Electronic Supplementary Material (ESI) for Chemical Communications.
This journal is © The Royal Society of Chemistry 2021

Supporting Information for

Spectroscopic discernibility of dopants and axial ligands in pyridinic FeN_4 environments relevant to single-atom catalysts

Charlotte Gallenkamp,[a,b] Ulrike I. Kramm[b] and Vera Krewald*[a]

a Technical University of Darmstadt, Department of Chemistry, Alarich-Weiss-Str. 4, 64287 Darmstadt, Germany.

b Technical University of Darmstadt, Department of Materials and Earth Sciences, Catalysts and Electrocatalysts Group, Otto-Bernd-Str. 3, 64287 Darmstadt, Germany.

Table of Contents

Computational details

All calculations were performed with version 4.2.1 of the ORCA quantum chemistry suite of programs.[1] The geometries were optimized with the TPSS[2] density functional using unrestricted Kohn-Sham density functional theory. Ahlrichs' def2-SVP basis set was used for carbon and hydrogen atoms, for all other elements def2-TZVP was used.[3] The split-RI-J approximation[4] with def2/J basis sets was used,[5] as well as Grimme's dispersion correction with Becke-Johnson damping (D3BJ).[6, 7] To include environmental effects the SMD model was employed,[8] choosing water as the model solvent. The grid was set to 6, and integration accuracy was increased to 6.0 in ORCA nomenclature. The convergence criteria for the SCF and the geometry optimization were set to "tight" in ORCA nomenclature.

To obtain NRVS and IR spectra, frequency calculations were performed using the exact same settings as the geometry optimization. The single point calculations for all other reported spectra used the B3LYP[9, 10] hybrid density functional with the chain-of-spheres approximation.[11] Similar to the geometry optimization, the convergence criteria for the SCF was set to "tight" in ORCA nomenclature, the grid was set to 6, Grimme's D3BJ dispersion correction[6, 7] and the SMD solvation model for water was employed.[8] Additionally, the gridX was set to 8 in ORCA nomenclature.

Electronic transitions for the UV-vis and iron K pre-edge X-ray absorption spectra[12, 13] were calculated with time-dependent density functional theory using the Tamm-Dancoff-approximation[14] as implemented in ORCA. The zeroth-order regular approximation for relativistic effects (ZORA)[15-17] and the scalar-relativistically recontracted def2-TZVP(-f) basis set was used, as well as the SARC/J auxiliary basis set.[18, 19] X-ray emission calculations were performed using the same settings using the one-electron DFT approach.[20] Because these exact settings have not been used in any previous calibration study, the X-ray spectra are not shifted in energy to align with experimental values. Even though the precise shift will depend on the choice of density functional, basis set and relativistic correction among other factors, we note that previous shifts were on the order of 33 eV (XAS) [13] and 182 eV (XES).[20, 21]

For the single-point calculations of hyperfine coupling constants and Mössbauer parameters, a setup recently calibrated[22] for Mössbauer spectroscopy was used wherein the CP(PPP)[23] basis set is chosen for Fe and def2-TZVP basis set for all other elements. Additionally, the integration grid for iron was set to 7.0 in ORCA nomenclature.

Visualizations were performed with gnuplot 5.4 for plotted spectra and UCSF Chimera 1.13.1 for chemical structures, molecular orbitals and difference densities associated with electronic transitions. All calculations for this research were conducted on the Lichtenberg high performance computer of the TU Darmstadt.

References

1. F. Neese, *WIREs Comput. Mol. Sci.*, 2012, **2**, 73-78.
2. J. Tao, J. P. Perdew, V. N. Staroverov and G. E. Scuseria, *Phys. Rev. Lett.*, 2003, **91**, 146401.
3. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
4. F. Neese, *J. Comput. Chem.*, 2003, **24**, 1740-1747.
5. F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057-1065.
6. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104-154119.
7. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.
8. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
9. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
10. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
11. F. Neese, F. Wennmohs, A. Hansen and U. Becker, *Chem. Phys.*, 2009, **356**, 98-109.
12. S. DeBeer George, T. Petrenko and F. Neese, *Inorg. Chim. Acta*, 2008, **361**, 965-972.
13. S. DeBeer George, T. Petrenko and F. Neese, *J. Phys. Chem. A*, 2008, **112**, 12936-12943.
14. S. Hirata and M. Head-Gordon, *Chem. Phys. Lett.*, 1999, **314**, 291-299.
15. E. van Lenthe, E. J. Baerends and J. G. Snijders, *J. Chem. Phys.*, 1994, **101**, 9783-9792.
16. E. van Lenthe, J. G. Snijders and E. J. Baerends, *J. Chem. Phys.*, 1996, **105**, 6505-6516.
17. C. van Wüllen, *J. Chem. Phys.*, 1998, **109**, 392-399.

18. D. A. Pantazis, X. Y. Chen, C. R. Landis and F. Neese, *J. Chem. Theory Comput.*, 2008, **4**, 908-919.
19. D. A. Pantazis and F. Neese, *WIREs Comput. Mol. Sci.*, 2014, **4**, 363-374.
20. N. Lee, T. Petrenko, U. Bergmann, F. Neese and S. DeBeer, *J. Am. Chem. Soc.*, 2010, **132**, 9715-9727.
21. K. M. Lancaster, K. D. Finkelstein and S. DeBeer, *Inorg. Chem.*, 2011, **50**, 6767-6774.
22. C. Gallenkamp, U. I. Kramm, J. Proppe and V. Krewald, *Int. J. Quantum Chem.*, 2020, DOI: 10.1002/qua.26394.
23. F. Neese, *Inorg. Chim. Acta*, 2002, **337**, 181-192.

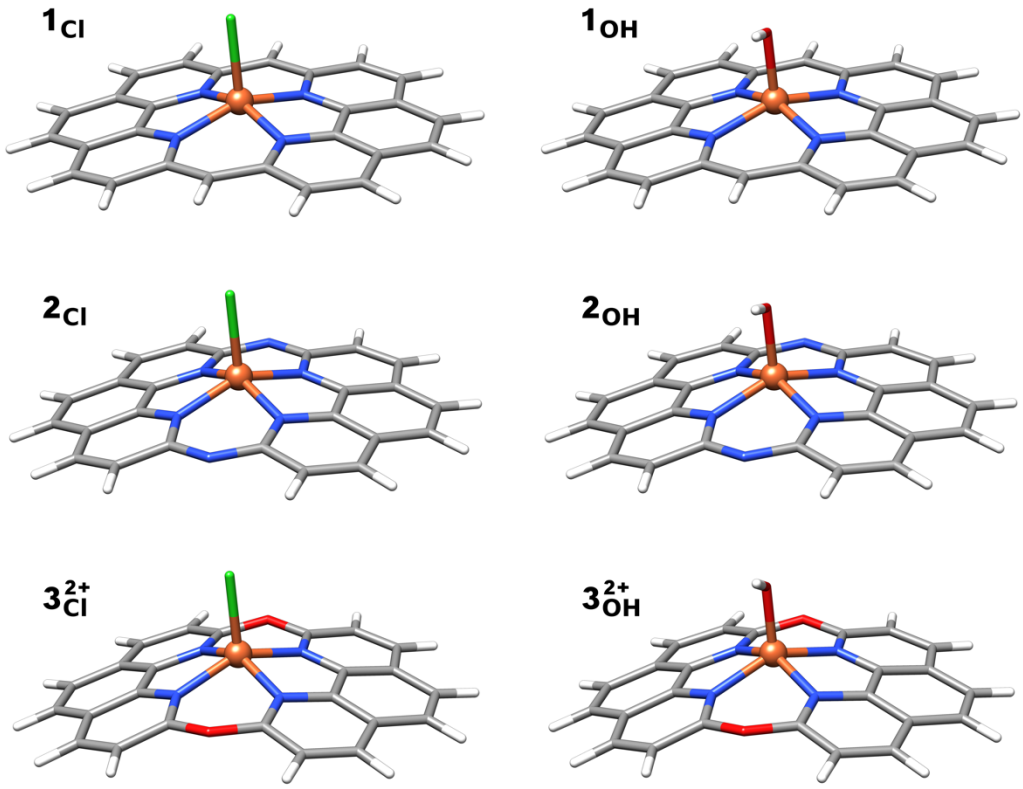


Figure S1. Representations of the [Fe{phen$_2$(CH)$_2$}*L*], [Fe{phen$_2$(N)$_2$}*L*] and [Fe{phen$_2$(O)$_2$}*L*]$^{2+}$ complexes with *L* = Cl^- (left) and OH^- (right). The elements are coloured as follows: Fe orange, N blue, C grey, H white, Cl green.

Table S1. All [Fe{phen$_2$A$_2$}L] complexes with A = C, N, O and L = Cl^-, OH^- with their relative electronic energies (kcal/mol), Mulliken spin populations, contact densities (au^{-3}), isomer shifts δ (mm/s) and quadrupole splitting values ΔE_Q (mm/s) from Mössbauer spectroscopy calculations.

	E_{rel}	Mulliken spin pop.		$\rho(0)$	δ	ΔE_Q
	(kcal/mol)	Fe	ring	(au^{-3})	(mm/s)	(mm/s)
1$_{Cl}$ (LS)	9.2	1.69	-0.37	11816.79145	0.453	-2.127
1$_{Cl}$ (IS)	0.0	2.70	-0.03	11817.05520	0.321	2.105
1$_{Cl}$ (HS)	6.0	4.10	0.51	11816.69270	0.502	0.604
1$_{OH}$ (LS)	7.4	1.18	-0.13	11817.07939	0.309	2.661
1$_{OH}$ (IS)	0.0	2.74	-0.06	11817.10670	0.295	1.559
1$_{OH}$ (HS)	4.3	4.18	0.46	11816.84288	0.427	-0.937
2$_{Cl}$ (LS)	16.5	1.31	-0.19	11816.98324	0.357	2.655
2$_{Cl}$ (IS)	0.0	2.74	-0.02	11817.06650	0.315	2.123
2$_{Cl}$ (HS)	6.8	4.14	0.55	11816.84931	0.424	-0.219
2$_{OH}$ (LS)	12.6	1.08	-0.08	11817.16910	0.264	2.909
2$_{OH}$ (IS)	0.0	2.76	-0.05	11817.10130	0.298	1.532
2$_{OH}$ (HS)	4.3	4.20	0.48	11816.91938	0.389	-0.784
3$_{Cl}$ (LS)	3.0	2.07	-1.13	11816.96138	0.368	2.455
3$_{Cl}$ (IS)	0.0	3.66	-0.77	11815.74647	0.976	4.251
3$_{Cl}$ (HS)	2.0	3.69	1.22	11815.75960	0.970	3.741
3$_{OH}$ (LS)	21.7	0.52	0.47	11816.66153	0.518	-1.673
3$_{OH}$ (IS)	0.0	3.62	-0.71	11815.69987	1.000	2.593
3$_{OH}$ (HS)	8.5	3.69	1.21	11815.79269	0.953	2.923
3$^{2+}_{Cl}$ (LS)	19.8	1.10	-0.08	11817.12406	0.286	3.067
3$^{2+}_{Cl}$ (IS)	0.0	2.71	-0.01	11817.07550	0.311	1.681
3$^{2+}_{Cl}$ (HS)	3.5	4.17	0.51	11816.91401	0.392	-0.288
3$^{2+}_{OH}$ (LS)	21.2	0.95	-0.01	11817.06034	0.318	-2.924
3$^{2+}_{OH}$ (IS)	0.9	2.69	-0.03	11817.06862	0.314	0.933
3$^{2+}_{OH}$ (HS)	0.0	4.22	0.44	11816.89219	0.403	-1.159

Table S2a. Selected interatomic distances (Å) and Fe-O-H angles (°) for all [Fe{phen$_2$A$_2$}L] complexes; A = C, N, O and L = Cl^-, OH^-.

	Fe-N	Fe-N	Fe-N	Fe-N	Fe-axial	O-H	Fe-O-H
1$_{Cl}$ (LS)	1.936	1.936	1.936	1.936	2.281		
1$_{Cl}$ (IS)	1.947	1.948	1.948	1.947	2.316		
1$_{Cl}$ (HS)	2.043	2.043	2.043	2.043	2.246		
1$_{OH}$ (LS)	1.939	1.939	1.941	1.941	1.882	0.979	107.87
1$_{OH}$ (IS)	1.946	1.948	1.948	1.947	1.935	0.977	108.89
1$_{OH}$ (HS)	2.045	2.049	2.048	2.045	1.879	0.975	114.88
2$_{Cl}$ (LS)	1.934	1.935	1.935	1.934	2.260		
2$_{Cl}$ (IS)	1.947	1.947	1.947	1.947	2.291		
2$_{Cl}$ (HS)	2.027	2.027	2.027	2.027	2.219		
2$_{OH}$ (LS)	1.936	1.935	1.942	1.943	1.868	0.980	109.28
2$_{OH}$ (IS)	1.943	1.947	1.947	1.944	1.928	0.977	110.72
2$_{OH}$ (HS)	2.032	2.035	2.035	2.033	1.860	0.976	115.68
3$_{Cl}$ (LS)	1.870	1.870	1.870	1.869	2.585		
3$_{Cl}$ (IS)	2.043	2.044	2.045	2.044	2.298		
3$_{Cl}$ (HS)	2.068	2.068	2.068	2.068	2.234		
3$_{OH}$ (LS)	1.873	1.882	1.882	1.873	2.103	0.974	101.611
3$_{OH}$ (IS)	2.089	2.090	2.095	2.095	1.894	0.975	110.639
3$_{OH}$ (HS)	2.074	2.077	2.076	2.074	1.878	0.975	111.756
3$^{2+}_{Cl}$ (LS)	1.943	1.944	1.945	1.945	2.170		
3$^{2+}_{Cl}$ (IS)	1.955	1.955	1.955	1.955	2.192		
3$^{2+}_{Cl}$ (HS)	2.039	2.039	2.039	2.039	2.154		
3$^{2+}_{OH}$ (LS)	1.967	1.939	1.984	1.946	1.786	0.983	116.056
3$^{2+}_{OH}$ (IS)	1.955	1.959	1.959	1.955	1.844	0.979	117.069
3$^{2+}_{OH}$ (HS)	2.049	2.059	2.052	2.056	1.804	0.978	119.638

Table S2b. Selected interatomic angles (°) for all [Fe{phen$_2$A$_2$}L] complexes; A = C, N, O and L = Cl^-, OH^-.

	cis N-atoms				*trans* N-atoms			
	N-Fe-N	N-Fe-N	N-Fe-N	N-Fe-N	N-Fe-N	N-Fe-N	C-A-C	C-A-C
1$_{Cl}$ (LS)	83.07	93.62	83.08	93.67	160.55	160.57	128.46	128.44
1$_{Cl}$ (IS)	83.46	90.79	83.46	90.82	154.18	154.19	126.75	126.76
1$_{Cl}$ (HS)	80.40	85.72	80.41	85.70	139.32	139.34	127.20	127.20
1$_{OH}$ (LS)	83.03	93.73	83.04	93.69	160.66	160.61	128.36	128.36
1$_{OH}$ (IS)	83.66	90.96	83.65	91.07	155.13	155.10	126.80	126.77
1$_{OH}$ (HS)	80.42	85.57	80.43	85.70	139.26	139.23	127.13	127.11
2$_{Cl}$ (LS)	83.43	91.48	83.45	91.56	155.81	155.82	125.89	125.86
2$_{Cl}$ (IS)	83.49	88.15	83.49	88.14	148.66	148.68	123.75	123.76
2$_{Cl}$ (HS)	80.99	82.70	81.00	82.66	135.73	135.75	123.54	123.55
2$_{OH}$ (LS)	83.49	91.74	83.49	91.68	156.43	156.38	125.79	125.80
2$_{OH}$ (IS)	83.77	88.36	83.77	88.51	149.79	149.78	123.78	123.76
2$_{OH}$ (HS)	80.98	82.48	80.97	82.55	135.45	135.48	123.44	123.42
3$_{Cl}$ (LS)	86.06	92.81	86.07	92.88	168.79	168.80	126.72	126.70
3$_{Cl}$ (IS)	80.33	83.81	80.30	83.88	136.43	136.42	123.76	123.80
3$_{Cl}$ (HS)	78.74	80.66	78.77	80.67	129.99	130.02	125.29	125.29
3$_{OH}$ (LS)	85.55	91.15	85.55	92.12	163.69	163.65	126.05	126.27
3$_{OH}$ (IS)	77.54	79.08	77.30	79.08	126.33	126.39	120.43	120.41
3$_{OH}$ (HS)	78.45	80.28	78.54	80.37	129.24	129.24	125.23	125.20
3$^{2+}_{Cl}$ (LS)	83.66	92.16	83.69	92.07	158.02	157.86	128.24	128.23
3$^{2+}_{Cl}$ (IS)	83.24	87.42	83.26	87.42	146.92	146.84	125.36	125.38
3$^{2+}_{Cl}$ (HS)	80.68	81.74	80.71	81.72	134.00	133.97	124.86	124.88
3$^{2+}_{OH}$ (LS)	82.97	87.10	82.78	87.22	153.54	135.42	124.46	124.68
3$^{2+}_{OH}$ (IS)	83.29	87.33	83.30	87.57	147.05	146.99	125.26	125.24
3$^{2+}_{OH}$ (HS)	80.14	81.04	80.18	81.14	132.26	132.52	124.35	124.32

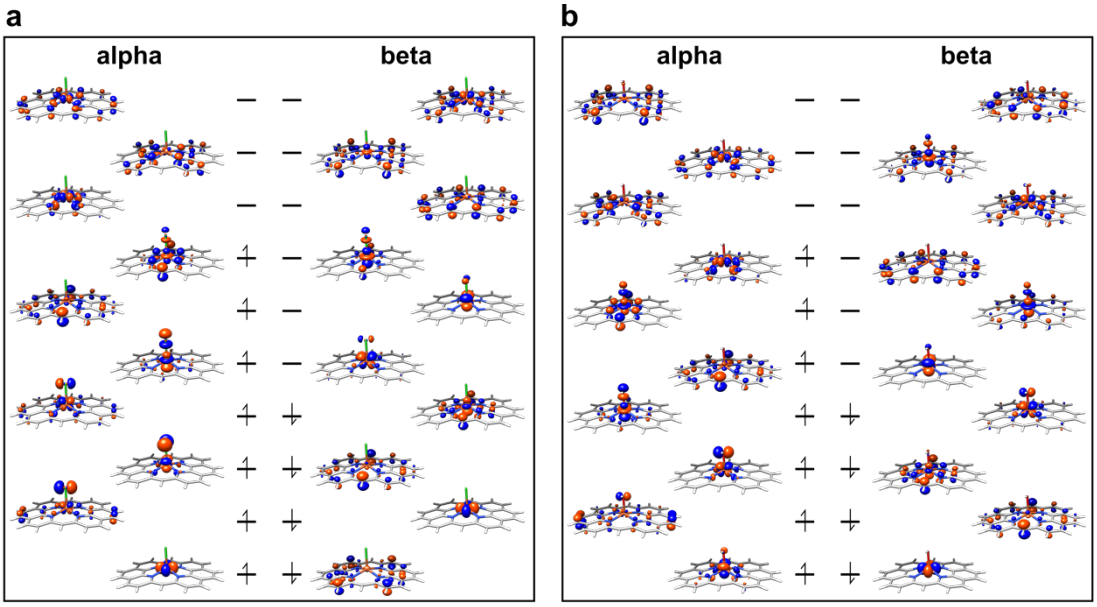


Figure S2a. Frontier molecular orbitals of the [Fe{phen$_2$(CH)$_2$}Cl] (**1$_{Cl}$**) and [Fe{phen$_2$(CH)$_2$}OH] (**1$_{OH}$**) complexes. Displayed are orbitals 116-125 for **1$_{Cl}$** and orbitals 113-122 for **1$_{OH}$**. The elements are coloured as follows: Fe orange, N blue, C grey, H white, O red, Cl green.

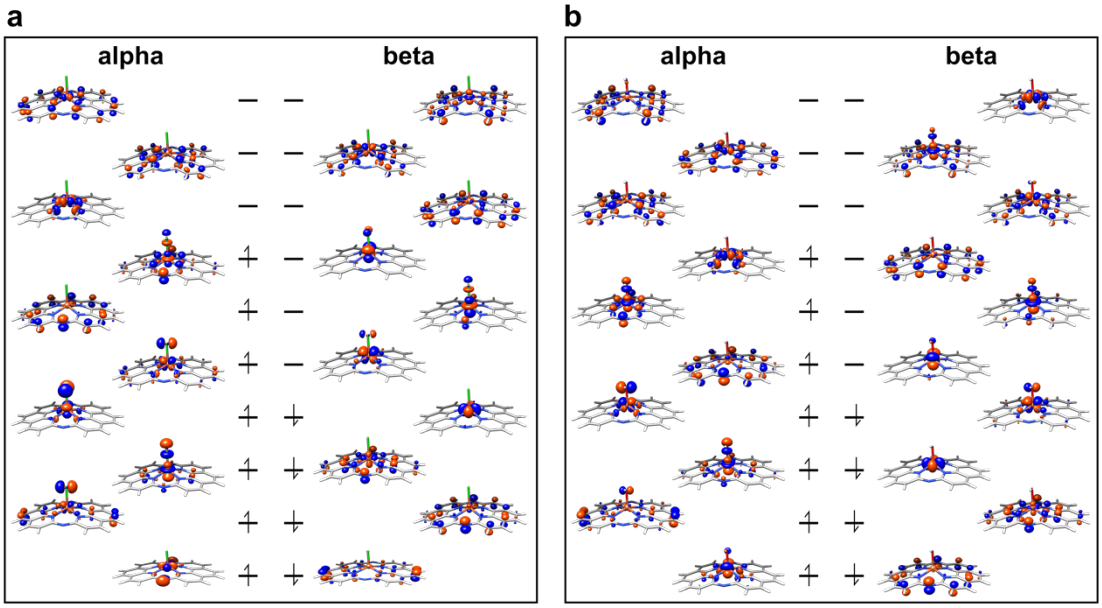


Figure S2b. Frontier molecular orbitals of the [Fe{phen$_2$(N)$_2$}Cl] (**2$_{Cl}$**) and [Fe{phen$_2$(N)$_2$}OH] (**2$_{OH}$**) complexes. Displayed are orbitals 116-125 for **2$_{Cl}$** and orbitals 113-122 for **2$_{OH}$**. The elements are coloured as follows: Fe orange, N blue, C grey, H white, O red, Cl green.

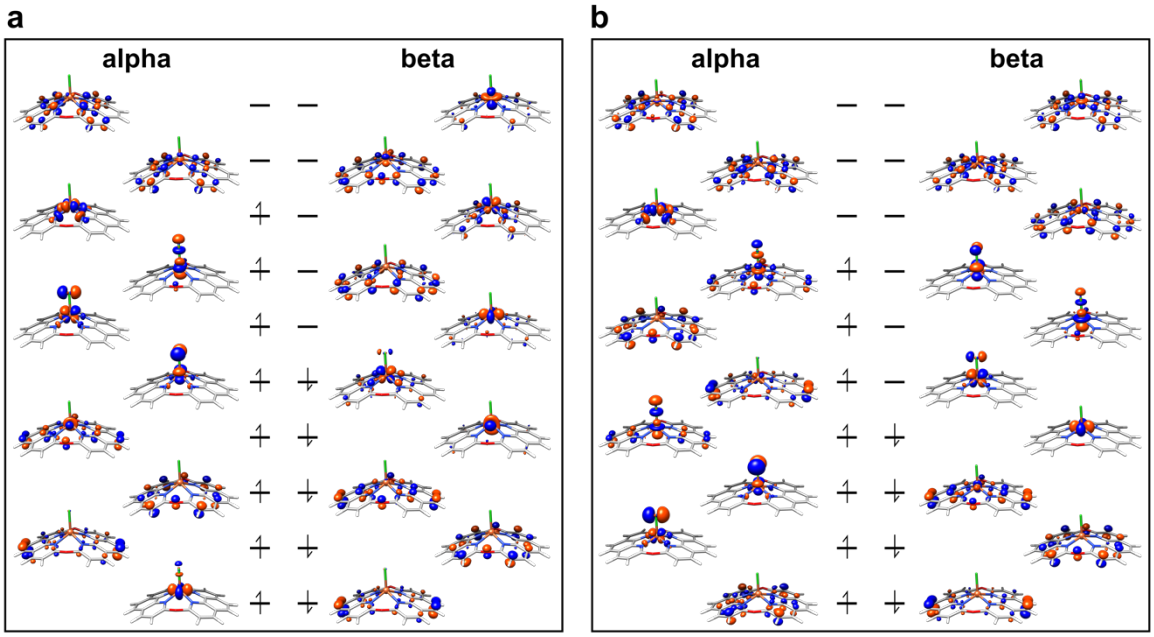


Figure S2c. Frontier molecular orbitals of the $[Fe\{phen_2(O)_2\}Cl]^{2+}$ ($\mathbf{3_{Cl}}$) and $[Fe\{phen_2(O)_2\}Cl]^{2+}$ ($\mathbf{3^{2+}_{Cl}}$) complexes. Displayed are orbitals 116-125 for $\mathbf{3_{Cl}}$ and orbitals 116-125 for $\mathbf{3^{2+}_{Cl}}$. The elements are coloured as follows: Fe orange, N blue, C grey, H white, O red, Cl green.

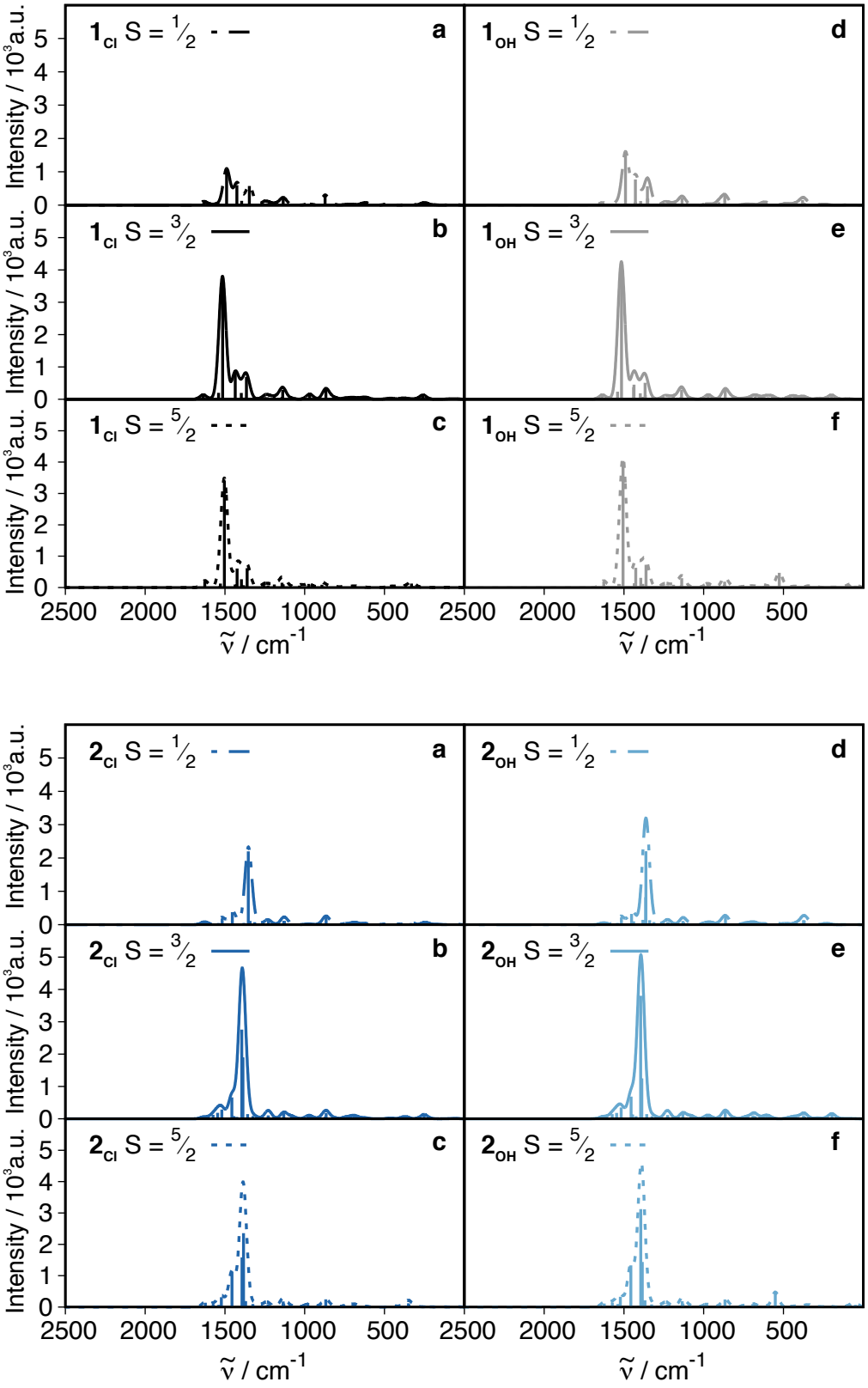


Figure S3a. IR spectra of complexes **1** and **2** in all spin states.

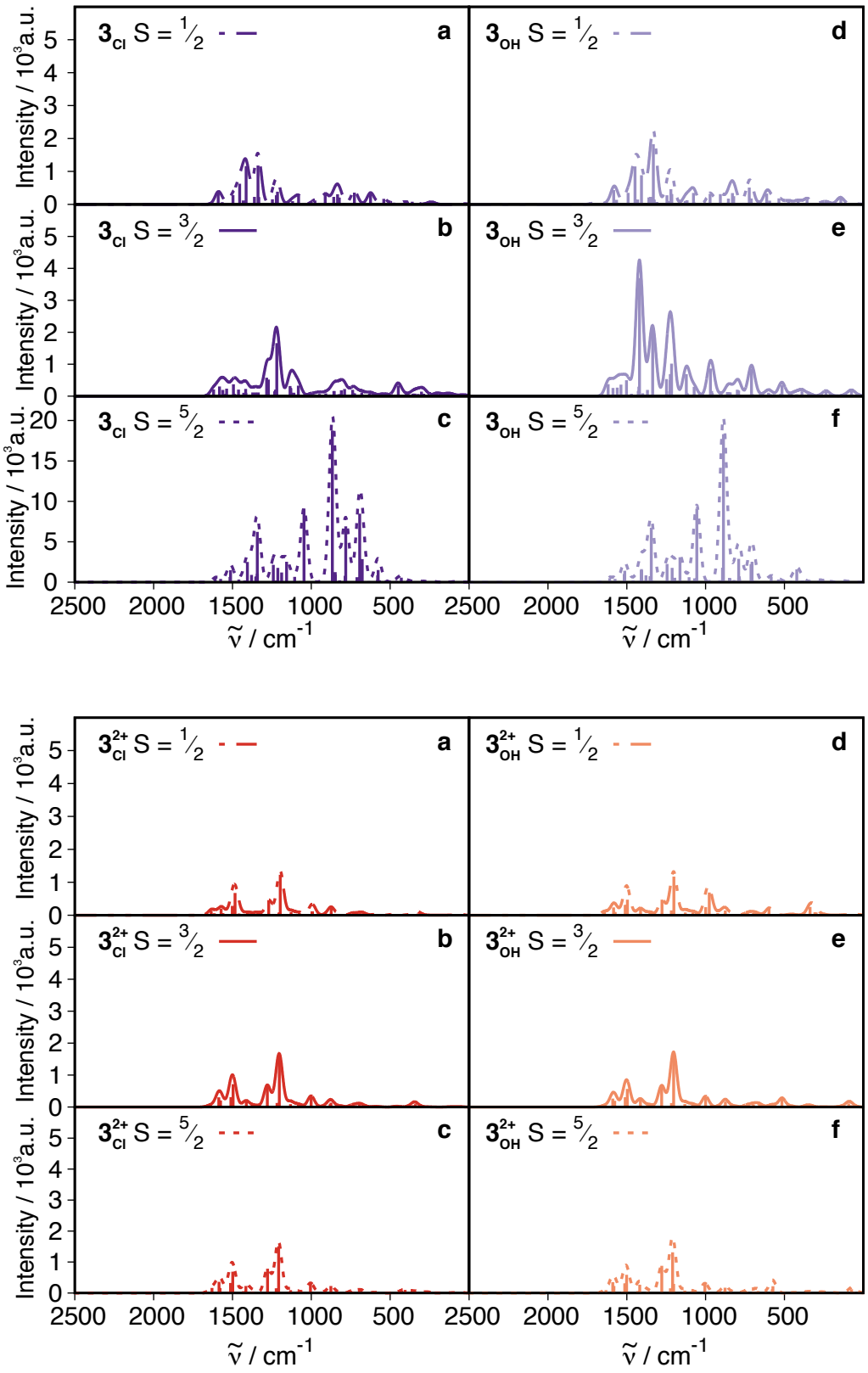
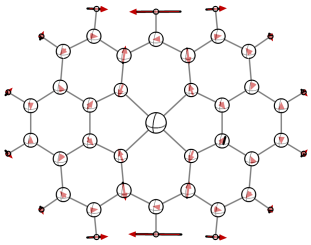
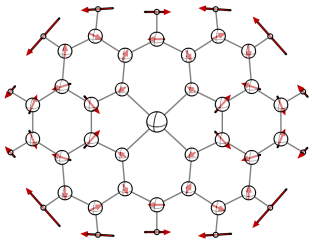
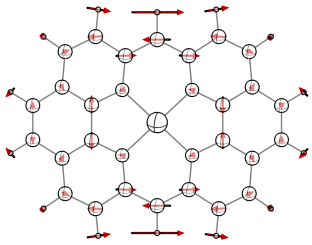
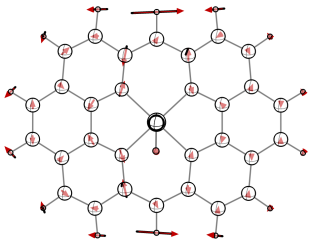
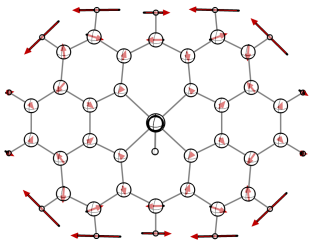
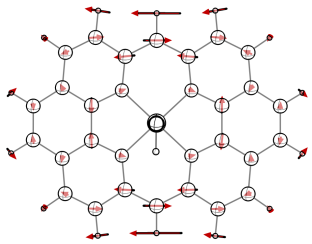
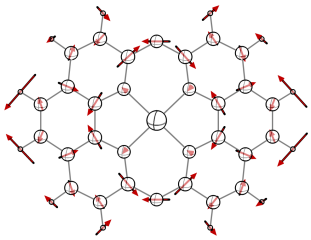
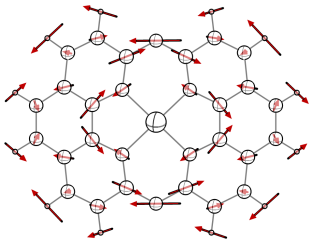
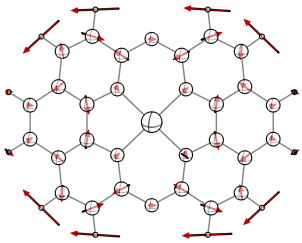
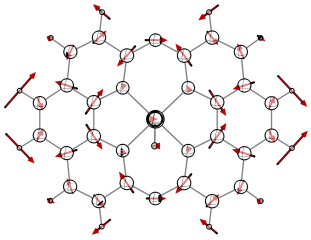
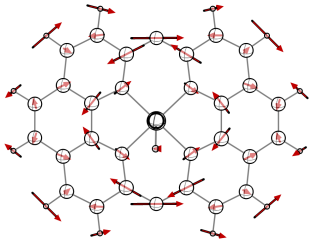
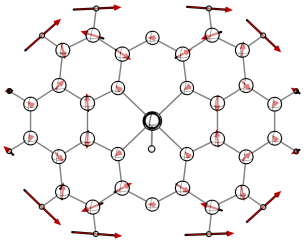
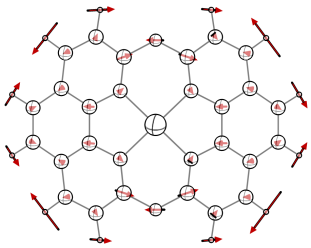
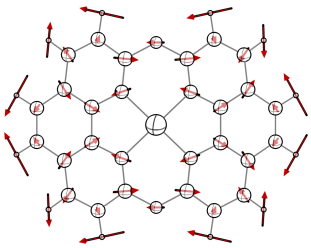
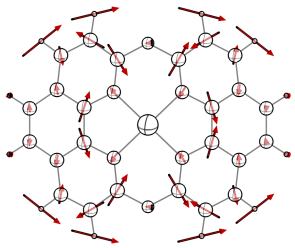
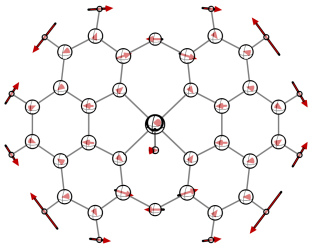
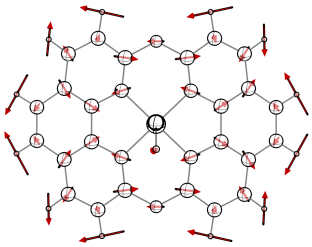
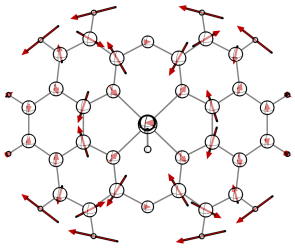


Figure S3b. IR spectra of complexes **3** and $\mathbf{3}^{2+}$ in all spin states.

Table S3. Sketches of the most relevant vibration modes for IR spectra of intermediate spin species in Figures S2a/b, including their band number, energy (E, cm^{-1}) and intensity (I, a.u.).

1_{Cl} S=3/2	 Band 102 E = 1365.27 cm^{-1} I = 691.70 a.u.	 Band 108 E = 1435.09 cm^{-1} I = 822.94 a.u.	 Band 115 E = 1514.57 cm^{-1} I = 3698.69 a.u.
1_{OH} S=3/2	 Band 105 E = 1367.05 cm^{-1} I = 510.15 a.u.	 Band 110 E = 1436.53 cm^{-1} I = 449.95 a.u.	 Band 117 E = 1515.21 cm^{-1} I = 4111.19 a.u.
2_{Cl} S=3/2	 Band 102 E = 1387.10 cm^{-1} I = 1899.07 a.u.	 Band 103 E = 1394.26 cm^{-1} I = 2759.57 a.u.	 Band 108 E = 1456.55 cm^{-1} I = 661.45 a.u.

2_{OH} S=3/2	 Band 104 E = 1387.50 cm^{-1} I = 1247.97 a.u.	 Band 105 E = 1395.47 cm^{-1} I = 3806.00 a.u.	 Band 110 E = 1455.43 cm^{-1} I = 684.25 a.u.
3_{Cl}^{2+} S=3/2	 Band 87 E = 1202.81 cm^{-1} I = 1553.06 a.u.	 Band 95 E = 1278.81 cm^{-1} I = 683.91 a.u.	 Band 109 E = 1496.07 cm^{-1} I = 713.63 a.u.
3_{OH}^{2+} S=3/2	 Band 89 E = 1202.58 cm^{-1} I = 1597.33 a.u.	 Band 97 E = 1278.57 cm^{-1} I = 672.66 a.u.	 Band 111 E = 1496.79 cm^{-1} I = 566.19 a.u.

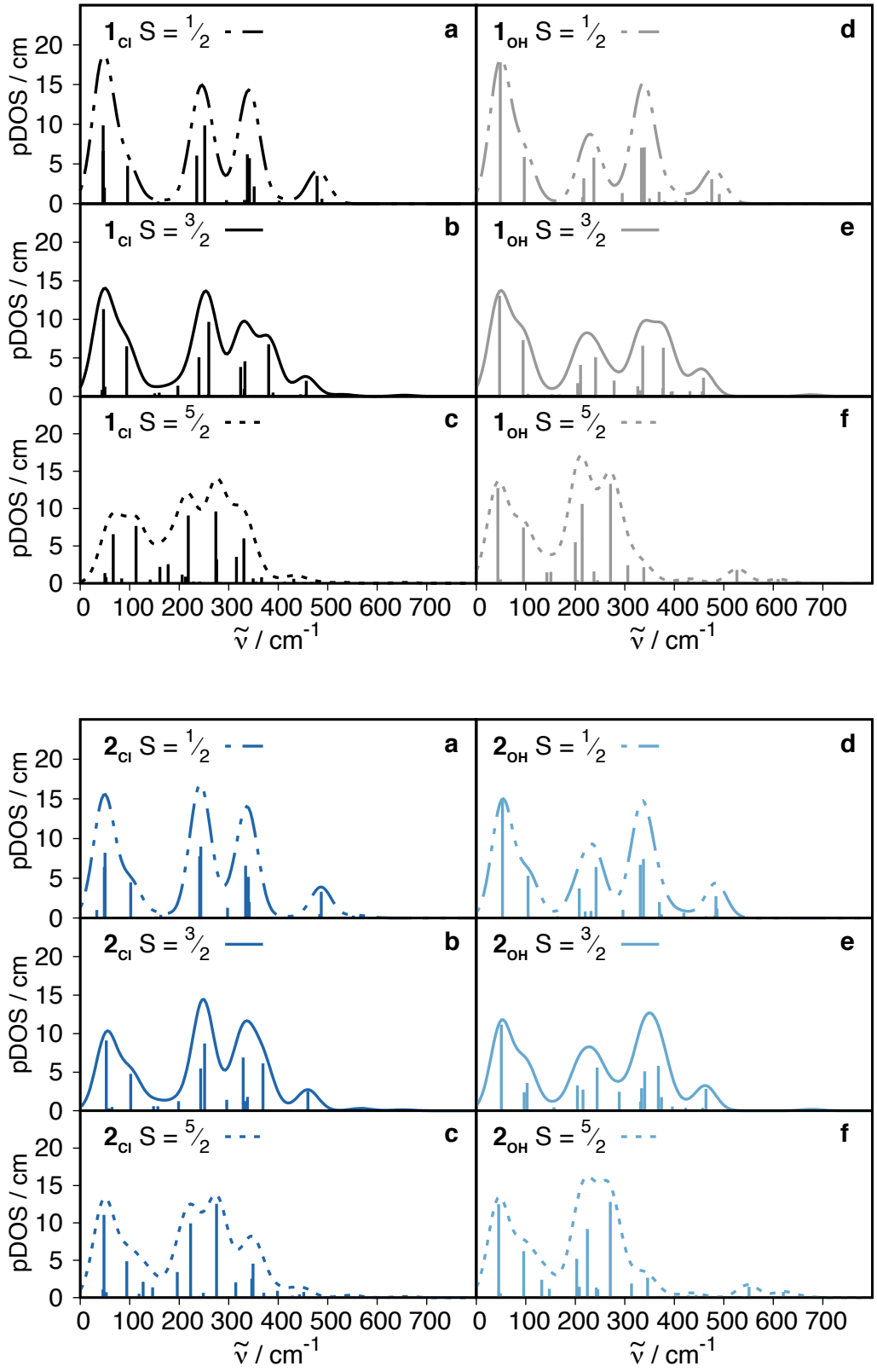


Figure S4a. NRVS spectra of complexes **1** and **2** in all spin states.

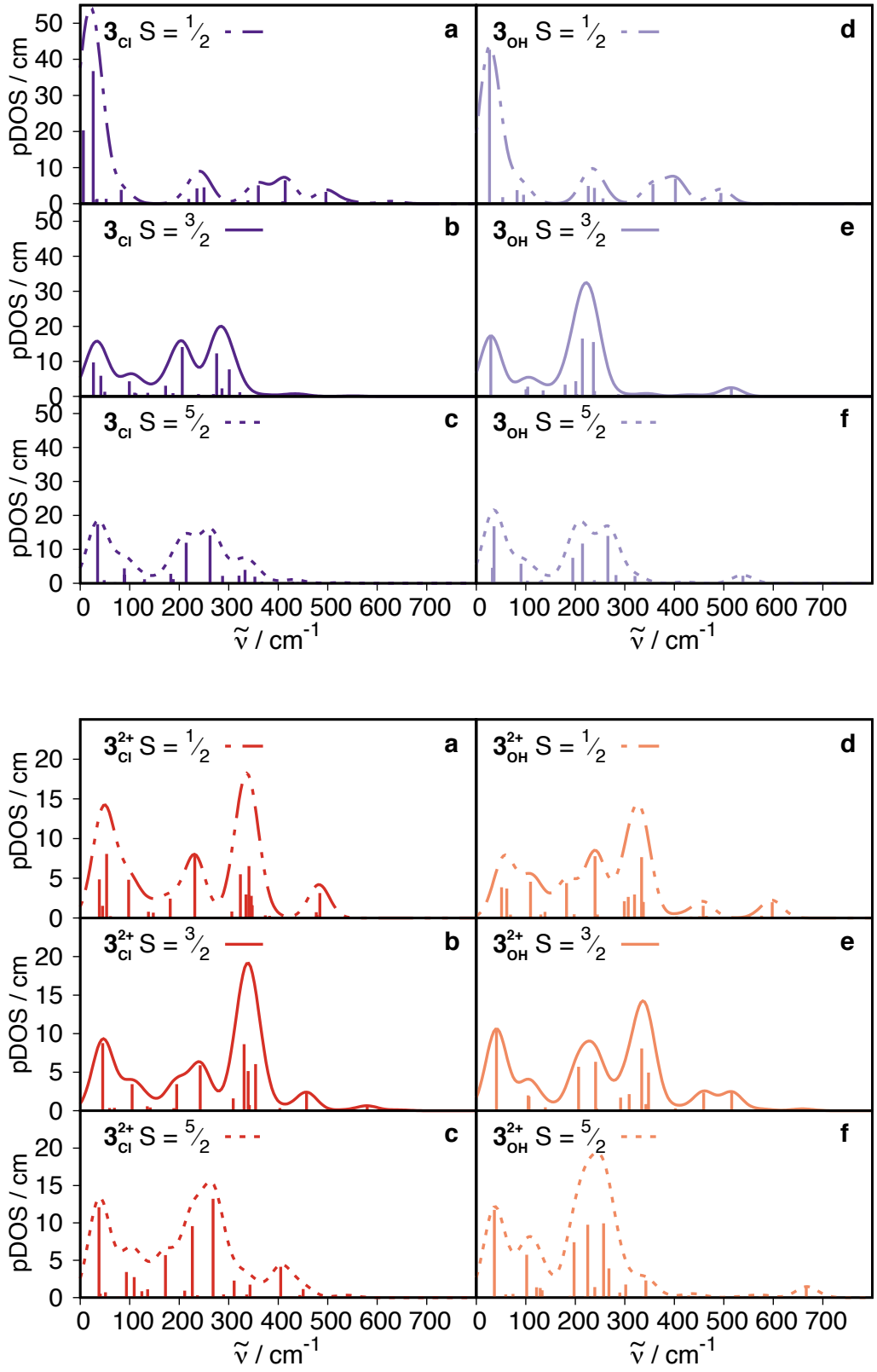
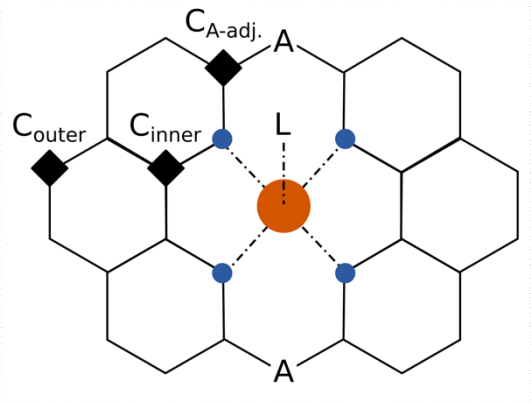


Figure S4b. NRVS spectra of complexes **3** and $\mathbf{3}^{2+}$ in all spin states.



Scheme S1. Generic structure of a [Fe{phen$_2$*A*$_2$}*L*] complex with black diamonds and labels highlighting the 'outer', 'inner' and 'adjacent' carbon atoms for which HFCs were computed.

Table S4. Selected hyperfine coupling constants (MHz) of all [Fe{phen$_2$*A*$_2$}*L*] complexes with *A* = C, N, O and *L* = Cl^-, OH^-.

	Fe	N	N	C_{outer}	C_{inner}	$C_{A\text{-}adj.}$	A (H)	
$\mathbf{1}_{Cl}$ (LS)	-14.7	-9.3	-9.3	-0.2	0.9	8.1	-9.3	(8.7)
$\mathbf{1}_{Cl}$ (IS)	-11.0	-0.5	-0.5	-0.0	-0.2	-1.4	2.2	(-1.5)
$\mathbf{1}_{Cl}$ (HS)	-16.7	9.7	9.7	0.1	-0.5	-0.5	2.0	(-1.6)
$\mathbf{1}_{OH}$ (LS)	-16.7	-4.7	-4.7	-0.2	-1.4	1.9	-1.4	(1.9)
$\mathbf{1}_{OH}$ (IS)	-14.6	-0.3	-0.7	0.0	-0.1	-1.0	1.9	(-1.1)
$\mathbf{1}_{OH}$ (HS)	-17.7	10.0	9.7	0.1	-0.3	0.0	1.6	(-1.1)
$\mathbf{2}_{Cl}$ (LS)	-15.9	-5.9	-5.9	-0.3	-1.5	3.0	-1.0	
$\mathbf{2}_{Cl}$ (IS)	-13.0	-0.1	-0.1	0.0	0.0	-0.5	0.7	
$\mathbf{2}_{Cl}$ (HS)	-17.0	10.4	10.4	0.1	-0.2	-0.2	0.6	
$\mathbf{2}_{OH}$ (LS)	-16.4	-3.3	-3.3	-0.2	-2.4	0.7	0.1	
$\mathbf{2}_{OH}$ (IS)	-15.6	0.0	-0.3	0.0	0.1	-0.3	0.6	
$\mathbf{2}_{OH}$ (HS)	-17.3	10.3	10.1	0.1	-0.1	0.0	0.5	
$\mathbf{3}_{Cl}$ (LS)	14.9	-8.9	-8.8	0.0	1.0	-1.5	-2.7	
$\mathbf{3}_{Cl}$ (IS)	-22.9	8.7	8.7	0.1	-1.3	1.0	-1.6	
$\mathbf{3}_{Cl}$ (HS)	-14.6	7.1	7.1	0.0	-0.9	-1.0	-0.3	
$\mathbf{3}_{OH}$ (LS)	11.9	-3.1	-3.5	0.1	2.2	1.9	-3.9	
$\mathbf{3}_{OH}$ (IS)	-24.0	9.4	9.4	0.2	-1.4	0.2	0.2	
$\mathbf{3}_{OH}$ (HS)	-13.4	7.0	6.9	0.0	-0.9	-1.0	-0.3	
$\mathbf{3}^{2+}_{Cl}$ (LS)	-14.6	-4.3	-4.2	-0.3	-2.6	0.8	-0.2	
$\mathbf{3}^{2+}_{Cl}$ (IS)	-15.1	0.0	0.0	0.0	0.2	0.6	-1.3	
$\mathbf{3}^{2+}_{Cl}$ (HS)	-16.5	10.0	10.0	0.1	-0.1	0.1	-0.7	
$\mathbf{3}^{2+}_{OH}$ (LS)	-17.3	-8.4	10.6	0.0	-1.9	1.6	-1.0	
$\mathbf{3}^{2+}_{OH}$ (IS)	-16.3	0.1	0.0	0.0	0.2	0.6	-1.3	
$\mathbf{3}^{2+}_{OH}$ (HS)	-15.3	9.6	9.6	0.1	-0.1	0.1	-0.6	

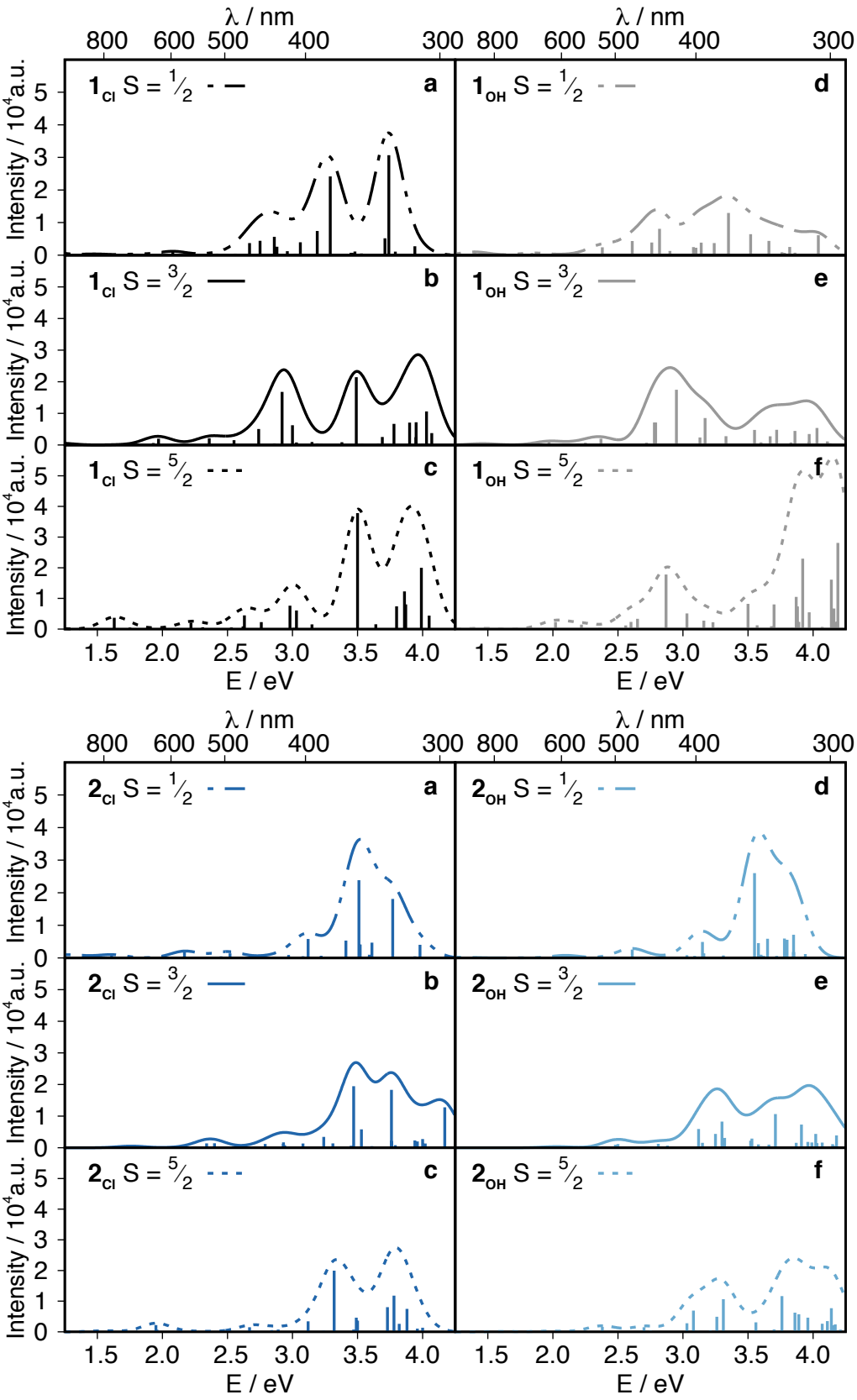


Figure S5a. UV-vis spectra of complexes **1** and **2**.

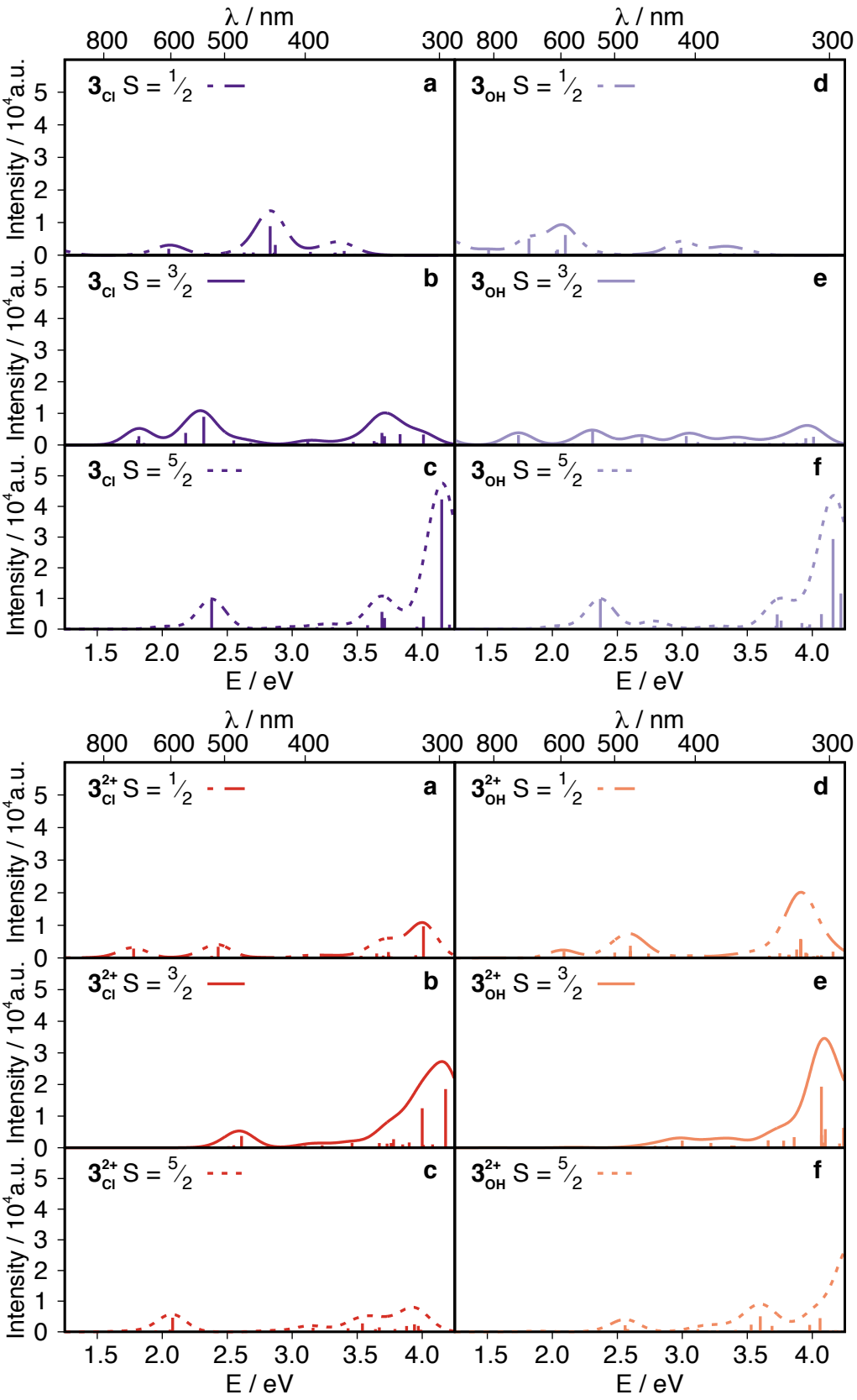
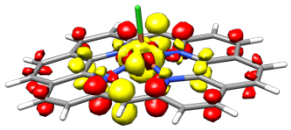
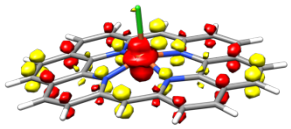
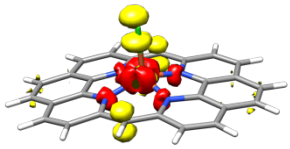
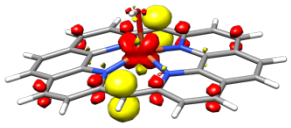
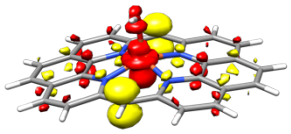
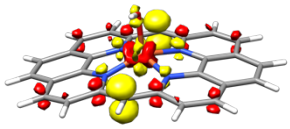
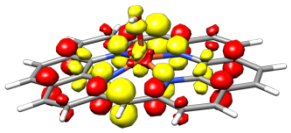
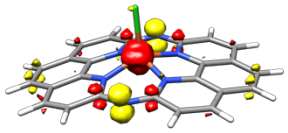
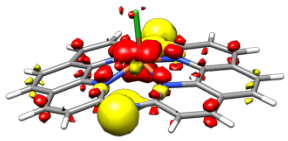
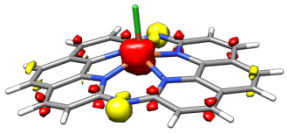
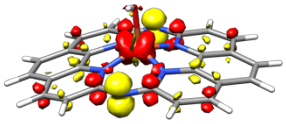


Figure S5b. UV-vis spectra of complexes **3** and $\mathbf{3}^{2+}$.

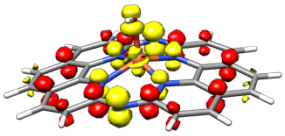
Table S5. Difference densities of most relevant transitions in the UV-vis spectra shown in Figure S3. Yellow isosurfaces correspond to the density loss in the ground state, red isosurfaces to the density gain in the excited state.

1_{Cl} S=3/2	 State 14 E = 2.92 eV I = 16771 a.u.	 State 35 E = 3.49 eV I = 21428 a.u.	 State 57 E = 4.03 eV I = 10613 a.u.
1_{OH} S=3/2	 State 20 E = 2.79 eV I = 7098 a.u.	 State 21 E = 2.78 eV I = 7109 a.u.	 State 24 E = 2.95 eV I = 17487 a.u.
	 State 29 E = 3.17 eV I = 8528 a.u.		
2_{Cl} S=3/2	 State 33 E = 3.47 eV I = 19476 a.u.	 State 43 E = 3.76 eV I = 18301 a.u.	 State 59 E = 4.17 eV I = 12761 a.u.

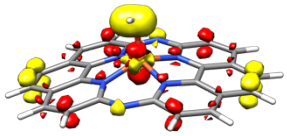
2_{OH}
S=3/2



State 26
E = 3.30 eV
I = 8283 a.u.

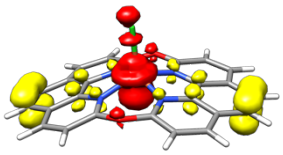


State 34
E = 3.71 eV
I = 10644 a.u.

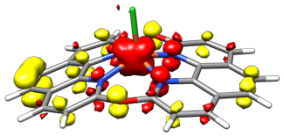


State 42
E = 3.91 eV
I = 7327 a.u.

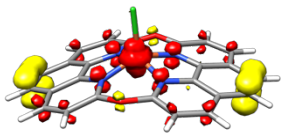
3_{Cl}^{2+}
S=3/2



State 16
E = 2.61 eV
I = 3731 a.u.

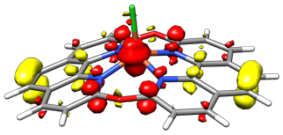


State 48
E = 4.00 eV
I = 12476 a.u.



State 56
E = 4.18 eV
I = 18550 a.u.

3_{OH}^{2+}
S=3/2



State 44
E = 4.07 eV
I = 19306 a.u.

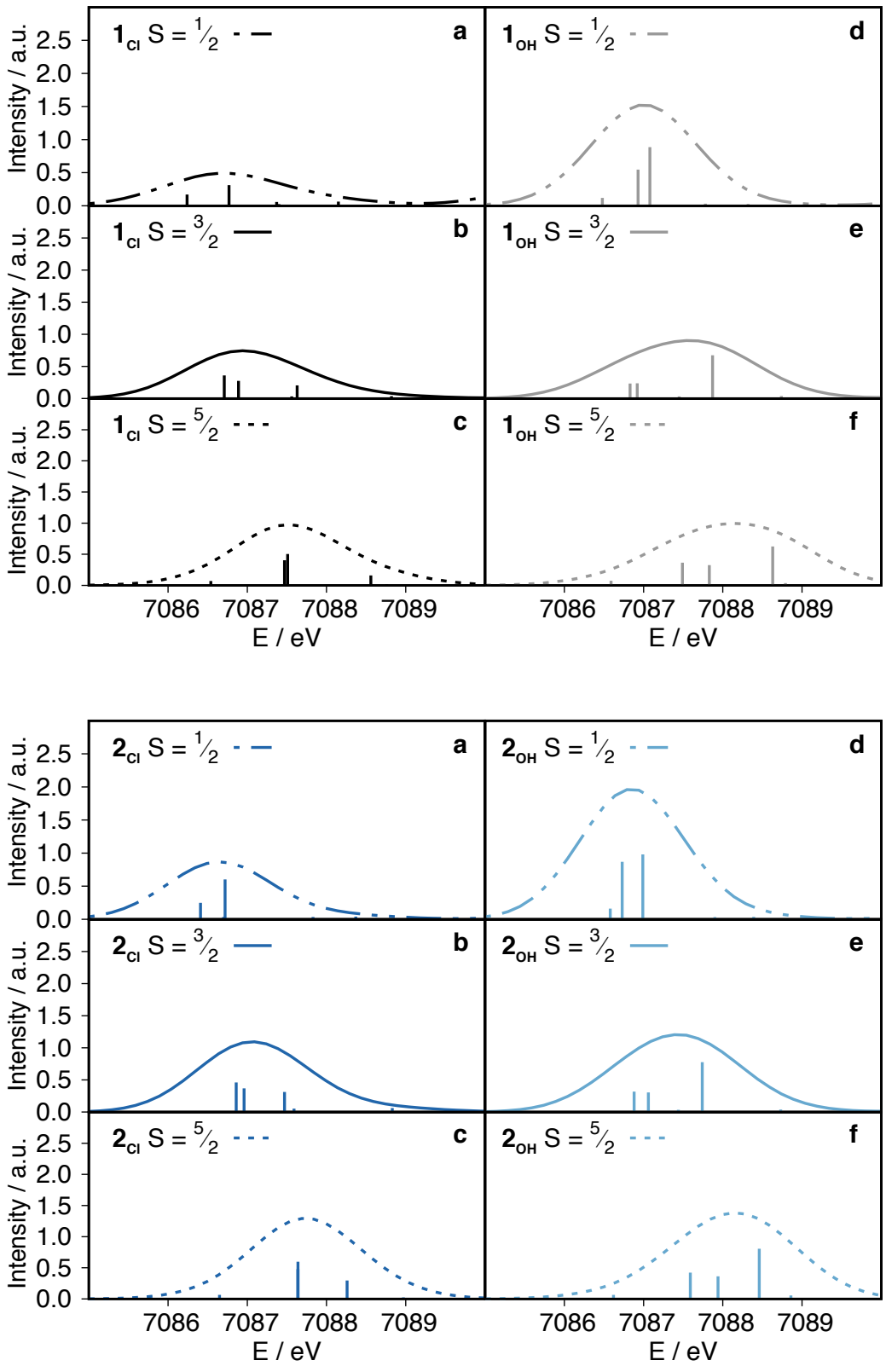


Figure S6a. Fe K pre-edge XAS of complexes **1** and **2**. Energy is not shifted to match experiment.

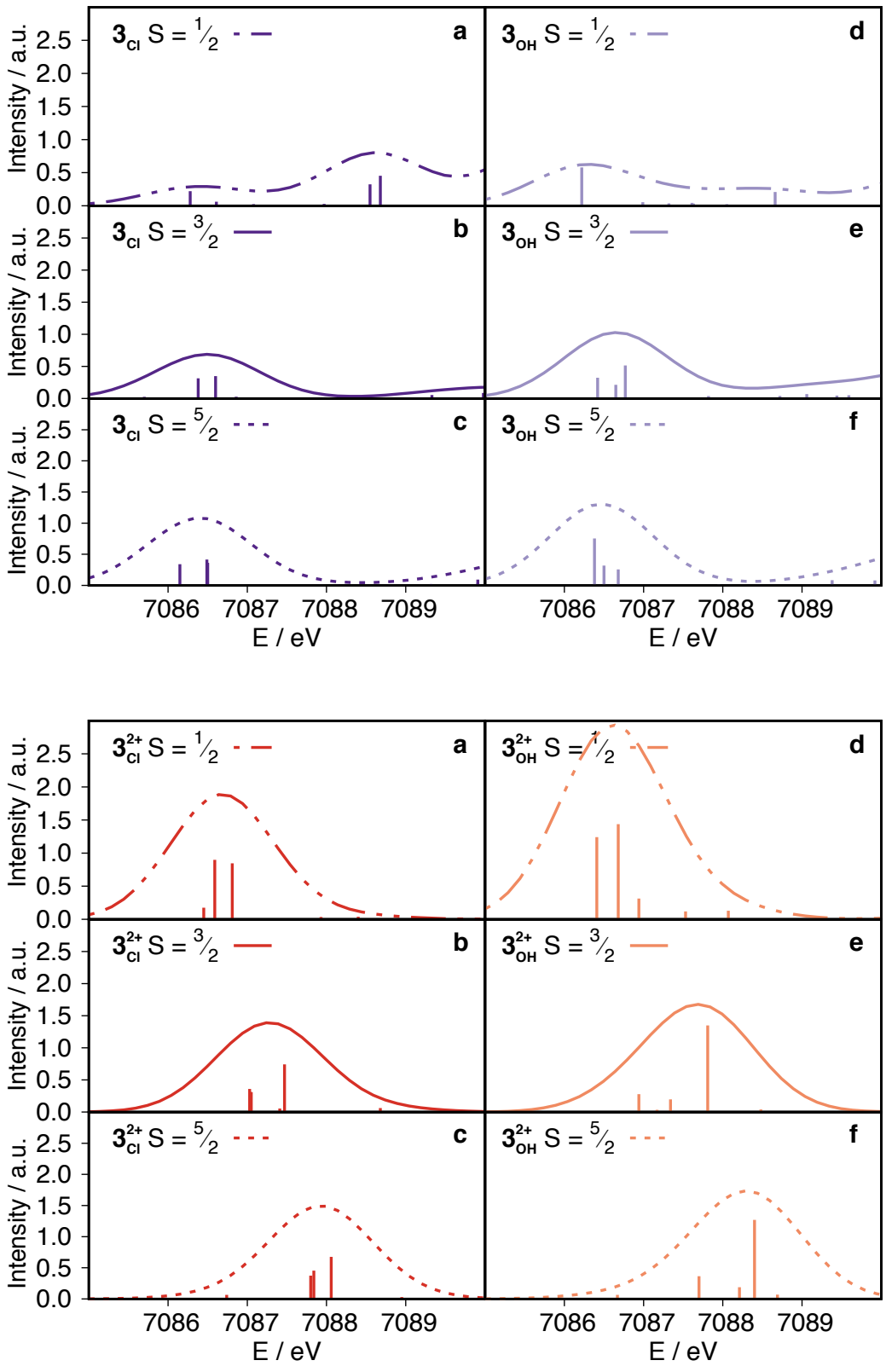
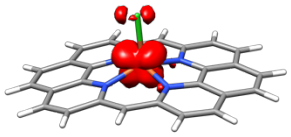
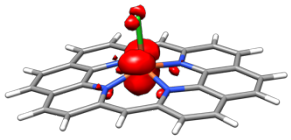
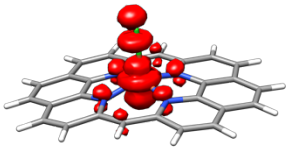
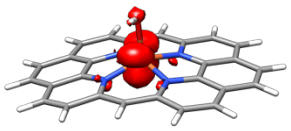
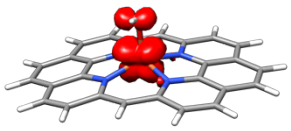
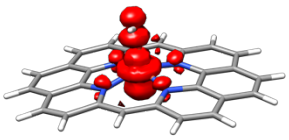
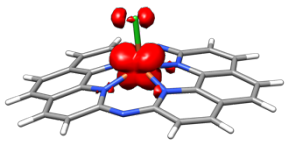
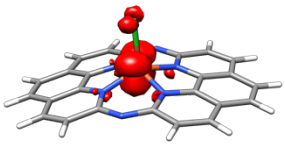
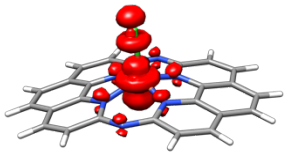
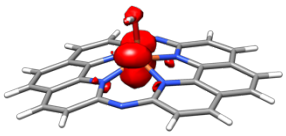
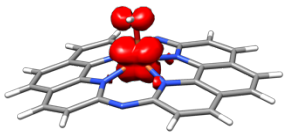
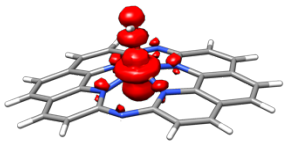
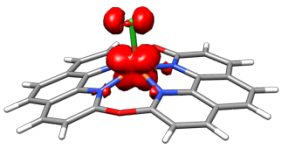
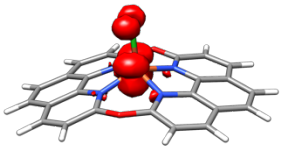
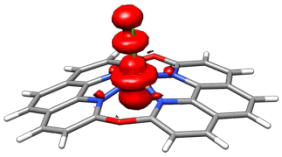
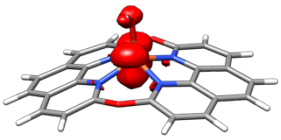
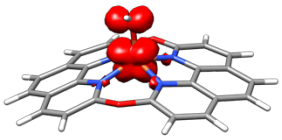
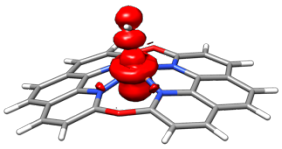


Figure S6b. Fe K pre-edge XAS of complexes **3** and $\mathbf{3}^{2+}$. Energy is not shifted to match experiment.

Table S6. Difference densities associated with the most relevant transitions in the Fe K pre-edge XAS spectra shown in Figures S6a/b.

1_{Cl} S=3/2	 State 1 E = 7086.71 eV I = 0.36 a.u.	 State 2 E = 7086.89 eV I = 0.27 a.u.	 State 4 E = 7087.63 eV I = 0.20 a.u.
1_{OH} S=3/2	 State 1 E = 7086.83 eV I = 0.24 a.u.	 State 2 E = 7086.92 eV I = 0.24 a.u.	 State 4 E = 7087.87 eV I = 0.67 a.u.
2_{Cl} S=3/2	 State 1 E = 7086.86 eV I = 0.46 a.u.	 State 2 E = 7086.96 eV I = 0.37 a.u.	 State 3 E = 7087.47 eV I = 0.31 a.u.
2_{OH} S=3/2	 State 1 E = 7086.88 eV I = 0.32 a.u.	 State 2 E = 7087.06 eV I = 0.31 a.u.	 State 4 E = 7087.74 eV I = 0.78 a.u.

3_{Cl}^{2+} S=3/2	 State 1 E = 7087.03 eV I = 0.36 a.u.	 State 2 E = 7087.05 eV I = 0.31 a.u.	 State 4 E = 7087.47 eV I = 0.74 a.u.
3_{OH}^{2+} S=3/2	 State 1 E = 7086.94 eV I = 0.28 a.u.	 State 3 E = 7087.34 eV I = 0.20 a.u.	 State 4 E = 7087.81 eV I = 1.35 a.u.

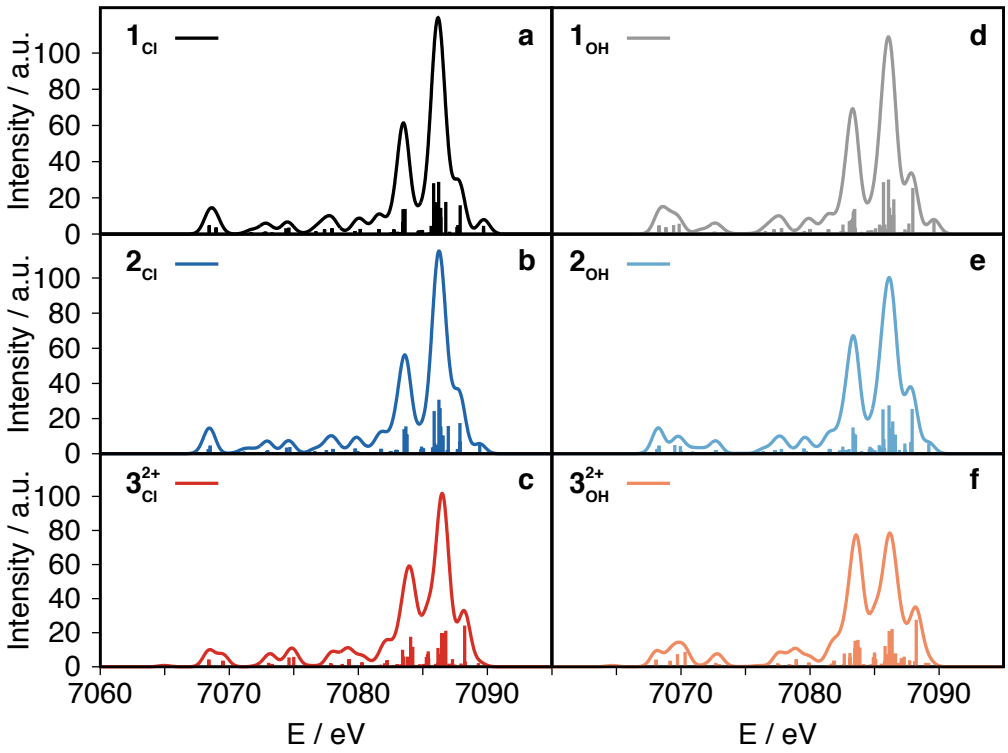


Figure S7. Valence-to-core XES traces of (a) $\mathbf{1}_{Cl}$, $\mathbf{2}_{Cl}$, $\mathbf{3}^{2+}_{Cl}$, (b) $\mathbf{1}_{OH}$, $\mathbf{2}_{OH}$, $\mathbf{3}^{2+}_{OH}$ in the IS states. Line spectra are broadened by 1.5 eV, energy is not shifted to match experiment.

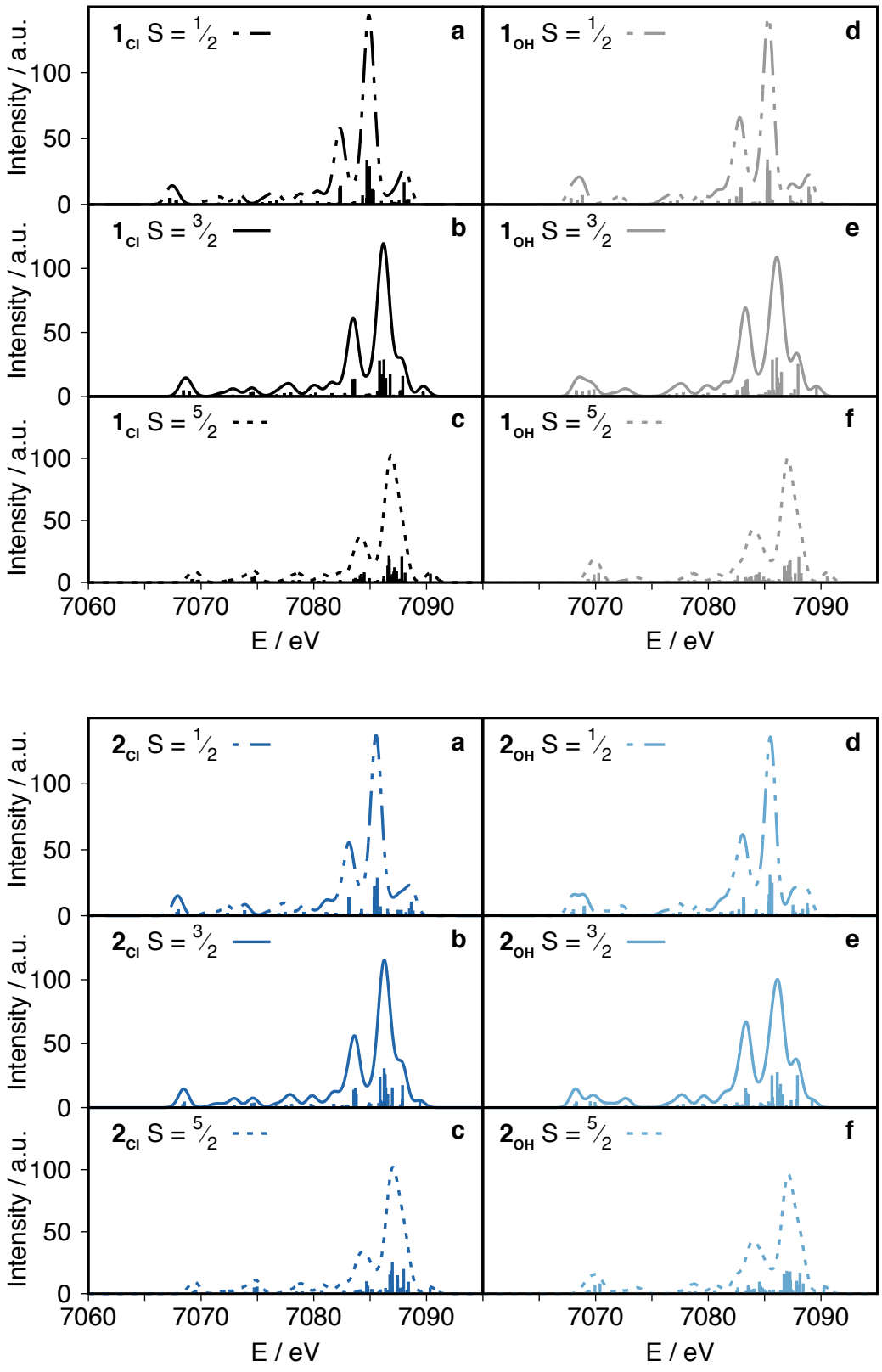


Figure S8a. Valence-to-core XES traces of complexes **1** and **2**. Energy is not shifted to match experiment.

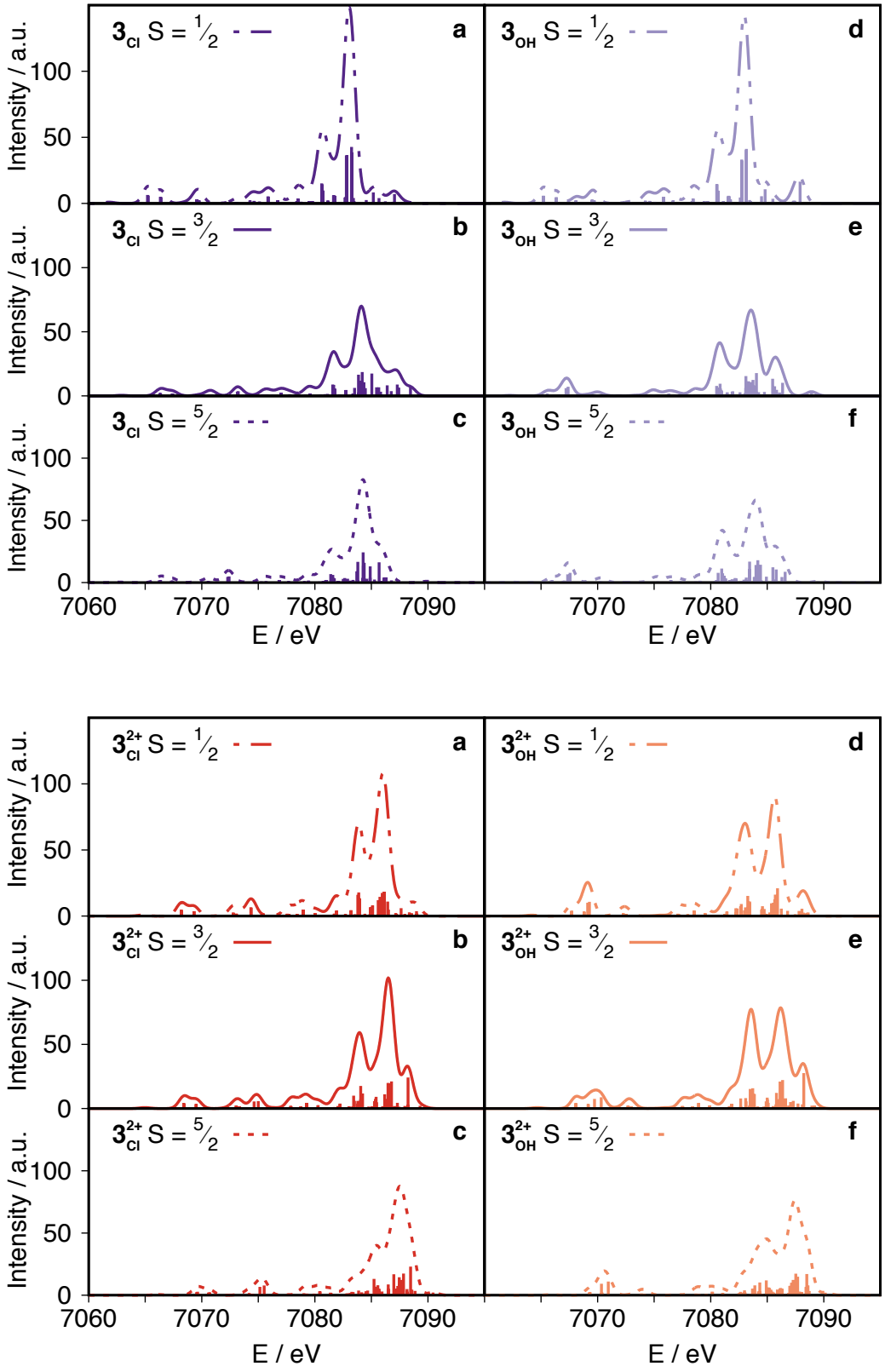
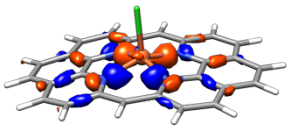
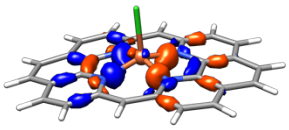
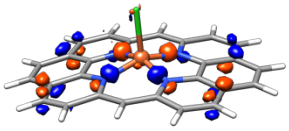
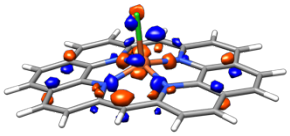
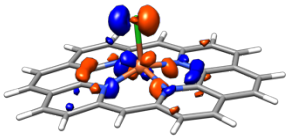
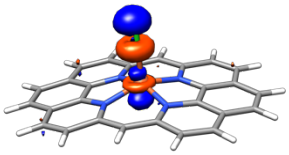
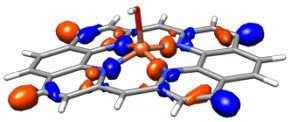
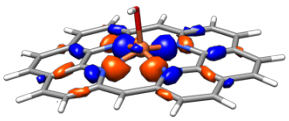
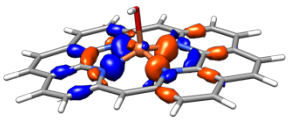
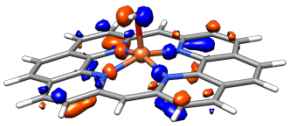
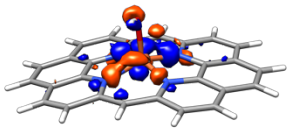
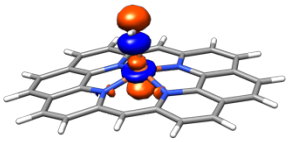
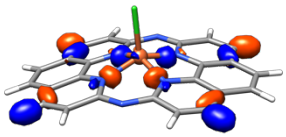
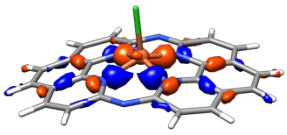
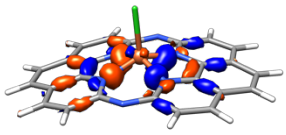
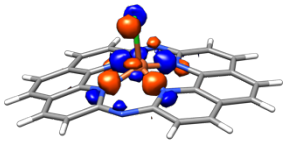
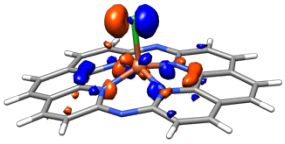
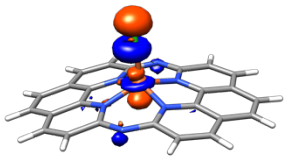
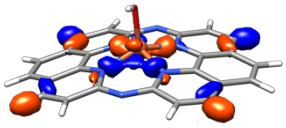
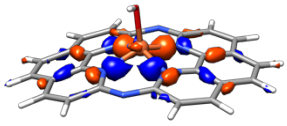
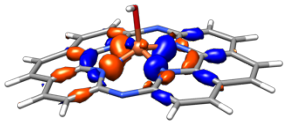
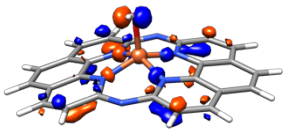
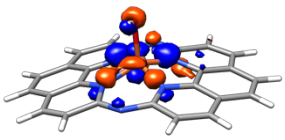
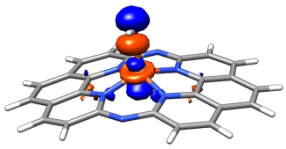
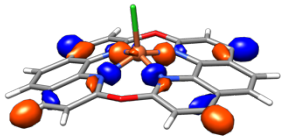
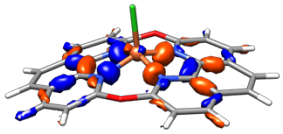
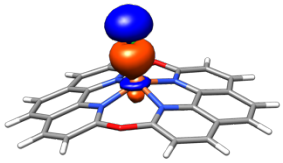
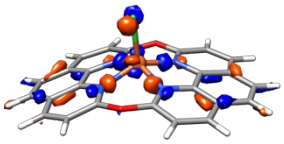
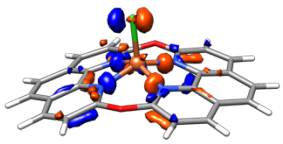
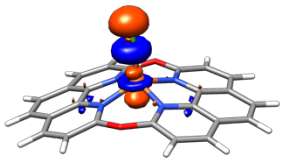
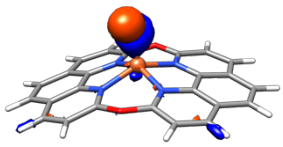
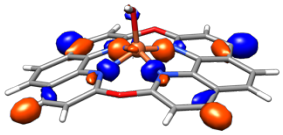
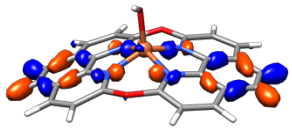
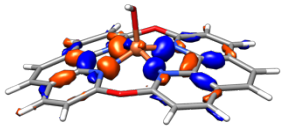
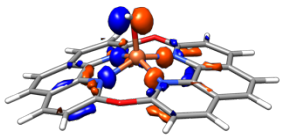
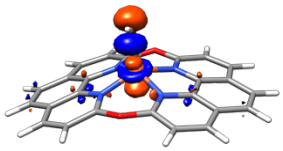


Figure S8b. Valence-to-core XES traces of complexes **3** and $\mathbf{3}^{2+}$. Energy is not shifted to match experiment.

Table S7. Orbitals associated with the most relevant transitions in the valence-to-core XES spectra shown in Figures S8a/b.

1$_{Cl}$ S=3/2	 103b E = 7085.84 eV I = 28.01 a.u.	 106b E = 7086.22 eV I = 28.81 a.u.	 107a E = 7086.04 eV I = 17.62 a.u.
	 110a E = 7086.39 eV I = 14.43 a.u.	 112a E = 7086.78 eV I = 17.62 a.u.	 117a E = 7087.90 eV I = 15.94 a.u.
1$_{OH}$ S=3/2	 86b E = 7083.46 eV I = 13.85 a.u.	 100b E = 7085.70 eV I = 28.67 a.u.	 103b E = 7086.08 eV I = 30.12 a.u.
	 105a E = 7086.17 eV I = 14.59 a.u.	 109a E = 7086.50 eV I = 19.20 a.u.	 114a E = 7087.96 eV I = 25.45 a.u.

2_{Cl} S=3/2	 90b E = 7083.69 eV I = 15.59 a.u.  100b E = 7085.88 eV I = 24.29 a.u.  104b E = 7086.34 eV I = 25.96 a.u.  107a E = 7086.25 eV I = 30.75 a.u.  110a E = 7086.97 eV I = 15.77 a.u.  116a E = 7087.88 eV I = 17.47 a.u.
2_{OH} S=3/2	 86a E = 7083.33 eV I = 14.95 a.u.  97b E = 7087.91 eV I = 25.47 a.u.  101b E = 7086.13 eV I = 27.51 a.u.  104a E = 7086.28 eV I = 14.51 a.u.  105a E = 7086.41 eV I = 18.43 a.u.  114a E = 7087.91 eV I = 27.51 a.u.

3_{Cl}^{2+} S=3/2	 90b E = 7084.06 eV I = 17.60 a.u.  106b E = 7086.47 eV I = 19.88 a.u.  107b E = 7086.59 eV I = 19.31 a.u.  109a E = 7086.48 eV I = 19.73 a.u.  110a E = 7086.78 eV I = 21.15 a.u.  116a E = 7088.24 eV I = 24.22 a.u.
3_{OH}^{2+} S=3/2	 84b E = 7083.49 eV I = 15.25 a.u.  87b E = 7083.72 eV I = 15.83 a.u.  100b E = 7085.82 eV I = 12.17 a.u.  103b E = 7086.14 eV I = 21.03 a.u.  106a E = 7086.36 eV I = 22.16 a.u.  113a E = 7088.24 eV I = 27.64 a.u.

Cartesian coordinates of all models in Å.

Coordinates for: **1**$_{Cl}$ S=1/2

Final Single Point Energy: -2942.19893943889 Eh

Fe	-0.08892185570378	0.10338037596046	-0.44163991925608
N	-0.34258538846133	-1.77135226626155	-0.85444979573799
N	-2.00333782595901	0.18285188594046	-0.72181376136279
N	0.14903379523266	2.00996483639403	-0.68195284055978
N	1.81065183215719	0.05647241240260	-0.81408866138084
Cl	-0.03307780054166	-0.00748144913858	1.83633673140665
C	2.01975921033289	-2.36958605414879	-0.94265323826789
C	-2.21334204464505	2.60933587235658	-0.60685927804911
C	-1.08864374512876	-4.46463300458719	-1.21901348856474
C	-2.11500500098413	-3.46460537156757	-1.14714964276696
C	-3.52418779503609	-3.67699202705916	-1.24953064582206
C	-1.66644952581247	-2.13679611533122	-0.96217648328232
C	-2.58650269290356	-1.05432458056026	-0.88896372478178
C	-4.42484271064764	-2.61744397939553	-1.17784615545393
C	-3.97899565549202	-1.27185943540201	-0.99880519779175
C	-4.80085598507120	-0.09812258549620	-0.92403663726870
C	0.64683095247189	-2.72602034700586	-0.96113914994522
C	0.23795961746405	-4.09935371585034	-1.13237963862486
C	-2.78908639536141	1.31557061263142	-0.68810297045570
C	-4.21906758291239	1.14321107318753	-0.77836884695659
C	-0.84185671269159	2.96854745837578	-0.65197962110665
C	1.46775351833597	2.38731949096695	-0.81281276878158
C	0.88400454948330	4.72783295491089	-0.81819973223813
C	1.91044388140834	3.72774507082339	-0.88828339780772
C	2.59439809367676	-1.07275888022574	-0.92443807006688
C	4.01928468301892	-0.88942801115382	-1.06098403640539
C	3.77489714759420	1.53528115201513	-1.03571561200249
C	2.38815634027608	1.30509279927310	-0.88576888118948
C	3.31409554304625	3.95225670042067	-1.03241397938138
C	4.21498187040195	2.89287697311491	-1.10357037410031
C	-0.43810647383464	4.35289973396659	-0.70838621254995
C	4.59662610005176	0.36155003060306	-1.11154300763325
H	-3.89384848440862	-4.69703026992659	-1.39423528079485
H	-5.49890052300697	-2.80877219811977	-1.26661547074457
H	-1.36446631387803	-5.51542735612391	-1.35032541819009
H	-5.88896338666521	-0.19355943253758	-0.99084857515505
H	3.67883007484297	4.98237695440707	-1.09504073996909
H	1.15595801380760	5.78696483614479	-0.86068595792985
H	-4.84161202043027	2.04136069810699	-0.73232522076404
H	1.02343933863269	-4.85767868796808	-1.19797974991227
H	4.64141349487306	-1.78636024756126	-1.13030811692313
H	5.68085803063317	0.46492276716483	-1.21788058559727
H	-1.22436983466158	5.11210977288369	-0.66636465733354
H	5.28431288856203	3.09456394177344	-1.22165848988857
H	-2.92103882651060	3.44238526949207	-0.58150093893242
H	2.72609769325932	-3.19968079471940	-1.02914624859658

Coordinates for: **1**$_{Cl}$ S=3/2

Final Single Point Energy: -2942.19644644500 Eh

Fe	-0.08673244243658	0.09835932879819	-0.33572478433007
N	-0.31502586249046	-1.76399415096207	-0.85664093104975
N	-1.99198545942430	0.20861517189619	-0.72386982672118
N	0.12195625256416	2.00315450823177	-0.68381310866959
N	1.79900332954545	0.03064719612003	-0.81616998265838
Cl	-0.03614121173055	-0.01030629721355	1.97760150236419
C	2.03439009831532	-2.38667891512189	-0.94419701304359
C	-2.22762533656469	2.62627207633764	-0.60567056002990
C	-1.08091377153201	-4.44706755795425	-1.22598407731366
C	-2.09837010330520	-3.43834762054032	-1.15331226390460
C	-3.50711370050400	-3.65978112872097	-1.25316846791704
C	-1.64104620126953	-2.11324690148316	-0.96972922837719
C	-2.55957367517725	-1.03278643941634	-0.89690987609391
C	-4.40509631536620	-2.60361522556423	-1.18159232062019
C	-3.95075304529063	-1.25963889860813	-1.00587580239175
C	-4.78266545663605	-0.09325349852033	-0.93131665544814
C	0.66168859359182	-2.72140936121050	-0.96626439075329
C	0.24546873220028	-4.09336588332165	-1.13935653021583
C	-2.78247248322384	1.32958714825117	-0.69264699412627
C	-4.21243250086599	1.14980976236376	-0.78462688960130
C	-0.85654430653179	2.96454555878770	-0.65664293741452
C	1.44243387788726	2.36453963661133	-0.82107533693946
C	0.87647561301662	4.71095568163837	-0.82613437788570
C	1.89405040763270	3.70212939026818	-0.89602095493438
C	2.58753672438685	-1.08646093972060	-0.92979267776998
C	4.01224171246905	-0.89563989786858	-1.06860637746449
C	3.74643268966399	1.52333381292852	-1.04258744927746
C	2.36103367536575	1.28412916154614	-0.89369472119065
C	3.29738818229361	3.93519198675957	-1.03697307224374
C	4.19533966566928	2.87896179363725	-1.10802513497581
C	-0.44548940159512	4.34770449328839	-0.71502296748060
C	4.57813722941680	0.35697135991329	-1.11940746862600
H	-3.86991702626034	-4.68280201391714	-1.39310743885473
H	-5.48062552182206	-2.78831758787622	-1.26477995030298
H	-1.36695989037739	-5.49482416171490	-1.36016500882409
H	-5.86965243492209	-0.19913787966060	-1.00131445123559
H	3.65572935973953	4.96771481159292	-1.09439277027603
H	1.15867127717625	5.76731732877876	-0.87218369478375
H	-4.83763966359075	2.04607202713624	-0.74402394870382
H	1.02834880334502	-4.85346693495370	-1.21115008561838
H	4.63658265126038	-1.79020159560656	-1.14459942640576
H	5.66103182826814	0.47100809311071	-1.22902875458389
H	-1.22935193585779	5.10932623871246	-0.67871565591215
H	5.26637185534833	3.07328546685269	-1.22175469468317
H	-2.93471134017019	3.45848200887541	-0.57695885658104
H	2.74024861660320	-3.21616428930497	-1.02821807504739

Coordinates for: **1**$_{Cl}$ S=5/2

Final Single Point Energy: -2942.17221407334 Eh

Fe	-0.07938727133437	0.08228258562039	0.00177371961380
N	-0.30128402799300	-1.78571618916405	-0.79541494117941
N	-2.00738354011753	0.22073228255741	-0.65918141871673
N	0.11106179740197	2.01902590354292	-0.61918065438439
N	1.81703525248793	0.01243781015924	-0.75461443755469
Cl	-0.02681460320611	-0.02420072325270	2.24448660499166
C	2.04595673471649	-2.40166326898133	-0.88384230146396
C	-2.23658603367223	2.63537130290958	-0.54340473402967
C	-1.07516591789508	-4.44014123845330	-1.25636039251575
C	-2.08383557138036	-3.42107230010440	-1.19623106893070
C	-3.48654231900763	-3.63550189547169	-1.35457393739211
C	-1.61990427183606	-2.10309834286391	-0.95719933733020
C	-2.54554186925992	-1.01452422377359	-0.88348001453532
C	-4.38473092819174	-2.57924742405304	-1.28280602719003
C	-3.93447551088377	-1.24468322380276	-1.04844094269177
C	-4.77716147516692	-0.08635081393709	-0.96078829546038
C	0.67138887935724	-2.74245051985510	-0.91406091171680
C	0.25324456585052	-4.10892356707421	-1.12154292391393
C	-2.79838425649506	1.33842798632526	-0.63765501242500
C	-4.22553774070217	1.15851654979895	-0.76427867860362
C	-0.86396482491227	2.98052293079330	-0.60184953060536
C	1.42183751520010	2.35335135880584	-0.80847113309248
C	0.86925176247024	4.70705824314393	-0.85655799925899
C	1.87750361126330	3.68918552094205	-0.93964223084441
C	2.60564227094564	-1.10045110436977	-0.87721765338964
C	4.02601195257149	-0.90624965164792	-1.05016314530185
C	3.72803249381994	1.51254404709425	-1.08614590180362
C	2.34738474874925	1.26467991287552	-0.88178252059361
C	3.27217318010641	3.92081367779290	-1.13944460307362
C	4.17024039064353	2.86441312286841	-1.21058254793640
C	-0.45256165195658	4.36150572054470	-0.69533205939716
C	4.57110458906084	0.35292082443685	-1.14959626926790
H	-3.84594526271017	-4.65300448737680	-1.53792438194624
H	-5.45715125132548	-2.75830954285247	-1.40906162590866
H	-1.37199256564038	-5.48048327747198	-1.42249685246388
H	-5.86076958340396	-0.20148167424722	-1.06358921526225
H	3.62532752430633	4.95195766106950	-1.24011059127579
H	1.16061644845259	5.75916702178966	-0.93528969877197
H	-4.86095520770712	2.04753828991900	-0.71829970580977
H	1.02793536607767	-4.87812278402397	-1.18830975243858
H	4.66059241474869	-1.79429902126469	-1.12022296579967
H	5.64916347786279	0.47930530417245	-1.29064204912376
H	-1.22785274913064	5.13182921954162	-0.65344927555568
H	5.23623246655218	3.05707575155022	-1.36765698410846
H	-2.94397361983133	3.46812053458002	-0.52012992305891
H	2.75188669992975	-3.23120142561597	-0.97288016739931

Coordinates for: **1_{OH}** S=1/2

Final Single Point Energy: -2557.79550838506 Eh

Fe	-0.07742990261247	0.09593768399091	-0.40128677492663
N	-0.32948221851530	-1.77873273394553	-0.82727780161632
N	-1.99323407284466	0.17519711724010	-0.68742852918241
N	0.16282209939519	2.00854922401579	-0.62571062185043
N	1.82833906001693	0.05218405460778	-0.76745921732599
O	-0.06240120299755	-0.02592828244843	1.47680145230594
H	-0.76812077003783	-0.64993371994118	1.74295567862302
C	2.03638859260243	-2.37443251109893	-0.92393327719031
C	-2.20311871894844	2.60475984538728	-0.56621518185360
C	-1.07440633769749	-4.46902382694644	-1.20994882763814
C	-2.10316721107771	-3.47128151609159	-1.13187506410434
C	-3.51302779738810	-3.68497765750084	-1.23860414615261
C	-1.65601389808871	-2.14535414364784	-0.93739892451173
C	-2.57663110642041	-1.06422096503042	-0.86019111056274
C	-4.41395557418659	-2.62691722646765	-1.16288441139132
C	-3.96779749877566	-1.28135889558898	-0.97519075422642
C	-4.78873297473710	-0.10657198257007	-0.89803008077053
C	0.66243919481790	-2.73059194314729	-0.94118489350885
C	0.25201853286361	-4.10304742572710	-1.12102479926720
C	-2.77745003086361	1.30952368546206	-0.65171213197429
C	-4.20748434842861	1.13452214902132	-0.74623065171295
C	-0.83159108561542	2.96447407896662	-0.61187567410818
C	1.48336585448592	2.38620900601104	-0.77515558482416
C	0.89283541001551	4.72416727537043	-0.80635689979136
C	1.92195545244466	3.72509741681325	-0.87334045370229
C	2.60916278959477	-1.07685584368850	-0.90304833833952
C	4.03227416641446	-0.88963887069079	-1.06283536747219
C	3.78534760192865	1.53643830562998	-1.03149994821042
C	2.40349517769797	1.30540466788992	-0.85320087987683
C	3.32382484033992	3.95265087447558	-1.04006723711268
C	4.22457751633460	2.89460337788130	-1.11650338929102
C	-0.42812521974074	4.34925551649228	-0.68519049462139
C	4.60665330200196	0.36207519267068	-1.12118339564185
H	-3.88083961984327	-4.70473967337030	-1.39044416198489
H	-5.48793946793364	-2.81732881923259	-1.25547356626133
H	-1.34838770839765	-5.51952318955069	-1.34830583512276
H	-5.87685418220171	-0.20083844155297	-0.96816818453378
H	3.68450085111302	4.98325351060279	-1.11801865552616
H	1.16252161579154	5.78330563561443	-0.86393004567678
H	-4.83157228290696	2.03168899571762	-0.69857112666787
H	1.03745241624068	-4.86115689559713	-1.19182152077053
H	4.65493850207656	-1.78511091851868	-1.14712029582911
H	5.68872371170446	0.46657575433859	-1.24797485320140
H	-1.21463583968382	5.10878082369407	-0.65019485700539
H	5.29182986823537	3.09535759900101	-1.25426540197999
H	-2.91195260586891	3.43704880039931	-0.54489385786882
H	2.74234641664824	-3.20364089156819	-1.02203604802840

Coordinates for: $\mathbf{1}_{OH}$ S=3/2

Final Single Point Energy: -2557.78706824387 Eh

Fe	-0.10649363301969	0.09522661907199	-0.32691340945565
N	-0.33539275705505	-1.76925570053841	-0.83521142808839
N	-2.01432065247597	0.20822074461576	-0.70599916808651
N	0.10531665238831	2.00388644947466	-0.65591238976551
N	1.78386820679104	0.02608242209402	-0.78608633256563
O	-0.05141052959600	-0.02164400100653	1.60372873050063
H	0.54522097265830	-0.75132955180312	1.85944511502958
C	2.01528227054781	-2.39275920902585	-0.90951513754923
C	-2.24607861211260	2.62820820385281	-0.60206920944734
C	-1.10299051859138	-4.44888619761128	-1.21301935042358
C	-2.12005435698752	-3.43914023164718	-1.14656436923546
C	-3.52888725358077	-3.65967528794494	-1.25845926118791
C	-1.66247809653437	-2.11531465264611	-0.95664756998620
C	-2.58017306363482	-1.03349712846577	-0.88834225943322
C	-4.42552964007538	-2.60268687198521	-1.19402793164062
C	-3.97021937149979	-1.25894547285982	-1.01230648571102
C	-4.80113380967487	-0.09122891770196	-0.94649132533593
C	0.64179581607985	-2.72677129180947	-0.93978313540908
C	0.22365670681900	-4.09809485806256	-1.11635267333985
C	-2.80215897251490	1.33135603069524	-0.68899234145837
C	-4.23159270896669	1.15179521892778	-0.79550094918792
C	-0.87373112717689	2.96512513441633	-0.64386892052966
C	1.42740372353812	2.36181857037559	-0.79469781629277
C	0.86350011137277	4.70820640510666	-0.81551630596968
C	1.88071248323686	3.69830270719950	-0.87645070350046
C	2.57060716468575	-1.09254994245329	-0.89560675762577
C	3.99604901990550	-0.90183990778749	-1.03048667678368
C	3.73120725710018	1.51840538729545	-1.01138248393681
C	2.34570390860600	1.28051813146206	-0.86363922799602
C	3.28521047268799	3.93049803053114	-1.01589079939661
C	4.18236963781611	2.87397940351851	-1.08055027336104
C	-0.45963115765644	4.34758869619686	-0.70826135247034
C	4.56195178413448	0.35092109786226	-1.08330711834362
H	-3.89133069302353	-4.68233114231952	-1.40247572806263
H	-5.50066826955726	-2.78524432830763	-1.28748932817459
H	-1.38972417581519	-5.49609223054121	-1.35078455151207
H	-5.88754498740664	-0.19595862105746	-1.02789437949309
H	3.64379103376518	4.96280514049692	-1.07718638852676
H	1.14699906251847	5.76409243149489	-0.86672043871801
H	-4.85729004974337	2.04820690677234	-0.76362769631691
H	1.00510304652605	-4.86019777557856	-1.18389061483679
H	4.62117850864121	-1.79625124032638	-1.10307988477394
H	5.64522308977418	0.46420316607160	-1.19095097688854
H	-1.24206745124464	5.11121611492725	-0.68104591331579
H	5.25396450647737	3.06661904925876	-1.19249920633711
H	-2.95247406062379	3.46142050851573	-0.58382436980952
H	2.72072180944902	-3.22315379138232	-0.98915734753754

Coordinates for: **1_{OH}** S=5/2

Final Single Point Energy: -2557.76425494459 Eh

Fe	-0.09893388738997	0.07703750925287	0.02807217021750
N	-0.31895137529970	-1.79191901917921	-0.77185816346552
N	-2.02753722099866	0.22013292247214	-0.64780684608475
N	0.09515344658577	2.01814785399189	-0.59454445276102
N	1.80336061588151	0.00567852432598	-0.72012279869554
O	-0.06880932182889	-0.01819487045820	1.90452791811918
H	0.48152702575924	-0.73541273878811	2.27013634225936
C	2.02943294119018	-2.40944908818641	-0.85690621457645
C	-2.25415644476678	2.63673353339133	-0.53987952478947
C	-1.09306403551238	-4.44053113088649	-1.26087532060372
C	-2.10122256946545	-3.42031309909159	-1.20357078828781
C	-3.50304836699227	-3.63374109894755	-1.37926075598779
C	-1.63839052355410	-2.10522059688290	-0.95085257566895
C	-2.56323433780489	-1.01574269907503	-0.88268800583459
C	-4.40010990394133	-2.57717494242172	-1.31326710933358
C	-3.94953922196573	-1.24374614838931	-1.06735584794096
C	-4.79180530569233	-0.08409324044553	-0.98817975684092
C	0.65434545351387	-2.74801301545415	-0.89399398709453
C	0.23480111672604	-4.11267711530589	-1.11369324308119
C	-2.81593485068519	1.33981152522026	-0.63861824239914
C	-4.24204844328696	1.16026358100539	-0.78343192310376
C	-0.88043422756248	2.97945759011534	-0.59103595591359
C	1.40817952797934	2.34886069906092	-0.78559303178770
C	0.85691114173097	4.70204890639025	-0.85195785472624
C	1.86486815974973	3.68273620667654	-0.92684739929819
C	2.58979987440825	-1.10826799636144	-0.84828082415446
C	4.01000605711010	-0.91392899356893	-1.02610920352328
C	3.71248127064228	1.50565351492801	-1.06530802485085
C	2.33306678766251	1.25942506971956	-0.85490598227357
C	3.26013937854869	3.91372307861770	-1.13025395811215
C	4.15701487537455	2.85709284259490	-1.19742304942748
C	-0.46583566145548	4.35963277455320	-0.69214725609881
C	4.55479552790061	0.34510773469094	-1.12863011560862
H	-3.86053760090032	-4.65021768064285	-1.57224082173685
H	-5.47134110032001	-2.75321545352613	-1.45388227067268
H	-1.39016432290221	-5.47936037753103	-1.43643336029355
H	-5.87423018916106	-0.19797967784102	-1.10520157429991
H	3.61271154311417	4.94446280023222	-1.23789398754401
H	1.14967338697866	5.75338756256609	-0.93721442664258
H	-4.87810594975799	2.04935404759705	-0.74522211866613
H	1.00848780848719	-4.88300181705625	-1.18066984265160
H	4.64450401103803	-1.80198741050215	-1.09844182458262
H	5.63249865329622	0.47098397617975	-1.27364458274678
H	-1.23971938885133	5.13194380196663	-0.65828540328347
H	5.22298394537616	3.04723360028582	-1.35820620881691
H	-2.96076954915666	3.47047108834350	-0.52589898540306
H	2.73464254715006	-3.23933831626438	-0.94940895321821

Coordinates for: **2**$_{Cl}$ S=1/2

Final Single Point Energy: -2974.38377212069 Eh

Fe	-0.08290664217348	0.09089899113739	-0.18768849409968
N	-0.31658036579862	-1.76579169056040	-0.67753363294629
N	-1.98186700868514	0.19354486233014	-0.54570372639486
N	0.13083668433800	1.98748817830067	-0.50752042026720
N	1.79706642804328	0.02826230464733	-0.63894451795538
Cl	-0.02682111604309	-0.01519945382087	2.06918947340351
N	2.01501699140620	-2.36558769150578	-0.87630130897004
N	-2.20573692557066	2.59875632756610	-0.54135170197347
C	-1.02482236421500	-4.40957927760172	-1.26816941760656
C	-2.06844454758640	-3.43004246465637	-1.16089966358983
C	-3.47422794607245	-3.62717831731739	-1.35489144247237
C	-1.64004014821293	-2.12254472642941	-0.86019431425783
C	-2.56127637621486	-1.03871717872087	-0.78715803987363
C	-4.37440537780658	-2.56839580746555	-1.28312672249878
C	-3.93821412725066	-1.23086477836854	-1.01210392691834
C	-4.73948148099887	-0.04063694876137	-0.97235108180717
C	0.69546669881749	-2.67715004880348	-0.87264365898188
C	0.29934810915512	-4.04020129543830	-1.13564846500215
C	-2.72708198510099	1.34858467929085	-0.60086048122214
C	-4.15104921108796	1.19413194435447	-0.78153048306569
C	-0.88660809883648	2.91124310376594	-0.56735498565572
C	1.44577878387960	2.36303329530108	-0.71295548157452
C	0.81827384798647	4.67747444640072	-0.86941269982762
C	1.86355725833385	3.69439371576201	-0.90377290024163
C	2.53634217951585	-1.11452476707364	-0.83856559478791
C	3.95104980248983	-0.94041162750680	-1.06716517971395
C	3.73343496060880	1.49517370186504	-1.05166852732882
C	2.36734876759060	1.27935536978370	-0.78587383835155
C	3.25983515562041	3.91239337196216	-1.13963919335375
C	4.16004818472059	2.85362922321963	-1.21093975069412
C	-0.49951662254439	4.29417131986357	-0.71479628366595
C	4.53296469239067	0.30840378278802	-1.16337538114678
H	-3.83819517691197	-4.63347140596372	-1.58382990003244
H	-5.43964970906528	-2.75000604987809	-1.45576107747587
H	-1.28176564564130	-5.45183380475147	-1.48041643851624
H	-5.82156628238849	-0.11272147818079	-1.11818810767280
H	3.61553840396372	4.93692874736175	-1.28560706342455
H	1.06802465409161	5.73586581658456	-0.99105291329762
H	-4.75659174323463	2.10372778544401	-0.78243421457821
H	1.09577367412968	-4.77977977840180	-1.24873277128267
H	4.55401291376750	-1.84421138297393	-1.18398533576519
H	5.60766324635424	0.39631367004233	-1.34966485796084
H	-1.29865468412301	5.03939317706491	-0.72043235340248
H	5.21695615546976	3.05345536397792	-1.41238280158194

Coordinates for: **2**$_{Cl}$ S=3/2

Final Single Point Energy: -2974.39136029273 Eh

Fe	-0.08193051308168	0.08796241651187	-0.11652186290274
N	-0.28721514927662	-1.74895215699230	-0.72752359503837
N	-1.96407106830749	0.22334584388853	-0.59430835234098
N	0.10012387616401	1.97576706457097	-0.55556641626563
N	1.77698802928685	0.00337460846150	-0.68828291956489
Cl	-0.02971010062891	-0.02244937470895	2.17164357604101
N	2.03117345241002	-2.38434745923655	-0.87439456345928
N	-2.22117923286706	2.61723963410605	-0.53659238616302
C	-1.01875059244839	-4.39506462309236	-1.26350188617384
C	-2.05096917939277	-3.40355876611710	-1.17615435201888
C	-3.45813319197792	-3.61132092537102	-1.35018683438128
C	-1.61041032192572	-2.09240941571887	-0.90534267269041
C	-2.52971880916149	-1.01114429498108	-0.83243151829398
C	-4.35568876944974	-2.55565307160420	-1.27907071168756
C	-3.91016651401176	-1.21680390040328	-1.02874796813024
C	-4.72365434717992	-0.03741959240710	-0.96965185744647
C	0.70841885794320	-2.67047903245589	-0.89085119225542
C	0.30546135507312	-4.03584798671241	-1.12993628223004
C	-2.71965249163145	1.36161336336687	-0.61870804529195
C	-4.14530662089089	1.19899588288425	-0.77674757524999
C	-0.89987797158770	2.90652817231186	-0.58463738813434
C	1.41490500834282	2.33752142192985	-0.75797783832052
C	0.81280728606512	4.66265449727777	-0.86575237732030
C	1.84580687977102	3.66961609145546	-0.92020783888148
C	2.52811159471040	-1.12555277707085	-0.85701765376669
C	3.94545178105504	-0.94549846580481	-1.06312971318388
C	3.70488384400851	1.48281602558575	-1.06829139709079
C	2.33416465298430	1.25621347145305	-0.83106343550274
C	3.24426183669197	3.89624597338396	-1.13600603633858
C	4.14168839052112	2.84051482250725	-1.20764507806454
C	-0.50496741250161	4.28943864163155	-0.70883369709225
C	4.51741681272261	0.30495233633569	-1.16110811595354
H	-3.81851250499298	-4.62416638991734	-1.55405403674825
H	-5.42499846095315	-2.73476165299354	-1.42663827236741
H	-1.28674263295716	-5.43818459062655	-1.45721584736944
H	-5.80708460499782	-0.12160900430475	-1.09831385959219
H	3.59743895763270	4.92478273371864	-1.25714064160632
H	1.07429560334275	5.72009516869544	-0.97009914946302
H	-4.75498974650657	2.10544192263806	-0.76110664911592
H	1.09942285878095	-4.78017033182739	-1.22602066816031
H	4.55283310597349	-1.84800319962417	-1.16412172111104
H	5.59400697018720	0.40292048697942	-1.33099707463559
H	-1.30075537410665	5.03787435593261	-0.69772891297957
H	5.20365846427828	3.03525528097811	-1.38545485949032

Coordinates for: **2**$_{Cl}$ S=5/2

Final Single Point Energy: -2974.36606918321 Eh

Fe	-0.07713718002623	0.07715591765391	0.10623311977883
N	-0.26285041234297	-1.75372478247574	-0.74460945904347
N	-1.96636033104119	0.24931283668669	-0.60796906135228
N	0.07523891873879	1.98228487118674	-0.56842662141607
N	1.77843788142114	-0.02111320442127	-0.70452864126172
Cl	-0.02281456831023	-0.02969520540028	2.32177890281003
N	2.04508692889150	-2.40047740198406	-0.88719449021742
N	-2.23570150182590	2.63447163214666	-0.54604472333581
C	-1.01521946834984	-4.38885488802981	-1.26848354319529
C	-2.03461045227846	-3.38360962799721	-1.18832265181257
C	-3.43848123310224	-3.59313167960682	-1.36731221566055
C	-1.58099895362503	-2.07203347121479	-0.91759075719365
C	-2.50588178048388	-0.98447640801514	-0.84373965818484
C	-4.33581254031268	-2.53773400526088	-1.29631426099215
C	-3.88883268623843	-1.20281697570027	-1.04121370954815
C	-4.71738563730419	-0.03441839134517	-0.97485530083095
C	0.72138472453352	-2.68425911040057	-0.90108565018490
C	0.31305200895015	-4.04876122520971	-1.13250194837918
C	-2.73202205106916	1.37733156945905	-0.62598194535858
C	-4.15706058358938	1.20882248555608	-0.77749255835680
C	-0.91326432329938	2.92117089732077	-0.59150289063071
C	1.38505520539794	2.31845881563865	-0.76910227798692
C	0.80882402285075	4.65687281144170	-0.87102538032800
C	1.82877938090611	3.65093362147196	-0.93283265137415
C	2.53988305403081	-1.14041881843622	-0.86690161653679
C	3.95697128948434	-0.95514536340405	-1.06584599076419
C	3.68285277238307	1.47007270112533	-1.08087125931684
C	2.30973812982624	1.23074451681339	-0.84306683118136
C	3.22360911400802	3.87973407321427	-1.15400111445508
C	4.12084009414305	2.82430676309784	-1.22570592582761
C	-0.51281424601022	4.30238733549501	-0.70939481254468
C	4.51077066135226	0.30246613174817	-1.16653040061612
H	-3.79715171352453	-4.60643268606150	-1.57252456348355
H	-5.40534295907634	-2.71507174899415	-1.44524692855931
H	-1.29972776181763	-5.42857385387319	-1.45758585758561
H	-5.79979243530210	-0.13561199429741	-1.10087670310569
H	3.57498639680856	4.90878506413228	-1.27695279945436
H	1.08675629922715	5.71049177857196	-0.97274289106616
H	-4.77810104858601	2.10750676898253	-0.75491615986650
H	1.09812522815086	-4.80348961054148	-1.22140123986104
H	4.57579720394341	-1.85073614713047	-1.15987202609327
H	5.58649605658161	0.41721130597007	-1.33213074869218
H	-1.29939439740012	5.06051031851752	-0.69126951236225
H	5.18290690039686	3.01732758820362	-1.40548392240507

Coordinates for: **2**$_{OH}$ S=1/2

Final Single Point Energy: -2589.98393051017 Eh

Fe	-0.07129704437537	0.08239754704243	-0.15847226402247
N	-0.30153021522960	-1.77319992934137	-0.65948171476255
N	-1.96985257465902	0.18590843205389	-0.51693822063401
N	0.14749258911354	1.99010995866103	-0.44775576801160
N	1.82175446989060	0.02388807792420	-0.59230115783002
O	-0.07535656127446	-0.05424485677905	1.70406686854423
H	-0.78149300300584	-0.67496471729248	1.98159841706674
N	2.03349478314986	-2.36830366805230	-0.86767803050922
N	-2.19257731226794	2.59427718752430	-0.50398614917073
C	-1.00897706069429	-4.41205957009130	-1.26634936348878
C	-2.05440345783118	-3.43550230539672	-1.15253356471320
C	-3.46124378288872	-3.63318290499106	-1.34835116092203
C	-1.62674998122255	-2.13021886821300	-0.84324130497081
C	-2.54900042486364	-1.04736220272725	-0.76422353727338
C	-4.36144257695488	-2.57625578656705	-1.27088483035654
C	-3.92513935664169	-1.23895368466246	-0.99173488920748
C	-4.72522284136779	-0.04840426024164	-0.94673658656164
C	0.71189207788518	-2.67985453002748	-0.86164891500533
C	0.31531526428501	-4.04143899207342	-1.13234137406348
C	-2.71278509391083	1.34161557428422	-0.56746710542814
C	-4.13654016258738	1.18598267558940	-0.74962198021298
C	-0.87303409112104	2.90764162215602	-0.52958250222767
C	1.46353568647550	2.36293624186352	-0.67164537263613
C	0.82803737517560	4.67279524457009	-0.86065018544450
C	1.87593794456643	3.69131291713575	-0.88828615123769
C	2.55357286783225	-1.11628653955311	-0.82486494500130
C	3.96430493816929	-0.93921553315255	-1.07995977178813
C	3.74404542291468	1.49727576924918	-1.04984081952869
C	2.38559083496994	1.27992331629924	-0.75153212360829
C	3.26858822218658	3.91236490414558	-1.14804374685793
C	4.16848532387742	2.85545850923367	-1.22583638475509
C	-0.48850766664357	4.29005700611812	-0.69583930686923
C	4.54217763284098	0.31080740793908	-1.18156981596573
H	-3.82376395333610	-4.63881117877379	-1.58295314485812
H	-5.42678570915576	-2.75680097731240	-1.44467095506568
H	-1.26387271721177	-5.45363068671282	-1.48496873082562
H	-5.80740583045809	-0.11876931352951	-1.09360800679704
H	3.61810914033195	4.93683061791508	-1.30943115001787
H	1.07519920843317	5.72976606935296	-1.00006625191140
H	-4.74359488453134	2.09474663235434	-0.74672827396842
H	1.11173261649395	-4.78043484055001	-1.25063095381385
H	4.56615719548133	-1.84113025588250	-1.21678757278110
H	5.61243548158631	0.40097233841174	-1.39179445059748
H	-1.28843110609115	5.03450362863847	-0.71185946483509
H	5.22172154791144	3.05347448229098	-1.44786861827752

Coordinates for: **2_{OH}** S=3/2

Final Single Point Energy: -2589.98409300420 Eh

Fe	-0.10268394922742	0.08363298492306	-0.11931375157583
N	-0.30833431919718	-1.75510083637562	-0.71354395040349
N	-1.98726228988012	0.22216141240818	-0.58699340526298
N	0.08256350146344	1.97569165962827	-0.53726353277876
N	1.76096446684138	-0.00223288023486	-0.66408122290511
O	-0.06544090253628	-0.01052198877612	1.80640001089633
H	0.52086101400908	-0.73238254498561	2.10582446635425
N	2.01139068594963	-2.39100071042871	-0.85096924002424
N	-2.23966204514137	2.61772560393945	-0.54165239416998
C	-1.04062948795207	-4.39771499897105	-1.25793594462291
C	-2.07232390102290	-3.40547564747829	-1.17460171758304
C	-3.47909513569687	-3.61238150740137	-1.35867325475746
C	-1.63190395196774	-2.09543254849031	-0.89828988684784
C	-2.55062778567698	-1.01249508903616	-0.83064416992852
C	-4.37534517041379	-2.55597497098942	-1.29427522691878
C	-3.92948539398554	-1.21715880366717	-1.04025856879325
C	-4.74171171766853	-0.03668962214484	-0.99102075811713
C	0.68749937194214	-2.67625220124931	-0.87405974533479
C	0.28378053390494	-4.04077824542755	-1.11718389290657
C	-2.73937261320593	1.36133889849727	-0.62408632892266
C	-4.16377605232523	1.19987783542841	-0.79574966203415
C	-0.91659874648206	2.90563675986636	-0.58035567504562
C	1.39922863117076	2.33380316446970	-0.73554800729675
C	0.80038351997029	4.65872070778989	-0.85791121891632
C	1.83278778928220	3.66478758526478	-0.90149114245705
C	2.51035194379662	-1.13187354968731	-0.83116425411455
C	3.92859377159148	-0.95262784648216	-1.03212517552155
C	3.69005698675624	1.47662221518884	-1.03716216724434
C	2.31846678052609	1.25127645128622	-0.80367898037447
C	3.23304454552625	3.89024232963780	-1.11163946191327
C	4.12963171917075	2.83418130544629	-1.17679486508484
C	-0.51916474934797	4.28767055204269	-0.70852764010678
C	4.50151520498670	0.29796797676183	-1.12738323735207
H	-3.83877621686713	-4.62496153049631	-1.56547097573592
H	-5.44386382329125	-2.73325095085773	-1.45025927765031
H	-1.30889226656347	-5.44024292554160	-1.45494291448995
H	-5.82403938346074	-0.11979150428555	-1.13006496093386
H	3.58718037623935	4.91841577116692	-1.23384708046759
H	1.06357513295474	5.71551942034409	-0.96542040077968
H	-4.77330724830801	2.10666425393423	-0.78892645255418
H	1.07662142571472	-4.78670623852771	-1.21106063582628
H	4.53655807895388	-1.85497881301864	-1.13197239272750
H	5.57882890024789	0.39518896116843	-1.29362330784507
H	-1.31371314001324	5.03766063417434	-0.70708611489094
H	5.19269912448022	3.02726003001636	-1.35027281523715

Coordinates for: **2$_{OH}$** S=5/2

Final Single Point Energy: -2589.96106738961 Eh

Fe	-0.09744831981518	0.06974220712615	0.13769168204357
N	-0.28030786557179	-1.76280079840663	-0.72129311298672
N	-1.98798593889996	0.24746701192530	-0.59395541139154
N	0.05873774478846	1.98087891910763	-0.54277539769873
N	1.76573830332025	-0.03006072738959	-0.66942294014942
O	-0.07870301908121	0.00017117677645	1.99591691653635
H	0.46181263729831	-0.71166218015506	2.38681626825315
N	2.02888038875774	-2.40999675397838	-0.86441041008132
N	-2.25344600464112	2.63450722724529	-0.54344871224728
C	-1.03312424572557	-4.38953746677891	-1.28024960495425
C	-2.05168951886347	-3.38352885982599	-1.19902643837855
C	-3.45419942339367	-3.59140145967780	-1.39709517704641
C	-1.59920022916234	-2.07564987719261	-0.90995914118835
C	-2.52388787626498	-0.98657944326308	-0.84092091381111
C	-4.35043052731323	-2.53595395113560	-1.33066822627466
C	-3.90372360169041	-1.20279396158633	-1.06138551054663
C	-4.73163607578891	-0.03340559552467	-1.00542564241025
C	0.70374531219614	-2.69137577847362	-0.88483664423973
C	0.29486628756141	-4.05319097045313	-1.13215512832785
C	-2.74979394299056	1.37621962414507	-0.62702570792000
C	-4.17305092898036	1.20939169116799	-0.79964419394823
C	-0.92890695998820	2.91849353055423	-0.58195251796579
C	1.37048490387112	2.31252583669143	-0.74408255572498
C	0.79640105576893	4.65014982468576	-0.86972241655913
C	1.81567125436314	3.64290724234626	-0.92039358057405
C	2.52427558097945	-1.14901093434509	-0.84048986255857
C	3.94074498630086	-0.96414179522340	-1.04557814724468
C	3.66695836790872	1.46156169931338	-1.05951794630789
C	2.29522922296819	1.22340652848314	-0.81337233111520
C	3.21094879770760	3.87080500528461	-1.14550006788223
C	4.10691254329346	2.81522257150348	-1.21283110284925
C	-0.52639129565287	4.29863175992196	-0.71016939532307
C	4.49413599867925	0.29364991248593	-1.14768390692253
H	-3.81043682588099	-4.60304032469547	-1.61489809111451
H	-5.41828350373933	-2.70975604552296	-1.49575786828873
H	-1.31792628739868	-5.42693016673415	-1.48197293577973
H	-5.81226934317134	-0.13330955700264	-1.14779548901407
H	3.56156673731148	4.89923755944782	-1.27653551780054
H	1.07581461440258	5.70267041512383	-0.97984166563307
H	-4.79391228723116	2.10856403214872	-0.78680296519072
H	1.07900883057776	-4.80864047842317	-1.22451193824577
H	4.55939034184202	-1.85949818064447	-1.14430791932065
H	5.56918722252744	0.40827682839318	-1.31846897328644
H	-1.31194240431946	5.05819956560145	-0.70235605567945
H	5.16875850838751	3.00560569578375	-1.39728463405394

Coordinates for: **3**$_{Cl}$ S=1/2

Final Single Point Energy: -3015.29787247667 Eh

Fe	-0.09267982093589	0.10938174376538	-0.56451524428745
N	-0.30424448058097	-1.72935346995329	-0.82913680752622
N	-1.95480333817344	0.21288654366228	-0.70344517939284
N	0.10989779662143	1.96574767335834	-0.66476835432993
N	1.76107700128672	0.02394821072441	-0.78995000894378
Cl	-0.05641525340738	0.01942376324551	2.01886759927268
O	1.98848715171966	-2.33484820331324	-0.90721357904924
O	-2.18239120185320	2.57118546615953	-0.58065334761128
C	-1.02895285672072	-4.41212421982795	-1.23908899119026
C	-2.06106179603771	-3.43169624493590	-1.13871934834981
C	-3.48573585322104	-3.63909899891047	-1.24264618325416
C	-1.63262817466240	-2.10606796985495	-0.93391719881175
C	-2.54935524665503	-1.02745150228097	-0.86291646696794
C	-4.38119718739240	-2.58588742051391	-1.17171326156846
C	-3.93782791883572	-1.22414001835350	-0.99084522899183
C	-4.74136291823525	-0.04571491425081	-0.94592943548921
C	0.63767758921915	-2.66459965539552	-0.96260270091411
C	0.31140740727598	-4.02513443065690	-1.15857527381832
C	-2.73070067757943	1.29763875049035	-0.69892854816332
C	-4.13638605736281	1.20635782430284	-0.80754626895995
C	-0.83457698369362	2.90735296468924	-0.66301920127988
C	1.43344859486105	2.35359707698952	-0.78719476249669
C	0.82203727743044	4.67716662899609	-0.84057600169831
C	1.85537298219010	3.69379824579297	-0.88067807816754
C	2.53397391393002	-1.05476808590590	-0.92639279924127
C	3.93345882836290	-0.95031766529389	-1.08919799015184
C	3.73225554453010	1.48628142232592	-1.02792152309939
C	2.35048160924244	1.27518199711238	-0.85797154393136
C	3.27461211305986	3.91329256776976	-1.02619394713723
C	4.17002645516544	2.86001367330562	-1.09679350066153
C	-0.51429005674983	4.28131138063722	-0.73910137362698
C	4.53434725203717	0.31057339617792	-1.13267487160879
H	-3.85758913299129	-4.65758563226946	-1.39147704232131
H	-5.45429409384678	-2.77962444095504	-1.26489591227117
H	-1.28133119333822	-5.46450564787370	-1.39558857819601
H	-5.82893600533503	-0.11615591980047	-1.03506644129632
H	3.64169969814232	4.94216346683532	-1.09288389846150
H	1.06983601362669	5.74021448691622	-0.90534445111807
H	-4.73075291072817	2.12245290723392	-0.79025104572174
H	1.11726998901039	-4.75621689881018	-1.25317116710821
H	4.52597932073961	-1.86237843648136	-1.18850609721215
H	5.61692548297523	0.39101339694269	-1.26416448702308
H	-1.32216892054924	5.01617134377308	-0.72681303918245
H	5.23828927501485	3.06417165841493	-1.21880133293794

Coordinates for: **3**$_{Cl}$ S=3/2

Final Single Point Energy: -3015.27440453571 Eh

Fe	-0.07175714030306	0.06201480161196	0.43328926695719
N	-0.27644180534205	-1.78772917655592	-0.41067100802784
N	-1.98180042310688	0.21868353052397	-0.27881131647446
N	0.10018580103392	1.98594472920569	-0.23783642634150
N	1.80585997119977	-0.02010498568809	-0.36991831330011
Cl	-0.02584196405905	-0.04921426164811	2.72813534265023
O	2.00989081234486	-2.36850670659719	-0.50265089074710
O	-2.18713727454567	2.56824020516728	-0.17709340206345
C	-0.96655333547587	-4.31782162265143	-1.39917889791258
C	-1.98980586924057	-3.35097425891347	-1.21842873750089
C	-3.38427229510281	-3.52892145376965	-1.53705636984218
C	-1.58327430761372	-2.07850534726908	-0.73696444697811
C	-2.50279975078620	-0.99711022197807	-0.66486635288661
C	-4.27700414981620	-2.47975773081880	-1.46578168245195
C	-3.85388283182353	-1.15981940035097	-1.07029050669706
C	-4.65143375760038	0.01367831466181	-1.10608305035064
C	0.66530863539553	-2.68033476132309	-0.69976252921283
C	0.37138738084449	-3.97354217151144	-1.16944180110565
C	-2.72654405254737	1.30856102262512	-0.43405838715680
C	-4.07947754968455	1.25891391498508	-0.81722122696611
C	-0.85125930614454	2.90001074556378	-0.39931955697693
C	1.39235288782906	2.30932037600289	-0.59072482183530
C	0.75229429369046	4.60042789422223	-1.00830136244961
C	1.78030202468656	3.62275757742373	-0.96578162777468
C	2.54010790782395	-1.08887597307925	-0.66269482419814
C	3.87441067511347	-1.00052981120404	-1.09993700997231
C	3.64393880855508	1.43086459470023	-1.10998238646874
C	2.31190041380052	1.22781402566824	-0.66201208595297
C	3.15982495829092	3.83292148750035	-1.32700109921883
C	4.05224465349586	2.78335277777761	-1.39585765535559
C	-0.57510324146616	4.23305509200517	-0.75477531436416
C	4.43619752117475	0.26762660313136	-1.29346166843776
H	-3.72229122187285	-4.51435386931837	-1.87286668000821
H	-5.32450850359273	-2.63160876005139	-1.74461320844399
H	-1.21743189964228	-5.31826879747238	-1.76331846457264
H	-5.70174083126754	-0.04790145425370	-1.40526768495634
H	3.48554211019125	4.84654074418213	-1.58096460198602
H	0.98943864063741	5.63177465624430	-1.28485140970224
H	-4.65384253923040	2.18452617558135	-0.89313282179963
H	1.18426225236876	-4.67852217173081	-1.35574646925914
H	4.44206502452730	-1.91374564884070	-1.29041690825301
H	5.47260976054081	0.35893120737477	-1.63106202538222
H	-1.39396334210048	4.95070679496978	-0.83772829403104
H	5.08692207637616	2.96313812788113	-1.70441419648998

Coordinates for: **3**$_{Cl}$ S=5/2

Final Single Point Energy: -3015.26470215455 Eh

Fe	-0.07587970313190	0.06855229020392	0.29090065688776
N	-0.26488418614986	-1.75188856914979	-0.67127341837903
N	-1.96218474871925	0.24408275592591	-0.53879829068301
N	0.07825970382676	1.97612252967629	-0.49272984769681
N	1.77590911830761	-0.02061276465359	-0.62426663999885
Cl	-0.03524192215693	-0.04257498846586	2.52162400021648
O	2.01435853631014	-2.36726123988474	-0.78015594078968
O	-2.20309185531940	2.59343882779263	-0.45083677611376
C	-1.00556277268739	-4.37296783637935	-1.31284285618780
C	-2.02209534903216	-3.38515743062651	-1.19612241528619
C	-3.43556009340652	-3.58389446292065	-1.39541000210533
C	-1.59010331500043	-2.07229388298380	-0.87979654473431
C	-2.50705685352604	-0.99412387646667	-0.80798468269747
C	-4.32980160317004	-2.53239390174905	-1.32514145800589
C	-3.89071197399846	-1.18770119374624	-1.04941373385117
C	-4.70504222782874	-0.02202594054116	-1.02257530975230
C	0.66184373185126	-2.68099663891409	-0.86154368051379
C	0.34387283842919	-4.02316975980436	-1.15978292046210
C	-2.73793058021694	1.31754903015501	-0.59552236477344
C	-4.13086325503972	1.23943611502094	-0.80927383894731
C	-0.85422232218300	2.91629314475527	-0.55777426165920
C	1.39412636472297	2.31708659468144	-0.72751926083075
C	0.79515211710573	4.64674150396869	-0.91997206442492
C	1.81399280292346	3.65477127952613	-0.93928518212996
C	2.54516854120812	-1.08227148140932	-0.82324289941595
C	3.92658923076412	-0.98132983712034	-1.09295924104928
C	3.68226571720248	1.45714203888551	-1.08516579976178
C	2.31082096865949	1.23871284480067	-0.79894815842797
C	3.21738003054013	3.87444206611943	-1.18259364706204
C	4.11136685033734	2.82275716756780	-1.25242462563864
C	-0.54716605534865	4.28124677754490	-0.74328692340836
C	4.49395308619645	0.29597549273591	-1.20901732089612
H	-3.79663893326222	-4.59265416574768	-1.61985039288846
H	-5.39646482883521	-2.71160037808242	-1.49384356844217
H	-1.27402402162950	-5.40570955655945	-1.55403967657175
H	-5.78137928751131	-0.10494288778333	-1.19989048427861
H	3.57017004064604	4.90046709988947	-1.32795393387436
H	1.05497157297914	5.69791059646439	-1.07589844090843
H	-4.72940155419282	2.15237973600274	-0.82989324424160
H	1.14376411859295	-4.75490535014138	-1.28996089584734
H	4.52055988843414	-1.88698865463121	-1.23138976007882
H	5.56106564600255	0.39730572846452	-1.42776161451762
H	-1.35089070127543	5.01970903466360	-0.77226958344513
H	5.16948645613784	3.01899895689981	-1.45303587062472

Coordinates for: **3$_{OH}$** S=1/2

Final Single Point Energy: -2630.87953311391 Eh

Fe	-0.09336740607587	0.07979501216674	-0.34309195989629
N	-0.30745211446162	-1.74339766255521	-0.71316159943383
N	-1.96032054802553	0.19183125386262	-0.55458627992287
N	0.10705639715837	1.94434118339443	-0.50392833350470
N	1.74980324925536	0.00074683848916	-0.66401624971582
O	0.03455734540978	-0.12902567962886	1.74607194550890
H	0.64655226723855	-0.88233756721858	1.83073668900192
O	1.98343189306986	-2.35750348470039	-0.79205161486461
O	-2.18619053158221	2.55142071187599	-0.44697896436689
C	-1.03238508267228	-4.40956222999534	-1.27970122757756
C	-2.05955547471837	-3.43335985643411	-1.15188343220651
C	-3.48020263691241	-3.63022073473910	-1.31642710756095
C	-1.63648749030144	-2.11753667708667	-0.86512098716327
C	-2.55172527250815	-1.04253645491585	-0.78505994384233
C	-4.37427256442979	-2.57713265894809	-1.24465033744457
C	-3.93416259530706	-1.22488288292030	-0.99727251541515
C	-4.73265018460890	-0.04574485070385	-0.97699562032125
C	0.63160951716723	-2.68065047662523	-0.88659273345233
C	0.30909917023041	-4.02482718019682	-1.15743155229484
C	-2.73324658331855	1.28192221280612	-0.60115318584704
C	-4.12816012619794	1.20270416201313	-0.79402660789305
C	-0.84056811711445	2.88637032740195	-0.55539442021634
C	1.42725319161509	2.33059224694412	-0.68970789916061
C	0.80534482247490	4.64922252755237	-0.84620783793437
C	1.83838746191822	3.66894367704846	-0.86075180042931
C	2.52533981998397	-1.07495994357994	-0.84231023187384
C	3.91077517105241	-0.97104336913052	-1.07433426306487
C	3.71433854661181	1.46174041923321	-1.01684562373340
C	2.34002225915806	1.25359172766113	-0.77075322856054
C	3.25032376045692	3.88701105761170	-1.06640250779503
C	4.14475369613851	2.83429983277721	-1.13888146910295
C	-0.52954059545846	4.25348496312821	-0.70867081122617
C	4.51259794105423	0.29170991121969	-1.15135588252929
H	-3.84756074822879	-4.64047882641855	-1.52236890054867
H	-5.44274113189644	-2.76082000532209	-1.39480223757286
H	-1.28258238516529	-5.45171680048993	-1.49619190752271
H	-5.81342400511659	-0.10873489143667	-1.13116830352533
H	3.60980479749291	4.91399922308495	-1.18461333532356
H	1.04811996831963	5.70817190553967	-0.97069932857562
H	-4.71458752506586	2.12385644284528	-0.80993698627970
H	1.11812422463742	-4.74843842319793	-1.27930847195567
H	4.49524782678696	-1.88472304537591	-1.20291807554266
H	5.58700614558444	0.37240411766986	-1.33776225460063
H	-1.34200588978262	4.98292018254296	-0.73138033901080
H	5.20637953613361	3.03577276475098	-1.31315526570199

Coordinates for: **3$_{OH}$** S=3/2

Final Single Point Energy: -2630.87095480741 Eh

Fe	-0.05921473312799	0.03780274558603	0.63431616916748
N	-0.24233990417402	-1.76124599169100	-0.41191127958961
N	-1.93689142951791	0.22792156964226	-0.26425732592820
N	0.09435376391525	1.95095660730190	-0.20459048562051
N	1.78782968360670	-0.03820349458576	-0.35044648878123
O	0.00351366828280	-0.06049131243927	2.52445176065481
H	-0.58167662821335	-0.76809094473591	2.85127412065481
O	2.02295171057000	-2.37754351813738	-0.31579172949681
O	-2.16740057923033	2.54553498923849	0.04502782666318
C	-0.91285221081751	-4.28753248383456	-1.43854080181131
C	-1.92831952930059	-3.30742292897021	-1.30980006407060
C	-3.31319273877094	-3.46816911738872	-1.67973856030114
C	-1.52770500442309	-2.04088370814802	-0.80229439980986
C	-2.44819939604258	-0.95993610564428	-0.72264062583164
C	-4.20552674139342	-2.41972386679072	-1.60334888293285
C	-3.79589302980601	-1.11323579797047	-1.14942631934703
C	-4.60482645642307	0.05000527934518	-1.12146161003998
C	0.69246078474341	-2.67870003791052	-0.62590953757762
C	0.41426155303459	-3.96461660440480	-1.12260671593526
C	-2.70258296967301	1.30937575724229	-0.33358930624659
C	-4.04882795923666	1.27890404942004	-0.73933406039755
C	-0.85074726138256	2.87933937799590	-0.28943909147394
C	1.35726848613050	2.27202721281924	-0.63338315241435
C	0.71221070180708	4.56609504589871	-1.02320116150343
C	1.73181425626893	3.58168453089899	-1.04056318209491
C	2.54194612157892	-1.10590896464408	-0.58113664939582
C	3.86358788840643	-1.03101476302027	-1.05732818399763
C	3.59859581743214	1.38932786979667	-1.20034777101965
C	2.27803113159931	1.19059223588718	-0.71237597199660
C	3.09406232595575	3.78280833932953	-1.46928879845902
C	3.98656283499685	2.73464370275555	-1.54556728247512
C	-0.59669337966282	4.20822256935872	-0.67494171702604
C	4.40314979701711	0.23065369964637	-1.33921059101978
H	-3.64575547924290	-4.44429328594746	-2.04712969421576
H	-5.24644701642863	-2.56352282951342	-1.91026324511288
H	-1.15723097030531	-5.28358411548825	-1.81927071476122
H	-5.65203386244622	-0.00270757384448	-1.43352489581081
H	3.40751590327866	4.79102745518999	-1.75826506707934
H	0.93784582545479	5.59464759186145	-1.31962432762109
H	-4.62977325025336	2.20325815183291	-0.76207144087481
H	1.22786371769464	-4.67898745160431	-1.26490148747017
H	4.43608458255025	-1.94783004752797	-1.21295209776027
H	5.43112950115083	0.31689659151440	-1.70336530136400
H	-1.41728279689078	4.92781087521030	-0.71112534512207
H	5.00894648653511	2.91012925529976	-1.89520584455671

Coordinates for: **3$_{OH}$** S=5/2

Final Single Point Energy: -2630.85624833810 Eh

Fe	-0.09465150564103	0.05544485636537	0.31540224523985
N	-0.27928232355726	-1.75697789528224	-0.67546555237109
N	-1.97621548484579	0.24104436175039	-0.54366160745551
N	0.06576376109508	1.97101636472156	-0.46939257834648
N	1.76360091659468	-0.02929697259136	-0.60169465473639
O	-0.11946698541954	0.00248206161287	2.19227181227992
H	0.43845347885965	-0.71704770564937	2.54089818438842
O	1.99954947486311	-2.37589337993836	-0.77365955859404
O	-2.21609641827047	2.58990700921231	-0.44885214986911
C	-1.02189721503677	-4.37653694938244	-1.32604466232882
C	-2.03692352248327	-3.38797564593744	-1.21008573123498
C	-3.45039871984372	-3.58493978241214	-1.41371905354148
C	-1.60430835000216	-2.07533780798521	-0.89018492807587
C	-2.52059761047334	-0.99599438175756	-0.81996530886414
C	-4.34352433189600	-2.53265572137318	-1.34622493248101
C	-3.90414601128073	-1.18814534910145	-1.06837968389678
C	-4.71733609358011	-0.02245726701607	-1.04590040686615
C	0.64600657384978	-2.68785651809175	-0.86438895730378
C	0.32821973309781	-4.02835550611666	-1.16810109975376
C	-2.75147504547304	1.31416685918886	-0.60378900988630
C	-4.14268119308539	1.23871247632366	-0.82808518333571
C	-0.86518548442001	2.91123313148419	-0.55097994990863
C	1.38270499779105	2.30987639434314	-0.70350104360279
C	0.78633679658080	4.63947687870411	-0.91390184116003
C	1.80406784890075	3.64735113589111	-0.92048678203721
C	2.53171035990294	-1.08988197015455	-0.81157018075108
C	3.91195241763148	-0.98983694442532	-1.08514554684254
C	3.67116486534070	1.44849570093589	-1.06203474089341
C	2.29910289683478	1.23060246893841	-0.77381113844933
C	3.20849703250662	3.86611135639726	-1.15999538746012
C	4.10181003926668	2.81415903668812	-1.22736091866519
C	-0.55777370652109	4.27456620543699	-0.74556461069930
C	4.48134425975096	0.28798895328102	-1.19361337474755
H	-3.81201942726797	-4.59331298964306	-1.63946891913218
H	-5.40988460731688	-2.71075250756593	-1.51858077245682
H	-1.29100672049036	-5.40848472415857	-1.57020025456971
H	-5.79277146725586	-0.10409900466849	-1.22959169657544
H	3.56193923784395	4.89190380531597	-1.30606678845162
H	1.04743124141365	5.68961292308346	-1.07501018137896
H	-4.74029715467061	2.15226294922939	-0.85178111684194
H	1.12755888630394	-4.76089141203226	-1.29773399820510
H	4.50420468013164	-1.89539851440158	-1.23190134137725
H	5.54809023168504	0.38958807789308	-1.41432881018363
H	-1.36144151697716	5.01260216428389	-0.78688304706153
H	5.16044438081048	3.00954433743393	-1.42656607271838

Coordinates for: $\mathbf{3}_{Cl}^{2+}$ S=1/2

Final Single Point Energy: -3014.97814994636 Eh

Fe	-0.05267629854250	0.07046421703062	-0.20322667973894
N	-0.29761082878922	-1.79797353983623	-0.67826489758169
N	-1.97220122322103	0.17372823976491	-0.49722500266923
N	0.16196904184842	1.98531342746187	-0.46746401921102
N	1.83704634613665	0.01334656062242	-0.65383943886785
Cl	0.02703997136843	-0.06463333455100	1.96084972714247
O	2.00105232399808	-2.34079599295865	-0.88431605188027
O	-2.14355195433944	2.53725205982038	-0.42671996468565
C	-0.99365893193408	-4.38250954729743	-1.43142910953650
C	-2.04017787520669	-3.42372640776161	-1.25261860367539
C	-3.45067516755702	-3.60827113206846	-1.47483472486757
C	-1.62504053870450	-2.13789773620474	-0.87023999150409
C	-2.54382273017943	-1.05613660067104	-0.77040855253527
C	-4.34579049344843	-2.55484839201254	-1.37656068416470
C	-3.91035142184199	-1.22253951033134	-1.04751533726061
C	-4.69466333518947	-0.02637995104659	-1.02418387186536
C	0.66563326523402	-2.68607626783879	-0.93704388260041
C	0.34119899689875	-4.01865322320757	-1.29208893593100
C	-2.70853349352232	1.28551565547584	-0.56589096594692
C	-4.10353363890202	1.21253651766028	-0.80205724561731
C	-0.81493472122878	2.89262686220294	-0.54402235122062
C	1.47147107913562	2.35160597451831	-0.72346670868979
C	0.80705759152243	4.64308701078438	-0.96853990429300
C	1.86027407607625	3.67517972184060	-0.98634338229881
C	2.55910591227245	-1.07872418225380	-0.91766603868080
C	3.93009074654126	-0.97176649681445	-1.25811675125511
C	3.73002669034642	1.47421845051119	-1.19378895826869
C	2.39031471086454	1.26996011215787	-0.82578770907178
C	3.24875048842342	3.89132579992956	-1.29988756702442
C	4.14365579919538	2.83790090088300	-1.39911237412059
C	-0.51392504941003	4.25917993504974	-0.76565965290235
C	4.50703911203680	0.28756430748913	-1.37937847665131
H	-3.81026658924128	-4.60153699168258	-1.75666037226059
H	-5.40653864969136	-2.72319315406443	-1.58088504242569
H	-1.24123237075314	-5.40820782724606	-1.71746514831771
H	-5.76928739175918	-0.07890852340736	-1.21808554704100
H	3.58894546816647	4.91224325631973	-1.49274234507832
H	1.03551932118069	5.69612401181863	-1.15279087867059
H	-4.68471399783856	2.13584996237769	-0.82578225583326
H	1.14931172788820	-4.72995585502547	-1.47078004384182
H	4.50171294990486	-1.88293725904161	-1.44218316306346
H	5.56183648636389	0.36759656333292	-1.65538880281927
H	-1.33074014888506	4.98218323501817	-0.79615492882601
H	5.18479174478250	3.03385614325156	-1.66914236434763

Coordinates for: $\mathbf{3}_{Cl}^{2+}$ S=3/2

Final Single Point Energy: -3014.99338956455 Eh

Fe	-0.08034476925292	0.08100623088914	0.04282466143154
N	-0.28194580287039	-1.75428367824217	-0.60038846387322
N	-1.96203968414648	0.22222274176528	-0.46948071817538
N	0.09769147038249	1.97106673778910	-0.42580379941473
N	1.77779762015501	-0.00577535689014	-0.55931429563822
Cl	-0.03445948998235	-0.02686721110613	2.23162350286659
O	1.99923389081418	-2.35250835156838	-0.66078871418997
O	-2.18319279512357	2.56711033269624	-0.33312569017174
C	-0.98353075630354	-4.35556728718382	-1.31213707416591
C	-2.01634946965198	-3.37582365856986	-1.20174216339328
C	-3.41975254312816	-3.56752789867897	-1.45155956834276
C	-1.59760310219227	-2.08157567462813	-0.84130801545537
C	-2.51453752573282	-1.00272808241160	-0.77036262088289
C	-4.31414293881875	-2.51511839221364	-1.38283204712272
C	-3.88023633737992	-1.18286273522186	-1.05787097047462
C	-4.68325628831472	-0.00261098283719	-1.02645868623981
C	0.66686569814115	-2.66800796529405	-0.78412673025479
C	0.34562373381100	-4.00515629150471	-1.11797516975605
C	-2.71871819757458	1.31474555686543	-0.52018390732974
C	-4.10901805752049	1.23545715410980	-0.77243821710343
C	-0.85656879358062	2.89584465996986	-0.48149113509733
C	1.40233884976252	2.32247184294042	-0.69155480568272
C	0.77256127645030	4.62930360072778	-0.91925923708440
C	1.80741158790704	3.64585668837558	-0.94629205082979
C	2.52874016478779	-1.08682777520121	-0.74976112970844
C	3.90653891821791	-0.98115201422447	-1.05501605765092
C	3.67101918275976	1.45298905211625	-1.09483734136817
C	2.31912153089915	1.24359108854410	-0.76491234977479
C	3.19878474106772	3.86335639745265	-1.23885676728530
C	4.09307090468773	2.81104502789877	-1.31009347024095
C	-0.54752196613777	4.25934802991133	-0.70108154516393
C	4.47154758372367	0.27674866910060	-1.21452569825612
H	-3.77066935716676	-4.56783230690389	-1.71866542329348
H	-5.37344198675749	-2.68204224696091	-1.59519020087412
H	-1.23660834697113	-5.38442367269705	-1.58115009069144
H	-5.75476116683948	-0.06846592368163	-1.23265123887822
H	3.53975453422243	4.88505848995311	-1.42558570154856
H	1.01577648814326	5.67936865893496	-1.10116452010147
H	-4.69455625443282	2.15612767365714	-0.78284941190371
H	1.15578129151351	-4.72641215485442	-1.23685491048608
H	4.48834707647180	-1.89550100181017	-1.18175490638431
H	5.53281999511136	0.36399865416396	-1.46174145967026
H	-1.36092064492295	4.98648755150773	-0.71752930740611
H	5.14222895332819	2.99952263729916	-1.55265546723085

Coordinates for: $\mathbf{3}_{Cl}^{2+}$ S=5/2

Final Single Point Energy: -3014.97193380798 Eh

Fe	-0.07596302784320	0.06943011349616	0.27638975102135
N	-0.25502830472892	-1.75849946421747	-0.60960106416862
N	-1.96283614213735	0.25014416229587	-0.47545278177712
N	0.07123868634658	1.97707362366889	-0.42893571892791
N	1.77932131744143	-0.03244643550937	-0.56410778368067
Cl	-0.03532845219684	-0.04166841299179	2.42721052461532
O	2.01533673902126	-2.37075678167160	-0.67460975068867
O	-2.19953334991037	2.58698548373510	-0.34444762944588
C	-0.97851790888528	-4.34627019212854	-1.32284422013926
C	-1.99876322173543	-3.35365323231984	-1.20930243718869
C	-3.39861603952152	-3.54835090606382	-1.46266731034775
C	-1.56726748457642	-2.05991053084951	-0.84583083550749
C	-2.48885368518591	-0.97578274141874	-0.77410010917328
C	-4.29278103816472	-2.49646789441583	-1.39327123980313
C	-3.85643586326157	-1.16853660275973	-1.06464107192920
C	-4.67458246578125	0.00145608735168	-1.03531431796969
C	0.68065937355005	-2.67950960042464	-0.79473878226486
C	0.35451853513506	-4.01458935435677	-1.13113587753772
C	-2.72890849468623	1.33103257758182	-0.52801219342533
C	-4.11825630941296	1.24658459967918	-0.78248059825791
C	-0.87029990021865	2.90884912480957	-0.48871034060316
C	1.37250757186544	2.30187166522905	-0.69376205191842
C	0.76743022911513	4.62122907747506	-0.93086488500424
C	1.78989882347957	3.62470940191530	-0.95429461319656
C	2.53911235435757	-1.10183171164378	-0.75740715955611
C	3.91555304007717	-0.99096568972231	-1.06571139175974
C	3.64723021003099	1.43959411950958	-1.10108172291698
C	2.29403510775579	1.21760542685987	-0.76689826510046
C	3.17720518137065	3.84527785429455	-1.25192412135456
C	4.07122644067986	2.79345125748202	-1.32255306981110
C	-0.55659267941185	4.27023295799108	-0.71304193323009
C	4.46262580444483	0.27374597240869	-1.22322630392103
H	-3.74691764340249	-4.54844844285759	-1.73409410673543
H	-5.35191839717919	-2.66065139748839	-1.60886474195560
H	-1.24821104711397	-5.37061363955644	-1.59325818681071
H	-5.74459333308156	-0.08146954226878	-1.24357184021800
H	3.51497832614484	4.86705430649718	-1.44431961174799
H	1.02705625817543	5.66672191151012	-1.11676790369707
H	-4.71362750368559	2.16090004485991	-0.79540958074627
H	1.15675433943659	-4.74417997318390	-1.25290121470001
H	4.50670902458912	-1.89881996494965	-1.19594349066279
H	5.52195253949185	0.37813553548177	-1.47248108673390
H	-1.36230944812459	5.00577474207061	-0.73342524923485
H	5.11967105529267	2.97921927857941	-1.57051659608635

Coordinates for: $\mathbf{3}_{OH}^{2+}$ S=1/2

Final Single Point Energy: -2630.56235132056 Eh

Fe	-0.08092805577610	0.07249314649874	0.13981561737456
N	-0.29207942080613	-1.80707924557032	-0.39845568072501
N	-1.88730858801468	0.22436724176102	-0.54920400299109
N	0.11310656264840	2.01326324740947	-0.22389811903060
N	1.69907126526173	-0.00204128479174	-0.64257564751704
O	-0.03168047149936	-0.02878242390775	1.92217993917343
H	-0.16637633007359	-0.92305510256675	2.30779491447155
O	1.98405547485887	-2.35740954589949	-0.58131040545873
O	-2.16555108641026	2.56855924903981	-0.26666225405932
C	-0.98040880745395	-4.38095998672193	-1.26555242159430
C	-2.00450952187641	-3.39368307155310	-1.16384169355076
C	-3.39750523496367	-3.56253489985864	-1.47906800070364
C	-1.58647950786884	-2.10956927065830	-0.75918057155852
C	-2.47073214658782	-1.00435976704240	-0.79519865074744
C	-4.27832967925843	-2.49842335452622	-1.43645451083985
C	-3.83301653183828	-1.16991810228505	-1.11184554834608
C	-4.62713602575031	0.01387589867089	-1.09452463151387
C	0.65180959945716	-2.70248141508686	-0.66478430818154
C	0.34574602579799	-4.02641858804372	-1.05805774198192
C	-2.66101100014497	1.31672509701606	-0.53661831927050
C	-4.04969876242301	1.23893813616775	-0.79481344735617
C	-0.83964878755410	2.92499429105878	-0.36878384584089
C	1.39094540369148	2.34446537333945	-0.61371532087297
C	0.76959419077149	4.65276014820213	-0.87842845348031
C	1.79504053895035	3.66062006280782	-0.91443049764126
C	2.47044450033276	-1.08684216844506	-0.76614163832133
C	3.84649366308128	-0.98228948199273	-1.07757913752657
C	3.61718211917401	1.44583332282766	-1.15305481356896
C	2.26959089241414	1.24744491203312	-0.79434671761113
C	3.17312749822795	3.86175927354148	-1.27252517704955
C	4.05192663751586	2.79956491825004	-1.36918966419313
C	-0.54774805706909	4.28166282165003	-0.64828031637198
C	4.41003327540373	0.26791467824687	-1.28438800022682
H	-3.75131210612328	-4.55577378624578	-1.76843628793825
H	-5.33365454638884	-2.64911864688128	-1.67918466527447
H	-1.23170875662474	-5.40212557064347	-1.56366541356277
H	-5.69491148041066	-0.04148637143942	-1.32218207506507
H	3.51693831494162	4.87853571923120	-1.48052938016519
H	1.01232795329940	5.69727869863686	-1.09029915860152
H	-4.63232588454600	2.16145809581535	-0.77361996680985
H	1.16377733287688	-4.73266759774395	-1.21025758779301
H	4.42889440254485	-1.90057338532406	-1.16923549284138
H	5.46680867466644	0.34851033312452	-1.55236792743192
H	-1.36866685501112	4.99882532271328	-0.70077735407618
H	5.09638653380422	2.97376363801567	-1.64142695453156

Coordinates for: $\mathbf{3}_{OH}^{2+}$ S=3/2

Final Single Point Energy: -2630.59402094118 Eh

Fe	-0.09760136627869	0.07047553904741	0.06057449096571
N	-0.29992334734978	-1.76419396737385	-0.58298825373478
N	-1.98051799985179	0.21654327884454	-0.45876570101439
N	0.08259927392686	1.96498683842891	-0.40412323424595
N	1.76395259020104	-0.01576940855530	-0.53009025663795
O	-0.09533293102889	0.01346441716075	1.90400718509213
H	0.48065955983783	-0.65424813160452	2.32814175867798
O	1.98195320311958	-2.36318541829814	-0.63856089529001
O	-2.19897612119918	2.56242040202383	-0.32581931022696
C	-0.99999956113827	-4.35841435865387	-1.32272383073540
C	-2.03190144629625	-3.37855321311356	-1.20989273821441
C	-3.43386861154798	-3.56785486003009	-1.47187378492569
C	-1.61426796782634	-2.08730128261830	-0.83571385044931
C	-2.53078756537234	-1.00667575373814	-0.76779517417518
C	-4.32722031567201	-2.51512647948176	-1.40517449146721
C	-3.89403663516087	-1.18447226168726	-1.07082962240354
C	-4.69611918294434	-0.00390743105043	-1.04600833790933
C	0.64805810171346	-2.67656863611099	-0.77143003817834
C	0.32858618341960	-4.01055462783604	-1.11951635331912
C	-2.73417955499972	1.30877165493471	-0.51778123045293
C	-4.12234705343316	1.23292547953219	-0.78529014420829
C	-0.86943947960171	2.88898974126899	-0.46972191640482
C	1.38789494589520	2.31361595624931	-0.66680844388147
C	0.76129679647892	4.62026633402383	-0.91022305536374
C	1.79489504642094	3.63586585171863	-0.92770879646126
C	2.51314792724880	-1.09605993456991	-0.72571009308667
C	3.89042603087059	-0.99213015399677	-1.03417942591716
C	3.65700297295265	1.44186281781752	-1.06856474609170
C	2.30511239015903	1.23351014919299	-0.73582966924833
C	3.18732184104969	3.85206514651084	-1.21843398461973
C	4.08075449497575	2.79949763979348	-1.28605058518289
C	-0.55983166267614	4.25173262606464	-0.69633076065140
C	4.45653066276813	0.26571440419067	-1.19128116438346
H	-3.78337985532184	-4.56645835430116	-1.74740509836106
H	-5.38497988720904	-2.67947454591016	-1.62746290398086
H	-1.25287108469296	-5.38465243295846	-1.60193570689981
H	-5.76564815612668	-0.06864166948692	-1.26293456723262
H	3.52887621888214	4.87319500355701	-1.40775543720347
H	1.00626088220021	5.66917173734335	-1.09666270617475
H	-4.70643340784150	2.15449023471725	-0.80145391840102
H	1.13861225192283	-4.73140026755838	-1.24194969313514
H	4.47127856857171	-1.90649184363822	-1.16534150022165
H	5.51743557949559	0.35284719085993	-1.44033248502074
H	-1.37271208909510	4.97928534955061	-0.72085333147464
H	5.13029297580106	2.98645779857088	-1.52851752895154

Coordinates for: $\mathbf{3}_{OH}^{2+}$ S=5/2

Final Single Point Energy: -2630.57750142368 Eh

Fe	-0.07903900468980	0.05978560308183	0.35140698013295
N	-0.25888246949695	-1.76200312307704	-0.56944856923257
N	-1.97305124723210	0.24665389867263	-0.43302637114484
N	0.06704917356396	1.96999377077608	-0.38485743655376
N	1.78169091064129	-0.04073531337159	-0.51838917324451
O	-0.06090527508558	0.01670789002108	2.15467348460860
H	0.01294373994182	-0.84149815434609	2.61705245057658
O	2.01293883898354	-2.37814526725968	-0.61989701298606
O	-2.20466870813331	2.58132387199995	-0.28537676435938
C	-0.97489236695226	-4.33614480239456	-1.34359230347577
C	-1.99459260663523	-3.34384297099311	-1.22909719625230
C	-3.38987630820223	-3.53408180909114	-1.51370748593738
C	-1.56826258531749	-2.05756671755684	-0.83336848660522
C	-2.49150145335877	-0.97340015804894	-0.76259375188010
C	-4.28381474175015	-2.48333390843785	-1.44725601193719
C	-3.85228987029222	-1.16067097207132	-1.08921263394347
C	-4.67032054128796	0.00900492392550	-1.06335667204004
C	0.67717952317474	-2.68088047251058	-0.76022027451803
C	0.35513946086744	-4.00951451210965	-1.12573461451217
C	-2.73484238772998	1.32645236230296	-0.49310702685696
C	-4.11852505392999	1.24995087783426	-0.78208928572531
C	-0.87417030662414	2.89947351148786	-0.44927072082837
C	1.36445587675225	2.29189617489361	-0.67176780883670
C	0.75489549663970	4.60752080205386	-0.93741105464845
C	1.77668294191088	3.61118897341282	-0.95982729082678
C	2.53751540141231	-1.10742108995931	-0.72223240115543
C	3.90714985993266	-1.00057489771727	-1.06158487616489
C	3.63380098600283	1.42824842694565	-1.11225258299716
C	2.28797454275524	1.20758200889885	-0.74636568179879
C	3.15926033976456	3.83078806967348	-1.28333033655740
C	4.05288121848099	2.78042286752005	-1.35718974959585
C	-0.56573490968887	4.25817285292526	-0.69882988985337
C	4.44912030288399	0.26357977649536	-1.23993359738305
H	-3.73220524020795	-4.53006932581221	-1.80740873864135
H	-5.33849329381312	-2.64243321646075	-1.68764450588131
H	-1.24186433726055	-5.35480024415099	-1.63748565101202
H	-5.73505738082282	-0.07037549580086	-1.29861389255537
H	3.49121634057509	4.85104205620851	-1.49361541923012
H	1.01156378498920	5.65023812628609	-1.14249955965379
H	-4.71204402404323	2.16544387775227	-0.79960995694715
H	1.15851018170108	-4.73745559597843	-1.25013720799577
H	4.49644731377471	-1.90870665244098	-1.19836029364141
H	5.50309334050467	0.36792079634196	-1.51122298859677
H	-1.37262374722508	4.99242928407113	-0.72136653182908
H	5.09672149977383	2.96385445483817	-1.62594243868563