1.348185	-0.539880
C	2.765511	3.218992	-1.992306
H	2.505757	3.821757	-2.875772
C	3.887276	3.550271	-1.206890
C	1.910224	2.139133	-1.687877
C	3.052407	-2.957415	2.160261
C	4.013029	-1.910788	2.306831
C	2.935362	-3.922335	3.216925
C	4.822855	-1.812917	3.454742
H	5.569238	-1.003709	3.521562
C	3.747177	-3.783914	4.351617
H	3.640582	-4.527576	5.161742
C	4.694748	-2.740470	4.504907
C	1.934113	-5.038901	3.065039
H	1.915855	-5.693438	3.959822
H	2.163609	-5.662519	2.174142
H	0.912178	-4.638769	2.893970
C	5.538014	-2.640316	5.757968
H	6.284901	-1.823882	5.681923
H	6.091554	-3.583583	5.959953
H	4.915107	-2.437286	6.657536
O	1.392104	0.305342	-0.203993
C	0.717375	1.813679	-2.549041
H	1.031424	1.534757	-3.578294
H	0.137049	0.968155	-2.137215
S	-0.443684	3.222581	-2.886305
C	3.543219	0.827326	1.495741
H	2.599154	0.628356	2.043886
H	4.303928	1.270776	2.167557
O	2.293184	-3.056116	1.085220
C	-2.695545	1.637131	7.201420
H	-3.740332	1.270770	7.132434
H	-2.742573	2.727738	7.420269
H	-2.229703	1.154642	8.088761
O	-0.638349	2.400559	0.186062
C	-0.672133	3.685301	-0.071622
C	-0.852379	4.627670	1.006316
C	-0.928534	5.998726	0.730126
C	-0.810936	6.518163	-0.580761
C	-0.603344	5.603010	-1.626984
C	-0.545391	4.208336	-1.406489
C	-0.987138	4.102739	2.410120
H	-1.082071	6.695086	1.573719
C	-0.905165	8.005736	-0.839444
H	-0.479639	5.970281	-2.659853
H	-1.160024	4.925126	3.132703
H	-1.824118	3.378058	2.494579
H	-0.080553	3.544051	2.721976
H	-0.630521	8.255962	-1.884421
H	-1.937167	8.386427	-0.667228
H	-0.236433	8.584353	-0.165425
C	-4.758961	1.925908	-1.133590
H	-5.124103	2.442298	-0.220163
C	-5.776545	0.826439	-1.479397
H	-5.590264	0.379018	-2.470274
H	-5.779631	0.043387	-0.698808
Br	-7.639566	1.539903	-1.515513
C	-4.535316	2.956921	-2.240805
H	-4.134066	2.465529	-3.147646
H	-5.493876	3.458672	-2.486762
H	-3.810366	3.723292	-1.902159
O	-3.528471	1.317690	-0.677928
C	-2.811000	0.504539	-1.556200
O	-3.229836	0.231569	-2.681563
O	-1.715260	0.070817	-1.018867
C	-4.625157	-5.301104	-0.337973
C	4.820045	4.740251	-1.526193
C	4.778939	5.753916	-0.352542
H	5.108386	5.291521	0.600782
H	5.447177	6.619550	-0.555908
H	3.749423	6.138560	-0.199045
C	4.399230	5.478137	-2.815132
H	4.423928	4.808385	-3.699864
H	3.376002	5.899009	-2.733350
H	5.095071	6.321191	-3.012725
C	6.272296	4.228457	-1.711556
H	6.646694	3.713209	-0.803016
H	6.334669	3.507641	-2.553493
H	6.962471	5.073436	-1.927478
C	-5.495930	-4.833320	-1.533344
H	-6.351803	-5.525828	-1.690066
H	-5.902286	-3.816363	-1.354325
H	-4.914524	-4.796757	-2.477316
C	-5.522788	-5.363418	0.916302
H	-4.964295	-5.719115	1.807306
H	-5.961694	-4.373508	1.159495
H	-6.363908	-6.068474	0.745455
C	-4.090060	-6.729175	-0.621356
H	-3.460701	-6.758415	-1.534533
H	-3.470084	-7.096024	0.223440
H	-4.930804	-7.442345	-0.768251

6-TS-CD

E: -7417.17077413 A.U.

Fe	1.792385	-1.680705	-0.526620
S	-2.223124	-0.379895	2.534815
S	4.239202	-0.867719	0.409669
C	3.706543	3.650623	-1.375062
C	2.099558	1.395990	-0.643384
C	3.312748	1.674487	0.049752
C	2.489846	3.367454	-2.026518
H	2.116438	4.030178	-2.821909
C	1.681116	2.262520	-1.686742
C	4.095252	2.776056	-0.333287
H	5.031644	2.958502	0.221073
O	1.362004	0.322677	-0.286467
C	3.708675	0.757938	1.171291
H	2.843807	0.535992	1.830899
H	4.557064	1.161575	1.757594
C	2.229801	-5.225337	2.510890
H	2.312197	-5.944102	3.350939
H	2.359754	-5.779337	1.556326
H	1.194232	-4.824645	2.485424
C	4.217776	-2.036352	1.758218
C	3.240192	-4.113491	2.633905
C	3.247188	-3.077438	1.640904
C	5.143858	-2.012234	2.818741
H	5.895228	-1.206185	2.862766
C	5.125978	-3.011396	3.809277
C	4.167146	-4.048096	3.684006
H	4.146555	-4.847041	4.446673
O	2.379265	-3.105747	0.644957
C	-3.016186	-3.742003	1.207342
H	-3.578613	-3.927031	2.135361
C	-1.929527	-2.846495	1.279632
C	-1.163275	-2.552015	0.115234
C	-2.617114	-4.084849	-1.131981
H	-2.867697	-4.550962	-2.099936
C	-3.386101	-4.390214	0.013027
C	-1.542241	-3.180153	-1.108766
C	0.073528	0.517308	3.702799
C	-1.308036	0.235563	3.938529
C	0.862190	0.918141	4.834682
C	-1.900612	0.376288	5.206002
H	-2.972991	0.148231	5.324533
C	0.240953	1.048732	6.087523
H	0.865427	1.366519	6.942140
C	-1.135215	0.799020	6.308734
C	2.333177	1.189620	4.647858
H	2.805169	1.521120	5.594915
H	2.504933	1.973568	3.879117
H	2.868417	0.283166	4.291198
C	-1.754028	0.994369	7.676403
H	-2.769598	0.551545	7.729439
H	-1.852624	2.072596	7.936255
H	-1.140709	0.527858	8.477513
O	-0.143511	-1.681882	0.176078
C	-0.764863	-2.874566	-2.351033
H	-1.242700	-3.288940	-3.259359
H	-0.601596	-1.784805	-2.475881
S	0.915315	-3.683156	-2.162350
C	-1.586944	-2.155368	2.559952
H	-0.491736	-2.073889	2.705962
H	-2.054361	-2.639153	3.439322
O	0.598112	0.408990	2.496952
C	6.098581	-2.994982	4.968907
H	6.831644	-2.168143	4.874409
H	6.671977	-3.945220	5.039603
H	5.575313	-2.865261	5.942275
O	2.635597	-1.310534	-2.235882
C	2.599418	-1.929083	-3.399273
C	3.370350	-1.441526	-4.507254
C	3.288933	-2.119125	-5.732690
C	2.490718	-3.273730	-5.932902
C	1.752351	-3.755866	-4.836698
C	1.800777	-3.094123	-3.595045
C	4.236861	-0.224747	-4.305712
H	3.882774	-1.731846	-6.580111
C	2.441973	-3.955809	-7.283330
H	1.131439	-4.661524	-4.939661
H	4.747101	0.070149	-5.244705
H	3.641698	0.636599	-3.934708
H	5.008093	-0.410600	-3.527390
H	1.847216	-4.891043	-7.245198
H	1.983075	-3.302168	-8.058331
H	3.458344	-4.219206	-7.649736
O	-3.752398	0.398810	-1.899894
C	-4.997689	1.175459	-2.005045
H	-5.752654	0.451137	-2.363934
C	-5.390690	1.654455	-0.610424
H	-5.785408	0.944676	0.123929
H	-5.455335	2.719960	-0.371618
Br	-7.882453	1.933076	-1.238236
O	-0.572718	2.323294	0.565806
C	-0.634173	3.624141	0.421468
C	-0.713135	4.255929	-0.869182
C	-0.628759	4.472350	1.589229
C	-0.803782	5.662159	-0.961553
C	-0.741445	5.859629	1.443232
C	-0.838659	6.485246	0.177226
H	-0.846079	6.115752	-1.965963
H	-0.752072	6.483355	2.354485
S	-0.834653	3.397758	-2.425381
C	-0.968092	7.987546	0.062048
H	-0.896727	8.324091	-0.992104
H	-1.944744	8.343478	0.459735
H	-0.178234	8.513879	0.641174
C	-0.534846	3.829481	2.945817
H	-1.382824	3.134910	3.123445
H	0.381364	3.210014	3.033739
H	-0.530056	4.588597	3.752980
Fe	-0.427061	0.443911	0.758021
C	0.379838	1.990787	-2.394480
H	-0.122492	1.098387	-1.980461
H	0.541687	1.815774	-3.480123
O	-1.912242	0.174214	-0.668715
C	-3.048253	0.722229	-0.792342
O	-3.608195	1.515022	0.034092
C	-4.800355	2.302470	-3.012366
H	-5.761031	2.841666	-3.131756
H	-4.016510	3.006011	-2.663096
H	-4.486968	1.891696	-3.993038
C	4.591143	4.865433	-1.734643
C	-4.570443	-5.377609	-0.084162
C	4.703862	5.799994	-0.501692
H	5.151043	5.278134	0.369327
H	5.343088	6.680589	-0.731611
H	3.703517	6.168426	-0.193320
C	6.005792	4.377296	-2.142060
H	6.662814	5.240012	-2.388076
H	6.495378	3.804004	-1.328121
H	5.956546	3.716443	-3.032688
C	4.006111	5.681979	-2.907019
H	3.911174	5.070615	-3.828565
H	3.004337	6.092531	-2.664507
H	4.672276	6.539424	-3.141212
C	-4.054847	-6.758095	-0.568114
H	-4.893789	-7.483347	-0.649486
H	-3.571412	-6.690896	-1.564427
H	-3.306714	-7.173413	0.139312
C	-5.614401	-4.835011	-1.094897
H	-6.471036	-5.537442	-1.189924
H	-6.010508	-3.851035	-0.768978
H	-5.177620	-4.699694	-2.105650
C	-5.272791	-5.575071	1.276275
H	-4.582643	-5.986499	2.042440
H	-5.692277	-4.624439	1.665702
H	-6.115093	-6.290352	1.166480

6-D

E: -4842.95170385 A.U.

Fe	1.079548	1.780997	0.348743
S	1.058124	-3.412580	0.900475
S	-0.465659	3.195624	2.079657
C	-4.568672	2.348495	-0.457849
C	-1.945942	1.245865	-0.126078
C	-2.602962	1.887510	0.962813
C	-3.902560	1.697353	-1.513646
H	-4.391607	1.591731	-2.493733
C	-2.608159	1.150521	-1.378134
C	-3.883375	2.432880	0.777229
H	-4.361624	2.929523	1.638144
O	-0.702738	0.748211	0.053037
C	-1.876580	1.973813	2.273562
H	-1.413807	1.004799	2.550350
H	-2.531993	2.338197	3.088111
C	4.163658	1.516933	3.881602
H	4.790481	1.405589	4.788555
H	4.701390	2.162996	3.155206
H	4.071299	0.524474	3.391343
C	0.595350	2.856042	3.473784
C	2.809154	2.088525	4.213600
C	1.868652	2.298180	3.151138
C	0.253270	3.190592	4.797752
H	-0.728574	3.646732	5.006315
C	1.161225	2.964347	5.848752
C	2.428420	2.417508	5.522294
H	3.156585	2.246079	6.334539
O	2.192979	1.988611	1.906123
C	4.497039	-2.542580	-0.294209
H	4.857831	-3.445898	0.225922
C	3.327586	-1.934073	0.196685
C	2.808038	-0.766326	-0.440547
C	4.713680	-0.860527	-1.987404
H	5.239092	-0.401723	-2.838573
C	5.221992	-2.031984	-1.392678
C	3.531170	-0.232332	-1.546027
C	-0.359749	-2.284203	2.946641
C	0.264747	-3.488272	2.501607
C	-0.922544	-2.276443	4.265730
C	0.305232	-4.649962	3.293799
H	0.797712	-5.554450	2.900443
C	-0.865567	-3.451707	5.032005
H	-1.310868	-3.430995	6.042439
C	-0.271981	-4.654881	4.577413
C	-1.563252	-1.015355	4.786906
H	-1.929452	-1.148928	5.824226
H	-2.423444	-0.706646	4.154056
H	-0.848058	-0.165548	4.774455
C	-0.258551	-5.891238	5.449785
H	0.301861	-6.720446	4.972976
H	-1.287684	-6.259492	5.655374
H	0.211796	-5.691685	6.436959
O	1.662035	-0.205889	-0.009772
C	3.057491	1.030545	-2.199650
H	3.623022	1.262141	-3.122423
H	1.971404	1.012980	-2.424294
S	3.351680	2.430727	-0.986111
C	2.624490	-2.491329	1.394635
H	2.283546	-1.690200	2.080063
H	3.251706	-3.217435	1.946339
O	-0.415109	-1.213328	2.170098
C	0.816483	3.310791	7.280605
H	-0.200039	3.745392	7.362001
H	1.531492	4.047718	7.706975
H	0.851975	2.414846	7.938246
O	0.500425	3.065069	-0.973041
C	1.191496	3.950346	-1.673254
C	0.539636	5.056043	-2.308666
C	1.319754	5.951450	-3.057693
C	2.722399	5.822273	-3.213326
C	3.354345	4.733928	-2.581916
C	2.601649	3.815119	-1.828205
C	-0.949174	5.221945	-2.140441
H	0.809413	6.802331	-3.542779
C	3.506739	6.831887	-4.022761
H	4.444790	4.596290	-2.667745
H	-1.323625	6.104838	-2.695554
H	-1.497831	4.322241	-2.491370
H	-1.218724	5.338025	-1.069055
H	4.584078	6.573785	-4.062152
H	3.137604	6.894135	-5.069666
H	3.423402	7.854330	-3.593638
O	0.364574	-2.594843	-4.023107
C	-0.141509	-3.798589	-4.672284
H	0.741451	-4.450605	-4.857314
O	-1.890636	-1.851097	-0.358218
C	-3.136243	-2.129839	-0.665811
C	-3.700077	-1.777984	-1.939725
C	-3.979595	-2.814954	0.281884
C	-5.036345	-2.113112	-2.243446
C	-5.293526	-3.143988	-0.075404
C	-5.850517	-2.812711	-1.333665
H	-5.443129	-1.806244	-3.221183
H	-5.917687	-3.677004	0.662872
S	-2.768982	-1.014508	-3.254953
C	-7.275452	-3.185827	-1.674197
H	-7.585112	-2.767628	-2.652818
H	-7.406474	-4.289414	-1.723990
H	-7.989077	-2.816521	-0.906453
C	-3.418570	-3.176188	1.630353
H	-2.518024	-3.819252	1.540031
H	-3.084927	-2.271654	2.179807
H	-4.167832	-3.707776	2.248905
Fe	-0.201757	-1.228300	0.206520
C	-1.914257	0.490448	-2.536437
H	-0.879482	0.211879	-2.269086
H	-1.873443	1.166909	-3.415829
O	0.492394	-1.805802	-1.911676
C	0.097469	-2.646169	-2.703459
O	-0.590748	-3.755118	-2.369597
C	-0.835503	-3.445565	-5.975071
H	-1.225312	-4.366794	-6.456031
H	-1.680255	-2.752945	-5.786967
H	-0.128576	-2.965230	-6.679904
C	-1.050709	-4.395866	-3.575519
H	-0.946807	-5.491058	-3.455446
H	-2.118924	-4.130752	-3.725422
C	6.504689	-2.743706	-1.877156
C	6.157420	-4.193769	-2.305095
H	7.068421	-4.729958	-2.648221
H	5.720267	-4.777444	-1.468870
H	5.422673	-4.196821	-3.137357
C	7.148147	-2.024798	-3.081963
H	6.464829	-1.986978	-3.955953
H	7.446639	-0.985249	-2.832992
H	8.063843	-2.566167	-3.399029
C	7.541639	-2.783421	-0.724250
H	8.471248	-3.296946	-1.051844
H	7.812082	-1.758069	-0.396656
H	7.154145	-3.327288	0.161773
C	-5.985954	2.947438	-0.596635
C	-6.553727	2.771760	-2.021230
H	-5.924210	3.276967	-2.783136
H	-6.642248	1.701783	-2.301943
H	-7.569023	3.216779	-2.080232
C	-6.941336	2.237295	0.398132
H	-6.605794	2.357072	1.448866
H	-7.967282	2.658252	0.323408
H	-6.997711	1.149460	0.185700
C	-5.940789	4.464022	-0.274643
H	-5.572375	4.658977	0.753533
H	-5.270264	5.000379	-0.978011
H	-6.954636	4.911832	-0.356342

Table_S 6**. Cartesian coordinates and energies (in A.U.) of species: 4, 4 with Fe1-S dissociated, 4-A.**

Complex 4

E: -7824.81650738 A.U.

Fe	1.602158	-0.136343	0.020433
Fe	-1.602607	0.136298	0.020474
S	-3.312290	-1.644871	1.021228
S	2.974496	-2.161105	-1.028417
S	3.312081	1.645540	1.019666
S	-2.975001	2.160301	-1.029606
C	-3.866420	-0.533839	2.307731
C	-3.060867	0.633746	2.510734
C	-5.026639	-0.795031	3.053773
H	-5.623911	-1.699073	2.866466
C	-3.496121	1.530360	3.537817
C	-5.410933	0.121996	4.047785
C	-4.648393	1.279583	4.295928
H	-4.953916	1.990779	5.075854
C	0.499697	5.508835	-0.078557
C	0.230694	2.645108	-0.010273
C	-0.502713	3.422425	-0.948794
C	1.226566	4.714662	0.835824
H	1.915118	5.196642	1.549433
C	1.102794	3.315482	0.896483
C	-0.364163	4.825874	-0.956308
H	-0.953766	5.387754	-1.696091
O	0.105496	1.301794	0.025217
C	3.061193	-0.632278	2.510476
C	3.496912	-1.528430	3.537767
C	3.866759	0.535114	2.306449
C	5.027379	0.796580	3.051776
H	5.624632	1.700480	2.863722
C	5.412096	-0.119975	4.046056
C	4.649589	-1.277375	4.295168
H	4.955453	-1.988207	5.075292
O	1.984401	-0.852003	1.794509
C	1.887359	2.519954	1.895094
H	1.276190	1.728073	2.373134
H	2.346471	3.161418	2.670821
C	-1.419611	2.746936	-1.922727
H	-0.961199	1.845919	-2.377537
H	-1.761158	3.436151	-2.717926
C	-3.710543	1.126143	-2.290445
C	-3.674557	-0.994216	-3.481069
C	-3.099467	-0.156958	-2.473435
C	-4.820108	1.551224	-3.038441
H	-5.266981	2.541497	-2.868627
C	-5.349194	0.685562	-4.012040
C	-4.778754	-0.581803	-4.239685
H	-5.197508	-1.251380	-5.003722
O	-2.066849	-0.528410	-1.755170
O	-1.984509	0.853260	1.794063
C	0.363289	-4.826255	-0.954524
H	0.952772	-5.388442	-1.694171
C	0.502071	-3.422826	-0.947419
C	-0.231165	-2.645146	-0.009067
C	-1.227247	-4.714317	0.837744
H	-1.915774	-5.196000	1.551579
C	-0.500620	-5.508842	-0.076531
C	-1.103241	-3.315143	0.897991
C	3.099271	0.155424	-2.473373
C	3.710442	-1.127502	-2.289483
C	3.674761	0.992309	-3.481079
C	4.820448	-1.552767	-3.036718
H	5.267375	-2.542899	-2.866235
C	4.779410	0.579717	-4.238943
H	5.198455	1.249011	-5.003068
C	5.349912	-0.687463	-4.010434
O	-0.105813	-1.301834	0.026116
C	-1.887447	-2.519189	1.896554
H	-1.276042	-1.727240	2.374178
H	-2.346445	-3.160354	2.672597
C	1.419140	-2.747812	-1.921531
H	0.960918	-1.846889	-2.376711
H	1.760655	-3.437367	-2.716446
O	2.066205	0.527008	-1.755805
C	0.668626	7.043848	-0.081749
C	-0.669893	-7.043815	-0.079439
C	2.157950	7.398949	-0.330354
H	2.298365	8.500896	-0.330771
H	2.821990	6.979037	0.452845
H	2.504250	7.007893	-1.309641
C	0.224655	7.608317	1.293404
H	-0.841351	7.374197	1.495316
H	0.824573	7.187329	2.126322
H	0.344706	8.712455	1.318748
C	-0.179840	7.717388	-1.181303
H	0.103745	7.367705	-2.195894
H	-1.265127	7.531638	-1.041648
H	-0.026775	8.816225	-1.154555
C	-0.226376	-7.608181	1.295903
H	-0.826330	-7.186888	2.128638
H	-0.346787	-8.712274	1.321394
H	0.839666	-7.374369	1.497985
C	-2.159259	-7.398567	-0.328313
H	-2.823344	-6.978348	0.454684
H	-2.505246	-7.007563	-1.307730
H	-2.299973	-8.500478	-0.328597
C	0.178650	-7.717769	-1.178673
H	-0.104708	-7.368312	-2.193404
H	1.263939	-7.532137	-1.038869
H	0.025417	-8.816574	-1.151671
Cl	-6.734048	1.188213	-4.961349
Cl	-2.977854	-2.571161	-3.752076
Cl	6.856205	0.180666	4.992431
Cl	2.563982	-2.972430	3.837295
Cl	-2.563127	2.974559	3.836177
Cl	-6.854541	-0.178281	4.995037
Cl	2.977985	2.569044	-3.753135
Cl	6.735324	-1.190357	-4.958799

Complex 4 with Fe1-S bond dissociated

E: -7824.80566504 A.U.

Fe	1.592965	0.581098	0.679602
Fe	-0.902793	-0.785169	-0.838470
S	0.657462	1.212337	3.176614
S	4.072919	0.679107	-0.443896
S	-0.912272	-3.240371	-1.694628
C	3.728891	-3.098518	-3.383073
C	1.999014	-1.528201	-1.700572
C	1.836641	-2.936534	-1.799782
C	3.914016	-1.708079	-3.217000
H	4.740486	-1.200628	-3.741340
C	3.080038	-0.920695	-2.403950
C	2.680973	-3.684231	-2.647198
H	2.506811	-4.769063	-2.705122
O	1.161075	-0.768071	-0.954345
C	3.035474	3.124013	0.191591
C	3.130475	4.542921	0.340211
C	4.214568	2.450467	-0.257123
C	5.415451	3.127732	-0.526480
H	6.307652	2.576876	-0.857804
C	5.458211	4.522641	-0.359989
C	4.320274	5.232844	0.068581
H	4.359246	6.323720	0.194684
O	1.923660	2.466448	0.430703
C	3.372809	0.533344	-2.184062
H	2.468174	1.172640	-2.228330
H	4.138493	0.919457	-2.883297
C	0.782559	-3.620386	-0.984326
H	0.775778	-3.264750	0.065678
H	0.897467	-4.720875	-0.999261
C	-1.955134	-3.808708	-0.350857
C	-3.006418	-3.340596	1.786054
C	-2.186273	-2.879099	0.711242
C	-2.499369	-5.103495	-0.357936
H	-2.308055	-5.787989	-1.196947
C	-3.294888	-5.508690	0.727058
C	-3.549000	-4.632999	1.799711
H	-4.174916	-4.953197	2.644149
O	-1.671902	-1.666048	0.693321
C	-2.445573	3.131551	2.223455
H	-2.814103	3.202173	3.260016
C	-1.628307	2.041294	1.886259
C	-1.139145	1.925862	0.555957
C	-2.269264	3.998506	-0.019297
H	-2.497790	4.751827	-0.788102
C	-2.807790	4.120244	1.276742
C	-1.426514	2.932288	-0.397461
C	1.940452	-1.193464	3.001489
C	1.138283	-0.369490	3.854601
C	2.359806	-2.450992	3.538834
C	0.793160	-0.758100	5.160391
H	0.200431	-0.094234	5.806156
C	2.008736	-2.856169	4.832453
H	2.345185	-3.830821	5.212101
C	1.225547	-2.006259	5.637552
O	-0.363323	0.856079	0.244273
C	-0.751886	2.895026	-1.746874
H	-0.079174	3.773607	-1.852276
H	-0.136753	1.985944	-1.854296
S	-1.823866	3.090545	-3.243292
C	-1.196240	1.008040	2.886425
H	-1.342667	-0.026242	2.514387
H	-1.699481	1.138214	3.863451
O	2.279176	-0.820022	1.786485
O	-1.868251	0.160957	-2.132832
C	-3.034100	0.617117	-2.537563
C	-4.222384	-0.183258	-2.493979
C	-5.451808	0.252244	-2.997477
C	-5.533708	1.547653	-3.541313
C	-4.415772	2.394541	-3.560537
C	-3.171983	1.946888	-3.069526
H	-6.332108	-0.403405	-2.961530
H	-4.509709	3.419807	-3.947130
C	-3.743335	5.277600	1.690950
C	4.659326	-3.903883	-4.315991
C	4.287077	-5.401545	-4.351484
H	4.375915	-5.876613	-3.352207
H	3.253079	-5.564096	-4.721053
H	4.972157	-5.943367	-5.035911
C	4.550578	-3.339347	-5.756558
H	3.511947	-3.418931	-6.139653
H	4.846296	-2.271189	-5.806580
H	5.215268	-3.902337	-6.445867
C	6.123400	-3.776517	-3.819520
H	6.808988	-4.344528	-4.483817
H	6.467959	-2.722041	-3.808573
H	6.233041	-4.176727	-2.790108
C	-3.999226	6.261633	0.529515
H	-3.062009	6.740670	0.177247
H	-4.479412	5.764086	-0.338364
H	-4.679039	7.071650	0.866144
C	-3.103403	6.065055	2.864022
H	-2.933116	5.422974	3.752565
H	-2.124508	6.495981	2.567677
H	-3.765485	6.899921	3.178652
C	-5.106590	4.691613	2.143978
H	-5.589696	4.124109	1.321494
H	-4.995330	4.003416	3.007152
H	-5.797323	5.505506	2.452049
Cl	1.719191	5.424980	0.867031
Cl	6.944305	5.392690	-0.686279
Cl	-3.345510	-2.252374	3.109264
Cl	-3.981959	-7.120436	0.747917
Cl	3.314757	-3.508907	2.527679
Cl	0.800248	-2.511642	7.260959
Cl	-4.111494	-1.791190	-1.816925
Cl	-7.065740	2.119380	-4.164701

4-A

E: -8017.87254351 A.U.

Fe	1.414945	0.989636	0.369772
Fe	-0.762187	-1.095760	-0.812993
S	0.712023	2.146819	2.678924
S	3.914966	1.440557	-0.564221
S	-0.238391	-3.652462	-1.041514
C	4.504557	-2.887125	-2.586235
C	2.345952	-1.370183	-1.416826
C	2.445001	-2.775970	-1.217207
C	4.424223	-1.482643	-2.719107
H	5.206312	-0.941256	-3.277173
C	3.380894	-0.722839	-2.159765
C	3.497033	-3.500955	-1.816046
H	3.526931	-4.586344	-1.637832
O	1.320611	-0.657054	-0.915584
C	2.254001	3.604238	-0.700512
C	2.003434	5.000775	-0.883749
C	3.622933	3.190206	-0.781769
C	4.675952	4.092594	-1.005164
H	5.716399	3.740159	-1.053222
C	4.374560	5.456144	-1.165787
C	3.043327	5.912615	-1.112593
H	2.814903	6.979329	-1.244402
O	1.292310	2.738498	-0.485789
C	3.393192	0.773624	-2.249728
H	2.394156	1.203909	-2.463907
H	4.132725	1.146253	-2.983585
C	1.483719	-3.465239	-0.299966
H	1.345023	-2.886249	0.635715
H	1.818079	-4.490818	-0.053591
C	-1.097214	-4.093465	0.463836
C	-2.031306	-3.338797	2.570349
C	-1.396377	-2.996909	1.334700
C	-1.413903	-5.425123	0.771641
H	-1.170377	-6.238350	0.072662
C	-2.048587	-5.700491	1.995331
C	-2.352530	-4.663313	2.897568
H	-2.846481	-4.884359	3.853853
O	-1.105207	-1.761548	1.007852
C	-2.792347	3.023231	1.877491
H	-2.993949	3.263603	2.934420
C	-1.817521	2.052099	1.601163
C	-1.527127	1.714274	0.247510
C	-3.188073	3.345416	-0.473564
H	-3.707215	3.833023	-1.312219
C	-3.512434	3.683654	0.853797
C	-2.204552	2.387601	-0.798894
C	2.270999	-0.083743	2.977894
C	1.644323	0.996246	3.680019
C	3.037093	-0.994404	3.773039
C	1.777396	1.172098	5.067415
H	1.295532	2.021328	5.573196
C	3.167574	-0.838766	5.158987
H	3.762712	-1.559107	5.737104
C	2.538280	0.245759	5.800327
O	-0.577560	0.783781	-0.008081
C	-1.818505	2.119844	-2.228924
H	-1.426063	3.045485	-2.702346
H	-1.031263	1.349063	-2.295855
S	-3.214389	1.677562	-3.370144
C	-1.023355	1.395241	2.690102
H	-0.909769	0.303829	2.530616
H	-1.442858	1.594186	3.694457
O	2.141493	-0.235783	1.682135
O	-2.485082	-0.790141	-1.547230
C	-3.763080	-0.575406	-1.714077
C	-4.757621	-1.464544	-1.175727
C	-6.130390	-1.279356	-1.370782
C	-6.565288	-0.169376	-2.116605
C	-5.643256	0.738560	-2.659550
C	-4.259235	0.540634	-2.483103
H	-6.849855	-1.993723	-0.948316
H	-5.999090	1.612297	-3.224495
O	-0.344777	-1.099301	-3.144422
C	-1.244009	-1.368869	-4.238645
C	0.221882	-1.381362	-4.455797
H	-1.856933	-0.502234	-4.547826
H	-1.777461	-2.335194	-4.167213
H	0.667765	-0.477298	-4.915072
C	1.004321	-2.656406	-4.631762
H	1.103140	-2.882722	-5.714813
H	2.025048	-2.562058	-4.208408
H	0.495906	-3.509119	-4.139551
C	5.670618	-3.667444	-3.232268
C	-4.584236	4.735093	1.217315
C	5.573463	-5.183650	-2.960087
H	5.618735	-5.414823	-1.875549
H	4.637368	-5.619909	-3.367113
H	6.422173	-5.708794	-3.445199
C	5.650932	-3.445895	-4.767195
H	4.705034	-3.819421	-5.212445
H	5.748101	-2.372997	-5.032941
H	6.492496	-3.986906	-5.250155
C	7.015564	-3.152650	-2.655173
H	7.167268	-2.072417	-2.857354
H	7.060014	-3.298160	-1.555913
H	7.868578	-3.700171	-3.109809
C	-5.241866	5.348759	-0.036585
H	-4.502712	5.872423	-0.677757
H	-5.751961	4.580971	-0.654121
H	-6.006037	6.094436	0.266498
C	-5.691892	4.063665	2.070913
H	-6.186734	3.244116	1.509424
H	-5.286677	3.631009	3.008705
H	-6.469148	4.805885	2.352666
C	-3.925162	5.878711	2.032225
H	-3.471448	5.508615	2.974479
H	-3.123467	6.374534	1.446292
H	-4.679994	6.647362	2.303775
Cl	0.353546	5.568570	-0.814179
Cl	5.668655	6.606560	-1.441816
Cl	-2.431060	-2.057937	3.688985
Cl	-2.461995	-7.353638	2.409388
Cl	-4.222428	-2.877533	-0.304706
Cl	-8.280819	0.090461	-2.353557
Cl	3.825474	-2.334950	2.975585
Cl	2.714720	0.441150	7.533695

Complete reference 21

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09 Revision A.1, Gaussian, Inc., Wallingford, CT, **2009**.