π-Complexed Polyfluoroarenes: A Reactivity, Bonding and Spectroscopic Study of (η^6-C_6F_6)Cr(η^6-C_6H_6) and Related Molecules

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Cartesian coordinates and total energies (E, in hartrees) of the B3LYP/6-31G* optimized geometries of all calculated structures.

C_6H_6 E = –232.243832			
C	0.000000	0.000000	1.396639
C	1.209525	0.000000	0.698319
C	1.209525	0.000000	-0.698319
C	0.000000	0.000000	-1.396639
C	-1.209525	0.000000	-0.698319
C	-1.209525	0.000000	0.698319
H	0.000000	0.000000	2.483620
H	2.150878	0.000000	1.241810
H	2.150878	0.000000	-1.241810
H	0.000000	0.000000	-2.483620
H	-2.150878	0.000000	-1.241810
H	-2.150878	0.000000	1.241810

C_6F_6 E = –827.588048			
C	-0.161811	1.494325	-0.000462
C	1.232177	1.494226	-0.000462
C	1.929258	2.701405	-0.000462
C	1.232350	3.908684	-0.000462
C	-0.161638	3.908783	-0.000462
C	-0.858718	2.701604	-0.000462
F	1.900174	5.065198	-0.000462
F	3.264740	2.701309	-0.000462
F	1.899836	0.337616	-0.000462
F	-0.829635	0.337811	-0.000462
F	-2.194201	2.701700	-0.000462
F	-0.829296	5.065393	-0.000462

Cr(C_6H_6) E = –1276.518219			
Cr	0.009566	0.004595	1.181109
H	2.453300	-0.706891	2.486659
C	1.416302	-0.395345	2.587519
C	-1.337191	0.429661	2.637959
C	0.370991	-1.381634	2.619115
C	1.084862	1.003484	2.581002
C	-0.291796	1.415944	2.606420
C	-1.005827	-0.969133	2.644129

Cr(C_6F_6) E = –1871.855384			
Cr	-0.001578	0.000365	0.811184
C	1.333364	0.341597	-0.688749
C	-1.414313	-0.368929	-0.608959
C	0.339123	1.354245	-0.671840
C	0.953708	-1.026131	-0.665859
C	-0.419982	-1.381658	-0.625506
C	-1.034728	0.998661	-0.632405
F	-0.776086	-2.677623	-0.449892

H	0.619476	-2.437505	2.540844	F	-2.713572	-0.704361	-0.417966
H	1.871409	1.746857	2.473818	F	-1.974680	1.961100	-0.465935
H	-0.543379	2.470290	2.518007	F	0.702459	2.653604	-0.542441
H	-1.796217	-1.713799	2.585141	F	2.641164	0.679044	-0.575761
H	-2.377400	0.740497	2.575151	F	1.902416	-1.984944	-0.531172

$Cr(C_6H_6)_2$ E = –1508.891147

Cr	0.000308	0.002020	0.998438
C	1.203790	0.670409	-0.658883
C	-1.281965	-0.697981	-0.585111
C	-0.010236	1.405174	-0.636525
C	1.174951	-0.748507	-0.644439
C	-0.067935	-1.432755	-0.607433
C	-1.253130	0.720931	-0.599750
H	2.182981	-1.276430	2.543258
C	1.254579	-0.715530	2.596586
C	-1.175276	0.750966	2.641379
C	0.012536	-1.401306	2.633262
C	1.281676	0.703420	2.582081
C	0.066767	1.436731	2.604462
C	-1.202377	-0.667986	2.655679
H	-0.009015	-2.486747	2.607134
H	2.230716	1.227384	2.517600
H	0.086500	2.521454	2.556329
H	-2.153179	-1.192658	2.647462
H	-2.105383	1.311251	2.622330
H	0.012600	2.490593	-0.610524
H	2.155226	1.193931	-0.650722
H	2.104364	-1.309942	-0.625350
H	-0.088981	-2.517448	-0.559177
H	-2.231629	-1.220797	-0.520509
H	-2.180733	1.283157	-0.546496

$Cr(C_6H_6)_2^+$ E = –1508.706667

Cr	0.000199	0.002207	0.998434
C	1.201990	0.672163	-0.676426
C	-1.280917	-0.699989	-0.602788
C	-0.013006	1.404939	-0.654446
C	1.175531	-0.746644	-0.662490
C	-0.065966	-1.432736	-0.625138
C	-1.254460	0.718862	-0.618195
H	2.178665	-1.279202	2.551063
C	1.253793	-0.717022	2.614606
C	-1.173463	0.752967	2.659773
C	0.010848	-1.400715	2.650919
C	1.283018	0.701645	2.599674
C	0.069380	1.436620	2.622352
C	-1.202758	-0.665775	2.673376
H	-0.012729	-2.484028	2.614827
H	2.230845	1.222528	2.523991
H	0.090597	2.519031	2.564431
H	-2.152871	-1.187627	2.653991
H	-2.101054	1.313515	2.630657
H	0.008151	2.488308	-0.618547
H	2.151014	1.195986	-0.656969
H	2.104208	-1.305364	-0.633078
H	-0.084922	-2.515178	-0.566895
H	-2.227606	-1.222936	-0.527155
H	-2.181331	1.277779	-0.554887

$(C_6F_6)Cr(C_6H_6)$ E = –2104.243624

Cr	0.000947	0.002563	0.979156
C	1.329420	0.336422	-0.636104
C	-1.406657	-0.363256	-0.560481
C	0.342036	1.346418	-0.621901
C	0.948721	-1.023520	-0.613432
C	-0.419194	-1.373156	-0.575640
C	-1.025986	0.996755	-0.583461

$(C_6F_6)Cr(C_6H_6)^+$ E = –2104.005737

Cr	0.003633	0.002552	1.025644
C	1.333470	0.339833	-0.682973
C	-1.412945	-0.367441	-0.603983
C	0.340351	1.352903	-0.665849
C	0.953310	-1.026578	-0.660191
C	-0.419802	-1.380437	-0.618837
C	-1.032806	0.999005	-0.627354

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H	2.436467	-0.693967	2.511469	H	2.437695	-0.698596	2.551416
C	1.399105	-0.385579	2.584069	C	1.400990	-0.388295	2.627872
C	-1.320198	0.420573	2.640366	C	-1.320261	0.424091	2.680638
C	0.370503	-1.361844	2.615500	C	0.369199	-1.363919	2.659301
C	1.068122	0.993706	2.579392	C	1.072354	0.993447	2.621554
C	-0.291559	1.396903	2.606916	C	-0.288474	1.399681	2.648050
C	-0.989243	-0.958782	2.644388	C	-0.991684	-0.957698	2.685724
H	0.621998	-2.415751	2.565995	H	0.618942	-2.418247	2.607016
H	1.852843	1.738592	2.502745	H	1.858293	1.736779	2.541173
H	-0.545636	2.449910	2.551131	H	-0.540718	2.452959	2.587072
H	-1.776507	-1.704372	2.616718	H	-1.780062	-1.702127	2.654296
H	-2.359899	0.728182	2.610093	H	-2.359384	0.733459	2.643728
F	-0.781378	-2.669792	-0.523788	F	-0.773627	-2.654768	-0.567632
F	-2.710196	-0.697762	-0.496339	F	-2.693105	-0.697087	-0.538163
F	-1.966465	1.960611	-0.541666	F	-1.958215	1.944153	-0.581748
F	0.706175	2.643507	-0.617142	F	0.695864	2.627784	-0.658610
F	2.634424	0.670873	-0.647393	F	2.615142	0.670078	-0.691235
F	1.890158	-1.987233	-0.600260	F	1.879841	-1.971530	-0.646579