Noncovalently bound complexes of polar molecules: Dipole-inside-of-dipole vs dipole-dipole systems

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Optimized coordinates (in Å)

Cs-$C_4H_4F_4$(all-*cis*)-I

1 C	6.0000	0.09487611	-1.08947754	0.44850971
2 C	6.0000	1.08947754	0.09487611	0.44850971
3 C	6.0000	-0.09487611	1.08947754	0.44850971
4 C	6.0000	-1.08947754	-0.09487611	0.44850971
5 H	1.0000	0.15469683	-1.77657139	1.27716035
6 F	9.0000	0.15626260	-1.79454866	-0.75856311
7 F	9.0000	1.79454866	0.15626260	-0.75856311
8 H	1.0000	1.77657139	0.15469683	1.27716035
9 F	9.0000	-0.15626260	1.79454866	-0.75856311
10 H	1.0000	-0.15469683	1.77657139	1.27716035
11 F	9.0000	-1.79454866	-0.15626260	-0.75856311
12 H	1.0000	-1.77657139	-0.15469683	1.27716035
13 Cs	55.0000	0.00000000	0.00000000	-3.07710468
14 I	53.0000	0.00000000	0.00000000	3.58625850

CsI-$C_4H_4F_4$(all-*cis*)

1 C	6.0000	1.05694936	3.07267560	-0.00120231
2 C	6.0000	0.01053032	3.38854296	1.07795365
3 C	6.0000	-1.04110596	3.10255883	-0.00450846
4 C	6.0000	0.01367667	3.36972365	-1.08869521
5 H	1.0000	1.30528049	2.01458891	0.00826895
6 F	9.0000	2.18712926	3.83463645	-0.00619897
7 F	9.0000	0.02902185	4.72029417	1.40897048
8 H	1.0000	0.00059477	2.79528254	1.98523485
9 F	9.0000	-2.14893247	3.89651752	-0.01300533
10 H	1.0000	-1.31970995	2.05200278	0.00413754
11 F	9.0000	0.03314981	4.69548671	-1.44288267
12 H	1.0000	0.00633883	2.76055734	-1.98539973
13 Cs	55.0000	0.01809851	-3.91179289	-0.01037846
14 I	53.0000	-0.04020690	-0.49773479	0.02141431

CsI:$C_4H_4F_4$(all-*cis*)

1 C	6.0000	-0.66823760	-1.53111127	-0.91326677
2 C	6.0000	-0.78655666	-3.06260866	-0.93047026
3 C	6.0000	-1.28172777	-2.93944741	0.51854747
4 C	6.0000	-0.62157881	-1.55747528	0.62116694
5 H	1.0000	-1.55097242	-1.00299261	-1.26107197
6 F	9.0000	0.44396298	-1.03027112	-1.54421403
7 F	9.0000	0.46228962	-3.63002589	-0.95710820
8 H	1.0000	-1.41063924	-3.54566930	-1.67318600
9 F	9.0000	-0.87193607	-3.89486120	1.39174257
10 H	1.0000	-2.36451608	-2.83872195	0.55580022
11 F	9.0000	0.69200072	-1.65992906	1.05781518
12 H	1.0000	-1.11186044	-0.75273237	1.15327728
13 Cs	55.0000	1.84644656	1.02135551	0.10566099
14 I	53.0000	-1.53653024	1.85748456	0.00275568

Cs-$C_4H_4F_4$(*cross*)-I

1 H	1.0000	1.99934665	0.14513010	0.00000000
2 H	1.0000	1.21054870	-1.51589001	0.00000000
3 F	9.0000	0.00015655	-0.77392184	-2.18748972
4 F	9.0000	0.00621290	1.24340091	-1.38576012
5 C	6.0000	1.07586208	-0.42085391	0.00000000
6 C	6.0000	0.00206558	-0.13099868	-1.02938310
7 C	6.0000	0.00206558	-0.13099868	1.02938310
8 C	6.0000	-1.07371358	-0.41396926	0.00000000
9 F	9.0000	0.00015655	-0.77392184	2.18748972
10 F	9.0000	0.00621290	1.24340091	1.38576012
11 H	1.0000	-1.21675877	-1.50782029	0.00000000
12 H	1.0000	-1.99295700	0.15887975	0.00000000
13 Cs	55.0000	0.00232821	3.68148092	0.00000000
14 I	53.0000	-0.00752105	-3.80885963	0.00000000

CsI-$C_4H_4F_4$(*cross*)

1 H	1.0000	-0.01931324	-3.94656953	-1.94730184
2 H	1.0000	0.00143643	-2.23081350	-1.34760939
3 F	9.0000	2.13122824	-2.77966815	-0.00321802
4 F	9.0000	1.44945600	-4.84365395	-0.00172864
5 C	6.0000	-0.01125437	-3.28668036	-1.08928418
6 C	6.0000	1.02448715	-3.54725272	-0.00248442
7 C	6.0000	-1.05270458	-3.52218240	-0.00226261
8 C	6.0000	-0.01100088	-3.28528486	1.08421417
9 F	9.0000	-2.14075088	-2.72817385	-0.00274203
10 F	9.0000	-1.50894068	-4.80793927	-0.00141630
11 H	1.0000	0.00177049	-2.22901446	1.34101272
12 H	1.0000	-0.01884589	-3.94398579	1.94314597
13 I	53.0000	0.03346694	0.39429506	0.00264373

14 Cs	55.0000	-0.01282301	3.78974613	-0.00254801

CsI:$C_4H_4F_4$(*cross*)

1 H	1.0000	-1.08694814	1.63117564	0.68948538
2 H	1.0000	-1.08560886	1.99561671	-1.05028750
3 F	9.0000	1.22835729	0.90102344	-1.32255078
4 F	9.0000	1.45301210	1.13985656	0.82563118
5 C	6.0000	-0.54746243	2.11218719	-0.11571774
6 C	6.0000	0.91185252	1.72913035	-0.28790355
7 C	6.0000	-0.05417585	3.54177646	0.07990503
8 C	6.0000	1.33651903	3.18076041	-0.44243487
9 F	9.0000	-0.70657513	4.50538185	-0.60265100
10 F	9.0000	-0.02897747	3.91731245	1.38282607
11 H	1.0000	1.43261067	3.44037931	-1.49104849
12 H	1.0000	2.18437576	3.51261846	0.14312928
13 Cs	55.0000	1.37326993	-1.90039192	0.08718709
14 I	53.0000	-1.97328360	-1.19206152	-0.01663691