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

Supporting Information

"Pnicogen bond" or "Chalcogen bond": Exploiting the effect of substitution on the formation of P…Se noncovalent bonds.

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Coordinates of optimized geometry for $XH_2P\ldots SeH_2$ complexes.

X= -H

P	2.42439100	0.07233500	-0.05399500
H	2.54095400	0.15394700	1.36453900
H	3.83400800	0.02165300	-0.26968900
H	2.27049100	-1.34526200	-0.05812100
Se	-1.21776600	-0.04361400	-0.01198400
H	-1.00129000	1.38891700	-0.22627000
H	-2.60598000	0.17858600	0.40692400

X= -F

P	1.69308900	0.05892700	-0.14870300
H	1.38503400	0.69266500	1.09376600
H	1.38904700	-1.24131200	0.35855100
Se	-1.60926100	-0.05179500	-0.02460700
H	-1.68328600	1.35216100	-0.43906300
H	-2.00287900	0.28661100	1.34673000
F	3.35895600	-0.02366800	0.07857800

X= $-CH_3$

P	1.81889500	0.03867900	0.09484900
H	1.83194700	-0.04501100	1.51910300
H	1.60284200	-1.36131000	-0.07720300
Se	-1.77037000	-0.03535200	-0.03831700
H	-1.53384100	1.40948900	-0.05911700
H	-3.18422300	0.15062900	0.30940500
C	3.67461100	0.04466400	-0.17731400
H	3.87417800	-0.09665000	-1.25038200
H	4.07053600	1.03057100	0.11000500
H	4.20006700	-0.73392500	0.39212200

X= -CF_3

P	0.64693200	-0.13154800	0.26707300
H	0.40556100	-0.66381800	-1.03066900
H	0.40379200	1.21643400	-0.11931900
Se	-2.96338000	0.06178100	0.00490900
H	-2.91088400	-1.30157800	0.54048700
H	-3.40029100	-0.42504500	-1.30696700
C	2.50998100	0.00970800	-0.02259500
F	3.09205800	0.75040700	0.96506600
F	2.87111200	0.58453900	-1.20526800
F	3.09159400	-1.22511900	0.00454100

X= -Cl

P	1.23410300	0.11079500	-0.18044900
H	0.95673500	0.48293200	1.16707000
H	0.96386300	-1.26709800	0.06355400
Se	-2.13641200	-0.05375600	-0.02125400
H	-2.17779400	1.39338400	-0.25047100
H	-2.49011800	0.11625900	1.39157900
Cl	3.34551700	-0.03292300	0.06221500

X= -OH

P	1.77352100	0.10456500	-0.06617600
H	1.43738900	-0.06102200	1.31029300
H	1.43283700	-1.24172700	-0.39279800
Se	-1.68458100	-0.02311100	-0.05361400
H	-1.65833900	1.36844000	0.40532600
H	-2.26880800	-0.47457900	1.21312100
O	3.47744200	-0.12005800	0.08650500
H	3.91032400	0.58666100	-0.41247500

X= -OCH_3

P	1.25598600	-0.18512600	0.06943400
H	0.83626000	-1.53139500	0.26707400
H	0.91462000	-0.19768700	-1.32416100
Se	-2.16489400	0.11480100	-0.03299700
H	-2.16843300	-0.00444300	1.42758200
H	-2.97402600	-1.09958500	-0.17731700
O	2.92959400	-0.56380000	-0.04001400
C	3.77961400	0.59416700	0.01818400
H	3.53546300	1.22916400	0.88777600
H	4.80971300	0.22498200	0.11347700
H	3.69858100	1.19802700	-0.90303400

X= -NH_2

P	1.80188300	0.04328600	-0.00191700
H	1.60205000	-0.04595400	1.40545800
H	1.51755700	-1.34503100	-0.21504800
Se	-1.72328300	-0.02570100	-0.05162100
H	-1.54764400	1.38281700	0.31068900
H	-2.90327500	-0.14874600	0.81124700
N	3.56017300	0.10399300	0.00751800
H	4.04254300	-0.73861200	0.31401900
H	3.93093300	0.39214000	-0.89512600

X= -$NHCH_3$

P	-1.27132800	-0.33894900	0.00784700
H	-1.16717100	0.38053000	1.23536900
H	-1.12416100	0.85352200	-0.78548000
Se	2.22164700	0.07404300	-0.05382900
H	2.17843600	-1.06262600	0.86929700
H	3.37755300	0.65276900	0.64006300
N	-3.00900100	-0.54802000	0.02512200
H	-3.29271300	-1.21978000	-0.68608500
C	-3.85551200	0.65025600	0.02288300
H	-3.67920700	1.31051900	-0.84854700
H	-4.91676700	0.35733200	0.03912300
H	-3.64596100	1.22909900	0.93559700

X = -CN

P	1.49183400	0.24133800	-0.07848900
H	1.20135600	-0.31650300	1.19856600
H	1.20465500	-0.95705000	-0.79100600
Se	-2.09303600	-0.04309600	-0.04619500
H	-2.11172900	1.27331100	0.59827600
H	-2.46152600	-0.70844400	1.20700200
C	3.28029200	-0.06615600	0.02443700
N	4.46731300	-0.14988600	0.05550000

Coordinates of optimized geometry for H_3P…SeHX complexes.

X= -F

P	-2.22317200	0.03897000	0.00000200
H	-3.02251300	0.53382800	1.06538900
H	-2.73622100	-1.28467300	-0.00041400
H	-3.02259300	0.53449700	-1.06501800

Se	0.58896600	-0.07564400	0.00000100
H	0.38819900	1.37748400	-0.00001000
F	2.41287400	0.09179900	-0.00000200

X= -CH_3

P	2.81642100	0.08812500	-0.05290800
H	4.23894400	-0.03404000	-0.04046000
H	2.61947900	-0.91773300	0.93808800
H	2.79828000	1.15856500	0.88841200
Se	-0.77266200	-0.15205900	-0.03973700
H	-0.56039200	0.65546200	-1.24406100
C	-2.66939100	0.30874400	0.15874600
H	-3.02107300	-0.22443400	1.05308300
H	-2.79188700	1.38850500	0.31011700
H	-3.24279800	-0.03066700	-0.71298600

X= -CF_3

P	3.67424800	-0.12241800	0.00006400
H	4.58422100	-0.44798600	1.04736300
H	3.99975800	1.26495800	0.00050600
H	4.58730400	-0.44817700	-1.04446300
Se	0.13055800	0.17093700	-0.00033000
H	0.34940700	-1.27704500	-0.00181900
C	-1.80793600	-0.06195900	0.00016000
F	-2.38658300	1.16605100	0.00133600
F	-2.26406200	-0.73191500	-1.08854000
F	-2.26332800	-0.73364400	1.08806200

X= -Cl

P	-2.76709300	0.06211900	-0.00007800
H	-3.60000000	0.51824700	1.05936600
H	-3.26131000	-1.27110400	-0.01142300
H	-3.59514200	0.53437800	-1.05625400
Se	0.27356000	-0.09619300	0.00054700
H	0.07940400	1.35690800	0.00265200
Cl	2.50484700	0.07060900	-0.00069200

X= -OH

P	2.51093800	0.04553400	0.00754200

H	2.95647900	-1.30666000	0.00854000
H	3.39080700	0.46517900	1.04622300
H	3.36572900	0.45647200	-1.05489800
Se	-0.69904600	-0.07348200	-0.00455700
H	-0.41152800	1.36921200	-0.02595800
O	-2.54358000	0.08980900	-0.09480600
H	-2.84933600	0.11270300	0.82634000

X= -OCH_3

P	2.88156500	0.21321400	0.03119800
H	3.57696100	1.45639800	0.01630000
H	3.34170300	-0.19871200	-1.25170000
H	3.89176600	-0.48487800	0.75335100
Se	-0.31013400	-0.24733000	-0.05074500
H	-0.08439800	0.28860900	1.30356900
O	-2.13265100	-0.46148700	0.12295700
C	-2.85939100	0.76984000	-0.04777300
H	-2.63952900	1.23605300	-1.02275200
H	-3.92462500	0.49970900	0.00342300
H	-2.62325000	1.48669900	0.75816500

X= -NH_2

P	-2.69981500	0.05935100	-0.00340100
H	-3.50519100	0.38260600	1.12777100
H	-2.95191500	-1.34065900	0.08357900
H	-3.74242100	0.29655600	-0.94683500
Se	0.75895700	-0.07345600	-0.01269700
H	0.43275400	1.35245800	-0.11793700
N	2.63274400	0.20649000	0.02767700
H	2.98944800	-0.20974200	0.89036400
H	3.04080100	-0.31940600	-0.74798800

X= -$NHCH_3$

P	3.07990500	0.18559500	0.06159800
H	3.65340100	1.42681200	0.46571100
H	3.21425100	0.45670900	-1.33118000
H	4.31009400	-0.53096200	0.14843300
Se	-0.35593600	-0.23645600	-0.06950600
H	-0.00228600	-0.56101400	1.31700400
N	-2.22055100	-0.42487400	0.19298700
H	-2.53268200	-1.10871500	-0.49978500
C	-2.95441000	0.84094100	0.00704500
H	-4.03160700	0.63017700	0.10608400
H	-2.65979700	1.53612900	0.80615000

H	-2.77781700	1.33491400	-0.96637500

X= -CN

P	2.98711800	-0.10002900	-0.00034900
H	3.85218700	-0.53143700	-1.04641700
H	3.85789800	-0.50937900	1.04981800
H	3.44970500	1.24704600	-0.01582700
Se	-0.49931100	0.13422500	0.00089100
H	-0.23713700	-1.30823600	0.00748500
C	-2.34106500	-0.10674700	-0.00041800
N	-3.52949200	-0.18867200	-0.00251600

Coordinates of optimized geometry for $XH_2P\ldots SeHX$ complexes

X= -F

P	-1.60635900	-0.32548700	0.05817200
H	-1.92117000	-1.18334100	1.14550800
H	-1.83051900	-1.24911600	-0.99582000
Se	0.88206600	0.07003500	-0.09630900
H	0.71072100	0.60600700	1.25784900
F	2.71694800	-0.03484700	0.13120200
F	-3.03404800	0.51568900	-0.02071500

X= $-CH_3$

P	-2.23320300	-0.11133000	-0.00086900
H	-2.15140700	-1.15747000	-0.96745100
H	-1.99626200	0.91860100	-0.95926400
Se	1.31183400	0.14711500	0.04168500
H	1.08253200	-0.72046700	1.19980600
C	3.21920700	-0.28103000	-0.13400000
H	3.58527000	0.29938900	-0.99249100
H	3.76848400	0.02147400	0.76651200
H	3.35974300	-1.35052800	-0.33503800
C	-4.10356400	0.02867000	0.06309100
H	-4.50402000	-0.83309400	0.61847500
H	-4.37066300	0.93929700	0.62063700
H	-4.57184700	0.06501500	-0.92998100

X= $-CF_3$

P	-1.54020000	-0.44441600	-0.38143300
H	-0.95660200	0.63523600	0.34023200
H	-1.48197700	-1.35161700	0.71507300

Se	2.03772000	-1.12779000	0.07808100
H	2.31266400	-1.25931600	-1.35647800
C	2.26361300	0.81032400	-0.00177600
C	-3.30327700	0.09669500	0.03205400
F	-4.19145200	-0.88818100	-0.29017100
F	-3.52081800	0.40608800	1.34151300
F	-3.64469500	1.20082900	-0.69283100
F	3.54094000	1.18437300	-0.24225400
F	1.89638100	1.32701400	1.19678600
F	1.49569400	1.38595100	-0.95901600

X= -Cl

P	1.77909000	0.48063100	0.07323200
H	2.03625500	1.43162200	1.10057400
H	1.94300200	1.40513200	-0.99594000
Se	-1.07289200	-0.05038500	-0.12272500
H	-0.84660000	-0.67120800	1.18676200
Cl	3.68967200	-0.38847300	0.00123900
Cl	-3.29794800	-0.06223000	0.10363000

X= -OH

P	2.14152700	-0.47745200	0.05187300
H	2.97987000	-0.81497700	-1.05103500
H	3.14603000	-0.73094500	1.03178100
Se	-0.95284500	-0.16670700	-0.09317500
H	-0.76980200	-0.68639400	1.27098900
O	-2.73135600	0.31133100	0.10743900
H	-2.72663400	1.23047400	0.42038700
O	2.26745600	1.22280800	-0.01842900
H	1.35554800	1.55854500	0.00564800

X= -OCH_3

P	2.12044300	-0.85352200	0.09586100
H	2.61300400	-1.35327100	-1.15447500
H	2.94647800	-1.70276900	0.88521600
Se	-0.94448000	-0.43343200	-0.12884100
H	-0.71329200	-0.44268400	1.32661700
O	-2.77497100	-0.18983600	-0.02976500
O	3.07750500	0.54382400	0.28516600
C	2.45564000	1.73976700	-0.23402000
H	1.41009200	1.82504800	0.10511600
H	3.04492300	2.58408500	0.14639000
H	2.47988100	1.74605300	-1.33719200
C	-3.14306200	1.17527700	0.23610700

H	-2.72769400	1.86093700	-0.52194700
H	-4.24215800	1.20662000	0.20005200
H	-2.80130100	1.49335900	1.23716400

X= -NH_2

P	2.32940200	-0.50752800	-0.05850000
H	3.57670800	-0.69710300	-0.72155800
H	2.86186000	-0.83022200	1.23287900
Se	-1.03533600	-0.20124500	0.07231200
H	-0.74552300	-0.35546000	-1.35752200
N	-2.79475700	0.44698200	-0.19961800
H	-3.43245300	-0.17361700	0.30350300
H	-2.86089100	1.36558200	0.24347500
N	2.29578800	1.24452900	-0.07623700
H	1.36266300	1.58302700	0.15546800
H	2.99082400	1.72249000	0.49363500

X= -$NHCH_3$

P	2.37342700	-1.02008800	-0.11625600
H	3.73249100	-1.10277500	-0.55219400
H	2.60164600	-1.82538400	1.04154700
Se	-0.93372500	-0.28051600	-0.02582700
H	-0.40930600	0.41840200	-1.20652400
N	-2.46715300	0.81594900	0.13978400
H	-2.44670700	1.18368300	1.09345300
C	-3.72364900	0.07354500	-0.07957900
H	-4.56320400	0.76407400	0.10087400
H	-3.75808000	-0.25158300	-1.12907100
H	-3.84912600	-0.81529200	0.56554100
N	2.54234900	0.57447600	0.68373700
H	1.63285100	0.75098300	1.12420300
C	2.75499500	1.63176200	-0.32606200
H	2.71483200	2.61311700	0.16905800
H	3.75919400	1.51216900	-0.76218400
H	2.01619600	1.62665000	-1.15354300

X= -CN

P	3.12589000	0.28915000	-0.15320700
H	2.81679600	0.95526000	1.06481100
H	4.16192200	-0.51641700	0.41013200

Se	-2.03480300	-0.12049300	-0.01973600
H	-1.09431600	-1.25944800	0.01838600
C	-0.61943200	1.06293900	0.03147500
N	0.29202600	1.83097300	0.06492000
C	1.85730600	-0.99181300	0.05601500
N	0.99130100	-1.80906500	0.07091600

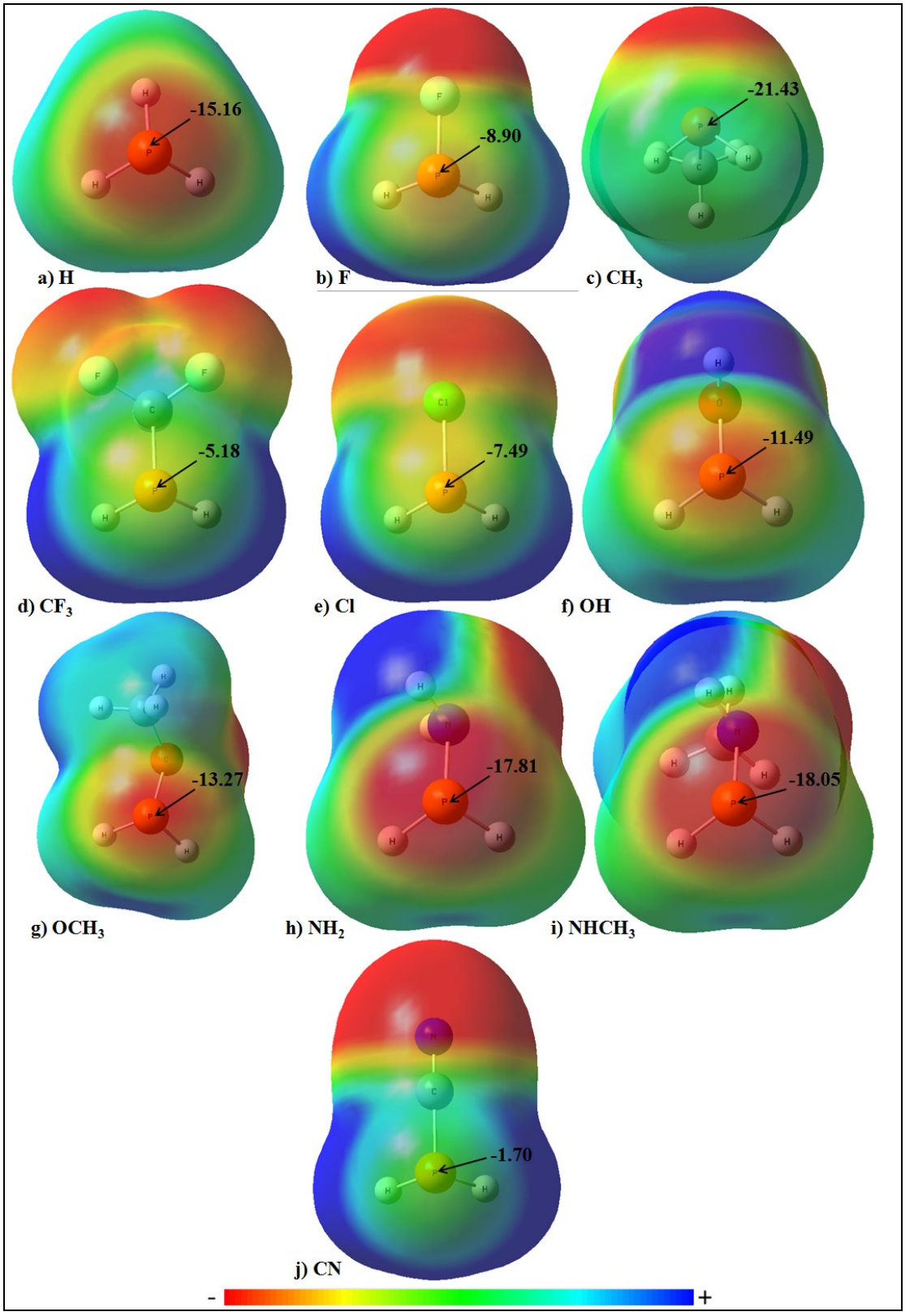

-15.16
a) H
-8.90
b) F
-21.43
c) CH3
-5.18
d) CF3
-7.49
e) Cl
-11.49
f) OH
-13.27
g) OCH3
-17.81
h) NH2
-18.05
i) NHCH3
-1.70
j) CN
-
+

Figure S1: Electrostatic potential maps for the electrostatic negative regions of monomers (a) H_3P, (b) FH_2P, (c) $(CH_3)H_2P$, (d) $(CF_3)H2P$, (e) $(OH)H_2P$, (f) $(OCH_3)H_2P$, (g) $(NH_2)H_2P$, (h) $(NHCH_3)H_2P$ and (i) $(CN)H_2P$ on the total density isosurface with potentials ranging from -12 kcal/mol(red) to 12 kcal/mol (blue). All energy values are reported in kcal/mol.

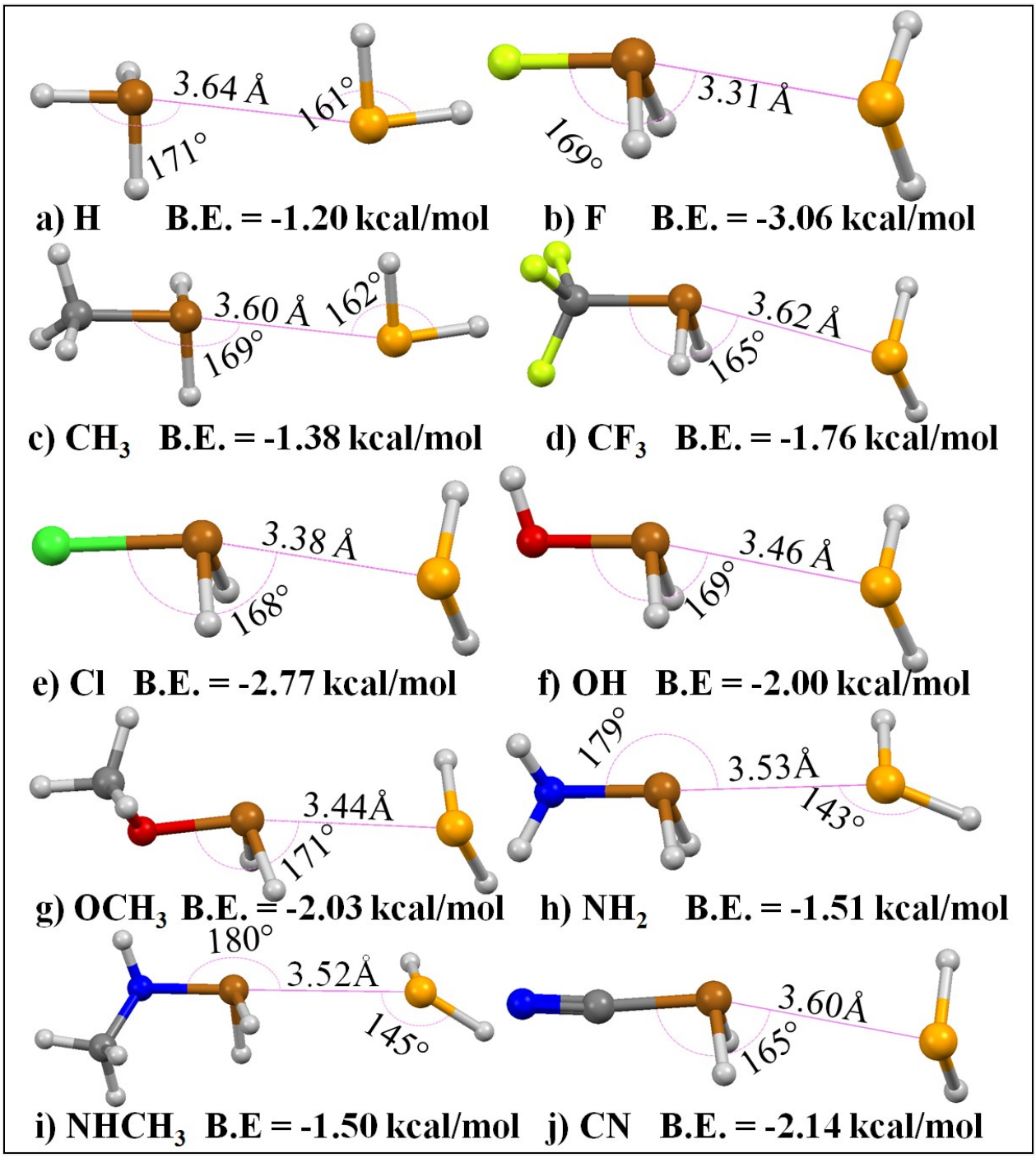


Figure S2: Optimized geometries of the $XH_2P\cdots SeH_2$ complex for X = (a) −H, (b) −F, (c) $-CH_3$, (d) $-CF_3$, (e) −Cl, (f) −OH, (g) $-OCH_3$, (h) $-NH_2$, (i) $-NHCH_3$, (j) −CN.

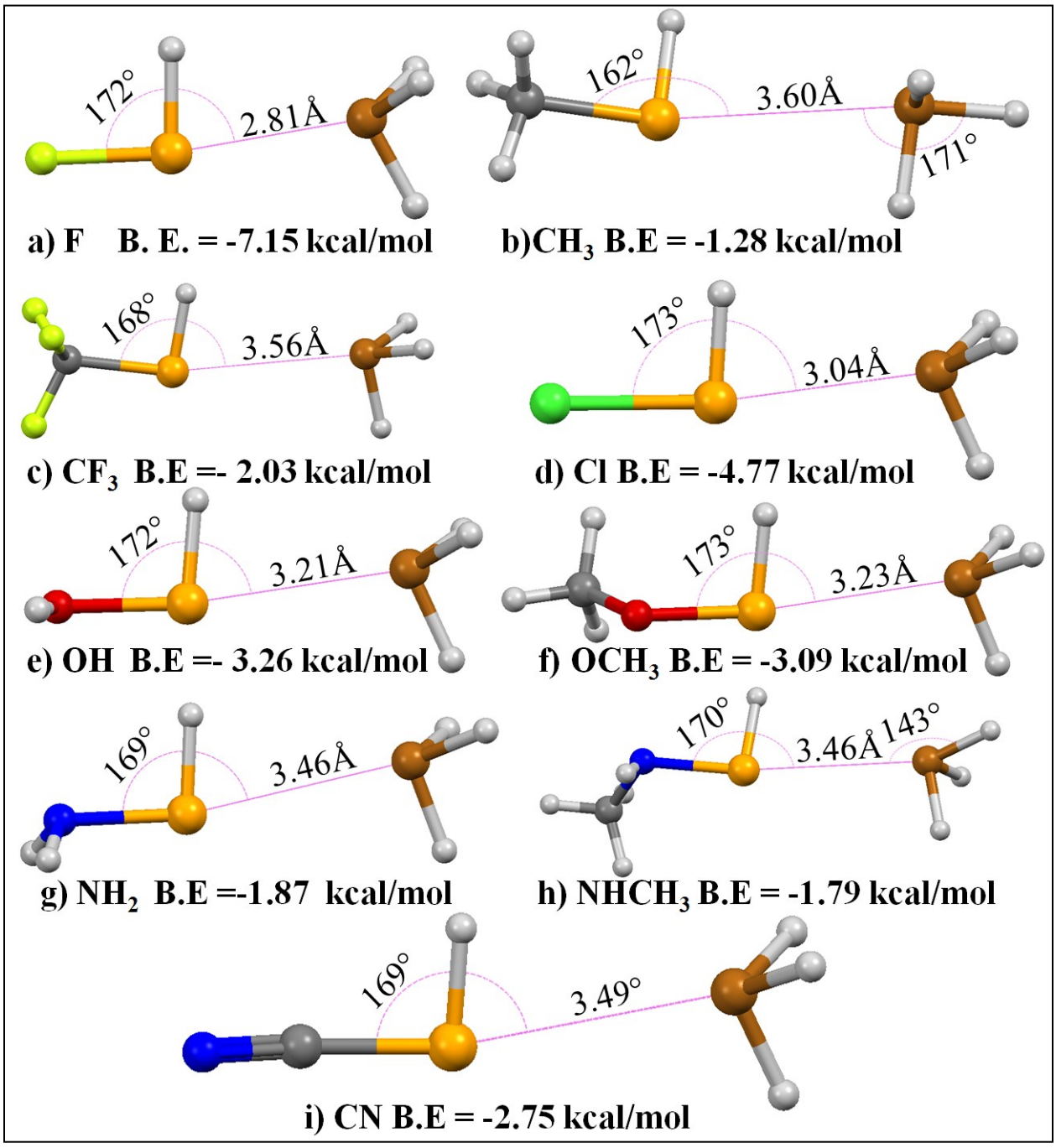


Figure S3: Optimized geometries of the $H_3P\cdots SeHX$ complex for X = (a) −F, (b) $-CH_3$, (c) $-CF_3$, (d) −Cl, (e) −OH, (f) $-OCH_3$, (g) $-NH_2$, (h) $-NHCH_3$, (i) −CN.

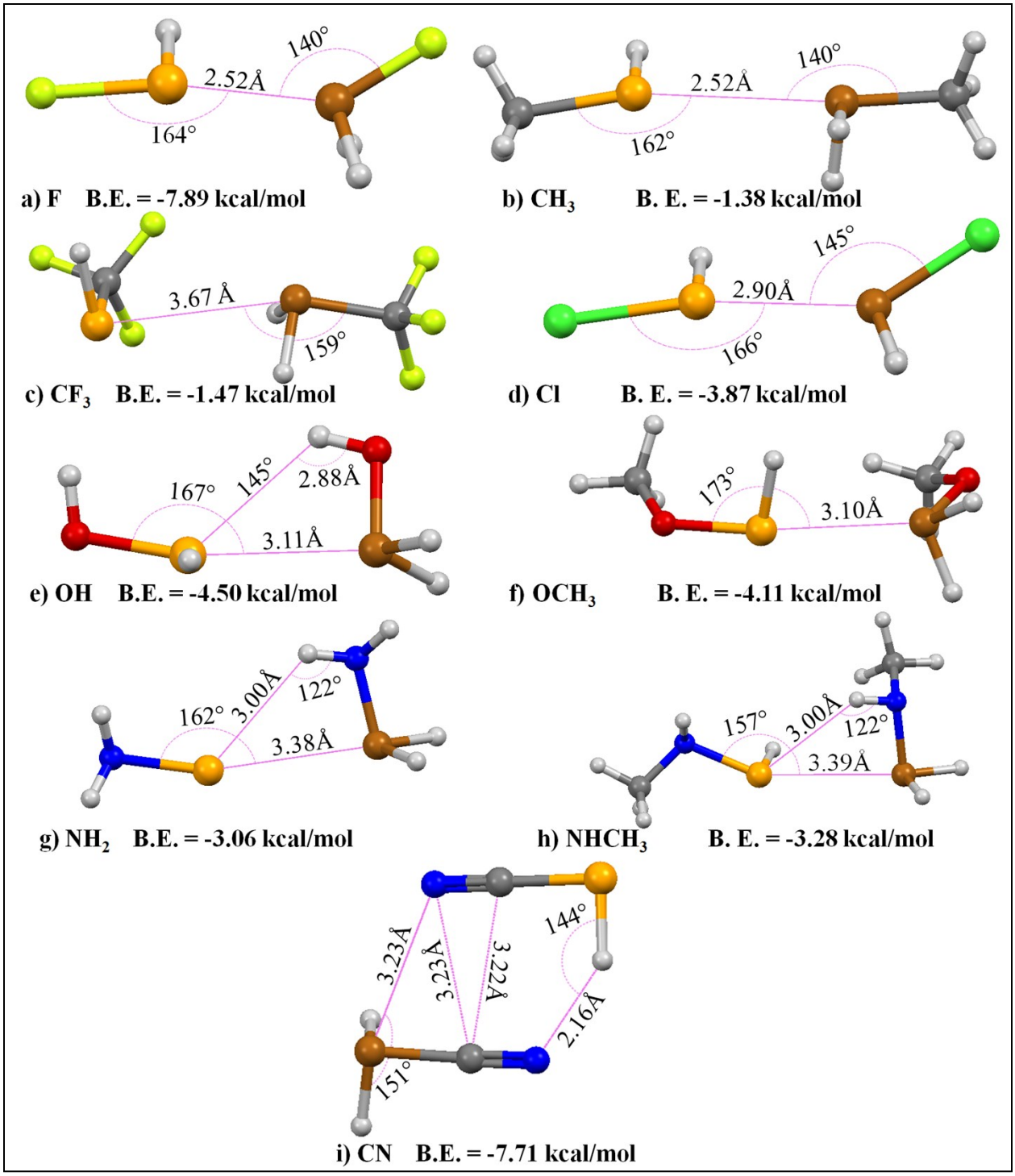


Figure S4: Optimized geometries of the $XH_2P\cdots SeHX$ complex for X = (a) −F, (b) $-CH_3$, (c) $-CF_3$, (d) −Cl, (e) −OH, (f) $-OCH_3$, (g) $-NH_2$, (h) $-NHCH_3$, (i) −CN.

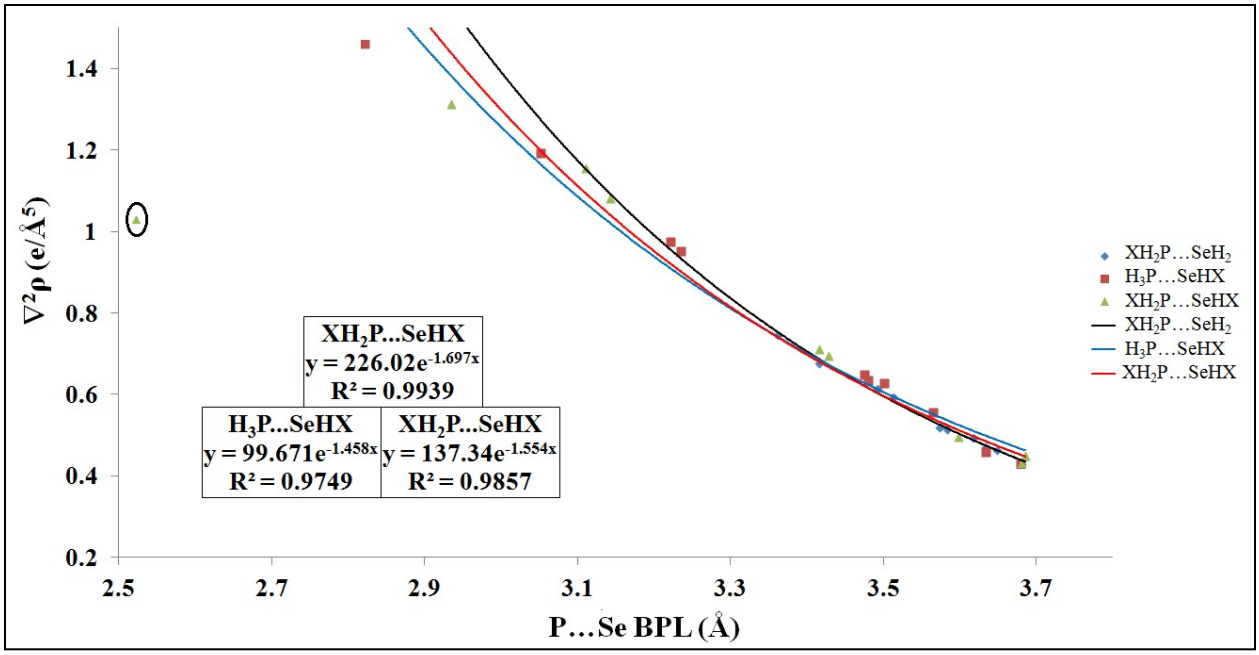


Figure S5: Plot showing variation of $\nabla^2\rho$ with increasing Bond Path Length (BPL) for different complexes of $XH_2P\cdots SeH_2$, $H_3P\cdots SeHX$ and $XH_2P\cdots SeHX$

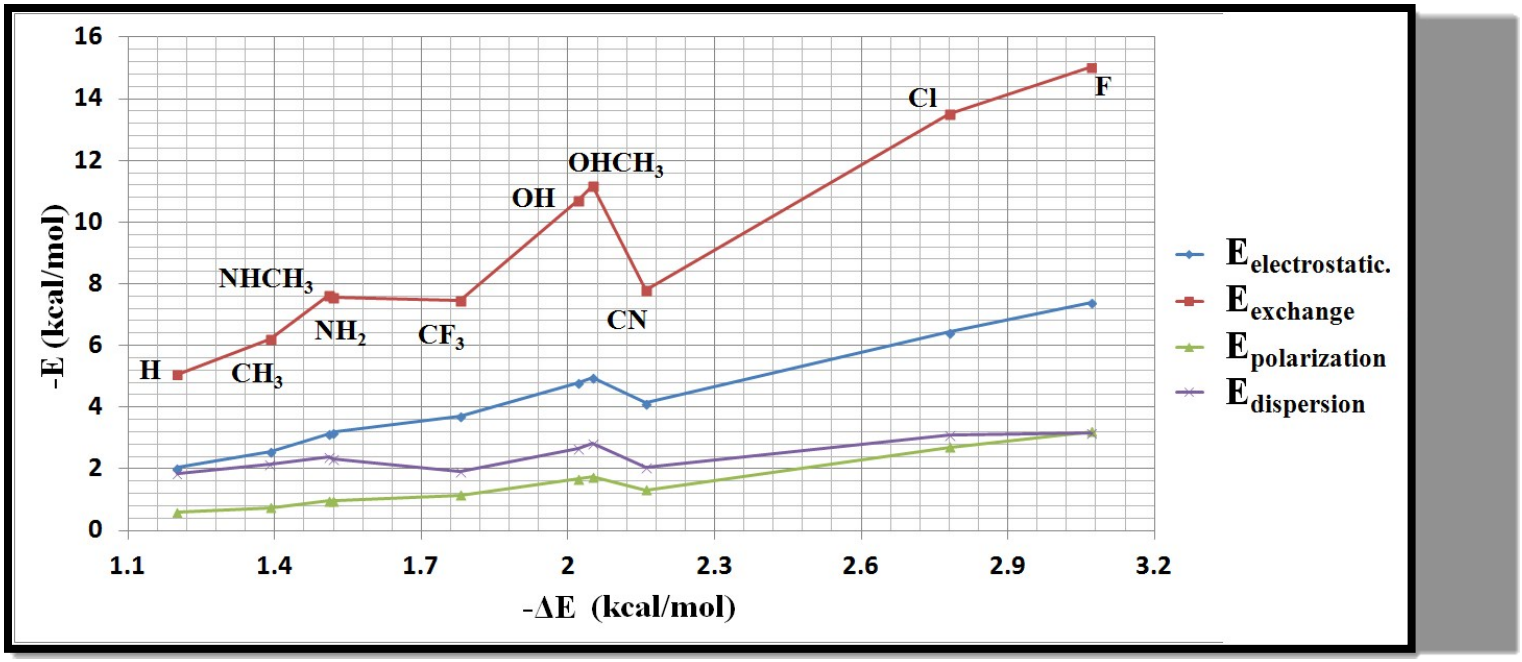


Figure S6: Variation of total binding energy obtained from LMOEDA with individual energy decomposition components for $XH_2P\ldots SeH_2$ complexes.

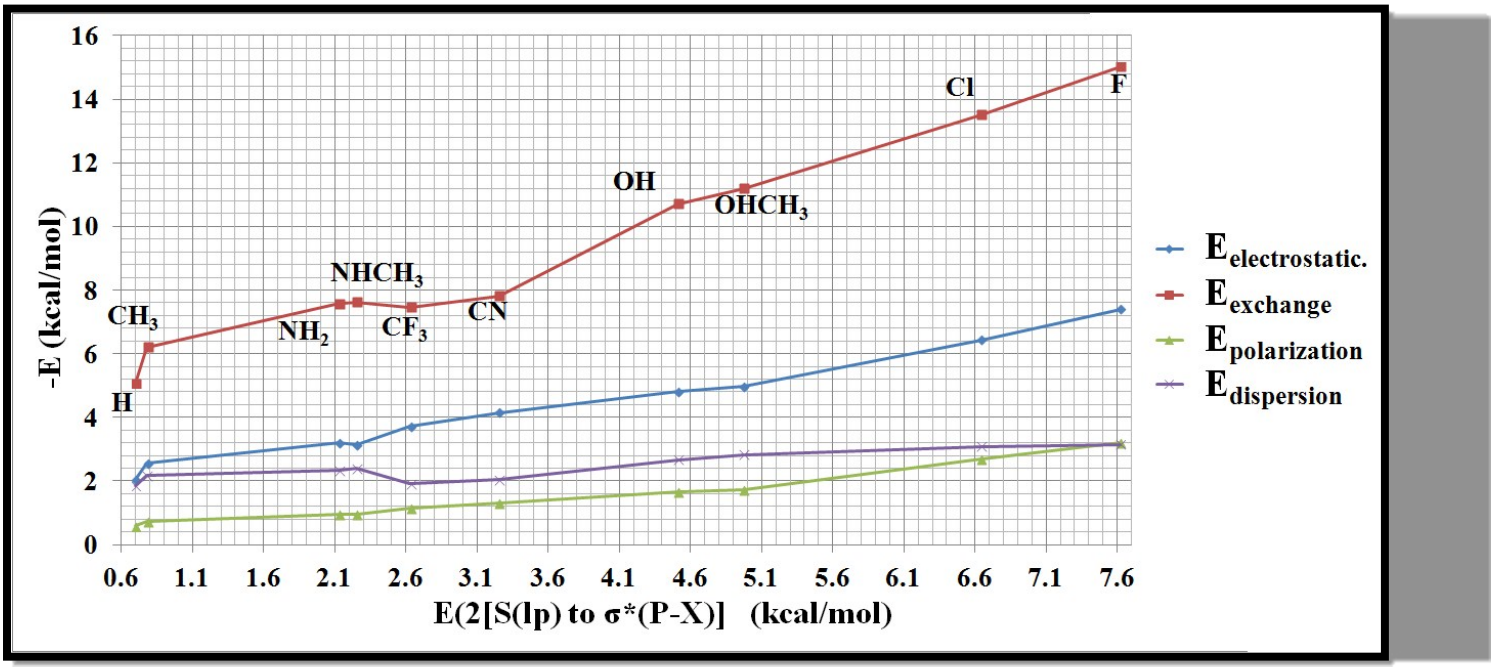


Figure S7: Variation of E(2) for S(*lp*) to σ*(P-X) charge transfer with energy decomposition components for $XH_2P\ldots SeH_2$ complexes.

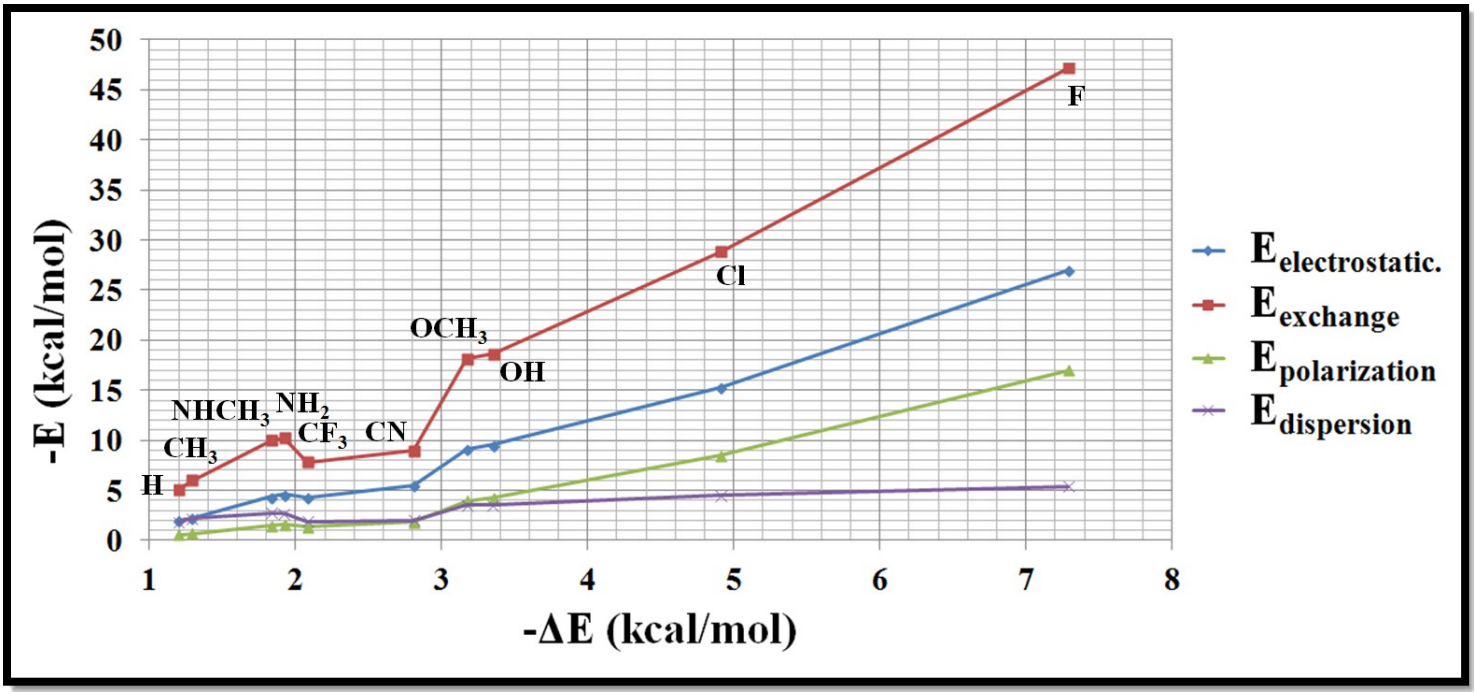


Figure S8: Variation of total binding energy obtained from LMOEDA with individual energy decomposition components for H_3P…SeHX complexes.

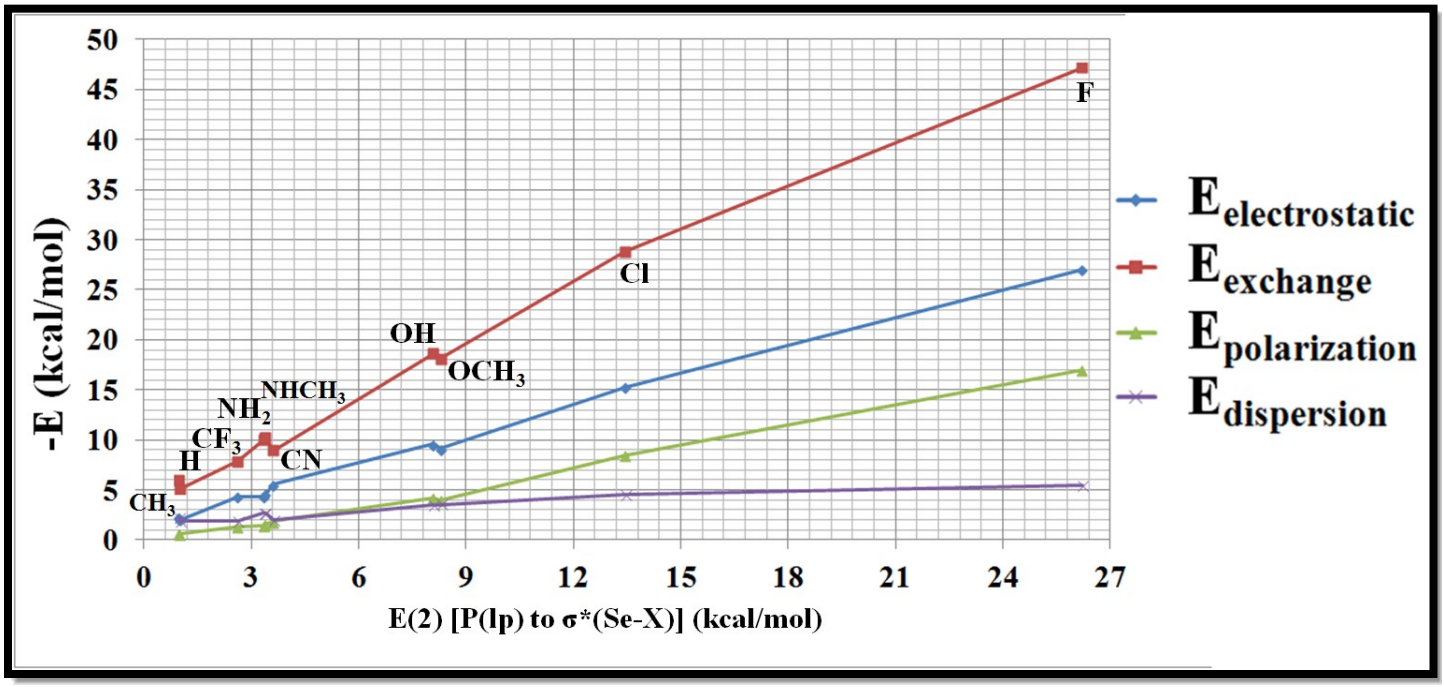


Figure S9: Variation of E(2) for S(*lp*) to σ*(P-X) charge transfer with energy decomposition components. for H_3P…SeHX complexes.

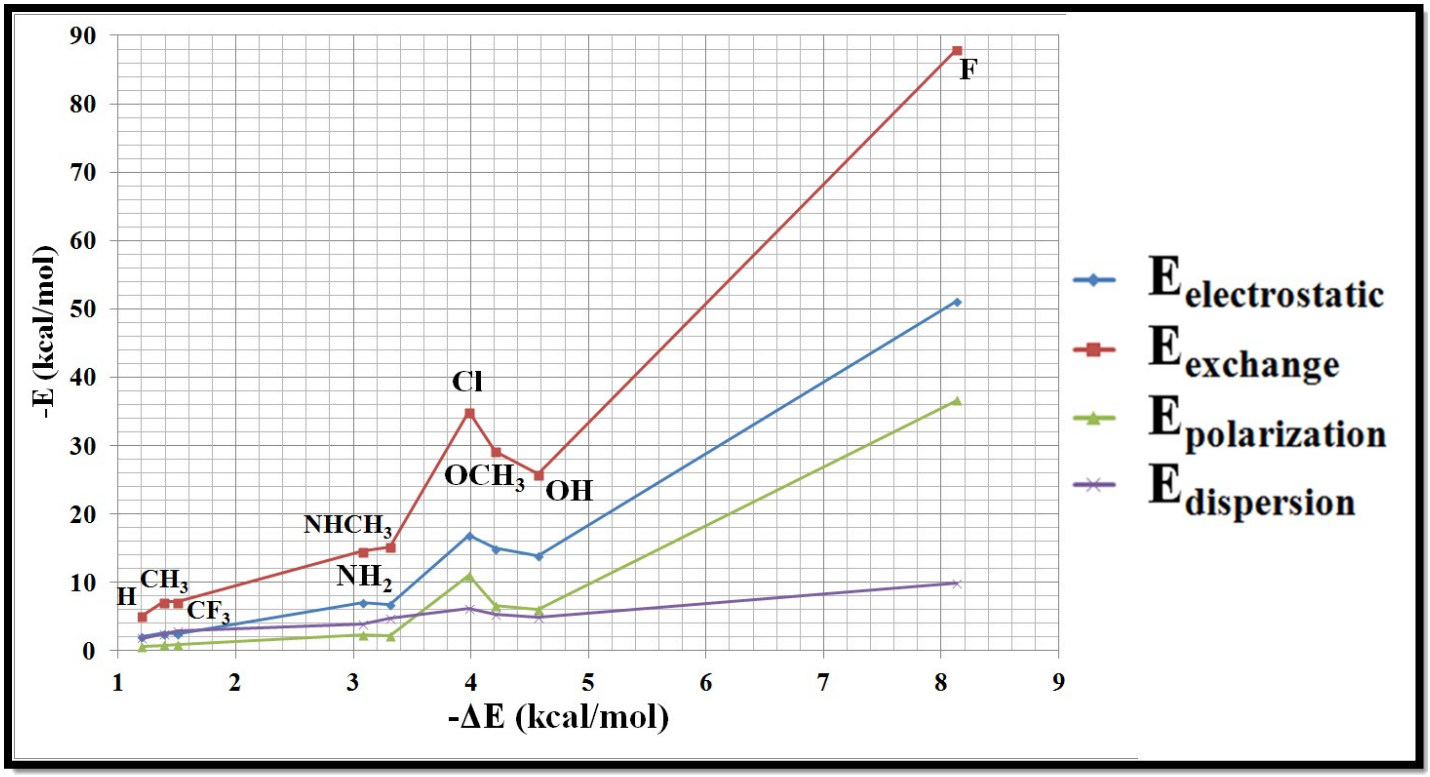


Figure S10: Variation of total binding energy obtained from LMOEDA with individual energy decomposition components for $XH_2P\ldots SeHX$ complexes.

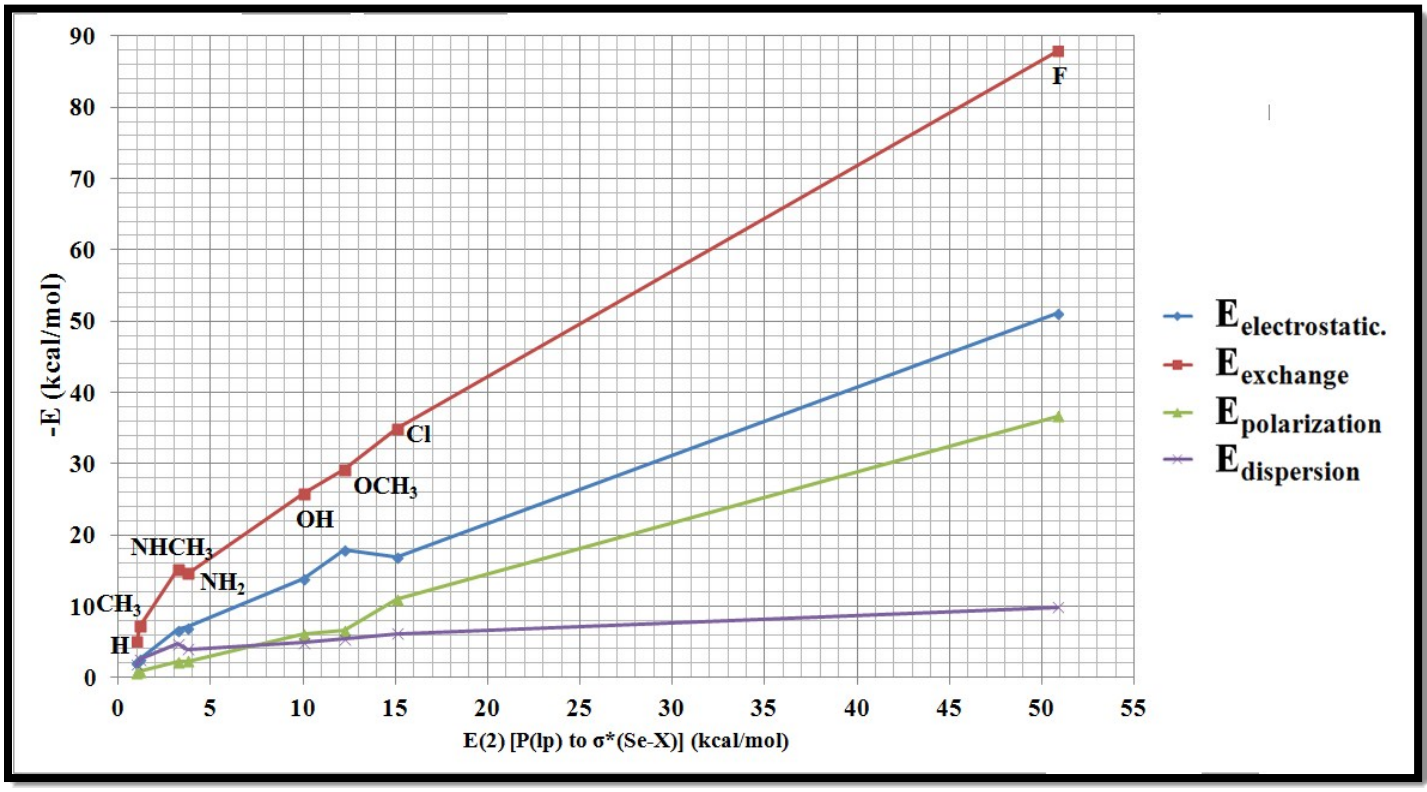


Figure S11: Variation of E(2) for P(*lp*) to σ*(Se-X) charge transfer with energy decomposition components for $XH_2P\ldots SeHX$ complexes.

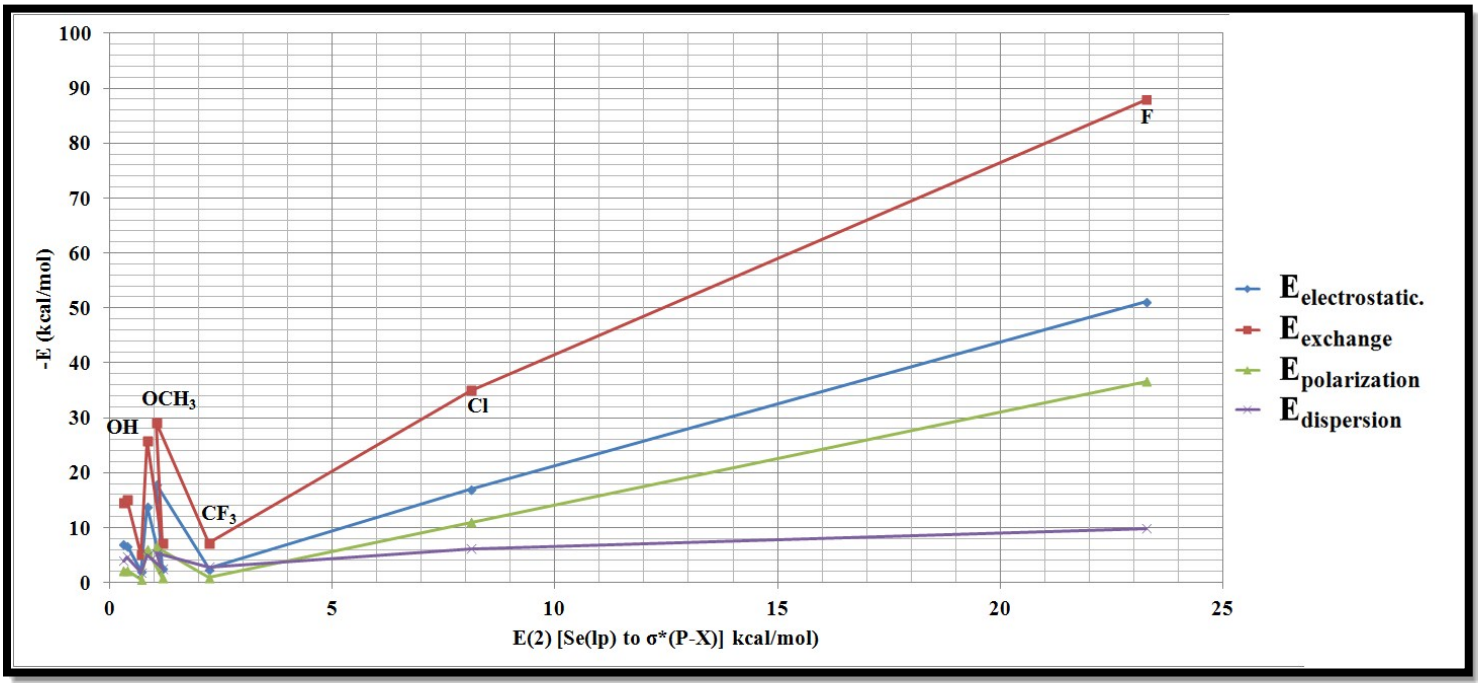


Figure S12: Variation of E(2) for S(*lp*) to σ*(P-X) charge transfer with energy decomposition components for $XH_2P\ldots SeHX$ complexes.

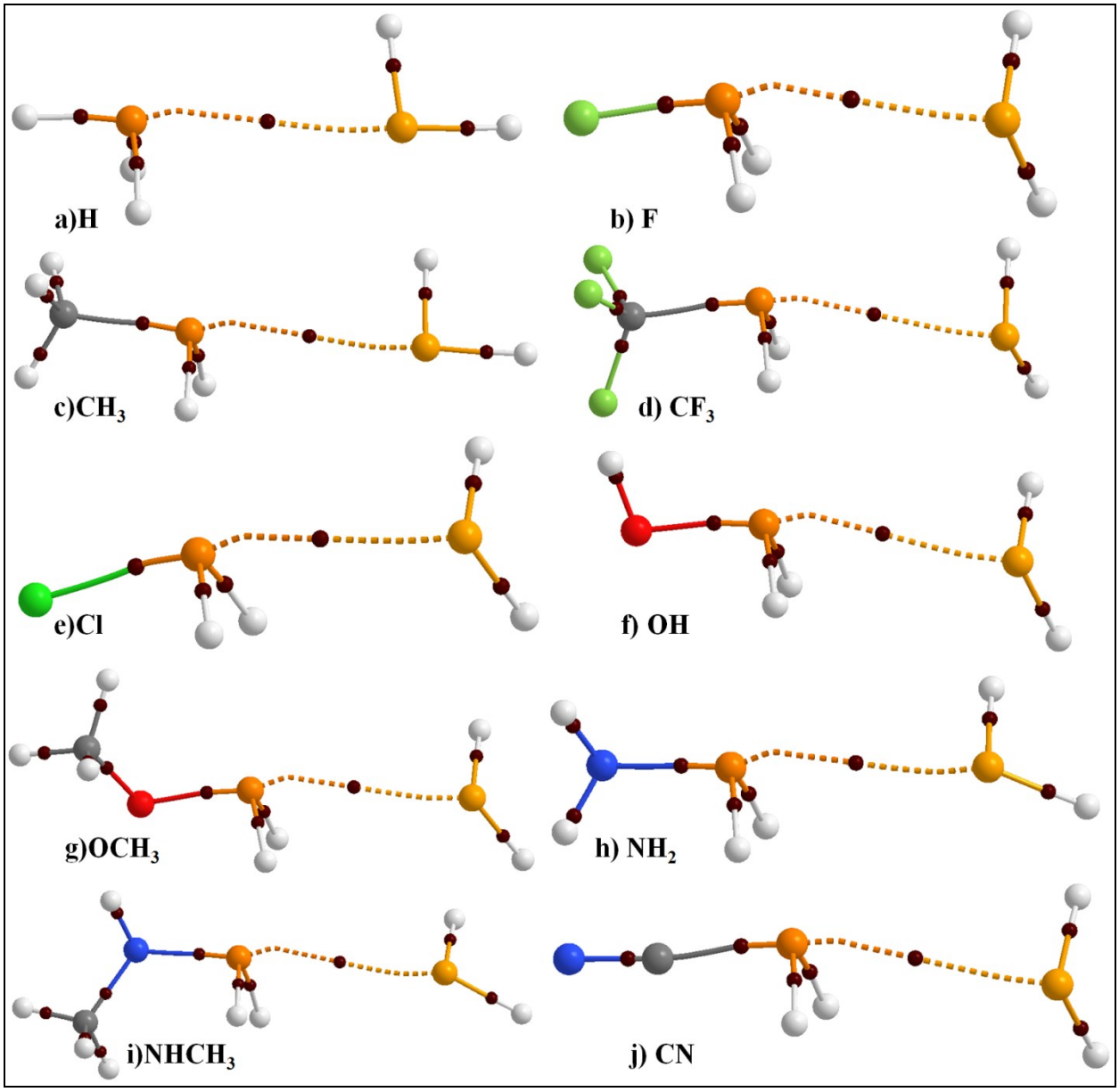


Figure S13: Molecular pairs representing bond critical point between Se and P in $XH_2P\ldots SeH_2$.

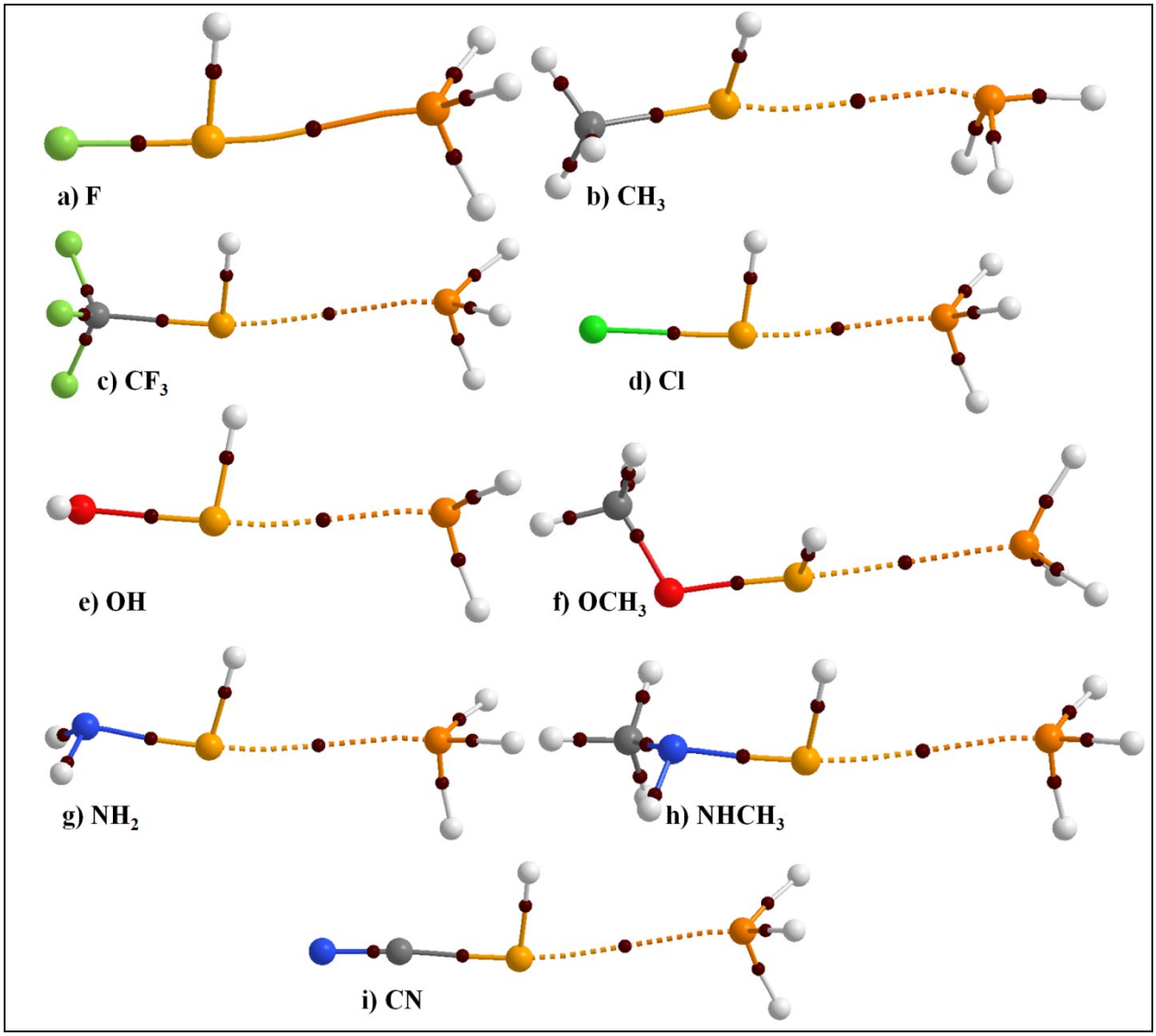


Figure S14: Molecular pairs representing bond critical point between Se and P in $H_3P\ldots SeHX$.

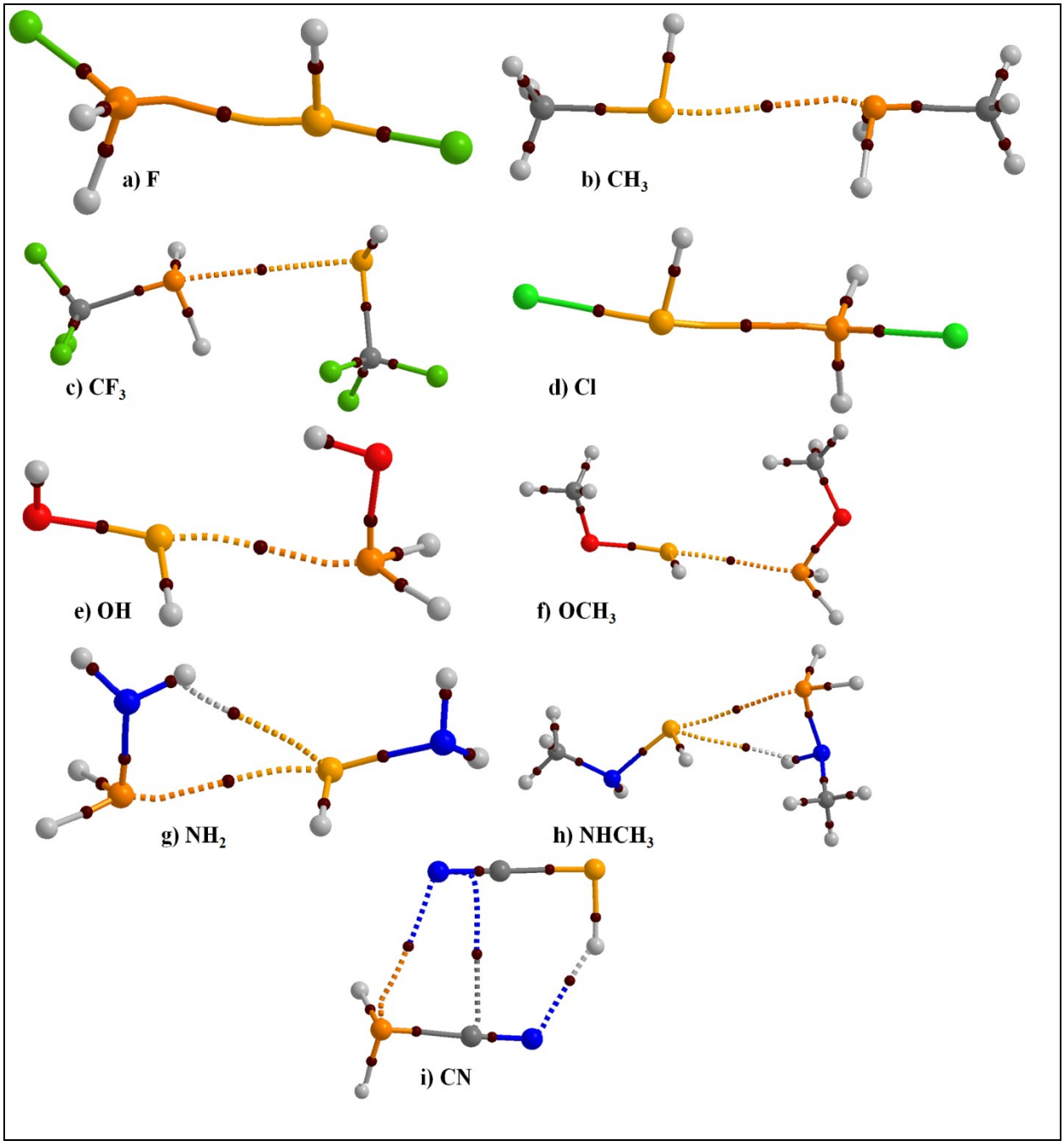


Figure S15: Molecular pairs representing bond critical point between Se and P in $XH_2P\ldots SeHX$. (No Se…P bcp was observed in case of X=-CN)

Table S1: Energies obtained from energy decomposition analysis for $XH_2P\ldots SeH_2$ interactions. Values shown in parenthesis are the percentage contribution towards stabilization. All energy values are reported in kcal/mol.

X	$E_{Electrostatic}$	$E_{Exchange}$	$E_{Repulsion}$	$E_{Polarization}$	$E_{Dispersion}$	E_{Total}
H	-2.04(21.38)	-5.07(53.14)	8.34	-0.59(6.18)	-1.84(19.28)	-1.20
F	-7.39(27.44)	-15.02(52.24)	25.68	-3.20(11.13)	-3.15(10.95)	-3.07
CH_3	-2.56(22.01)	-6.20(53.31)	10.24	-0.74(6.36)	-2.13(18.31)	-1.39
CF_3	-3.71(26.05)	-7.46(52.38)	12.46	-1.15(8.07)	-1.92(13.48)	-1.78
Cl	-6.43(24.98)	-13.52(52.52)	22.95	-2.70(10.48)	-3.09(12.00)	-2.78
OH	-4.80(24.18)	-10.71(53.95)	17.83	-1.67(8.41)	-2.67(13.45)	-2.02
OCH_3	-4.96(23.94)	-11.19(54.03)	18.66	-1.73(8.35)	-2.83(13.66)	-2.05
NH_2	-3.19(22.72)	-7.57(53.91)	12.51	-0.96(6.83)	-2.32(16.52)	-1.52
$NHCH_3$	-3.14(22.53)	-7.62(54.00)	12.60	-0.96(6.80)	-2.39(16.93)	-1.51
CN	-4.14(27.05)	-7.81(51.04)	13.13	-1.31(8.56)	-2.04(13.33)	-2.16

Table S2: Energies obtained from energy decomposition analysis for $H_3P\ldots SeHX$ interactions. Values shown in parenthesis are the percentage contribution towards stabilization. All energy values are reported in kcal/mol.

X	$E_{Electrostatic}$	$E_{Exchange}$	$E_{Repulsion}$	$E_{Polarization}$	$E_{Dispersion}$	E_{Total}
F	-26.98(27.94)	-47.18(48.86)	89.25	-16.98(17.58)	-5.41	-7.23(5.60)
CH_3	-2.23(20.01)	-6.02(54.04)	9.83	-0.69(6.19)	-2.20	-1.29(19.74)
CF_3	-4.31(27.96)	-7.84(50.87)	13.33	-1.37(8.89)	-1.89	-2.08(12.26)
Cl	-15.31(26.79)	-28.85(50.49)	52.24	-8.49(14.85)	-4.49	-4.91(7.85)
OH	-9.57(26.64)	-18.61(51.82)	32.56	-4.23(11.77)	-3.50	-3.35(9.74)
OCH_3	-9.11(26.20)	-18.14(52.17)	31.61	-3.97(11.41)	-3.55	-3.17(10.20)
NH_2	-4.59(24.08)	-10.23(53.67)	17.14	-1.56(8.18)	-2.68	-1.92(14.06)
$NHCH_3$	-4.34(23.38)	-10.00(53.87)	16.73	-1.48(7.97)	-2.74	-1.83(14.76)
CN	-5.54(30.15)	-8.97(48.82)	15.55	-1.84(10.01)	-2.02	-2.81(10.99)

Table S3: Energies obtained from energy decomposition analysis for $XH_2P\ldots SeHX$ interactions. Values shown in parenthesis are the percentage contribution towards stabilization. All energy values are reported in kcal/mol.

X	$E_{Electrostatic}$	$E_{Exchange}$	$E_{Repulsion}$	$E_{Polarization}$	$E_{Dispersion}$	E_{Total}
F	-51.11(27.55)	-87.91(47.39)	177.36	-36.63(19.74)	-9.84(5.30)	-8.13
CH_3	-2.60(19.80)	-7.16(54.53)	11.74	-0.84(6.39)	-2.53(19.26)	-1.39
CF_3	-2.55(18.91)	-7.14(52.69)	11.98	-0.94(6.97)	-2.85(21.14)	-1.50
Cl	-16.96(24.55)	-34.95(50.59)	65.10	-10.99(15.90)	-6.18(8.94)	-3.98
OH	-13.90(27.43)	-25.84(50.99)	46.10	-6.02(11.88)	-4.91(9.69)	-4.57
OCH_3	-14.97(26.69)	-29.16(52.00)	51.87	-6.56(11.69)	-5.38(9.59)	-4.21
NH_2	-7.08(25.40)	-14.58(52.31)	24.78	-2.29(8.21)	-3.92(14.06)	-3.08

$NHCH_3$	-6.76(23.45)	-15.17(52.63)	25.52	-2.17(7.52)	-4.72(16.37)	-3.31
CN	-11.08(28.07)	-18.58(47.07)	31.78	-4.64(11.75	-5.17(13.09)	-7.69

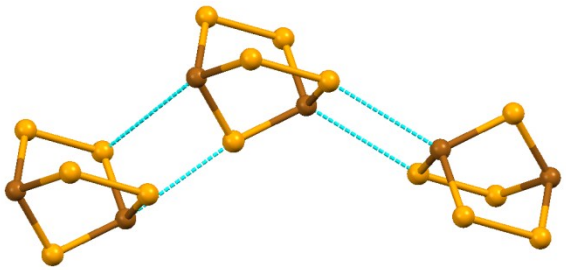
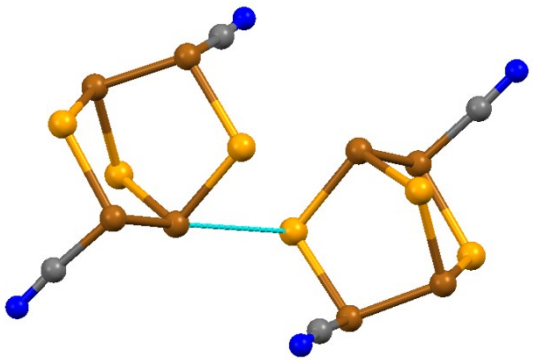
Table S4: Topological parameters and E(2) energies for hydrogen bonds observed in some $XH_2P\ldots SeHX$ complexes.

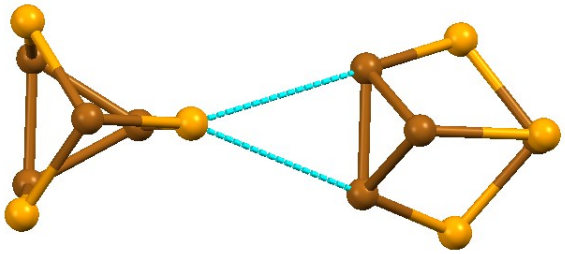
X	**Interaction**	**Bond Distance (Å)**	**Angle(°)**	**BPL(Å)**	**ρ (e/Å^3)**	**$\nabla^2\rho$(e/Å^5)**	**$\lvert V_b\rvert/G_b$**	**E(2) (kcal/mol)**
OH	O-H...Se	2.88	145		-	-	-	1.95
NH_2	N-H...Se	3.00	122	3.06	0.055	0.577	0.872	1.54
$NHCH_3$	N-H...Se	3.00	122	3.08	0.062	0.589	0.865	2.19

Table S5: Topological parameters and E(2) energies for $(CN)H_2P/HSe(CN)$ complex.

Interaction	**Bond Distance (Å)**	**Angle(°)**	**BPL(Å)**	**ρ (e/Å^3)**	**$\nabla^2\rho$(e/Å^5)**	**$\lvert V_b\rvert/G_b$**	**E(2) (kcal/mol)**
Se-H...N	2.16	144	2.18	0.126	1.251	0.946	4.57
H-P...N	3.23	151	3.33	0.054	0.656	0.810	-
C...C	3.22	-	-	-	-	-	-
C...N	3.23	-	3.79	0.050	0.585	0.752	-

Table S6: Crystal structure of the molecules retrieved from CSD containing P…Se contact

 **HEBTIR**	 **REQQIN**



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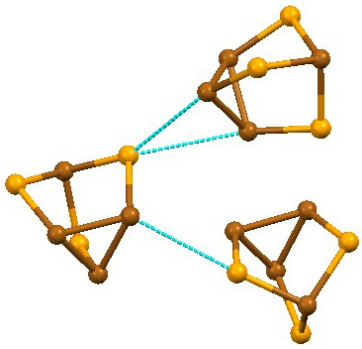

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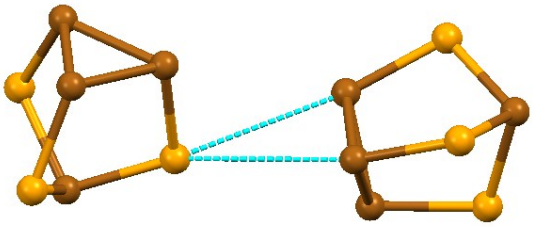

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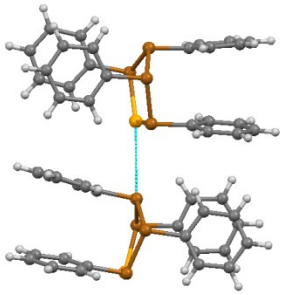

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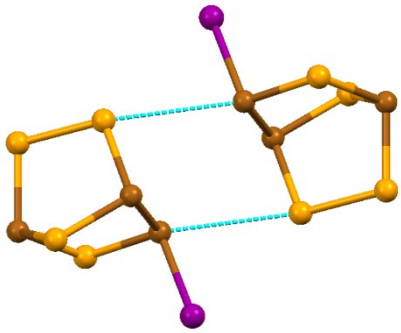

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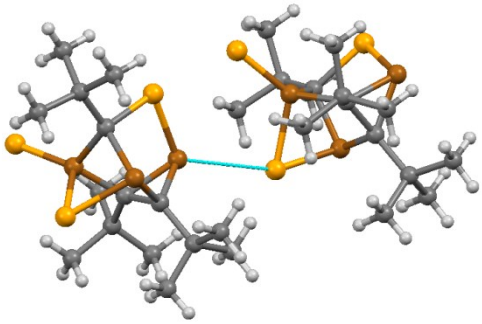

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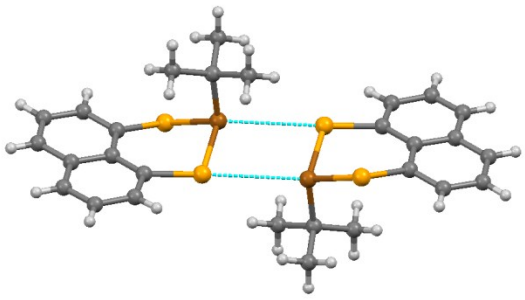

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