Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Table S1 Total energy (E_{total}, Hartree), vibrational frequencies (ν, cm^{-1}) of C=S(Se) and H-M stretch vibrations, and SCS-MP2 energy ($E_{SCS-MP2}$, Hartree) in the complexes and monomers

	E_{total}	$\nu_{C=S(Se)}$	ν_{H-M}	$E_{SCS-MP2}$
F_2CS-HLi	-643.2149714	1383.32	1434.31	-0.8544665
F_2CS-HNa	-797.6198813	1380.93	1188.78	-0.8552125
F_2CS-HBeH	-651.0314977	1397.04	2273.69	-0.8912355
F_2CS-HMgH	-835.9953568	1393.43	1664.53	-0.8889203
F_2CS-$HMgCH_3$	-875.2319698	1392.82	1642.21	-1.0698128
F_2CSe-HLi	-2645.5988299	1313.24	1443.49	-0.8979413
F_2CSe-HNa	-2800.0040337	1309.26	1196.95	-0.8988305
F_2CSe-HBeH	-2653.4137855	1331.98	2274.82	-0.9340426
F_2CSe-HMgH	-2838.3780917	1327.30	1661.91	-0.9319366
F_2CSe-$HMgCH_3$	-2877.6148236	1326.22	1645.58	-1.1129363
F_2CSe-HLi-OH_2	-2721.9553458	1307.51	1391.15	-1.1628111
HLi-OH_2	-84.3703778	--	1356.70	-0.2978593
F_2CS	-635.1964816	1401.56	--	-0.8169315
F_2CSe	-2637.5777905	1337.34	--	-0.8588907
HLi	-8.0150132	--	1415.31	-0.0338199
HNa	-162.4195527	--	1161.15	-0.0341013
HBeH	-15.8334668	--	2266.59	-0.0724961
HMgH	-200.7967717	--	1658.03	-0.0695852
$HMgCH_3$	-240.0332696	--	1630.64	-0.2503432
H_2O	-76.3289921	--	--	-0.2659570

Note: $E_{SCS-MP2}$ was calculated according to Ref [J. Chem. Phys. 2003, 118, 9095].

Table S2 The Cartesian coordinates of the complexes and monomers

F_2CS-HLi			
C	0.00000000	0.77855200	0.00000000
S	-0.00002800	-0.81703400	0.00000000
F	-1.05879800	1.57260500	0.00000000
F	1.05882500	1.57256800	0.00000000
Li	0.00007900	-5.37758500	0.00000000
H	-0.00002800	-3.77256500	0.00000000
F_2CS-HNa			
C	0.00036500	1.66898600	0.00000000
S	0.00000000	0.07309200	0.00000000
F	1.05938700	2.46412200	0.00000000
F	-1.05829200	2.46460700	0.00000000
Na	-0.00103500	-4.78849100	0.00000000
H	-0.00065900	-2.86855500	0.00000000
F_2CS-HBeH			
C	0.00004500	-1.02679900	0.00000000
S	0.00000000	0.56937300	0.00000000
F	-1.05840300	-1.81118900	0.00000000
F	1.05853600	-1.81113000	0.00000000
Be	-0.00022300	4.94203100	0.00000000
H	-0.00000200	3.61232100	0.00000000
H	-0.00057100	6.27125600	0.00000000
F_2CS-HMgH			
C	0.00054000	1.85201100	0.00000000
S	0.00000000	0.25582900	0.00000000
F	1.05949800	2.63819200	0.00000000
F	-1.05788600	2.63890800	0.00000000
Mg	-0.00125500	-4.47864800	0.00000000
H	-0.00076900	-2.77116500	0.00000000
H	-0.00191900	-6.18429700	0.00000000
F_2CS-HMgCH_3			
C	2.72479800	0.00182200	-0.00008300
S	1.12867600	-0.00630400	0.00077000
F	3.51719600	-1.05284600	-0.00053600
F	3.50641700	1.06450700	-0.00051600
Mg	-3.60146300	-0.00737400	0.00023900
H	-1.88898600	-0.02069600	0.00023000
C	-5.69952100	0.00937700	-0.00058000
H	-6.11054300	-0.63961800	-0.77743200
H	-6.09737300	1.01146500	-0.17711700
H	-6.10852900	-0.33395200	0.95257300

F_2CSe-HLi

C	0.00002600	-1.09507500	0.00000000
F	1.05996800	-1.88688400	0.00000000
F	-1.05989100	-1.88691700	0.00000000
Li	-0.00020000	5.06230900	0.00000000
H	-0.00025100	3.45739000	0.00000000
Se	0.00000000	0.64383400	0.00000000

F_2CSe-HNa

C	-1.62978100	-0.50386000	0.00000000
F	-2.00026600	-1.77527600	0.00000000
F	-2.74460100	0.20971500	0.00000000
Na	4.53360800	1.12436300	0.00000000
H	2.61280300	1.09604300	0.00000000
Se	0.00000000	0.10732900	0.00000000

F_2CSe-HBeH

C	0.00069000	-1.26752900	0.00000000
F	1.06079600	-2.04828500	0.00000000
F	-1.05879300	-2.04913000	0.00000000
Be	-0.00369100	4.76754500	0.00000000
H	-0.00255300	3.43763200	0.00000000
H	-0.00484100	6.09609800	0.00000000
Se	0.00000000	0.46700000	0.00000000

F_2CSe-HMgH

C	0.00563300	1.86141700	0.00000000
F	-1.05155100	2.64846500	0.00000000
F	1.06790000	2.64159100	0.00000000
Mg	-0.01295700	-4.50299500	0.00000000
H	-0.00829900	-2.79506100	0.00000000
H	-0.01715800	-6.20765700	0.00000000
Se	0.00000000	0.12528400	0.00000000

F_2CSe-HMgCH_3

C	-2.53878600	-0.00170200	-0.00008100
F	-3.32540200	1.05634500	-0.00005400
F	-3.32057100	-1.06331400	-0.00004500
Mg	3.81620000	0.00262000	0.00091700
H	2.10327900	0.00861500	0.00240400
Se	-0.80259600	0.00227300	-0.00008800
C	5.91339200	-0.00446600	-0.00089400
H	6.32180300	0.93668500	-0.37629200
H	6.31563100	-0.80196200	-0.62994300
H	6.31926200	-0.15232000	1.00255500

F_2CSe-HLi-OH_2

C	2.08013200	0.00018000	0.00045400
F	2.87425500	1.06028000	-0.01149500

F	2.87484700	-1.05947100	0.01308500
Li	-4.05603700	0.00001300	0.00000400
H	-2.42829100	-0.00007000	-0.00042200
Se	0.33947100	-0.00031100	-0.00068200
O	-6.00070500	0.00019000	0.00063200
H	-6.58155300	-0.15583700	-0.74971700
H	-6.58113500	0.15657400	0.75123000
$HLi\text{-}OH_2$			
Li	1.35573000	0.00002800	-0.00001000
H	2.98347600	-0.00005400	0.00004900
O	-0.58893900	-0.00000800	-0.00002800
H	-1.16954400	0.76657500	0.00010200
H	-1.16961100	-0.76654000	0.00010200
F_2CS			
C	0.00000000	0.00000000	-0.28634700
S	0.00000000	0.00000000	1.30926200
F	0.00000000	1.05842300	-1.06833900
F	0.00000000	-1.05842300	-1.06833900
F_2CSe			
C	0.00000000	0.00000000	-0.77398000
F	0.00000000	1.05979700	-1.55284700
F	0.00000000	-1.05979700	-1.55284700
Se	0.00000000	0.00000000	0.95868000
HLi			
Li	0.00000000	0.00000000	0.40116200
H	0.00000000	0.00000000	-1.20348600
HNa			
Na	0.00000000	0.00000000	0.15991600
H	0.00000000	0.00000000	-1.75907500
HBeH			
Be	0.00000000	0.00000000	0.00008100
H	0.00000000	0.00000000	-1.32962900
H	0.00000000	0.00000000	1.32930600
HMgH			
Mg	0.00000000	0.00000000	0.00013100
H	0.00000000	0.00000000	-1.70735200
H	0.00000000	0.00000000	1.70578000
$HMgCH_3$			
Mg	-0.83636300	0.00000600	0.00000600
H	-2.54813000	-0.00003800	-0.00004000
C	1.26284700	-0.00000200	-0.00000600
H	1.66915800	0.88097400	-0.50255100
H	1.66912600	-0.87573000	-0.51166700
H	1.66912300	-0.00527300	1.01423000

H_2O

O	0.00000000	0.00000000	0.11835100
H	0.00000000	0.75804300	-0.47340600
H	0.00000000	-0.75804300	-0.47340600