

Supporting Information

Electronic and Steric Effects on Oxygen Reactivities of NiFeSe Complexes Related to O₂-Damaged [NiFeSe]-Hydrogenases' Active Site

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I. Mass Spectra of three NiFeSe complexes (before and after O₂ reaction)

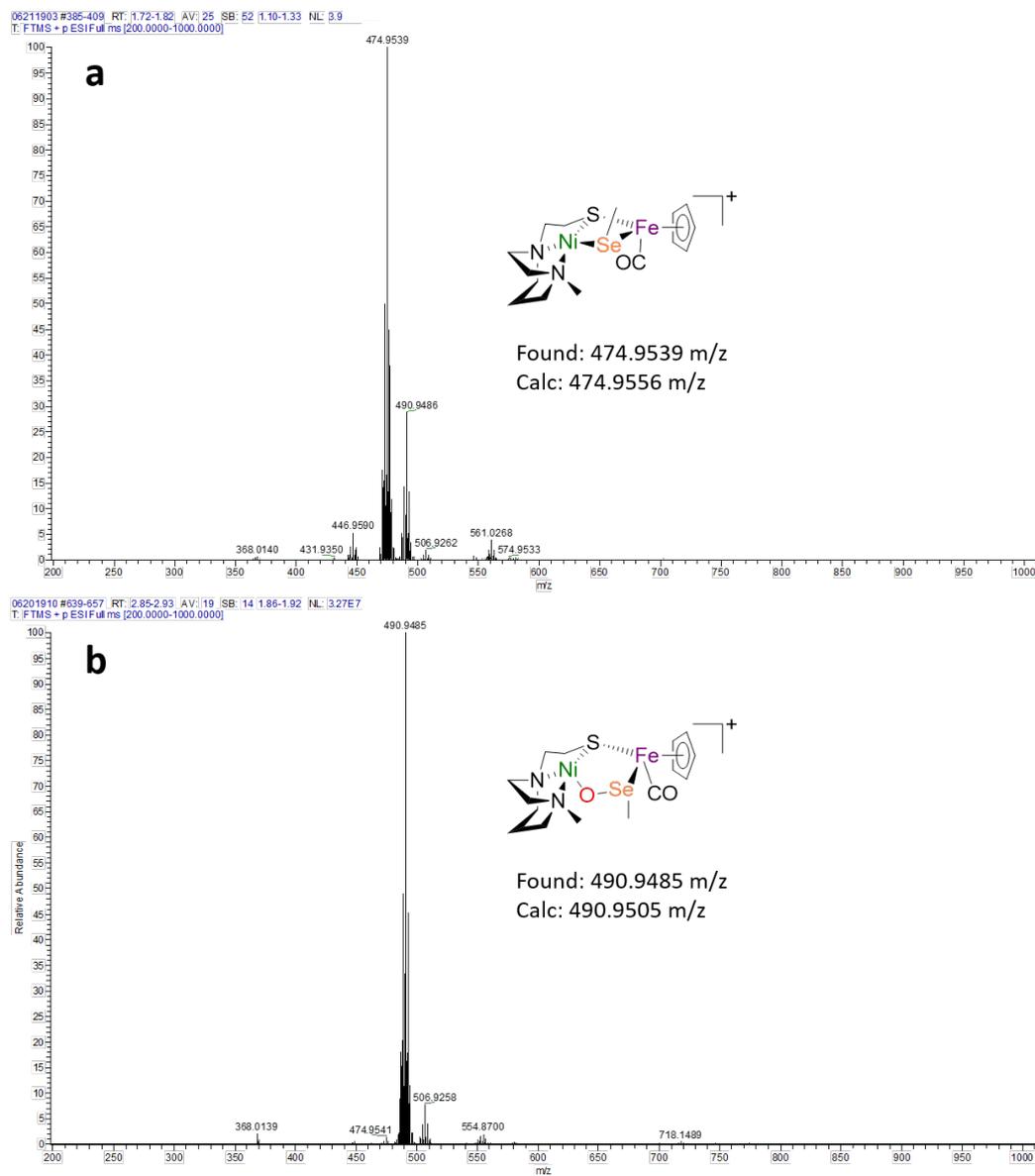


Figure S1. The high resolution ⁺ESI-MS of NiSe(CH₃)FeCp (a) and its 1-O uptake species (b).

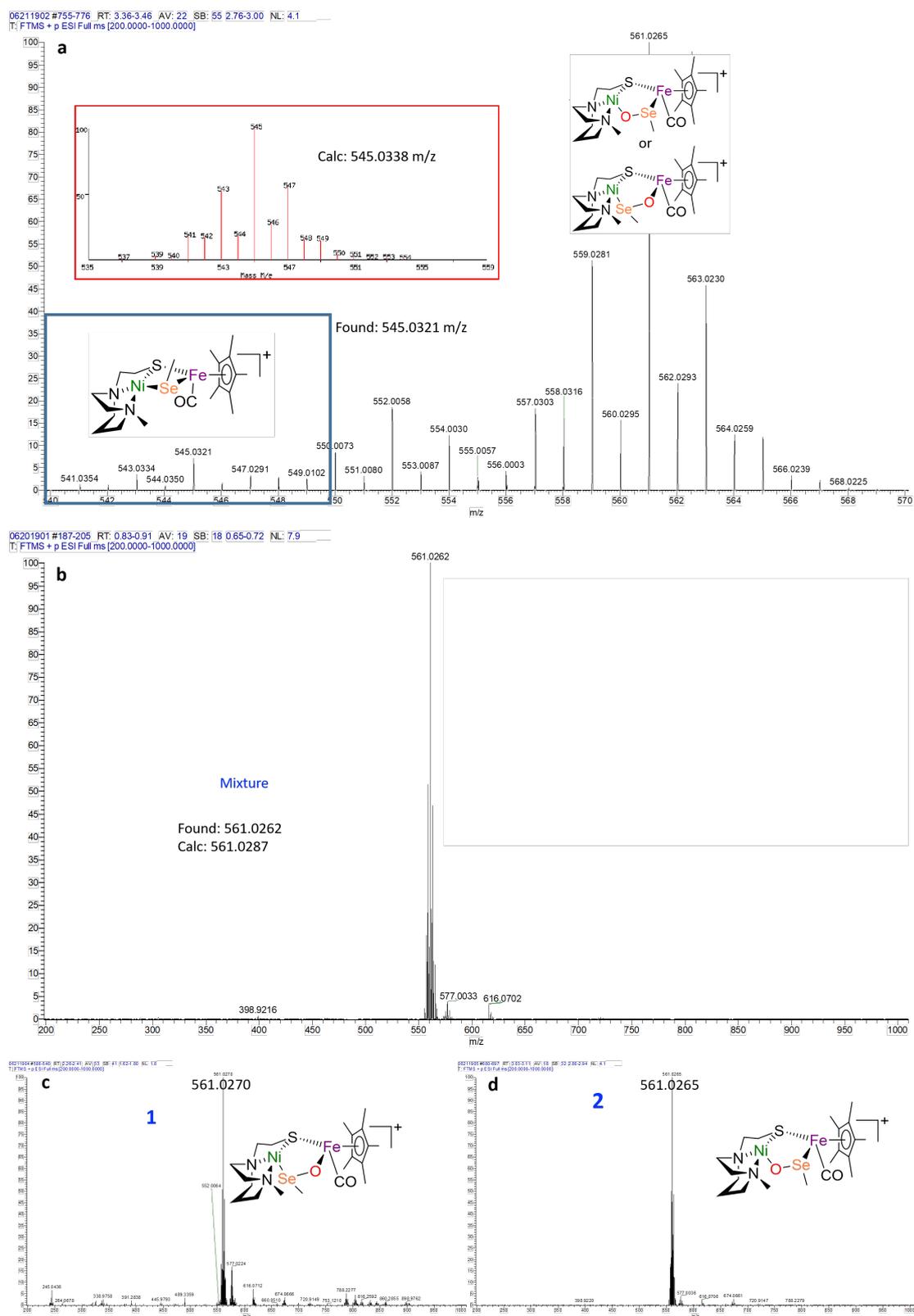


Figure S2. The high resolution of $^+$ ESI-MS of $\text{NiSe}(\text{CH}_3)\text{FeCp}^*$ (a) and its 1-O uptake species: the mixture (b), portion 1 (c), portion 2 (d),.

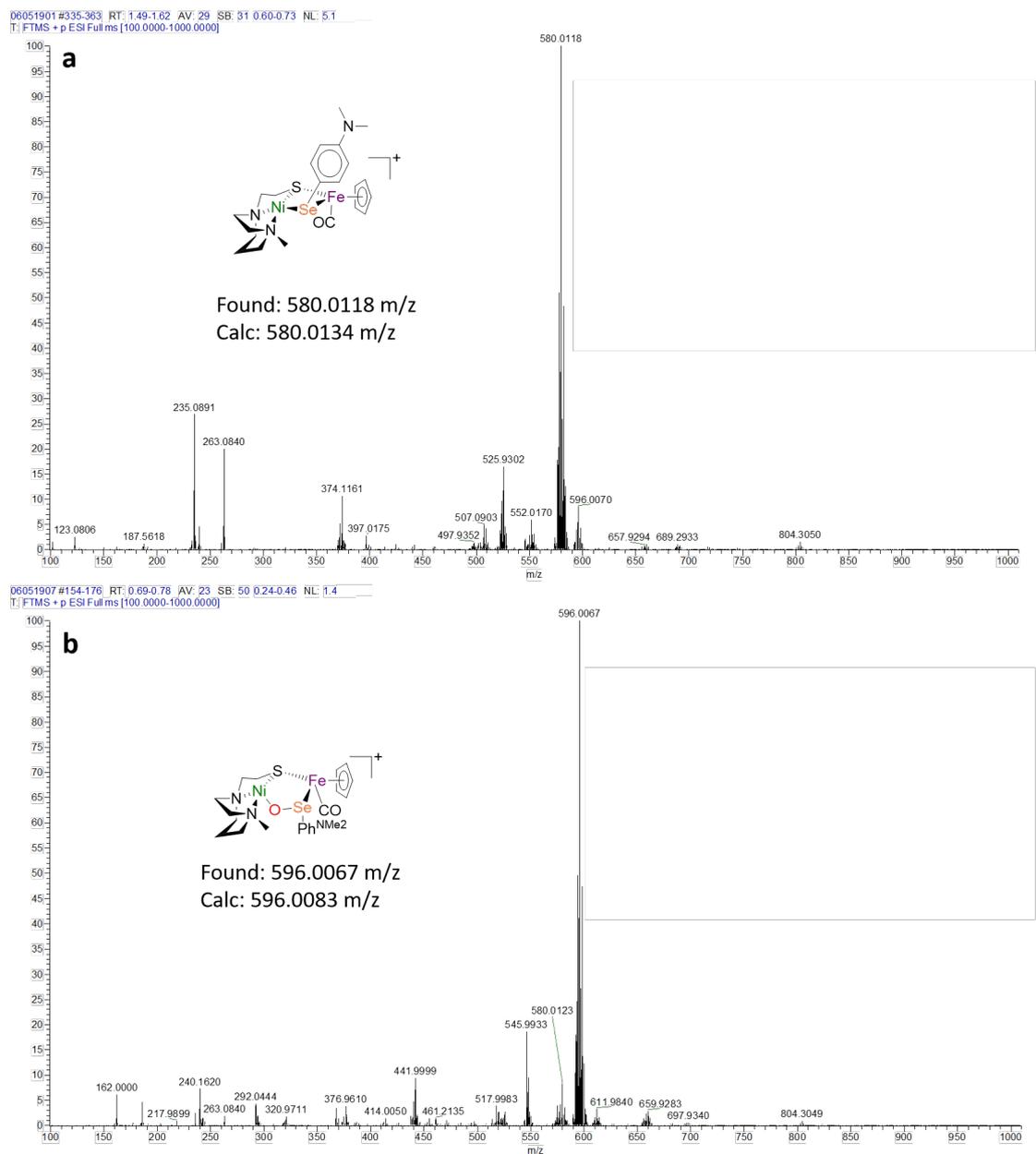
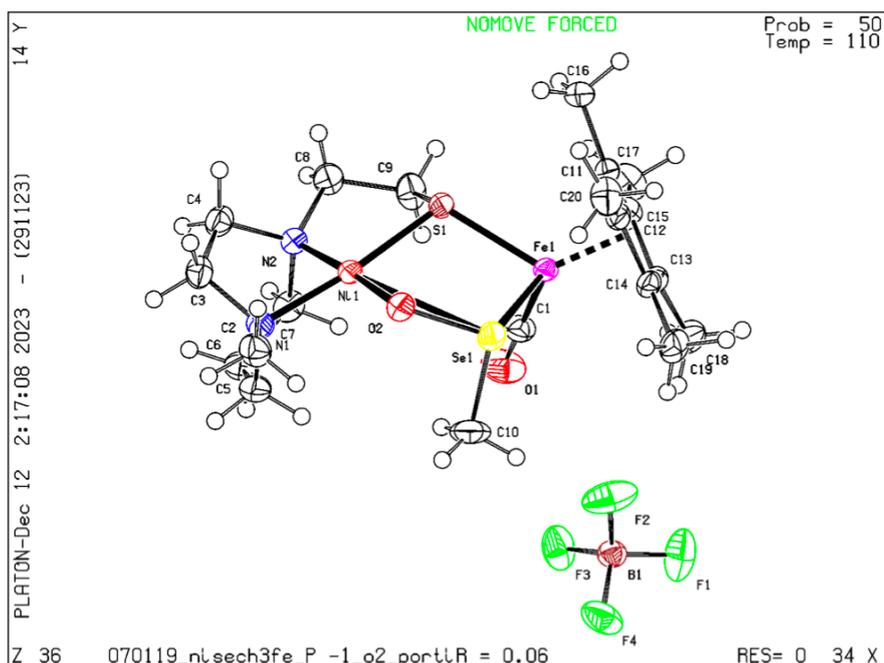


Figure S3. The high resolution ⁺ESI-MS of NiSe(Ph^{NMe2})FeCp (a) and its 1-O uptake species (b).

II. Crystal structure



Bond precision: C-C = 0.0063 Å

Wavelength=1.54184

Cell: a=10.9842 (6) b=11.3750 (3) c=11.6936 (6)
 alpha=74.651 (3) beta=63.420 (5) gamma=87.908 (3)
 Temperature: 110 K

	Calculated	Reported
Volume	1254.34 (12)	1254.34 (11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H35 Fe N2 Ni O2 S Se, B F4	C20 H35 Fe N2 Ni O2 S Se, B F4
Sum formula	C20 H35 B F4 Fe N2 Ni O2 S Se	C20 H35 B F4 Fe N2 Ni O2 S Se
Mr	647.87	647.89
Dx, g cm ⁻³	1.715	1.715
Z	2	2
Mu (mm ⁻¹)	8.457	8.457
F000	660.0	660.0
F000'	652.42	
h, k, lmax	13, 14, 14	13, 14, 14
Nref	5396	5246
Tmin, Tmax	0.919, 0.919	0.332, 1.000
Tmin'	0.919	

Correction method= # Reported T Limits: Tmin=0.332 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.972

Theta(max)= 78.335

R(reflections)= 0.0580 (5068)

wR2(reflections)=
0.1681 (5246)

S = 1.044

Npar= 305