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

Noncovalent Interaction with Inverted Carbon: A Carbo-hydrogen Bond or a New Type of Hydrogen Bond?

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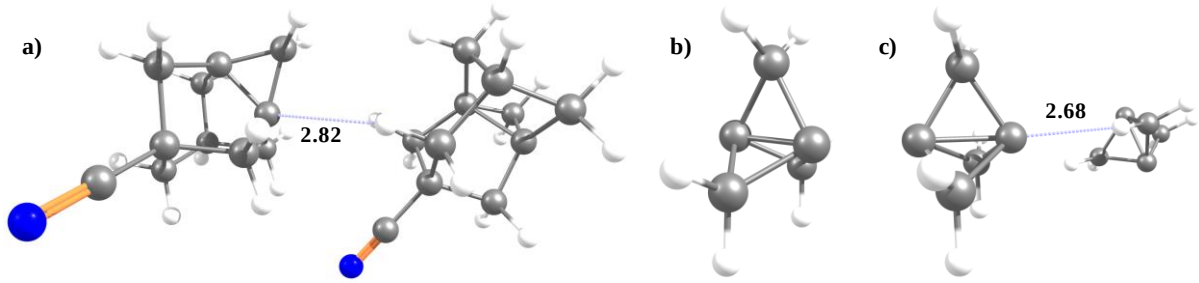

Fig-S1. a) Fully optimized structure of 5-cyano-1,3-dehydroademantane, b) [1.1.1]propellane (PPL), c) [1.1.1]propellane dimer (PPL•••PPL) at B97-D3/aug-cc-pVTZ level of theory. The C^{i}•••H distances mentioned in a) and c) are in Å.

Tab-S1. Comparison of the crystal structure data of didehydroademantane at different level of theory

Bonds	RMSD values at b97-d3/ aug-cc-pVDZ (Å)	RMSD values at b97-d3/ def2-TZVPP (Å)	RMSD values at b97-d3/ aug-cc-PVTZ (Å)
C-C	0.01606	0.01347	0.01346
C-X (X=H,N)	0.10181	0.09529	0.09496

Tab-S2. Dispersion contribution in interaction energy by DFT method

System	$\Delta E_{BSSE/wD}$ (kJ/mol)	$\Delta E_{BSSE/woD}$ (kJ/mol)	E(Disp) (kJ/mol)	%Disp
PPL-NH_3	-7.64	-2.88	-4.77	62
PPL-PH_3	-3.92	0.86	-4.78	122
PPL-AsH_3	-3.57	1.24	-4.81	135
PPL-H_2O	-15.16	-9.04	-6.12	40
PPL-H_2S	-10.51	-3.43	-7.08	67
PPL-H_2Se	-9.74	-2.16	-7.59	78
PPL-HF	-31.27	-24.26	-7.01	22

PPL-HCl	-23.84	-14.41	-9.43	40
PPL-HBr	-24.22	-12.72	-11.50	47
CH_4-H_2O	-5.15	0.43	-5.57	108
CH_3CN-H_2O	-7.99	-4.21	-3.79	47
H_2O-H_2O	-19.44	-14.25	-5.19	27
C_3H_6-H_2O	-11.45	-2.63	-8.83	77
Benzene-H_2O	-14.44	-1.82	-12.63	87
LiH-C_2H_2	-16.30	-13.60	-2.70	17

Tab-S3. Details of donor-acceptor NBO and interaction energies for the PPL-HX complexes. The values in parenthesis denote the percentage of back donation. For the numbering, refer to the optimized Cartesian coordinates and atom numbering of the complexes.

System	Front Donation		Back Donation	
	Interaction	ΔE^2 (kJ/mol)	Interaction	ΔE^2 (kJ/mol)
PPL-NH_3	σ(C1-C2) $\rightarrow$ σ*(H12-N13)	1.72	σ (H12-N13) $\rightarrow$ σ*(C1-C2)	1.34 (44)
	σ (C2-C3) $\rightarrow$ σ*(H12-N13)	0.50	σ (N13-H14) $\rightarrow$$\sigma$*(C1-C2)	0.42
	σ (C2-C4) $\rightarrow$ σ*(H12-N13)	0.50	σ (N13-H15) $\rightarrow$ σ*(C1-C2)	0.42
	σ (C2-C5) $\rightarrow$ σ*(H12-N13)	0.50	Lp1(N13) $\rightarrow$ σ*(C1-C2)	0.67
	Total	3.22	Total	2.85 (47)
PPL-PH_3	σ (C1-C2) $\rightarrow$ σ*(H12-P13)	1.42	σ (H12-P13) $\rightarrow$ σ*(C1-C2)	0.84 (41)
	σ (C1-C4) $\rightarrow$ σ*(H12-P13)	0.21	Lp1(P13) $\rightarrow$ σ*(C1-C2)	1.00
	σ (C2-C3) $\rightarrow$ σ*(H12-P13)	0.33		
	σ (C2-C4) $\rightarrow$ σ*(H12-P13)	0.33		
	σ (C2-C5) $\rightarrow$ σ*(H12-P13)	0.33		
	Total	2.62	Total	1.84 (41)
PPL-AsH_3	σ (C1-C2) $\rightarrow$ σ*(H12-As13)	1.42	σ (H12-As13) $\rightarrow$ σ*(C1-C2)	0.67 (32)
	σ (C2-C3) $\rightarrow$ σ*(H12-As13)	0.33	σ (As13-H14) $\rightarrow$ σ*(C1-C2)	0.21
	σ (C2-C4) $\rightarrow$ σ*(H12-As13)	0.29	σ (As13-H15) $\rightarrow$ σ*(C1-C2)	0.21
	σ (C2-C5) $\rightarrow$ σ*(H12-As13)	0.38	Lp1(As13) $\rightarrow$ σ*(C1-C2)	1.00
	Total	2.42	Total	2.09 (46)
PPL-H_2O	σ (C1-C2) $\rightarrow$ σ*(H12-O13)	7.03	σ (H12-O13) $\rightarrow$ σ*(C1-C2)	4.27 (38)
	σ (C1-C3) $\rightarrow$ σ*(H12-O13)	1.09	σ (H12-O13) $\rightarrow$ σ*(C1-C3)	0.25
	σ (C1-C4) $\rightarrow$ σ*(H12-O13)	1.09	σ (H12-O13) $\rightarrow$ σ*(C1-C4)	0.29
	σ (C1-C5) $\rightarrow$ σ*(H12-O13)	1.09	σ (H12-O13) $\rightarrow$ σ*(C1-C5)	0.29
	σ (C2-C3) $\rightarrow$ σ*(H12-O13)	1.46	σ (O13-H14) $\rightarrow$ σ*(C1-C2)	0.63
	σ (C2-C4) $\rightarrow$ σ*(H12-O13)	1.42	Lp1(O13) $\rightarrow$ σ*(C1-C2)	1.80
	σ (C2-C5) $\rightarrow$ σ*(H12-O13)	1.42		
	Total	14.60	Total	7.53 (34)
PPL-H_2S	σ (C1-C2) $\rightarrow$ σ*(H12-S13)	6.32	σ (H12-S13) $\rightarrow$ σ*(C1-C2)	3.81 (38)
	σ (C1-C3) $\rightarrow$ σ*(H12-S13)	1.46	σ (H12-S13) $\rightarrow$ σ*(C1-C3)	0.33
	σ (C1-C4) $\rightarrow$ σ*(H12-S13)	1.51	σ (H12-S13) $\rightarrow$ σ*(C1-C4)	0.38
	σ (C1-C5) $\rightarrow$ σ*(H12-S13)	1.51	σ (H12-S13) $\rightarrow$ σ*(C1-C5)	0.38
	σ (C2-C3) $\rightarrow$ σ*(H12-S13)	0.96	σ (S13-H14) $\rightarrow$ σ*(C1-C2)	0.46
	σ (C2-C4) $\rightarrow$ σ*(H12-S13)	0.92	Lp1(S13) $\rightarrow$ σ*(C1-C2)	2.68
	σ (C2-C5) $\rightarrow$ σ*(H12-S13)	0.92		
	Total	13.60	Total	8.04 (37)
PPL-H_2Se	σ (C1-C2) $\rightarrow$ σ*(H12-Se13)	7.36	σ (H12-Se13) $\rightarrow$ σ*(C1-C2)	4.31 (37)
	σ (C1-C3) $\rightarrow$ σ*(H12-Se13)	1.92	σ (H12-Se13) $\rightarrow$ σ*(C1-C3)	0.38
	σ (C1-C4) $\rightarrow$ σ*(H12-Se13)	1.97	σ (H12-Se13) $\rightarrow$ σ*(C1-C4)	0.38

	σ (C1-C5) → σ*(H12-Se13)	1.97	σ (H12-Se13) → σ*(C1-C5)	0.38
	σ (C2-C3) → σ*(H12-Se13)	1.09	σ (Se13-H14) → σ*(C1-C2)	0.50
	σ (C2-C4) → σ*(H12-Se13)	1.09	Lp1(Se13) → σ*(C1-C2)	3.22
	σ (C2-C5) → σ*(H12-Se13)	1.09		
	Total	16.49	Total	9.17 (36)
PPL-HF	σ (C1-C2) → σ*(H12-F13)	23.77	σ (H12-F13) → σ*(C1-C2)	8.66 (27)
	σ (C1-C3) → σ*(H12-F13)	7.20	σ (H12-F13) → σ*(C1-C3)	0.46
	σ (C1-C4) → σ*(H12-F13)	7.15	σ (H12-F13) → σ*(C1-C4)	0.46
	σ (C1-C5) → σ*(H12-F13)	7.15	σ (H12-F13) → σ*(C1-C5)	0.46
	σ (C2-C3) → σ*(H12-F13)	3.14	Lp3(F13) → σ*(C1-C2)	2.18
	σ (C2-C4) → σ*(H12-F13)	3.14		
	σ (C2-C5) → σ*(H12-F13)	3.14		
	Total	54.69	Total	12.22 (18)
PPL-HCl	σ (C1-C2) → σ*(H12-Cl13)	25.86	σ (H12-Cl13) → σ*(C1-C2)	12.47 (33)
	σ (C1-C3) → σ*(H12-Cl13)	10.50	σ (H12-Cl13) → σ*(C1-C3)	0.67
	σ (C1-C4) → σ*(H12-Cl13)	10.42	σ (H12-Cl13) → σ*(C1-C4)	0.67
	σ (C1-C5) → σ*(H12-Cl13)	10.42	σ (H12-Cl13) → σ*(C1-C5)	0.67
	σ (C2-C3) → σ*(H12-Cl13)	2.47	Lp3(Cl13) → σ*(C1-C2)	4.85
	σ (C2-C4) → σ*(H12-Cl13)	2.51		
	σ (C2-C5) → σ*(H12-Cl13)	2.51		
	Total	64.69	Total	19.33 (23)
PPL-HBr	σ (C1-C2) → σ*(H12-Br13)	43.26	σ (H12-Br13) → σ*(C1-C2)	25.23 (37)
	σ (C1-C3) → σ*(H12-Br13)	19.96	σ (H12-Br13) → σ*(C1-C3)	1.09
	σ (C1-C4) → σ*(H12-Br13)	19.92	σ (H12-Br13) → σ*(C1-C4)	1.09
	σ (C1-C5) → σ*(H12-Br13)	19.92	σ (H12-Br13) → σ*(C1-C5)	1.09
	σ (C2-C3) → σ*(H12-Br13)	3.35	Lp3(Br13) → σ*(C1-C2)	6.49
	σ (C2-C4) → σ*(H12-Br13)	3.35		
	σ (C2-C5) → σ*(H12-Br13)	3.35		
	Total	113.11	Total	34.99 (24)

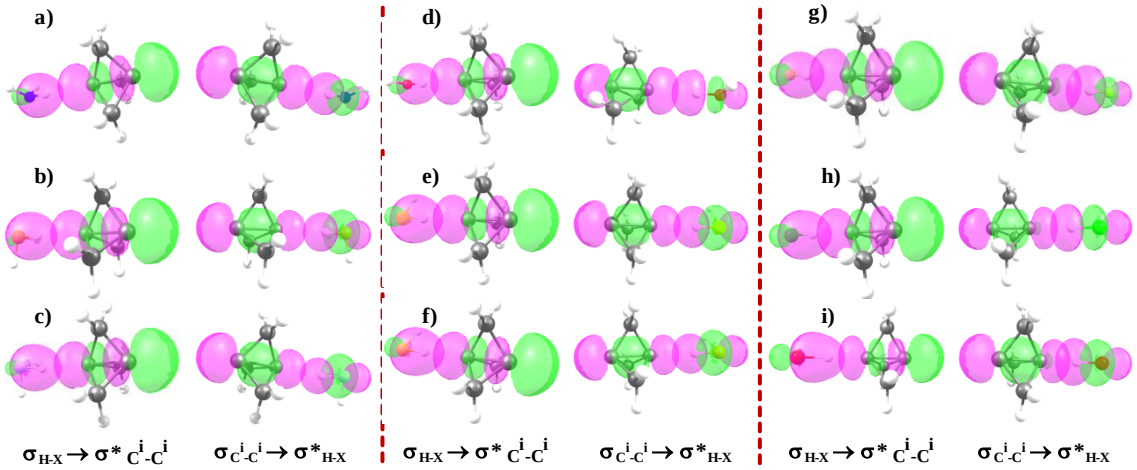

Fig-S2. Overlap of $\sigma_{C^i-C^i}$ orbital with σ^*_{X-H} orbital and overlap of σ_{X-H} orbital with $\sigma^*_{C^i-C^i}$ orbital for **a.** PPL•••NH_3, **b**. PPL•••PH_3, **c.** PPL•••AsH_3**, d.** PPL•••H_2O, e. PPL•••H_2S, **f.** PPL•••H_2Se, **g.** PPL•••HF, **h.** PPL•••HCl, **i.** PPL•••HBr complexes.

Tab-S4: Topological parameters: electron density (ρ), laplacian of electron density ($\nabla^2\rho$), ellipticity (ε) and $-G_c/V_c$ at bond critical point (BCP). All are in atomic units.

System	ρ	$\nabla^2\rho$	ε	$-G_c/V_c$
PPL-NH_3	0.009	0.028	0.021	1.179
PPL-PH_3	0.008	0.021	0.003	1.226
PPL-AsH_3	0.007	0.019	0.004	1.227
PPL-H_2O	0.020	0.047	0.009	0.915
PPL-H_2S	0.017	0.040	0.006	1.017
PPL-H_2Se	0.017	0.041	0.005	1.005
PPL-HF	0.037	0.050	0.000	0.704
PPL-HCl	0.036	0.050	0.000	0.725
PPL-HBr	0.049	0.039	0.000	0.622

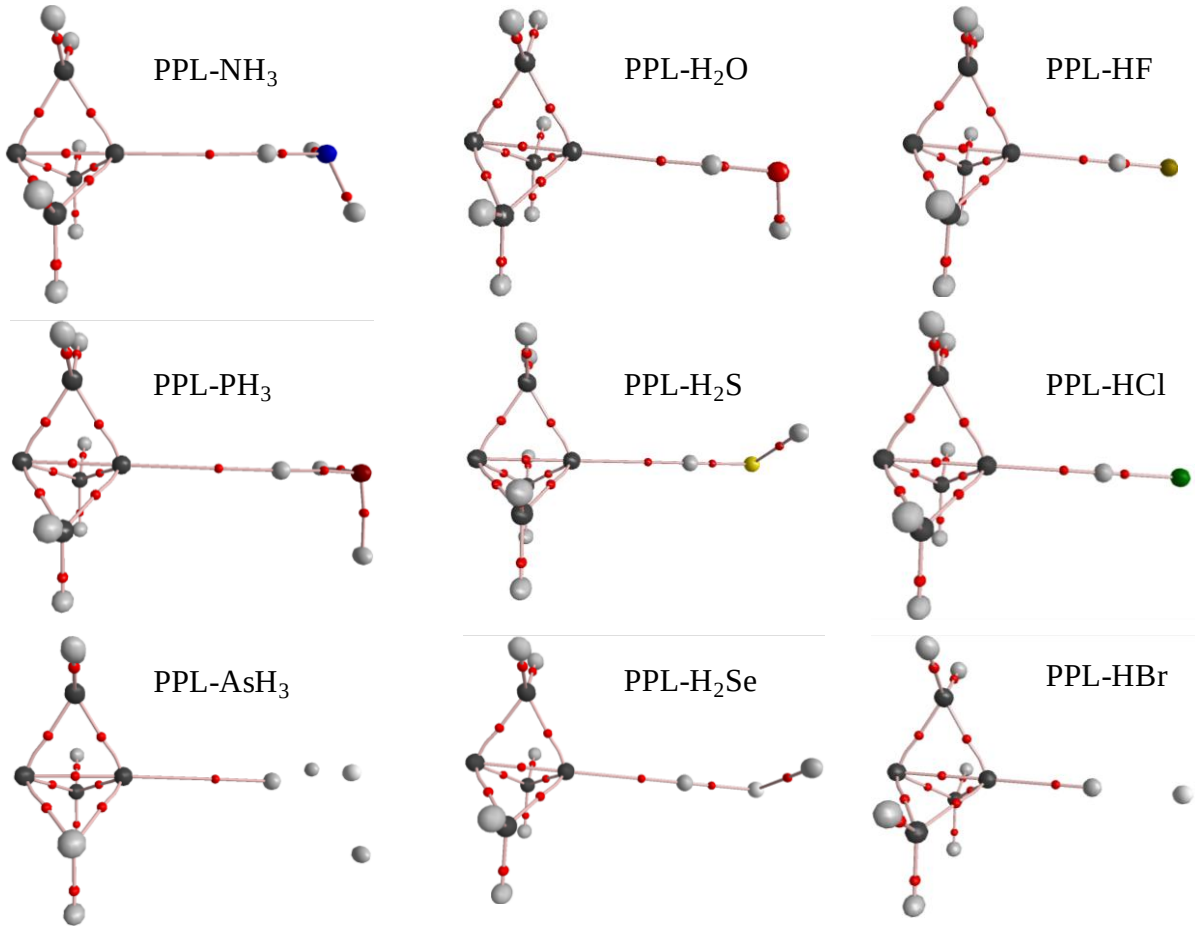

Fig-S3. Molecular graphs for the PPL•••HX complexes.

Tab-S5a. Change in bonded hydrogen energy (ΔE_H), volume (ΔV_H), population (ΔN_H), dipolar polarisation (ΔM_H), and mutual penetration (Δr_H). All are in atomic units.

System	ΔE_H	ΔV_H	ΔN_H	ΔM_H	Δr_H
PPL-NH_3	-0.018	-2.230	0.016	-0.021	0.536

PPL-PH_3	-0.001	-4.075	-0.026	-0.006	0.504
PPL-AsH_3	-0.028	-1.251	0.038	0.051	0.538
PPL-H_2O	0.002	-6.072	0.001	-0.022	0.741
PPL-H_2S	0.014	-7.822	-0.046	-0.005	0.757
PPL-H_2Se	0.007	-8.293	-0.032	-0.012	0.854
PPL-HF	-0.051	-3.795	0.081	-0.015	0.881
PPL-HCl	0.024	-11.332	-0.034	-0.036	1.017
PPL-HBr	0.028	-16.358	-0.053	-0.064	1.160

Tab-S5b. Change in bonded inverted carbon energy (ΔE_C^i), volume (ΔV_C^i), population (ΔN_C^i), dipolar polarisation (ΔM_C^i), and mutual penetration (Δr_C^j). All are in atomic units.

System	ΔE_C^i	ΔV_C^i	ΔN_C^i	ΔM_C^i	Δr_C^i
PPL-NH_3	0.016	-7.924	-0.118	-0.072	0.708
PPL-PH_3	0.079	-6.708	-0.088	-0.114	0.600
PPL-AsH_3	0.116	-6.622	-0.111	-0.095	0.578
PPL-H_2O	-0.068	-12.281	-0.068	-0.110	1.063
PPL-H_2S	-0.022	-11.480	-0.093	-0.108	0.968
PPL-H_2Se	-0.051	-11.839	-0.075	-0.126	0.993
PPL-HF	-0.065	-15.567	-0.034	-0.098	1.321
PPL-HCl	0.022	-16.490	-0.041	-0.130	1.324
PPL-HBr	0.054	-20.171	-0.045	-0.171	1.472

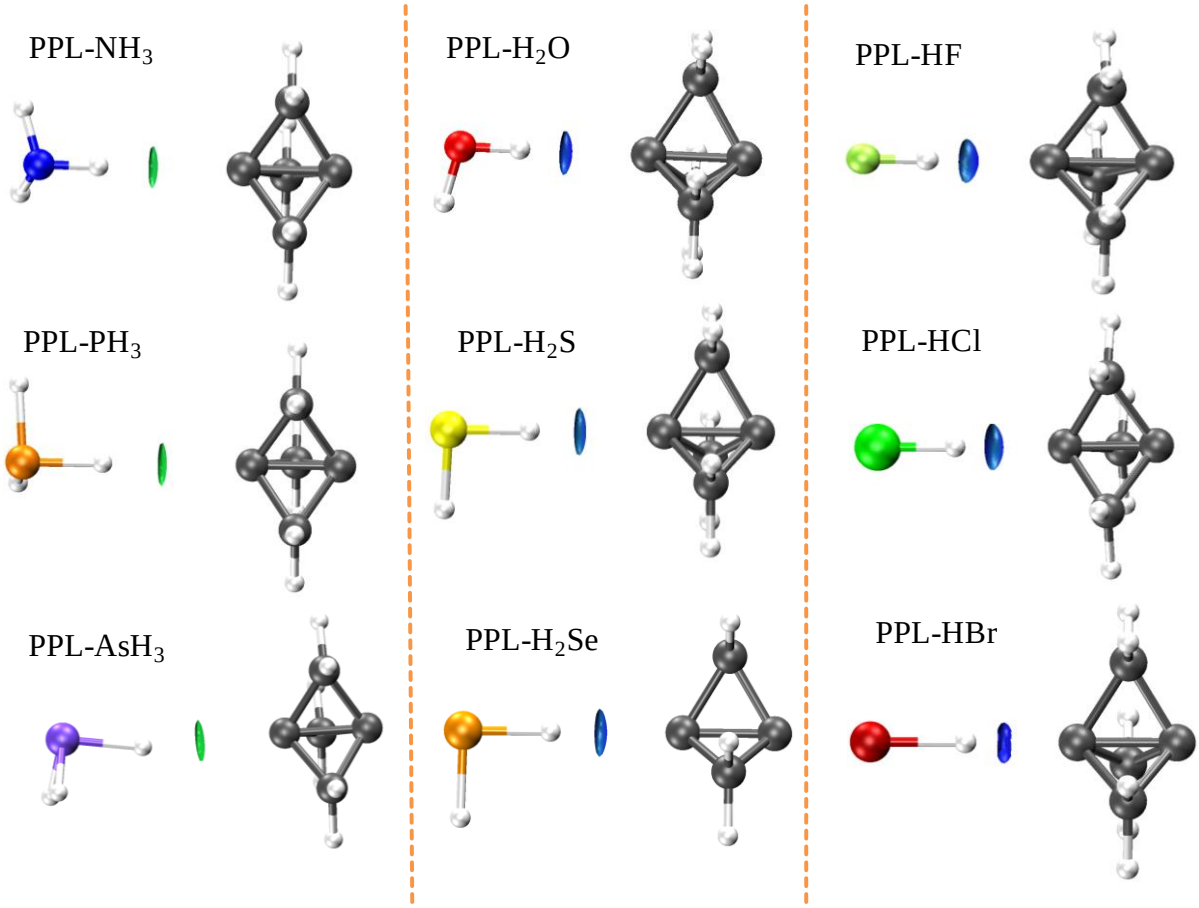

Fig-S4a. RDG isosurfaces in real 3D space for PPL•••HX complexes.

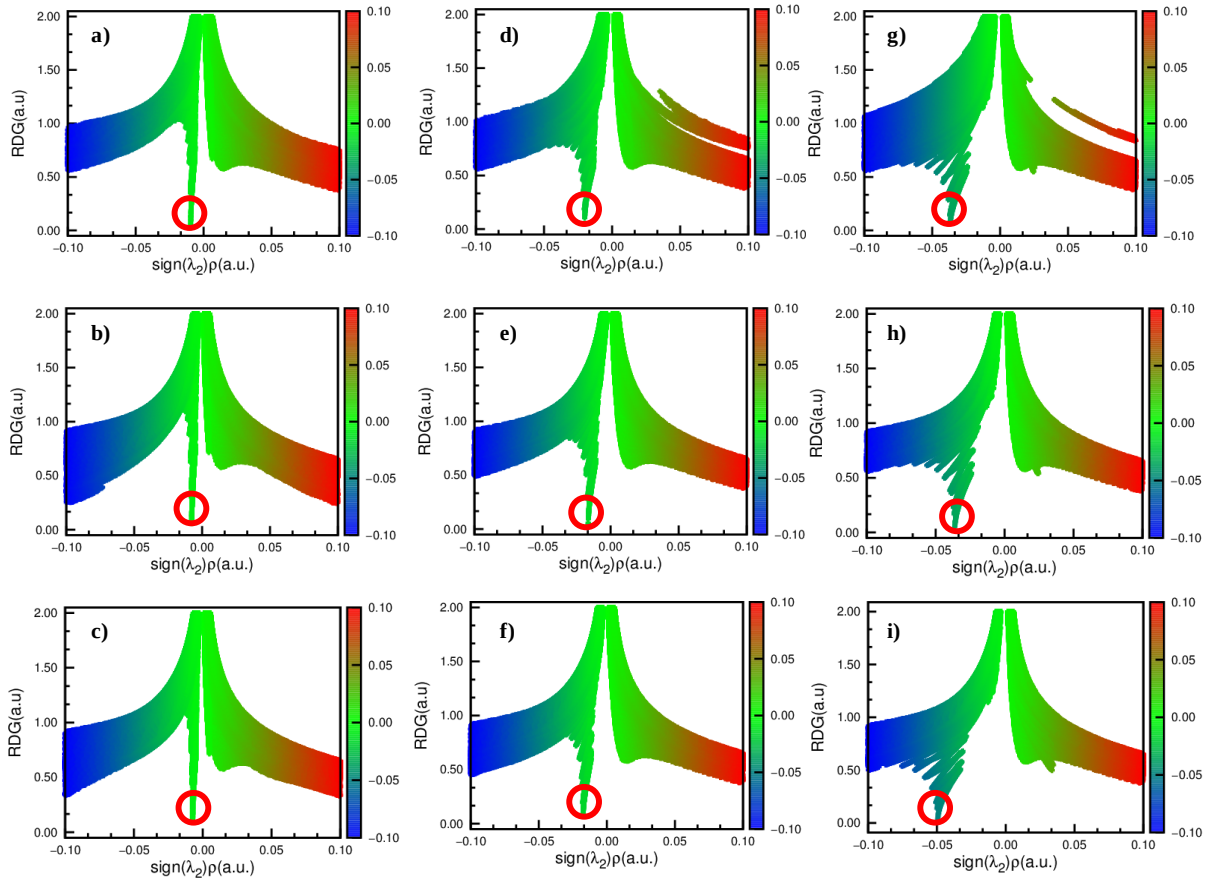

Fig-S4b. RDG versus sign(λ_2)ρ plots for **a.** PPL•••NH_3, **b**. PPL•••PH_3, **c.** PPL•••AsH_3**, d.** PPL•••H_2O, e. PPL•••H_2S, **f.** PPL•••H_2Se, **g.** PPL•••HF, **h.** PPL•••HCl, **i.** PPL•••HBr complexes. BCPs are indicated by the red circles.

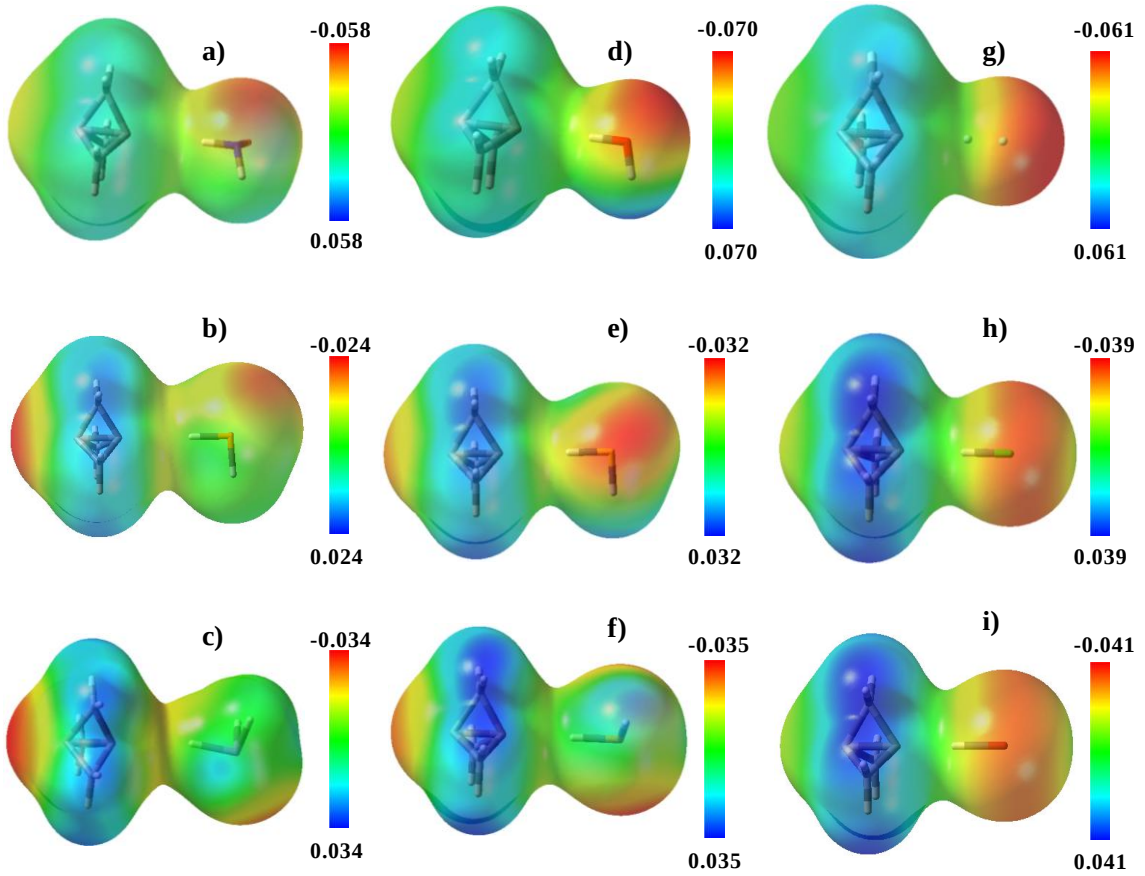

Fig-S5. MESP isosurfaces of **a.** PPL•••NH_3, **b**. PPL•••PH_3, **c.** PPL•••AsH_3, **d.** PPL•••H_2O, e. PPL•••H_2S, **f.** PPL•••H_2Se, **g.** PPL•••HF, **h.** PPL•••HCl, **i.** PPL•••HBr complexes.

Tab-S6a. LMOEDA analyses of PPL···HX complexes and complexes possessing different type of non-covalent interactions.

System	E(Electrostatic) (kJ/mol)	E(Exchange) (kJ/mol)[a]	E(Repulsion) (kJ/mol)	E(Polarisation) (kJ/mol)[b]	E(Dispersion) (kJ/mol)	E(Total) (kJ/mol)
PPL-NH_3	-9.83	-16.99	28.24	-3.14	-7.20	-8.95
PPL-PH_3	-4.98	-17.45	27.74	-2.51	-8.54	-5.73
PPL-AsH_3	-4.35	-17.61	27.82	-2.55	-8.87	-5.56
PPL-H_2O	-23.89	-38.33	67.36	-11.21	-10.29	-16.36
PPL-H_2S	-17.66	-41.38	69.91	-9.37	-14.43	-12.89
PPL-H_2Se	-18.03	-48.12	80.79	-10.92	-16.19	-12.47
PPL-HF	-43.89	-65.02	121.38	-33.18	-9.75	-30.46
PPL-HCl	-42.47	-91.34	164.43	-35.77	-21.13	-26.32
PPL-HBr	-56.19	-145.23	263.26	-60.25	-28.33	-26.78
CH4-H_2O	-2.55	-6.32	10.59	-1.46	-3.85	-3.60
CH_3CN-H_2O	-9.58	-6.23	10.25	-1.17	-2.01	-8.74
H_2O-H_2O	-31.34	-30.33	54.43	-8.08	-4.39	-19.75

C_3H_6-H_2O	-11.21	-17.53	30.00	-4.14	-7.99	-10.88
Benzene-H_2O	-12.59	-19.50	32.47	-4.27	-10.25	-14.14
LiH-C_2H_2	-26.74	-31.55	54.48	-9.54	-4.77	-18.07

Tab-S6b. SAPT(2) analyses of PPL···HX complexes and complexes possessing different type of non-covalent interactions.

System	E(Electrostatic) (kJ/mol)	E(Exchange) (kJ/mol)[a]	E(Induction) (kJ/mol)	E(Dispersion) (kJ/mol)[b]	E(Charge Transfer) (kJ/mol)	E(Total) (kJ/mol)
PPL-NH_3	-9.35	11.68	-3.02	-7.52	-0.57	-8.21
PPL-PH_3	-5.15	10.41	-2.45	-8.19	-0.33	-5.38
PPL-AsH_3	-4.63	10.31	-2.53	-8.45	-0.33	-5.30
PPL-H_2O	-22.53	30.53	-10.67	-12.12	-2.51	-14.79
PPL-H_2S	-17.18	28.74	-9.05	-14.79	-1.56	-12.28
PPL-H_2Se	-17.67	32.99	-10.58	-16.77	-1.82	-12.04
PPL-HF	-40.49	59.01	-31.15	-16.00	-7.19	-28.64
PPL-HCl	-40.23	72.85	-34.28	-25.21	-6.83	-26.87
PPL-HBr	-53.85	117.11	-56.98	-36.69	-12.31	-30.41
CH4-H_2O						
CH_3CN-H_2O	-8.89	4.70	-1.22	-3.30	-0.21	-8.70
H_2O-H_2O	-32.46	28.19	-8.30	-6.59	-2.59	-19.16
C_3H_6-H_2O	-11.96	14.24	-4.03	-7.73	-1.00	-9.49
Benzene-H_2O	-12.10	14.16	-3.95	-10.85	-0.98	-12.74
LiH-C_2H_2	-24.21	22.78	-8.91	-6.40	-0.96	-16.74

Coordinates of the optimized structures:

5-cyano-1,3-dehydroademantane (H-position optimized)

C	1.245765000	4.298110000	4.921706000
H	1.751354600	4.273759000	3.952438000
H	1.148473700	5.344035800	5.232857400
C	0.020239000	2.114773000	4.467970000
H	-0.959442200	1.627543900	4.528007500
H	0.334880200	2.082448800	3.418429400
C	1.968520000	3.715015000	7.413417000

H	1.845696800	4.753236700	7.723501500
H	2.689870200	3.161612300	8.014767400
C	-0.491166000	3.667008000	6.401982000
H	-0.597585800	4.706245700	6.733588100
H	-1.410848500	3.130802400	6.649913500
C	1.040374000	1.340582000	5.338859000
H	1.112722500	0.306503000	4.972219400
C	-0.142552000	3.609305000	4.893502000
C	0.661126000	1.463112000	6.822322000
H	-0.340574200	1.094048700	7.061843500
H	1.378833200	0.930892700	7.458501200
C	2.377856000	2.097018000	5.356561000
H	3.115488300	1.572704400	5.977033500
H	2.818725000	2.231401800	4.362746500
C	1.915325000	3.405012000	5.954146000
C	-1.113298000	4.279772000	4.009042000
N	-1.862878000	4.809253000	3.319057000
C	0.751404000	2.973881000	6.937968000
C	0.511885000	1.542190000	10.822041000
H	1.012997000	1.570785000	9.851108900
H	0.414818800	0.496058700	11.132399500
C	-0.713641000	3.725527000	10.368305000
H	-1.693800900	4.212852900	10.426872300
H	-0.395003300	3.754244300	9.321036700
C	1.234640000	2.125285000	13.313753000
H	1.110301600	1.086061400	13.619366200
H	1.953255300	2.676536500	13.920116900

C	-1.225046000	2.173292000	12.302317000
H	-1.333211900	1.134857400	12.634902300
H	-2.146898600	2.709054000	12.544442400
C	0.306494000	4.499718000	11.239195000
H	0.378910000	5.533800600	10.871021700
C	-0.876432000	2.230995000	10.793838000
C	-0.072754000	4.377188000	12.722657000
H	-1.077004300	4.746994500	12.953497100
H	0.640801000	4.910050900	13.362133200
C	1.643976000	3.743282000	11.256896000
H	2.380998300	4.267179400	11.878315000
H	2.082174800	3.611474200	10.263676600
C	1.181445000	2.435288000	11.854482000
C	-1.847178000	1.560528000	9.909377000
N	-2.596757000	1.031047000	9.219392000
C	0.017525000	2.866419000	12.838304000

5-cyano-1,3-dehydroademantane (fully optimized)

C	1.164346500	4.230481700	4.989539000
H	1.603463500	4.238850900	3.988297100
H	1.080765600	5.265968200	5.337525200
C	-0.078965600	2.036955200	4.544410400
H	-1.045438300	1.535434800	4.663909700
H	0.158620600	2.044958800	3.474531100
C	2.077980600	3.592647900	7.415479500
H	1.970065700	4.624000200	7.752414700
H	2.842202700	3.030971600	7.952600200

C	-0.461105900	3.540899700	6.575891300
H	-0.557266600	4.572075100	6.934777600
H	-1.348956400	2.984484400	6.882613800
C	1.020572000	1.239899700	5.319487800
H	1.070179500	0.215865000	4.926560100
C	-0.233803900	3.531696100	5.030495500
C	0.743555900	1.335360500	6.841668300
H	-0.235165200	0.953352200	7.141575400
H	1.509935300	0.795372100	7.411469200
C	2.358999600	2.020973900	5.262279400
H	3.145995400	1.489252900	5.810350500
H	2.719564700	2.205079700	4.245070800
C	1.906773300	3.309353800	5.951244300
C	-1.267682000	4.224040400	4.266110200
N	-2.079731600	4.797325700	3.666298600
C	0.834550000	2.854611700	6.998687200
C	0.608348800	1.727504700	10.665491900
H	1.182974100	1.865783600	9.747244700
H	0.511922400	0.653542100	10.859088800
C	-0.629510800	3.939838900	10.323694600
H	-1.619650000	4.408515600	10.348358200
H	-0.226672100	4.068144500	9.315177000
C	1.128251300	2.051612300	13.267494000
H	1.007154400	0.983658600	13.447800700
H	1.783818300	2.549482700	13.981272700
C	-1.255661500	2.172121200	12.067372300
H	-1.369174700	1.102560100	12.275172500

H	-2.201531900	2.669326300	12.298576200
C	0.310777700	4.644864600	11.354019900
H	0.381240100	5.712892400	11.108223200
C	-0.804719800	2.392250800	10.586980500
C	-0.182676300	4.342147100	12.792221700
H	-1.209205900	4.670639800	12.983148200
H	0.468092300	4.815052500	13.537194600
C	1.669360100	3.899086200	11.399177800
H	2.348045600	4.365691200	12.123030700
H	2.178938300	3.858334200	10.431753700
C	1.166304000	2.523548700	11.840661500
C	-1.688571700	1.796874700	9.589908500
N	-2.376703000	1.306402000	8.793778800
C	-0.062763000	2.817713100	12.764886500

$CH_3OH•••H_2O$ (H-bonded system)

O	-3.078737200	1.659388600	-5.533507900
H	-2.689981400	2.526775800	-5.318001900
H	-2.347636400	1.145848200	-5.895328900
C	-2.980399600	4.380757400	-3.385402900
H	-2.299480500	3.835597700	-2.727309100
H	-3.092654900	5.407534200	-3.011308900
H	-3.956011200	3.876375100	-3.380315100
O	-2.382273300	4.361733100	-4.698239200
H	-2.942430100	4.877684500	-5.291083400

$H_2O•••CH_3OH$ (C-bonded system)

O	-2.048408600	1.392613900	-7.887268200
H	-2.608254000	0.878676900	-8.482156100
H	-1.390044200	1.795807800	-8.466227500
C	-2.023957000	3.110301600	-5.117944900
H	-2.859273600	3.491932800	-5.710023500
H	-1.099352300	3.238304000	-5.700783100
H	-2.184927300	2.037314700	-4.945926600
O	-1.999370000	3.863424100	-3.894845000
H	-1.306776300	3.496287500	-3.333460600

H_2O•••H_2O

O	0.331316500	1.941709300	-0.266708200
H	0.223243200	2.609998700	-0.955359100
H	-0.105188600	2.316341600	0.508959700
O	-1.595339600	-0.163433900	-1.119390400
H	-0.877656600	0.430731500	-0.840101700
H	-1.176629800	-1.027508200	-1.206292400

CH_4•••H_2O

C	-0.309480000	-0.132305700	3.580224200
H	-0.479063800	-0.238086000	4.655048500
H	-0.329946800	-1.122271900	3.115361400
H	0.665099800	0.336106000	3.415307900
H	-1.099062800	0.493368100	3.152749300
O	0.000329200	-0.000153400	-0.000095100
H	-0.000402900	0.000349700	0.965362500
H	-0.366973700	0.859374900	-0.239649600

H_2O•••CH_3CN

O	-2.024267600	1.539001500	-7.915708500
H	-2.607970100	0.866449700	-8.287908400
H	-1.347954800	1.667556300	-8.592310700
C	-2.051651100	3.144152100	-5.103153500
H	-2.864407100	3.509398100	-5.738135100
H	-1.107933300	3.288904400	-5.637534200
H	-2.192935100	2.070689300	-4.946683100
C	-2.032558400	3.853882600	-3.828131500
N	-2.013128500	4.417473000	-2.815044700

C_3H_6•••H_2O

C	0.684612700	-1.059084000	-0.135096000
C	-0.067174000	-1.232879400	1.172179400
C	1.431751000	-1.076933500	1.173623600
H	0.778856900	-1.920970300	-0.789064400
H	0.592716300	-0.109648300	-0.655257700
H	-0.477199700	-2.212670700	1.399524400
H	-0.668014300	-0.402206100	1.531156700
H	1.844795500	-0.140080200	1.535639100
H	2.032334100	-1.951905000	1.404516800
H	-1.735057300	-1.601867200	-0.605080500
O	-2.537877100	-1.910771300	-1.049106800
H	-2.862613600	-1.136298700	-1.523514100

Benzene•••H_2O

C	0.781143600	-0.612057900	-1.211452200
C	0.478029000	0.753136600	-1.211882700
C	0.327004800	1.436402500	0.000000000
C	0.478029000	0.753136600	1.211882700
C	0.781143600	-0.612057900	1.211452200
C	0.933044700	-1.294231500	0.000000000
H	0.897393800	-1.142635800	-2.152965000
H	0.355818100	1.282968300	-2.152864500
H	0.089161300	2.496964100	0.000000000
H	0.355818100	1.282968300	2.152864500
H	0.897393800	-1.142635800	2.152965000
H	1.170897900	-2.355066300	0.000000000
O	-2.786501900	-0.275241400	0.000000000
H	-2.627169600	-1.226508300	0.000000000
H	-1.897331400	0.106585200	0.000000000

LiH•••C_2H_2

Li	-0.723601500	0.000000000	-3.031740200
H	-0.723601500	0.000000000	-4.641561200
C	-0.723601500	0.000000000	-8.948816500
C	-0.723601500	0.000000000	-7.741532900
H	-0.723601500	0.000000000	-6.662998900
H	-0.723601500	0.000000000	-10.015261200

[1.1.1]propellane (PPL)

C	-0.001648900	0.000000000	-1.675864000
C	0.001579000	0.000000000	-3.245194100

C	-1.301199100	0.000000100	-2.463245500
C	0.651671300	-1.126467500	-2.459320900
C	0.651671300	1.126467500	-2.459320800
H	-1.884817400	0.917863600	-2.464474500
H	0.150757200	-2.092544300	-2.460493500
H	1.738413300	1.172256200	-2.457013500
H	-1.884817500	-0.917863500	-2.464474500
H	1.738413200	-1.172256300	-2.457013500
H	0.150757300	2.092544300	-2.460493500

PPL•••PPL

C	-0.387031200	1.555146100	-4.286172300
C	-1.158358400	2.523584900	-5.246483400
C	-1.868333400	1.363835700	-4.569788300
C	0.029055200	1.714080600	-5.739209700
C	-0.481388700	3.044169700	-3.991364400
H	-2.564273500	1.600765400	-3.768022400
H	-0.175438500	0.883036400	-6.410814600
H	0.422517200	3.636546600	-4.117395000
H	-2.152962300	0.518146700	-5.192188000
H	0.954375300	2.250328600	-5.938737200
H	-1.121746600	3.350008100	-3.166690700
H	0.970895700	-0.822708800	-0.822529500
C	0.889749900	0.246037800	-1.011210700
H	0.577515900	0.517815300	-2.017206300
C	1.897909900	1.150202100	-0.321386800
C	1.038075700	2.401861200	-0.368082400

H	0.733230900	2.759145400	-1.348742700
H	1.244085800	3.178505400	0.365865800
C	1.518700600	0.756553000	1.095922900
H	1.625093200	-0.291577100	1.368274300
H	1.745130100	1.463761400	1.891414700
C	0.398299200	1.117320500	0.134204700

PPL•••NH_3

C	0.285009300	0.094733400	0.023919300
C	1.847464700	-0.005126500	0.085200500
C	0.987973800	-1.255109000	0.054766900
C	1.067984300	0.697501300	1.181381400
C	1.155898400	0.691566600	-1.072217500
H	0.985735300	-1.838709800	-0.862880100
H	0.997058300	0.199072400	2.145862700
H	1.226209900	1.776018000	-1.118848800
H	0.914817600	-1.834949500	0.972059700
H	1.134702000	1.782283300	1.227206600
H	1.159965900	0.187783300	-2.036278400
H	-2.213812200	0.254121700	-0.077928600
N	-3.231283400	0.319145100	-0.106995700
H	-3.481566800	1.152337400	0.420917500
H	-3.585646100	-0.472258900	0.425601500

PPL•••PH_3

C	0.316334900	0.090490800	0.029395300
C	1.879807500	-0.018644600	-0.010996600

C	1.007838100	-1.262753200	0.008290600
C	1.172606600	0.682312400	1.136564000
C	1.115119700	0.688163300	-1.117218800
H	0.943116300	-1.843459600	-0.909379800
H	1.161566700	0.178759400	2.100769000
H	1.189023700	1.772679400	-1.162676700
H	0.990063300	-1.847796900	0.925362400
H	1.249029000	1.766566600	1.183949800
H	1.054434700	0.189739000	-2.082220700
H	-2.364939600	0.277864600	0.103828200
P	-3.789709000	0.377681200	0.141303300
H	-3.777454500	1.428407900	1.109974200
H	-3.922049700	-0.643774500	1.132087300

PPL•••AsH_3

C	0.438044000	0.089180900	-0.002033300
C	1.999785500	-0.015485000	0.093030200
C	1.131866200	-1.261868400	0.044931800
C	1.194086200	0.690431100	1.170768500
C	1.330690200	0.681841300	-1.079541400
H	1.148089000	-1.848221900	-0.871409100
H	1.101189700	0.192759200	2.133698000
H	1.406035900	1.766186300	-1.126428600
H	1.036729400	-1.841657400	0.960575400
H	1.263241900	1.775157100	1.218041800
H	1.354965700	0.176685300	-2.042765300
H	-2.277879200	0.250906800	-0.075247000

As	-3.768398700	0.347706700	-0.404474400
H	-3.981176300	1.469912100	0.615163500
H	-4.126758500	-0.725125200	0.627457500

PPL•••H_2O

C	0.191321600	0.130181000	0.000001500
C	1.747197500	0.284143200	0.000003000
C	1.107710500	-1.088943100	0.000004500
C	0.916193400	0.856824300	1.128653800
C	0.916195500	0.856826700	-1.128647700
H	1.162010400	-1.668197400	-0.918538200
H	0.962100300	0.355299200	2.092700400
H	0.806538700	1.937955800	-1.173859200
H	1.162008600	-1.668194300	0.918544900
H	0.806536200	1.937955200	1.173866600
H	0.962104300	0.355302100	-2.092696400
H	-1.925409000	-0.083239900	-0.000000100
O	-2.895824000	-0.173897600	-0.000000700
H	-3.216993900	0.735564800	-0.000004200

PPL•••H_2S

C	0.219770800	0.104916900	0.000001700
C	1.781023700	-0.011267900	0.000000800
C	0.910065700	-1.252734100	-0.000000100
C	1.054023000	0.695771100	1.128079800
C	1.054021500	0.695770200	-1.128077900
H	0.865407800	-1.833440200	-0.918351200

H	1.013630000	0.194360700	2.092541900
H	1.132857300	1.779624200	-1.174564100
H	0.865407600	-1.833445800	0.918347400
H	1.132859200	1.779625300	1.174563200
H	1.013627100	0.194356900	-2.092538400
H	-2.045284000	0.276606300	0.000003100
S	-3.398742200	0.379928700	0.000003600
H	-3.357017400	1.726898000	-0.000003700

PPL•••H_2Se

C	0.234964800	0.099290600	0.000000500
C	1.797197500	-0.013708800	-0.000000400
C	0.927637800	-1.256688700	0.000000300
C	1.067424000	0.692199100	1.127640000
C	1.067422600	0.692199600	-1.127639700
H	0.884255800	-1.837628100	-0.918314400
H	1.028344600	0.191905000	2.092678100
H	1.143988000	1.776332400	-1.172878000
H	0.884256300	-1.837627200	0.918315300
H	1.143989700	1.776331900	1.172878900
H	1.028342000	0.191906100	-2.092678200
H	-2.018625300	0.263501900	0.000001300
Se	-3.500131600	0.372251600	0.000001900
H	-3.427257600	1.844778300	-0.000004800

PPL•••HF

C	0.146762800	0.098408000	0.000001900

C	1.701813200	-0.006276100	0.000000100
C	0.861523000	-1.258116000	0.000000700
C	0.992135300	0.696241400	1.130304100
C	0.992132600	0.696241600	-1.130302400
H	0.816934800	-1.836648800	-0.919173100
H	0.951975100	0.193829300	2.093761700
H	1.059368200	1.780468100	-1.173295400
H	0.816936400	-1.836651000	0.919172400
H	1.059371000	1.780468400	1.173295900
H	0.951970000	0.193828400	-2.093759400
H	-1.689749200	0.220547700	0.000003400
F	-2.639874300	0.284355800	0.000004400

PPL•••HCl

C	0.160359800	0.098101800	0.000003100
C	1.718581600	-0.007165000	0.000001300
C	0.870506900	-1.257146000	0.000000000
C	1.000936700	0.695125100	1.129538500
C	1.000933700	0.695123500	-1.129535100
H	0.827124100	-1.836382700	-0.918935000
H	0.961100200	0.192315500	2.093008800
H	1.070003600	1.779315400	-1.174297300
H	0.827124200	-1.836391900	0.918928900
H	1.070006700	1.779317400	1.174295700
H	0.961094100	0.192308800	-2.093002600
H	-1.724675800	0.221519400	0.000005800
Cl	-3.045619500	0.310220800	0.000009700

PPL•••HBr

C	0.154310200	0.097365600	0.000000800
C	1.713780900	-0.007132900	-0.000001100
C	0.865181800	-1.257258200	0.000000600
C	0.995548500	0.695271500	1.128957700
C	0.995545900	0.695272400	-1.128957600
H	0.819422300	-1.836107700	-0.919043800
H	0.955232200	0.193535500	2.092888500
H	1.061030000	1.779736700	-1.171530700
H	0.819425200	-1.836103800	0.919048300
H	1.061032700	1.779735300	1.171533200
H	0.955227600	0.193539300	-2.092889600
H	-1.605043100	0.214332600	0.000005400
Br	-3.093216300	0.314076000	0.000010000

H_2O

H	-1.928482100	-0.081098200	-0.000000100
O	-2.889232900	-0.172404600	-0.000000700
H	-3.215029200	0.736033200	-0.000004200

CH_3OH

H	-1.977402900	-0.165145500	-0.209677300
O	-2.859200300	-0.125054300	0.178593300
C	-3.351002100	1.213176100	0.029386800
H	-3.426278200	1.511290000	-1.027769100

H	-4.353794900	1.229283400	0.466200600
H	-2.726282200	1.945873000	0.563237000

CH_4

H	4.696703400	0.000793300	0.000157000
C	5.790411600	0.000896200	0.000480100
H	6.155596400	-0.010793800	1.031000600
H	6.156535800	-0.885564600	-0.524746000
H	6.156365600	0.899143300	-0.504407300

CH_3CN

C	-2.050998600	3.142573300	-5.106073800
H	-2.867137000	3.512674900	-5.735772000
H	-1.104255700	3.292043900	-5.636135700
H	-2.194271200	2.069303000	-4.941721300
C	-2.032124700	3.852190000	-3.830752800
N	-2.013822800	4.415708700	-2.818218600

C_3H_6

C	1.731329500	0.000000000	-5.369265800
C	0.992606800	-0.154564800	-4.062070900
C	2.470052200	0.154564800	-4.062070900
H	1.918136100	-0.892777400	-5.959671900
H	1.544523000	0.892777400	-5.959671900
H	0.678933500	-1.152071600	-3.766845700
H	0.305324600	0.633517600	-3.766845300
H	2.783725600	1.152071600	-3.766845700
H	3.157334500	-0.633517600	-3.766845300

Benzene

C	0.781051400	-0.611847700	-1.211124500
C	0.477538000	0.753238200	-1.211104700
C	0.326650200	1.435840700	0.000000000
C	0.477538000	0.753238200	1.211104700
C	0.781051400	-0.611847700	1.211124500
C	0.933482000	-1.294107400	0.000000000
H	0.897528400	-1.142686000	-2.152808700
H	0.356263000	1.283030900	-2.152750400
H	0.089340000	2.496856500	0.000000000
H	0.356263000	1.283030900	2.152750400
H	0.897528400	-1.142686000	2.152808700
H	1.170641900	-2.355169800	0.000000000

LiH

Li	0.027830800	0.000000000	-2.733137900
H	0.027830800	0.000000000	-4.349534400

C_2H_2

C	0.240685200	-0.148255900	-1.561227300
C	0.240685200	-0.148255900	-0.356395500
H	0.240685200	-0.148255900	-2.627813600
H	0.240685200	-0.148255900	0.710289800

NH_3

H	-2.215920800	0.254218800	-0.077752200

N	-3.230853100	0.319229200	-0.105306600
H	-3.480522000	1.153541500	0.420745700
H	-3.584768800	-0.473314500	0.425503100

PH_3

H	-2.366161900	0.277902100	0.104545300
P	-3.790759900	0.377747500	0.141300500
H	-3.775452800	1.428314400	1.109174700
H	-3.920010300	-0.643864800	1.131311300

AsH_3

H	-1.867602400	0.231864300	-0.085354700
As	-3.355354600	0.326238800	-0.433480800
H	-3.574223600	1.445485800	0.587789600
H	-3.714887500	-0.749913500	0.594236100

H_2S

H	-2.050795400	0.279826400	0.000003100
S	-3.395028700	0.378031100	0.000003700
H	-3.354259200	1.725287700	-0.000003700

H_2Se

H	-2.025379900	0.267967700	0.000001300
Se	-3.496270300	0.369996600	0.000001900
H	-3.422944600	1.842674900	-0.000004800

HF

H	-1.682631400	0.220546900	0.000003200
F	-2.606406800	0.282484500	0.000004400

HCl

H	-1.702699300	0.221087500	0.000005800
Cl	-2.983680400	0.306767200	0.000009700

HBr

H	-1.631739000	0.216341300	0.000005600
Br	-3.054642000	0.311513600	0.000009900