Supporting Information

Nature and Strength of M-H•••S and M-H•••Se (M=Mn, Fe & Co) Hydrogen Bond

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Table S1. Topological parameters like electron density (electrondensity ρ_C(au), Eigen values of electron density Hessian matrixes λ_1, λ_2 and λ_3, Kinetic energy density G_C(au), potential energy density V_C(au), H_C(au) (Sum of G_C and V_C, negative of ratio of G_C and V_C at bond critical points of H-bond complexes.

complexes	ρ_H(a.u.)	λ1	λ2	λ3	G_C	V_C	H_C	$-G_C/V_C$
Mn-H···SH_2	0.006	-0.004	-0.004	0.023	0.003	-0.003	0.000	1.154
Fe-H···SH_2	0.007	-0.005	-0.005	0.027	0.004	-0.003	0.000	1.137
Co-H···SH_2	0.011	-0.009	-0.009	0.041	0.006	-0.005	0.000	1.053
Mn-H···SMe_2	0.013	-0.010	-0.010	0.047	0.007	-0.007	0.000	0.995
Fe-H···SMe_2	0.017	-0.015	-0.015	0.062	0.008	-0.009	0.000	0.956
Co-H···SMe_2	0.030	-0.037	-0.037	0.117	0.013	-0.016	-0.003	0.834
Mn-H···SeH_2	0.007	-0.004	-0.004	0.024	0.003	-0.003	0.000	1.128
Fe-H···SeH_2	0.008	-0.005	-0.005	0.029	0.004	-0.004	0.000	1.118
Co-H···SeH_2	0.012	-0.010	-0.009	0.043	0.006	-0.006	0.000	1.031
Mn-H···$SeMe_2$	0.013	-0.010	-0.010	0.045	0.006	-0.006	0.000	0.977
Fe-H···$SeMe_2$	0.018	-0.016	-0.016	0.063	0.008	-0.009	-0.001	0.918
Co-H···$SeMe_2$	0.028	-0.032	-0.032	0.100	0.012	-0.014	-0.003	0.819
Co-H···OH_2	0.012	-0.013	-0.012	0.056	0.008	-0.008	0.000	0.998
Mn-H···OMe_2	0.012	-0.011	-0.011	0.052	0.008	-0.008	0.000	0.956
Fe-H···OMe_2	0.014	-0.014	-0.014	0.061	0.009	-0.009	-0.001	0.935
Co-H···OMe_2	0.019	-0.024	-0.023	0.096	0.013	-0.013	-0.001	0.961

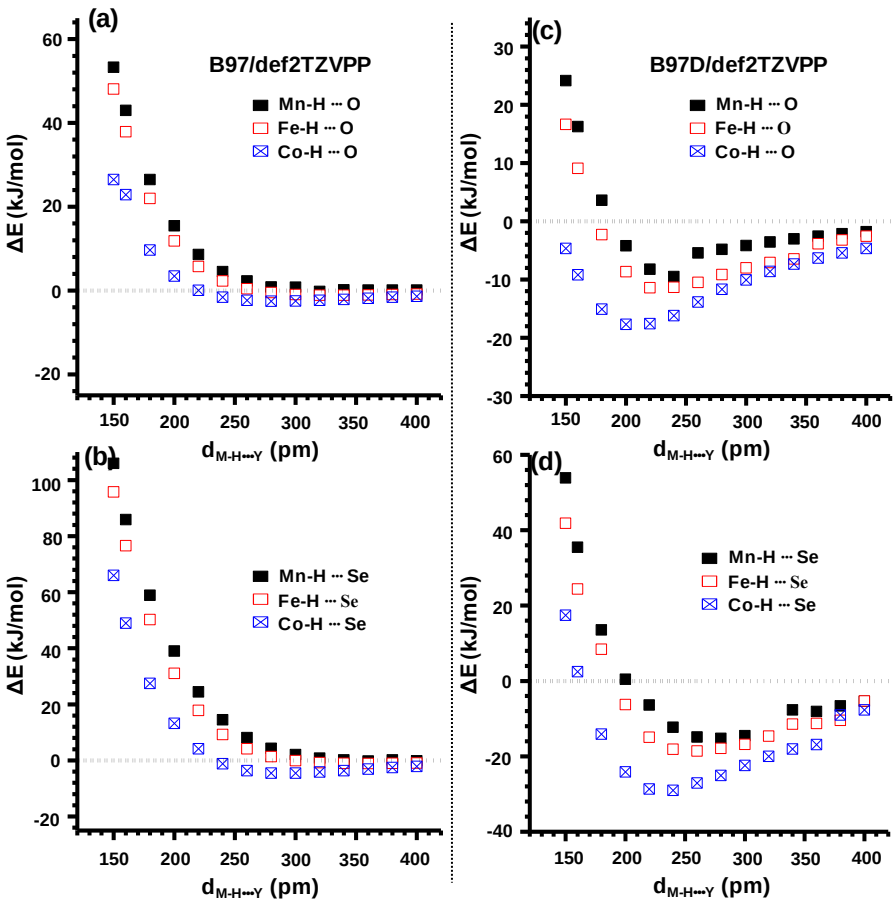

Figure S1. Potential energy surface (PES) curve of M-H•••Y H-Bond dimers: (a), (c) $Mn(CO)_5H$•••DME, $Fe(CO)_4H_2$•••DME , $Co(CO)_4H$•••DME representing M-H•••O HBs; (b), (d) $Mn(CO)_5H$•••DMSe, $Fe(CO)_4H_2$•••DMSe , $Co(CO)_4H$•••DMSe representing M-H•••Se HBs, respectively. Left part of the plot (a,b) represents PES without dispersion and right part of the plot (c,d) represents PES with dispersion . BSSE is added to dimerisation energy.

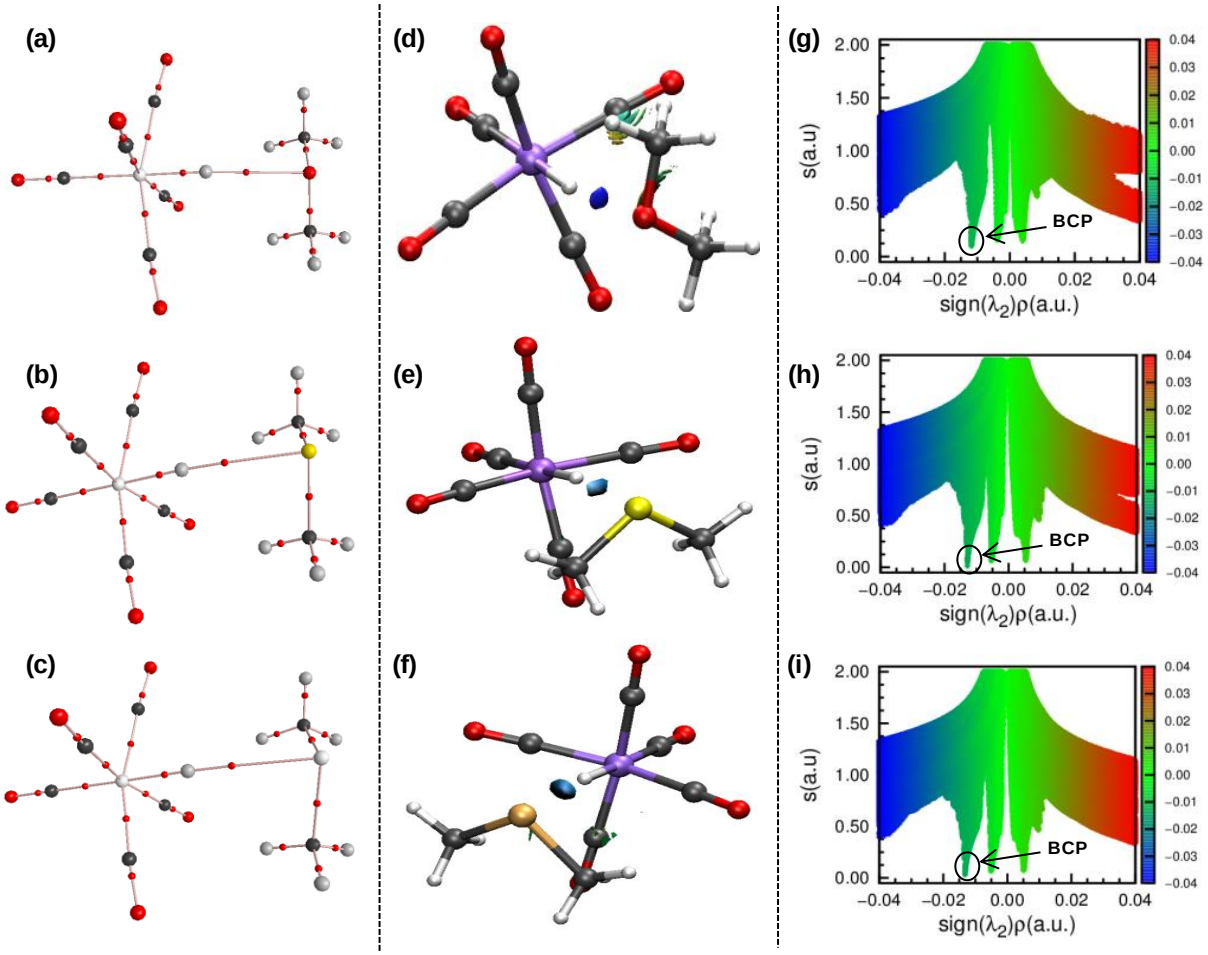

Figure S2. Molecular graph of H-bond interaction obtained from AIM analysis showing the presence of bond critical points for (a) $Mn(CO)_5H$•••DME, (b) $Mn(CO)_5H$•••DMS, (c) $Mn(CO)_5H$•••DMSe; Colored isosurfaces of the reduced electron density gradient (3D-NCI-plot) for H-bond complexes of (d)$Mn(CO)_5H$•••DME, (e) $Mn(CO)_5H$•••DMS, (f) $Mn(CO)_5H$•••DMSe; Plots of the reduced density gradient(RDG) versus the sign of the second eigen value of the electron-density Hessian matrix (λ2) times electron density (sign(λ2)ρ) for H-bond complexes of (g) $Mn(CO)_5H$•••DME, (h) $Mn(CO)_5H$•••DMS, (i) $Mn(CO)_5H$•••DMSe.

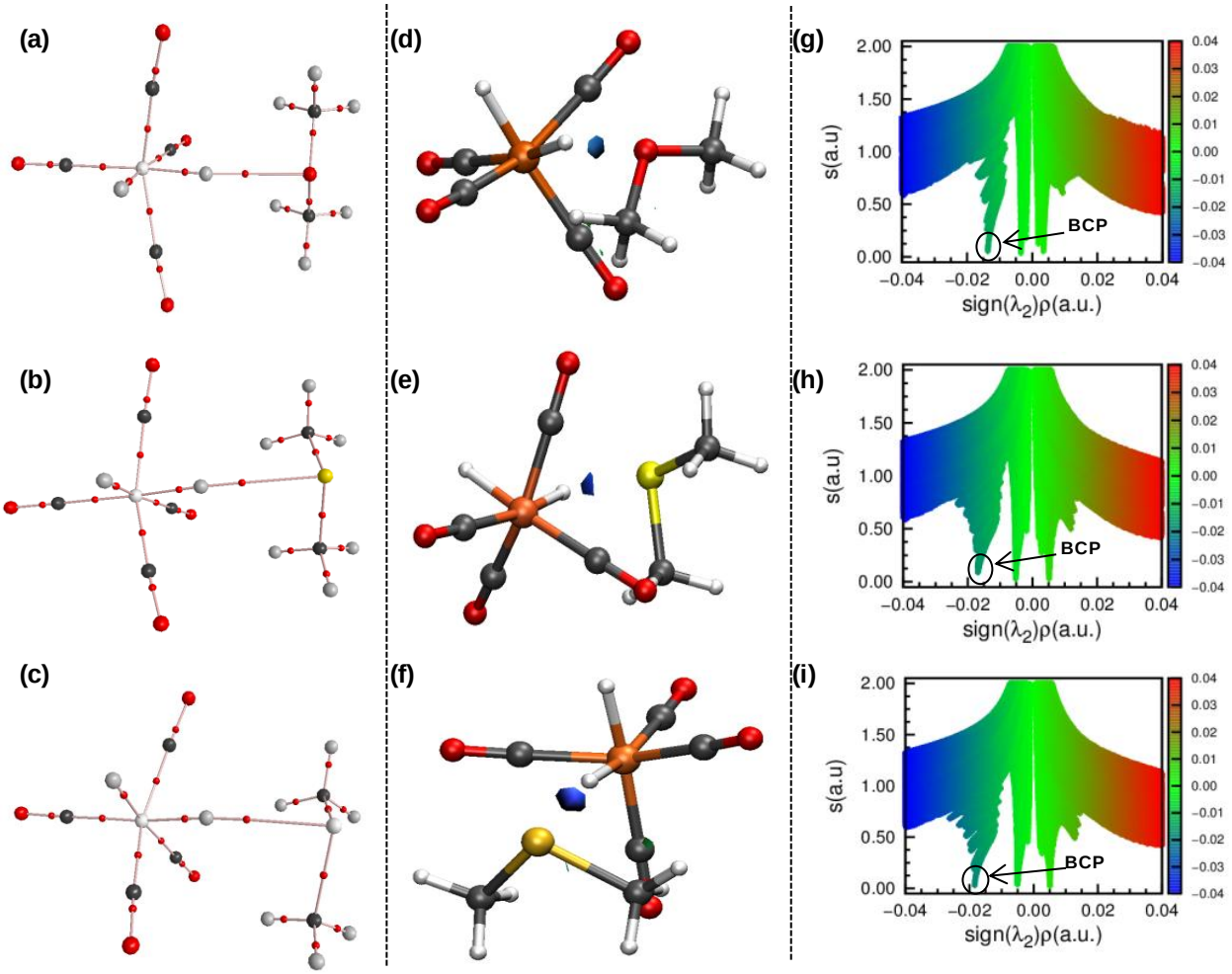

Figure S3. Molecular graph of H-bond interaction obtained from AIM analysis showing the presence of bond critical points for (a) $Fe(CO)_4H_2$•••DME, (b) $Fe(CO)_4H_2$•••DMS, (c) $Fe(CO)_4H_2$•••DMSe; Colored isosurfaces of the reduced electron density gradient (3D-NCI-plot) for H-bond complexes of (d) $Fe(CO)_4H$•••DME, (e) $Fe(CO)_4H_2$•••DMS, (f) $Fe(CO)_4H_2$•••DMSe; Plots of the reduced density gradient(RDG) versus the sign of the second eigen value of the electron-density Hessian matrix (λ2) times electron density (sign(λ2)ρ) for H-bond complexes of (g) $Fe(CO)_4H_2$•••DME, (h) $Fe(CO)_4H_2$•••DMS, (i) $Fe(CO)_4H_2$•••DMSe.

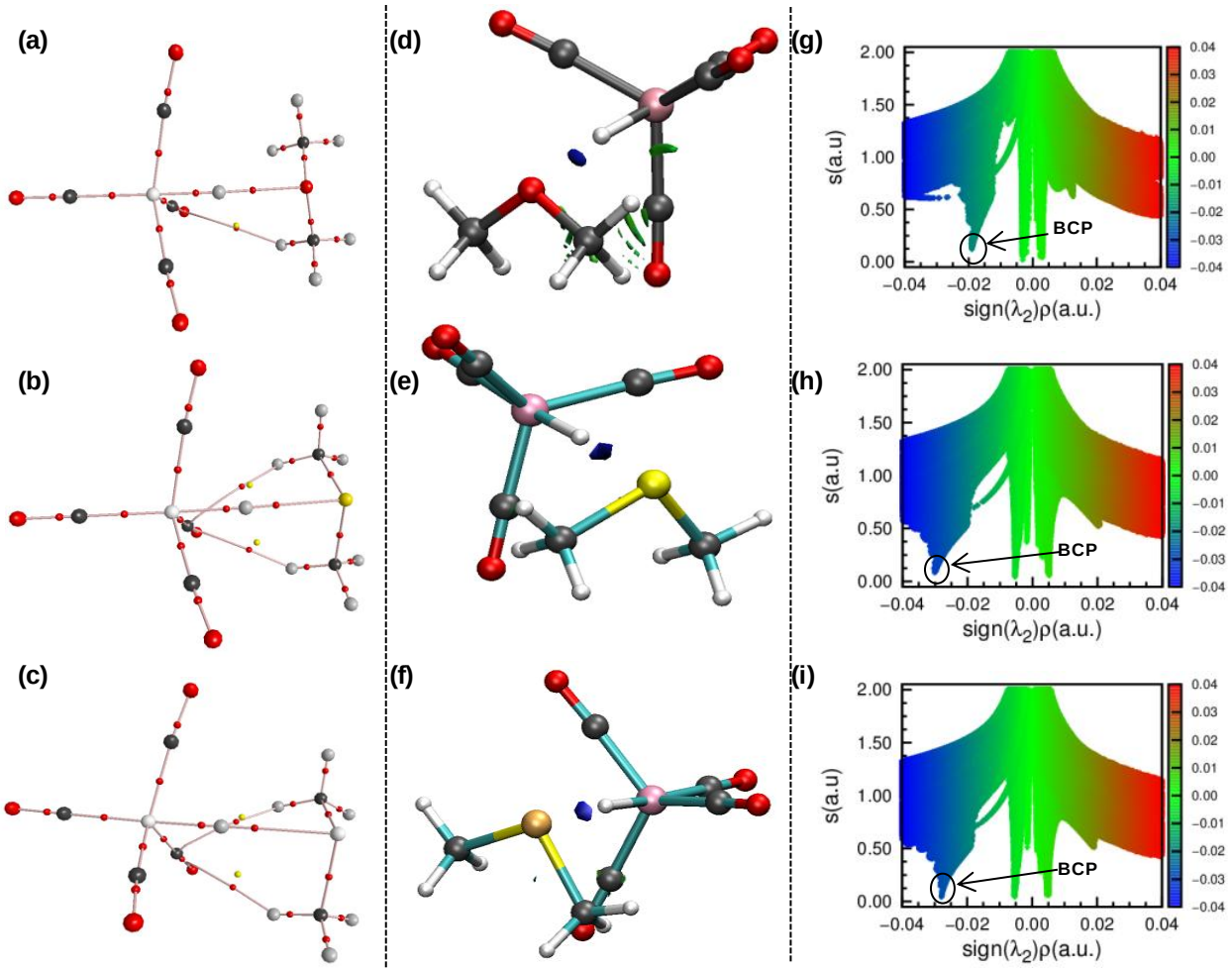

Figure S4. Molecular graph of H-bond interaction obtained from AIM analysis showing the presence of bond critical points for (a) $Co(CO)_4H$•••DME, (b) $Co(CO)_4H$•••DMS, (c) $Co(CO)_4H$•••DMSe; Colored isosurfaces of the reduced electron density gradient (3D-NCI-plot) for H-bond complexes of (d) $Co(CO)_4H$•••DME, (e) $Co(CO)_4H$•••DMS, (f) $Co(CO)_4H$•••DMSe; Plots of the reduced density gradient(RDG) versus the sign of the second eigen value of the electron-density Hessian matrix (λ2) times electron density (sign(λ2)ρ) for H-bond complexes of (g) $Co(CO)_4H$•••DME, (h) $Co(CO)_4H$•••DMS, (i) $Co(CO)_4H$•••DMSe.

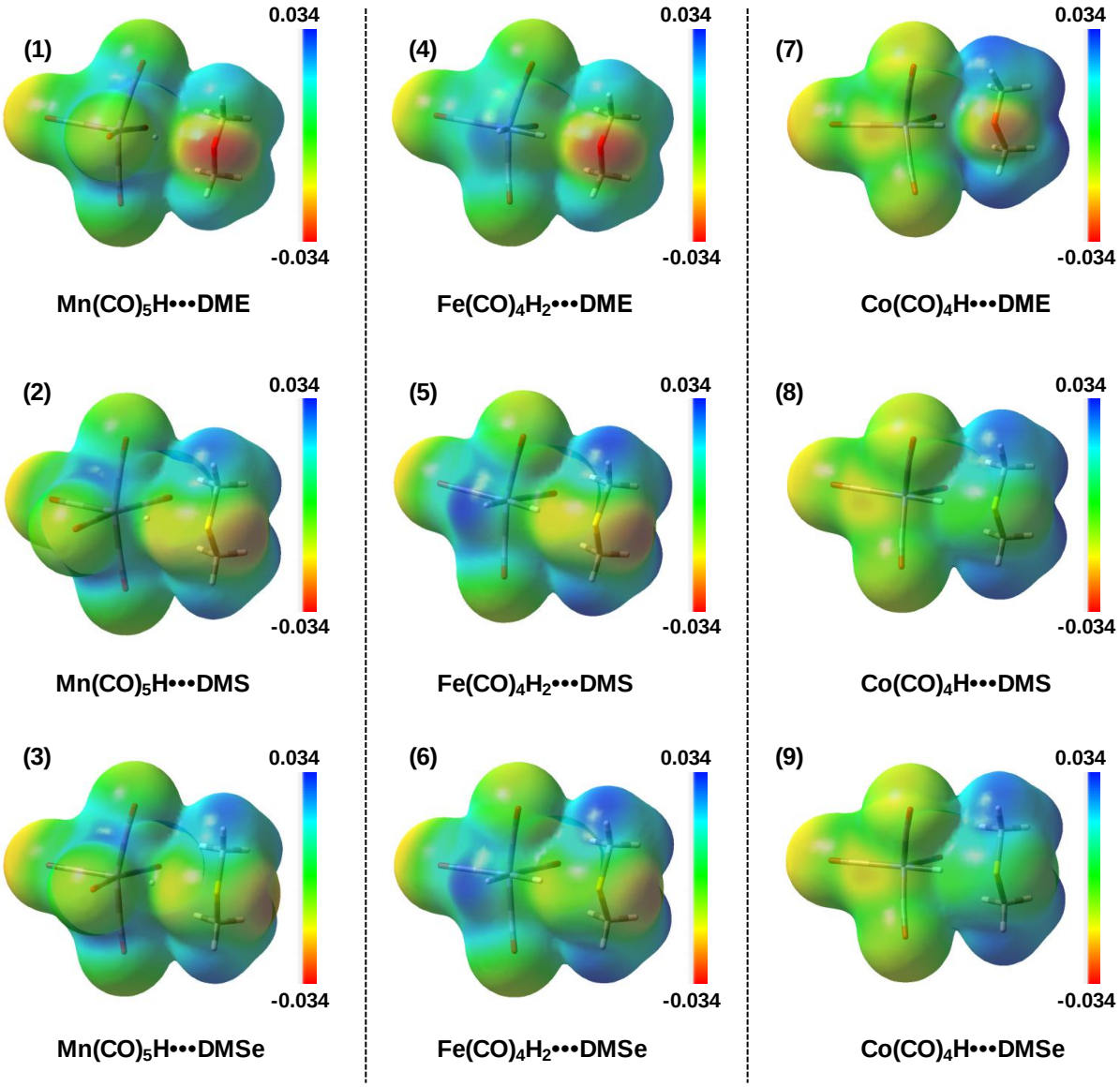

Figure S5. MESP surface of M-H•••Y HB dimer mapped on 0.001 a.u. electron density surface. The points 1 to 9 in above figure are as follows 1:$Mn(CO)_5H$•••DME, 2:$Mn(CO)_5H$•••DMS, 3:$Mn(CO)_5H$•••DMSe, 4:$Fe(CO)_4H_2$•••DME, 5:$Fe(CO)_4H_2$•••DMS, 6:$Fe(CO)_4H_2$•••DMSe, 7:$Co(CO)_4H$•••DME, 8:$Co(CO)_4H$•••DMS, and 9:$Co(CO)_4H$•••DMSe.

Table S2. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis at MP2/aug-cc-pVDZ. LP1 and LP2 are two lone pair electrons on donor atoms O, S, Se that donate to antibonding σ^*_{M-H} orbital; Frequency shifts ($\Delta\nu$) of H-bonded complexes; 1H NMR chemical shifts (σ); change in M-H bond length (Δd) between H-bonded complexes and monomers.

H-bond complex	LP1(S)→σ_{M-H}* (kJ/mol)	LP2(P)→σ_{M-H}* (kJ/mol)	E_{DA} (kJ/mol)	Freq shift($\Delta\nu$) cm^{-1}	chem shift(σ) ppm	Δd(M-H) pm
$Mn(CO)_5H$-DME	3.68	4.39	8.08	15.91	1.10	-0.40
$Mn(CO)_5H$-DMS	4.44	12.59	17.03	-67.87	2.09	0.59
$Mn(CO)_5H$-DMSe	4.64	15.94	20.59	-89.81	2.44	0.83
$Fe(CO)_4H_2$-DME	5.82	5.36	11.17	-9.73	1.77	0.01
$Fe(CO)_4H_2$-DMS	7.2	21.05	28.24	-152.24	3.52	1.51
$Fe(CO)_4H_2$-DMSe	8.03	29.75	37.78	-195.54	4.29	1.95
$Co(CO)_4H$-DME	10.08	42.19	19.2	-93.31	3.65	0.81
$Co(CO)_4H$-DMS	13.22	55.32	65.65	-404.6	7.90	4.81
$Co(CO)_4H$-DMSe	11.84	49.54	68.83	-407.65	7.85	4.96

NB: E_{DA} is 2nd order perturbation energy between donor and acceptor

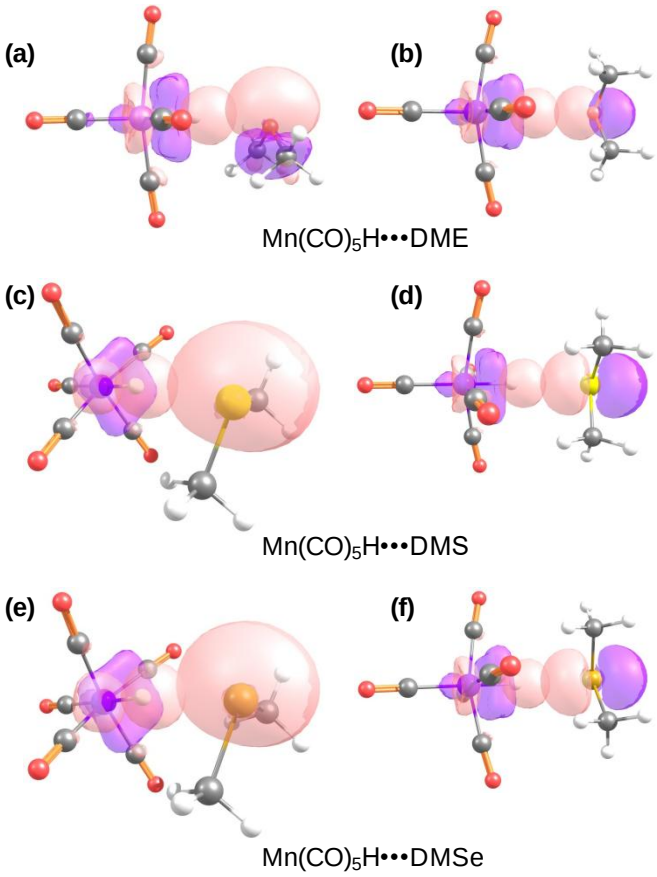

Figure S6. (a,b) Overlap of SP and P type Oxygen lone pair and M-H σ* orbital of $Mn(CO)_5H$•••DME H-bond complex, (c,d) Overlap of S and P type Sulfur lone pair and M-H σ* orbital of $Mn(CO)_5H$•••DMS H-bond complex, (e,f) Overlap of S and P type Selenium lone pair and M-H σ* orbital of $Mn(CO)_5H$•••DMSe H-bond complex.

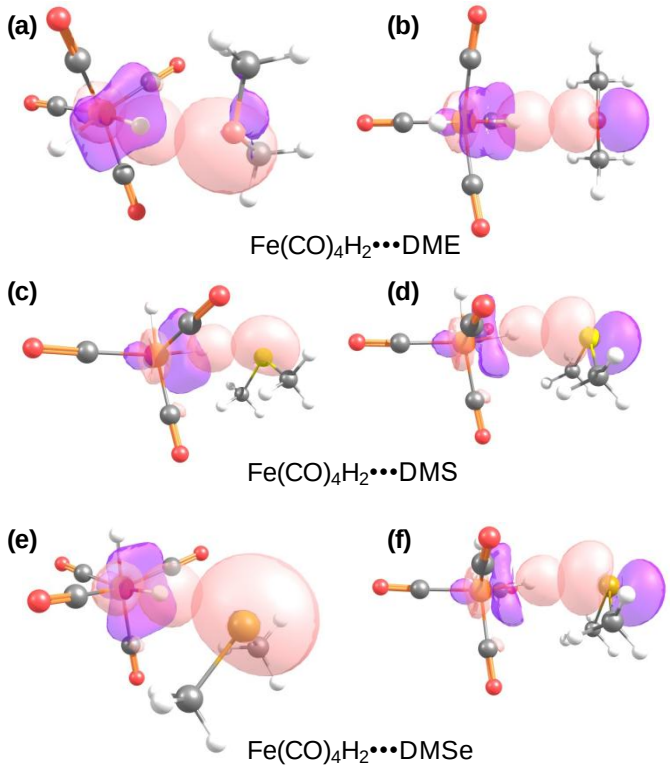

Figure S7. (a,b) Overlap of S and P type Oxygen lone pair and M-H σ* orbital of $Fe(CO)_4H_2$•••DME H-bond complex, (c,d) Overlap of S and P type Sulfur lone pair and M-H σ* orbital of $Fe(CO)_4H_2$•••DMS H-bond complex, (e,f) Overlap of S and P type Selenium lone pair and M-H σ* orbital of $Fe(CO)_4H_2$•••DMSe H-bond complex.

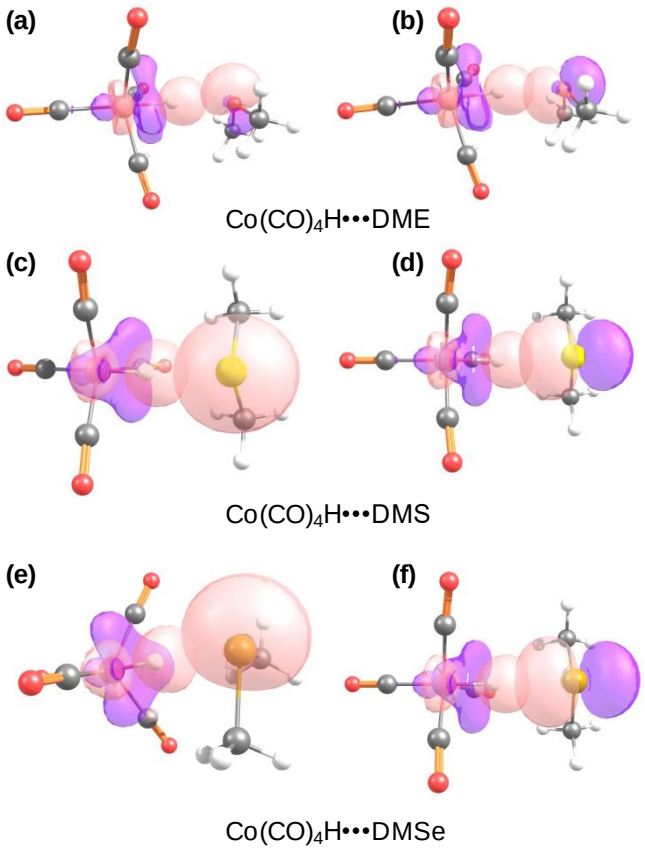

Figure S8. (a,b) Overlap of S and P type Oxygen lone pair and M-H σ* orbital of $Co(CO)_4H$•••DME H-bond complex, (c,d) Overlap of S and P type Sulfur lone pair and M-H σ* orbital of $Co(CO)_4H$•••DMS H-bond complex, (e,f) Overlap of S and P type Selenium lone pair and M-H σ* orbital of $Co(CO)_4H$•••DMSe H-bond complex.

Table S3. Experimental and computational frequencies of M-H bond and carbonyls (A1, B1, B2 and E are irreducible representations of point groups) of transition metal hydrides.

	Frequency (cm^{-1})								
M-H	**Expt[a]**	**B97D[b]**	**M06[c]**	**wB97XD[c]**	**HF[c]**	**B3LYPD[c]**	**B3LYP[c]**	**B2PLYP[c]**	**MP2[c]**
$HMn(CO)_5$									
Mn-H	1784	1768	1752	1835	1484	1803	1821	1954	2339
CO(A1)	2125	2106	2251	2231	2431	2185	2184	2132	2101
CO(A1)	2020	2007	2158	2133	2370	2087	2086	2033	1938
CO(B1)	2054	2033	2177	2159	2383	2112	2111	2065	2071
CO(E)	2029	2012	2176	2142	2387	2096	2095	2017	1966
$H_2Mn(CO)_4$									
Fe-H	1895	1894	1962	1989	1613	1936	1948	1994	1433
CO(A1)	2127	2104	2218	2233	2463	2183	2184	2160	2100
CO(A1)	2060	2040	2156	2171	2449	2121	2121	2115	2052
CO(B1)	2060	2032	2149	2167	2444	2117	2117	2144	2298
CO(B2)	2060	2032	2152	2166	2440	2114	2114	2045	1950
$HCo(CO)_4$									
Co-H	1934	1956	1840	2040	1555	2012	2017	2024	2926
CO(A1)	2123	2102	2247	2232	2459	2180	2181	2276	2108
CO(A1)	2062	2048	2200	2176	2420	2126	2126	2119	1949
CO(E)	2043	2026	2168	2156	2396	2104	2105	2041	2036
RMSD		**20**	**110**	**105**	**347**	**59**	**60**	**78**	**338**

a: Gas phase experimental frequency, b: Frequency calculation for this project,
c: Frequency calculation at various functional

Table S4. Comparision of Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis at MP2/aug-cc-pVDZ and B97D/aug-cc-pVDZ.

H-bond complex	E_{DA} (MP2/aug-cc-pVDZ) (kJ/mol)	E_{DA} (B97D/aug-cc-pVDZ) (kJ/mol)
$Mn(CO)_5H$-DME	8.08	6.82
$Mn(CO)_5H$-DMS	17.03	14.85
$Mn(CO)_5H$-DMSe	20.59	17.99
$Fe(CO)_4H_2$-DME	11.17	9.58
$Fe(CO)_4H_2$-DMS	28.24	23.43
$Fe(CO)_4H_2$-DMSe	37.78	30.59
$Co(CO)_4H$-DME	19.20	17.15
$Co(CO)_4H$-DMS	65.65	48.99
$Co(CO)_4H$-DMSe	68.83	52.89

NB: E_{DA} is 2nd order perturbation energy between donor and acceptor

Table S5. Topological parameters like electron density, ρ_H(au), Laplacian of electron density, $\nabla^2\rho_H$(au), change in bonded hydrogen charge, Δq_H, energy, ΔE_H, dipolar polarization, $\Delta|M_H|$, volume, ΔV_H, population, ΔN_H, and mutual penetration, Δr_H of metal hydride on complexation with H-bond acceptors H_2O, H_2S, H_2Se, DME, DMS and DMSe by AIM theory at B97D/aug-cc-pVDZ. All the values are in atomic units.

complexes	ρ_H	$\nabla^2\rho_H$	Δq_H	ΔE_H	$\Delta\|M_H\|$	ΔV_H	ΔN_H	Δr_H
$Co(CO)_4H$-DME	0.024	0.053	0.07	0.02	-0.09	-15.78	-0.05	2.12
$Co(CO)_4H$-DMS	0.035	0.050	0.06	0.02	-0.08	-19.08	-0.03	2.55
$Co(CO)_4H$-DMSe	0.033	0.040	0.04	0.02	-0.07	-17.30	-0.02	2.70
$Co(CO)_4H$-H_2O	0.015	0.032	0.05	0.01	-0.06	-9.26	-0.04	1.83
$Co(CO)_4H$-H_2S	0.013	0.026	0.02	0.01	-0.03	-6.22	0.00	1.67
$Co(CO)_4H$-H_2Se	0.014	0.026	0.02	0.01	-0.03	-6.32	0.00	1.85

Table S6. Topological parameters like electron density (electrondensity ρ_C(au), Eigen values of electron density Hessian matrixes λ_1, λ_2 and λ_3, Kinetic energy density G_C(au), potential energy density V_C(au), H_C(au) (Sum of G_C and V_C, negative of ratio of G_C and V_C at bond critical points of H-bond complexes at B97D/aug-cc-pVDZ.

System	ρ_H	$\lambda 1$	$\lambda 2$	$\lambda 3$	G_H	V_H	H_H	G_C/V_C
$Co(CO)_4H$-DME	0.024	-0.028	-0.027	0.107	0.014	-0.015	-0.0007	0.952
$Co(CO)_4H$-DMS	0.035	-0.041	-0.041	0.131	0.015	-0.017	-0.0023	0.863
$Co(CO)_4H$-DMSe	0.033	-0.035	-0.034	0.109	0.012	-0.015	-0.0026	0.829
$Co(CO)_4H$-H_2O	0.015	-0.015	-0.014	0.062	0.009	-0.009	-0.0005	0.948
$Co(CO)_4H$-H_2S	0.013	-0.011	-0.011	0.047	0.006	-0.006	0.0004	1.079
$Co(CO)_4H$-H_2Se	0.014	-0.012	-0.011	0.049	0.006	-0.006	0.0003	1.046

Optimized Co-ordinates

DME:

O	1.595458600	-0.000604400	2.246573900
C	2.274372100	-1.176518500	1.834354100
H	3.288173600	-1.233252500	2.268461400
H	1.687865500	-2.031867700	2.183225100
H	2.365744500	-1.227732400	0.735055400
C	2.272967700	1.175875000	1.833672100
H	3.286272600	1.234714300	2.268683400
H	2.365220800	1.225819300	0.734406200
H	1.684906500	2.030785100	2.181012200

DMS:

S	1.457086000	0.002523400	2.675569200
C	2.257535700	-1.380218000	1.801877100
H	3.344739800	-1.356545100	1.941651000
H	1.864573500	-2.308564900	2.227808600
H	2.024869700	-1.354709000	0.730998000
C	2.264849400	1.384249200	1.807039400
H	3.352060400	1.353026000	1.945116800
H	2.030503800	1.365247100	0.736382800
H	1.878484900	2.313065800	2.237952200

DMSe:

Se	1.384451400	0.003100600	2.773641900
C	2.266420000	-1.466619800	1.788257400
H	3.349457100	-1.416006400	1.930932300
H	1.884463000	-2.404950000	2.198768200

H	2.018275200	-1.402772500	0.725333100
C	2.275869300	1.471673100	1.795115000
H	3.358577300	1.412668100	1.936922600
H	2.026661300	1.415010000	0.732028500
H	1.900858000	2.410575700	2.210685300

H2O:

O	-0.6192357	0.0000000	-1.9883936
H	-0.6192357	0.7602249	-1.3957748
H	-0.6192357	-0.7602249	-1.3957748

H2S:

S	-0.6192357	0.0000000	-2.2156272
H	-0.6192357	0.9679186	-1.2821579
H	-0.6192357	-0.9679186	-1.2821579

H2Se:

Se	-0.6192357	0.0000000	-2.2824392
H	-0.6192357	1.0502913	-1.2487519
H	-0.6192357	-1.0502913	-1.2487519

$HMn(CO)_5$:

Mn	0.000000100	-0.000000100	0.130419500
H	-0.000000300	0.000000100	1.704375800
C	-1.839638600	0.000000000	0.353812400
O	-2.969779700	0.000000000	0.551415400
C	0.000000500	-0.000000100	-1.728159100
O	0.000000200	0.000000000	-2.878274100
C	0.000000000	-1.839616200	0.353841500

O	-0.000000100	-2.969804500	0.551372900
C	0.000000000	1.839628300	0.353843100
O	-0.000000100	2.969792600	0.551371300
C	1.839617800	0.000000000	0.353811100
O	2.969800100	0.000000000	0.551417000

$HMn(CO)_5$-DME:

Mn	-0.038569900	-0.000075500	0.345129700
H	0.191177900	-0.002117600	1.898168000
C	-1.833497000	-0.001963100	0.785042100
O	-2.934560500	-0.003365200	1.113788300
C	-0.282479000	0.001024600	-1.499996000
O	-0.432079300	0.001304400	-2.640616100
C	-0.001658600	-1.823590500	0.639247800
O	0.027625800	-2.939321100	0.910328200
C	-0.004554100	1.823221800	0.641757900
O	0.022923400	2.938779700	0.913755900
C	1.815364800	0.001350900	0.302708900
O	2.962144600	0.002017400	0.333901600
O	0.134334600	0.000693700	4.319408000
C	-0.653927800	1.178123600	4.423386400
H	-1.168396900	1.232594200	5.397685900
H	0.021600300	2.032697000	4.323923400
H	-1.414011600	1.225473300	3.625430700
C	-0.652439800	-1.177495500	4.426193500
H	-1.166580600	-1.230444300	5.400767700
H	-1.412648100	-1.227553900	3.628497700
H	0.024253100	-2.031350400	4.328478300

$HMn(CO)_5$-DMS:

Mn	-0.028287200	0.000391600	0.362191300
H	0.313656300	-0.001757700	1.904599700
C	-1.791069900	-0.002458600	0.912658200
O	-2.871489000	-0.004925200	1.305660400
C	-0.385713500	0.004027400	-1.462937400
O	-0.606685600	0.007070200	-2.591947700
C	0.026174800	-1.825798600	0.639064300
O	0.072240700	-2.945389600	0.891793700
C	0.023811500	1.825938000	0.643897500
O	0.068589300	2.945019100	0.898797100
C	1.820714000	0.001289800	0.214608400
O	2.967235800	0.001310600	0.182236300
S	0.479192700	0.000639400	4.587235700
C	-0.691826000	1.380983800	4.410929700
H	-1.453279900	1.350752100	5.197806400
H	-0.122602000	2.310872900	4.499869100
H	-1.176667500	1.354583500	3.429540500
C	-0.690844800	-1.381988500	4.422181100
H	-1.455189100	-1.342919600	5.205881400
H	-1.172136500	-1.366979300	3.438752000
H	-0.121804800	-2.310657800	4.524182400

$HMn(CO)_5$-DMSe:

Mn	-0.031241700	0.000928500	0.354822400
H	0.320119300	-0.000455000	1.897590500
C	-1.792207600	-0.003119300	0.911310400

O	-2.870708700	-0.007391800	1.310158900
C	-0.389520400	0.005310000	-1.470356200
O	-0.608312100	0.009632000	-2.599853200
C	0.024849900	-1.824271200	0.636235600
O	0.073534200	-2.942396100	0.895443900
C	0.022507900	1.825718200	0.639751700
O	0.070080600	2.943698800	0.899793700
C	1.817605800	0.000773600	0.210598500
O	2.964521700	-0.000672400	0.185804200
Se	0.595043200	0.000536900	4.637773800
C	-0.706524600	1.467586000	4.411553200
H	-1.466595400	1.415156800	5.194916300
H	-0.155146200	2.407517800	4.492650400
H	-1.169719200	1.397332700	3.424612500
C	-0.705639500	-1.469290400	4.424626100
H	-1.468731800	-1.406848400	5.204312700
H	-1.165145400	-1.411597600	3.435116000
H	-0.154752500	-2.408145600	4.520151100

$HMn(CO)_5$-H_2S:

Mn	-0.0188047	0.0004694	0.4215187
H	0.3038788	-0.0020164	1.9605445
C	-1.7792437	-0.0016272	0.9909988
O	-2.8503528	-0.0029982	1.4049177
C	-0.3800225	0.0033998	-1.4034695
O	-0.6023199	0.0052247	-2.5317936
C	0.0305891	-1.8327484	0.6690345
O	0.0715815	-2.9569567	0.8973249

C 0.0283511 1.8328416 0.6755191

O 0.0679986 2.9562739 0.9078896

C 1.8299730 0.0019001 0.2728225

O 2.9763041 0.0026897 0.2392779

S 0.4988503 0.0015777 4.9939640

H -0.2376379 0.9685354 4.4188336

H -0.2374114 -0.9681568 4.4232256

$HMn(CO)_5$-H_2Se:

Mn -0.0296955 0.0004836 0.3393930

H 0.2863331 -0.0019236 1.8801504

C -1.7929582 -0.0014366 0.9007383

O -2.8664324 -0.0025786 1.3085332

C -0.3870398 0.0031671 -1.4862741

O -0.6068464 0.0047640 -2.6152520

C 0.0223895 -1.8297956 0.6019660

O 0.0667639 -2.9510349 0.8448077

C 0.0200693 1.8298942 0.6082064

O 0.0630059 2.9503389 0.8550004

C 1.8185048 0.0019729 0.1887582

O 2.9650188 0.0028562 0.1524941

Se 0.6265637 0.0014051 4.9528536

H -0.2894748 1.0514153 4.4727805

H -0.2892997 -1.0520472 4.4800148

$H_2Fe(CO)_4$:

Fe 0.000032000 0.000013500 0.284466300

H	-1.003341800	-0.000082700	1.425146000
C	0.000084900	1.738687500	0.736693400
O	0.000124000	2.818400700	1.123401300
C	1.392491500	0.000111100	-0.898709400
O	2.290986600	0.000126600	-1.611941600
C	-1.392787500	0.000111100	-0.898276800
O	-2.291519900	0.000126800	-1.611208600
H	1.003721200	-0.000082600	1.424878700
C	0.000084900	-1.738784200	0.736239100
O	0.000124100	-2.818627900	1.122585300

$H_2Fe(CO)_4$-DME:

Fe	-0.838260200	0.000207600	-0.682315900
H	-2.056310400	-0.001554300	0.227908000
C	-0.891942700	1.721923400	-0.189387700
O	-0.927203000	2.788582000	0.234261500
C	0.749354900	0.002594800	-1.572012800
O	1.771095400	0.004118200	-2.098132500
C	-1.977006200	-0.001598400	-2.115331000
O	-2.720297400	-0.002778800	-2.989668900
H	-0.088213300	0.000990100	0.638914000
C	-0.886688300	-1.721726200	-0.189925800
O	-0.918565700	-2.788518000	0.233607600
O	1.596807000	-0.000604200	2.247511400
C	2.275587800	-1.179403400	1.833690100
H	3.287488300	-1.232075700	2.268656000
H	1.687123000	-2.032733200	2.182628300
H	2.365281900	-1.227603700	0.735527600

C	2.274190900	1.178779800	1.833066200
H	3.285599400	1.233690400	2.268982100
H	2.364639300	1.225455700	0.734931800
H	1.684270100	2.031712400	2.180454900

$H_2Fe(CO)_4$-DMS:

Fe	-0.808673100	-0.001615900	-0.673581900
H	-2.077494000	-0.003879700	0.165521300
C	-0.887011700	1.715822400	-0.170783000
O	-0.943333100	2.777987400	0.262977700
C	0.816639900	0.000942000	-1.489353300
O	1.859123200	0.002316300	-1.975144100
C	-1.872456000	-0.003703400	-2.163052800
O	-2.572516600	-0.005258500	-3.072573600
H	-0.135862900	0.000554100	0.705359800
C	-0.881482900	-1.719523900	-0.171602200
O	-0.934687700	-2.782256900	0.261199500
S	1.460147300	0.002485600	2.670275000
C	2.258594300	-1.381855000	1.802098900
H	3.344353800	-1.355084600	1.942057900
H	1.863547700	-2.308722200	2.227860800
H	2.023715200	-1.353352600	0.733000200
C	2.265844200	1.385882900	1.807226400
H	3.351636000	1.351557300	1.945530300
H	2.029348900	1.363901200	0.738287900
H	1.877521400	2.313261800	2.238062200

$H_2Fe(CO)_4$-DMSe:

Fe	-0.807192000	-0.001344900	-0.675921500
H	-2.078523700	-0.003583000	0.159435300
C	-0.885413300	1.714617800	-0.169082900
O	-0.941620000	2.774900400	0.269986400
C	0.820216100	0.000062500	-1.486866300
O	1.863945300	-0.000335200	-1.970670400
C	-1.869914300	-0.004241900	-2.167171000
O	-2.572782200	-0.007064400	-3.074685500
H	-0.145239300	0.001431700	0.713061800
C	-0.879439300	-1.718057300	-0.171403900
O	-0.932118300	-2.779605900	0.264998300
Se	1.388218500	0.003069900	2.767653000
C	2.267145700	-1.467745600	1.788791900
H	3.349027400	-1.414593600	1.931292500
H	1.883414100	-2.404891500	2.198942400
H	2.017181400	-1.401134600	0.727279600
C	2.276542500	1.472809300	1.795594500
H	3.358112700	1.411228400	1.937373900
H	2.025523500	1.413357000	0.733857400
H	1.899872500	2.410579300	2.210903700

$H_2Fe(CO)_4$-H_2S:

Fe	-1.5956354	-0.2018353	-0.2190483
H	-0.2145142	0.4055156	-0.0456680
C	-0.8324616	-1.3263160	0.9502153
O	-0.2888446	-1.9575251	1.7400211
C	-1.0012053	-0.9470037	-1.7712119
O	-0.5664564	-1.3895396	-2.7380570

C	-1.8648753	1.4782214	-0.7906035
O	-1.9699675	2.5837971	-1.0784769
C	-3.3182340	-0.8216769	-0.2034120
O	-4.4035714	-1.1910386	-0.1586155
H	-1.8715475	0.5121001	1.0937941
S	2.6999126	0.4578846	-0.6778214
H	2.4772847	-0.8490447	-0.4510732
H	2.1457851	0.3927371	-1.9016739

$H_2Fe(CO)_4$-H_2Se:

Fe	-1.5959257	-0.2021852	-0.2191773
H	-0.2144558	0.4054504	-0.0458573
C	-0.8324443	-1.3263073	0.9501052
O	-0.2889846	-1.9569969	1.7404915
C	-1.0009502	-0.9472619	-1.7714333
O	-0.5667557	-1.3897017	-2.7384708
C	-1.8644054	1.4776058	-0.7906784
O	-1.9694265	2.5834304	-1.0784376
C	-3.3186399	-0.8218757	-0.2035678
O	-4.4041939	-1.1905692	-0.1581772
H	-1.8712339	0.5119082	1.0938079
Se	2.7282743	0.5068899	-0.6419408
H	2.4772838	-0.9264133	-0.4076528
H	2.1175240	0.4223016	-1.9806442

$HCo(CO)_4$:

Co	-0.000119600	0.000000000	-0.144295300
H	0.000275400	-0.000000100	-1.625015500

C	-0.891700700	-1.544581500	-0.425059800
O	-1.453456100	-2.518288300	-0.657015200
C	-0.891701700	1.544583200	-0.425060300
O	-1.453455200	2.518286800	-0.657014400
C	1.783171800	-0.000000100	-0.425176300
O	2.907292500	0.000000000	-0.657328000
C	-0.000138000	0.000000100	1.669008200
O	-0.000168500	0.000000000	2.814918900

$HCo(CO)_4$-DME:

Co	-1.404508800	-0.159686600	-0.050008200
H	0.049131400	0.150024000	-0.137754700
C	-0.757869300	-1.165541400	1.295488700
O	-0.272027800	-1.788873900	2.130114800
C	-1.079326500	-0.748750300	-1.716522300
O	-0.796929600	-1.104324600	-2.773994700
C	-1.409100700	1.623805500	0.185843600
O	-1.331713300	2.763093700	0.318694900
C	-3.183867700	-0.519068900	0.090560200
O	-4.304921500	-0.743406100	0.181705800
O	2.062514900	0.588678600	-0.478331900
C	2.604299100	-0.678758400	-0.841268600
H	3.634390000	-0.573716000	-1.217653600
H	2.609052600	-1.297098300	0.060656200
H	1.992966200	-1.168734000	-1.615730900
C	1.987556900	1.481109800	-1.587104400
H	1.551753500	2.414450600	-1.220556600
H	2.989011600	1.682111900	-1.999814200

H	1.350764000	1.072199700	-2.387828200

$HCo(CO)_4$-DMS:

Co	-1.358251000	-0.153103100	-0.072828000
H	0.124357700	0.215165200	-0.010902500
C	-0.759823500	-1.165154200	1.287722400
O	-0.296204500	-1.789232900	2.135943100
C	-0.953078400	-0.719526400	-1.729445900
O	-0.656234700	-1.070739100	-2.786525500
C	-1.403500000	1.626392700	0.174997500
O	-1.340724100	2.766426200	0.319509400
C	-3.138616400	-0.549768100	-0.033989300
O	-4.259057000	-0.795316500	0.000514800
S	2.254428900	0.764490500	-0.101865000
C	2.626155300	-0.880693300	-0.780991400
H	3.483873700	-0.831373000	-1.459128300
H	2.870633400	-1.531901200	0.063004900
H	1.756953400	-1.285905900	-1.307510100
C	1.892382000	1.661504000	-1.641254400
H	1.645632300	2.690701800	-1.365795200
H	2.766072100	1.662363600	-2.300341100
H	1.036177600	1.213185600	-2.154623000

$HCo(CO)_4$-DMSe:

Co	-1.373050100	-0.151036700	-0.060572700
H	0.107626700	0.224081800	0.034225100
C	-0.801257400	-1.166091900	1.310167500
O	-0.354723400	-1.790787600	2.166933300

C	-0.929381400	-0.706998300	-1.710793700
O	-0.606266400	-1.050497000	-2.762636600
C	-1.437246600	1.627631400	0.194842200
O	-1.385982900	2.767246400	0.346372300
C	-3.151724300	-0.559544100	-0.062372000
O	-4.270863300	-0.813048400	-0.052649300
Se	2.342901500	0.815788000	-0.009192700
C	2.673115500	-0.967939800	-0.785100500
H	3.475176000	-0.904052600	-1.523824200
H	2.975359100	-1.621570900	0.036567800
H	1.756343600	-1.345296800	-1.242261400
C	1.881359400	1.735472100	-1.692258300
H	1.682095500	2.779578400	-1.440079000
H	2.721142200	1.673103600	-2.387758600
H	0.986554900	1.281478800	-2.123119800

$HCo(CO)_4$-H_2O:

Co	-1.3964913	-0.0657537	0.0026014
H	0.0408034	0.2984703	-0.0567630
C	-0.7683811	-1.0673149	1.3622358
O	-0.3008560	-1.6837808	2.2117902
C	-0.9787080	-0.5841105	-1.6648705
O	-0.6223315	-0.8866023	-2.7165138
C	-1.5237811	1.7090694	0.3029400
O	-1.5443061	2.8417508	0.4888558
C	-3.1571690	-0.5186906	0.0631465
O	-4.2666659	-0.8047895	0.1034701
O	2.2932272	0.3896196	-0.6501048

H	2.4854556	-0.5391732	-0.4732279
H	2.1296997	0.4205272	-1.6004488

$HCo(CO)_4$- H_2S:

Co	-1.4284423	-0.1085916	-0.0378442
H	-0.0028031	0.3092157	-0.0574440
C	-0.7990314	-1.1043706	1.3263713
O	-0.3293663	-1.7124842	2.1805939
C	-0.9560953	-0.6047332	-1.6995806
O	-0.5674534	-0.8923715	-2.7432875
C	-1.6290614	1.6574035	0.2720998
O	-1.6937717	2.7871224	0.4671408
C	-3.1742015	-0.6216606	-0.0293902
O	-4.2744292	-0.9436857	-0.0276549
S	2.6270461	0.4721845	-0.6274090
H	2.4695021	-0.8549706	-0.4758267
H	2.1467645	0.4369430	-1.8834047

$HCo(CO)_4$- H_2Se:

Co	-1.4306437	-0.1085225	-0.0374766
H	-0.0029709	0.3107515	-0.0562259
C	-0.7999418	-1.1042921	1.3257966
O	-0.3288296	-1.7123791	2.1795080
C	-0.9575990	-0.6051694	-1.6997279
O	-0.5689735	-0.8924206	-2.7434821
C	-1.6296390	1.6569391	0.2720937
O	-1.6928370	2.7871508	0.4664203
C	-3.1766947	-0.6220779	-0.0291601

O	-4.2767247	-0.9451773	-0.0273525
Se	2.6578333	0.5206386	-0.5894275
H	2.4733631	-0.9335148	-0.4349787
H	2.1223166	0.4680751	-1.9616224