Dipoles Inside Dipoles:

Insertion Complexes of Polar vs Nonpolar Molecules in Ion-Pairs

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Optimized energies and atomic coordinates

Cs-$C_6H_6F_6$-I

E = -861.68859250

C	0.70528945	-0.21092732	1.26365397
C	-0.56381250	-0.98471297	1.03482127
C	-1.34962400	-0.53164622	-0.16485269
C	-0.46807206	-0.51344123	-1.38295571
C	0.79914666	0.27661489	-1.20862992
C	1.53681720	-0.20187128	0.01090843
F	0.40246464	1.11072791	1.65359292
F	-1.36073922	-0.89681191	2.16110742
F	-1.88442887	0.75359650	0.06467383
F	-1.17970057	-0.00627389	-2.45403298
F	0.50254931	1.65085018	-1.08922907
F	2.65362028	0.58822442	0.20956805
H	1.26773560	-0.64278940	2.08637500
H	-0.26876796	-2.02646569	0.84419671
H	-2.20224210	-1.18473377	-0.32636349
H	-0.16771423	-1.55444265	-1.57067967
H	1.42646016	0.18398253	-2.09011638
H	1.82522732	-1.24489812	-0.18377997
Cs	-0.95700014	3.37415834	0.62160327
I	1.05169166	-3.70361572	-0.68384490

Cs-$C_6H_6F_6$-Cl

E = -865.62419355

C	0.93172784	-1.04218139	1.11744842
C	-0.33808980	-1.81654435	0.89104562
C	-1.12161320	-1.36145150	-0.30987920
C	-0.24352705	-1.34344720	-1.53104733

C	1.02711554	-0.55785026	-1.35472322
C	1.76700288	-1.03021870	-0.13333655
F	0.62646122	0.28087249	1.50690205
F	-1.13691853	-1.71638636	2.01782042
F	-1.65337984	-0.07346664	-0.07864250
F	-0.95758618	-0.81874962	-2.59530320
F	0.73210567	0.81877200	-1.23895854
F	2.87369356	-0.22238933	0.06801285
H	1.49328033	-1.46966163	1.94273862
H	-0.04343014	-2.85642590	0.70023448
H	-1.97843238	-2.00910135	-0.46983369
H	0.05373251	-2.38308507	-1.72102325
H	1.65450673	-0.65125425	-2.23613341
H	2.05926339	-2.07088280	-0.32645976
Cs	-0.72057596	2.54189236	0.46885933
Cl	1.17771270	-4.11905589	-0.76502732

Cs-C_6H_{12}-I

E = -266.72519354

C	1.27025628	-1.87466413	0.04289177
C	2.42775468	-0.99324053	0.48155886
C	2.22007576	0.44462513	0.03576966
C	0.90728090	0.99121970	0.57790028
C	-0.23214486	0.09516270	0.12374773
C	-0.04777874	-1.34051457	0.58460298
H	1.42428170	-2.90314559	0.36844868
H	1.20695026	-1.86274614	-1.04689233
H	3.36024563	-1.37660181	0.06996678
H	2.52471929	-1.02958966	1.57419813
H	2.16363319	0.47490983	-1.05404543
H	3.05230723	1.07113919	0.35571794
H	0.74644945	2.01111322	0.22750789
H	1.00061748	1.03352969	1.67697398
H	-0.20484358	0.08087444	-0.97672099
H	-1.22367469	0.50212626	0.35123807
H	-0.87844715	-1.95637015	0.23884409
H	-0.00874934	-1.43082225	1.68401324
Cs	-1.37962542	0.57203200	2.98880469
I	0.39594369	-0.17285499	-3.37883123

Cs-C_6H_{12}-Cl

E = -270.654889630737

C	1.38080663	-1.92196181	-1.03699678
C	2.54084711	-1.04277793	-0.59971260
C	2.32979240	0.39552844	-1.04334302
C	1.02241488	0.93909528	-0.48421598
C	-0.12100261	0.04655401	-0.93926716
C	0.06905860	-1.38940088	-0.47761895
H	1.53708845	-2.95297453	-0.71963975
H	1.30615527	-1.88968474	-2.12587622
H	3.47149440	-1.42492496	-1.01700393
H	2.64312587	-1.08189044	0.49306976
H	2.25148671	0.41953731	-2.13221389
H	3.16515851	1.02215939	-0.73081262
H	0.86036080	1.96307218	-0.82231488
H	1.12783186	0.97097229	0.61489685
H	-0.07671429	0.02551328	-2.04348529
H	-1.11252967	0.45311482	-0.70780046
H	-0.76562505	-2.00720677	-0.81034052
H	0.12481448	-1.48045806	0.62183220
Cs	-1.21838503	0.50401446	1.93255977
Cl	0.65152363	-0.27645130	-4.02406007