Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

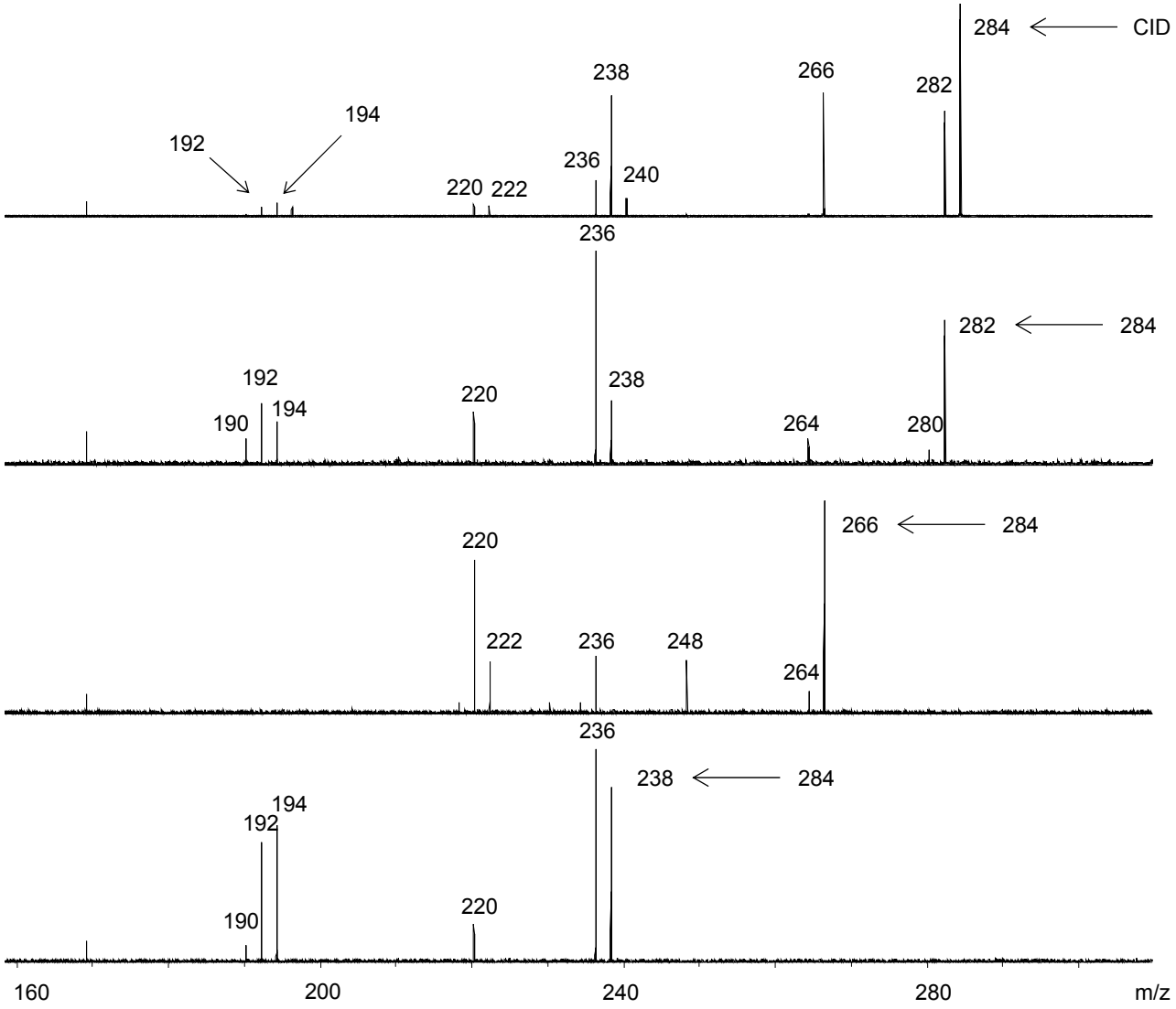




**Figure S1.** SORI/CID MS/MS spectra of $[Mn(Pro-H)(Pro)]^+$

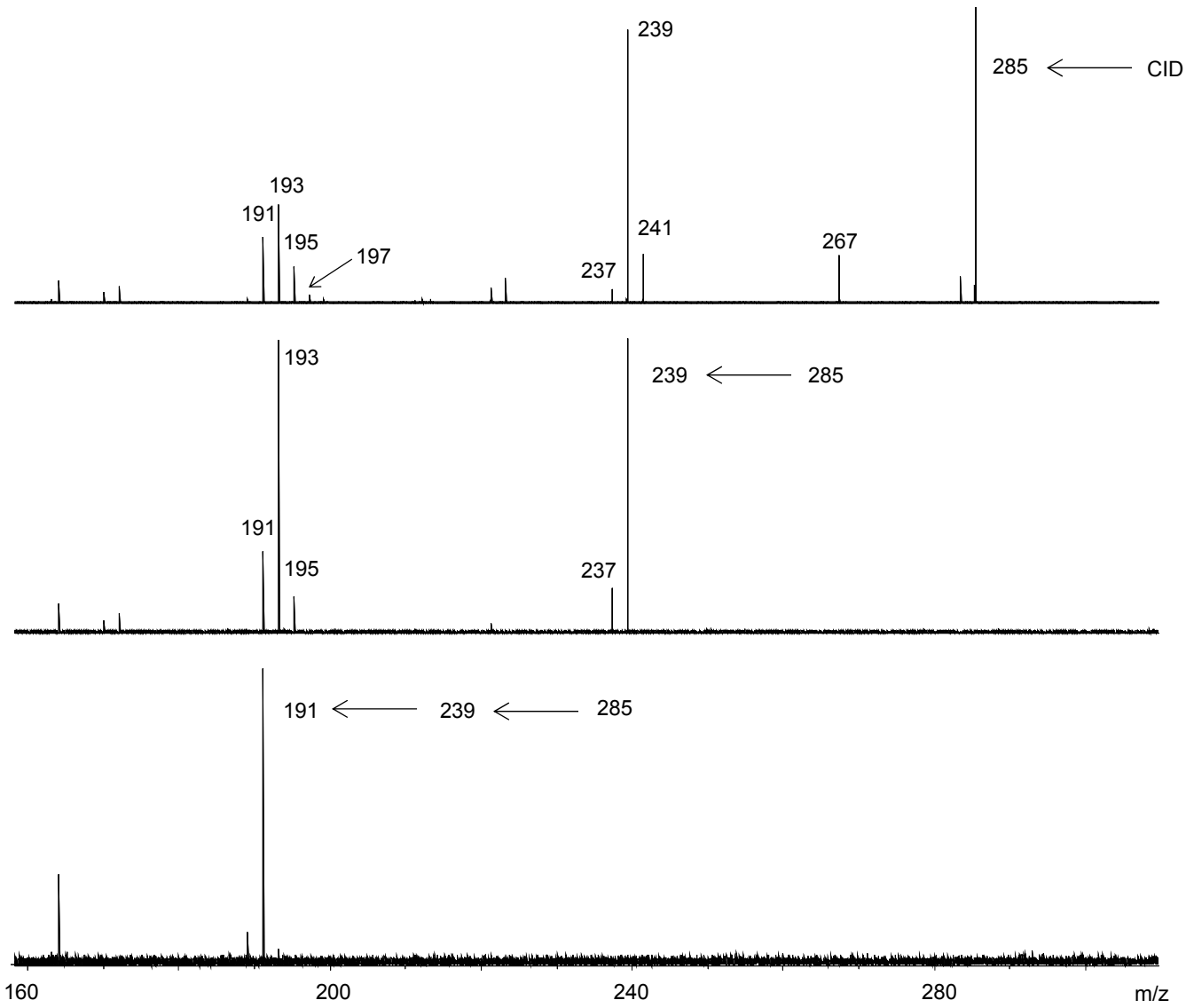



**Figure S2.** SORI/CID MS/MS spectra of $[Fe(Pro\text{-}H)(Pro)]^+$

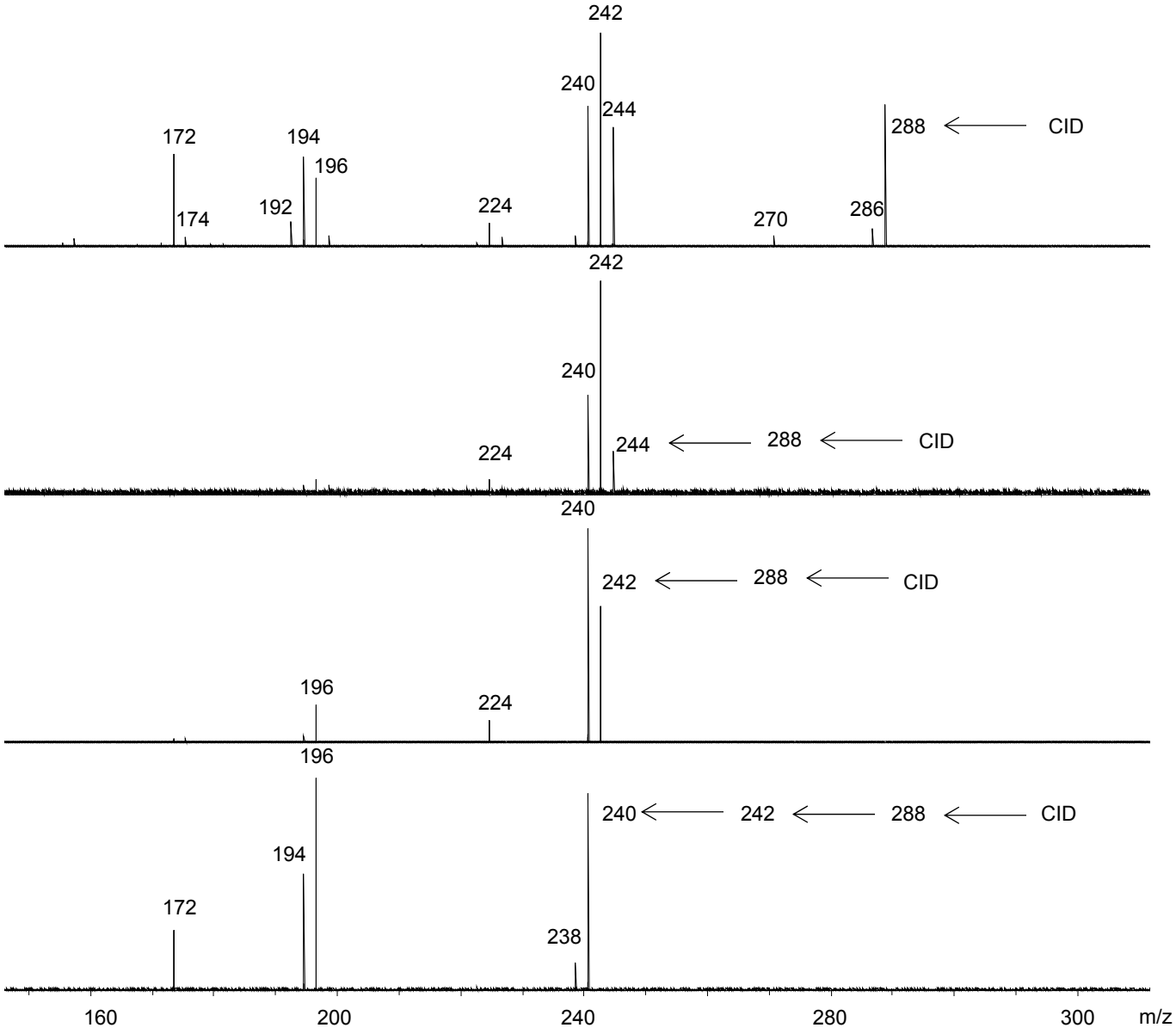



**Figure S3.** SORI/CID MS/MS spectra of $[Co(Pro\text{-}H)(Pro)]^+$

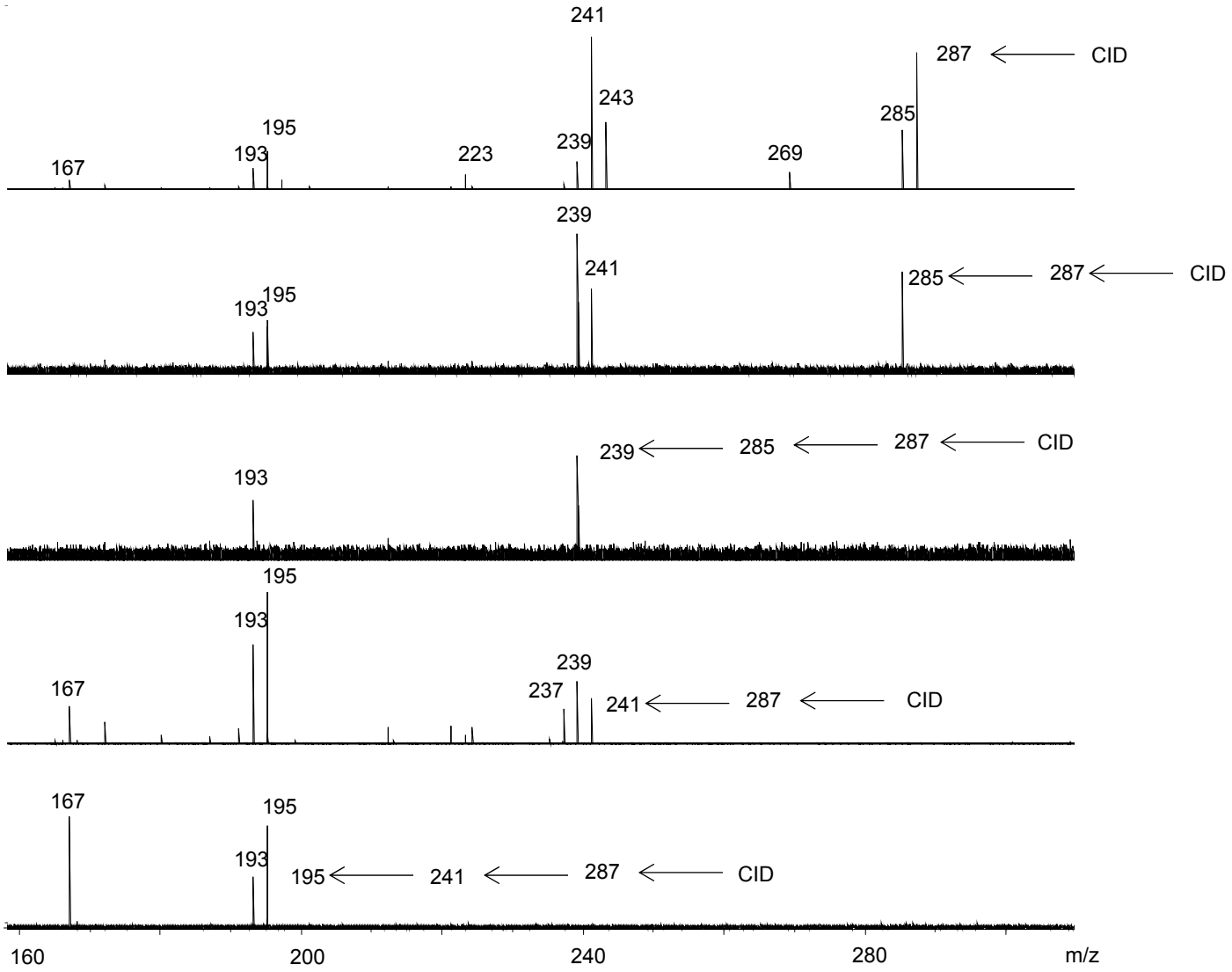



**Figure S4.** SORI/CID MS/MS spectra of $[Ni(Pro\text{-}H)(Pro)]^+$

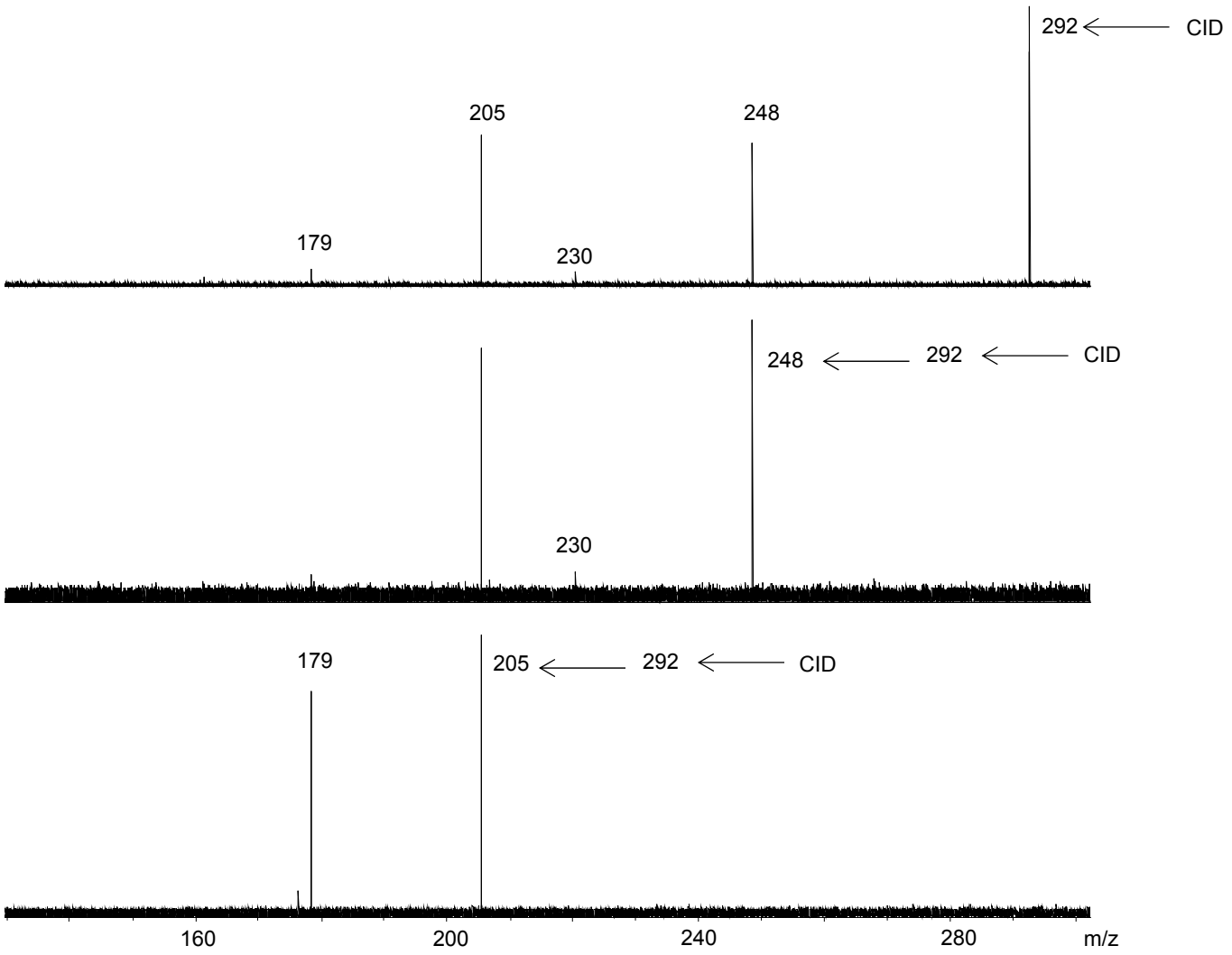



**Figure S5.** SORI/CID spectrum of the $[Cu(Pro\text{-}H)(Pro)]^+$

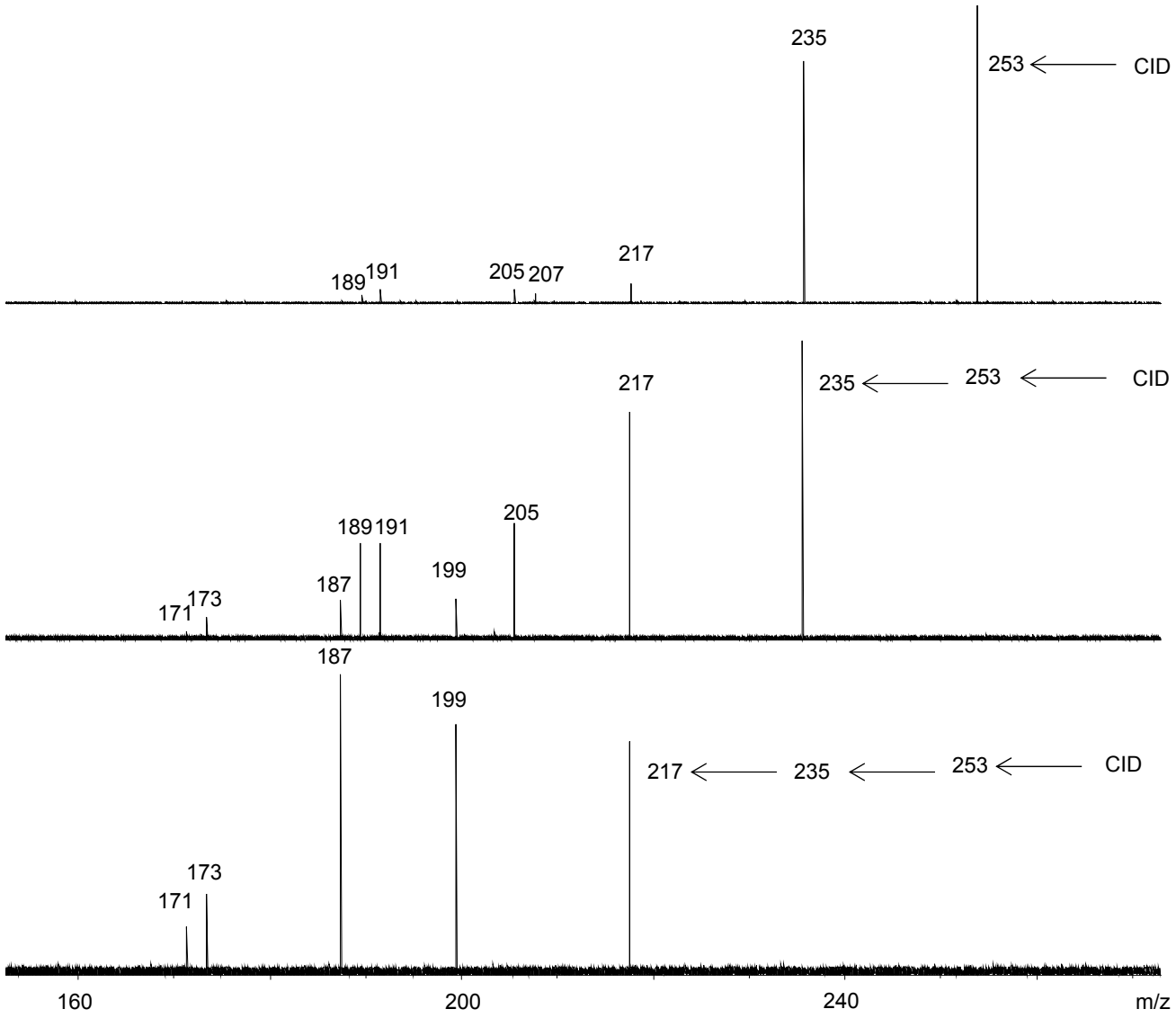



**Figure S6.** SORI/CID spectrum of the [Mg(Pro-H)(Pro)]$^+$

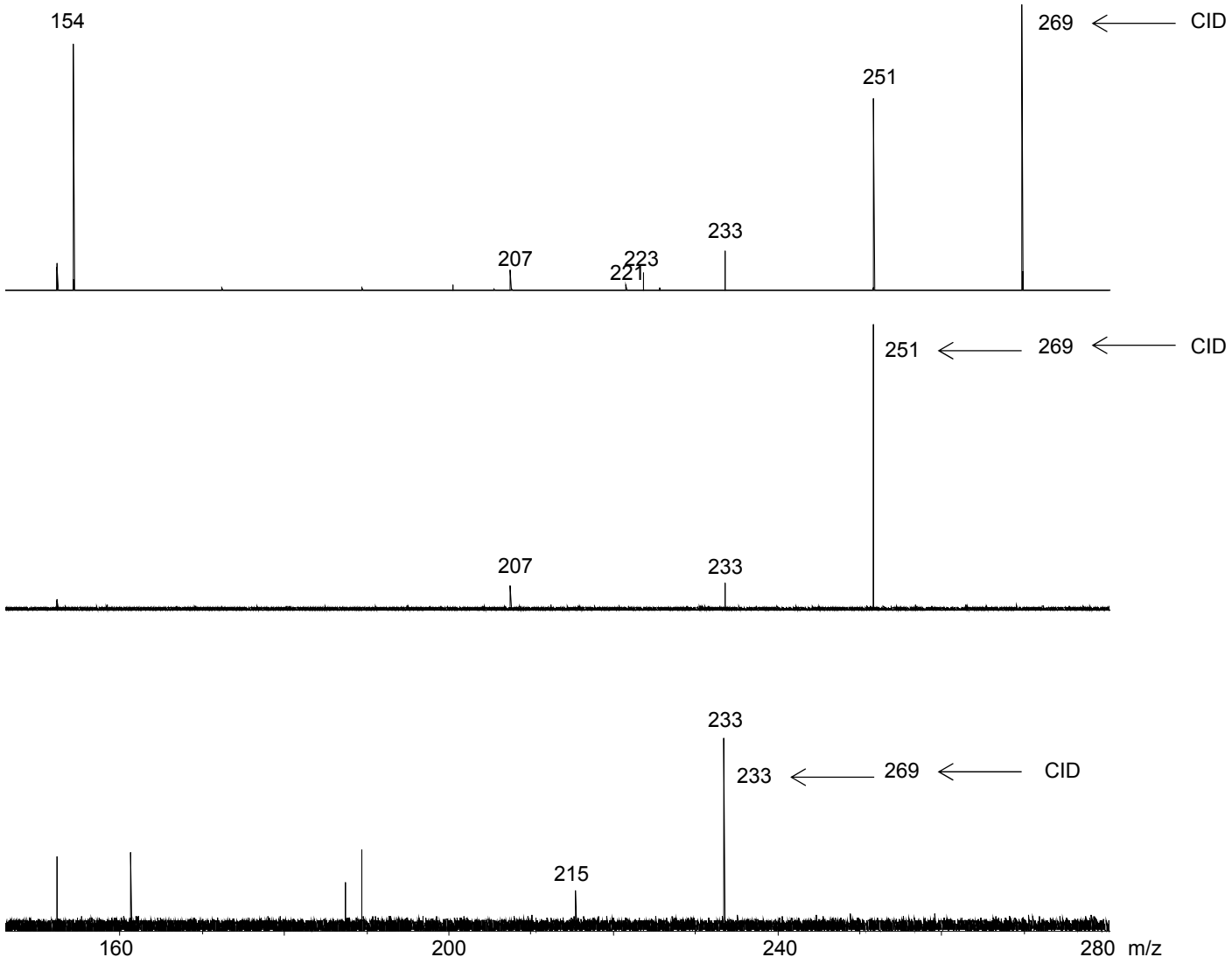



**Figure S7.** SORI/CID spectrum of the [Ca(Pro-H)(Pro)]$^+$

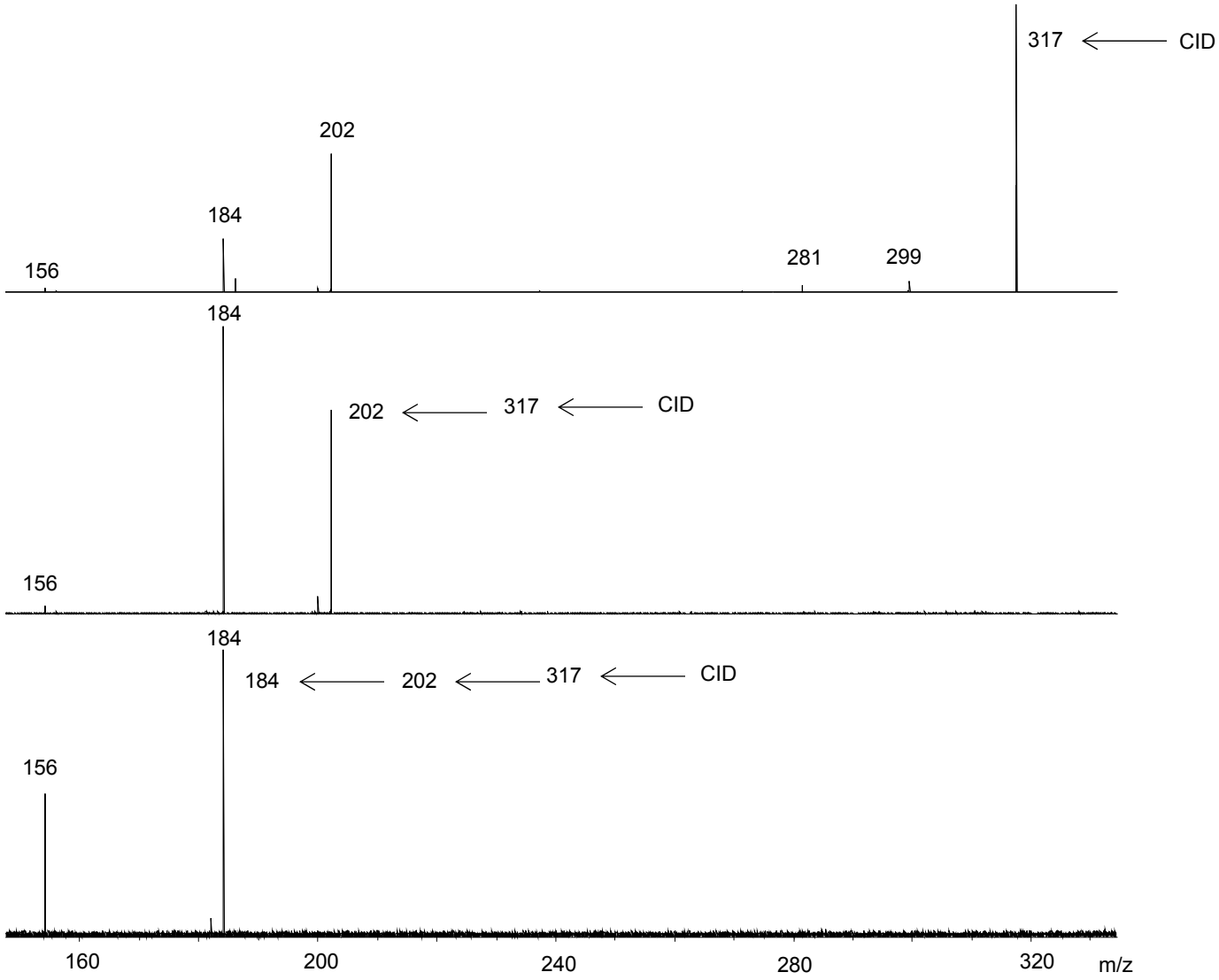



**Figure S8.** SORI/CID spectrum of the [Sr(Pro-H)(Pro)]$^+$

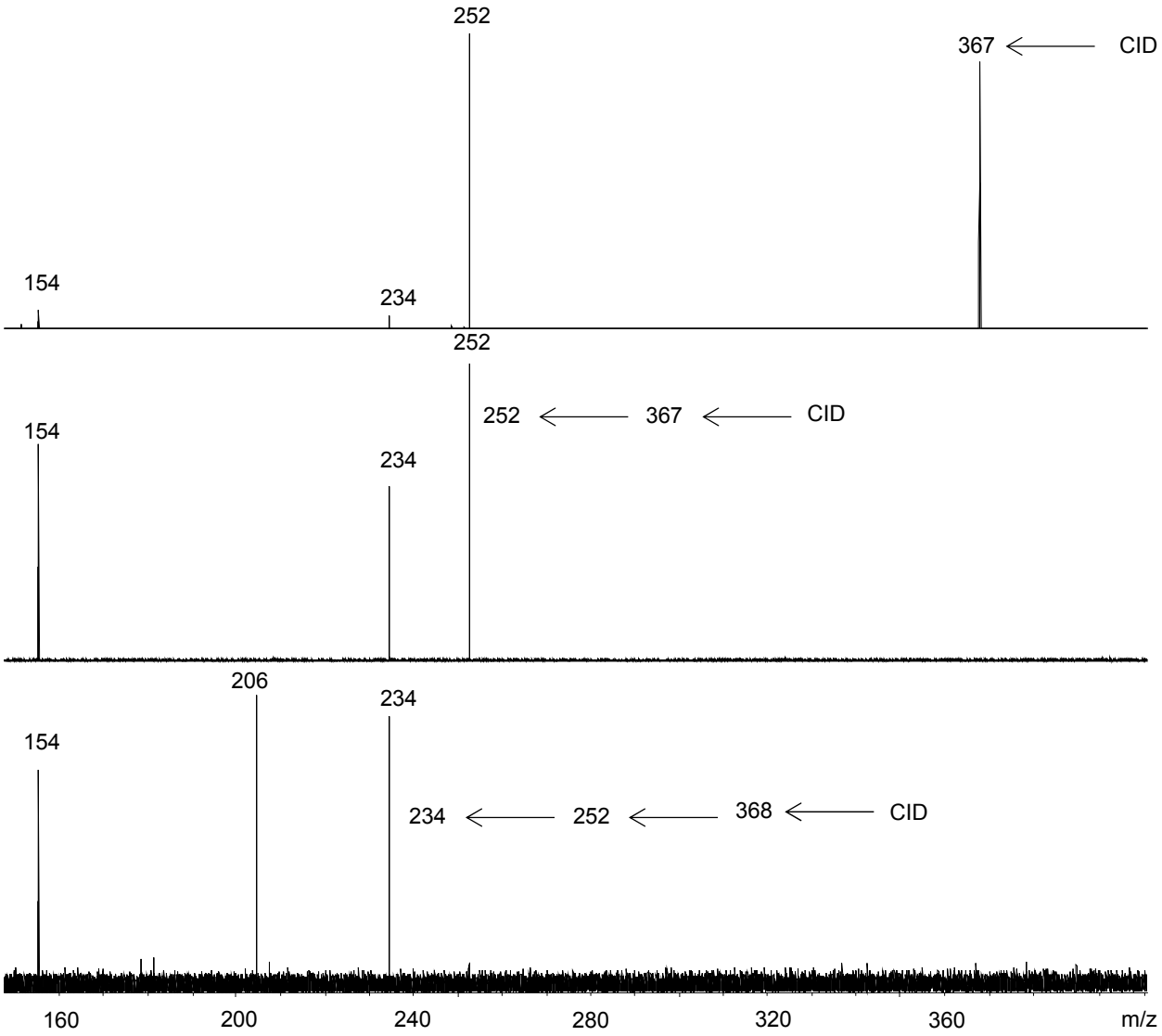



**Figure S9.** SORI/CID spectrum of the [Ba(Pro-H)(Pro)]$^+$

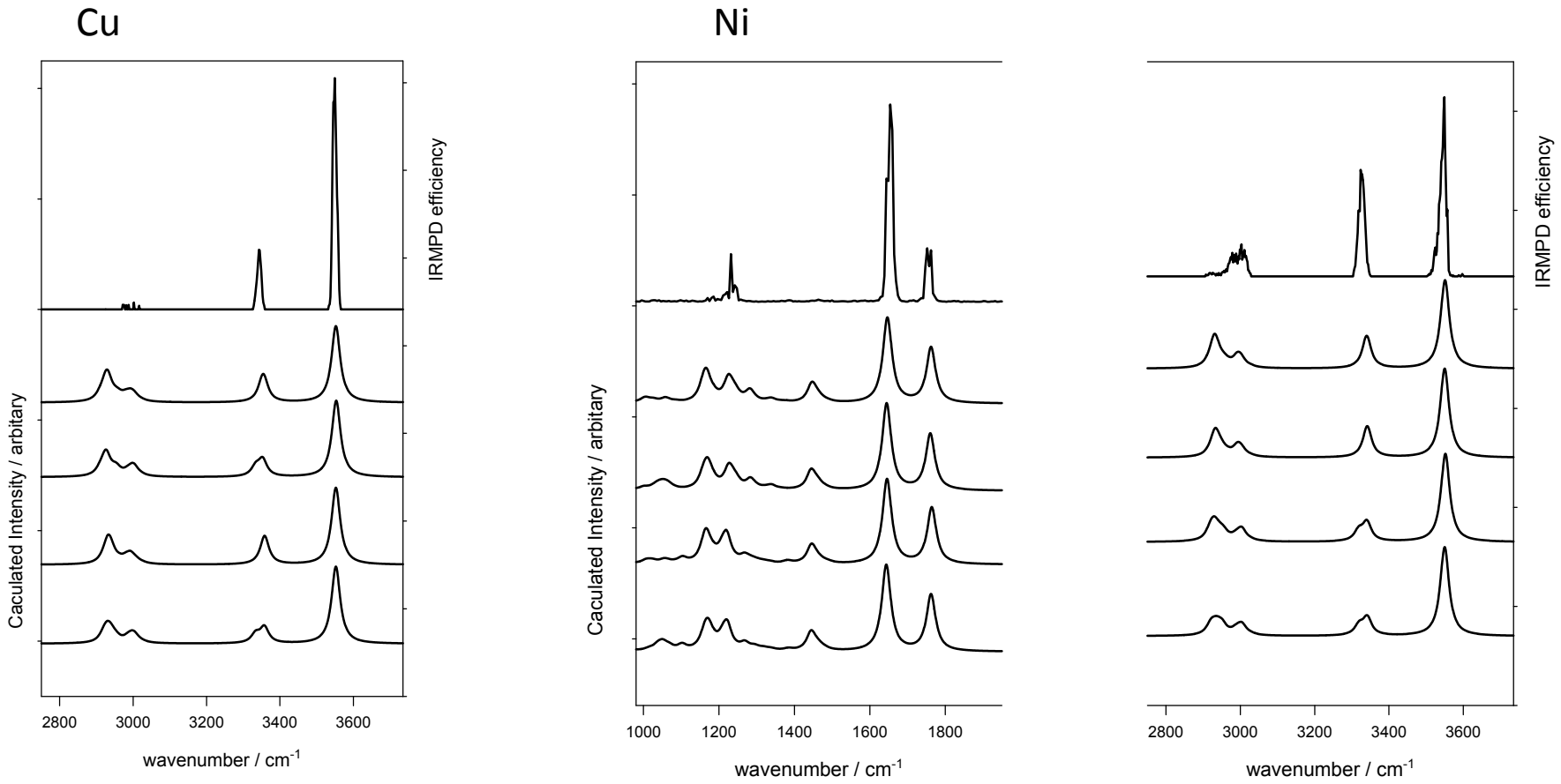



**Fig. S10.** IRMPD spectra for $[Cu(Pro_2\text{-}H)]^+$ and $[Ni(Pro_2\text{-}H)]^+$ compared with the computed spectra for the four NO-NO-CS structures. Structures can be seen in Figure S12a) and S13a).

NO-NO-CS

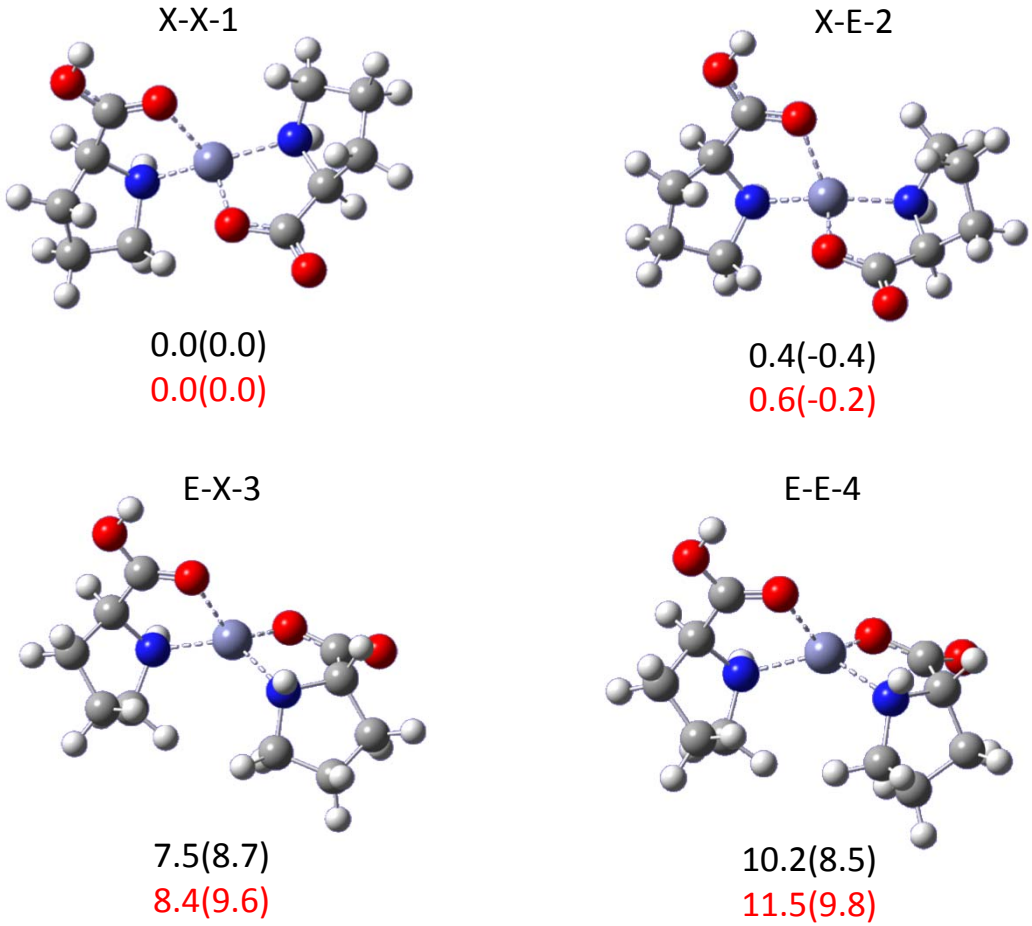



**Figure S11a).** Relative 298 K Gibbs energies (and enthalpies) computed at the B3LYP/6-311++G(3d,3p)//6- 31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) are reported for the NO-NO-CS $[Zn(Pro)_2\text{-}H]^+$ complexes.

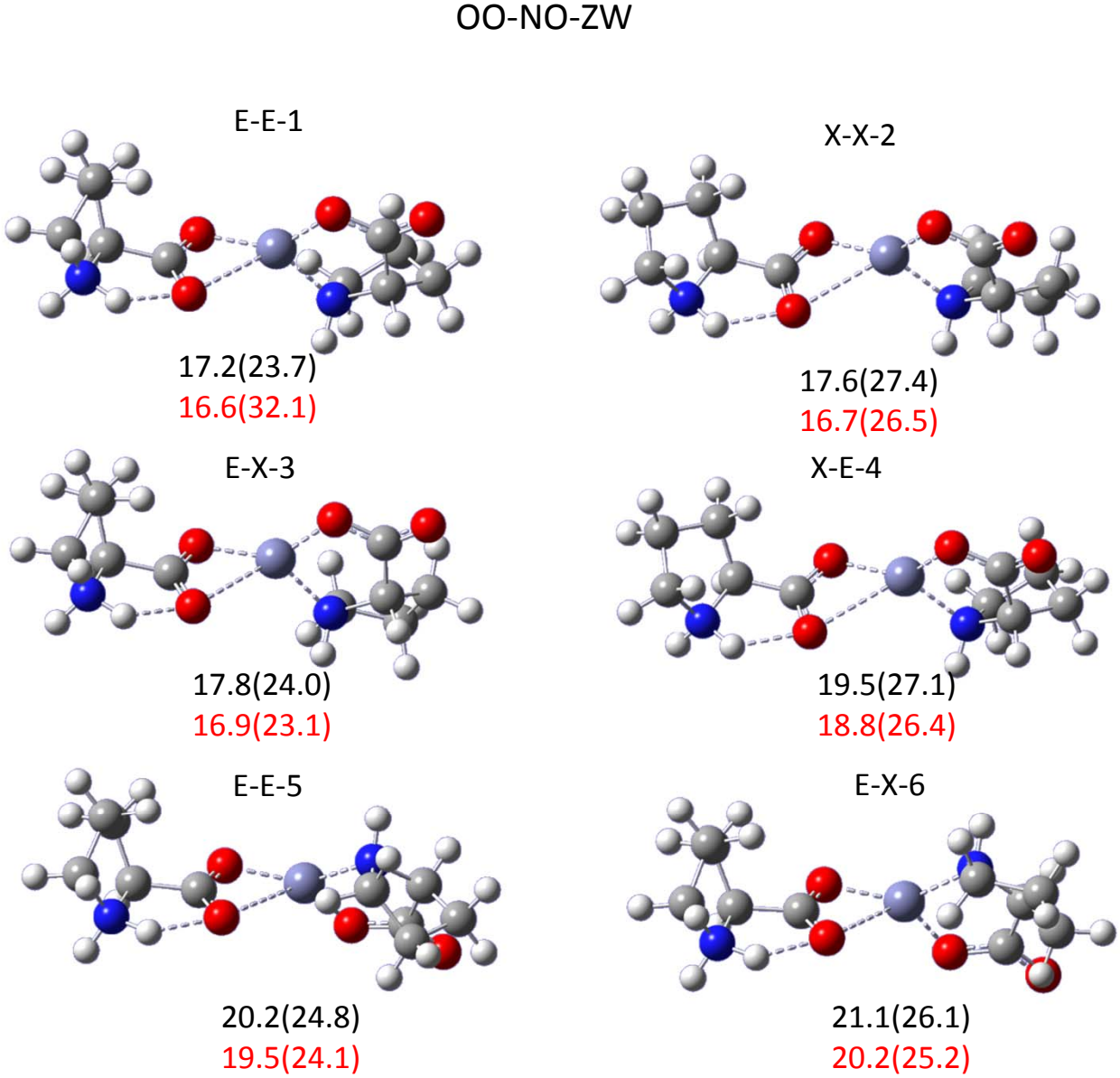
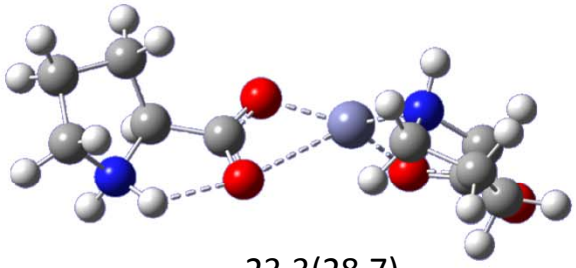



**Figure S11b).** Relative 298 K Gibbs energies (and enthalpies) computed at the B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color)are reported for the OO-NO-ZW $[Zn(Pro)_2-H]^+$ complexes.

OO-NO-ZW

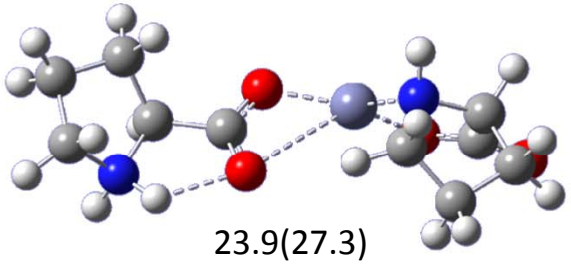
X-X-7



23.3(28.7)

22.2(27.6)

X-E-8



23.9(27.3)

23.1(26.5)

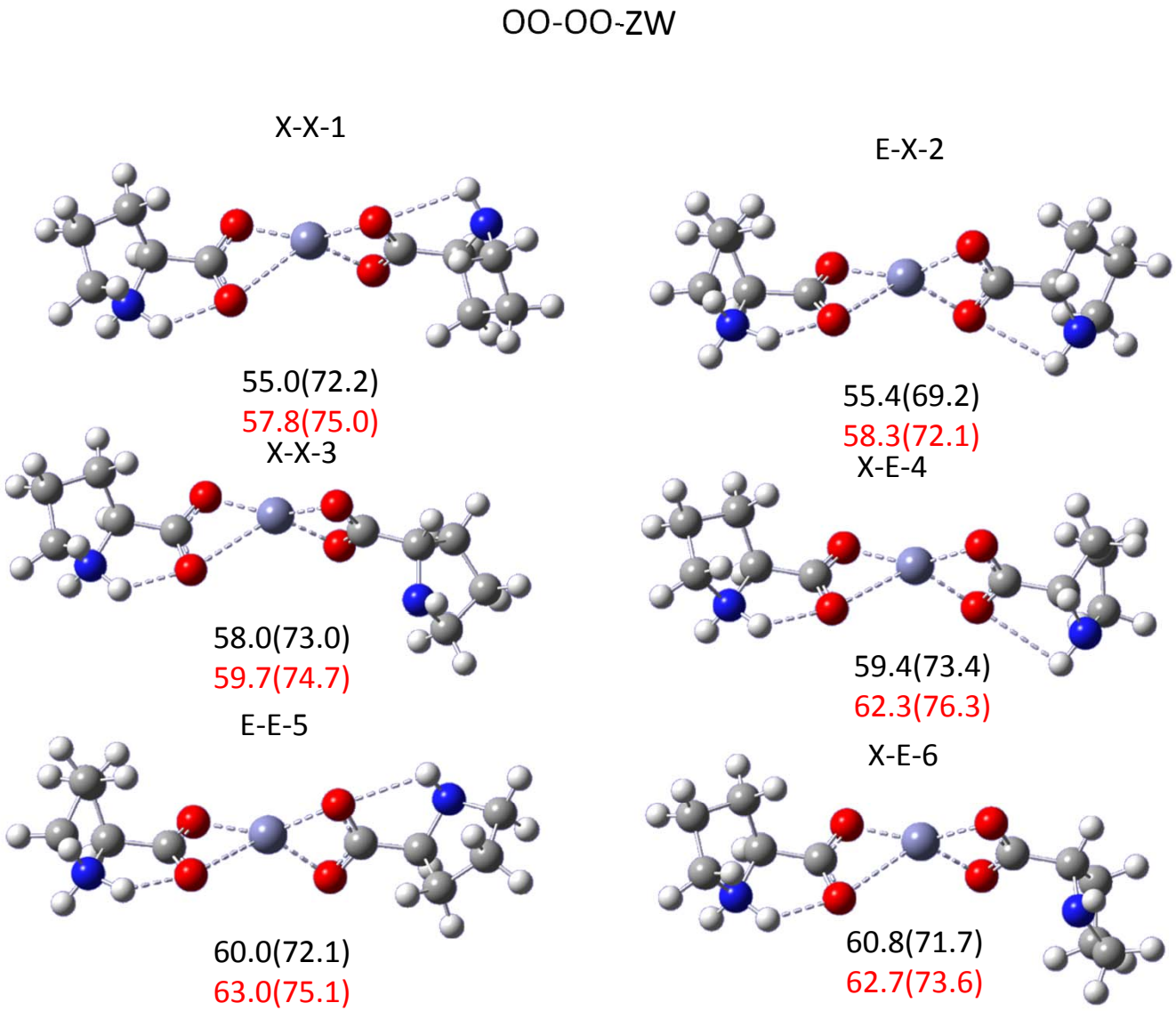



**Figure S11c).** Relative 298 K Gibbs energies (and enthalpies) computed at the B3LYP/6-311++G(3d,3p)//6- 31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) are reported for the OO-OO-ZW $[Zn(Pro)_2\text{-}H]^+$ complexes.

NO-OO-CS

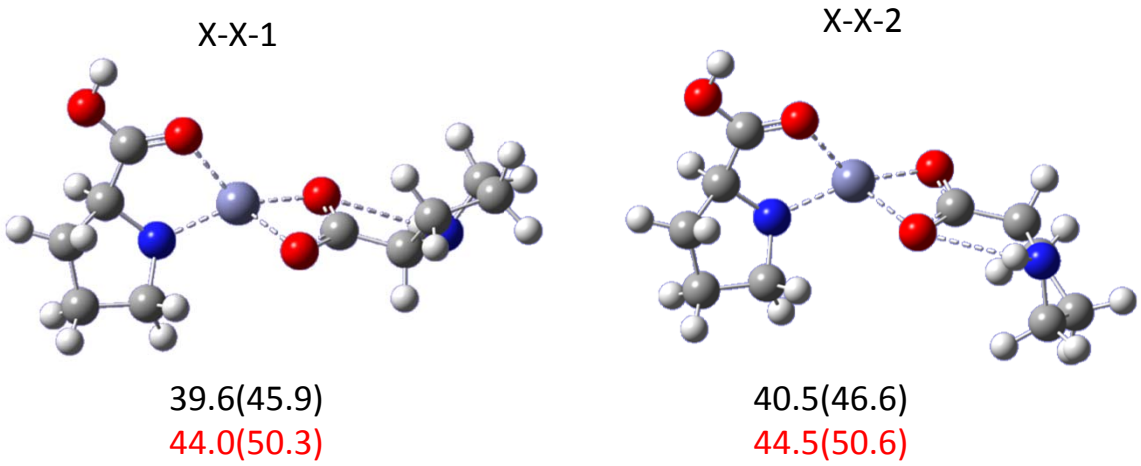



**Figure S11d).** Relative 298 K Gibbs energies (and enthalpies) computed at the B3LYP/6-311++G(3d,3p)//6- 31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color)are reported for the NO-OO-CS $[Zn(Pro)_2-H]^+$ complexes.

NO-NO-CS

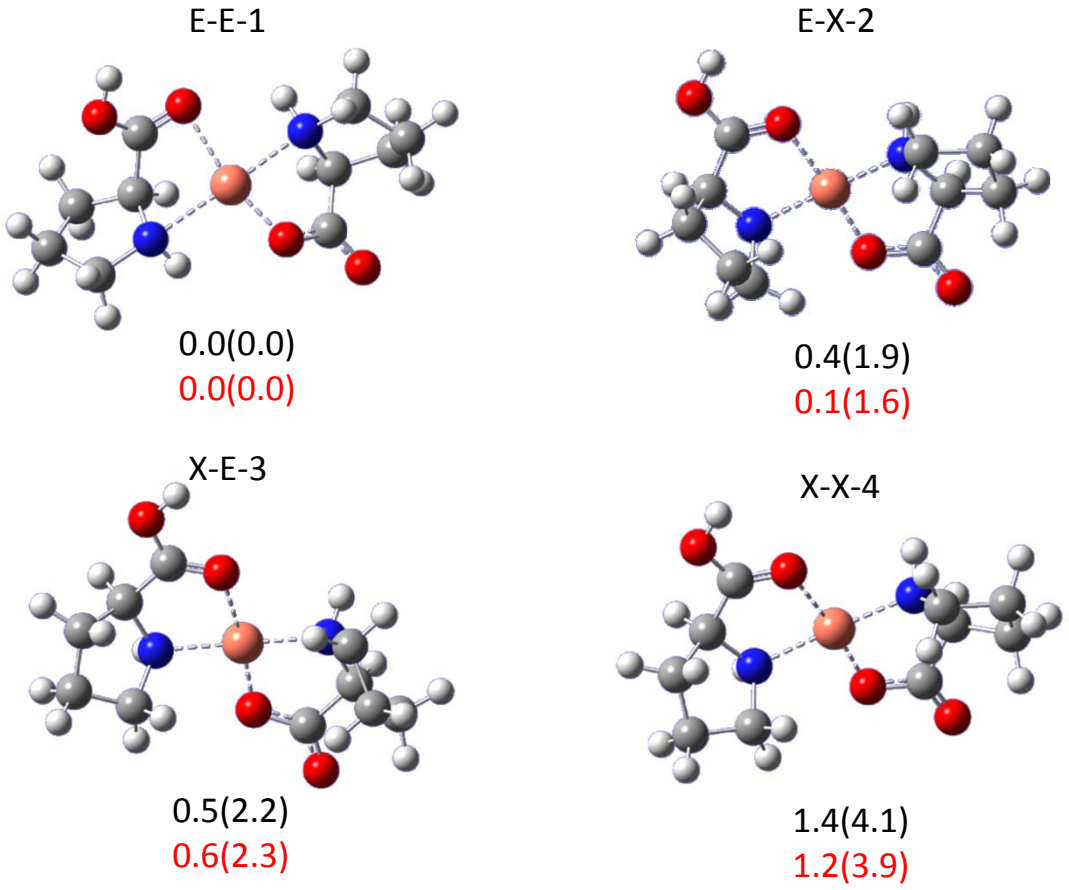



**Figure S12a).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-NO-CS isomers of the $[Cu(Pro)_2-H]^+$ complex. The structures are all doublets.

OO-NO-ZW

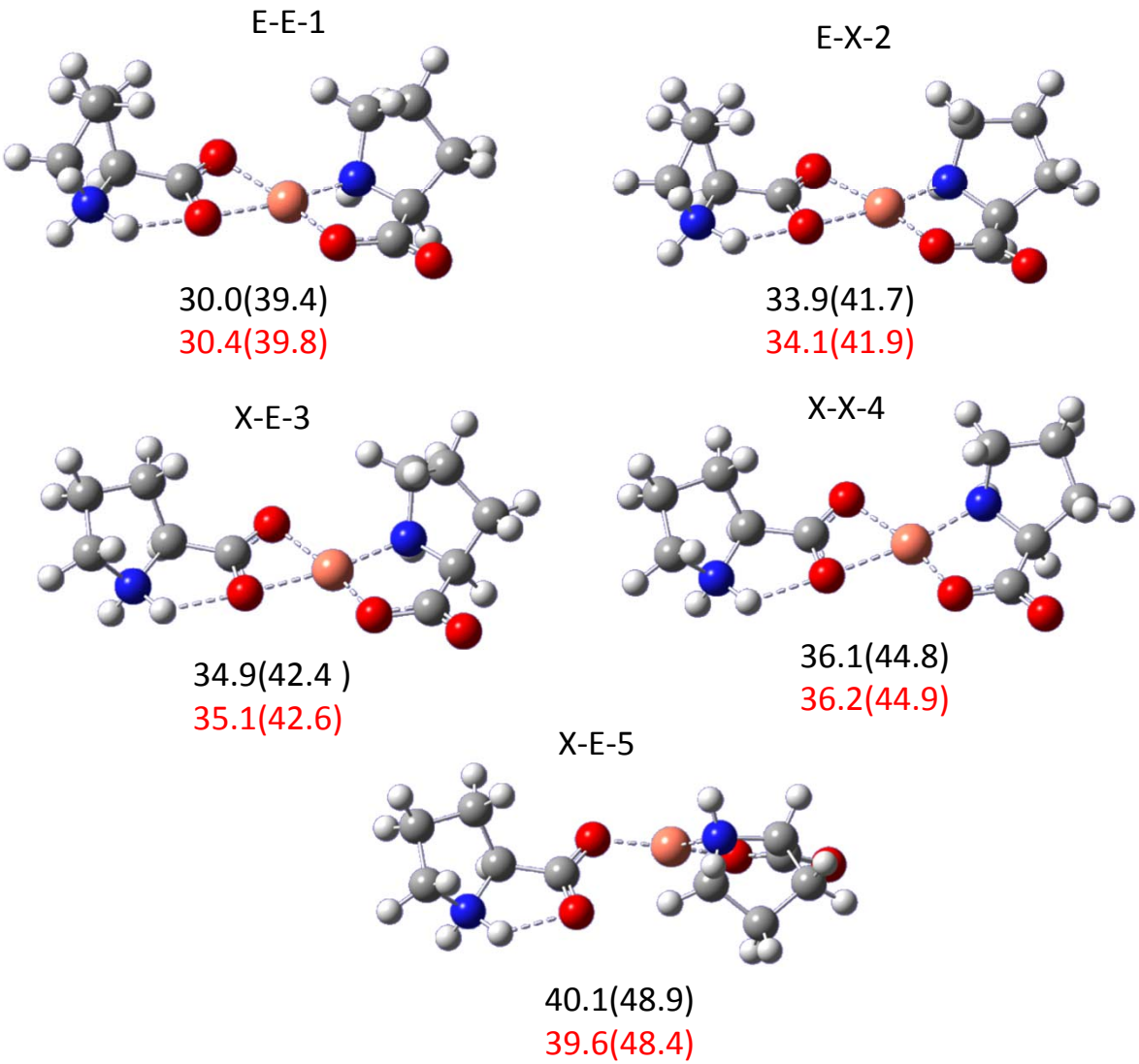



**Figure S12b).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-NO-ZW isomers of the $[Cu(Pro)_2-H]^+$ complex. The structures are all doublets.

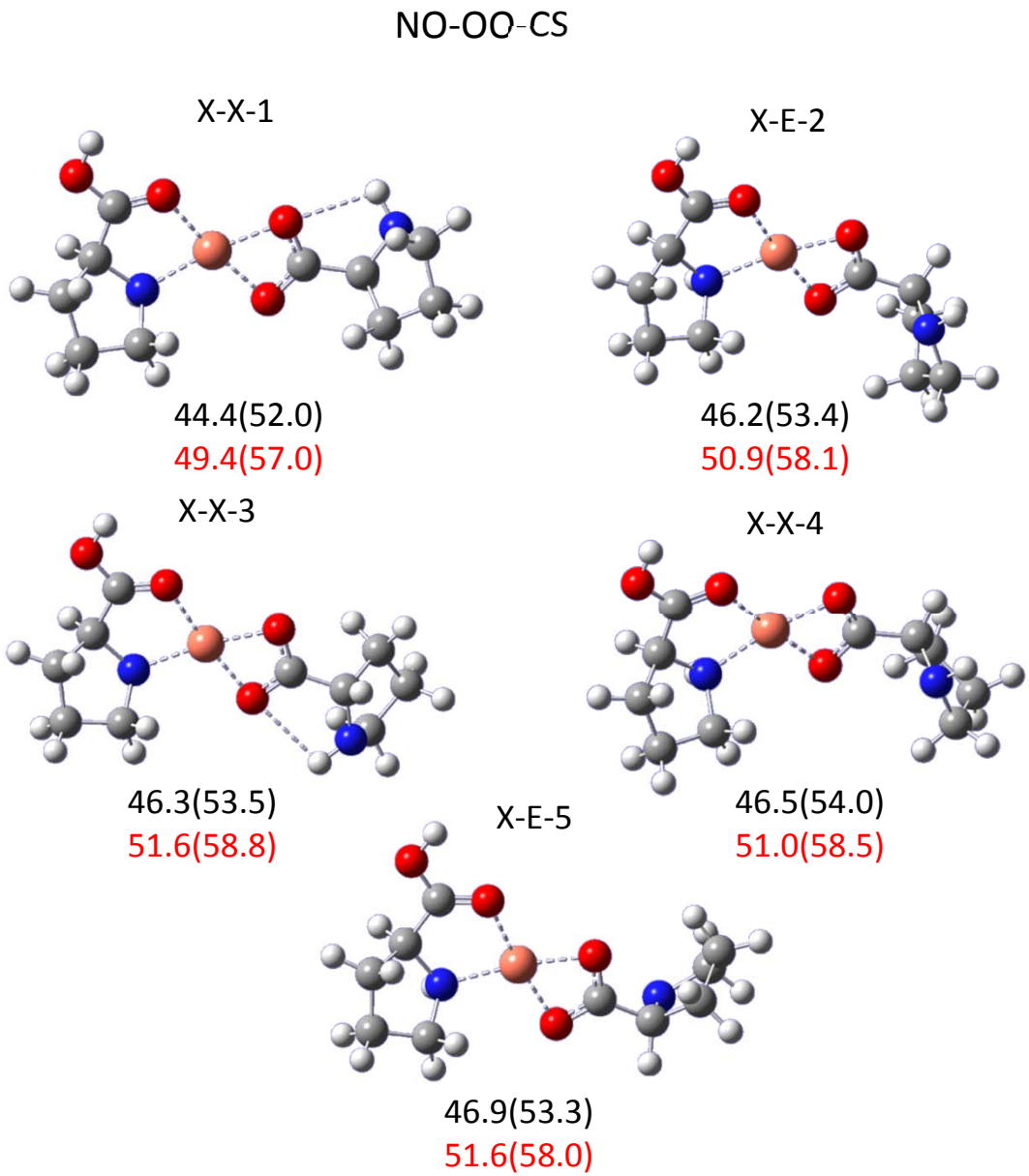



**Figure S12c).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-OO-CS isomers of the $[Cu(Pro)_2-H]^+$ complex. The structures are all doublets.

OO-OO-ZW

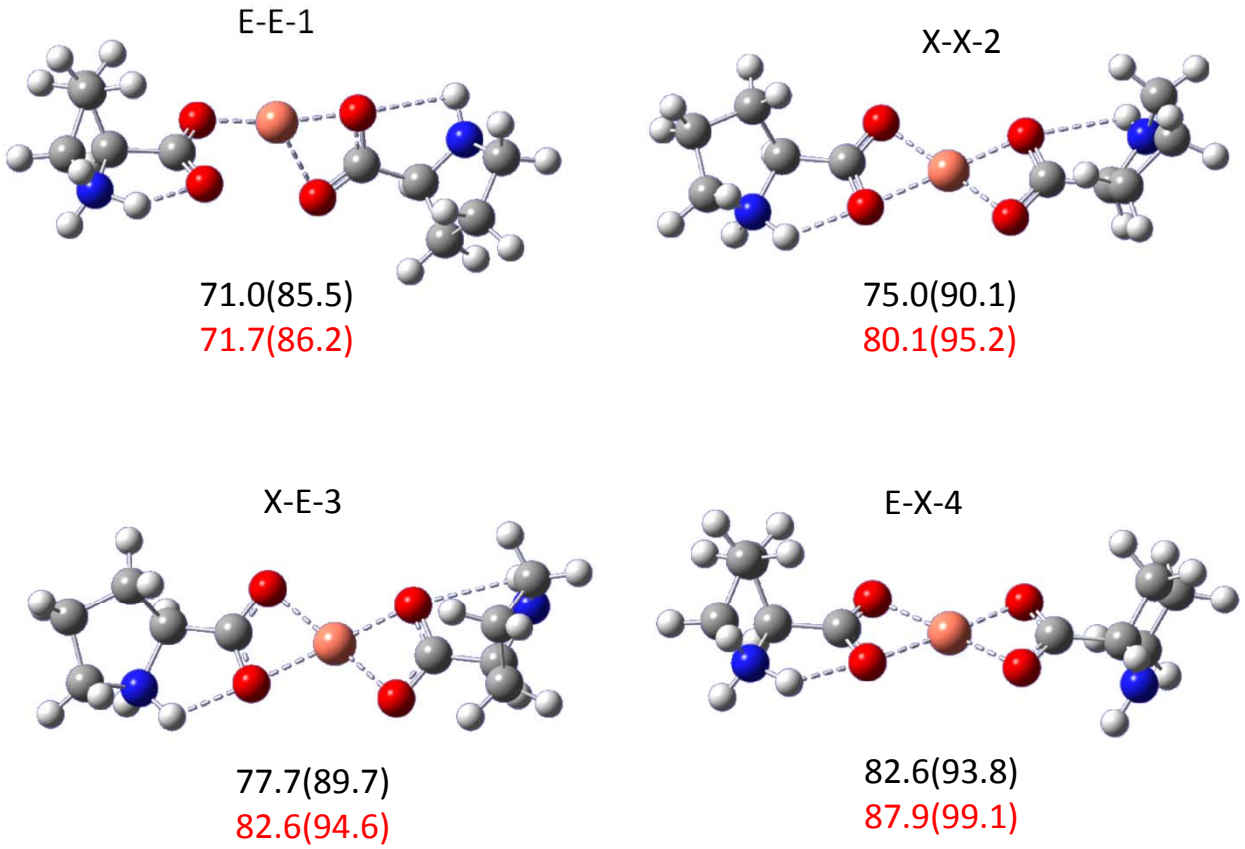



**Figure S12d).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-OO-ZW isomers of the $[Cu(Pro)_2\text{-}H]^+$ complex. The structures are all doublets.

NO-NO-CS

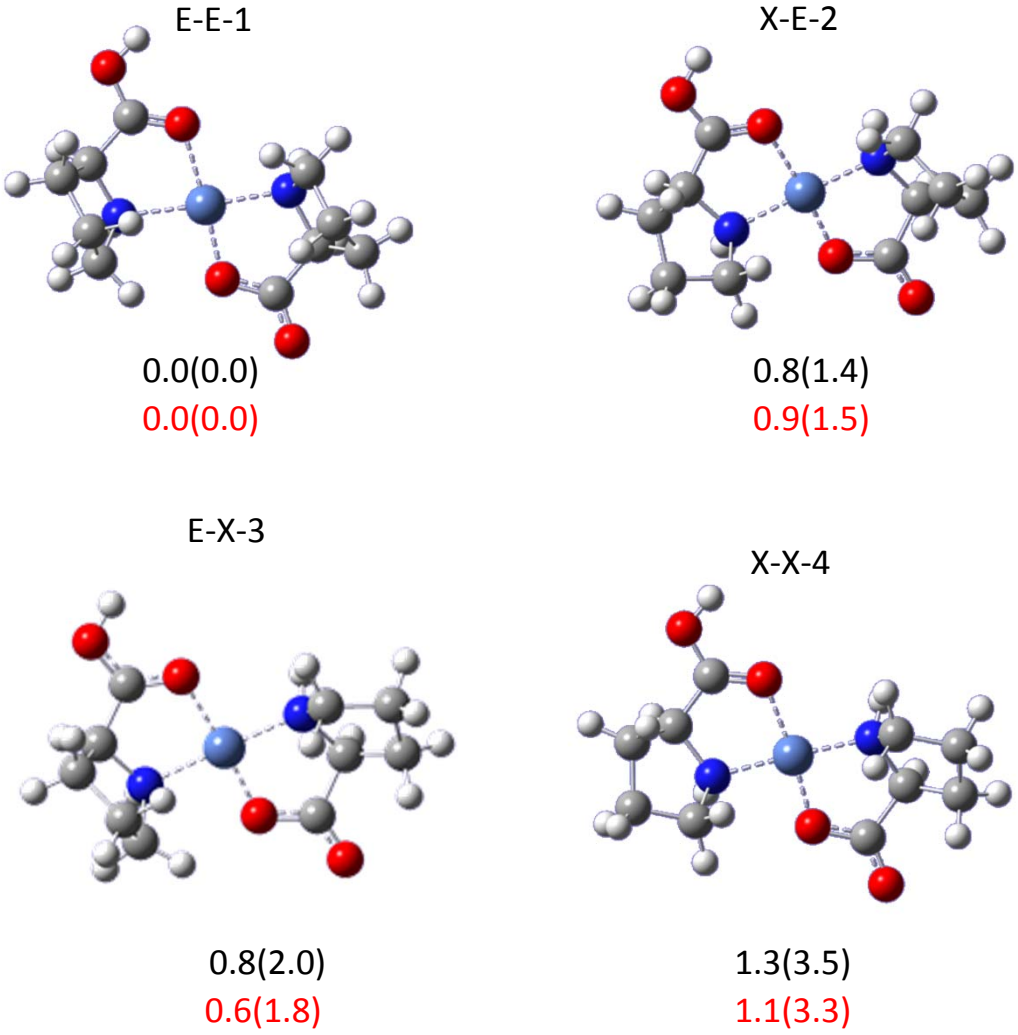



**Figure S13a).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-NO-CS isomers of the $[Ni(Pro)_2-H]^+$ complex. The structures are all singlets.

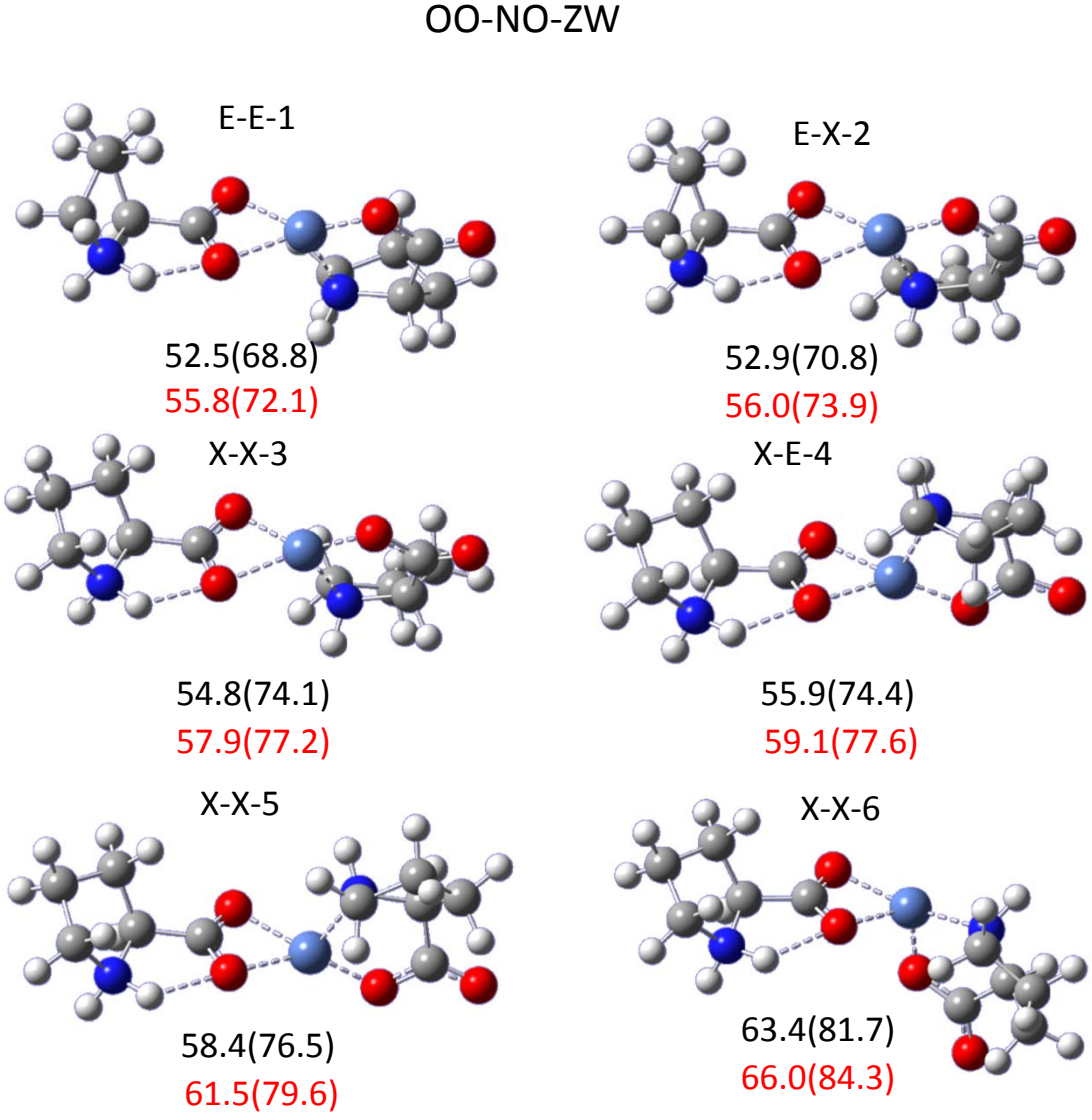



**Figure S13b).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-NO-ZW isomers of the $[Ni(Pro)_2-H]^+$ complex. The structures are all triplets.

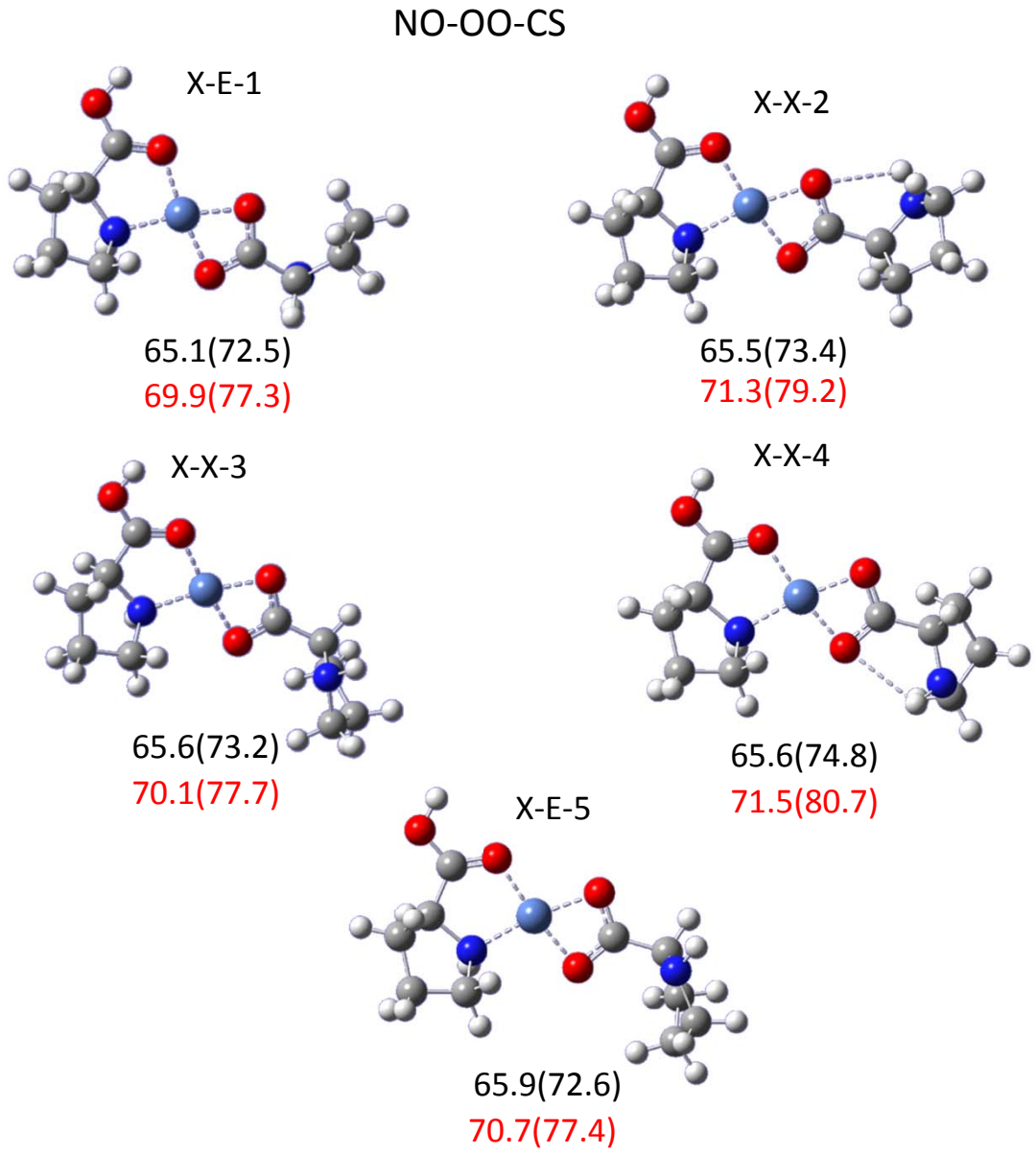



**Figure S13c).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-OO-CS isomers of the $[Ni(Pro)_2-H]^+$ complex. The structures are all singlets.

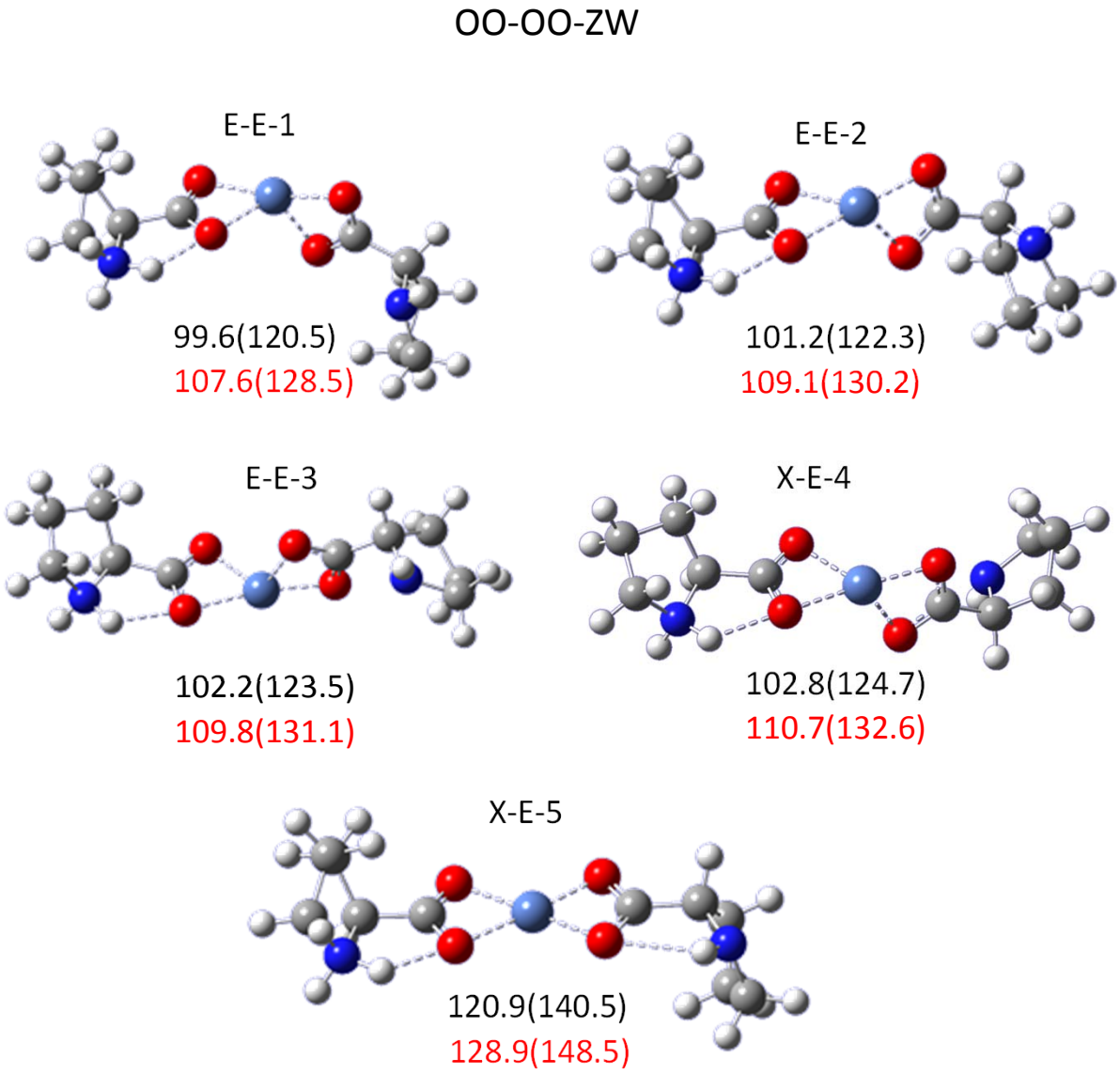



**Figure S13d).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-OO-ZW isomers of the $[Ni(Pro)_2-H]^+$ complex. The structures are all triplets.

NO-NO-CS

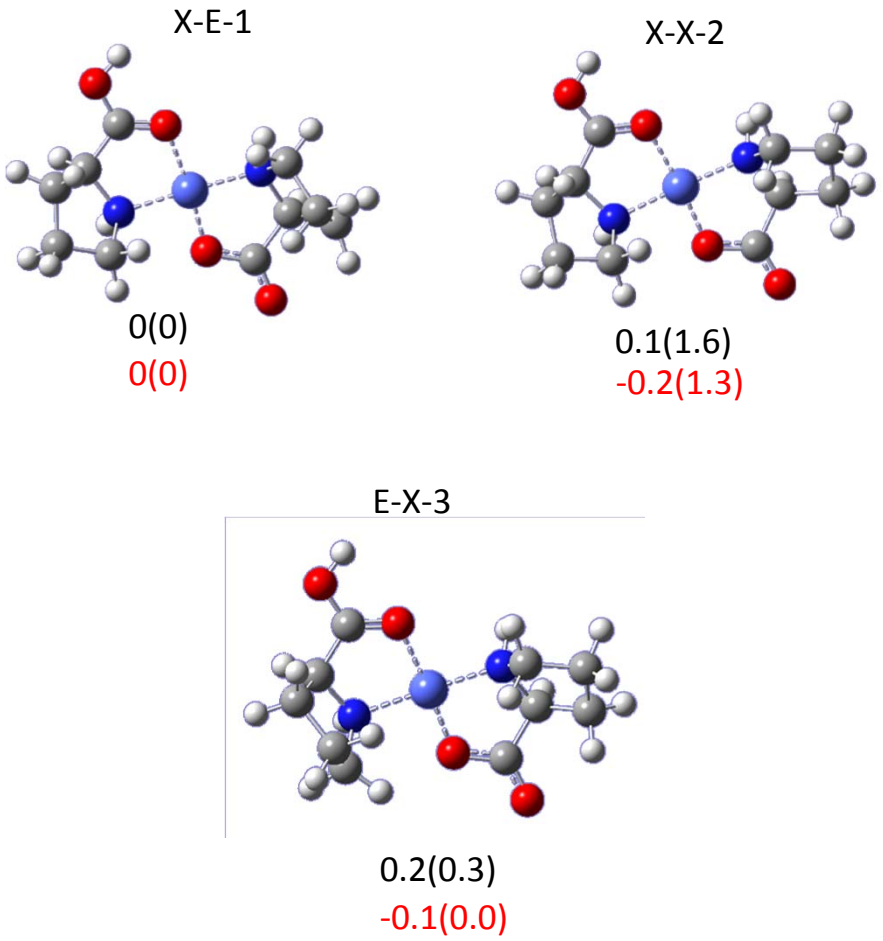



**Figure S14a).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-NO-CS isomers of the $[Co(Pro)_2-H]^+$ complex. The structures are all doublets.

OO-NO-ZW

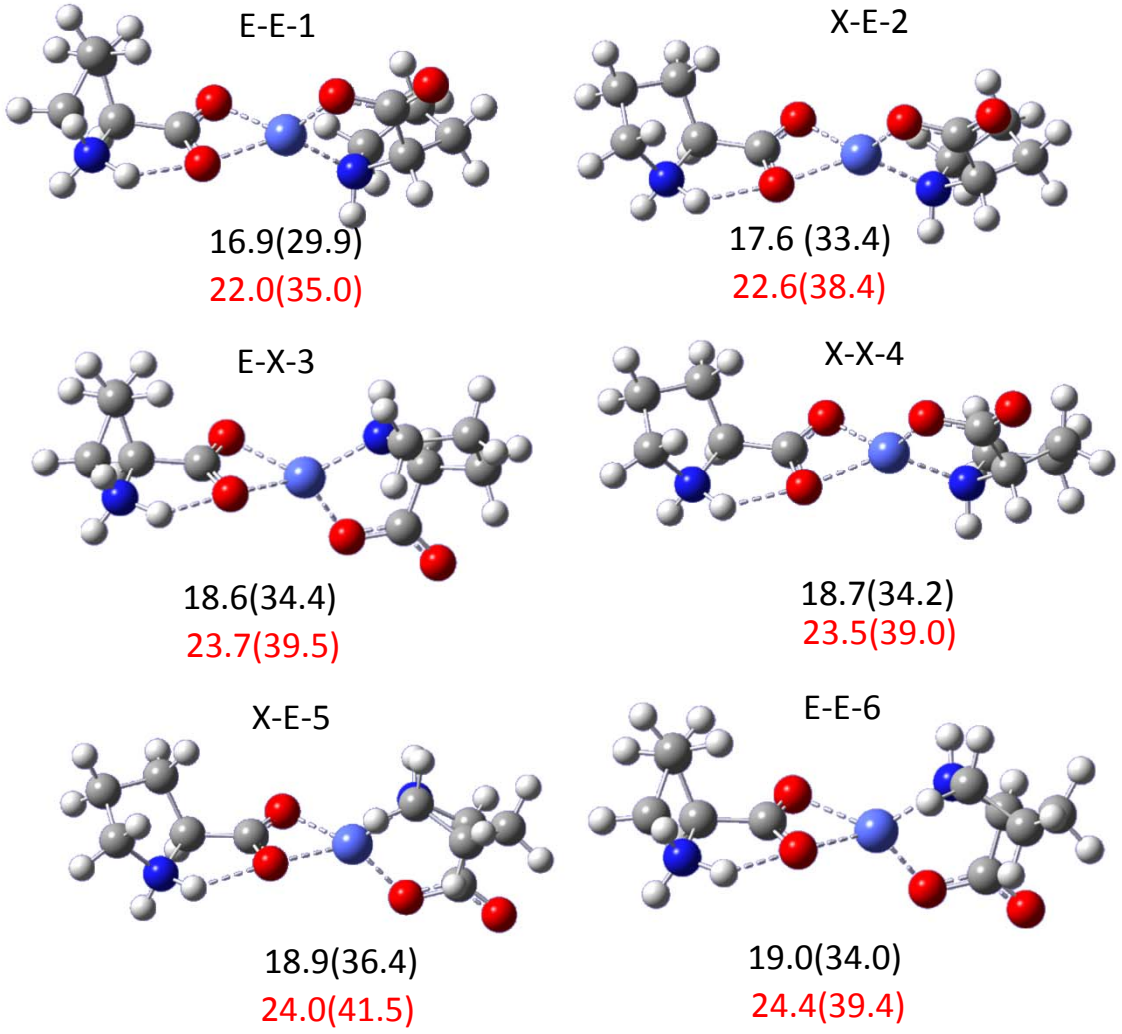
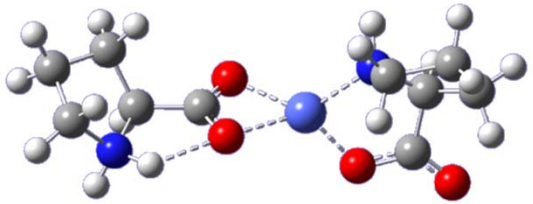



**Figure S14b).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-NO-ZW isomers of the $[Co(Pro)_2-H]^+$ complex. The structures are all quartets.

OO-NO-ZW

X-X-7



21.3(36.7)

26.2(41.6)

NO-OO-CS

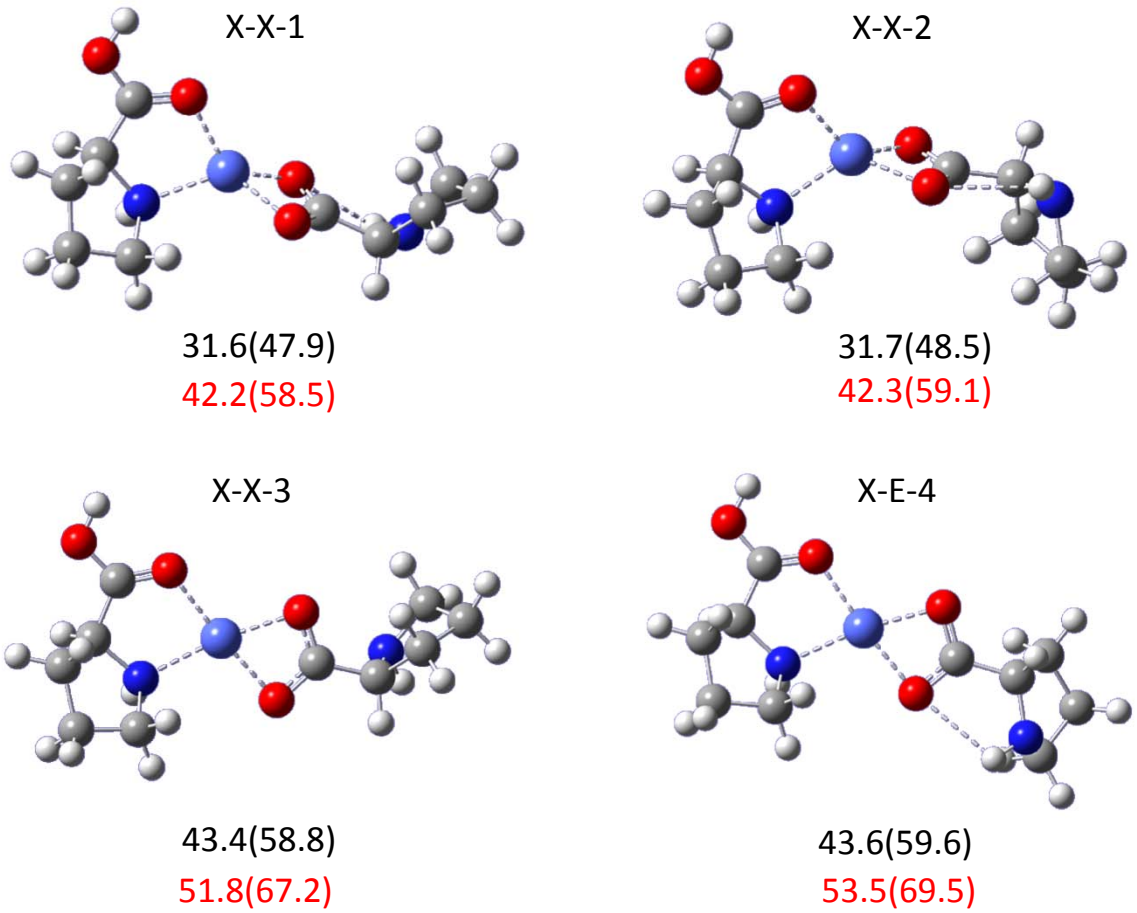



**Figure S14c).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-OO-CS isomers of the $[Co(Pro)_2-H]^+$ complex. The structures are all quartets.

OO-OO-ZW

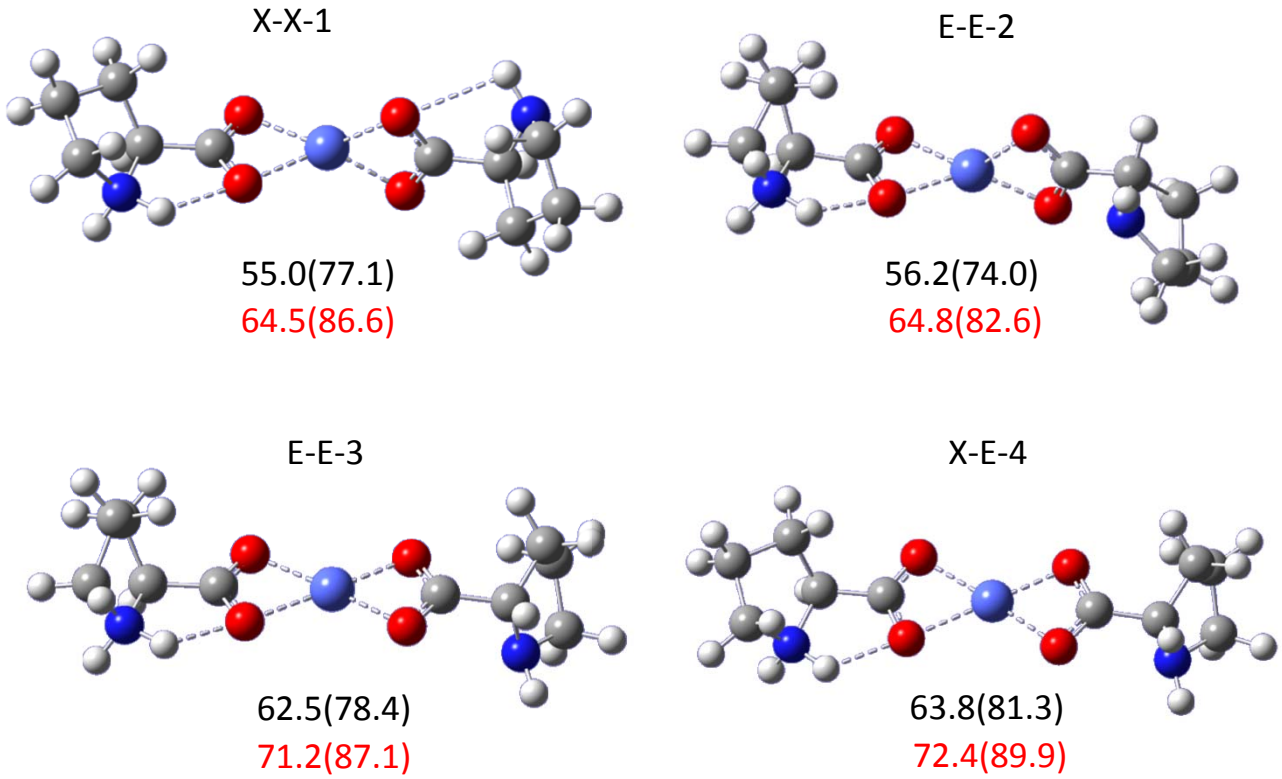



**Figure S14d).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-OO-ZW isomers of the $[Co(Pro)_2-H]^+$ complex. The structures are all quartets.

NO-NO-CS

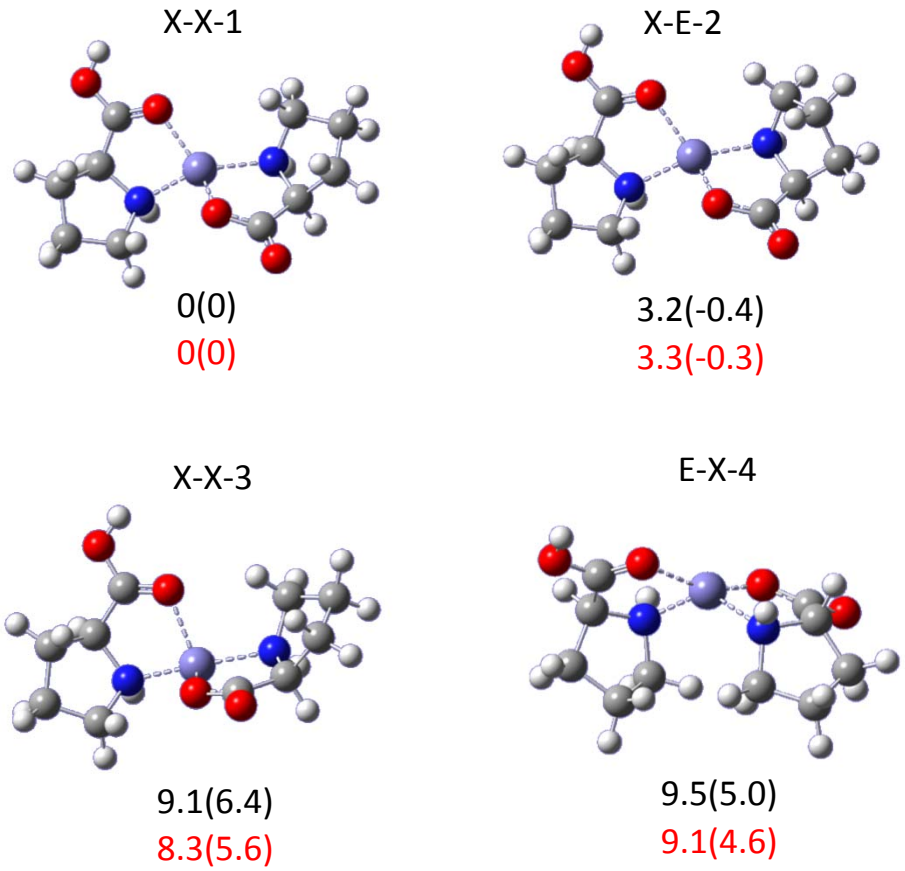



**Figure S15a).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-NO-CS isomers of the $[Fe(Pro)_2-H]^+$ complex. The structures are all quintets.

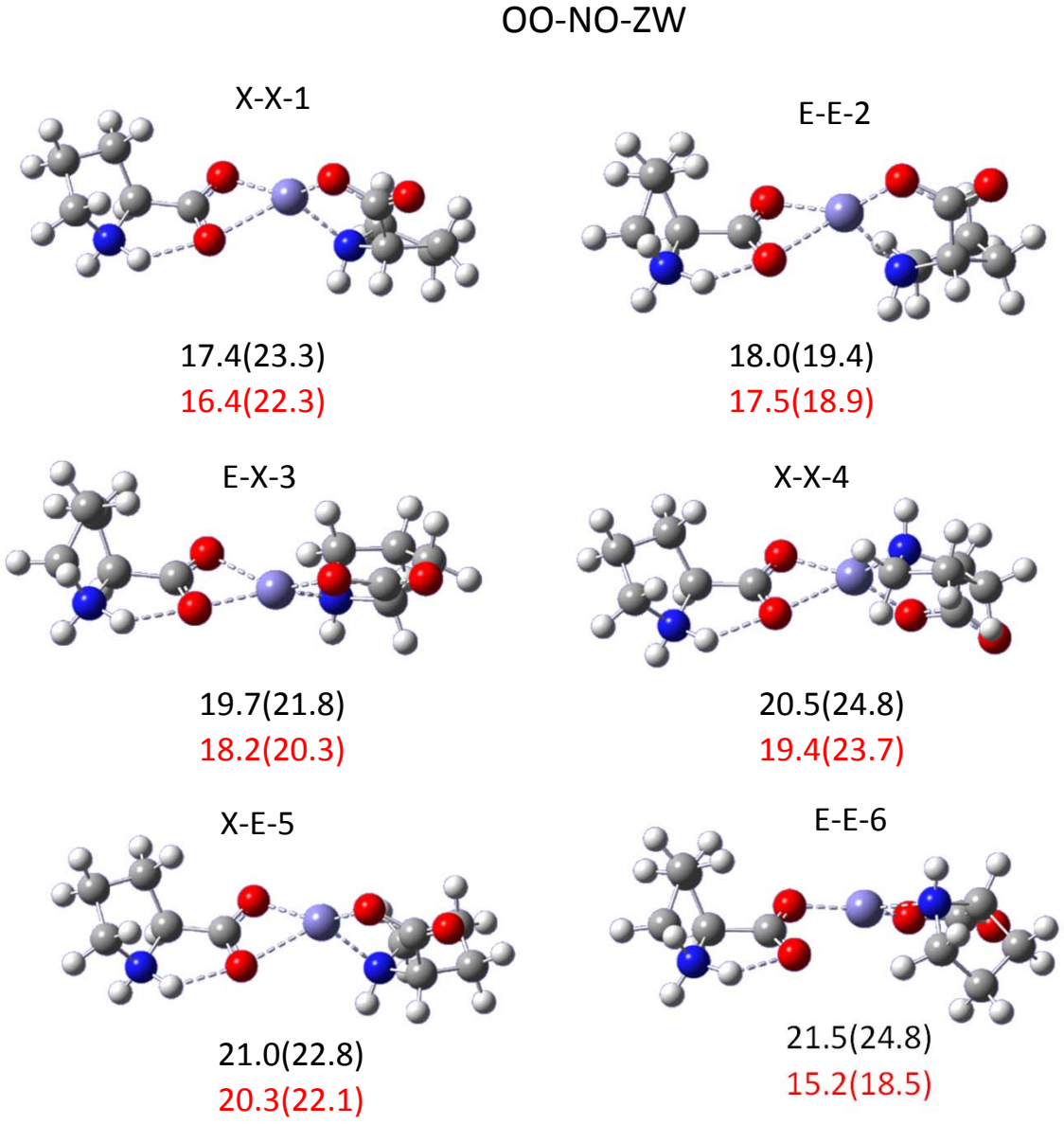
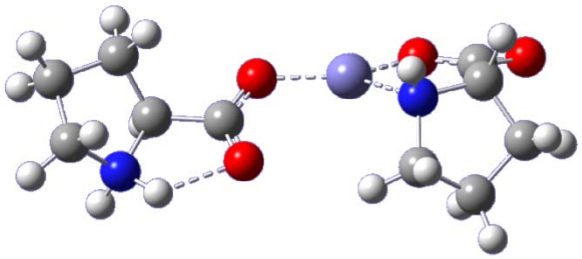



**Figure S15b).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-NO-ZW isomers of the $[Fe(Pro)_2\text{-}H]^+$ complex. The structures are all quintets.

OO-NO-ZW

X-E-7



23.6(28.0)

16.8(21.2)

NO-OO-CS

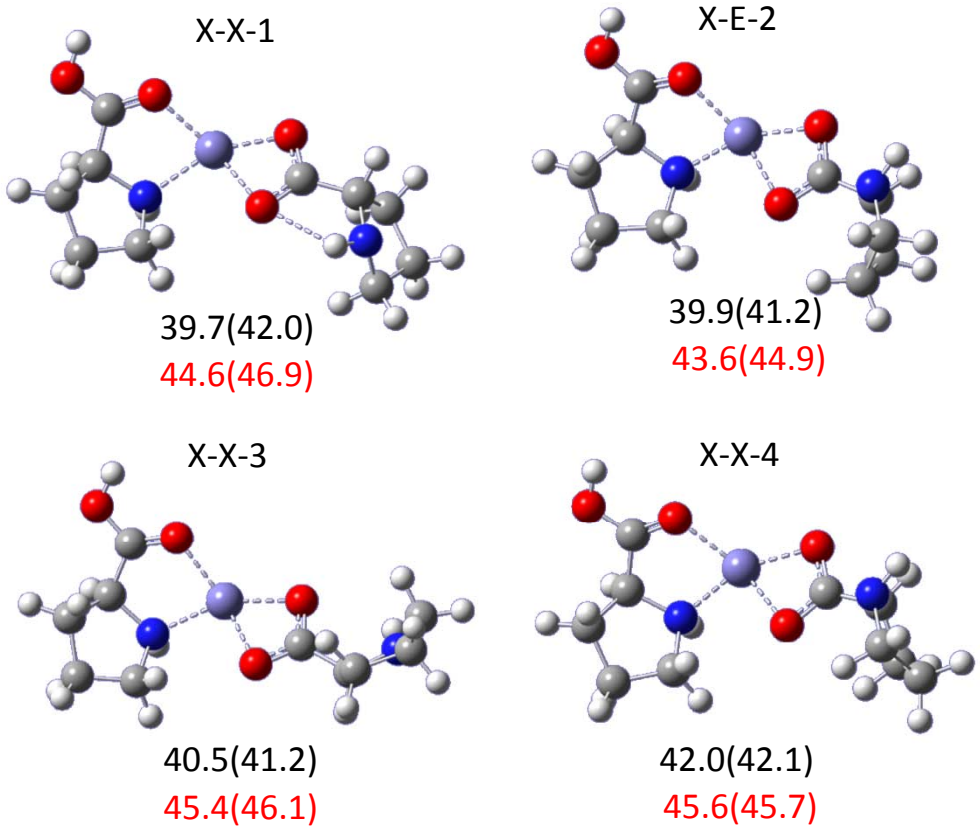



**Figure S15c).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-OO-CS isomers of the $[Fe(Pro)_2-H]^+$ complex. The structures are all quintets.

OO-OO-ZW

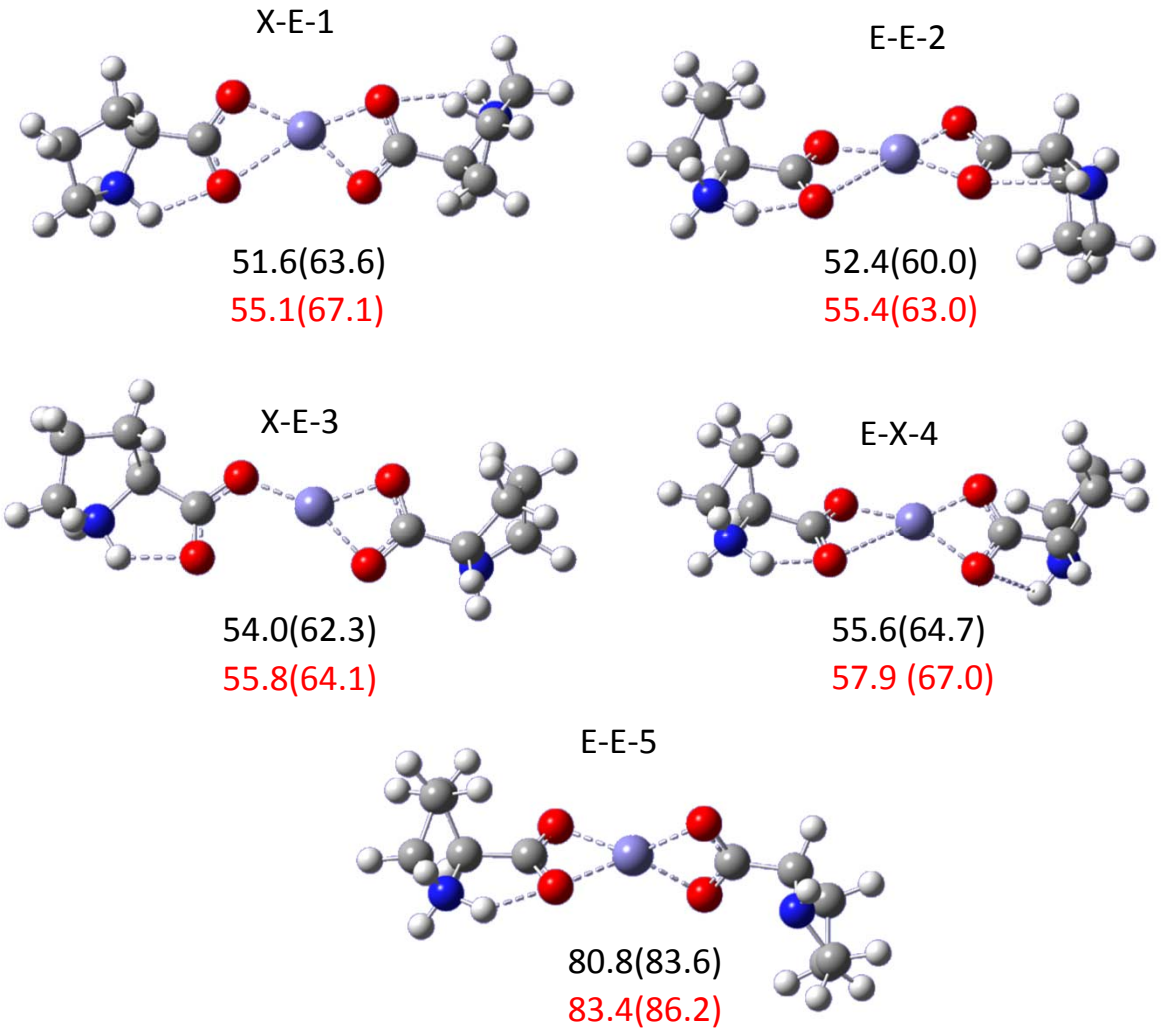



**Figure S15d).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-OO-ZW isomers of the $[Fe(Pro)_2-H]^+$ complex. The structures are all quintets.

NO-NO-CS

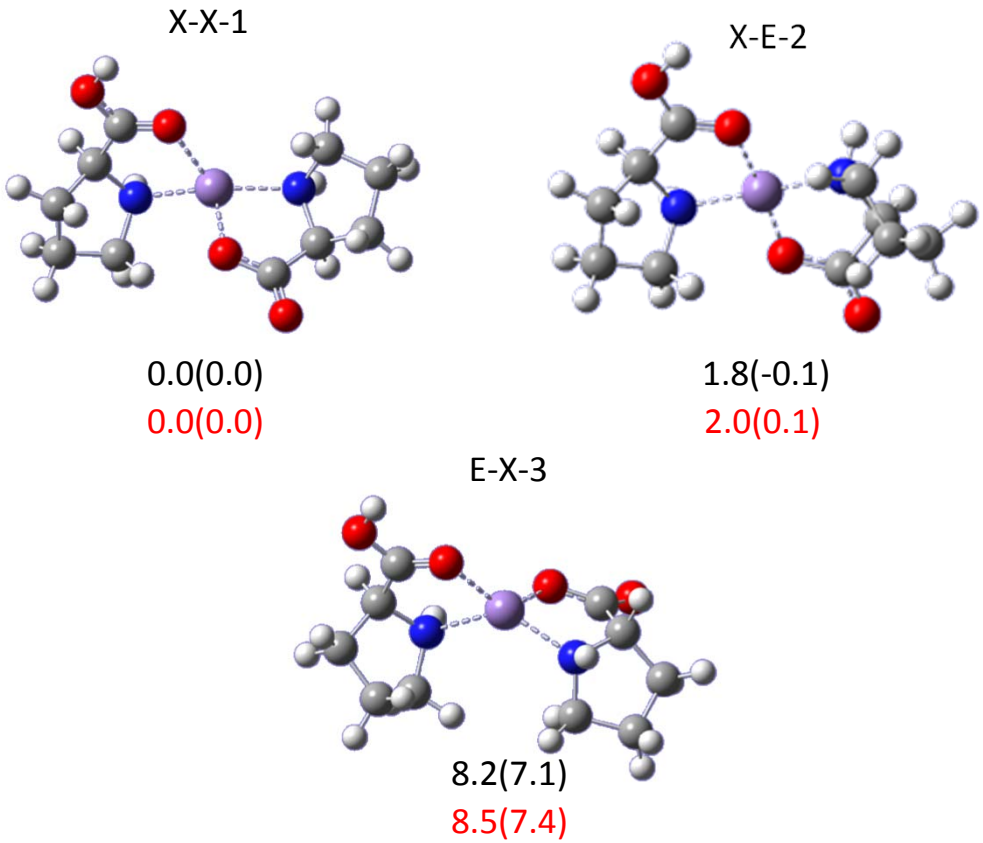



**Figure S16a).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-NO-CS isomers of the $[Mn(Pro)_2-H]^+$ complex. The structures are all sextets.

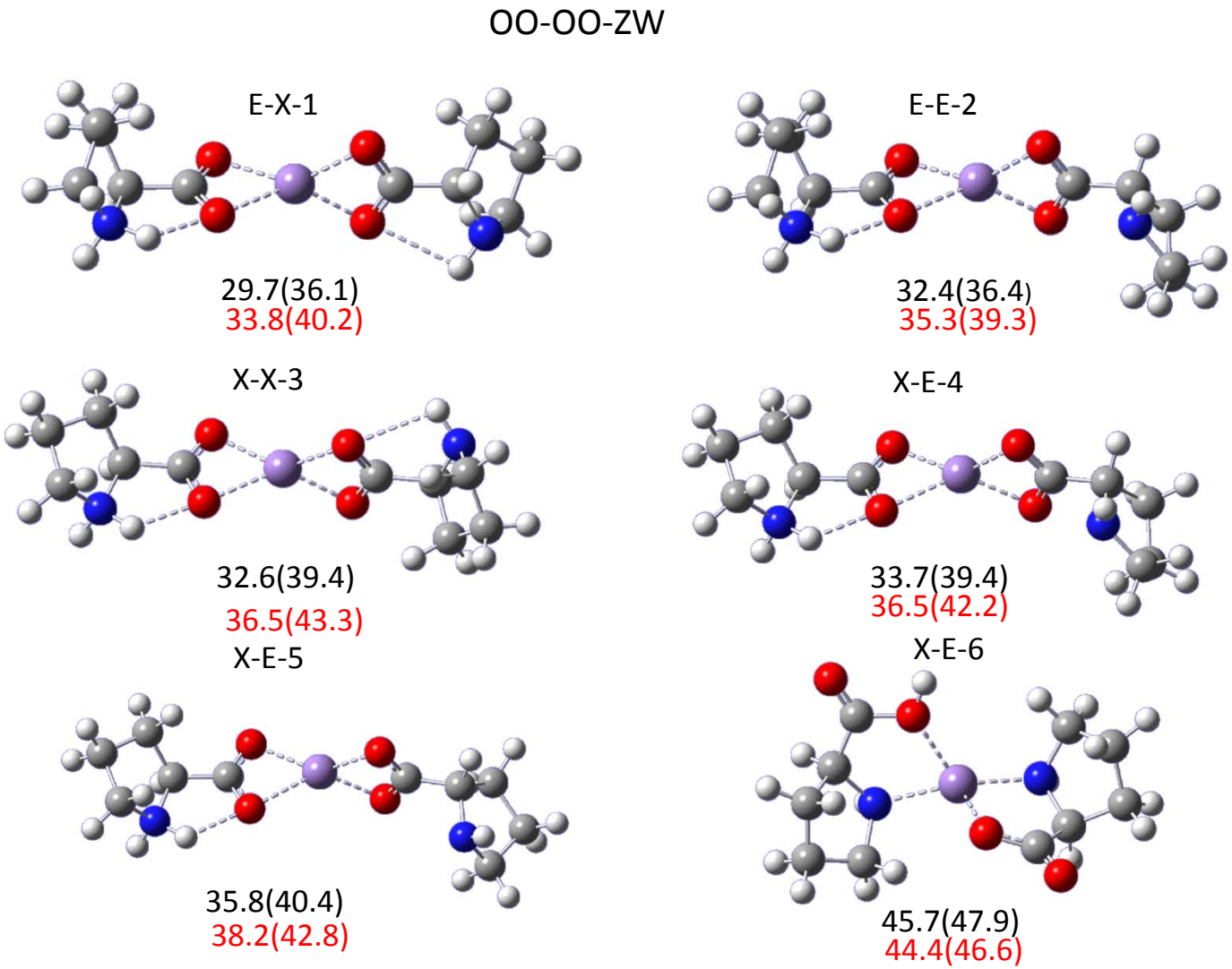



**Figure S16b).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-OO-ZW isomers of the $[Mn(Pro)_2\text{-}H]^+$ complex. The structures are all sextets.

OO-NO-ZW

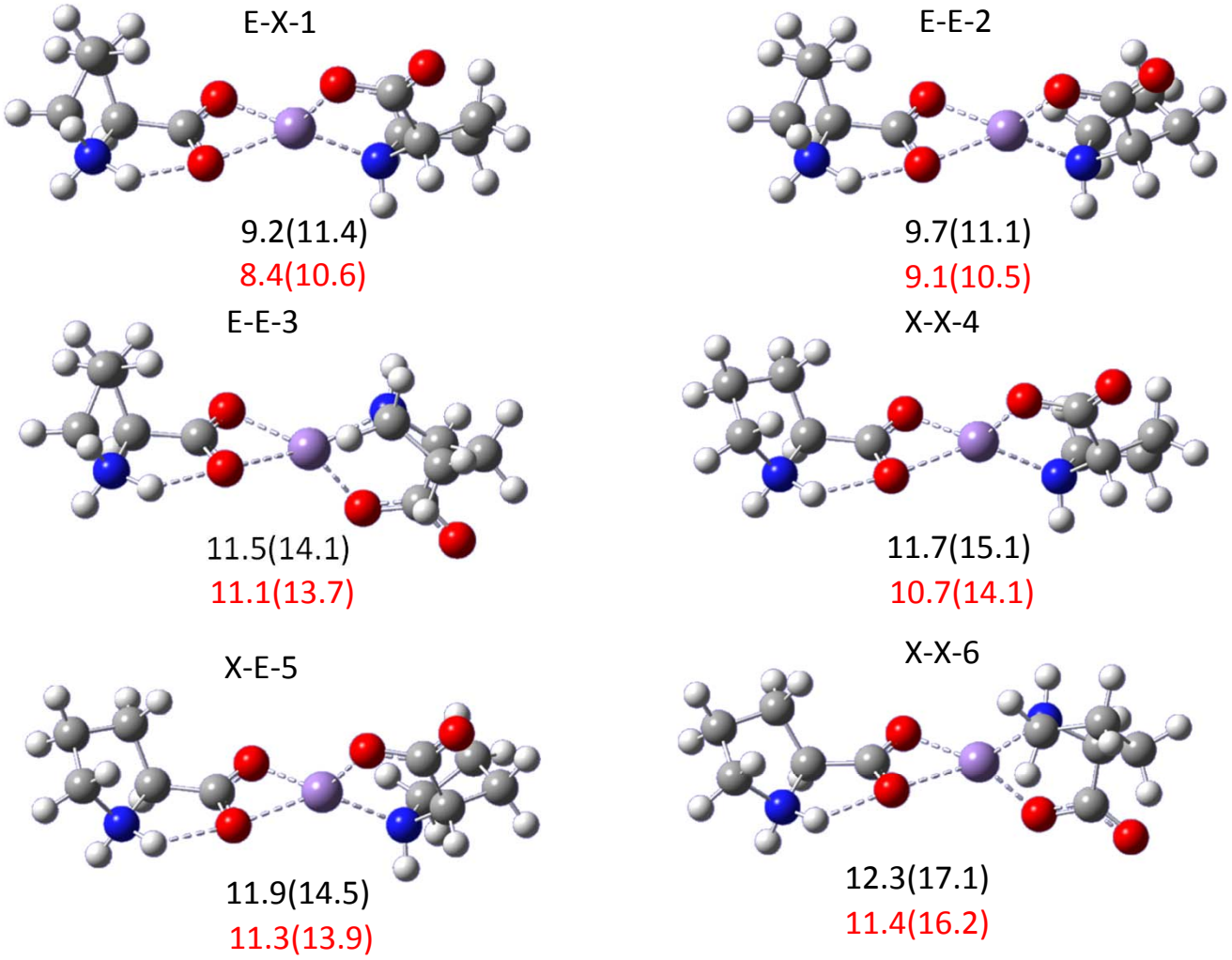
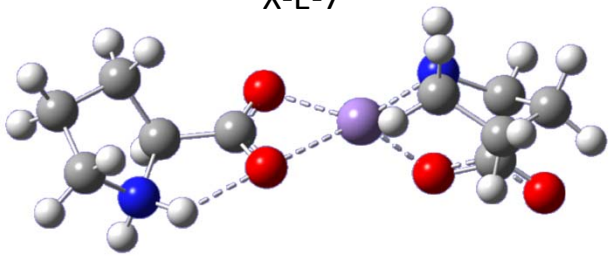



**Figure S16c).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the OO-NO-ZW isomers of the $[Mn(Pro)_2-H]^+$ complex. The structures are all sextets.

OO-NO-ZW

X-E-7



13.5(16.7)
12.9(16.1)

NO-OO-CS

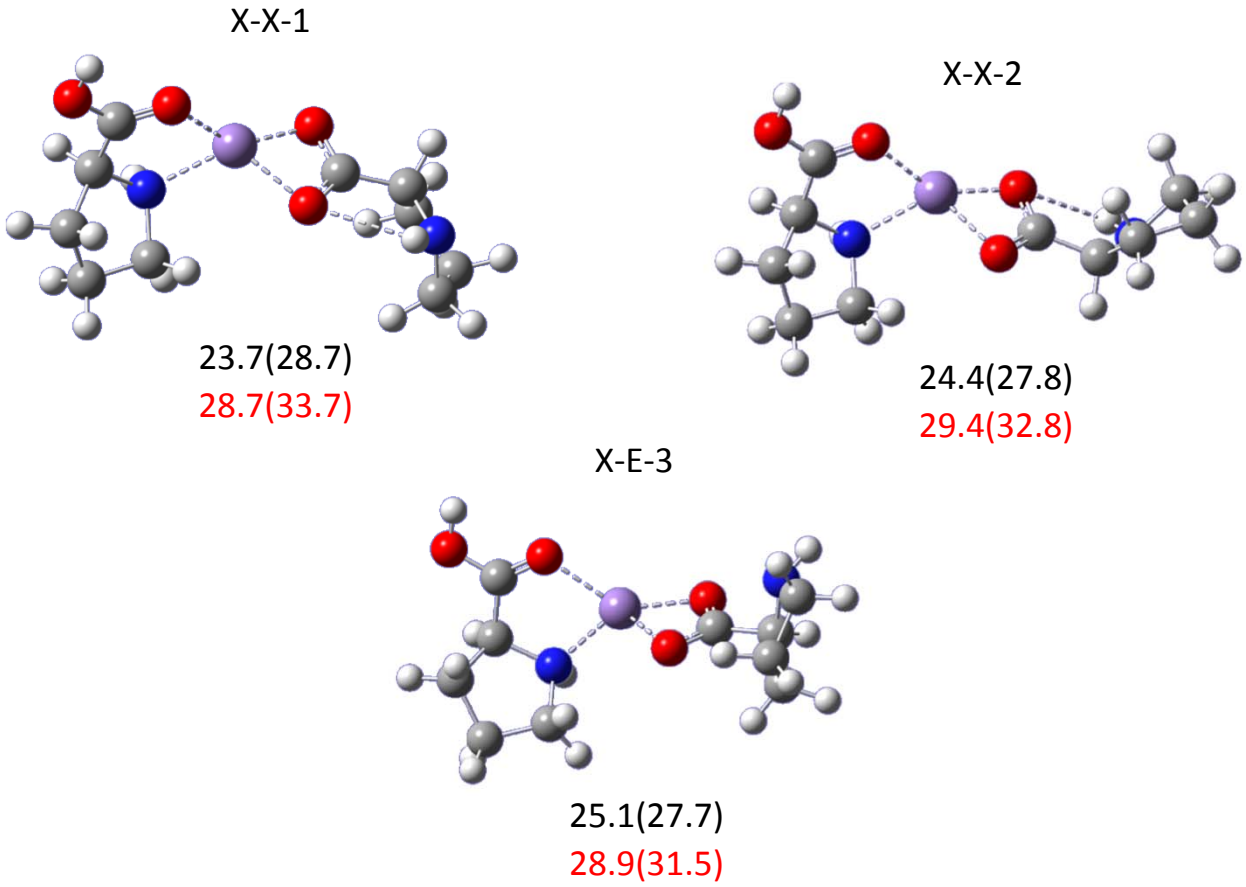



**Figure S16d).** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) (black color) and B3LYP/6- 31+G(d,p) (red color) for conformers of the NO-OO-CS isomers of the $[Mn(Pro)_2-H]^+$ complex. The structures are all sextets.

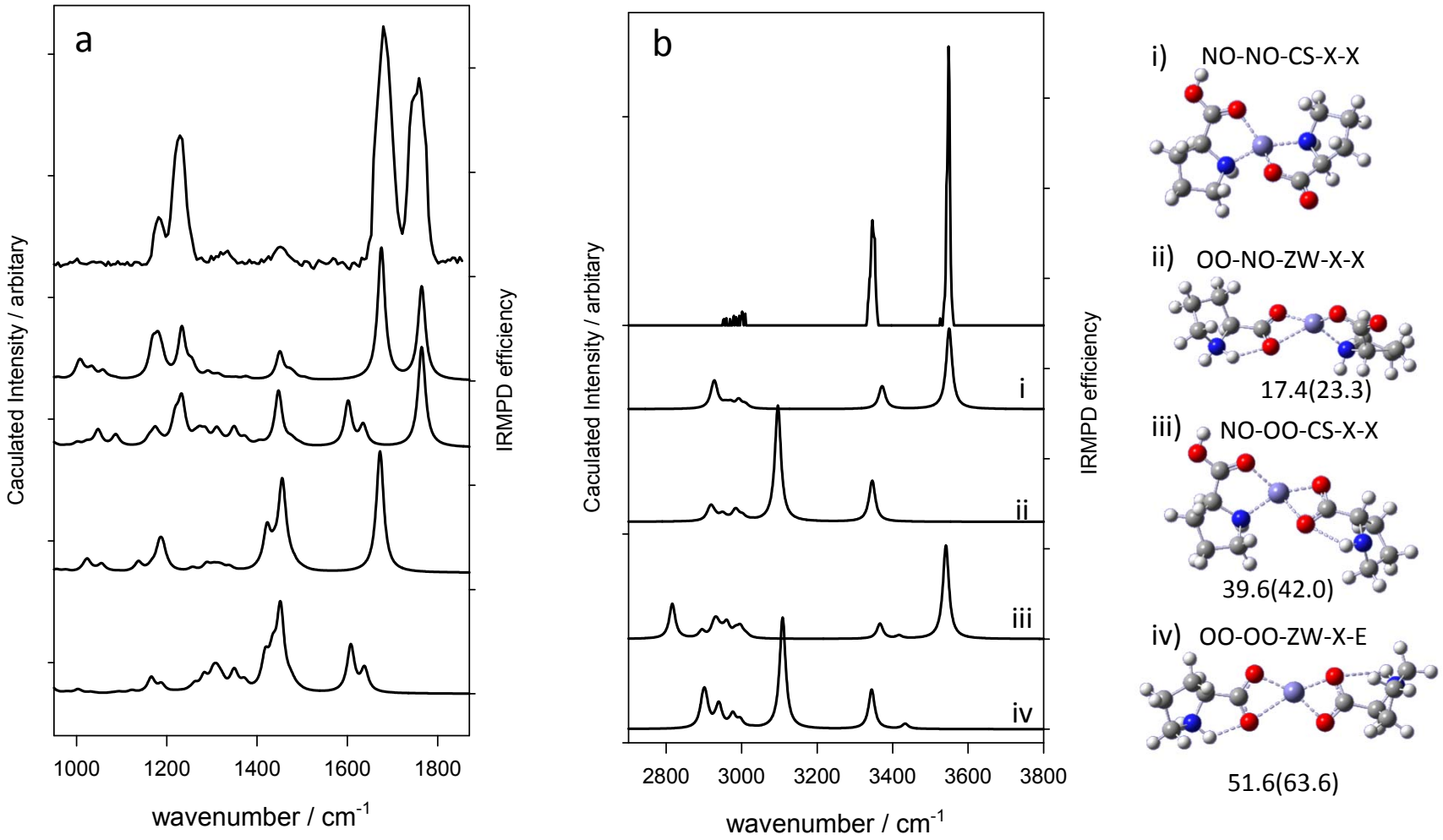



**Fig. S17.** Comparison of the experimental IRMPD spectrum and calculated absorbance spectra of the lowest energy structures of each form of the $[Fe(Pro)_2\text{-}H]^+$ in a) 1000 to 2000 $cm^{-1}$ region and b) 2800 to 3800 $cm^{-1}$ region.

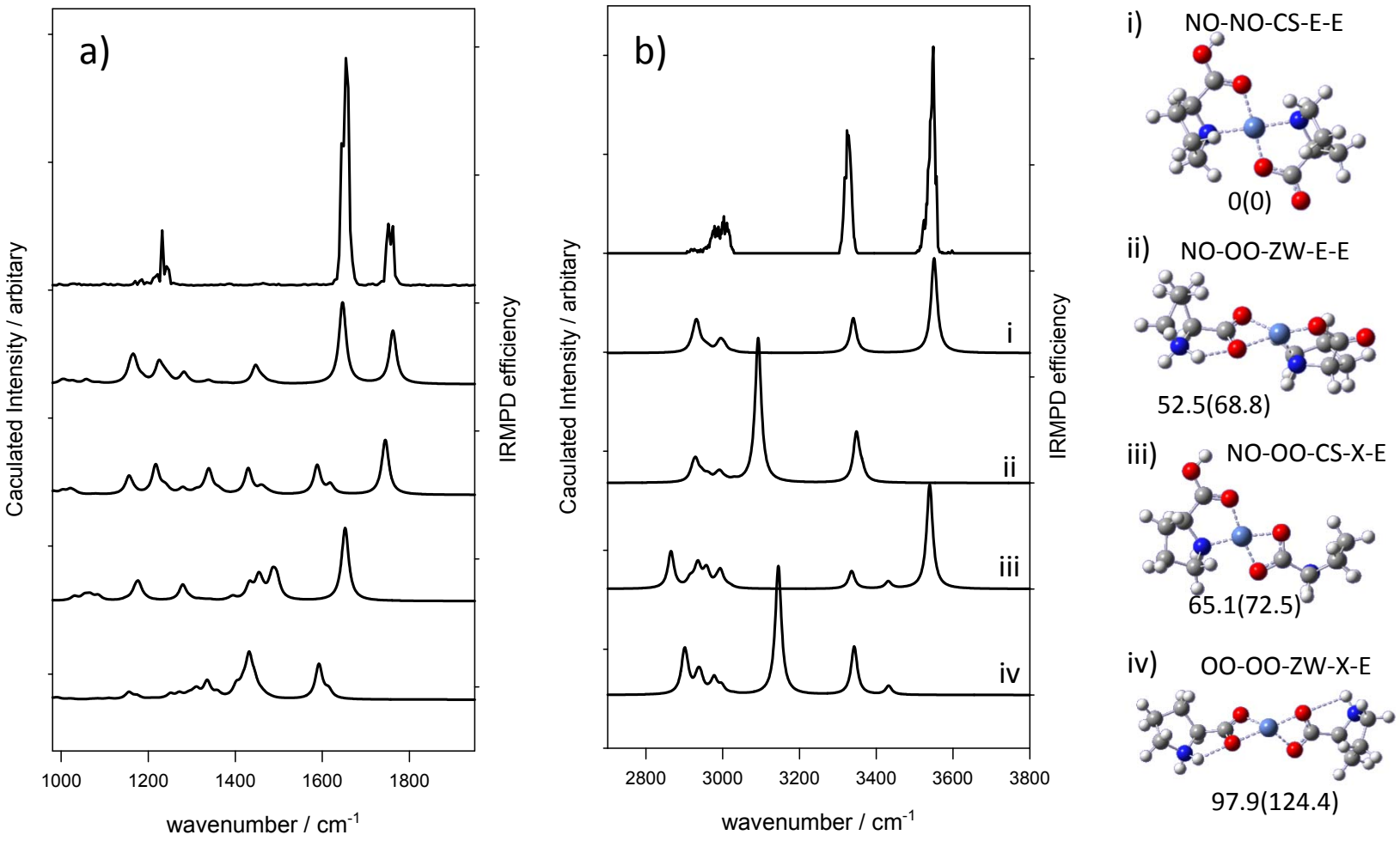



**Fig. S18.** Comparison of the experimental IRMPD spectrum and calculated absorbance of the lowest energy structures of each form of the $[Ni(Pro)_2\text{-}H]^+$ in a) 1000 to 2000 $cm^{-1}$ region and b) 2800 to 3800 $cm^{-1}$ region.

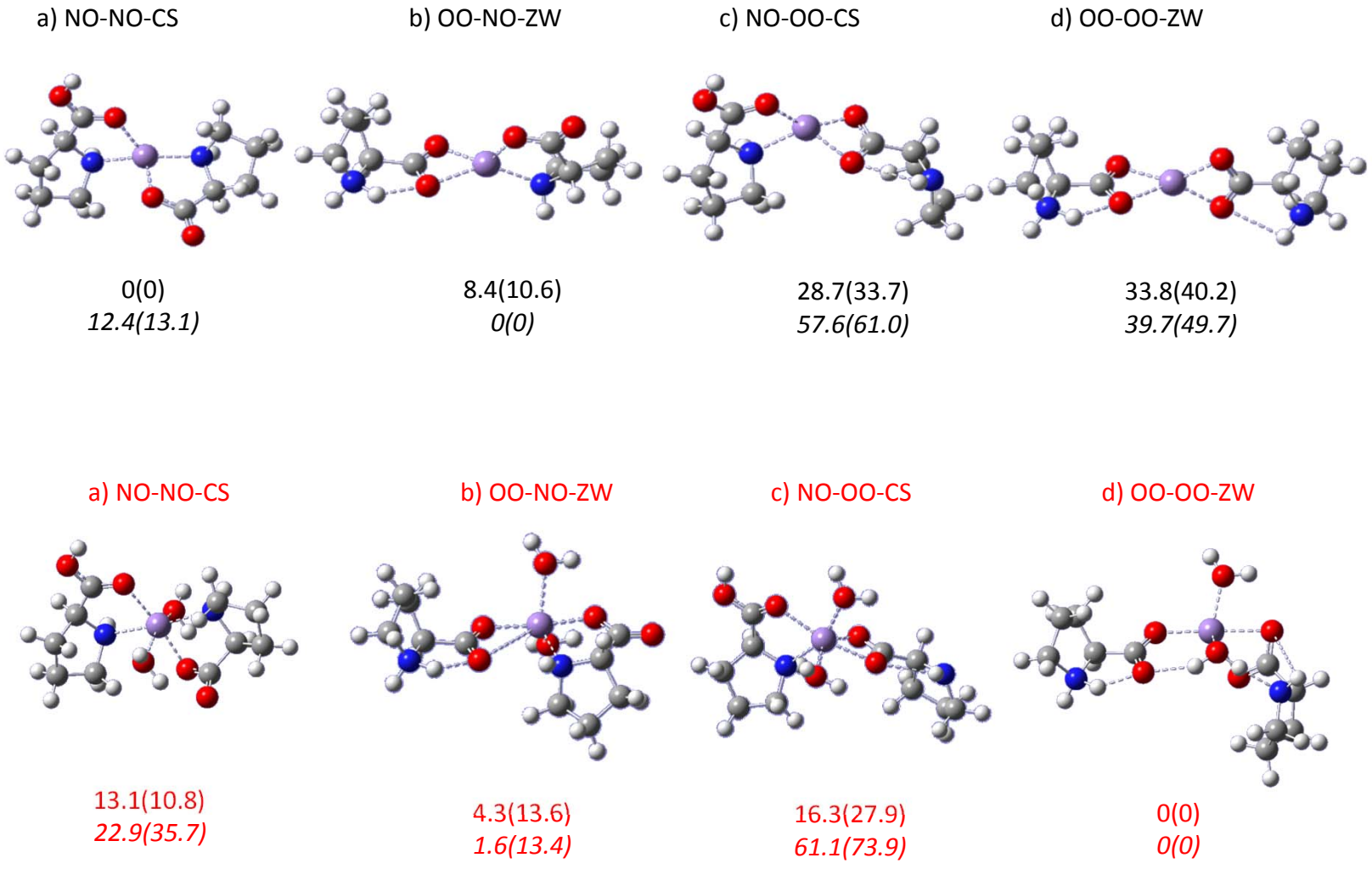



**Figure S19.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6- 31+G(d,p) for the lowest energy conformers of the $[Mn(Pro)_2\text{-}H]^+$ complex (black color) along with same complexes containing two explicit water molecules (red color) and using a PCM model (red italics). Values in black italics are bare ion PCM model calculations. The structures are all sextets.

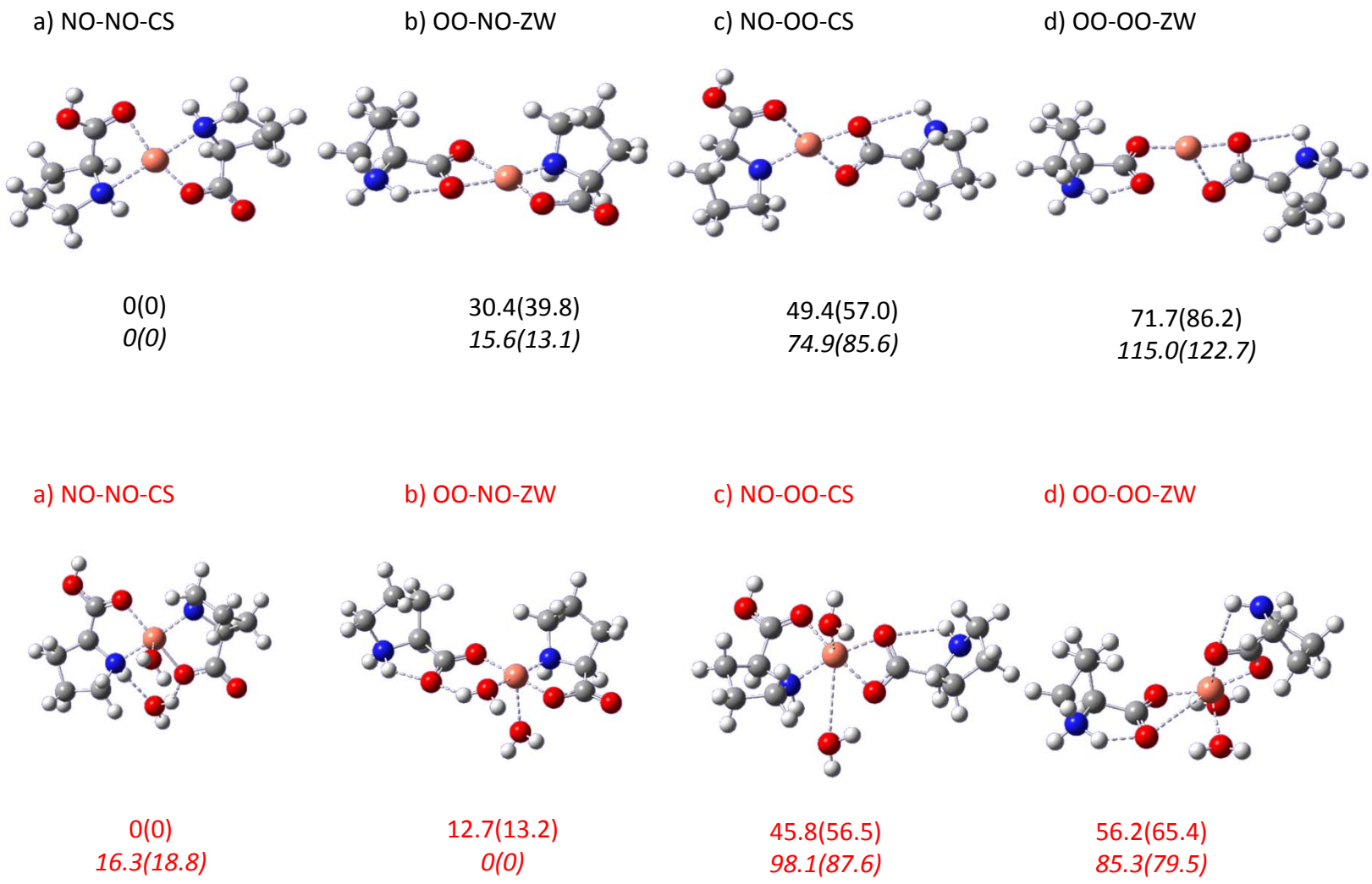



**Figure S20.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6- 31+G(d,p) for the lowest energy conformers of the $[Cu(Pro)_2\text{-}H]^+$ complex (black color) along with same complexes containing two explicit water molecules (red color) and using a PCM model (red italics). Values in black italics are bare ion PCM model calculations. The structures are all doublets.

NO-NO-CS

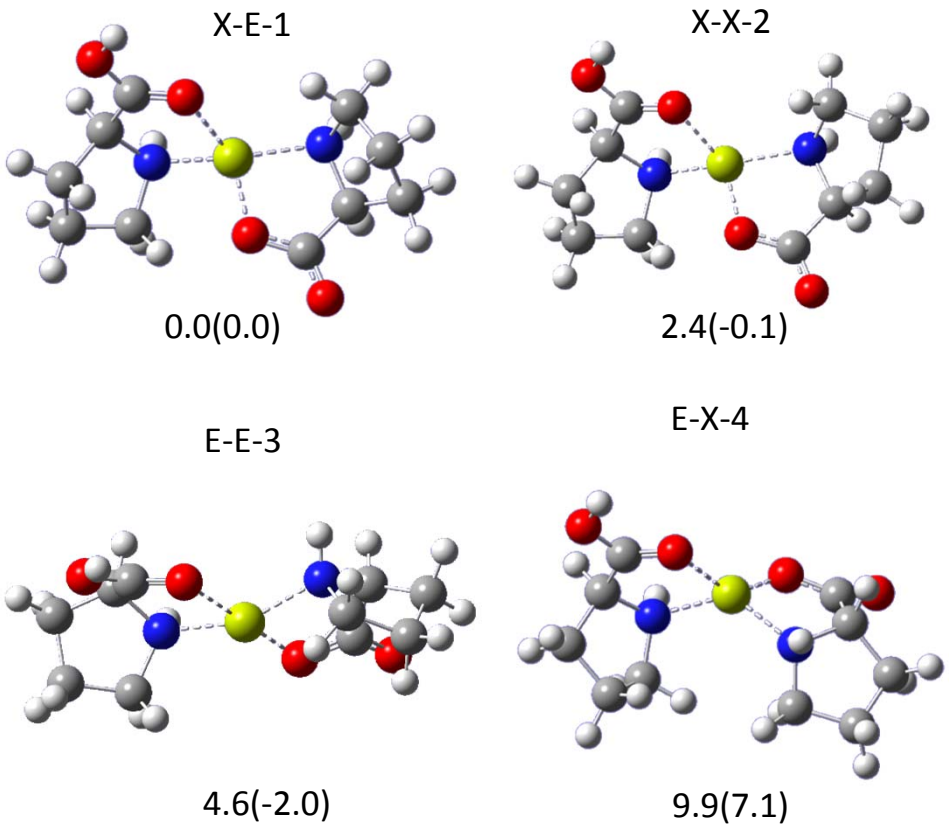



**Fig. S21. a.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) for conformers of the NO-NO-CS isomers of the $[Mg(Pro)_2-H]^+$ complex.

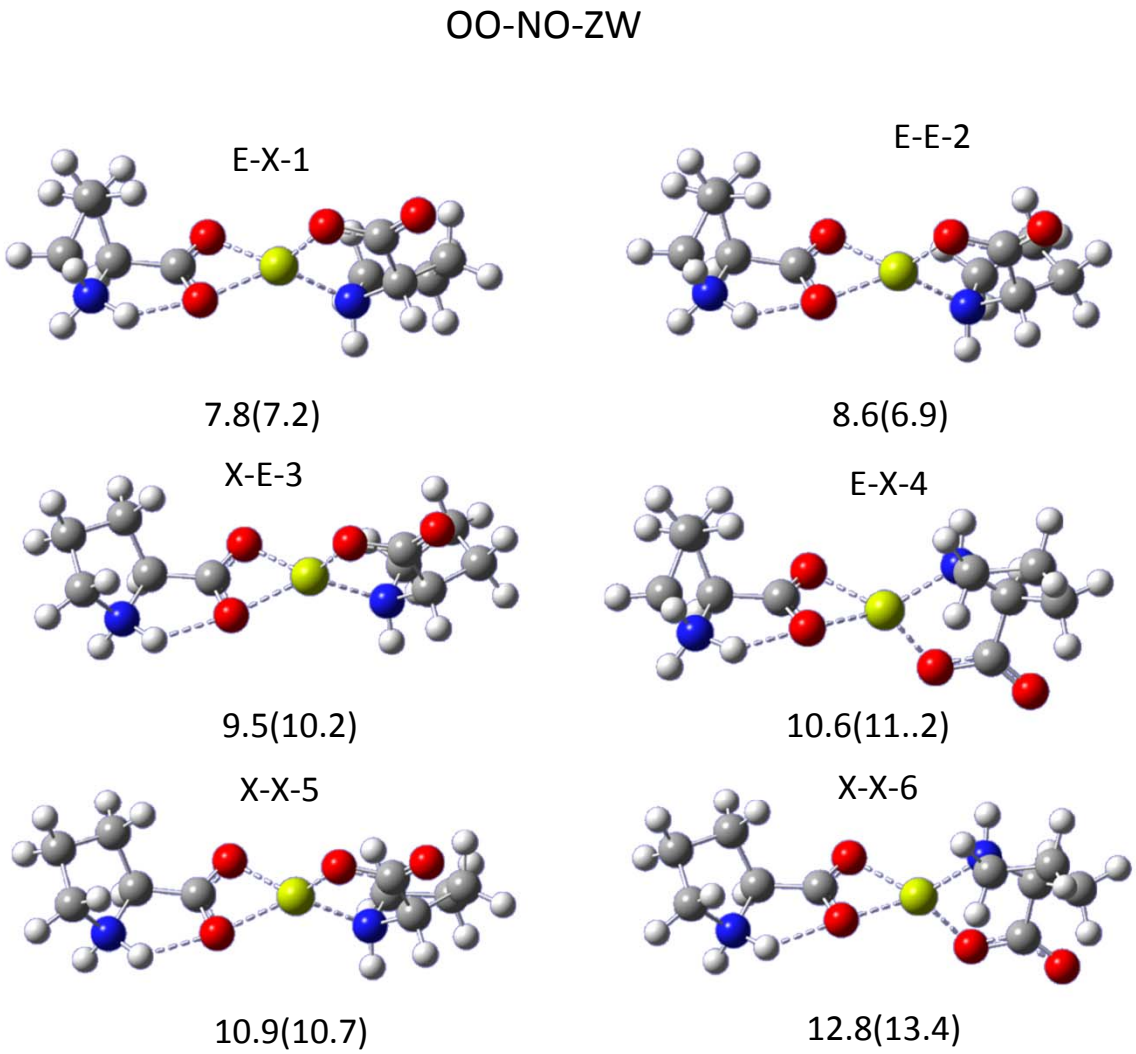



**Fig. S21. b.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) for conformers of the OO-NO-ZW isomers of the $[Mg(Pro)_2-H]^+$ complex.

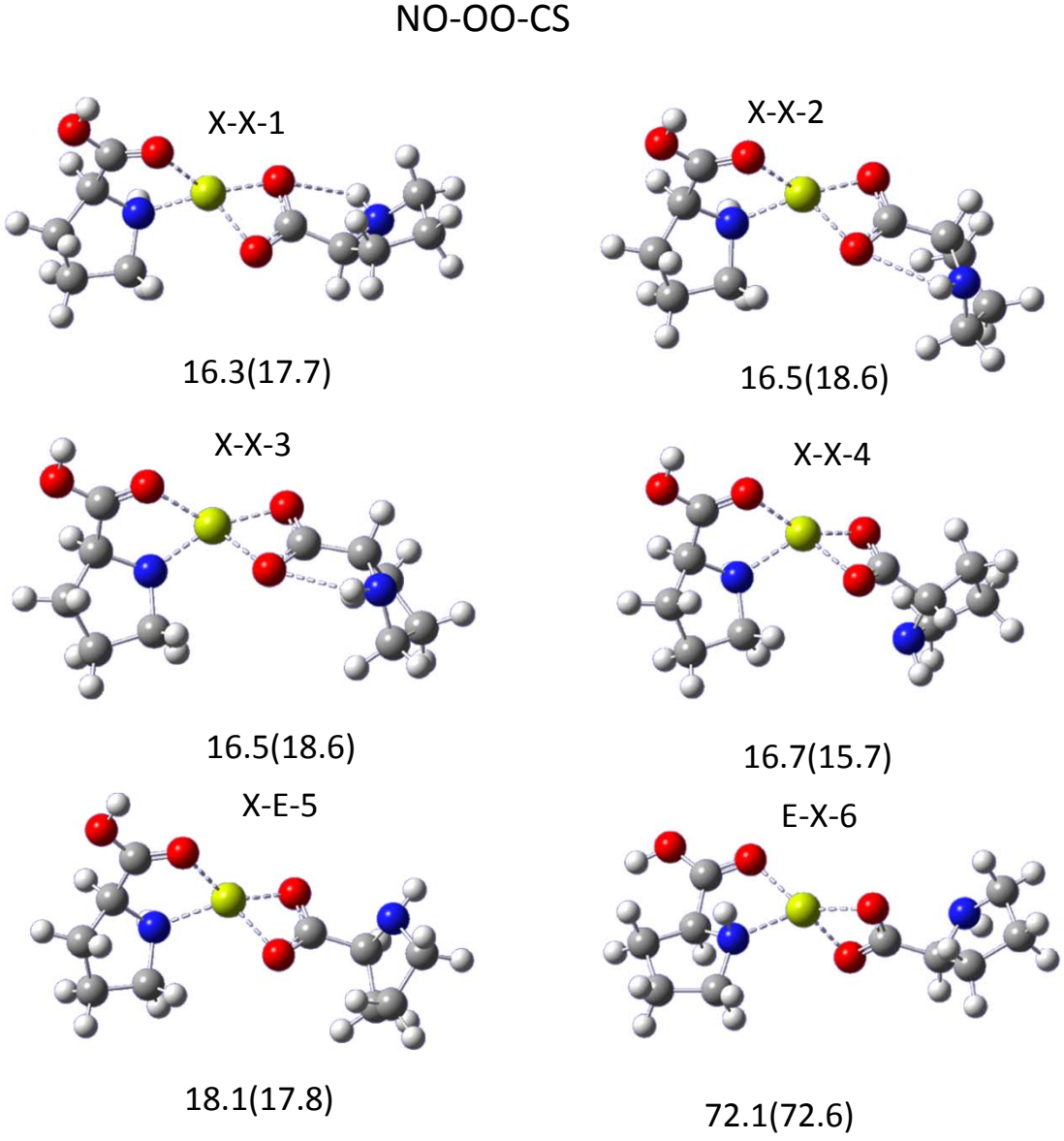



**Fig. S21. c.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the NO-OO-CS isomers of the $[Mg(Pro)_2-H]^+$ complex.

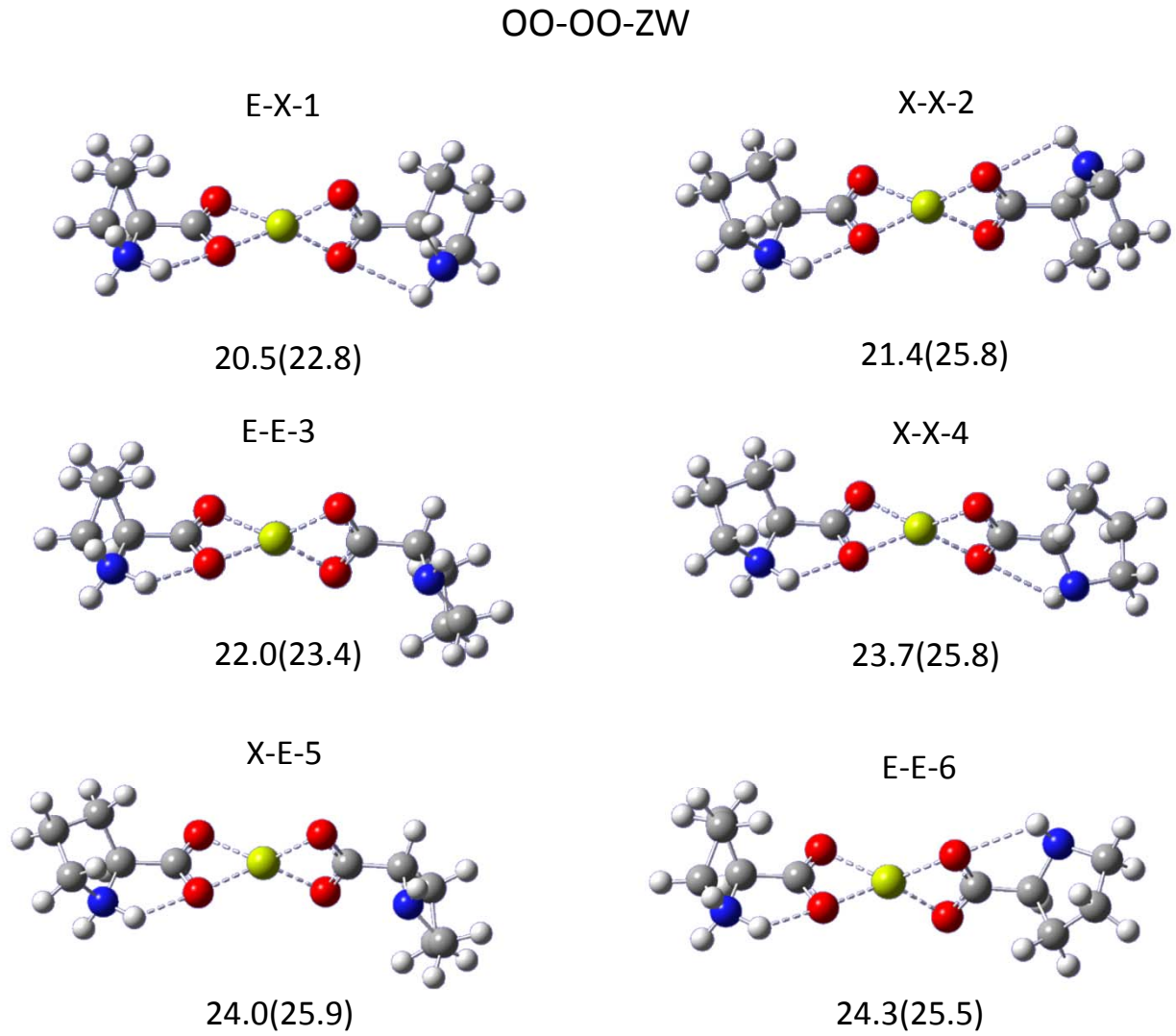
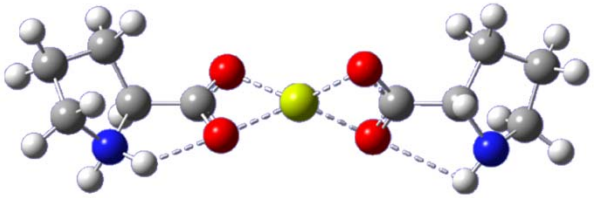



**Fig. S21. d.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) for conformers of the OO-OO-ZW isomers of the $[Mg(Pro)_2-H]^+$ complex.

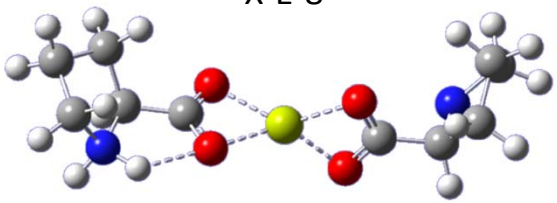
OO-OO-ZW

X-X-7



24.4(27.6)

X-E-8



24.7(26.3)

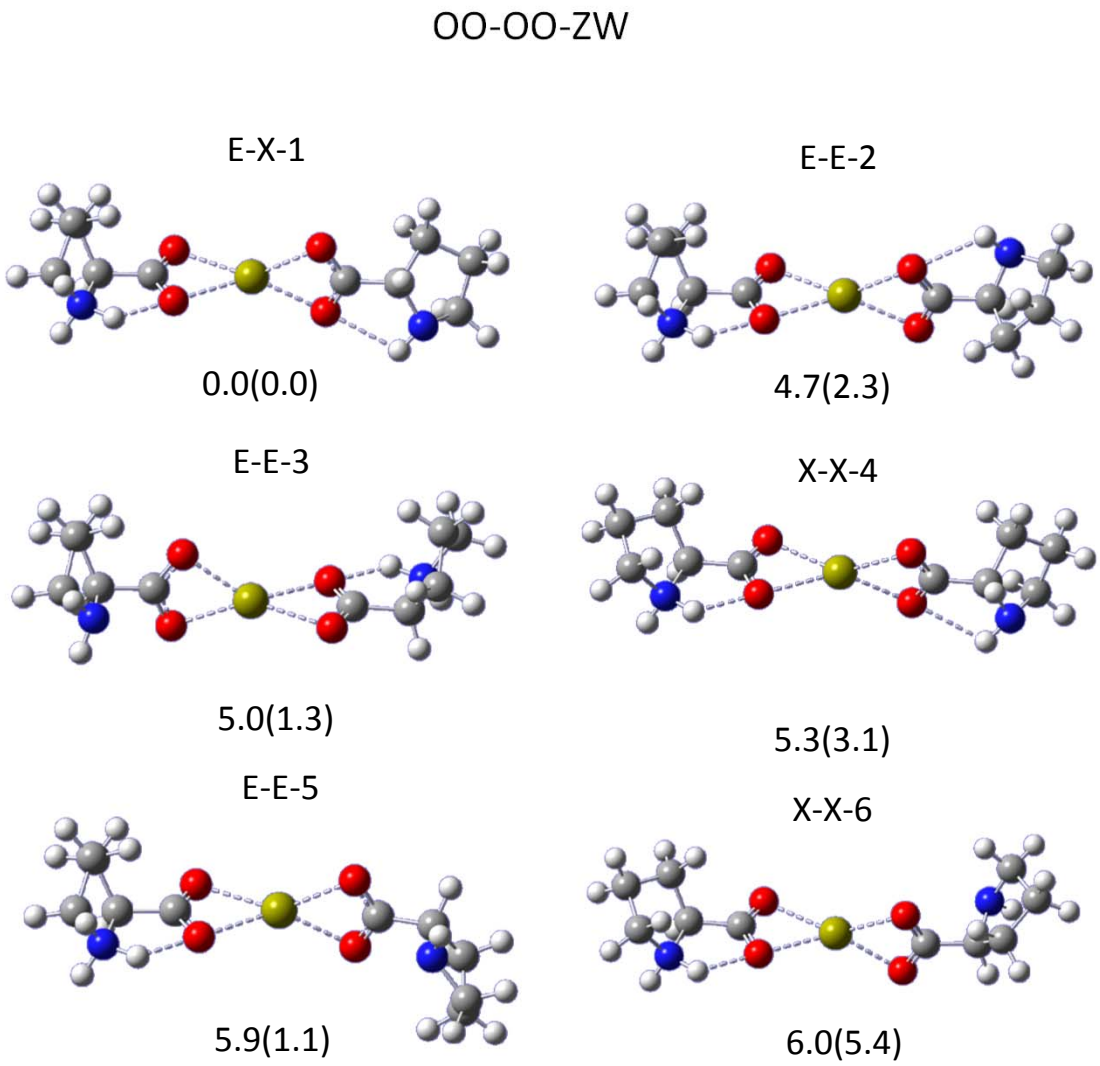
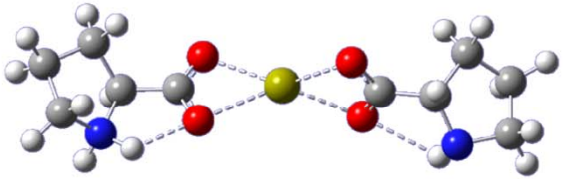



**Fig. S22. a.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) for conformers of the OO-OO-ZW isomers of the $[Ca(Pro)_2-H]^+$ complex.

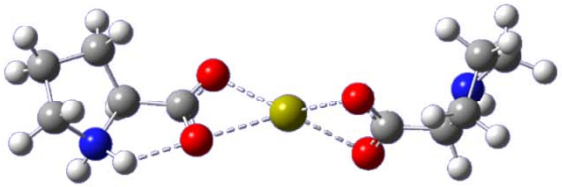
OO-OO-ZW

X-E-7



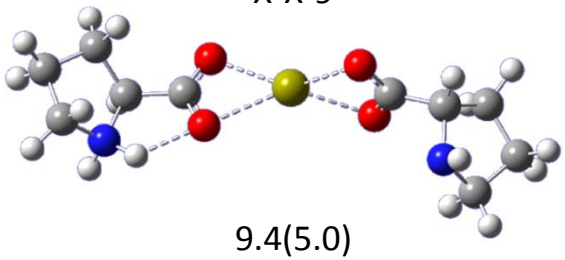
6.9(4.6)

X-E-8



7.8(4.5)

X-X-9



9.4(5.0)

OO-NO-ZW

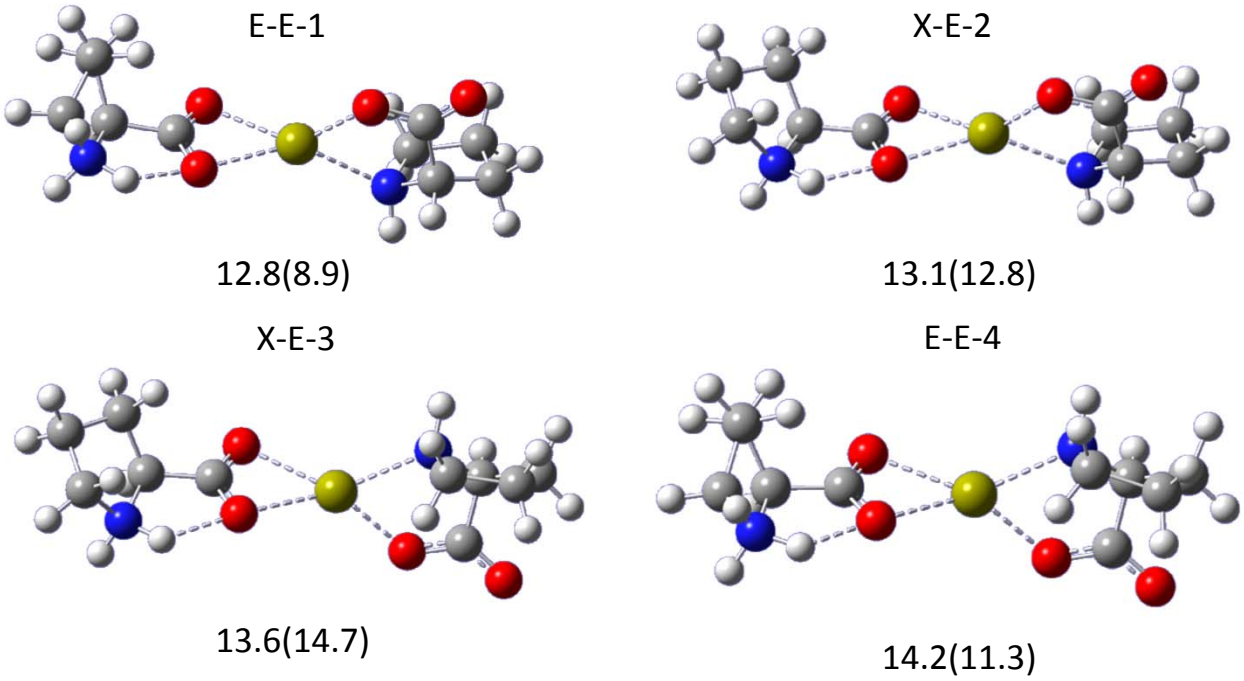



**Fig. S22. b.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)//6-31+G(d,p) for conformers of the OO-NO-ZW isomers of the $[Ca(Pro)_2-H]^+$ complex.

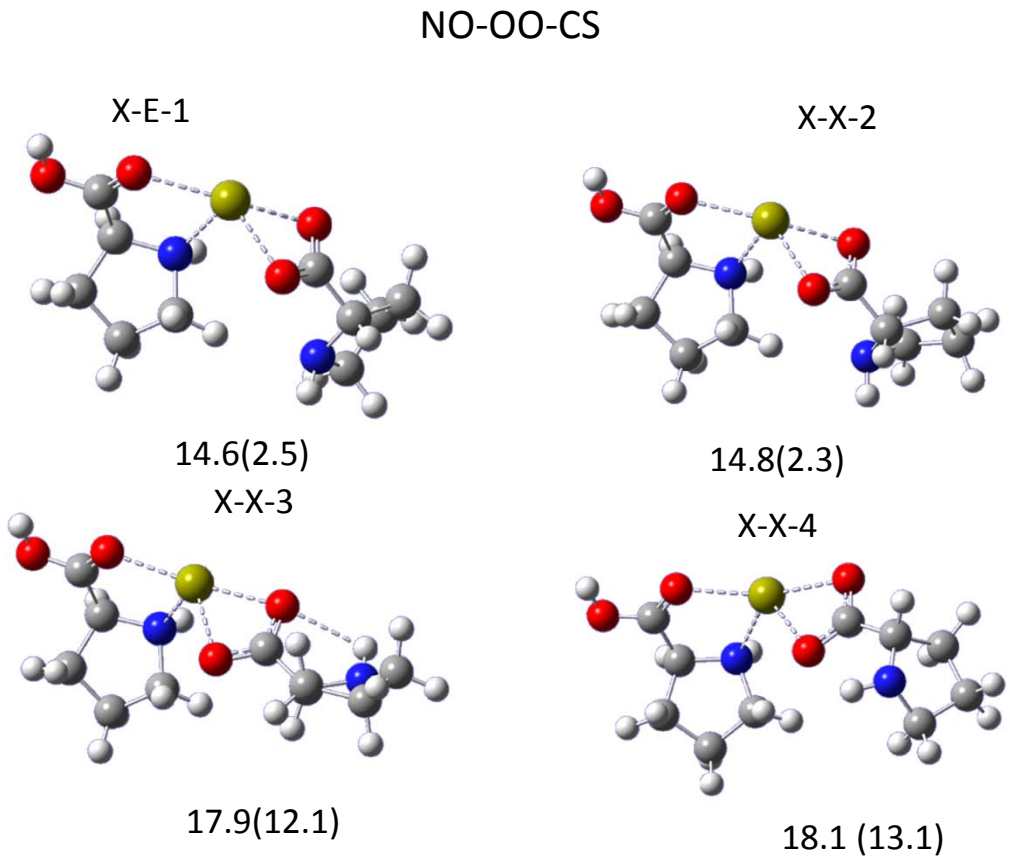
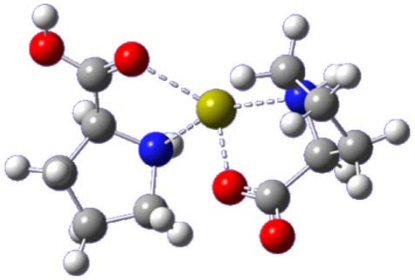



**Fig. S22. c.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the NO-OO-CS isomers of the $[Ca(Pro)_2-H]^+$ complex.

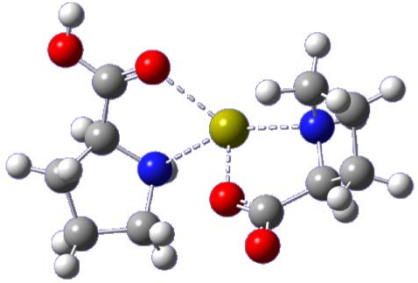
NO-NO-CS

X-X-1



31.2(16.2)

X-X-2

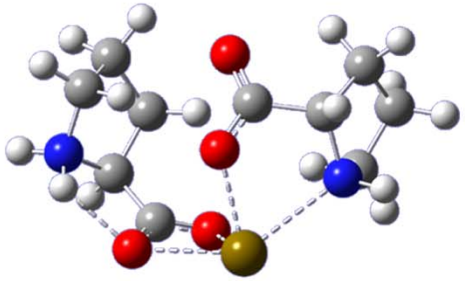


25.5(18.7)

**Fig. S22. d.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the NO-NO-CS isomers of the $[Ca(Pro)_2-H]^+$ complex.

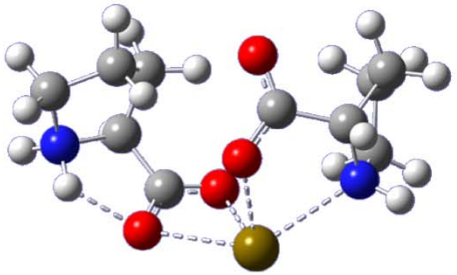
OO-NO-ZW

X-X-1



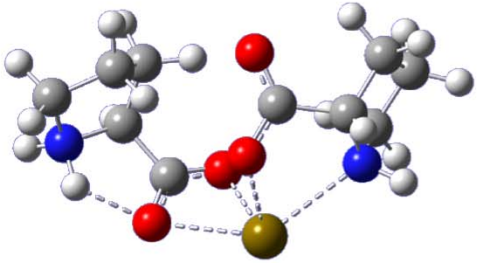
0(0)

E-E-2



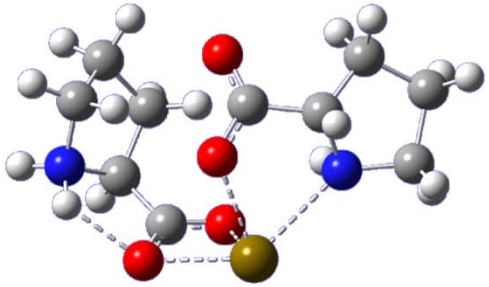
2.4(5.6)

E-X-3



6.7(6.5)

X-E-4



11.4(10.9)

**Fig. S23. a.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the OO-NO-ZW isomers of the $[Sr(Pro)_2-H]^+$ complex.

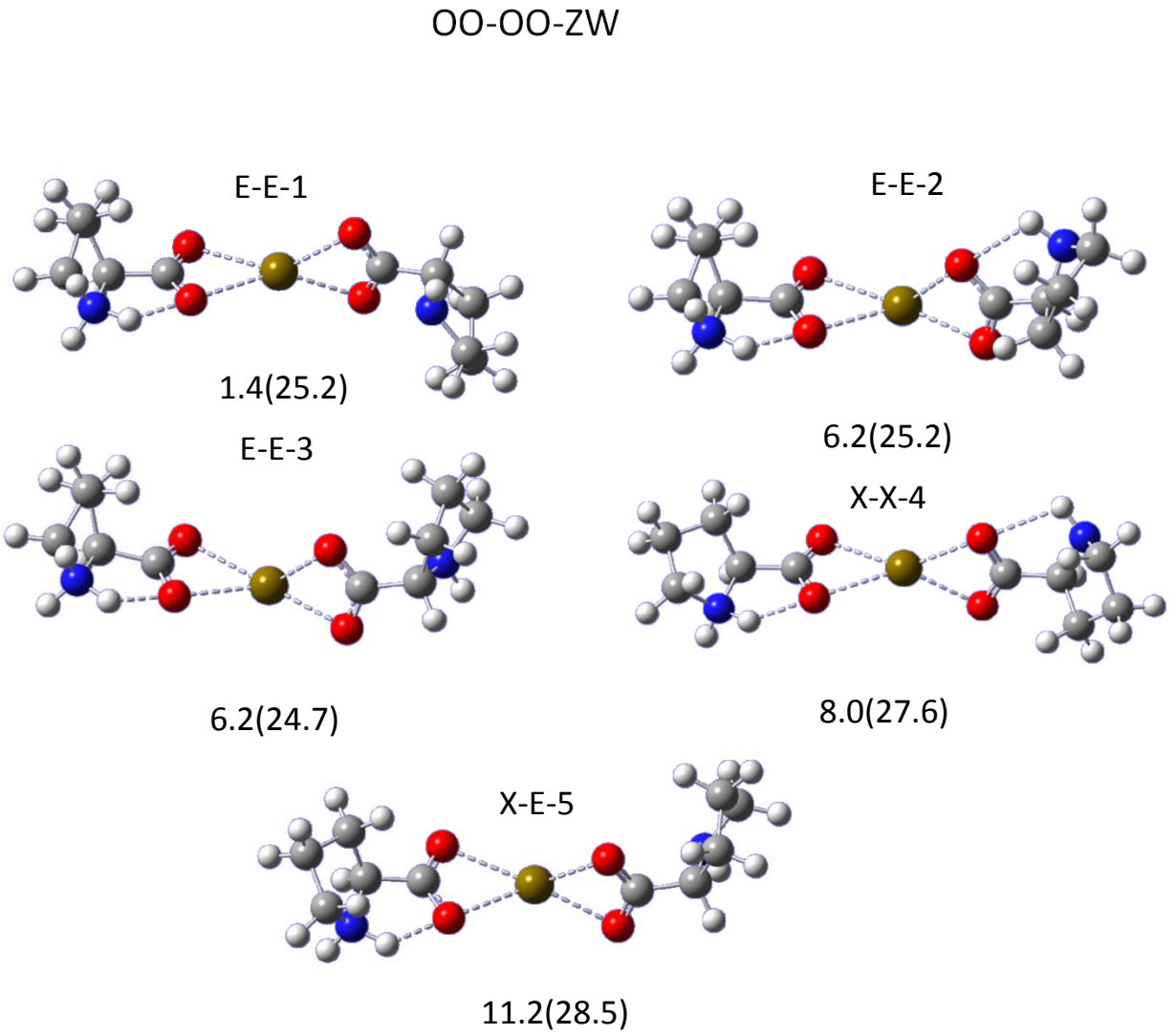



**Fig. S23. b.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the OO-OO-ZW isomers of the $[Sr(Pro)_2\text{-}H]^+$ complex.

NO-OO-CS

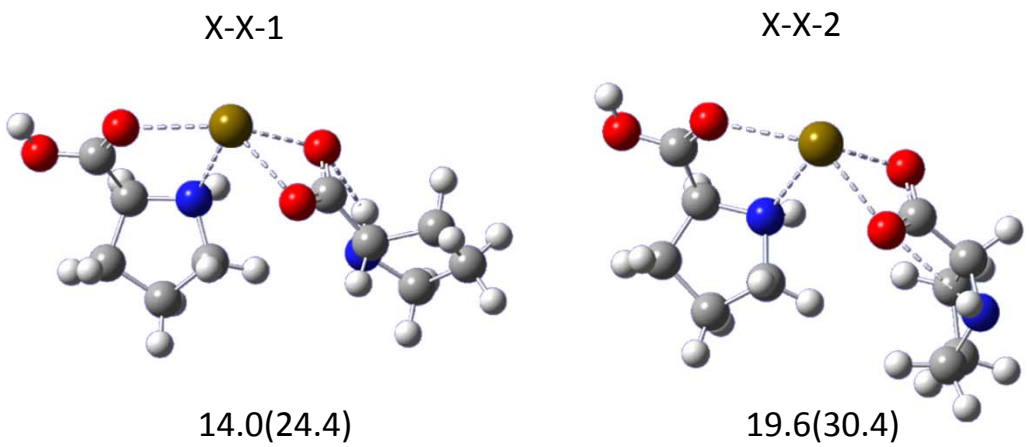



**Fig. S23. c.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the NO-OO-CS isomers of the $[Sr(Pro)_2-H]^+$ complex.

NO-NO-CS

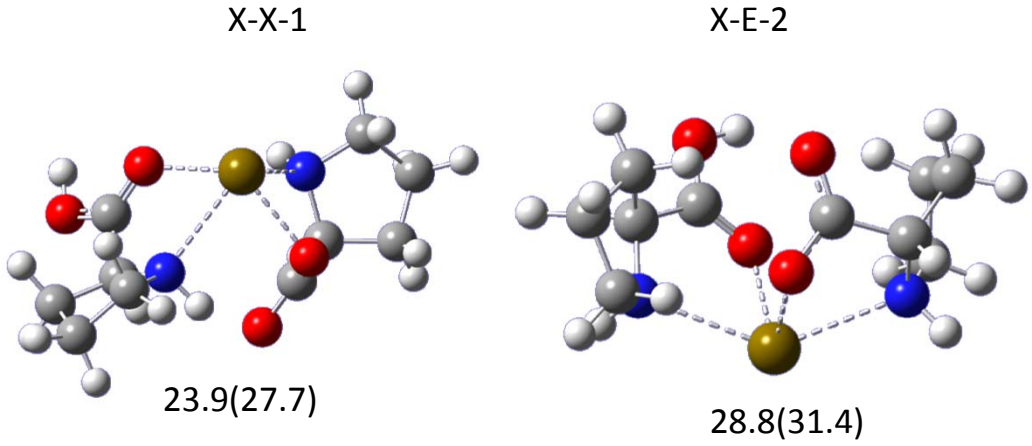



**Fig. S23. d.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the NO-NO-CS isomers of the $[Sr(Pro)_2-H]^+$ complex.

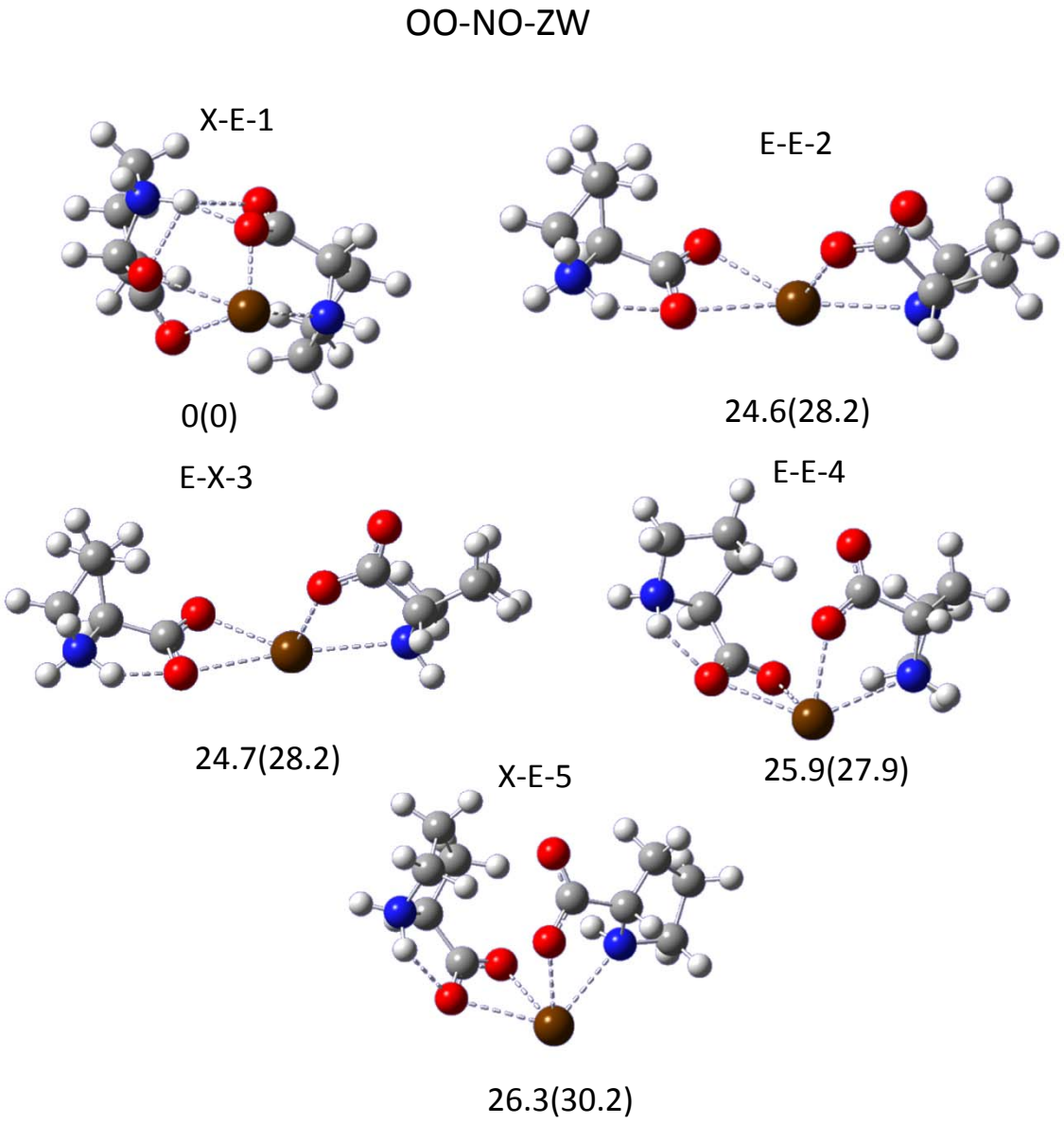



**Fig. S24. a.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the OO-NO-ZW isomers of the $[Ba(Pro)_2-H]^+$ complex.

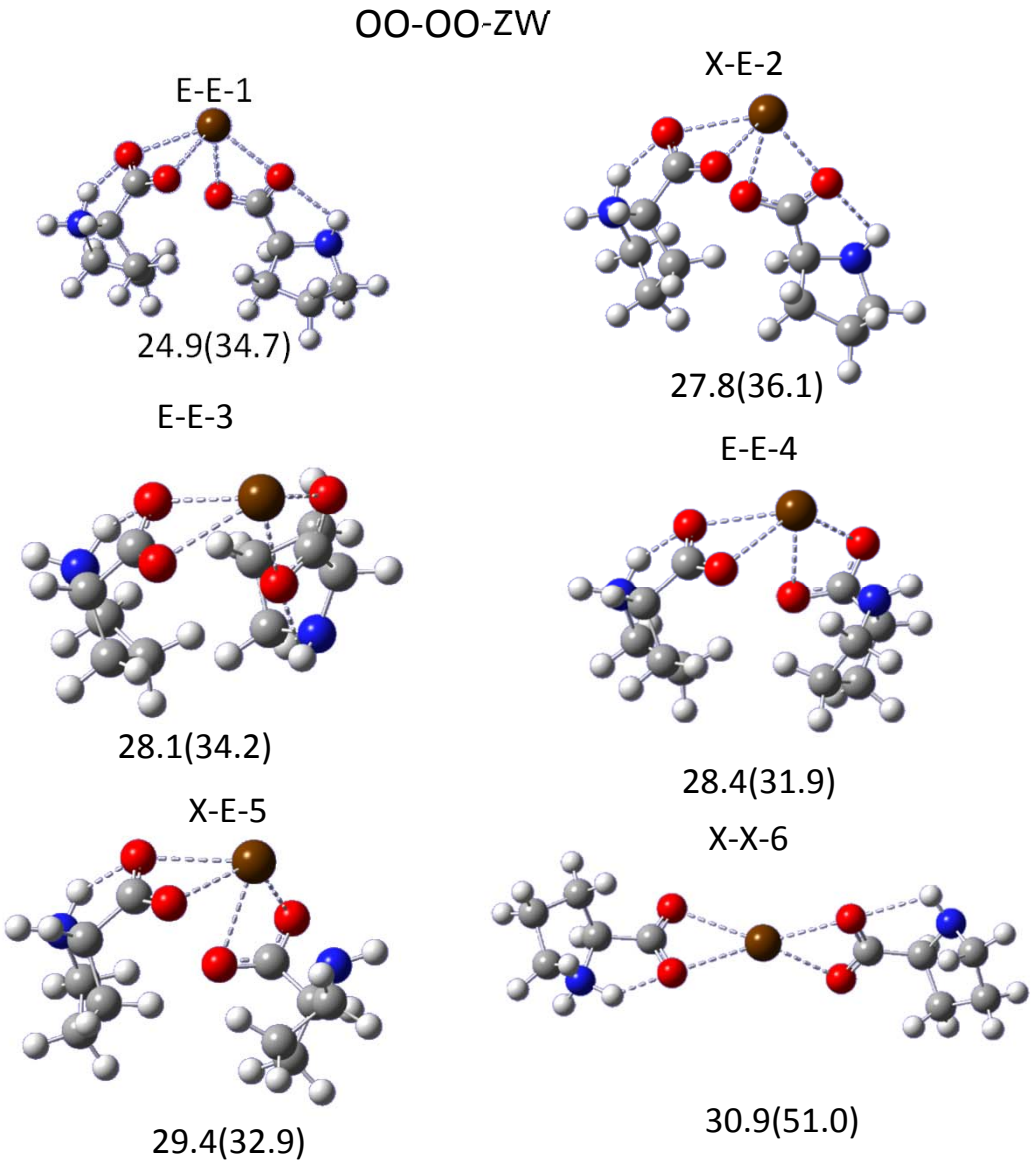
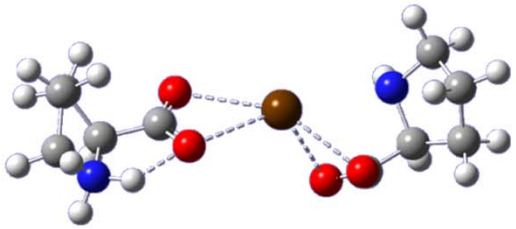



**Fig. S24. b.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the OO-OO-ZW isomers of the $[Ba(Pro)_2-H]^+$ complex.

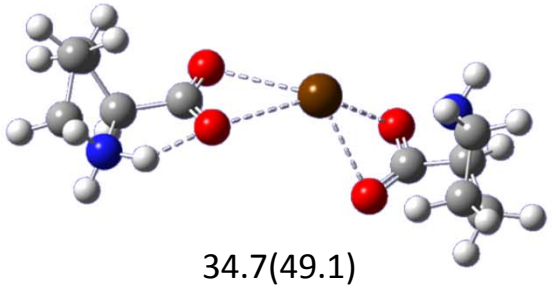
OO-OO-ZW

E-E-7



31.4(48.5)

E-E-8



34.7(49.1)

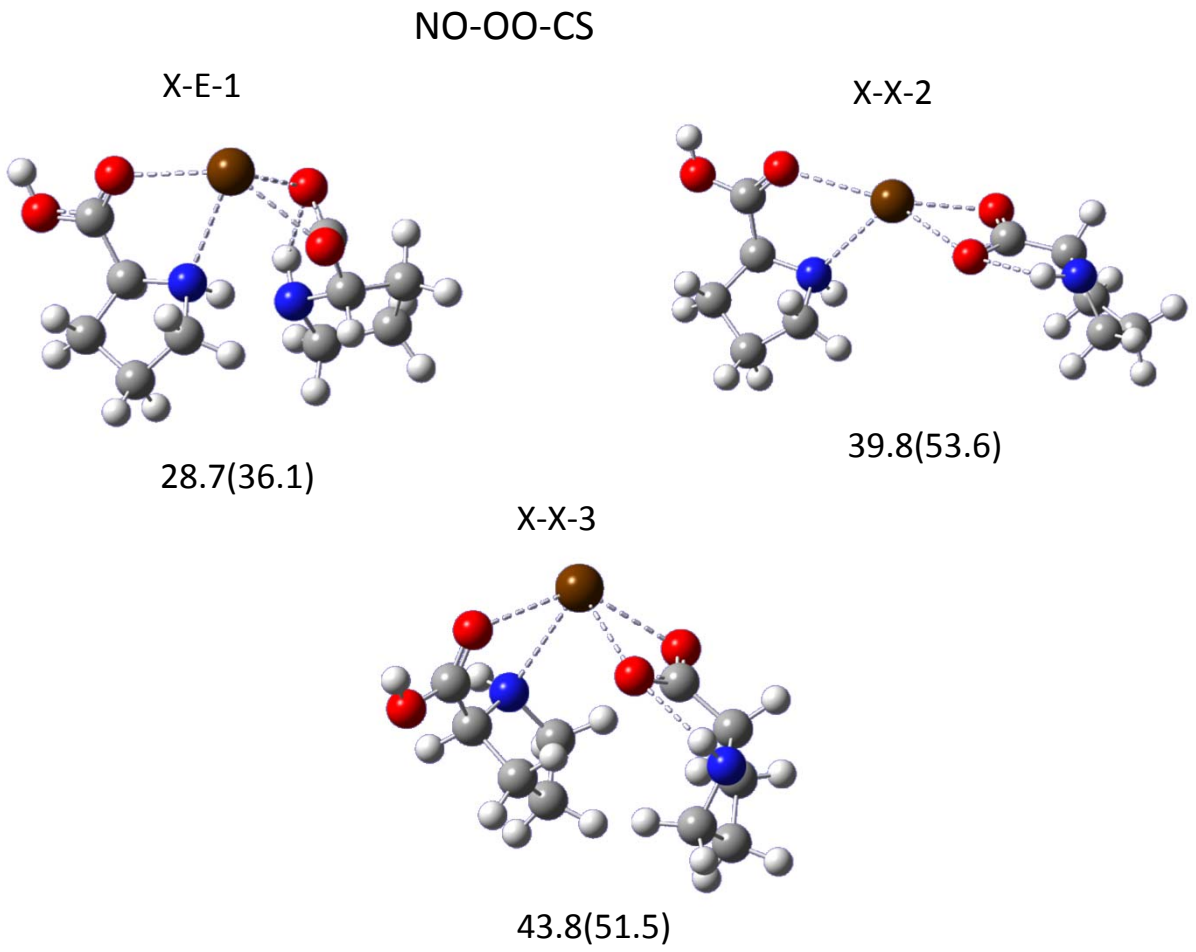



**Fig. S24. c.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the NO-OO-CS isomers of the $[Ba(Pro)_2-H]^+$ complex.

NO-NO-CS

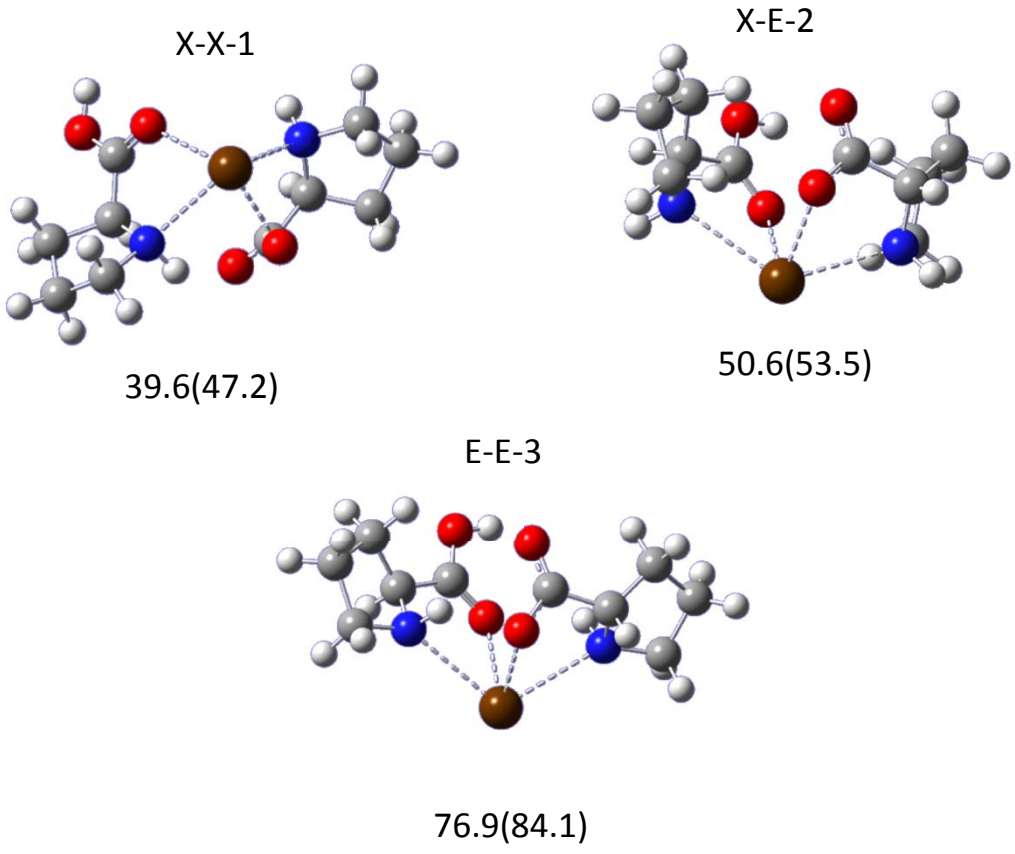



**Fig. S24. d.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6-311++G(3d,3p)// 6-31+G(d,p) for conformers of the NO-NO-CS isomers of the $[Ba(Pro)_2-H]^+$ complex.

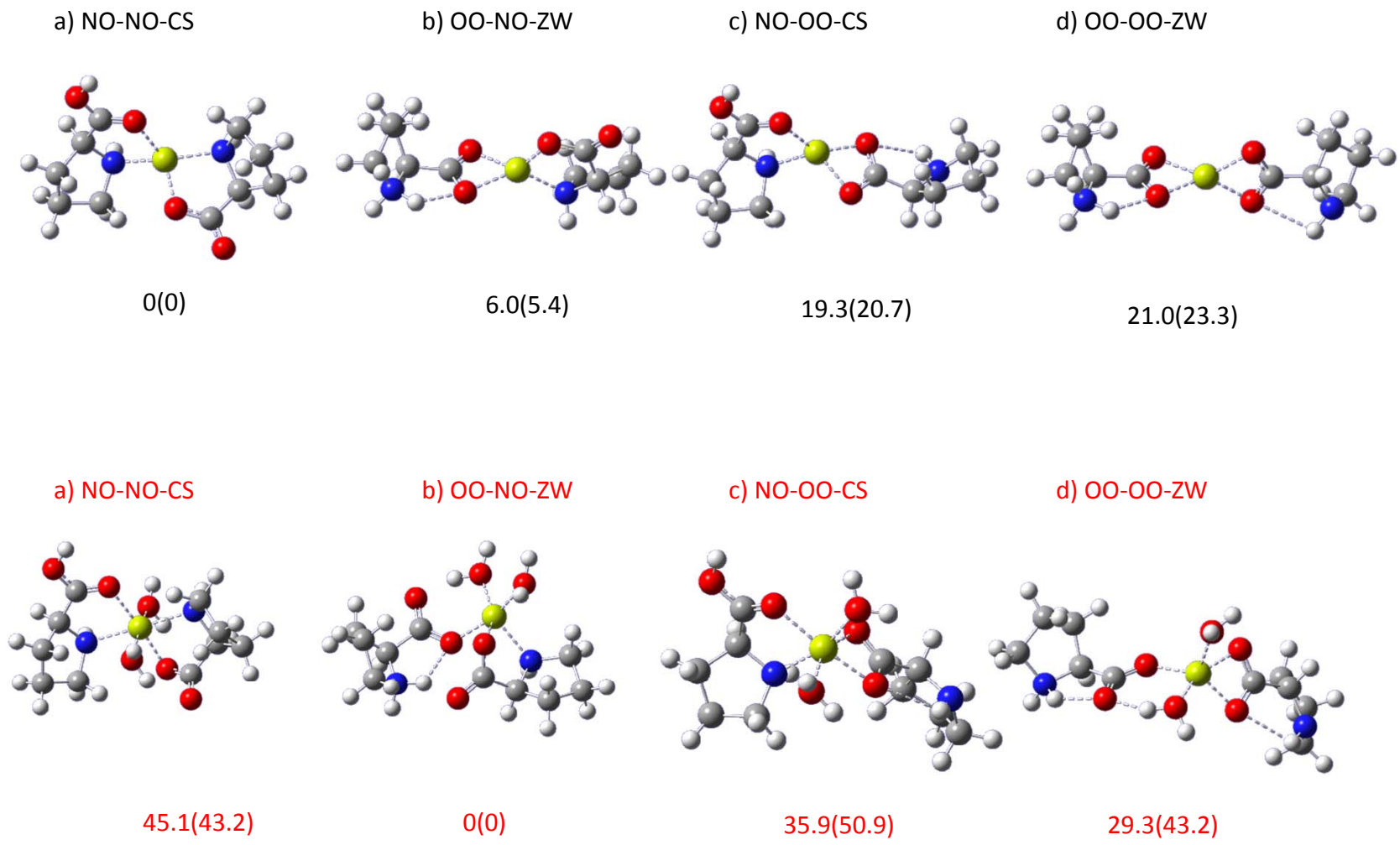



**Figure S25.** Relative 298 K Gibbs free energies and (enthalpies) computed using B3LYP/6- 31+G(d,p) for the lowest energy conformers of the $[Mg(Pro)_2\text{-}H]^+$ complex (black color) along with same complexes containing two explicit water molecules (red color).

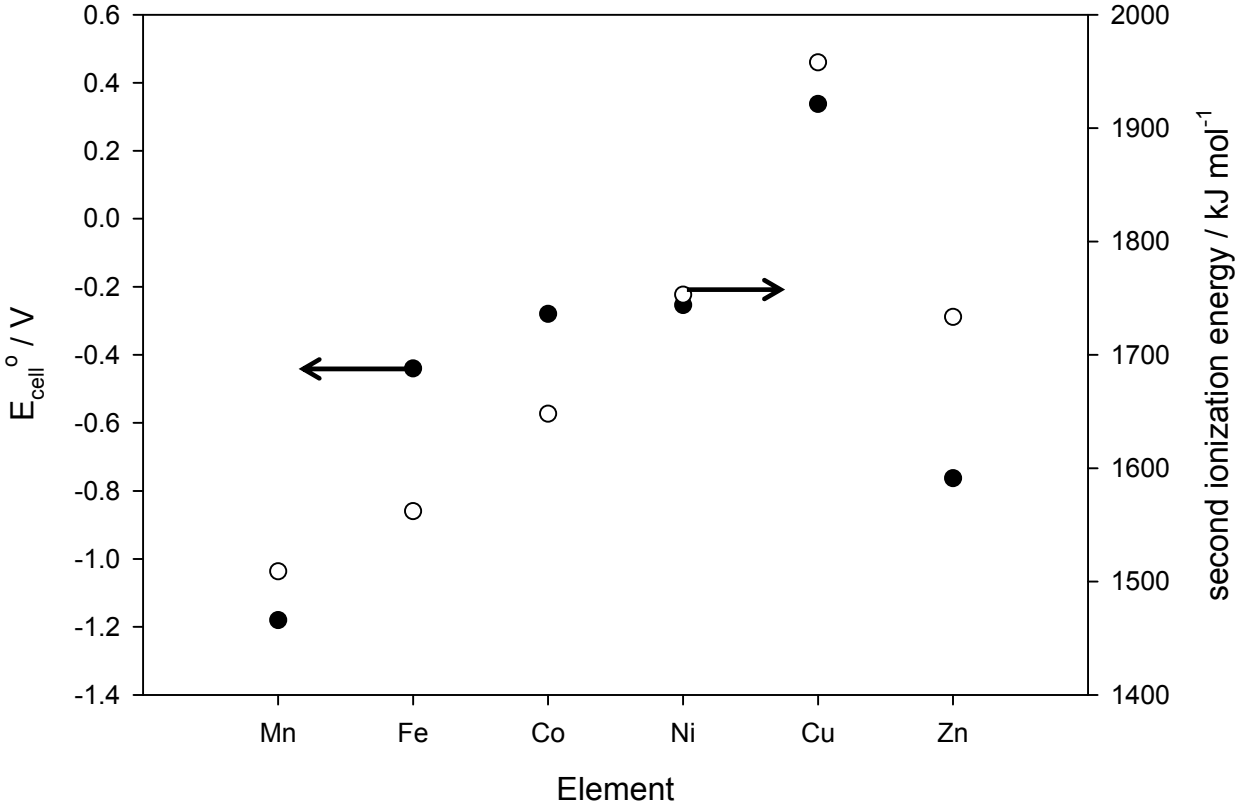



**Figure S26.** Plot of standard reduction potentials and 2-electron ionization energies for the transition metals of topic to this study.

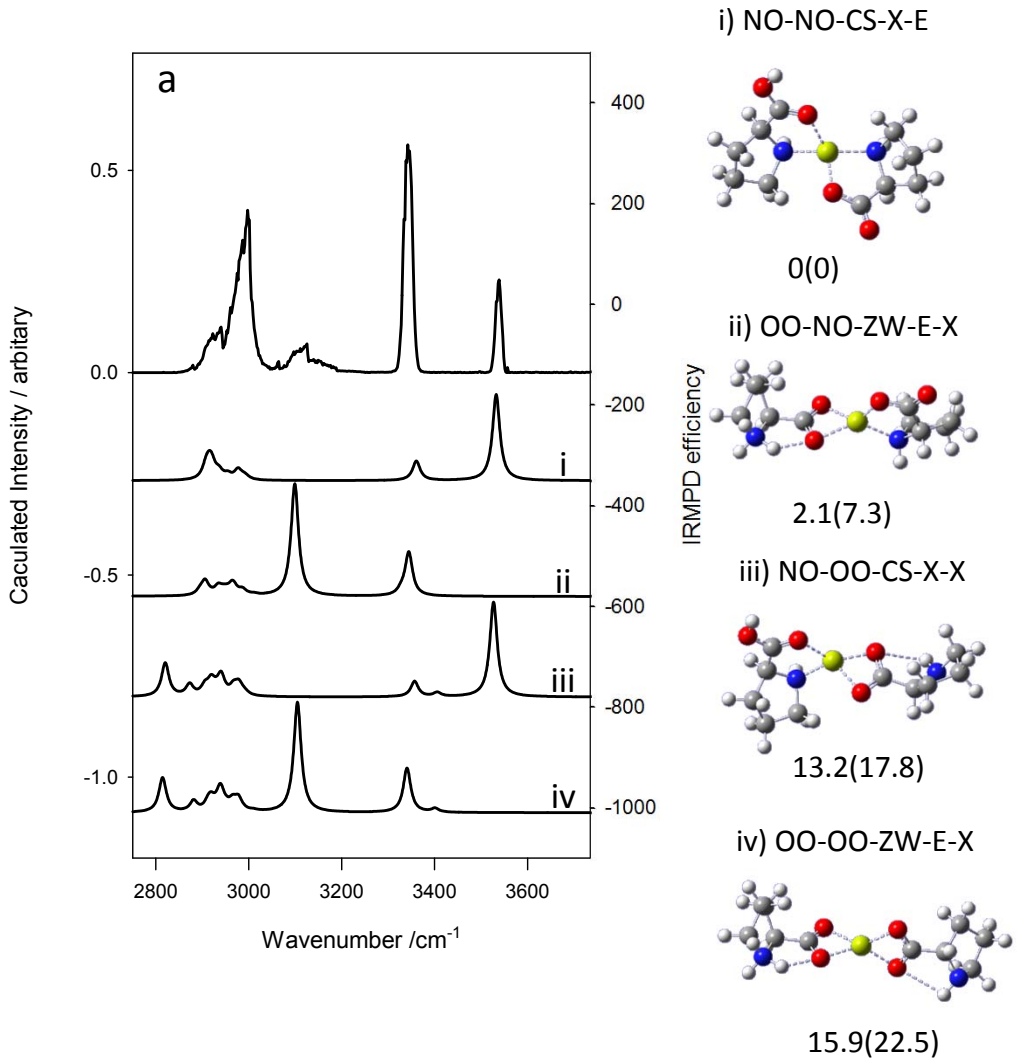



**Figure S27.** Comparison of the experimental IRMPD spectrum and calculated IR spectra of the lowest energy structures of each form of the $[Mg(Pro)_2\text{-}H]^+$ complexes in the 2700 to 3800 $cm^{-1}$ region. Energies are B3LYPD3/cc-PVTZ 298 K Gibbs energies (and enthalpies) and in kJ $mol^{-1}$.

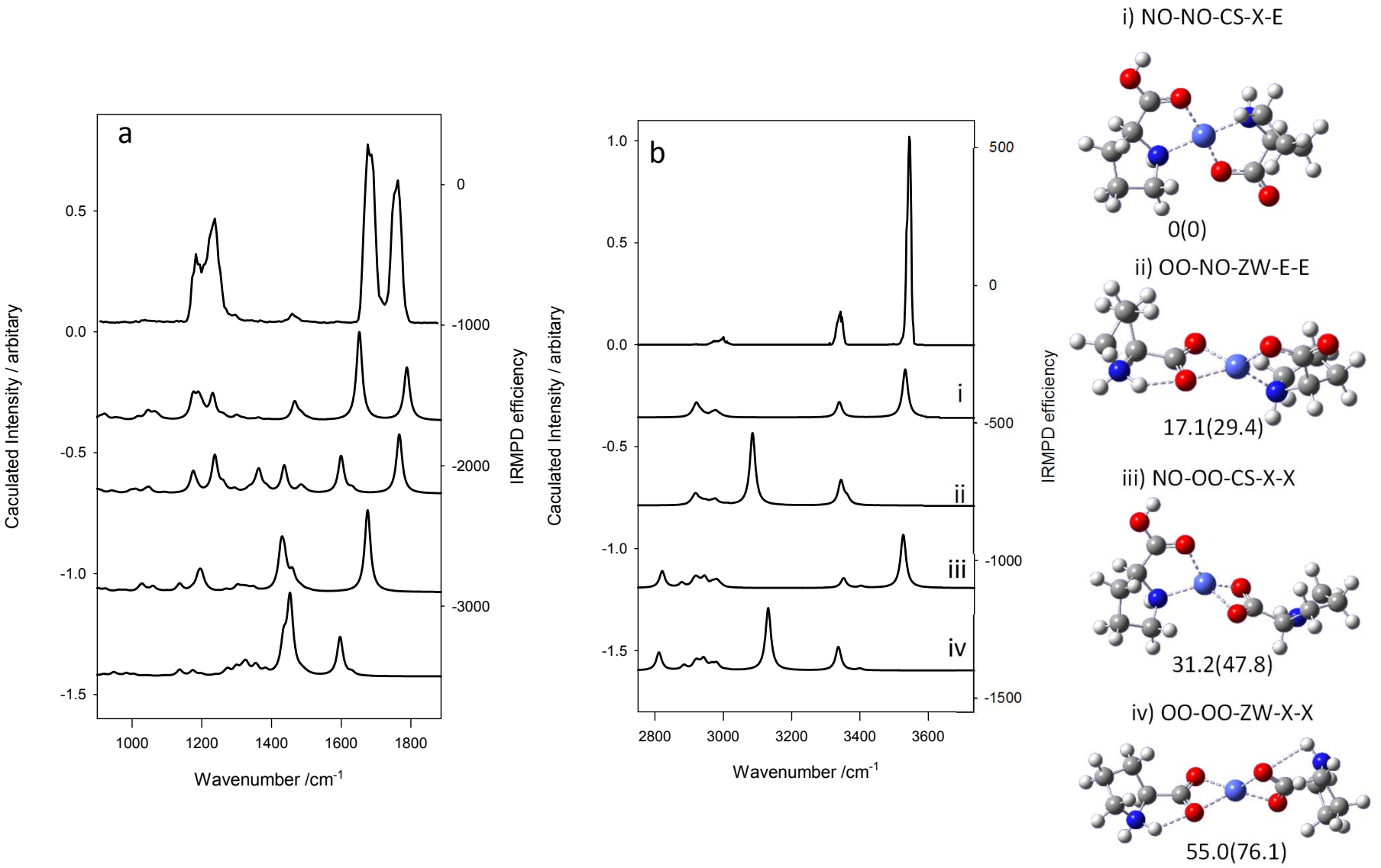



**Figure. S28.** Comparison of the experimental IRMPD spectrum and calculated IR spectra for the lowest energy structures of each form of the $[Co(Pro)_2\text{-}H]^+$ complex in the a) 1000 to 2000 $cm^{-1}$ region and b) 2800 to 3800 $cm^{-1}$ region. Energies are UB3LYPD3/cc-pVTZ 298 K Gibbs energies (and enthalpies) and in kJ $mol^{-1}$.

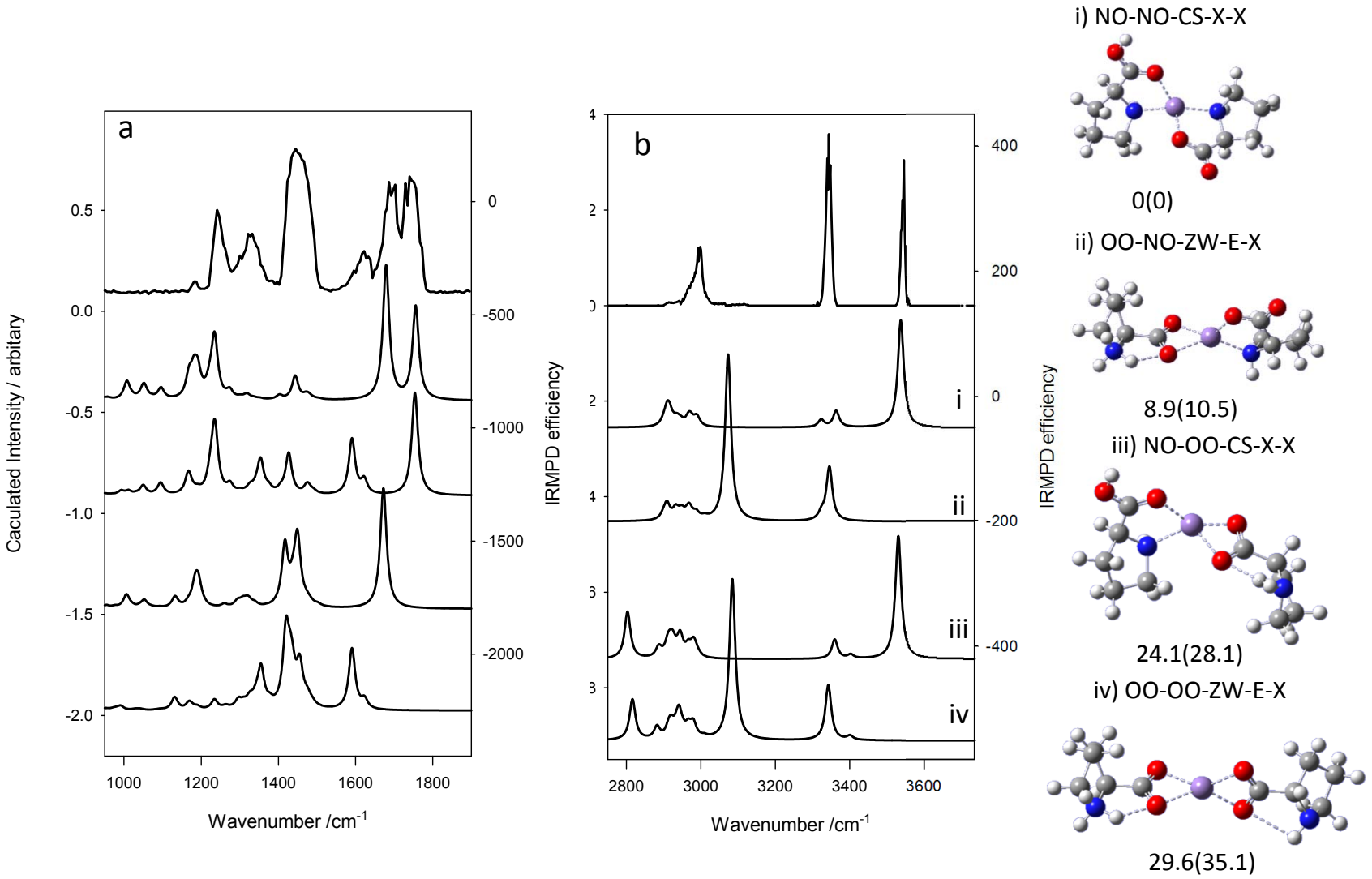



**Figure. S29.** Comparison of the experimental IRMPD spectrum and calculated IR spectra for the lowest energy structures of each form of the $[Mn(Pro)_2\text{-}H]^+$ complex in the a) 1000 to 2000 $cm^{-1}$ region and b) 2800 to 3800 $cm^{-1}$ region. Energies are UB3LYPD3/cc-pVTZ 298 K Gibbs energies (and enthalpies) and in kJ $mol^{-1}$.

**Table S1.** UB3LYP/6- 31+G(d,p) relative Gibbs energies (and enthalpies) at 298 K for quartet and doublet $[Mn(Pro)_2\text{-}H]^+$ complexes corresponding. All energies are relative to the lowest energy sextet complex in Figure S16.

| Structure | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Quartet | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Doublet |
|---|---|---|
| OO-OO-ZW | 165.4(164.4) | 313.0(314.3) |
| OO-OO-ZW | 166.5(160.4) | 316.6(314.4) |
| OO-NO-ZW | 122.2(113.9) | 206.5(197.3) |
| OO-NO-ZW | 122.8(115.3) | 206.9(195.8) |
| OO-NO-ZW | 124.3(116.9) | 208.5(200.4) |
| OO-NO-ZW | 125.1(118.4) | 260.5(252.8) |
| OO-NO-ZW | 133.7(127.9) | 275.4(264.7) |
| NO-OO-CS | 137.3(133.5) | 329.8(320.6) |
| NO-NO-CS | 85.0(74.4) | 222.2(210.0) |
| NO-NO-CS | 85.4(76.1) | 225.8(213.6) |
| NO-NO-CS | 86.8(74.4) | 238.4(226.7) |
| NO-NO-CS | 146.6(135.7) | 247.8(238.8) |
| NO-NO-CS | 167.2(160.7) | 261.4(251.7) |

**Table S2.** UB3LYP/6- 31+G(d,p) relative Gibbs energies (and enthalpies) at 298 K for quartet and doublet $[Fe(Pro)_2\text{-}H]^+$ complexes corresponding. All energies are relative to the lowest energy quintent complex in Figure S15.

| Structure | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Triplet | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Singlet |
|---|---|---|
| OO-OO-ZW | 122.2(120.1) | 261.5(175.6) |
| OO-OO-ZW | 123.8(120.1) | 284.0(278.8) |
| OO-OO-ZW | 121.3(115.2) | 309.2(300.9) |
| OO-NO-ZW | 78.0(70.5) | 205.6(16.7) |
| OO-NO-ZW | 77.5(65.7) | 207.3(197.2) |
| OO-NO-ZW | 79.4(68.7) | 189.1(171.2) |
| OO-NO-ZW | 77.5(65.7) | 209.9(200.8) |
| OO-NO-ZW | 79.4(68.7) | 207.2(197.7) |
| NO-OO-CS | 83.5(78.5) | 240.0(228.2) |
| NO-OO-CS | 80.7(75.0) | 217.2(205.3) |
| NO-OO-CS | 90.6(82.7) | 238.5(228.6) |
| NO-NO-CS | 29.8(15.8) | 157.5(138.9) |
| NO-NO-CS | 33.0(19.5) | 156.9(136.0) |
| NO-NO-CS | 33.3(19.4) | 149.7(134.0) |
| NO-NO-CS | 91.4(79.4) | 280.4(265.6) |
| NO-NO-CS | 101.8(92.1) | 188.9(175.6) |
| NO-NO-CS | 112.0(102.5) | 204.6(185.3) |

**Table S3.** UB3LYP/6- 31+G(d,p) relative Gibbs energies (and enthalpies) at 298 K for quartet and doublet $[Co(Pro)_2\text{-}H]^+$ complexes corresponding. All energies are relative to the lowest energy quintent complex in Figure S14.

| Structure | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Quartet | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Doublet |
|---|---|---|
| OO-OO-ZW | 64.5(86.6) | 111.6(122.0) |
| OO-OO-ZW | 64.8(82.6) | 116.1 (124.2) |
| OO-OO-ZW | 71.2(87.1) | 125.3(129.8) |
| OO-OO-ZW | 72.4(89.9) | 124.2(129.5) |
| OO-NO-ZW | 22.0(35.0) | 50.4(52.1) |
| OO-NO-ZW | 22.6(38.4) | 50.4(53.9) |
| OO-NO-ZW | 23.7(39.5) | 52.4(55.1) |
| NO-OO-CS | 42.2(58.5) | 62.2(66.7) |
| NO-OO-CS | 42.3(59.1) | 64.3(70.3) |
| NO-OO-CS | 51.8(67.2) | 64.4(69.0) |
| NO-NO-CS | 9.1(19.2) | 0(0) |
| NO-NO-CS | 10.0(20.0) | -0.2(1.3) |
| NO-NO-CS | 40.5(52.4) | -0.1(0) |

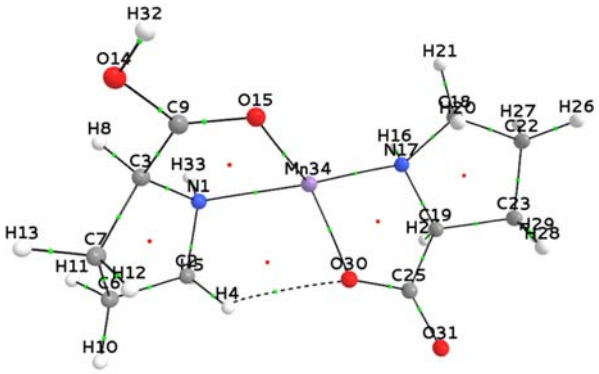
**Table S4.** UB3LYP/6- 31+G(d,p) relative Gibbs energies (and enthalpies) at 298 K for quartet and doublet [Co(Pro)2-H]+ complexes corresponding. All energies are relative to the lowest energy singlet complex in Figure S13.

| Structure | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Triplet | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ Singlet |
|---|---|---|
| OO-OO-ZW | 107.6(128.5) | 125.8(137.9) |
| OO-OO-ZW | 109.1(130.2) | 126.7(136.8) |
| OO-OO-ZW | 109.8(131.1) | 127.6(137.0) |
| OO-OO-ZW | 110.7(132.6) | 128.3(140.6) |
| OO-OO-ZW | 128.9(148.5) | 128.3(150.9) |
| OO-NO-ZW | 55.8(72.1) | 59.8(64.6) |
| OO-NO-ZW | 56.0(73.9) | 61.3(66.9) |
| OO-NO-ZW | 57.9(77.2) | 61.9(67.6) |
| OO-NO-ZW | 59.1(77.6) | 63.7(70.0) |
| OO-NO-ZW | 61.5(79.6) | 104.6(117.9) |
| NO-OO-CS | 75.8(94.1) | 69.9(77.3) |
| NO-OO-CS | 88.8(107.0) | 70.1(77.7) |
| NO-OO-CS | 90.3(108.2) | 70.7(77.4) |
| NO-OO-CS | 91.1(107.6) | 71.3(79.2) |
| NO-NO-CS | 27.6(36.1) | 0(0) |
| NO-NO-CS | 27.6(40.2) | 0.6(1.8) |
| NO-NO-CS | 28.2(34.6) | 0.9(1.5) |
| NO-NO-CS | 65.0(80.8) | 1.1(3.3) |

**Table. S5** Topological Analysis of the lowest energy $[Mn(Pro)_2\text{-}H]^+$ structures.

**$[Mn(Pro)_2\text{-}H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

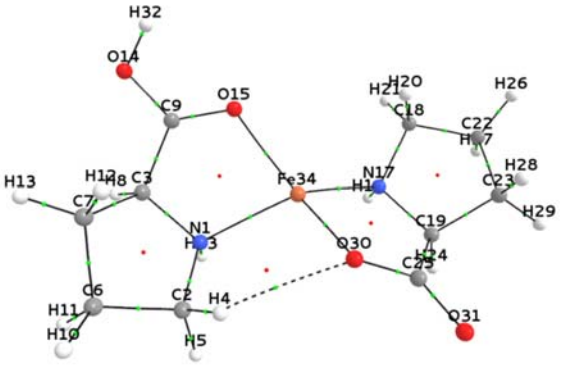



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – H(33) | 0.342 | -1.796 | 0.0332 |
| O(14) – H(32) | 0.350 | -2.098 | 0.0129 |
| C(25) – O(31) | 0.414 | 0.075 | 0.1207 |
| C(25) – O(30) | 0.321 | -0.454 | 0.0058 |
| C(23) – H(29) | 0.282 | -0.997 | 0.0082 |
| C(23) – H(28) | 0.282 | -0.993 | 0.0127 |
| C(22) – H(26) | 0.280 | -0.981 | 0.0022 |
| C(19) – C(25) | 0.248 | -0.584 | 0.0937 |
| H(4) – O(30) | 0.011 | 0.037 | 0.2549 |
| O(30) – Mn(34) | 0.099 | 0.559 | 0.0867 |
| C(19) – H(24) | 0.284 | -1.014 | 0.0381 |
| C(19) – C(23) | 0.237 | -0.521 | 0.0329 |
| C(22) – H(27) | 0.278 | -0.952 | 0.0080 |
| C(18) – H(21) | 0.284 | -1.018 | 0.0268 |
| C(22) – C(23) | 0.241 | -0.537 | 0.0033 |
| C(18) – H(20) | 0.283 | -0.998 | 0.0301 |
| C(18) – C(22) | 0.249 | -0.576 | 0.0188 |
| N(17) – C(19) | 0.231 | -0.531 | 0.0266 |
| N(17) – C(18) | 0.242 | -0.605 | 0.0366 |
| H(16) – N(17) | 0.341 | -1.779 | 0.0282 |
| N(17) – Mn(34) | 0.071 | 0.271 | 0.0288 |
| C(9) – O(14) | 0.327 | -0.359 | 0.0065 |
| C(9) – O(15) | 0.391 | -0.068 | 0.0591 |
| O(15) – Mn(34) | 0.058 | 0.281 | 0.0762 |
| C(7) – H(13) | 0.283 | -1.010 | 0.0086 |
| C7() – H(12) | 0.280 | -0.973 | 0.0119 |
| C(6) – H(11) | 0.279 | -0.963 | 0.0090 |
| C6() – H(10) | 0.281 | -0.995 | 0.0008 |
| C(3) – C(9) | 0.265 | -0.678 | 0.1125 |
| C(3) – H(8) | 0.285 | -1.024 | 0.0303 |
| C(3) – C(7) | 0.234 | -0.509 | 0.0165 |
| C(2) – H(5) | 0.285 | -1.029 | 0.0321 |
| C(6) – C(7) | 0.243 | -0.548 | 0.0013 |
| C(2) – H(4) | 0.289 | -1.071 | 0.0317 |
| C(2) – C(6) | 0.249 | -0.577 | 0.0223 |
| N(1) – C(3) | 0.251 | -0.625 | 0.0155 |
| N(1) – Mn(34) | 0.059 | 0.211 | 0.0447 |
| N(1) – C(2) | 0.230 | -0.540 | 0.0364 |

**Table. S6** Topological Analysis of the lowest energy $[Fe(Pro)_2\text{-}H]^+$ structures.

**$[Fe(Pro)_2\text{-}H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

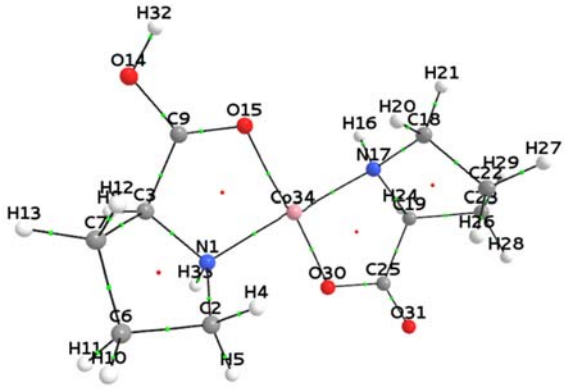



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – Fe(34) | 0.065 | 0.210 | 0.1184 |
| N(1) – C(2) | 0.231 | -0.548 | 0.0332 |
| N(1) – C(3) | 0.253 | -0.640 | 0.0159 |
| C(2) – C(6) | 0.249 | -0.577 | 0.0230 |
| C(2) – H(4) | 0.289 | -1.064 | 0.0325 |
| C(6) – C(7) | 0.243 | -0.546 | 0.0014 |
| C(2) – H(5) | 0.286 | -1.038 | 0.0309 |
| C(6) – H(11) | 0.279 | -0.964 | 0.0092 |
| C(3) – C(7) | 0.234 | -0.509 | 0.0154 |
| C(3) – H(8) | 0.284 | -1.024 | 0.0295 |
| C(3) – C(9) | 0.266 | -0.681 | 0.1126 |
| C(6) – H(10) | 0.281 | -0.994 | 0.0011 |
| C(7) – H(12) | 0.280 | -0.968 | 0.0122 |
| C(7) – H(13) | 0.283 | -1.011 | 0.0086 |
| O(15) – Fe(34) | 0.065 | 0.321 | 0.1874 |
| C(9) – O(15) | 0.388 | -0.078 | 0.0581 |
| C(9) – O(14) | 0.328 | -0.348 | 0.0055 |
| O(14) – H(32) | 0.349 | -2.099 | 0.0128 |
| N(17) – Fe(34) | 0.076 | 0.260 | 0.0745 |
| H(16) – N(17) | 0.342 | -1.791 | 0.0293 |
| N(17) – C(18) | 0.242 | -0.601 | 0.0343 |
| N(17) – C(19) | 0.232 | -0.533 | 0.0269 |
| C(18) – H(20) | 0.283 | -0.997 | 0.0309 |
| C(22) – C(23) | 0.243 | -0.545 | 0.0032 |
| C(18) – H(21) | 0.284 | -1.020 | 0.0267 |
| C(22) – H(27) | 0.278 | -0.953 | 0.0073 |
| C(18) – C(22) | 0.249 | -0.576 | 0.0196 |
| C(19) – C(23) | 0.238 | -0.527 | 0.0281 |
| C(19) – H(24) | 0.286 | -1.024 | 0.0386 |
| H(4) – O(30) | 0.010 | 0.036 | 0.3789 |
| O(30) – Fe(34) | 0.115 | 0.629 | 0.0867 |
| C(19) – C(25) | 0.253 | -0.605 | 0.0959 |
| C(22) – H(26) | 0.280 | -0.981 | 0.0026 |
| C(23) – H(28) | 0.281 | -0.975 | 0.0125 |
| C(23) – H(29) | 0.283 | -1.004 | 0.0060 |
| C(25) – O(30) | 0.315 | -0.464 | 0.0054 |
| C(25) – O(31) | 0.416 | 0.091 | 0.1236 |
| N(1) – (H33) | 0.343 | -1.802 | 0.0330 |

**Table. S7** Topological Analysis of the lowest energy $[Co(Pro)_2 -H]^+$ structures.

**$[Co(Pro)_2 -H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

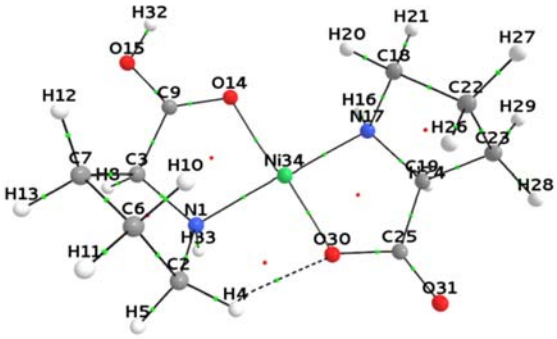



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – Co(34) | 0.0928 | 0.482 | 0.116 |
| N(1) – C(2) | 0.2386 | -0.591 | 0.019 |
| N(1) – C(3) | 0.2536 | -0.639 | 0.014 |
| C(2) – C(6) | 0.2501 | -0.581 | 0.022 |
| C(2) – H(4) | 0.2851 | -1.020 | 0.033 |
| C(6) – C(7) | 0.2417 | -0.540 | 0.003 |
| C(2) – H(5) | 0.2886 | -1.071 | 0.025 |
| C(6) – H(11) | 0.2791 | -0.965 | 0.009 |
| C(3) – C(7) | 0.2320 | -0.500 | 0.014 |
| C(3) – H(8) | 0.2837 | -1.022 | 0.027 |
| C(3) – C(9) | 0.2671 | -0.691 | 0.108 |
| C(7) – H(13) | 0.2833 | -1.012 | 0.010 |
| C(6) – H(10) | 0.2807 | -0.992 | 0.002 |
| C(7) – H(12) | 0.2802 | -0.972 | 0.013 |
| O(15) – Co(34) | 0.0811 | 0.459 | 0.685 |
| C(9) – O(15) | 0.3859 | -0.160 | 0.057 |
| C(9) – O(14) | 0.3305 | -0.331 | 0.003 |
| N(17) – Co(34) | 0.1013 | 0.497 | 0.116 |
| H(16) – N(17) | 0.3419 | -1.800 | 0.024 |
| N(17) – C(18) | 0.2364 | -0.572 | 0.005 |
| N(17) – C(19) | 0.2362 | -0.562 | 0.027 |
| C(18) – H(21) | 0.2843 | -1.013 | 0.030 |
| C(18) – H(20) | 0.2847 | -1.018 | 0.032 |
| C(18) – C(22) | 0.2484 | -0.575 | 0.017 |
| C(22) – C(23) | 0.2428 | -0.544 | 0.001 |
| C(19) – C(23) | 0.2450 | -0.557 | 0.022 |
| C(19) – H(24) | 0.2844 | -1.021 | 0.035 |
| O(30) – Co(34) | 0.1338 | 0.743 | 0.434 |
| C(19) – C(25) | 0.2540 | -0.612 | 0.095 |
| C(23) – H(28) | 0.2831 | -1.016 | 0.003 |
| C(22) – H(26) | 0.2785 | -0.957 | 0.009 |
| C(22) – H(27) | 0.2805 | -0.985 | 0.004 |
| C(23) – H(29) | 0.2793 | -0.964 | 0.012 |
| N(1) – H(33) | 0.3410 | -1.811 | 0.028 |
| C(25) – O(30) | 0.3145 | -0.542 | 0.002 |
| C(25) – O(31) | 0.4175 | 0.123 | 0.116 |
| O(14) – H(32) | 0.3487 | -2.098 | 0.012 |

**Table. S8** Topological Analysis of the lowest energy $[Ni(Pro)_2\text{-}H]^+$ structures.

**$[Ni(Pro)_2\text{-}H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

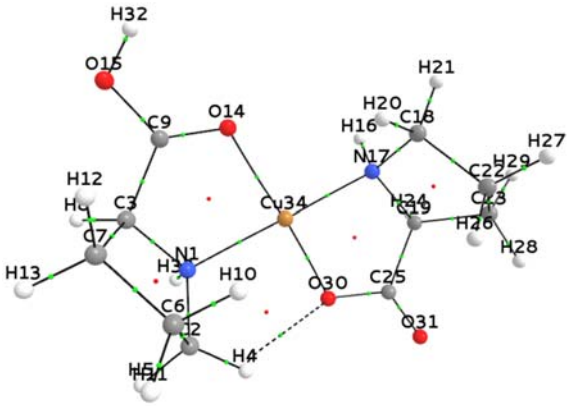



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – C(2) | 0.237 | -0.584 | 0.014 |
| N(1) – Ni(34) | 0.091 | 0.376 | 0.101 |
| N(1) – C(3) | 0.251 | -0.629 | 0.009 |
| C(2) – H(4) | 0.291 | -1.099 | 0.026 |
| C(2) – H(5) | 0.284 | -1.008 | 0.033 |
| C(2) – C(6) | 0.252 | -0.591 | 0.022 |
| C(7) – H(13) | 0.283 | -0.999 | 0.014 |
| C(3) – C(7) | 0.228 | -0.486 | 0.019 |
| C(6) – C(7) | 0.241 | -0.539 | 0.002 |
| C(3) – H(8) | 0.285 | -1.036 | 0.028 |
| C(3) – C(9) | 0.267 | -0.690 | 0.110 |
| C(6) – H(10) | 0.278 | -0.954 | 0.010 |
| C(6) – H(11) | 0.281 | -0.996 | 0.002 |
| C(7) – H(12) | 0.282 | -0.996 | 0.013 |
| O(14) – Ni(34) | 0.076 | 0.458 | 0.037 |
| C(9) – O(14) | 0.387 | -0.107 | 0.075 |
| C(9) – O(15) | 0.329 | -0.342 | 0.003 |
| N(17) – Ni(34) | 0.107 | 0.430 | 0.100 |
| H(16) – N(17) | 0.342 | -1.805 | 0.022 |
| N(17) – C(18) | 0.235 | -0.566 | 0.003 |
| N(17) – C(19) | 0.235 | -0.556 | 0.026 |
| C(18) – H(21) | 0.284 | -1.014 | 0.031 |
| C(18) – H(20) | 0.286 | -1.027 | 0.032 |
| C(18) – C(22) | 0.249 | -0.577 | 0.017 |
| C(22) – C(23) | 0.243 | -0.543 | 0.001 |
| C(23) – H(29) | 0.279 | -0.965 | 0.012 |
| C(19) – C(23) | 0.245 | -0.558 | 0.022 |
| C(19) – H(24) | 0.285 | -1.024 | 0.036 |
| O(30) – Ni(34) | 0.130 | 0.709 | 0.077 |
| H(4) – O(30) | 0.013 | 0.050 | 0.416 |
| C(19) - C25) | 0.255 | -0.616 | 0.095 |
| C(23) – H(28) | 0.283 | -1.016 | 0.003 |
| C(22) – H(26) | 0.279 | -0.958 | 0.009 |
| C(22) – H(27) | 0.281 | -0.987 | 0.004 |
| N(1) – H(33) | 0.340 | -1.806 | 0.024 |
| C(25) – O(30) | 0.316 | -0.498 | 0.015 |
| C(25) – O(31) | 0.417 | 0.104 | 0.114 |
| O(15) – H(32) | 0.349 | -2.098 | 0.013 |

**Table. S9** Topological Analysis of the lowest energy $[Cu(Pro)_2\text{-}H]^+$ structures.

**$[Cu(Pro)_2\text{-}H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

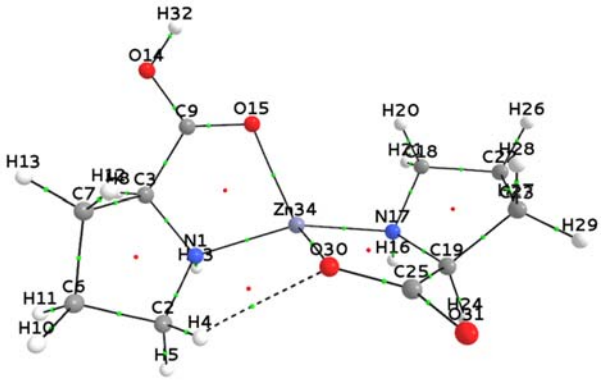



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – C(2) | 0.239 | -0.592 | 0.0163 |
| N(1) – Cu(34) | 0.081 | 0.233 | 0.0089 |
| N(1) – C(3) | 0.255 | -0.655 | 0.0147 |
| C(2) – H(4) | 0.290 | -1.097 | 0.0266 |
| C(2) – H(5) | 0.283 | -1.007 | 0.0329 |
| C(2) – C(6) | 0.252 | -0.590 | 0.0222 |
| C(3) – C(7) | 0.228 | -0.483 | 0.0191 |
| C(6) – C(7) | 0.241 | -0.538 | 0.0012 |
| C(3) – H(8) | 0.285 | -1.035 | 0.0278 |
| C(3) – C(9) | 0.265 | -0.678 | 0.1095 |
| C(6) – H(10) | 0.277 | -0.944 | 0.0108 |
| C(7) – H(13) | 0.283 | -1.000 | 0.0138 |
| C(6) – H(11) | 0.281 | -0.997 | 0.0018 |
| C(7) – H(12) | 0.282 | -0.995 | 0.0129 |
| O(14) – Cu(34) | 0.070 | 0.290 | 0.0102 |
| C(9) – O(14) | 0.391 | -0.089 | 0.0598 |
| C(9) - O(15) | 0.327 | -0.351 | 0.0093 |
| N(17) – Cu(34) | 0.094 | 0.268 | 0.0195 |
| H(16) – N(17) | 0.342 | -1.801 | 0.0262 |
| N(17) – C(18) | 0.236 | -0.573 | 0.0065 |
| N(17) – C(19) | 0.237 | -0.571 | 0.0302 |
| C(18) – H(21) | 0.285 | -1.015 | 0.0301 |
| C(18) – H(20) | 0.285 | -1.017 | 0.0333 |
| C(18) – C(22) | 0.248 | -0.573 | 0.0171 |
| C(22) – C(23) | 0.243 | -0.543 | 0.0011 |
| C(19) – C(23) | 0.245 | -0.557 | 0.0226 |
| C(19) – H(24) | 0.284 | -1.021 | 0.0358 |
| O(30) – Cu(34) | 0.115 | 0.489 | 0.0121 |
| H(4) – O(30) | 0.013 | 0.048 | 0.2998 |
| C(19) – C(25) | 0.251 | -0.596 | 0.0954 |
| C(23) – H(28) | 0.283 | -1.019 | 0.0032 |
| C(22) – H(26) | 0.278 | -0.955 | 0.0093 |
| C(22) – H(27) | 0.281 | -0.986 | 0.0044 |
| C(23) – H(29) | 0.279 | -0.963 | 0.0120 |
| C(25) – O(30) | 0.321 | -0.464 | 0.0060 |
| C(25) – O(31) | 0.414 | 0.083 | 0.1099 |
| O(15) – H(32) | 0.350 | -2.099 | 0.0130 |
| N(1) – H(33) | 0.340 | -1.800 | 0.0278 |

**Table. S10** Topological Analysis of the lowest energy $[Zn(Pro)_2\text{-}H]^+$ structures.

**$[Zn(Pro)_2\text{-}H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

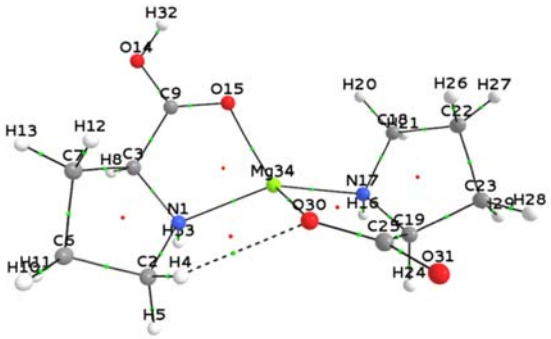



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – Zn(34) | 0.0792 | 0.227 | 0.0191 |
| N(1) – C(2) | 0.2267 | -0.522 | 0.0353 |
| N(1) – C(3) | 0.2500 | -0.629 | 0.0088 |
| C(2) – H(4) | 0.2904 | -1.083 | 0.0321 |
| C(2) – H(5) | 0.2859 | -1.034 | 0.0338 |
| C(2) – C(6) | 0.2486 | -0.576 | 0.0222 |
| C(6) – C(7) | 0.2433 | -0.547 | 0.0006 |
| C(3) – C(7) | 0.2354 | -0.515 | 0.0176 |
| C(3) – H(8) | 0.2852 | -1.030 | 0.0307 |
| C(3) – C(9) | 0.2643 | -0.673 | 0.1114 |
| C(6) – H(10) | 0.2813 | -0.998 | 0.0016 |
| C(6) – H(11) | 0.2794 | -0.966 | 0.0098 |
| C(7) - H(12) | 0.2804 | -0.978 | 0.0116 |
| C(7) – H(13) | 0.2831 | -1.012 | 0.0087 |
| O(15) – Zn(34) | 0.0644 | 0.259 | 0.0268 |
| C(9) – O(15) | 0.3930 | -0.068 | 0.0619 |
| C(9) – O(14) | 0.3271 | -0.359 | 0.0066 |
| N(17) – Zn(34) | 0.0896 | 0.247 | 0.0074 |
| H(16) – N(17) | 0.3425 | -1.800 | 0.0260 |
| N(17) – C(18) | 0.2378 | -0.583 | 0.0320 |
| N(17) – C(19) | 0.2274 | -0.511 | 0.0258 |
| C(18) – H(20) | 0.2849 | -1.015 | 0.0316 |
| C(22) – C(23) | 0.2435 | -0.547 | 0.0033 |
| C(18) – H(21) | 0.2846 | -1.022 | 0.0286 |
| C(18) – C(22) | 0.2495 | -0.579 | 0.0201 |
| C(19) – C(23) | 0.2396 | -0.533 | 0.0298 |
| C(19) – H(24) | 0.2858 | -1.026 | 0.0409 |
| O(30) – Zn(34) | 0.1061 | 0.429 | 0.0427 |
| H(4) – O(30) | 0.0115 | 0.040 | 0.4892 |
| C(19) – C(25) | 0.2470 | -0.577 | 0.0919 |
| C(23) – H(29) | 0.2829 | -1.008 | 0.0055 |
| C(22) – H(26) | 0.2799 | -0.981 | 0.0031 |
| C(22) – H(27) | 0.2780 | -0.954 | 0.0075 |
| C(23) – H(28) | 0.2802 | -0.973 | 0.0131 |
| C(25) – O(30) | 0.3247 | -0.448 | 0.0127 |
| C(25) – O(31) | 0.4131 | 0.053 | 0.1218 |
| O(14) – H(32) | 0.3494 | -2.100 | 0.0129 |
| N(1) – H(33) | 0.3425 | -1.806 | 0.0295 |

**Table. S11** Topological Analysis of the lowest energy $[Mg(Pro)_2\text{-}H]^+$ structures.

**$[Mg(Pro)_2\text{-}H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

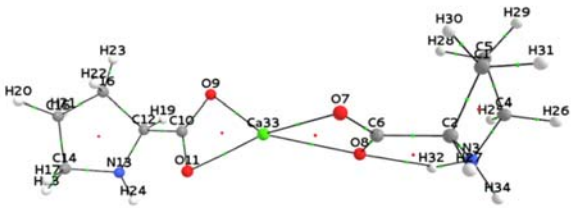



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – C(2) | 0.229 | -0.531 | 0.0372 |
| N(1) – C(3) | 0.251 | -0.626 | 0.0168 |
| N(1) – Mg(34) | 0.036 | 0.213 | 0.0357 |
| C(2) – H(4) | 0.289 | -1.074 | 0.0317 |
| C(6) – C(7) | 0.243 | -0.547 | 0.0011 |
| C(2) – H(5) | 0.286 | -1.032 | 0.0323 |
| C(2) – C(6) | 0.249 | -0.577 | 0.0228 |
| C(3) – C(7) | 0.233 | -0.506 | 0.0158 |
| C(3) – H(8) | 0.285 | -1.028 | 0.0300 |
| C(3) – C(9) | 0.265 | -0.678 | 0.1135 |
| C(6) – H(10) | 0.281 | -0.997 | 0.0009 |
| C(6) – H(11) | 0.279 | -0.964 | 0.0094 |
| C(7) – H(12) | 0.280 | -0.972 | 0.0124 |
| C(7) – H(13) | 0.283 | -1.012 | 0.0090 |
| C(9) – O(15) | 0.388 | -0.100 | 0.0473 |
| C(9) – O(14) | 0.329 | -0.343 | 0.0074 |
| O(15) – Mg(34) | 0.040 | 0.288 | 0.0115 |
| N(17) – Mg(34) | 0.043 | 0.267 | 0.0397 |
| H(16) – N(17) | 0.342 | -1.785 | 0.0318 |
| N(17) – C(18) | 0.232 | -0.541 | 0.0140 |
| N(17) – C(19) | 0.230 | -0.524 | 0.0378 |
| C(18) – H(21) | 0.285 | -1.018 | 0.0298 |
| C(18) – H(20) | 0.283 | -0.999 | 0.0345 |
| C(18) – C(22) | 0.245 | -0.558 | 0.0164 |
| C(22) – C(23) | 0.243 | -0.545 | 0.0010 |
| C(19) – C(23) | 0.247 | -0.567 | 0.0230 |
| C19) – H(24) | 0.283 | -1.006 | 0.0372 |
| O(30) – Mg(34) | 0.061 | 0.513 | 0.0573 |
| H(4) – O(30) | 0.011 | 0.039 | 0.2571 |
| C(19) – C(25) | 0.242 | -0.553 | 0.0923 |
| C(22) – H(26) | 0.279 | -0.965 | 0.0103 |
| C(22) – H(27) | 0.280 | -0.981 | 0.0062 |
| C(23) – H(28) | 0.284 | -1.025 | 0.0018 |
| C(23) – H(29) | 0.278 | -0.952 | 0.0116 |
| C(25) – O(30) | 0.327 | -0.438 | 0.0071 |
| C(25) – O(31) | 0.412 | 0.060 | 0.1177 |
| O(14) – H(32) | 0.349 | -2.100 | 0.0125 |
| N(1) – H(33) | 0.342 | -1.790 | 0.0348 |

**Table. S12** Topological Analysis of the lowest energy $[Ca(Pro)_2 -H]^+$ structures.

**$[Ca(Pro)_2 -H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level

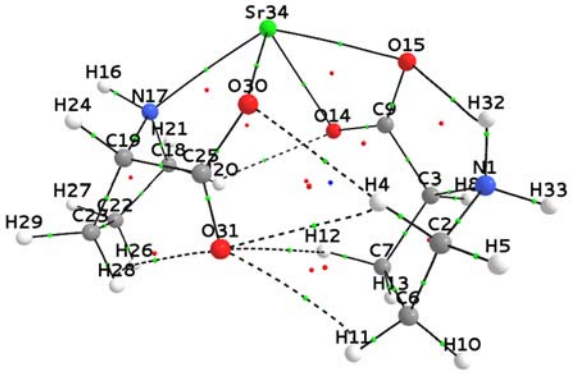



| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| C(1) – C(2) | 0.242 | -0.544 | 0.0242 |
| C(2) – N(3) | 0.227 | -0.522 | 0.0187 |
| N(3) – C(4) | 0.224 | -0.515 | 0.0123 |
| C(1) – C(5) | 0.242 | -0.540 | 0.0015 |
| C(4) – C(5) | 0.249 | -0.579 | 0.0194 |
| C(2) – C(6) | 0.254 | -0.616 | 0.0953 |
| O(8) – Ca(33) | 0.030 | 0.142 | 0.0032 |
| C(6) – O(7) | 0.380 | -0.238 | 0.0613 |
| C(6) – O(8) | 0.362 | -0.333 | 0.0332 |
| O(7) – Ca(33) | 0.032 | 0.155 | 0.0342 |
| N(3) – H(32) | 0.323 | -1.751 | 0.0022 |
| O(9) – Ca(33) | 0.043 | 0.225 | 0.0487 |
| O(9) – C(10) | 0.357 | -0.361 | 0.0102 |
| C(10) – O(11) | 0.355 | -0.341 | 0.0052 |
| C(10) – C(12) | 0.261 | -0.651 | 0.0997 |
| O(11) – Ca(33) | 0.042 | 0.219 | 0.0448 |
| N(13) – C(14) | 0.263 | -0.714 | 0.0412 |
| C(12) – N(13) | 0.272 | -0.733 | 0.0629 |
| C(14) – H(18) | 0.283 | -1.005 | 0.0273 |
| C(12) – C(16) | 0.232 | -0.502 | 0.0166 |
| C(15) – H(21) | 0.279 | -0.958 | 0.0039 |
| C(14) – C(15) | 0.248 | -0.575 | 0.0212 |
| C(15) – C(16) | 0.243 | -0.543 | 0.0033 |
| C(14) – H(17) | 0.276 | -0.936 | 0.0264 |
| C(12) – H(19) | 0.282 | -0.988 | 0.0351 |
| C(15) – H(20) | 0.279 | -0.961 | 0.0014 |
| C(16) – H(22) | 0.277 | -0.941 | 0.0076 |
| C(16) – H(23) | 0.281 | -0.984 | 0.0056 |
| N(13) – H(24) | 0.343 | -1.785 | 0.0502 |
| C(4) – H(25) | 0.288 | -1.067 | 0.0330 |
| C(4) – H(26) | 0.288 | -1.053 | 0.0346 |
| C(2) – H(27) | 0.287 | -1.056 | 0.0384 |
| C(5) – H(28) | 0.280 | -0.973 | 0.0125 |
| C(5) – H(29) | 0.282 | -1.003 | 0.0047 |
| C(1) – H(30) | 0.283 | -1.021 | 0.0073 |
| C(1) – H(31) | 0.281 | -0.985 | 0.0146 |
| O(8) – H(32) | 0.035 | 0.111 | 0.1071 |
| N(3) – H(34) | 0.340 | -1.852 | 0.0029 |

**Table. S13** Topological Analysis of the lowest energy $[Sr(Pro)_2\text{-}H]^+$ structures.

**$[Sr(Pro)_2\text{-}H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2 \rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level



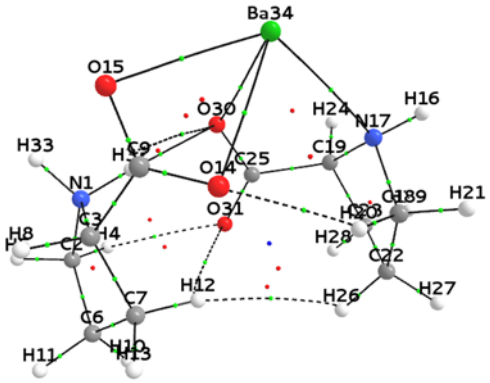

| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| C(25) – O(30) | 0.336 | -0.342 | 0.003 |
| H(28) – O(31) | 0.016 | 0.065 | 2.574 |
| C(25) – O(31) | 0.395 | 0.090 | 0.085 |
| N(1) – H(32) | 0.327 | -1.782 | 0.004 |
| O(14) – Sr(34) | 0.036 | 0.154 | 0.040 |
| O(15) – Sr(34) | 0.032 | 0.139 | 0.035 |
| O(30) – Sr(34) | 0.055 | 0.256 | 0.082 |

| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – (C2) | 0.224 | -0.502 | 0.0356 |
| N(1) – (C3) | 0.230 | -0.547 | 0.0042 |
| C(2) – (H4) | 0.290 | -1.113 | 0.0291 |
| C(2) – (H5) | 0.286 | -1.045 | 0.0376 |
| C(2) – (C6) | 0.252 | -0.597 | 0.0199 |
| C(3) – (C7) | 0.238 | -0.535 | 0.0306 |
| C(6) – (C7) | 0.239 | -0.534 | 0.0076 |
| C(3) – (C9) | 0.254 | -0.621 | 0.0847 |
| C(3) – (H8) | 0.285 | -1.036 | 0.0365 |
| N(1) – H(33) | 0.342 | -1.850 | 0.0013 |
| C(6) – H(10) | 0.278 | -0.955 | 0.0155 |
| C(6) – H(11) | 0.284 | -1.031 | 0.0014 |
| H(12) – O(31) | 0.008 | 0.029 | 0.2886 |
| C(7) – H(12) | 0.286 | -1.029 | 0.0120 |
| C(7) – H(13) | 0.282 | -0.996 | 0.0139 |
| C(9) – O(14) | 0.374 | -0.150 | 0.0564 |
| O(15) – H(32) | 0.031 | 0.101 | 0.1825 |
| C(9) – O(15) | 0.363 | -0.219 | 0.0405 |
| N(17) – Sr(34) | 0.031 | 0.109 | 0.0223 |
| H(16) – N(17) | 0.340 | -1.746 | 0.0351 |
| O(14) – H(20) | 0.008 | 0.028 | 0.1539 |
| N(17) – C(18) | 0.249 | -0.646 | 0.0413 |
| N(17) – C(19) | 0.243 | -0.595 | 0.0286 |
| C(18) – H(20) | 0.284 | -1.014 | 0.0272 |
| C(18) – H(21) | 0.282 | -0.998 | 0.0267 |
| C(18) – C(22) | 0.247 | -0.570 | 0.0185 |
| C(22) – C(23) | 0.236 | -0.519 | 0.0028 |
| C(19) – C(23) | 0.241 | -0.539 | 0.0273 |
| C(19) – C(25) | 0.246 | -0.579 | 0.0754 |
| C(19) – H(24) | 0.283 | -0.999 | 0.0253 |
| H(4) – O(31) | 0.010 | 0.036 | 0.1792 |
| H(11) – O(31) | 0.009 | 0.033 | 0.3380 |
| C(22) – H(26) | 0.280 | -0.974 | 0.0020 |
| C(22) – H(27) | 0.278 | -0.954 | 0.0084 |
| C(23) – H(28) | 0.284 | -1.012 | 0.0071 |
| C(23) – H(29) | 0.280 | -0.970 | 0.0127 |
| H(4) – O(30) | 0.009 | 0.030 | 0.1771 |

**Table. S14** Topological Analysis of the lowest energy $[Ba(Pro)_2-H]^+$ structures.

**$[Ba(Pro)_2-H]^+$**

Electron densities $\rho$(e a.u.$^{-3}$), Laplacian of the charge density $\nabla^2\rho$ (e a.u.$^{-5}$) and ellipticity $\varepsilon$ at the bond critical points, computed for geometries optimized at the B3LYP/6-31+G(d,p) level




| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| C(25) – O(31) | 0.395 | 0.076 | 0.087 |
| N(1) – H(32) | 0.310 | -1.659 | 0.002 |
| N(1) – H(33) | 0.341 | -1.852 | 0.005 |
| O(14) – Ba(34) | 0.034 | 0.132 | 0.037 |
| O(15) – Ba(34) | 0.036 | 0.138 | 0.046 |
| N(17) – Ba(34) | 0.028 | 0.090 | 0.023 |
| O(30) – Ba(34) | 0.043 | 0.173 | 0.072 |

| Bond | $\rho$ | $\nabla^2\rho$ | $\varepsilon$ |
|---|---|---|---|
| N(1) – C(2) | 0.228 | -0.544 | 0.026 |
| N(1) – C(3) | 0.232 | -0.554 | 0.010 |
| C(2) – H(4) | 0.292 | -1.106 | 0.029 |
| C(2) – H(5) | 0.287 | -1.040 | 0.037 |
| C(2) – C(6) | 0.241 | -0.549 | 0.022 |
| C(3) – C(7) | 0.252 | -0.598 | 0.024 |
| C(6) – C(7) | 0.241 | -0.539 | 0.004 |
| C(3) – C(9) | 0.257 | -0.639 | 0.054 |
| C(3) – H(8) | 0.285 | -1.027 | 0.028 |
| C(9) – O(30) | 0.011 | 0.039 | 0.748 |
| C(6) – H(10) | 0.282 | -1.003 | 0.007 |
| C(6) – H(11) | 0.281 | -0.974 | 0.013 |
| C(7) - H(12) | 0.283 | -0.999 | 0.010 |
| C(7) – H(13) | 0.281 | -0.993 | 0.005 |
| C(9) - O(14) | 0.370 | -0.159 | 0.061 |
| C(9) - O(15) | 0.365 | -0.225 | 0.053 |
| H(16) – N(17) | 0.341 | -1.756 | 0.038 |
| O(14) – H(20) | 0.009 | 0.030 | 0.093 |
| N(17) – C(18) | 0.242 | -0.602 | 0.035 |
| N(17) – C(19) | 0.249 | -0.628 | 0.038 |
| C(18) – H(20) | 0.286 | -1.024 | 0.030 |
| C(18) – H(21) | 0.283 | -1.003 | 0.029 |
| H(12) – H(26) | 0.002 | 0.007 | 0.520 |
| C(18) – C(22) | 0.237 | -0.527 | 0.019 |
| C(22) – C(23) | 0.240 | -0.535 | 0.002 |
| C(19) – C(23) | 0.249 | -0.578 | 0.017 |
| C(19) – C(25) | 0.249 | -0.600 | 0.072 |
| C(19) – H(24) | 0.281 | -0.991 | 0.023 |
| H(4) – O(31) | 0.012 | 0.041 | 0.231 |
| H(12) – O(31) | 0.007 | 0.026 | 0.208 |
| C(22) – H(26) | 0.281 | -0.977 | 0.010 |
| C(22) – H(27) | 0.280 | -0.977 | 0.007 |
| C(23) – H(28) | 0.283 | -1.010 | 0.001 |
| C(23) – H(29) | 0.278 | -0.951 | 0.010 |
| O(30) – H(32) | 0.041 | 0.105 | 0.050 |
| C(25) – O(30) | 0.333 | -0.345 | 0.003 |

**Table S15.** Comparison of the three levels calculations, UB3LYPD3/6-311++G(3d,3p)//6-31+G(d,p), UB3LYPD3/6-31+G(d,p), and UB3LYPD3/cc-PVTZ, relative Gibbs energies (and enthalpies) of the lowest energy structures of each forms of the [Co(Pro)2-H]+ complex at 298 K.

| Structure | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ B3LYP/6-311++G(3d,3p)// 6-31+G(d,p | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ B3LYP/6-31+G(d,p) | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ UB3LYP/cc-PVTZ |
|---|---|---|---|
| Co-NO-NO-CS-X-E | 0(0) | 0(0) | 0(0) |
| Co-OO-NO-ZW-E-E | 16.9(29.9) | 22.0(35.0) | 17.1(29.4) |
| Co- NO-OO-CS-X-X | 31.6(47.9) | 42.2(58.5) | 31.2(47.8) |
| Co- OO-OO-ZW-E-X | 55.0(77.1) | 64.5(86.6) | 55.0(76.1) |

**Table S16.** Comparison of the three levels calculations, UB3LYPD3/6-311++G(3d,3p)//6-31+G(d,p), UB3LYPD3/6-31+G(d,p), and UB3LYPD3/cc-PVTZ, relative Gibbs energies (and enthalpies) of the lowest energy structures of each forms of the [Mn(Pro)2-H]+ complex at 298K.

| Structure | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ B3LYP/6-311++G(3d,3p)// 6-31+G(d,p | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ B3LYP/6-31+G(d,p) | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ UB3LYP/cc-PVTZ |
|---|---|---|---|
| Mn-NO-NO-CS-X-X | 0(0) | 0(0) | 0(0) |
| Mn- OO-NO-ZW-E-X | 9.2(11.4) | 8.4(10.6) | 8.9(10.5) |
| Mn- NO-OO-CS-X-X | 23.6(28.7) | 28.6(33.7) | 24.1(28.1) |
| Mn- OO-OO-ZW-E-X | 29.7(36.1) | 33.8(40.2) | 29.6(35.1) |

**Table S17.** Comparison of the three levels calculations , B3LYPD3/6-311++G(3d,3p)//6-31+G(d,p), B3LYPD3/6-31+G(d,p), and B3LYPD3/cc-PVTZ, relative Gibbs energies (and enthalpies) of the lowest energy structures of each forms of the [Mg(Pro)2-H]+ complex at 298 K.

| Structure | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ B3LYP/6-311++G(3d,3p)// 6-31+G(d,p | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ B3LYP/6-31+G(d,p) | $\Delta_{rel}G(\Delta_{rel}H)$/kJ mol$^{-1}$ UB3LYP/cc-PVTZ |
|---|---|---|---|
| Mg-NO-NO-CS-X-E | 0(0) | 0(0) | 0(0) |
| Mg-OO-NO-ZW-E-X | 7.8(7.2) | 6.0(5.4) | 2.1(7.3) |
| Mg-NO-OO-CS-X-X | 16.3(17.7) | 19.3(20.7) | 13.2(17.8) |
| M-OO-OO-ZW-E-X | 20.5(22.8) | 21.0(23.3) | 15.9(22.5) |

Mn-NO-NO-CS-X-X

1 6

| | | | |
|---|---|---|---|
| N | -1.96482300 | -0.38702200 | -1.08455200 |
| C | -2.16409700 | -1.86462100 | -0.76489900 |
| C | -3.01720900 | 0.37758900 | -0.33424100 |
| H | -1.40055000 | -2.16429900 | -0.04270600 |
| H | -2.02663700 | -2.44826600 | -1.67713300 |
| C | -3.56582600 | -1.95375400 | -0.16009600 |
| C | -3.66978000 | -0.64561400 | 0.63393400 |
| H | -3.77480900 | 0.77010600 | -1.02092800 |
| C | -2.40887500 | 1.55041000 | 0.40020000 |
| H | -3.68449000 | -2.83635600 | 0.47273800 |
| H | -4.33215100 | -1.98919300 | -0.94290900 |
| H | -3.08747200 | -0.71512100 | 1.56002000 |
| H | -4.68878900 | -0.35273000 | 0.89093400 |
| O | -3.30193900 | 2.33957400 | 0.95773400 |
| O | -1.19100000 | 1.74598000 | 0.49500100 |
| H | 2.35318700 | 0.58331100 | -1.89999100 |
| N | 2.12047800 | 0.52703100 | -0.90814900 |
| C | 2.74771800 | 1.72752800 | -0.24799300 |
| C | 2.85798000 | -0.68519400 | -0.33955000 |
| H | 2.27750400 | 1.86029100 | 0.73367300 |
| H | 2.55728000 | 2.62064600 | -0.84802800 |
| C | 4.21952900 | 1.34419400 | -0.09561200 |
| C | 4.14623500 | -0.13308300 | 0.33031900 |
| H | 3.09261500 | -1.35018300 | -1.17585000 |
| C | 1.98973400 | -1.51122400 | 0.64251800 |
| H | 4.74092200 | 1.97002700 | 0.63310900 |
| H | 4.73164500 | 1.45510600 | -1.05900500 |
| H | 4.05847300 | -0.22579100 | 1.41606000 |
| H | 5.02605700 | -0.70508100 | 0.03191100 |
| O | 0.70914300 | -1.18933300 | 0.69364200 |
| O | 2.52036000 | -2.39949000 | 1.27718600 |
| H | -2.86701700 | 3.06150800 | 1.44937200 |
| H | -2.12950500 | -0.24997900 | -2.07984200 |
| Mn | 0.05436700 | 0.26098800 | -0.41074000 |

Mn-OO-NO-ZW-E-X

1 6

| | | | |
|---|---|---|---|
| N | 4.18395800 | -0.29959200 | -1.05811500 |
| C | 4.95201500 | 0.92084200 | -0.54442800 |
| C | 3.50802200 | -0.97716500 | 0.13613900 |
| H | 4.84454000 | 1.73084700 | -1.26657700 |
| H | 6.00282500 | 0.63292800 | -0.47213800 |
| C | 4.33535200 | 1.18119200 | 0.83048900 |
| C | 4.05947600 | -0.23328300 | 1.36539400 |
| H | 3.73527700 | -2.04541400 | 0.13062200 |
| C | 2.00156400 | -0.78107300 | -0.05366900 |
| H | 3.40595900 | 1.75289200 | 0.73450800 |
| H | 5.01478800 | 1.75086000 | 1.46766600 |
| H | 3.33889200 | -0.26201800 | 2.18415100 |
| H | 4.98442900 | -0.70948500 | 1.70515100 |
| O | 1.21637500 | -1.13396600 | 0.86383500 |
| O | 1.59501200 | -0.22836900 | -1.12527800 |
| H | -2.60418500 | -1.26300000 | -1.51231400 |
| N | -2.46210900 | -0.80812000 | -0.61008900 |
| C | -3.08462000 | -1.69881700 | 0.43034200 |
| C | -3.29640300 | 0.46911600 | -0.60669100 |
| H | -2.69427500 | -1.40039700 | 1.41072000 |
| H | -2.80098700 | -2.73795800 | 0.24640800 |
| C | -4.58144300 | -1.40277700 | 0.33086200 |
| C | -4.61695700 | 0.12403400 | 0.13548800 |
| H | -3.47854100 | 0.74774300 | -1.64880800 |
| C | -2.55046800 | 1.66596600 | 0.03725200 |
| H | -5.13195400 | -1.72996000 | 1.21671600 |
| H | -5.00355300 | -1.92446000 | -0.53669700 |
| H | -4.63732300 | 0.64455400 | 1.09639200 |
| H | -5.49013500 | 0.45871300 | -0.42677500 |
| O | -1.26048700 | 1.49221400 | 0.25688700 |
| O | -3.17846000 | 2.67746300 | 0.27745700 |
| H | 3.39535000 | -0.01833000 | -1.67308700 |
| H | 4.78573000 | -0.93795900 | -1.58118900 |
| Mn | -0.44234100 | -0.20010000 | -0.15790400 |

Mn-NO-OO-CS-X-X

1 6

| | | | |
|---|---|---|---|
| N | -1.92929200 | 0.71325700 | 0.89620800 |
| C | -1.58808700 | 2.05518800 | 0.27758600 |
| C | -3.31680900 | 0.35643100 | 0.44447900 |
| H | -1.00683800 | 1.88044100 | -0.63382700 |
| H | -0.96510100 | 2.62230000 | 0.97144700 |
| C | -2.94038300 | 2.69072600 | -0.04442400 |
| C | -3.76607100 | 1.48891700 | -0.52337100 |
| H | -3.99457600 | 0.30264700 | 1.30272000 |
| C | -3.31660100 | -1.00188300 | -0.22184400 |
| H | -2.86382200 | 3.47400700 | -0.80228200 |
| H | -3.38332500 | 3.13100900 | 0.85615400 |
| H | -3.50240000 | 1.23412000 | -1.55605300 |
| H | -4.84556100 | 1.63994500 | -0.48048700 |
| O | -4.51074400 | -1.41593900 | -0.57710100 |
| O | -2.28874500 | -1.65983000 | -0.43368100 |
| H | 3.32595300 | -0.26644400 | -2.07176100 |
| N | 3.96652600 | -0.20706300 | -1.28784600 |
| C | 4.44835900 | 1.15334500 | -1.01430400 |
| C | 3.42803100 | -0.77264300 | -0.05825100 |
| H | 3.63726300 | 1.90321400 | -0.98979200 |
| H | 5.17244800 | 1.45865900 | -1.77489300 |
| C | 5.06464400 | 0.99298100 | 0.37768700 |
| C | 4.04485300 | 0.09000600 | 1.09862100 |
| H | 3.72048000 | -1.82519100 | 0.05329600 |
| C | 1.92037100 | -0.76606100 | 0.04551600 |
| H | 5.21525900 | 1.94530500 | 0.89316600 |
| H | 6.03182100 | 0.48760600 | 0.29643400 |
| H | 3.26816400 | 0.69840500 | 1.57495200 |
| H | 4.48473700 | -0.53928000 | 1.87412300 |
| O | 1.17409400 | -0.16323800 | -0.80908400 |
| O | 1.33506900 | -1.38799700 | 1.01118600 |
| H | -4.46287600 | -2.28731800 | -1.01485400 |
| H | -1.94780800 | 0.82820000 | 1.90849700 |
| Mn | -0.46766800 | -0.83747900 | 0.26055600 |

Mn-OO-OO-ZW-E-X

1 6

| | | | |
|---|---|---|---|
| C | -4.60008500 | 1.03773200 | -0.83407700 |
| C | -3.90660400 | -0.33890500 | -0.84757700 |
| N | -4.54541600 | -1.10598100 | 0.31281600 |
| C | -5.50254500 | -0.16217300 | 1.04056900 |
| C | -5.00414900 | 1.22521100 | 0.63755600 |
| C | -2.40893700 | -0.26423700 | -0.55235900 |
| O | -1.65719900 | 0.35572900 | -1.35072700 |
| O | -1.96473400 | -0.82350000 | 0.50026800 |
| O | 1.53783400 | 0.91351100 | 0.86308000 |
| C | 2.37254000 | 0.01573300 | 0.47227100 |
| O | 1.91985800 | -0.93617700 | -0.26362900 |
| C | 3.82540700 | 0.09202300 | 0.88367100 |
| N | 4.63441700 | -1.06260200 | 0.51244400 |
| C | 5.41597200 | -0.72286700 | -0.68556600 |
| C | 5.80572000 | 0.73040600 | -0.40470100 |
| C | 4.51207300 | 1.32056800 | 0.18976700 |
| H | 4.82705600 | -0.78779100 | -1.61739000 |
| H | 6.27693900 | -1.39108400 | -0.77743300 |
| H | 3.81042800 | 0.22813800 | 1.97333000 |
| H | 6.13468200 | 1.26647200 | -1.29897200 |
| H | 6.61389000 | 0.75942100 | 0.33271400 |
| H | 3.87107200 | 1.71433000 | -0.60599800 |
| H | 4.68469400 | 2.13267400 | 0.89819100 |
| H | 4.08859100 | -1.91173900 | 0.41173400 |
| H | -5.46954200 | -0.38290400 | 2.10803000 |
| H | -6.50528200 | -0.36098900 | 0.65656500 |
| H | -4.05471600 | -0.89012700 | -1.77855600 |
| H | -4.14324700 | 1.51706500 | 1.24867100 |
| H | -5.78158900 | 1.98027900 | 0.77034900 |
| H | -3.92718400 | 1.81025200 | -1.20977600 |
| H | -5.48328400 | 1.01361600 | -1.47951200 |
| H | -3.74590700 | -1.37544600 | 0.91800300 |
| Mn | 0.05790900 | -0.07427000 | -0.14886000 |
| H | -5.00974300 | -1.96277800 | 0.00547300 |

Fe-NO-NO-CS-X-X

1 5

| | | | |
|---|---|---|---|
| N | -1.83036800 | -0.54867700 | -0.91554800 |
| C | -2.11552000 | -1.96909200 | -0.44781000 |
| C | -2.96021500 | 0.31700400 | -0.45087400 |
| H | -1.45802600 | -2.19095600 | 0.39594000 |
| H | -1.87322300 | -2.66622300 | -1.25151700 |
| C | -3.58844000 | -1.96058400 | -0.03463300 |
| C | -3.76805200 | -0.55299500 | 0.54923100 |
| H | -3.60371000 | 0.61188500 | -1.28682600 |
| C | -2.41534700 | 1.57362200 | 0.18475800 |
| H | -3.81750900 | -2.74551400 | 0.68994000 |
| H | -4.24196900 | -2.09895500 | -0.90341100 |
| H | -3.32245700 | -0.49454100 | 1.54925700 |
| H | -4.80485700 | -0.22039700 | 0.61790200 |
| O | -3.33267600 | 2.46403500 | 0.48826900 |
| O | -1.21089000 | 1.74434600 | 0.42525300 |
| H | 2.03279700 | 0.81341100 | -1.79644100 |
| N | 1.97469300 | 0.66138100 | -0.79077200 |
| C | 2.58638000 | 1.86276400 | -0.11382000 |
| C | 2.86965800 | -0.53191200 | -0.45669400 |
| H | 2.16093700 | 1.94499000 | 0.89334500 |
| H | 2.32968400 | 2.76763200 | -0.66949900 |
| C | 4.07948800 | 1.54208100 | -0.04003800 |
| C | 4.07646400 | 0.04995900 | 0.32201900 |
| H | 3.19421700 | -0.98645900 | -1.39649800 |
| C | 2.13216200 | -1.62244800 | 0.34351300 |
| H | 4.60369600 | 2.15827300 | 0.69491200 |
| H | 4.54819900 | 1.70994700 | -1.01724000 |
| H | 3.92387200 | -0.08216000 | 1.39815300 |
| H | 5.00042300 | -0.46708600 | 0.05990100 |
| O | 0.87207100 | -1.34451900 | 0.66227900 |
| O | 2.71651800 | -2.64125400 | 0.64050900 |
| H | -2.93430500 | 3.24077800 | 0.92432600 |
| H | -1.81001800 | -0.53737500 | -1.93290500 |
| Fe | 0.05085900 | 0.17009900 | -0.07267300 |

Fe-OO-NO-ZW-X-X

1 5

| | | | |
|---|---|---|---|
| N | -4.01108300 | -0.22818300 | 1.26648200 |
| C | -5.02954000 | 0.82644700 | 0.84902500 |
| C | -3.39953500 | -0.82284200 | -0.00349800 |
| H | -4.49984000 | 1.78127300 | 0.82087200 |
| H | -5.82399300 | 0.87355000 | 1.59467500 |
| C | -5.45209200 | 0.36680400 | -0.54488100 |
| C | -4.13243100 | -0.11687200 | -1.16820300 |
| H | -3.57698300 | -1.90057400 | -0.00226800 |
| C | -1.90115500 | -0.54059500 | 0.04905700 |
| H | -5.91311800 | 1.17911200 | -1.11104600 |
| H | -6.18019400 | -0.44951100 | -0.47700600 |
| H | -3.53933900 | 0.73172500 | -1.52291200 |
| H | -4.27150500 | -0.79788700 | -2.00865400 |
| O | -1.19411400 | -0.92772100 | -0.93550100 |
| O | -1.43461800 | 0.09530100 | 1.02565700 |
| H | 2.12802800 | -1.26063500 | 1.40487100 |
| N | 2.28562300 | -0.81570800 | 0.50078800 |
| C | 3.09193400 | -1.76837400 | -0.33438900 |
| C | 3.18869800 | 0.38639200 | 0.73441100 |
| H | 3.00486200 | -1.45519400 | -1.38145500 |
| H | 2.68687700 | -2.77888500 | -0.24048700 |
| C | 4.52548100 | -1.59176700 | 0.16850600 |
| C | 4.63051000 | -0.06957300 | 0.37911400 |
| H | 3.10015200 | 0.67181500 | 1.78672900 |
| C | 2.73392100 | 1.61505700 | -0.08468100 |
| H | 5.26767500 | -1.97403200 | -0.53695200 |
| H | 4.65407500 | -2.13168900 | 1.11448000 |
| H | 4.95543600 | 0.43462900 | -0.53470200 |
| H | 5.33996000 | 0.20127500 | 1.16270600 |
| O | 1.53055300 | 1.51801400 | -0.64201000 |
| O | 3.45747900 | 2.58348900 | -0.16262400 |
| H | -3.21115600 | 0.17018500 | 1.79534800 |
| H | -4.44605700 | -0.95246100 | 1.84082200 |
| Fe | 0.53823800 | -0.03446900 | -0.40872500 |

Fe-NO-OO-CS-X-X

1 5

| | | | |
|---|---|---|---|
| N | -1.81080100 | 0.72951400 | 0.82885200 |
| C | -1.56347200 | 2.04596000 | 0.11921400 |
| C | -3.24006500 | 0.34854000 | 0.57516700 |
| H | -1.10466800 | 1.83429600 | -0.85090500 |
| H | -0.85269600 | 2.63640300 | 0.69864400 |
| C | -2.95143700 | 2.66424800 | -0.04130600 |
| C | -3.82416600 | 1.44321600 | -0.36481400 |
| H | -3.80218600 | 0.31546000 | 1.51399500 |
| C | -3.28898800 | -1.02940700 | -0.04225500 |
| H | -2.98287200 | 3.42019700 | -0.82952000 |
| H | -3.27643300 | 3.13467000 | 0.89364200 |
| H | -3.69696500 | 1.15251500 | -1.41366900 |
| H | -4.88984300 | 1.59093500 | -0.18449500 |
| O | -4.49987100 | -1.49429100 | -0.23286300 |
| O | -2.26994800 | -1.66039800 | -0.36333500 |
| H | 3.18319800 | 0.98020500 | -1.82128900 |
| N | 3.86224600 | 0.54962700 | -1.20327300 |
| C | 4.43235300 | 1.46374900 | -0.20501000 |
| C | 3.35972000 | -0.63262700 | -0.52009000 |
| H | 3.66501100 | 2.04458000 | 0.33797900 |
| H | 5.11805400 | 2.16779800 | -0.68448500 |
| C | 5.13209900 | 0.48869100 | 0.74521400 |
| C | 4.12372000 | -0.67347200 | 0.85120400 |
| H | 3.56425300 | -1.54272200 | -1.10023600 |
| C | 1.86938100 | -0.64626600 | -0.28061700 |
| H | 5.36171700 | 0.92906000 | 1.71907100 |
| H | 6.06665700 | 0.14281900 | 0.29360800 |
| H | 3.42814900 | -0.50617300 | 1.68015900 |
| H | 4.59223500 | -1.64536500 | 1.01421700 |
| O | 1.10986300 | 0.34999600 | -0.55231800 |
| O | 1.29522800 | -1.69681200 | 0.20637000 |
| H | -4.47610600 | -2.37820700 | -0.64718000 |
| H | -1.69147600 | 0.87785700 | 1.82943000 |
| Fe | -0.45935300 | -0.80508000 | 0.10341900 |

Fe-OO-OO-ZW-X-E

1 5

| | | | |
|---|---|---|---|
| N | 4.52672200 | 0.86928700 | -0.56351400 |
| C | 5.46625500 | 1.02185400 | 0.62893000 |
| C | 3.81462000 | -0.47916000 | -0.43875800 |
| H | 4.91906300 | 1.57999400 | 1.39166300 |
| H | 6.34421400 | 1.59164800 | 0.32278600 |
| C | 5.72749300 | -0.42201800 | 1.05421500 |
| C | 4.35677100 | -1.09364600 | 0.87150100 |
| H | 4.07173400 | -1.08865000 | -1.30794900 |
| C | 2.31777300 | -0.19709800 | -0.43215300 |
| H | 6.09064200 | -0.47592200 | 2.08287500 |
| H | 6.48194500 | -0.88413600 | 0.40761100 |
| H | 3.69287300 | -0.84612600 | 1.70602700 |
| H | 4.40845300 | -2.18054700 | 0.79716600 |
| O | 1.52754700 | -1.19929900 | -0.38176200 |
| O | 1.91508200 | 0.98767700 | -0.45158200 |
| N | -4.86426800 | -0.21281100 | -0.82688600 |
| C | -5.44419400 | -0.93157300 | 0.33634900 |
| C | -3.93607300 | 0.80595100 | -0.37741500 |
| H | -5.21910700 | -2.00313600 | 0.30139000 |
| H | -6.53450500 | -0.81951700 | 0.32363800 |
| C | -4.83064900 | -0.25656400 | 1.57969100 |
| C | -4.41112200 | 1.12900400 | 1.06196300 |
| H | -3.96646000 | 1.70444000 | -1.00901400 |
| C | -2.47997700 | 0.37893100 | -0.36216000 |
| H | -3.94818400 | -0.81210100 | 1.91972500 |
| H | -5.52910000 | -0.19981100 | 2.41848500 |
| H | -3.64031500 | 1.62114900 | 1.65908500 |
| H | -5.27355200 | 1.79860300 | 0.99266900 |
| O | -2.11291300 | -0.81749300 | -0.66411300 |
| O | -1.54507000 | 1.20873600 | -0.06093300 |
| H | 5.03683300 | 0.93399000 | -1.44656800 |
| Fe | -0.21659000 | -0.24763000 | -0.37636400 |
| H | 3.77284200 | 1.58215100 | -0.57776400 |
| H | -4.47576100 | -0.83001900 | -1.52942600 |

Co-NO-NO-CS-X-E

1 2

| | | | |
|---|---|---|---|
| N | 1.61116000 | 0.95008700 | -0.40237600 |
| C | 1.77883100 | 1.83986800 | 0.80638300 |
| C | 2.81225000 | 0.05234400 | -0.45802900 |
| H | 1.28768000 | 1.35434100 | 1.65472500 |
| H | 1.27384400 | 2.78700200 | 0.61909200 |
| C | 3.29113500 | 1.91114200 | 1.01184500 |
| C | 3.73684300 | 0.46768700 | 0.72466500 |
| H | 3.33262400 | 0.16974300 | -1.41459500 |
| C | 2.32625900 | -1.37169100 | -0.37805500 |
| H | 3.56242100 | 2.23806100 | 2.01836300 |
| H | 3.74481000 | 2.60709000 | 0.29694100 |
| H | 3.54896200 | -0.16848000 | 1.59621900 |
| H | 4.79023800 | 0.36754000 | 0.45964400 |
| O | 3.26549800 | -2.28460500 | -0.38249200 |
| O | 1.11616000 | -1.65967800 | -0.30666000 |
| H | -1.74192300 | -1.78449900 | -1.11111600 |
| N | -1.74723600 | -1.08306700 | -0.37092900 |
| C | -2.01765100 | -1.77493900 | 0.95309300 |
| C | -2.88920100 | -0.10887200 | -0.61484700 |
| H | -1.08119900 | -1.90682000 | 1.50005700 |
| H | -2.44116300 | -2.76409200 | 0.75267400 |
| C | -3.03737700 | -0.87482600 | 1.65264700 |
| C | -3.91736900 | -0.39546700 | 0.48859800 |
| H | -3.28979100 | -0.26205000 | -1.62065700 |
| C | -2.35308500 | 1.33125500 | -0.55406700 |
| H | -2.53666300 | -0.02344200 | 2.12847800 |
| H | -3.59364900 | -1.41219600 | 2.42386000 |
| H | -4.50312800 | 0.49815100 | 0.71140700 |
| H | -4.60357000 | -1.18918800 | 0.17454000 |
| O | -1.02024500 | 1.42708300 | -0.53355200 |
| O | -3.09483600 | 2.28582200 | -0.53863600 |
| H | 2.88475300 | -3.18206200 | -0.33208700 |
| H | 1.59627000 | 1.54815400 | -1.22911700 |
| Co | -0.06645900 | -0.09460600 | -0.40437000 |

Co-OO-NO-ZW-E-E

1 4

| | | | |
|---|---|---|---|
| N | 4.08117500 | -0.19049900 | -1.03631100 |
| C | 4.92376600 | 0.89458900 | -0.36188000 |
| C | 3.34434400 | -0.97095700 | 0.05583300 |
| H | 4.89826300 | 1.79218600 | -0.98062300 |
| H | 5.94723200 | 0.51818100 | -0.30514300 |
| C | 4.28887100 | 1.03146000 | 1.02199400 |
| C | 3.90698600 | -0.41478500 | 1.37711400 |
| H | 3.51589300 | -2.04132700 | -0.07711500 |
| C | 1.85607500 | -0.67415000 | -0.12869500 |
| H | 3.40189700 | 1.67263800 | 0.97768800 |
| H | 4.98674600 | 1.47313900 | 1.73615600 |
| H | 3.16329300 | -0.49158600 | 2.17183300 |
| H | 4.78913000 | -0.98912600 | 1.67625600 |
| O | 1.02559200 | -1.10271400 | 0.71154700 |
| O | 1.49833700 | 0.03851300 | -1.12411600 |
| H | -2.30646600 | -1.15394400 | -1.74380000 |
| N | -2.27669700 | -0.80052400 | -0.78965100 |
| C | -2.74223500 | -1.90562400 | 0.14783800 |
| C | -3.27183200 | 0.35126400 | -0.66937400 |
| H | -1.89103200 | -2.29782300 | 0.70937800 |
| H | -3.16549700 | -2.71790400 | -0.45066200 |
| C | -3.81339300 | -1.25028700 | 1.02535500 |
| C | -4.47529500 | -0.24552400 | 0.07197900 |
| H | -3.52292400 | 0.70609100 | -1.67303800 |
| C | -2.66651100 | 1.56381100 | 0.08783000 |
| H | -3.35202800 | -0.72389800 | 1.86899000 |
| H | -4.50947000 | -1.98768500 | 1.43181400 |
| H | -5.04428700 | 0.53633400 | 0.57709400 |
| H | -5.13911900 | -0.76124500 | -0.63105600 |
| O | -1.35596700 | 1.53912600 | 0.28298200 |
| O | -3.39805200 | 2.46630100 | 0.43770600 |
| H | 3.32527900 | 0.22337000 | -1.61521500 |
| H | 4.64479000 | -0.79572400 | -1.63600600 |
| Co | -0.46803600 | 0.00618200 | -0.27732300 |

Co-NO-OO-CS-X-X

1 4

| | | | |
|---|---|---|---|
| N | -2.14988100 | -0.72767700 | -0.75236000 |
| C | -2.38834800 | -2.01816300 | 0.00976300 |
| C | -3.32470300 | 0.17430700 | -0.47953700 |
| H | -1.83896600 | -1.96453300 | 0.95432000 |
| H | -1.98870300 | -2.85320900 | -0.56780500 |
| C | -3.89749500 | -2.05436300 | 0.24703900 |
| C | -4.22410200 | -0.58266200 | 0.53785600 |
| H | -3.87767700 | 0.36672000 | -1.40452300 |
| C | -2.83591100 | 1.50321700 | 0.05057300 |
| H | -4.17232000 | -2.71433100 | 1.07316000 |
| H | -4.42326700 | -2.39756800 | -0.65116900 |
| H | -3.93811900 | -0.32493100 | 1.56376500 |
| H | -5.27496800 | -0.32134100 | 0.40608100 |
| O | -3.78853000 | 2.38206300 | 0.25076300 |
| O | -1.64335600 | 1.74042300 | 0.29499800 |
| H | 3.61408700 | -0.46369000 | -1.89575700 |
| N | 4.12889400 | -0.52776000 | -1.02421900 |
| C | 4.92314200 | 0.67015600 | -0.71340200 |
| C | 3.29025300 | -0.84481000 | 0.12302200 |
| H | 4.35224000 | 1.60764200 | -0.82994100 |
| H | 5.80067000 | 0.71972100 | -1.36390700 |
| C | 5.27345700 | 0.43990200 | 0.75869000 |
| C | 3.95750100 | -0.11178200 | 1.34126600 |
| H | 3.25560200 | -1.92823600 | 0.30161100 |
| C | 1.84945600 | -0.41535400 | -0.00124000 |
| H | 5.60249400 | 1.34933700 | 1.26809200 |
| H | 6.06899900 | -0.30740000 | 0.83648300 |
| H | 3.31955200 | 0.70802500 | 1.68795800 |
| H | 4.09959200 | -0.79119900 | 2.18337300 |
| O | 1.42371700 | 0.29781600 | -0.98464400 |
| O | 0.97491200 | -0.76184400 | 0.87943000 |
| H | -3.42610900 | 3.21763400 | 0.60312900 |
| H | -2.13960100 | -0.94375100 | -1.74849800 |
| Co | -0.38370600 | 0.22217900 | -0.17588400 |

Co-OO-OO-ZW-X-X

1 4

| | | | |
|---|---|---|---|
| C | 4.44429200 | -0.11039600 | 1.14154300 |
| C | 3.80419600 | -0.39890300 | -0.23464300 |
| N | 4.13400700 | 0.83179400 | -1.08457400 |
| C | 4.98277300 | 1.77934900 | -0.23866100 |
| C | 5.59347700 | 0.85656200 | 0.81457800 |
| C | 2.29197800 | -0.54831500 | -0.20456200 |
| O | 1.57431400 | 0.33998900 | -0.75800400 |
| O | 1.77695800 | -1.53527100 | 0.39185600 |
| O | -1.67273400 | -0.07874600 | 0.89493700 |
| C | -2.42349000 | -0.60766100 | -0.00339400 |
| O | -1.81528600 | -1.27924100 | -0.91854400 |
| C | -3.92283100 | -0.46682400 | -0.00447500 |
| N | -4.48555400 | 0.11950000 | 1.20642800 |
| C | -4.83782700 | 1.52116100 | 0.93923900 |
| C | -5.36345000 | 1.44519800 | -0.49633000 |
| C | -4.36610900 | 0.48473300 | -1.17161100 |
| H | -3.97098900 | 2.20284300 | 0.99372800 |
| H | -5.58905300 | 1.86459900 | 1.65614200 |
| H | -4.31218700 | -1.48017300 | -0.17064600 |
| H | -5.40198500 | 2.41936200 | -0.99109600 |
| H | -6.37004000 | 1.01560900 | -0.49892100 |
| H | -3.50458200 | 1.04124300 | -1.55599500 |
| H | -4.78945000 | -0.07864700 | -2.00492700 |
| H | -3.89980200 | -0.00763900 | 2.02462100 |
| H | 4.29804300 | 2.50676500 | 0.20255200 |
| H | 5.69331200 | 2.29551000 | -0.88509300 |
| H | 4.24987200 | -1.27560600 | -0.71003400 |
| H | 5.93385200 | 1.41791200 | 1.68744600 |
| H | 6.45582700 | 0.31939200 | 0.40398200 |
| H | 3.71487300 | 0.36681200 | 1.80394300 |
| H | 4.77132200 | -1.03617100 | 1.61649100 |
| H | 3.22486700 | 1.24450400 | -1.35966600 |
| Co | -0.10337200 | -0.86448600 | -0.04657000 |
| H | 4.62393200 | 0.56247600 | -1.94018100 |

Ni-NO-NO-E-E

1 1

| | | | |
|---|---|---|---|
| N | 1.64354800 | 1.06511300 | -0.58991600 |
| C | 1.67767400 | 2.16329600 | 0.44450400 |
| C | 2.86700000 | 0.21886400 | -0.37461600 |
| H | 0.66608600 | 2.54437400 | 0.57924800 |
| H | 2.32873100 | 2.97107400 | 0.09152000 |
| C | 2.28134800 | 1.45502600 | 1.65094200 |
| C | 3.42078600 | 0.62708000 | 1.03104000 |
| H | 3.61577600 | 0.38213300 | -1.15542500 |
| C | 2.44824500 | -1.22841200 | -0.41763400 |
| H | 1.53012100 | 0.80553100 | 2.11600400 |
| H | 2.64064000 | 2.15313800 | 2.40965100 |
| H | 3.71244300 | -0.24013100 | 1.62719900 |
| H | 4.31269200 | 1.24189200 | 0.88796900 |
| O | 1.25397600 | -1.57331400 | -0.43256800 |
| O | 3.43336200 | -2.09559100 | -0.41197500 |
| H | -1.56933300 | -1.81055600 | -1.16086200 |
| N | -1.60876400 | -1.12634500 | -0.40519200 |
| C | -1.78259200 | -1.85703200 | 0.91534000 |
| C | -2.82401100 | -0.22899000 | -0.59253600 |
| H | -0.81817000 | -1.94283400 | 1.41952700 |
| H | -2.15515600 | -2.86475900 | 0.70651000 |
| C | -2.82598500 | -1.03159000 | 1.66878700 |
| C | -3.78258400 | -0.59262000 | 0.54955100 |
| H | -3.25230100 | -0.40002200 | -1.58370900 |
| C | -2.37041200 | 1.23770500 | -0.53179800 |
| H | -2.35933500 | -0.15757900 | 2.13791600 |
| H | -3.31523500 | -1.61398500 | 2.45257400 |
| H | -4.40916900 | 0.26255700 | 0.80999600 |
| H | -4.43479900 | -1.42127500 | 0.25411800 |
| O | -1.04865100 | 1.40429100 | -0.55092200 |
| O | -3.15880000 | 2.15372200 | -0.47792400 |
| H | 3.09591900 | -3.01100800 | -0.42208200 |
| H | 1.64287000 | 1.47251500 | -1.52627700 |
| Ni | 0.00102900 | -0.05840200 | -0.49116100 |

Ni-OO-NO-ZW-E-E

1 3

| | | | |
|---|---|---|---|
| N | 3.88071200 | -0.29491900 | -1.18917400 |
| C | 4.96588700 | 0.63073900 | -0.63514300 |
| C | 3.17713800 | -0.96794900 | -0.00710000 |
| H | 5.00667000 | 1.53002000 | -1.25065400 |
| H | 5.91434400 | 0.09453000 | -0.70797000 |
| C | 4.54320400 | 0.84576900 | 0.81817000 |
| C | 3.98409300 | -0.52644000 | 1.22791200 |
| H | 3.16375300 | -2.04987000 | -0.15594500 |
| C | 1.74053900 | -0.44436700 | -0.00419400 |
| H | 3.77136400 | 1.62019000 | 0.88379400 |
| H | 5.38776000 | 1.16110900 | 1.43416500 |
| H | 3.34459500 | -0.49614500 | 2.11157500 |
| H | 4.79460300 | -1.23707700 | 1.41623500 |
| O | 0.96395100 | -0.74997900 | 0.93371200 |
| O | 1.36691800 | 0.31952500 | -0.95230100 |
| H | -1.59501300 | -0.93504000 | -1.73091700 |
| N | -1.87127900 | -0.71073300 | -0.77692300 |
| C | -2.11987300 | -1.99117200 | -0.00677100 |
| C | -3.17023300 | 0.07879600 | -0.79890900 |
| H | -1.26280000 | -2.20599600 | 0.63527200 |
| H | -2.24213500 | -2.81537800 | -0.71737700 |
| C | -3.42215600 | -1.72929200 | 0.75466800 |
| C | -4.23038500 | -0.87948700 | -0.23664000 |
| H | -3.38465100 | 0.39291100 | -1.82423700 |
| C | -3.05109300 | 1.37041800 | 0.04458100 |
| H | -3.22235700 | -1.16027600 | 1.67012900 |
| H | -3.92154600 | -2.65829600 | 1.03878400 |
| H | -5.05144000 | -0.32352300 | 0.21879700 |
| H | -4.63864500 | -1.50788600 | -1.03589600 |
| O | -1.82225500 | 1.68454700 | 0.44756500 |
| O | -4.03753300 | 2.03105800 | 0.28471400 |
| H | 3.13149400 | 0.24249300 | -1.66644100 |
| H | 4.25837900 | -0.97105400 | -1.85536700 |
| Ni | -0.49256300 | 0.49127000 | 0.09463400 |

Ni-NO-OO-CS-X-E

1 1

| | | | |
|---|---|---|---|
| N | 1.98502700 | 0.77085300 | -0.59099000 |
| C | 2.39632400 | 1.93662400 | 0.28431700 |
| C | 3.13717300 | -0.20342500 | -0.60989400 |
| H | 2.00875200 | 1.75728700 | 1.29057100 |
| H | 1.93964500 | 2.84849400 | -0.10106500 |
| C | 3.92447700 | 1.90149800 | 0.26608800 |
| C | 4.22650700 | 0.39546200 | 0.32004300 |
| H | 3.51927300 | -0.31696000 | -1.62946600 |
| C | 2.60493900 | -1.53462400 | -0.15124500 |
| H | 4.36145700 | 2.44503100 | 1.10693700 |
| H | 4.31175400 | 2.34227700 | -0.65962300 |
| H | 4.10330500 | 0.01945600 | 1.34130700 |
| H | 5.22814900 | 0.12751400 | -0.01886200 |
| O | 3.47367800 | -2.51505200 | -0.12118200 |
| O | 1.41869700 | -1.67596200 | 0.18703300 |
| H | -3.90889900 | 1.45082000 | -1.60421000 |
| N | -3.73237800 | 0.61000100 | -1.06793300 |
| C | -4.89197800 | -0.30488600 | -0.98116600 |
| C | -3.23008700 | 0.89561800 | 0.29323400 |
| H | -4.92180500 | -0.95876900 | -1.85729900 |
| H | -5.84345000 | 0.24575700 | -0.92795700 |
| C | -4.64617400 | -1.06635800 | 0.32483100 |
| C | -4.07622200 | 0.02549600 | 1.24811300 |
| H | -3.26337700 | 1.96231100 | 0.54499400 |
| C | -1.77975400 | 0.49239500 | 0.25037400 |
| H | -3.90296800 | -1.85510100 | 0.17025600 |
| H | -5.55614800 | -1.52222600 | 0.72236900 |
| H | -3.49673100 | -0.37239400 | 2.08458000 |
| H | -4.88317000 | 0.64156800 | 1.65678800 |
| O | -0.84608900 | 1.30276600 | -0.12912900 |
| O | -1.34676300 | -0.68442100 | 0.51363200 |
| H | 3.05716300 | -3.34217600 | 0.18891100 |
| H | 1.83105600 | 1.11971000 | -1.53801700 |
| Ni | 0.35928800 | -0.10371500 | -0.00817000 |

Ni-OO-OO-ZW-E-E

1 3

| | | | |
|---|---|---|---|
| C | -4.62274000 | -0.46351500 | 0.48695000 |
| C | -3.38813100 | 0.33142100 | 0.95698300 |
| N | -3.53234500 | 1.70255100 | 0.29097900 |
| C | -4.76352600 | 1.66748000 | -0.61349200 |
| C | -4.97149400 | 0.17498300 | -0.86783100 |
| C | -2.06920800 | -0.25286200 | 0.46271300 |
| O | -1.69845400 | -1.39046600 | 0.85890300 |
| O | -1.36132300 | 0.42292100 | -0.34808100 |
| O | 1.66219600 | -0.48613700 | 0.76954700 |
| C | 2.30884300 | -0.70172600 | -0.31259100 |
| O | 1.63115700 | -1.21841100 | -1.27900300 |
| C | 3.76016300 | -0.31597200 | -0.50208600 |
| N | 3.71573300 | 1.05789200 | -1.04844300 |
| C | 4.54693300 | 1.94553100 | -0.21038900 |
| C | 4.48753200 | 1.28028900 | 1.16792100 |
| C | 4.55555500 | -0.21642300 | 0.81708700 |
| H | 4.13837400 | 2.96057800 | -0.21418600 |
| H | 5.58862500 | 1.99245700 | -0.56498300 |
| H | 4.19454100 | -1.03666700 | -1.20440400 |
| H | 3.53520400 | 1.50870800 | 1.65743600 |
| H | 5.30057500 | 1.59907000 | 1.82501000 |
| H | 4.15398600 | -0.86335300 | 1.60032900 |
| H | 5.59110400 | -0.51611300 | 0.62673000 |
| H | 3.93484100 | 1.09323800 | -2.03661300 |
| H | -4.56556200 | 2.27271100 | -1.49883500 |
| H | -5.59095500 | 2.10332700 | -0.04957800 |
| H | -3.33542600 | 0.45215100 | 2.04093000 |
| H | -4.29685900 | -0.17793000 | -1.65520900 |
| H | -5.99545000 | -0.03511400 | -1.18341200 |
| H | -4.39396600 | -1.52892700 | 0.42689400 |
| H | -5.44093300 | -0.33220000 | 1.20139800 |
| H | -2.66141000 | 1.81956000 | -0.26186700 |
| Ni | 0.04293600 | -1.15772900 | -0.16792300 |
| H | -3.57476300 | 2.46333700 | 0.97194900 |

Cu-NO-NO-CS-E-E

1 2

| | | | |
|---|---|---|---|
| N | 1.874572 | -0.730016 | 1.188541 |
| C | 2.145719 | -1.832157 | 0.198940 |
| C | 2.901497 | 0.332304 | 0.969301 |
| H | 1.234824 | -2.415518 | 0.065662 |
| H | 2.943995 | -2.480331 | 0.578426 |
| C | 2.605468 | -1.050946 | -1.026356 |
| C | 3.538704 | 0.016163 | -0.426854 |
| H | 3.663763 | 0.336314 | 1.754165 |
| C | 2.219842 | 1.681503 | 0.975312 |
| H | 1.741533 | -0.587568 | -1.519599 |
| H | 3.110645 | -1.680866 | -1.761160 |
| H | 3.643089 | 0.908944 | -1.047036 |
| H | 4.540069 | -0.390761 | -0.267720 |
| O | 0.989826 | 1.819588 | 0.926841 |
| O | 3.048914 | 2.701728 | 1.005618 |
| H | -2.033612 | 1.484735 | 1.468842 |
| N | -1.857809 | 0.819946 | 0.717056 |
| C | -2.039380 | 1.515411 | -0.618069 |
| C | -2.859191 | -0.316386 | 0.788790 |
| H | -1.065311 | 1.779895 | -1.036430 |
| H | -2.604479 | 2.439116 | -0.459553 |
| C | -2.840986 | 0.518583 | -1.458399 |
| C | -3.780266 | -0.119118 | -0.423769 |
| H | -3.393850 | -0.268753 | 1.741484 |
| C | -2.133632 | -1.679201 | 0.749271 |
| H | -2.180038 | -0.241344 | -1.891979 |
| H | -3.368365 | 1.011337 | -2.278140 |
| H | -4.210195 | -1.070914 | -0.740392 |
| H | -4.598907 | 0.564978 | -0.175614 |
| O | -0.818331 | -1.636516 | 0.893242 |
| O | -2.761391 | -2.707214 | 0.606880 |
| H | 2.563194 | 3.547383 | 0.981645 |
| H | 1.919117 | -1.093116 | 2.140828 |
| Cu | -0.022833 | 0.046876 | 0.941830 |

Cu-OO-NO-ZW-E-E

1 2

| | | | |
|---|---|---|---|
| N | 4.02794400 | 0.96135600 | -0.34179200 |
| C | 4.85796200 | 0.67607300 | 0.90724500 |
| C | 3.33052000 | -0.33522400 | -0.76283900 |
| H | 4.83038500 | 1.55292100 | 1.55512200 |
| H | 5.88400800 | 0.49428300 | 0.58042900 |
| C | 4.21079100 | -0.58506500 | 1.47907400 |
| C | 3.85741100 | -1.39763700 | 0.22216900 |
| H | 3.56314000 | -0.55663900 | -1.80636400 |
| C | 1.83086800 | -0.07426200 | -0.62762700 |
| H | 3.31092700 | -0.32905800 | 2.04857600 |
| H | 4.89341600 | -1.11393600 | 2.14726800 |
| H | 3.10537500 | -2.16956900 | 0.39380900 |
| H | 4.74845900 | -1.87837900 | -0.19285400 |
| O | 1.00466900 | -0.98658100 | -0.90152300 |
| O | 1.45042000 | 1.06590500 | -0.22481400 |
| H | -2.21633100 | -0.94284800 | -1.81972800 |
| N | -2.19202200 | -0.75757300 | -0.81791400 |
| C | -2.24581400 | -2.05629500 | -0.04930900 |
| C | -3.38324100 | 0.08749200 | -0.40312600 |
| H | -1.23220700 | -2.39521100 | 0.17702000 |
| H | -2.73461500 | -2.81606000 | -0.66864600 |
| C | -3.10154400 | -1.71584800 | 1.17080600 |
| C | -4.17868600 | -0.79560900 | 0.57563600 |
| H | -3.96402700 | 0.35939200 | -1.28831500 |
| C | -2.91605000 | 1.40718600 | 0.25092500 |
| H | -2.50644800 | -1.17780800 | 1.91878800 |
| H | -3.51076600 | -2.61030100 | 1.64569800 |
| H | -4.69810700 | -0.18073400 | 1.31260700 |
| H | -4.92510300 | -1.38684800 | 0.03480200 |
| O | -1.61617700 | 1.64047800 | 0.22492500 |
| O | -3.73013100 | 2.16188900 | 0.74223200 |
| H | 3.24529400 | 1.61447400 | -0.13394400 |
| H | 4.58767300 | 1.36762800 | -1.09387400 |
| Cu | -0.54055400 | 0.29047700 | -0.41368100 |

Cu-NO-OO-CS-X-X

1 2

| | | | |
|---|---|---|---|
| N | -2.09973000 | -0.78771000 | -0.64913400 |
| C | -2.13767600 | -2.03926400 | 0.19972100 |
| C | -3.32429000 | 0.01635600 | -0.31960100 |
| H | -1.55177100 | -1.85774900 | 1.10588000 |
| H | -1.66950000 | -2.85740700 | -0.34858600 |
| C | -3.61780500 | -2.22708900 | 0.53180300 |
| C | -4.09237800 | -0.78538100 | 0.76956000 |
| H | -3.94514800 | 0.14229900 | -1.21237300 |
| C | -2.89914700 | 1.39112700 | 0.14539700 |
| H | -3.77158800 | -2.86715100 | 1.40378900 |
| H | -4.14835700 | -2.67587700 | -0.31568900 |
| H | -3.79768200 | -0.44747600 | 1.76916100 |
| H | -5.17040700 | -0.64817000 | 0.67526700 |
| O | -3.90028200 | 2.19220600 | 0.43434600 |
| O | -1.71435200 | 1.72656500 | 0.25693100 |
| H | 3.65039300 | 1.83694000 | -0.52426700 |
| N | 4.14200900 | 0.96196900 | -0.37666900 |
| C | 4.74872100 | 0.80006700 | 0.94957700 |
| C | 3.36861500 | -0.22912900 | -0.70353800 |
| H | 4.04806200 | 1.02649200 | 1.77162900 |
| H | 5.61539600 | 1.45965400 | 1.04918900 |
| C | 5.11323900 | -0.68706600 | 0.94829500 |
| C | 3.89098500 | -1.33921400 | 0.27180600 |
| H | 3.52387800 | -0.52631900 | -1.74969300 |
| C | 1.88257200 | -0.03422600 | -0.54525000 |
| H | 5.29342200 | -1.08394200 | 1.95055500 |
| H | 6.01350400 | -0.84577800 | 0.34693700 |
| H | 3.12463900 | -1.57827200 | 1.01634800 |
| H | 4.12600600 | -2.26143100 | -0.26220000 |
| O | 1.38005200 | 1.07864000 | -0.15235900 |
| O | 1.03837700 | -0.96301900 | -0.80917100 |
| H | -3.57295800 | 3.06202300 | 0.73308100 |
| H | -2.13999800 | -1.06472300 | -1.62948500 |
| Cu | -0.41211100 | 0.29292600 | -0.34219100 |

Cu-OO-OO-ZW-E-E

1 2

| | | | |
|---|---|---|---|
| C | -4.57823900 | -1.03935500 | -0.15429900 |
| C | -3.76655500 | -0.07561400 | 0.73031000 |
| N | -4.43427500 | 1.28275000 | 0.53543600 |
| C | -5.54604900 | 1.13356100 | -0.48993100 |
| C | -5.14978400 | -0.12971900 | -1.25564200 |
| C | -2.30745600 | 0.12797300 | 0.26226200 |
| O | -1.98096400 | 1.24934100 | -0.15379800 |
| O | -1.58541700 | -0.92334400 | 0.35755500 |
| O | 2.09378700 | -1.03868500 | -0.47466100 |
| C | 2.51792800 | -0.36610600 | 0.54393200 |
| O | 1.69015500 | 0.11017600 | 1.34850900 |
| C | 4.03458800 | -0.19755300 | 0.71978200 |
| N | 4.71674200 | -0.66811100 | -0.46065900 |
| C | 5.07178000 | 0.41717400 | -1.37753500 |
| C | 4.53553900 | 1.68693200 | -0.68303200 |
| C | 4.44811700 | 1.28507500 | 0.80169100 |
| H | 4.64211800 | 0.25106900 | -2.37149100 |
| H | 6.16481800 | 0.44930700 | -1.48954800 |
| H | 4.31353900 | -0.77002700 | 1.61269300 |
| H | 3.53829600 | 1.92812800 | -1.06779600 |
| H | 5.17658200 | 2.55490600 | -0.84974700 |
| H | 3.73305700 | 1.87576700 | 1.37725300 |
| H | 5.42652200 | 1.35362800 | 1.28631200 |
| H | -5.60191700 | 2.04426800 | -1.08771600 |
| H | -6.48200700 | 0.99842400 | 0.05690900 |
| H | -3.77173900 | -0.34515700 | 1.78787000 |
| H | -4.38625300 | 0.10354900 | -2.00524000 |
| H | -6.00639000 | -0.56977600 | -1.77024000 |
| H | -3.94220200 | -1.84088500 | -0.53308100 |
| H | -5.38581200 | -1.49320500 | 0.42871000 |
| H | -3.63460300 | 1.85618800 | 0.16687000 |
| Cu | 0.24886000 | -0.86377900 | 0.00517800 |
| H | -4.75867000 | 1.69778200 | 1.40970600 |
| H | 4.48073700 | -1.58096400 | -0.83115700 |

Zn-NO-NO-CS-X-X

1 1

| | | | |
|---|---|---|---|
| N | -1.87602700 | -0.31082000 | -1.08631700 |
| C | -2.19903200 | -1.79246600 | -0.88574500 |
| C | -2.84668600 | 0.48057000 | -0.25933000 |
| H | -1.41066100 | -2.22706000 | -0.26738600 |
| H | -2.20385800 | -2.28980600 | -1.85720300 |
| C | -3.54589400 | -1.80781000 | -0.15998900 |
| C | -3.47601300 | -0.54854200 | 0.71333900 |
| H | -3.62635400 | 0.92136800 | -0.88913400 |
| C | -2.13784000 | 1.60178000 | 0.46845100 |
| H | -3.67803500 | -2.71726800 | 0.43046500 |
| H | -4.37920800 | -1.73639900 | -0.86801100 |
| H | -2.81073500 | -0.71339400 | 1.56878100 |
| H | -4.44174000 | -0.20328500 | 1.08519200 |
| O | -2.95975400 | 2.43995500 | 1.06135200 |
| O | -0.90817800 | 1.70874000 | 0.52828700 |
| H | 2.13584800 | 0.30824400 | -1.96471100 |
| N | 1.96129500 | 0.41257400 | -0.96662500 |
| C | 2.54466100 | 1.73905400 | -0.53289400 |
| C | 2.74700200 | -0.68512000 | -0.23711900 |
| H | 1.98162600 | 2.09097700 | 0.33718400 |
| H | 2.42812000 | 2.46869100 | -1.33749100 |
| C | 3.98666200 | 1.40926700 | -0.15008100 |
| C | 3.83330700 | 0.06303500 | 0.57079300 |
| H | 3.20072100 | -1.32711600 | -0.99660000 |
| C | 1.87921300 | -1.60032700 | 0.66575500 |
| H | 4.43573600 | 2.18276900 | 0.47827900 |
| H | 4.60381300 | 1.30543200 | -1.05067100 |
| H | 3.49221400 | 0.21623600 | 1.60026200 |
| H | 4.75386800 | -0.51974000 | 0.61841600 |
| O | 0.59080000 | -1.32969000 | 0.73381500 |
| O | 2.44518300 | -2.49940100 | 1.25498900 |
| H | -2.46502100 | 3.12132600 | 1.55443700 |
| H | -2.00861500 | -0.06885700 | -2.06621900 |
| Zn | 0.04462400 | 0.09207100 | -0.39305400 |

Zn-OO-NO-ZW-E-E

1 1

| | | | |
|---|---|---|---|
| N | 4.28596900 | -0.39450100 | -1.02456100 |
| C | 5.17044100 | 0.72702900 | -0.48308500 |
| C | 3.43431900 | -0.93293800 | 0.12460600 |
| H | 5.26052700 | 1.50201800 | -1.24505300 |
| H | 6.15330700 | 0.29567600 | -0.28175800 |
| C | 4.45984600 | 1.14886100 | 0.80264700 |
| C | 3.94494100 | -0.18414000 | 1.37007300 |
| H | 3.54403300 | -2.01724500 | 0.19099100 |
| C | 1.98177100 | -0.58664800 | -0.24197900 |
| H | 3.62979500 | 1.82737100 | 0.57858900 |
| H | 5.14118800 | 1.66444800 | 1.48240700 |
| H | 3.14661400 | -0.07025800 | 2.10481800 |
| H | 4.75877100 | -0.74847600 | 1.83601400 |
| O | 1.10487400 | -0.89167200 | 0.64322300 |
| O | 1.74906500 | -0.02769600 | -1.32664600 |
| H | -2.14774900 | -1.27842200 | -1.60584300 |
| N | -2.29110800 | -0.87869200 | -0.68074300 |
| C | -3.00257200 | -1.90118200 | 0.19369800 |
| C | -3.19824300 | 0.34180200 | -0.79982900 |
| H | -2.29706200 | -2.34902800 | 0.89803200 |
| H | -3.39956500 | -2.69507000 | -0.44580400 |
| C | -4.13343600 | -1.11332700 | 0.86067100 |
| C | -4.54866400 | -0.11938800 | -0.23250000 |
| H | -3.25818700 | 0.63230800 | -1.85221700 |
| C | -2.64700600 | 1.58824800 | -0.03897400 |
| H | -3.76265100 | -0.57611900 | 1.74154900 |
| H | -4.94526600 | -1.76823800 | 1.18519300 |
| H | -5.12317500 | 0.73093800 | 0.13653900 |
| H | -5.13565500 | -0.62548500 | -1.00709500 |
| O | -1.41147600 | 1.52136300 | 0.42346800 |
| O | -3.37518100 | 2.55434700 | 0.06332900 |
| H | 3.57785400 | -0.03107800 | -1.69788500 |
| H | 4.82841300 | -1.12364300 | -1.49040000 |
| Zn | -0.57472900 | -0.11726600 | 0.12166900 |

Zn-NO-OO-CS-X-X

1 1

| | | | |
|---|---|---|---|
| N | -2.19895500 | -0.74373900 | -0.76113000 |
| C | -2.41149900 | -2.02043800 | 0.03796000 |
| C | -3.33482300 | 0.18583000 | -0.43580500 |
| H | -1.79633700 | -1.96642200 | 0.94077800 |
| H | -2.07300800 | -2.87150500 | -0.55499100 |
| C | -3.90113300 | -2.01507200 | 0.37724100 |
| C | -4.17443800 | -0.53095100 | 0.65875300 |
| H | -3.94466600 | 0.36326500 | -1.32719300 |
| C | -2.79761700 | 1.52397300 | 0.02857200 |
| H | -4.13266300 | -2.65257900 | 1.23369000 |
| H | -4.49446200 | -2.36329300 | -0.47575400 |
| H | -3.81088800 | -0.25912500 | 1.65606600 |
| H | -5.22616900 | -0.24853200 | 0.59542300 |
| O | -3.73430800 | 2.41308000 | 0.25873100 |
| O | -1.59367700 | 1.75594000 | 0.19656700 |
| H | 3.65070200 | -0.62928500 | -1.79749500 |
| N | 4.15732600 | -0.63661800 | -0.91933700 |
| C | 5.01090600 | 0.54563500 | -0.72256700 |
| C | 3.29179800 | -0.80143300 | 0.24344100 |
| H | 4.50486600 | 1.49124600 | -0.98343700 |
| H | 5.91601600 | 0.46276000 | -1.33082100 |
| C | 5.28813700 | 0.49168200 | 0.78146500 |
| C | 3.91466000 | 0.10663000 | 1.35988100 |
| H | 3.27432900 | -1.84826700 | 0.57503800 |
| C | 1.84477900 | -0.42534600 | 0.03201600 |
| H | 5.65834400 | 1.43852600 | 1.18337800 |
| H | 6.02648700 | -0.28762400 | 0.99544400 |
| H | 3.30299100 | 1.00426100 | 1.50270800 |
| H | 3.96352500 | -0.41399000 | 2.31791300 |
| O | 1.44726200 | 0.18450400 | -1.02897500 |
| O | 0.96107900 | -0.71233500 | 0.91841400 |
| H | -3.35041300 | 3.25534300 | 0.56988500 |
| H | -2.24223900 | -0.97221500 | -1.75336200 |
| Zn | -0.39875000 | 0.15557800 | -0.28358800 |

Zn-OO-OO-ZW-X-X

1 1

| | | | |
|---|---|---|---|
| C | 4.43316000 | -0.40556300 | 1.09734100 |
| C | 3.83519600 | -0.32871300 | -0.32447700 |
| N | 4.41432300 | 0.95424100 | -0.92238400 |
| C | 5.35103200 | 1.57931900 | 0.10692000 |
| C | 5.74118800 | 0.39476000 | 0.98982400 |
| C | 2.31379200 | -0.19327200 | -0.37070700 |
| O | 1.80568900 | 0.86584800 | -0.76619000 |
| O | 1.66207500 | -1.22384200 | 0.04130300 |
| O | -1.83364900 | -0.32858700 | 0.94144200 |
| C | -2.51574700 | -0.60288000 | -0.10971700 |
| O | -1.87034100 | -1.01806000 | -1.14269100 |
| C | -4.02308100 | -0.46401100 | -0.15806600 |
| N | -4.65848600 | -0.15958500 | 1.11464700 |
| C | -4.87380000 | 1.29155600 | 1.18900100 |
| C | -5.33453200 | 1.60882900 | -0.23629500 |
| C | -4.41166100 | 0.72783400 | -1.10464800 |
| H | -3.95322600 | 1.85200800 | 1.43018400 |
| H | -5.62577800 | 1.52407300 | 1.94819900 |
| H | -4.38750200 | -1.41613000 | -0.56398100 |
| H | -5.25133000 | 2.66979700 | -0.48677800 |
| H | -6.37837900 | 1.30563600 | -0.36039200 |
| H | -3.51780600 | 1.28244000 | -1.40732300 |
| H | -4.88996700 | 0.36543800 | -2.01625200 |
| H | -4.16263500 | -0.54172700 | 1.91284500 |
| H | 4.76759200 | 2.32235200 | 0.65486600 |
| H | 6.17336400 | 2.07442300 | -0.41059300 |
| H | 4.15198300 | -1.17197200 | -0.94209900 |
| H | 6.11566500 | 0.72608600 | 1.96088200 |
| H | 6.52788600 | -0.19957100 | 0.51161000 |
| H | 3.75420100 | 0.06232900 | 1.81767500 |
| H | 4.57883700 | -1.44308200 | 1.40069800 |
| H | 3.59224900 | 1.55044900 | -1.13831500 |
| Zn | -0.19638800 | -0.84326700 | -0.09745000 |
| H | 4.90214200 | 0.76286900 | -1.79954500 |

Mg-NO-NO-CS-X-E

1 1

| | | | |
|---|---|---|---|
| N | 1.90240500 | 0.48798000 | -1.06522300 |
| C | 2.11649000 | 1.93346500 | -0.62250300 |
| C | 2.94079500 | -0.35001100 | -0.37836400 |
| H | 1.34130100 | 2.18777100 | 0.10517500 |
| H | 2.00491600 | 2.59089200 | -1.48662300 |
| C | 3.50889300 | 1.95038000 | 0.00963600 |
| C | 3.58818300 | 0.57651600 | 0.68763700 |
| H | 3.70491900 | -0.68929300 | -1.08541500 |
| C | 2.30259600 | -1.57154000 | 0.24280600 |
| H | 3.62753200 | 2.77185000 | 0.71997800 |
| H | 4.28843500 | 2.04476800 | -0.75488900 |
| H | 2.99213900 | 0.57111700 | 1.60782800 |
| H | 4.60000700 | 0.25064400 | 0.93317600 |
| O | 3.16493500 | -2.44277300 | 0.71059800 |
| O | 1.07541600 | -1.72789900 | 0.33089200 |
| H | -2.15964500 | -0.68905400 | -2.06101000 |
| N | -1.99730200 | -0.59578600 | -1.06060900 |
| C | -2.58842600 | -1.83114500 | -0.38507300 |
| C | -2.81017800 | 0.60652800 | -0.57900500 |
| H | -1.80072700 | -2.39936100 | 0.11966300 |
| H | -3.02268200 | -2.47539800 | -1.15420400 |
| C | -3.65917100 | -1.30117200 | 0.58193400 |
| C | -4.12568500 | 0.00335700 | -0.07785900 |
| H | -2.94973600 | 1.28688000 | -1.42504600 |
| C | -2.07733300 | 1.43241100 | 0.52844400 |
| H | -3.22036300 | -1.08751400 | 1.56292000 |
| H | -4.46346200 | -2.02595700 | 0.72798800 |
| H | -4.62811600 | 0.68540800 | 0.60915200 |
| H | -4.79593000 | -0.20521100 | -0.91976700 |
| O | -0.78824600 | 1.20776700 | 0.65558900 |
| O | -2.72902600 | 2.24167900 | 1.15979600 |
| H | 2.70912600 | -3.19357700 | 1.13638300 |
| H | 2.06599100 | 0.43160500 | -2.06848900 |
| Mg | -0.04925400 | -0.18532100 | -0.38224300 |

Mg-OO-NO-ZW-E-X

1 1

| | | | |
|---|---|---|---|
| N | 4.02700600 | -0.31938900 | -1.08509700 |
| C | 4.86882100 | 0.83826400 | -0.53861300 |
| C | 3.33147500 | -1.00219800 | 0.09447400 |
| H | 4.80410000 | 1.67563500 | -1.23412600 |
| H | 5.90118900 | 0.48664700 | -0.48437000 |
| C | 4.27682700 | 1.08797000 | 0.84862900 |
| C | 3.92962300 | -0.32599200 | 1.34181200 |
| H | 3.50709200 | -2.07944300 | 0.05349200 |
| C | 1.83440700 | -0.73442800 | -0.06619300 |
| H | 3.37971900 | 1.71267900 | 0.77922800 |
| H | 4.99079200 | 1.59922800 | 1.49747000 |
| H | 3.21504100 | -0.34300300 | 2.16616000 |
| H | 4.83025600 | -0.86125400 | 1.65762100 |
| O | 1.03945900 | -1.07930500 | 0.84414600 |
| O | 1.43537200 | -0.12635300 | -1.11577100 |
| H | -2.49199600 | -1.23264400 | -1.58856200 |
| N | -2.35963100 | -0.81238400 | -0.66901200 |
| C | -2.91187800 | -1.78698200 | 0.33662300 |
| C | -3.26983300 | 0.41749400 | -0.59757100 |
| H | -2.51051600 | -1.52728500 | 1.32393400 |
| H | -2.58577200 | -2.80039000 | 0.08940900 |
| C | -4.42262500 | -1.55826500 | 0.29416500 |
| C | -4.52926400 | -0.02708200 | 0.19515000 |
| H | -3.52186200 | 0.69744500 | -1.62451900 |
| C | -2.58668600 | 1.66396400 | 0.03713300 |
| H | -4.93321800 | -1.96447700 | 1.17126300 |
| H | -4.84463100 | -2.04417800 | -0.59424200 |
| H | -4.51342900 | 0.43185000 | 1.18751600 |
| H | -5.44548400 | 0.30642400 | -0.29440400 |
| O | -1.29638900 | 1.57605600 | 0.26204600 |
| O | -3.29352000 | 2.62873300 | 0.26261100 |
| H | 3.25270300 | 0.02710000 | -1.68233300 |
| H | 4.58718700 | -0.97062000 | -1.63811300 |
| Mg | -0.45811500 | -0.05173500 | -0.18371500 |

Mg-NO-OO-CS-X-X

1 1

| | | | |
|---|---|---|---|
| N | -2.15590200 | -0.68632500 | -0.80756900 |
| C | -2.25873400 | -1.98767600 | -0.03249200 |
| C | -3.39861200 | 0.10369900 | -0.51543500 |
| H | -1.70023600 | -1.88237800 | 0.90353400 |
| H | -1.79339000 | -2.78749700 | -0.61084400 |
| C | -3.75371500 | -2.16600900 | 0.23018400 |
| C | -4.21754500 | -0.73057800 | 0.51386800 |
| H | -3.98261900 | 0.25523300 | -1.42887700 |
| C | -3.02483400 | 1.46794400 | 0.02282500 |
| H | -3.95307000 | -2.84140400 | 1.06549100 |
| H | -4.25619300 | -2.56621000 | -0.65771700 |
| H | -3.95330800 | -0.44023500 | 1.53710800 |
| H | -5.28924600 | -0.57138000 | 0.38696600 |
| O | -4.04797400 | 2.26056400 | 0.22486300 |
| O | -1.85615800 | 1.80278800 | 0.27314700 |
| H | 3.49357600 | -0.29753900 | -1.88660100 |
| N | 4.03474100 | -0.49971000 | -1.05333600 |
| C | 5.02793700 | 0.54137100 | -0.73945700 |
| C | 3.19701100 | -0.73416600 | 0.11961600 |
| H | 4.63536100 | 1.56413600 | -0.87333400 |
| H | 5.90898500 | 0.42789100 | -1.37755900 |
| C | 5.31846200 | 0.27950500 | 0.74015700 |
| C | 3.91740900 | -0.00951700 | 1.30578200 |
| H | 3.11687100 | -1.80875500 | 0.33597800 |
| C | 1.77276100 | -0.24765900 | 0.00103700 |
| H | 5.80405400 | 1.12345600 | 1.23727000 |
| H | 5.96259000 | -0.59987000 | 0.84390800 |
| H | 3.40764800 | 0.93183800 | 1.54090200 |
| H | 3.91622200 | -0.61947500 | 2.21093000 |
| O | 1.37996600 | 0.46532900 | -0.99707300 |
| O | 0.90864400 | -0.55320700 | 0.90554400 |
| H | -3.76207600 | 3.12113100 | 0.58742000 |
| H | -2.14931100 | -0.91127100 | -1.80143700 |
| Mg | -0.42619900 | 0.44160800 | -0.17626300 |

Mg-OO-OO-ZW-E-X

1 1

| | | | |
|---|---|---|---|
| C | -4.47826400 | 1.06225100 | -0.84335100 |
| C | -3.80060200 | -0.32248200 | -0.87747300 |
| N | -4.45150800 | -1.10173700 | 0.26734200 |
| C | -5.40125100 | -0.15838000 | 1.00808900 |
| C | -4.88606800 | 1.22956700 | 0.62963900 |
| C | -2.30358600 | -0.26605900 | -0.58223000 |
| O | -1.53871600 | 0.35845100 | -1.36043000 |
| O | -1.86325900 | -0.85045300 | 0.46521700 |
| O | 1.43157300 | 0.85999100 | 0.87678900 |
| C | 2.27223800 | -0.02133400 | 0.46201400 |
| O | 1.83491600 | -0.97827100 | -0.27865000 |
| C | 3.72939400 | 0.07794000 | 0.85731000 |
| N | 4.55766400 | -1.05888100 | 0.46820200 |
| C | 5.35672700 | -0.68040200 | -0.70682000 |
| C | 5.70785100 | 0.77649400 | -0.39559100 |
| C | 4.38600100 | 1.32613200 | 0.17263800 |
| H | 4.78918500 | -0.74182600 | -1.65216700 |
| H | 6.23441900 | -1.32756100 | -0.79232100 |
| H | 3.72411000 | 0.20330700 | 1.94836900 |
| H | 6.04775200 | 1.33282200 | -1.27333800 |
| H | 6.49589100 | 0.81254800 | 0.36328900 |
| H | 3.74807000 | 1.69318200 | -0.63861100 |
| H | 4.51677300 | 2.14755200 | 0.87939600 |
| H | 4.01706100 | -1.90582800 | 0.32895900 |
| H | -5.37417000 | -0.39760800 | 2.07170300 |
| H | -6.40453200 | -0.34043400 | 0.61729700 |
| H | -3.95102800 | -0.85558100 | -1.81867900 |
| H | -4.02515600 | 1.50300200 | 1.24926900 |
| H | -5.65600400 | 1.99070100 | 0.77124500 |
| H | -3.79551400 | 1.83328200 | -1.20413000 |
| H | -5.35873600 | 1.05818600 | -1.49281400 |
| H | -3.66183000 | -1.39420500 | 0.87279600 |
| Mg | 0.03551000 | -0.15006300 | -0.10754200 |
| H | -4.92626200 | -1.94656100 | -0.05733400 |

Ca-OO-OO-ZW-E-X

1 1

| | | | |
|---|---|---|---|
| C | -4.93059900 | 1.00355700 | -0.76598500 |
| C | -4.23456700 | -0.37054600 | -0.77519000 |
| N | -4.77012700 | -1.08368000 | 0.46742500 |
| C | -5.66872200 | -0.11273700 | 1.22884400 |
| C | -5.21587600 | 1.25706900 | 0.72354800 |
| C | -2.70889000 | -0.28529200 | -0.61118800 |
| O | -2.04694300 | 0.29921300 | -1.50160400 |
| O | -2.19899300 | -0.81419000 | 0.43372400 |
| O | 1.78063900 | 0.98374200 | 0.68607400 |
| C | 2.58997000 | 0.04323700 | 0.36038100 |
| O | 2.18263600 | -0.96833000 | -0.31692700 |
| C | 4.03792400 | 0.14771900 | 0.79952200 |
| N | 4.84402100 | -1.05362000 | 0.56433600 |
| C | 5.90433700 | -0.74579100 | -0.41183900 |
| C | 6.18047100 | 0.73904100 | -0.15833500 |
| C | 4.76458600 | 1.30167500 | 0.04321200 |
| H | 5.57929800 | -0.89254100 | -1.45645400 |
| H | 6.77937900 | -1.37965700 | -0.23771200 |
| H | 3.99893700 | 0.38326600 | 1.87224700 |
| H | 6.71559100 | 1.22105200 | -0.98135300 |
| H | 6.77341800 | 0.85947400 | 0.75508800 |
| H | 4.29142100 | 1.47157900 | -0.93169500 |
| H | 4.72718000 | 2.24100100 | 0.59850600 |
| H | 4.26708300 | -1.83795200 | 0.28035700 |
| H | -5.54574300 | -0.28348400 | 2.29898600 |
| H | -6.69931300 | -0.33090100 | 0.94076500 |
| H | -4.45796000 | -0.96293800 | -1.66473100 |
| H | -4.31061300 | 1.57943100 | 1.24935000 |
| H | -5.98529000 | 2.01468000 | 0.88552500 |
| H | -4.29365600 | 1.75858300 | -1.22953900 |
| H | -5.86383600 | 0.95207000 | -1.33505200 |
| H | -3.90964600 | -1.31385500 | 1.00560200 |
| Ca | 0.03075800 | -0.12159600 | -0.32621900 |
| H | -5.24918300 | -1.95785100 | 0.24422400 |

Ca-OO-NO-ZW-E-E

1 1

| | | | |
|---|---|---|---|
| N | 4.44604200 | -0.17432000 | -1.10749800 |
| C | 5.26616400 | 0.99171800 | -0.55941800 |
| C | 3.82393400 | -0.92224100 | 0.07235700 |
| H | 5.16609600 | 1.84131700 | -1.23586800 |
| H | 6.30905000 | 0.66895000 | -0.53083400 |
| C | 4.69644900 | 1.19737100 | 0.84418400 |
| C | 4.41149000 | -0.23692500 | 1.31980000 |
| H | 4.06708100 | -1.98460100 | 0.00505700 |
| C | 2.30102000 | -0.75196000 | -0.05459400 |
| H | 3.77556400 | 1.78906500 | 0.80214100 |
| H | 5.40408400 | 1.72522600 | 1.48666700 |
| H | 3.71034300 | -0.29511900 | 2.15375700 |
| H | 5.33771500 | -0.73732400 | 1.61864500 |
| O | 1.57329700 | -1.22164900 | 0.85177700 |
| O | 1.86450400 | -0.11897100 | -1.07459000 |
| H | -2.99785200 | -1.49069500 | -1.46838500 |
| N | -2.76086700 | -0.91991900 | -0.65698900 |
| C | -3.38603400 | -1.59946800 | 0.53810200 |
| C | -3.54740300 | 0.36621100 | -0.81213700 |
| H | -2.78285700 | -1.38233800 | 1.42884200 |
| H | -3.36823000 | -2.68169900 | 0.38444100 |
| C | -4.81743900 | -1.01496900 | 0.70313100 |
| C | -4.98562300 | -0.03937100 | -0.48125000 |
| H | -3.43115700 | 0.71810000 | -1.84418800 |
| C | -2.99835800 | 1.50971000 | 0.11080800 |
| H | -4.89533000 | -0.47392300 | 1.64948900 |
| H | -5.57741300 | -1.80014300 | 0.70589300 |
| H | -5.58968700 | 0.83232100 | -0.22732300 |
| H | -5.43929500 | -0.54361500 | -1.34260200 |
| O | -1.71396600 | 1.46610300 | 0.32792800 |
| O | -3.78312500 | 2.35531000 | 0.51139100 |
| H | 3.61939700 | 0.15777100 | -1.64602100 |
| H | 4.99942700 | -0.78284600 | -1.71292700 |
| Ca | -0.41070200 | -0.23737900 | -0.14466600 |

Ca-NO-OO-CS-X-E

1 1

| | | | |
|---|---|---|---|
| N | -1.22971100 | -0.55514500 | -0.50928400 |
| C | -0.75181800 | -1.43136200 | 0.61968700 |
| C | -2.68630700 | -0.81838400 | -0.67117200 |
| H | -0.87420900 | -0.88716000 | 1.56488400 |
| H | 0.31777400 | -1.62501800 | 0.49727900 |
| C | -1.68333900 | -2.64246300 | 0.57949900 |
| C | -3.04948000 | -2.00000900 | 0.28822000 |
| H | -2.91567000 | -1.09017100 | -1.70764000 |
| C | -3.48548700 | 0.43447500 | -0.36806000 |
| H | -1.68265800 | -3.21254000 | 1.51200600 |
| H | -1.39092700 | -3.31925800 | -0.23188500 |
| H | -3.49325900 | -1.61715200 | 1.21363300 |
| H | -3.77470900 | -2.67438500 | -0.16957400 |
| O | -4.78662500 | 0.26278500 | -0.49388900 |
| O | -2.98769700 | 1.51718500 | -0.03165600 |
| H | 2.82731900 | -1.53468300 | 1.54608500 |
| N | 2.76932400 | -1.11079000 | 0.62627200 |
| C | 3.62569000 | -1.80344700 | -0.36468700 |
| C | 3.17457100 | 0.32769400 | 0.67877500 |
| H | 3.08373900 | -2.64310700 | -0.81257900 |
| H | 4.54775400 | -2.19757600 | 0.08941900 |
| C | 3.96652900 | -0.69953300 | -1.36823900 |
| C | 4.20643400 | 0.51166900 | -0.45116400 |
| H | 3.57571200 | 0.59670200 | 1.66155600 |
| C | 1.88259600 | 1.11546800 | 0.48822000 |
| H | 3.11209900 | -0.50638200 | -2.02588100 |
| H | 4.83152300 | -0.94690500 | -1.98888000 |
| H | 4.08911100 | 1.46792100 | -0.96443000 |
| H | 5.21563600 | 0.46997500 | -0.02805700 |
| O | 1.53716100 | 1.52449900 | -0.67498300 |
| O | 1.11021000 | 1.26781300 | 1.49948300 |
| H | -5.26453900 | 1.08735800 | -0.28713400 |
| H | -0.74927100 | -0.86307500 | -1.35301900 |
| Ca | -0.62067200 | 1.83070500 | 0.08435900 |

Ca-NO-NO-CS-X-X

1 1

| | | | |
|---|---|---|---|
| N | -2.25520400 | -0.56101800 | -1.06202400 |
| C | -2.14601300 | -1.97196300 | -0.50401900 |
| C | -3.35443700 | 0.12889400 | -0.31362100 |
| H | -1.29005100 | -2.02438600 | 0.17700600 |
| H | -1.95873200 | -2.66909800 | -1.32357200 |
| C | -3.46193800 | -2.21118100 | 0.23758700 |
| C | -3.75625500 | -0.83273300 | 0.84219800 |
| H | -4.22180100 | 0.29939900 | -0.96079800 |
| C | -2.91614100 | 1.47761100 | 0.21662400 |
| H | -3.37463700 | -2.99051200 | 0.99837900 |
| H | -4.25718000 | -2.50060600 | -0.45917400 |
| H | -3.12027300 | -0.66074900 | 1.71888200 |
| H | -4.79438800 | -0.68115600 | 1.14174000 |
| O | -3.91365300 | 2.18101500 | 0.71658600 |
| O | -1.74885500 | 1.88453500 | 0.21929700 |
| H | 2.94022200 | 1.23511100 | -1.69688200 |
| N | 2.50014200 | 0.86686800 | -0.85327600 |
| C | 3.02048800 | 1.69720100 | 0.29329000 |
| C | 3.11751900 | -0.49946700 | -0.62941100 |
| H | 2.27709900 | 1.68977300 | 1.10113900 |
| H | 3.13746300 | 2.73249300 | -0.03748200 |
| C | 4.34162300 | 1.03663900 | 0.77917200 |
| C | 4.53467200 | -0.18887900 | -0.14166300 |
| H | 3.10523700 | -1.04168600 | -1.58249200 |
| C | 2.28787200 | -1.36376000 | 0.38293200 |
| H | 4.24173900 | 0.71816200 | 1.81954100 |
| H | 5.18406000 | 1.73019500 | 0.72362900 |
| H | 4.96452400 | -1.04457500 | 0.37998100 |
| H | 5.17593200 | 0.05983300 | -0.99492800 |
| O | 0.99858600 | -1.15849300 | 0.34876200 |
| O | 2.87840000 | -2.17418500 | 1.07763800 |
| H | -3.58874800 | 3.02553000 | 1.08051100 |
| H | -2.55022200 | -0.63422100 | -2.03303100 |
| Ca | 0.03475200 | 0.55592000 | -0.62610700 |

Sr-OO-NO-ZW-X-X

1 1

| | | | |
|---|---|---|---|
| N | 3.46531200 | 0.16237500 | -0.23996600 |
| C | 2.93498600 | 1.35293300 | -1.02583000 |
| C | 2.66733800 | 0.12222200 | 1.05777200 |
| H | 1.99611700 | 1.03587000 | -1.48810500 |
| H | 3.66638900 | 1.63436000 | -1.78504700 |
| C | 2.67887600 | 2.38024700 | 0.07032000 |
| C | 2.06795200 | 1.54246700 | 1.21357700 |
| H | 3.34527500 | -0.15136900 | 1.87077400 |
| C | 1.63424300 | -1.00489900 | 0.88606700 |
| H | 3.61349600 | 2.86260900 | 0.38023900 |
| H | 1.98389000 | 3.14372400 | -0.28222700 |
| H | 0.98515100 | 1.49069400 | 1.09913200 |
| H | 2.28611100 | 1.95382500 | 2.20043600 |
| O | 0.58673100 | -0.97752200 | 1.58295900 |
| O | 1.86742300 | -1.87190100 | -0.01631400 |
| H | -3.54400700 | -0.54332300 | -0.13764100 |
| N | -2.58108900 | -0.24902700 | 0.03282900 |
| C | -2.55616200 | 0.35398200 | 1.40391300 |
| C | -2.32180300 | 0.92813700 | -0.87858600 |
| H | -1.50734600 | 0.48921800 | 1.69013800 |
| H | -3.01667400 | -0.32894900 | 2.12406900 |
| C | -3.27747200 | 1.70115200 | 1.26147100 |
| C | -2.90839700 | 2.17388300 | -0.16910800 |
| H | -2.80114900 | 0.72560500 | -1.84222200 |
| C | -0.79737000 | 1.02357600 | -1.18023300 |
| H | -2.97516100 | 2.41409500 | 2.03317300 |
| H | -4.35907800 | 1.55344400 | 1.35786700 |
| H | -2.15506200 | 2.96389600 | -0.15998200 |
| H | -3.78268200 | 2.55670700 | -0.70127600 |
| O | -0.23862200 | -0.11176500 | -1.48816000 |
| O | -0.20749400 | 2.10214200 | -1.12280200 |
| H | 3.29126900 | -0.74407300 | -0.70855900 |
| H | 4.46571700 | 0.26208300 | -0.05912500 |
| Sr | -0.64419200 | -2.03372900 | -0.30587700 |

Sr-OO-OO-ZW-E-E

1 1

| | | | |
|---|---|---|---|
| C | 5.09999500 | -0.70992600 | 0.47888500 |
| C | 4.26088500 | -0.26130300 | -0.73020800 |
| N | 4.55649100 | 1.23101000 | -0.87494600 |
| C | 5.44192200 | 1.66197000 | 0.28880100 |
| C | 5.21733500 | 0.56519500 | 1.33128100 |
| C | 2.74014000 | -0.38226800 | -0.50427300 |
| O | 2.06402000 | 0.70104100 | -0.53952400 |
| O | 2.26833100 | -1.52366600 | -0.29971300 |
| O | -2.45435200 | -0.86159200 | -0.64983300 |
| C | -2.78276900 | -0.53466000 | 0.54447200 |
| O | -1.90674400 | -0.48827100 | 1.48177900 |
| C | -4.20157600 | -0.07513700 | 0.85526300 |
| N | -4.16214000 | 1.40374800 | 0.68857800 |
| C | -5.26297000 | 1.81459600 | -0.20611100 |
| C | -5.43496700 | 0.59991100 | -1.12224400 |
| C | -5.26615400 | -0.57536600 | -0.14306800 |
| H | -4.99139200 | 2.72698700 | -0.74700900 |
| H | -6.19900000 | 2.00831300 | 0.34303800 |
| H | -4.42431300 | -0.36839400 | 1.88758900 |
| H | -4.63765000 | 0.57807600 | -1.87225800 |
| H | -6.39912700 | 0.59275100 | -1.63784500 |
| H | -4.96742800 | -1.50341800 | -0.63515200 |
| H | -6.20382400 | -0.75775400 | 0.39297200 |
| H | -4.16792400 | 1.88533700 | 1.58013700 |
| H | 5.15569400 | 2.66818300 | 0.59782500 |
| H | 6.47264800 | 1.67196100 | -0.07248800 |
| H | 4.51996700 | -0.77999800 | -1.65544300 |
| H | 4.29316900 | 0.75102500 | 1.88941200 |
| H | 6.03975400 | 0.52408500 | 2.04848400 |
| H | 4.61473700 | -1.54168800 | 0.99228000 |
| H | 6.08769700 | -1.04521700 | 0.14714100 |
| H | 3.60597200 | 1.65901400 | -0.82096600 |
| Sr | -0.13595000 | -0.63733900 | -0.10662100 |
| H | 4.96558200 | 1.46814000 | -1.78002200 |

Sr-NO-OO-CS-X-X

1 1

| | | | |
|---|---|---|---|
| N | -1.17400500 | -0.79836400 | -0.49069700 |
| C | -0.48088800 | -1.64930500 | 0.54519800 |
| C | -2.59030400 | -1.25495100 | -0.55997500 |
| H | -0.50402000 | -1.12385800 | 1.50662600 |
| H | 0.56536700 | -1.78662500 | 0.25702500 |
| C | -1.30640500 | -2.93501400 | 0.60865700 |
| C | -2.74355700 | -2.41401000 | 0.47422700 |
| H | -2.83069300 | -1.62368800 | -1.56403200 |
| C | -3.54479600 | -0.11320700 | -0.27710500 |
| H | -1.14861600 | -3.49410100 | 1.53459200 |
| H | -1.05246200 | -3.59200100 | -0.23150800 |
| H | -3.09533500 | -2.02119100 | 1.43520700 |
| H | -3.46635500 | -3.15772800 | 0.13486500 |
| O | -4.81474700 | -0.47185400 | -0.35842900 |
| O | -3.19710600 | 1.03766200 | 0.00820700 |
| H | 2.67562100 | -0.73961100 | -1.44408200 |
| N | 2.84577400 | -1.18336900 | -0.54116600 |
| C | 4.21256000 | -1.74987300 | -0.53481300 |
| C | 2.91199700 | -0.10348800 | 0.45945500 |
| H | 4.40894900 | -2.26210900 | -1.48026600 |
| H | 4.26830200 | -2.49881600 | 0.26297100 |
| C | 5.19461400 | -0.57418900 | -0.24752400 |
| C | 4.28881800 | 0.58618300 | 0.25105300 |
| H | 2.86381600 | -0.54604200 | 1.46029100 |
| C | 1.72587600 | 0.82204700 | 0.31085300 |
| H | 5.73978800 | -0.28005600 | -1.14896600 |
| H | 5.93864800 | -0.85607500 | 0.50305800 |
| H | 4.19137300 | 1.36189900 | -0.51583000 |
| H | 4.65615200 | 1.05865700 | 1.16596700 |
| O | 1.35770200 | 1.17343100 | -0.86535400 |
| O | 1.07155300 | 1.19035100 | 1.34627900 |
| H | -5.39521500 | 0.28555400 | -0.15979400 |
| H | -0.72490800 | -0.99358100 | -1.38385800 |
| Sr | -0.79314500 | 1.81630600 | -0.00881600 |

Sr-NO-NO-CS-X-X

1 1

| | | | |
|---|---|---|---|
| N | 1.79580400 | -0.77195600 | -0.26653900 |
| C | 2.97309000 | -1.31342700 | -1.00783700 |
| C | 2.33298600 | 0.05751600 | 0.84574700 |
| H | 3.25060000 | -0.61433200 | -1.80834300 |
| H | 2.71100000 | -2.27099400 | -1.46471700 |
| C | 4.09346300 | -1.39742600 | 0.03514300 |
| C | 3.88417500 | -0.10676600 | 0.84190100 |
| H | 1.90231100 | -0.30067600 | 1.78957800 |
| C | 1.88807500 | 1.49763300 | 0.71300900 |
| H | 5.09047400 | -1.45944200 | -0.40878800 |
| H | 3.94579200 | -2.27865800 | 0.66935400 |
| H | 4.35714200 | 0.74102500 | 0.33429900 |
| H | 4.28521800 | -0.14858300 | 1.85574000 |
| O | 2.46135600 | 2.30608300 | 1.59010000 |
| O | 1.05578700 | 1.90354500 | -0.10732400 |
| H | -2.14996900 | 1.67065000 | 0.83187800 |
| N | -2.25662600 | 0.83496500 | 0.26049000 |
| C | -3.60850600 | 0.89520600 | -0.38625200 |
| C | -2.27389200 | -0.35867600 | 1.20942800 |
| H | -3.57803900 | 0.32919100 | -1.32748200 |
| H | -3.86862400 | 1.93215500 | -0.61747500 |
| C | -4.55769800 | 0.20333800 | 0.59546400 |
| C | -3.69410600 | -0.96055600 | 1.10697500 |
| H | -2.05608600 | -0.01138300 | 2.22213700 |
| C | -1.16001200 | -1.32435400 | 0.77214300 |
| H | -5.48647100 | -0.12866700 | 0.12355200 |
| H | -4.81781600 | 0.88790700 | 1.41184400 |
| H | -3.69342400 | -1.77630400 | 0.37695300 |
| H | -4.02885500 | -1.36099000 | 2.06633600 |
| O | -1.15528600 | -1.58081900 | -0.50363700 |
| O | -0.29715700 | -1.69310100 | 1.57951100 |
| H | 2.12536700 | 3.21385500 | 1.48008800 |
| H | 1.28931100 | -1.54805900 | 0.17344800 |
| Sr | -0.31145300 | 0.31688500 | -1.48656800 |

Ba-OO-NO-ZW-X-E

1 1

| | | | |
|---|---|---|---|
| N | -2.56023400 | -0.92729000 | 0.82460300 |
| C | -3.73185700 | 0.03008200 | 0.97496700 |
| C | -2.37259500 | -1.20209200 | -0.65988100 |
| H | -3.40548800 | 0.82249700 | 1.64646500 |
| H | -4.57113100 | -0.51571100 | 1.40865600 |
| C | -4.01349500 | 0.54537000 | -0.45580400 |
| C | -2.78894900 | 0.12104000 | -1.29005900 |
| H | -3.05805700 | -2.01266900 | -0.92924300 |
| C | -0.92777100 | -1.68200100 | -0.83808100 |
| H | -4.15438100 | 1.62769600 | -0.45919500 |
| H | -4.92453000 | 0.08507100 | -0.85048300 |
| H | -1.97644000 | 0.84385700 | -1.18582200 |
| H | -3.01086600 | 0.00501700 | -2.35243700 |
| O | -0.16520200 | -1.09210100 | -1.65313000 |
| O | -0.54296900 | -2.58485500 | -0.03027400 |
| H | 2.91924100 | 1.92396700 | 0.03675100 |
| N | 1.99236400 | 1.51888600 | -0.09102800 |
| C | 1.50159000 | 1.96257500 | -1.44909600 |
| C | 1.09891600 | 2.21478600 | 0.89421700 |
| H | 0.88428400 | 1.16921700 | -1.88206800 |
| H | 2.36396700 | 2.11376600 | -2.10402600 |
| C | 0.66456300 | 3.25514200 | -1.23320300 |
| C | 0.82239300 | 3.58402600 | 0.26546600 |
| H | 1.61615000 | 2.27705200 | 1.85888800 |
| C | -0.18480200 | 1.38293000 | 1.13378100 |
| H | -0.38684700 | 3.06312800 | -1.46368300 |
| H | 1.00024100 | 4.07260900 | -1.87565200 |
| H | -0.06539100 | 4.05448700 | 0.69028800 |
| H | 1.68251300 | 4.24132500 | 0.43568200 |
| O | -0.00006400 | 0.10257000 | 1.32157200 |
| O | -1.29307100 | 1.91935100 | 1.13806300 |
| H | -1.66921200 | -0.48326700 | 1.17297200 |
| H | -2.66988500 | -1.80012200 | 1.34225600 |
| Ba | 1.76791800 | -1.31535600 | 0.16271300 |

Ba-OO-OO-ZW-E-E

1 1

| | | | |
|---|---|---|---|
| C | -2.181653 | 1.505129 | -0.768182 |
| C | -3.171614 | 0.334565 | -0.886768 |
| N | -3.861648 | 0.275028 | 0.475031 |
| C | -3.174181 | 1.270291 | 1.405924 |
| C | -1.826612 | 1.523164 | 0.728061 |
| C | -2.475870 | -1.030678 | -1.065588 |
| O | -1.705386 | -1.173196 | -2.044697 |
| O | -2.693553 | -1.908670 | -0.168431 |
| O | 0.302048 | -1.070736 | 0.755837 |
| C | 1.481321 | -0.930798 | 0.274240 |
| O | 1.928465 | -1.724043 | -0.619578 |
| C | 2.319936 | 0.240717 | 0.738159 |
| N | 3.753235 | 0.028083 | 0.528914 |
| C | 4.308122 | 1.335602 | 0.147878 |
| C | 3.225781 | 2.004475 | -0.722445 |
| C | 1.912188 | 1.553090 | -0.049363 |
| H | 5.268189 | 1.209860 | -0.359844 |
| H | 4.488645 | 1.926255 | 1.055856 |
| H | 2.109344 | 0.383474 | 1.803706 |
| H | 3.283791 | 1.611581 | -1.744005 |
| H | 3.319182 | 3.093936 | -0.774843 |
| H | 1.116121 | 1.366924 | -0.777863 |
| H | 1.543703 | 2.305726 | 0.654918 |
| H | 3.870388 | -0.636067 | -0.233783 |
| H | -3.117056 | 0.834743 | 2.404417 |
| H | -3.795787 | 2.168213 | 1.434208 |
| H | -3.917284 | 0.464926 | -1.673860 |
| H | -1.114685 | 0.725030 | 0.964547 |
| H | -1.396364 | 2.474606 | 1.048558 |
| H | -1.321399 | 1.338260 | -1.417946 |
| H | -2.665570 | 2.439471 | -1.071263 |
| H | -3.691492 | -0.712723 | 0.769270 |
| Ba | -0.277675 | -3.059124 | -0.802227 |
| H | -4.868619 | 0.430507 | 0.417301 |

Ba-NO-OO-CS-X-E

1 1

| | | | |
|---|---|---|---|
| N | -0.61445700 | -0.96684600 | 0.43095100 |
| C | -0.74770200 | -1.34322000 | 1.86928100 |
| C | -1.50448500 | -1.86601700 | -0.34081400 |
| H | -1.53358300 | -0.73514800 | 2.34369600 |
| H | 0.19123800 | -1.13603100 | 2.38671900 |
| C | -1.16873000 | -2.81641800 | 1.85944100 |
| C | -2.14592800 | -2.86492600 | 0.67585000 |
| H | -0.92192500 | -2.41863000 | -1.08800100 |
| C | -2.55960500 | -1.09087800 | -1.10187800 |
| H | -1.62628200 | -3.14213400 | 2.79741900 |
| H | -0.29615400 | -3.45031300 | 1.66523300 |
| H | -3.13561700 | -2.51060800 | 0.98700900 |
| H | -2.27341900 | -3.85670500 | 0.23900200 |
| O | -3.32570400 | -1.86944900 | -1.85360300 |
| O | -2.71937900 | 0.13118500 | -1.04114800 |
| H | 2.06048400 | -0.80729500 | -1.41647500 |
| N | 2.27387000 | -1.18593800 | -0.49107700 |
| C | 3.44729200 | -2.08504900 | -0.62538200 |
| C | 2.80561600 | -0.03891000 | 0.29016500 |
| H | 3.32380000 | -2.72794900 | -1.50086700 |
| H | 3.48545700 | -2.73164400 | 0.25744200 |
| C | 4.70833900 | -1.16968100 | -0.69720200 |
| C | 4.19377200 | 0.24704900 | -0.31772300 |
| H | 2.90127100 | -0.34839900 | 1.33608500 |
| C | 1.78097600 | 1.07930400 | 0.22811300 |
| H | 5.15027000 | -1.17177600 | -1.69738600 |
| H | 5.47938300 | -1.51499100 | -0.00260900 |
| H | 4.06969100 | 0.87304300 | -1.20760600 |
| H | 4.85440200 | 0.77182900 | 0.37731900 |
| O | 1.32870600 | 1.41646500 | -0.92100200 |
| O | 1.28898700 | 1.54187000 | 1.30602000 |
| H | -3.99414900 | -1.33366200 | -2.31751200 |
| H | 0.35699800 | -1.17779900 | 0.14465700 |
| Ba | -0.98474800 | 1.86463600 | 0.10992000 |

Ba-NO-NO-CS-X-X

1 1

| | | | |
|---|---|---|---|
| N | -1.87432900 | 0.15791000 | -0.80258300 |
| C | -3.03577800 | -0.33736400 | -1.59619000 |
| C | -2.42590400 | 0.95652500 | 0.32349600 |
| H | -3.33444900 | -1.32836600 | -1.22700300 |
| H | -2.74930600 | -0.43661600 | -2.64644200 |
| C | -4.15570200 | 0.67933100 | -1.34422800 |
| C | -3.97417700 | 0.99544300 | 0.14757900 |
| H | -2.00492500 | 1.96894700 | 0.27497000 |
| C | -1.99640600 | 0.40307400 | 1.66432900 |
| H | -5.15087900 | 0.29049400 | -1.57581100 |
| H | -3.98782100 | 1.57577700 | -1.95160900 |
| H | -4.44912400 | 0.22173700 | 0.76133200 |
| H | -4.38868700 | 1.95792800 | 0.45139600 |
| O | -2.57428300 | 1.01974200 | 2.68658600 |
| O | -1.17906600 | -0.50862400 | 1.82762200 |
| H | 2.21375400 | 0.52406400 | 1.88136400 |
| N | 2.31270400 | 0.25144600 | 0.90572000 |
| C | 3.69229100 | -0.30214000 | 0.72517100 |
| C | 2.23282700 | 1.52317500 | 0.07473400 |
| H | 3.68355500 | -1.02285400 | -0.10480800 |
| H | 4.00957200 | -0.82751600 | 1.63077500 |
| C | 4.56558700 | 0.89782500 | 0.34673900 |
| C | 3.62675700 | 1.69539600 | -0.57182600 |
| H | 1.98879000 | 2.36279500 | 0.73002400 |
| C | 1.09841900 | 1.36165200 | -0.95012500 |
| H | 5.49829500 | 0.60581000 | -0.14376400 |
| H | 4.82039700 | 1.47438100 | 1.24424200 |
| H | 3.62088900 | 1.25640400 | -1.57467300 |
| H | 3.89878100 | 2.74930200 | -0.66215100 |
| O | 1.13474400 | 0.24419100 | -1.61295100 |
| O | 0.19308700 | 2.20444300 | -1.01726300 |
| H | -2.25065700 | 0.64679200 | 3.52598300 |
| H | -1.32736600 | 0.81300400 | -1.37155600 |
| Ba | 0.32995000 | -1.54666200 | -0.14204000 |