

Electrostatically enhanced F...F interactions through hydrogen bonding,
halogen bonding and metal coordination: An ab initio study.

A. Bauzá and A. Frontera*

Department of Chemistry Universitat de les Illes Balears, Crta. de Valldemossa km 7.5,
07122 Palma (Balears), Spain. E-mail: toni.frontera@uib.es;

Fax: +34 971 173426

Electronic Supplementary Information

Cartesian coordinates

7.

C	0.0000000	0.0000000	-0.2244916
C	1.2023658	0.0000000	0.4605613
C	-1.1413299	0.0000000	1.8514733
C	-1.2023658	0.0000000	0.4605613
H	2.1453680	0.0000000	-0.0716926
H	-2.0586620	0.0000000	2.4321310
H	-2.1453680	0.0000000	-0.0716926
F	0.0000000	0.0000000	-1.5640974
N	0.0000000	0.0000000	2.5524488
C	1.1413299	0.0000000	1.8514733
H	2.0586620	0.0000000	2.4321310
F	0.0000000	0.0000000	-4.5921792
H	0.0000000	0.0000000	-5.5166265

8.

C	0.0000000	0.0000000	-0.8154219
C	1.2154598	0.0000000	-0.1464470
C	1.2144026	0.0000000	1.2430581
C	0.0000000	0.0000000	1.9390716
C	-1.2144026	0.0000000	1.2430581
C	-1.2154598	0.0000000	-0.1464470
H	2.1385607	0.0000000	-0.7134574
H	2.1489831	0.0000000	1.7918484
H	-2.1489831	0.0000000	1.7918484
H	-2.1385607	0.0000000	-0.7134574
C	0.0000000	0.0000000	3.3693797
N	0.0000000	0.0000000	4.5424454
F	0.0000000	0.0000000	-2.1560660
F	0.0000000	0.0000000	-5.1524459
H	0.0000000	0.0000000	-6.0769671

9.

C	0.0000000	0.0000000	-1.5887915
C	1.2151497	0.0000000	-0.9187869
C	1.2139612	0.0000000	0.4702861
C	0.0000000	0.0000000	1.1739032
C	-1.2139612	0.0000000	0.4702861
C	-1.2151497	0.0000000	-0.9187869
H	2.1386191	0.0000000	-1.4855147
H	-2.1498288	0.0000000	1.0175018
H	-2.1386191	0.0000000	-1.4855147

F	0.0000000	0.0000000	-2.9296320
H	2.1498288	0.0000000	1.0175018
C	0.0000000	0.0000000	2.5939429
C	0.0000000	0.0000000	3.8190517
C	0.0000000	0.0000000	5.1858392
N	0.0000000	0.0000000	6.3646001
F	0.0000000	0.0000000	-5.9306832
H	0.0000000	0.0000000	-6.8552030

10.

C	0.1202924	-0.2823450	0.0000000
C	1.3303154	0.3997349	0.0000000
C	0.2325233	2.4101927	0.0000000
C	-1.0150942	1.7916754	0.0000000
C	-1.0822745	0.4020511	0.0000000
H	2.2655082	-0.1512298	0.0000000
H	0.3121932	3.4924479	0.0000000
H	-1.9202133	2.3873851	0.0000000
H	-2.0207320	-0.1394733	0.0000000
N	1.3906208	1.7360095	0.0000000
F	0.1244386	-1.6229404	0.0000000
F	0.1292109	-4.7495624	0.0000000
H	0.1332114	-5.6739458	0.0000000

11.

C	0.7182854	-0.0458942	0.0000000
C	0.4228075	-1.4018893	0.0000000
C	-0.9141652	-1.7935987	0.0000000
C	-1.9321439	-0.8455381	0.0000000
C	-1.6012145	0.5145167	0.0000000
C	-0.2649892	0.9292977	0.0000000
H	1.2308896	-2.1235653	0.0000000
H	-1.1616965	-2.8488276	0.0000000
H	0.0034279	1.9787604	0.0000000
F	2.0023093	0.3370147	0.0000000
C	-2.6414915	1.4973074	0.0000000
N	-3.4978694	2.2991904	0.0000000
H	-2.9734639	-1.1443308	0.0000000
F	4.8619387	1.1905245	0.0000000
H	5.7473759	1.4570321	0.0000000

12.

C	-1.2988737	-0.5203244	0.0008611
C	0.0844927	-0.5709834	0.0014413
C	0.7940670	0.6387386	0.0000667
C	0.1079518	1.8628193	-0.0018128
C	-1.2825503	1.8705233	-0.0023221
C	-2.0016151	0.6767870	-0.0009854
H	0.5963060	-1.5259929	0.0029183
H	0.6695634	2.7896049	-0.0029260
H	-1.8152672	2.8146291	-0.0038352

H	-3.0849581	0.6600085	-0.0013617
C	2.2145272	0.6203018	0.0005381
C	3.4397484	0.6089630	0.0009251
F	-1.9837236	-1.6725564	0.0021744
C	4.8064087	0.5967443	0.0013462
N	5.9851970	0.5868149	0.0017061
F	-3.4303015	-4.2945663	0.0006769
H	-3.8009726	-5.1415111	0.0005891

13.

C	-0.0046582	-1.7177744	0.0000000
C	1.2021481	-1.0399077	0.0000000
C	-1.1481004	0.3553313	0.0000000
C	-1.2075243	-1.0329360	0.0000000
H	2.1427053	-1.5757126	0.0000000
H	-2.0566206	0.9479869	0.0000000
H	-2.1511644	-1.5632923	0.0000000
F	-0.0085310	-3.0560944	0.0000000
N	0.0033449	1.0396519	0.0000000
C	1.1507846	0.3486848	0.0000000
H	2.0627288	0.9360554	0.0000000
H	0.0063436	2.6983955	0.0000000
F	0.0085439	3.6596116	0.0000000

14.

C	-0.0041360	-1.9026826	0.0000000
C	1.2031758	-1.2239296	0.0000000
C	-1.1569139	0.1678158	0.0000000
C	-1.2085159	-1.2187565	0.0000000
H	2.1438005	-1.7597717	0.0000000
H	-2.0590330	0.7696522	0.0000000
H	-2.1514197	-1.7505827	0.0000000
F	-0.0069956	-3.2379765	0.0000000
N	0.0017467	0.8417741	0.0000000
C	1.1575075	0.1628460	0.0000000
H	2.0621795	0.7608601	0.0000000
I	0.0070296	3.2058458	0.0000000
F	0.0115747	5.1849053	0.0000000

15.

C	0.0000000	0.0000000	-2.4679986
C	1.2166527	0.0000000	-1.8014041
C	1.2165540	0.0000000	-0.4123742
C	0.0000000	0.0000000	0.2795957
C	-1.2165540	0.0000000	-0.4123742
C	-1.2166527	0.0000000	-1.8014041
H	2.1396244	0.0000000	-2.3684590
H	2.1509698	0.0000000	0.1365817
H	-2.1509698	0.0000000	0.1365817
H	-2.1396244	0.0000000	-2.3684590
C	0.0000000	0.0000000	1.7079420

N	0.0000000	0.0000000	2.8773542
F	0.0000000	0.0000000	-3.8094966
F	0.0000000	0.0000000	5.6219967
H	0.0000000	0.0000000	4.6819180

16.

C	0.0000000	0.0000000	-2.6240543
C	1.2170494	0.0000000	-1.9576354
C	1.2177077	0.0000000	-0.5689549
C	0.0000000	0.0000000	0.1217392
C	-1.2177077	0.0000000	-0.5689549
C	-1.2170494	0.0000000	-1.9576354
H	2.1397947	0.0000000	-2.5250622
H	2.1519640	0.0000000	-0.0196877
H	-2.1519640	0.0000000	-0.0196877
H	-2.1397947	0.0000000	-2.5250622
C	0.0000000	0.0000000	1.5476179
N	0.0000000	0.0000000	2.7170772
F	0.0000000	0.0000000	-3.9645814
I	0.0000000	0.0000000	5.1987953
F	0.0000000	0.0000000	7.1460864

17.

C	0.0000000	0.0000000	-3.3549763
C	1.2160009	0.0000000	-2.6870570
C	1.2151774	0.0000000	-1.2982563
C	0.0000000	0.0000000	-0.5968335
C	-1.2151774	0.0000000	-1.2982563
C	-1.2160009	0.0000000	-2.6870570
H	2.1394879	0.0000000	-3.2536345
H	-2.1510099	0.0000000	-0.7511015
H	-2.1394879	0.0000000	-3.2536345
F	0.0000000	0.0000000	-4.6974099
H	2.1510099	0.0000000	-0.7511015
C	0.0000000	0.0000000	0.8222287
C	0.0000000	0.0000000	2.0474067
C	0.0000000	0.0000000	3.4114105
N	0.0000000	0.0000000	4.5866938
H	0.0000000	0.0000000	6.4114948
F	0.0000000	0.0000000	7.3500837

18.

C	0.0000000	0.0000000	-3.4903142
C	1.2162102	0.0000000	-2.8224588
C	1.2157668	0.0000000	-1.4338198
C	0.0000000	0.0000000	-0.7330286
C	-1.2157668	0.0000000	-1.4338198
C	-1.2162102	0.0000000	-2.8224588
H	2.1396071	0.0000000	-3.3891600

H	-2.1516033	0.0000000	-0.8866689
H	-2.1396071	0.0000000	-3.3891600
F	0.0000000	0.0000000	-4.8321385
H	2.1516033	0.0000000	-0.8866689
C	0.0000000	0.0000000	0.6850468
C	0.0000000	0.0000000	1.9111460
C	0.0000000	0.0000000	3.2713207
N	0.0000000	0.0000000	4.4471673
I	0.0000000	0.0000000	6.9295042
F	0.0000000	0.0000000	8.8755111

19.

C	-1.1748884	-1.0165468	0.0000000
C	0.2032619	-1.1758636	0.0000000
C	0.4884715	1.1127564	0.0000000
C	-0.8846835	1.3339045	0.0000000
C	-1.7481765	0.2433348	0.0000000
H	0.6506227	-2.1639794	0.0000000
H	1.1933492	1.9366412	0.0000000
H	-1.2719854	2.3454713	0.0000000
H	-2.8260388	0.3530086	0.0000000
N	1.0208605	-0.1169154	0.0000000
F	-1.9546498	-2.1044015	0.0000000
H	2.6751655	-0.3187674	0.0000000
F	3.6286913	-0.4286426	0.0000000

20.

C	-1.3548300	-0.9965158	0.0000000
C	0.0225631	-1.1566907	0.0000000
C	0.3021213	1.1479351	0.0000000
C	-1.0715391	1.3571796	0.0000000
C	-1.9306035	0.2632447	0.0000000
H	0.4846938	-2.1377865	0.0000000
H	1.0131335	1.9661315	0.0000000
H	-1.4625159	2.3672801	0.0000000
H	-3.0086865	0.3696724	0.0000000
N	0.8264155	-0.0860939	0.0000000
F	-2.1296820	-2.0836388	0.0000000
I	3.1733877	-0.3817192	0.0000000
F	5.1355421	-0.6289986	0.0000000

21.

C	1.9101732	0.9778936	0.0000000
C	2.4976573	-0.2793171	0.0000000
C	1.6734178	-1.4023655	0.0000000
C	0.2890249	-1.2671240	0.0000000
C	-0.2690909	0.0160992	0.0000000
C	0.5376692	1.1591550	0.0000000
H	3.5778459	-0.3632505	0.0000000
H	2.1173454	-2.3909591	0.0000000
H	0.1135226	2.1559206	0.0000000
F	2.6999655	2.0613466	0.0000000
C	-1.6905762	0.1665192	0.0000000

N	-2.8540556	0.2852020	0.0000000
H	-0.3575481	-2.1363142	0.0000000
H	-4.6550431	0.4632397	0.0000000
F	-5.5903079	0.5539545	0.0000000

22.

C	2.0442701	1.0149122	0.0000000
C	2.6590341	-0.2295028	0.0000000
C	1.8604687	-1.3709527	0.0000000
C	0.4734985	-1.2674169	0.0000000
C	-0.1116018	0.0041082	0.0000000
C	0.6681411	1.1661379	0.0000000
H	3.7408568	-0.2893196	0.0000000
H	2.3266817	-2.3492071	0.0000000
H	0.2215717	2.1530982	0.0000000
F	2.8096658	2.1145818	0.0000000
C	-1.5337934	0.1219776	0.0000000
N	-2.6998273	0.2129997	0.0000000
H	-0.1538856	-2.1505299	0.0000000
I	-5.1812116	0.3742071	0.0000000
F	-7.1238688	0.4949060	0.0000000

23.

C	-2.7355331	-1.0448656	0.0000000
C	-1.3555817	-1.1481657	0.0000000
C	-0.6044440	0.0362468	0.0000000
C	-1.2436822	1.2852652	0.0000000

C	-2.6328823	1.3434795	0.0000000
C	-3.3945698	0.1764962	0.0000000
H	-0.8785746	-2.1210086	0.0000000
H	-0.6486753	2.1909228	0.0000000
H	-3.1310026	2.3061364	0.0000000
H	-4.4777794	0.1997281	0.0000000
C	0.8136032	-0.0335780	0.0000000
C	2.0377076	-0.0887014	0.0000000
F	-3.4634602	-2.1724158	0.0000000
C	3.4003703	-0.1492198	0.0000000
N	4.5745950	-0.2005760	0.0000000
H	6.4011138	-0.2723436	0.0000000
F	7.3387954	-0.3074004	0.0000000

24.

C	-2.8710560	-1.0388376	0.0000000
C	-1.4910840	-1.1425281	0.0000000
C	-0.7404328	0.0423869	0.0000000
C	-1.3788799	1.2920160	0.0000000
C	-2.7680615	1.3499793	0.0000000
C	-3.5296833	0.1829467	0.0000000
H	-1.0142147	-2.1154453	0.0000000
H	-0.7837796	2.1976041	0.0000000
H	-3.2662003	2.3125981	0.0000000
H	-4.6129165	0.2063383	0.0000000
C	0.6766770	-0.0275485	0.0000000
C	1.9017159	-0.0830011	0.0000000

F	-3.5988787	-2.1656898	0.0000000
C	3.2605747	-0.1440816	0.0000000
N	4.4353476	-0.1961679	0.0000000
I	6.9184856	-0.2967225	0.0000000
F	8.8623866	-0.3738471	0.0000000

25.

C	-0.0022857	-0.8557625	0.0000000
C	1.2041051	-0.1759692	0.0000000
C	-1.1457191	1.2189486	0.0000000
C	-1.2047858	-0.1691111	0.0000000
H	2.1443861	-0.7123038	0.0000000
H	-2.0542164	1.8117025	0.0000000
H	-2.1481062	-0.7000815	0.0000000
F	-0.0060848	-2.1910434	0.0000000
N	0.0055763	1.9038232	0.0000000
C	1.1529485	1.2124049	0.0000000
H	2.0648145	1.7999613	0.0000000
H	0.0095032	3.5574948	0.0000000
F	0.0114128	4.5197538	0.0000000
F	-0.0144602	-5.1475988	0.0000000
H	-0.0170883	-6.0722187	0.0000000

26.

C	0.0104665	-1.0224372	0.0000000
C	1.2139237	-0.3356772	0.0000000
C	-1.1527295	1.0439474	0.0000000
C	-1.1969185	-0.3426051	0.0000000
H	2.1571872	-0.8669129	0.0000000
H	-2.0576782	1.6414984	0.0000000
H	-2.1370807	-0.8793109	0.0000000
F	0.0142152	-2.3544439	0.0000000
N	0.0025698	1.7240175	0.0000000
C	1.1617585	1.0506046	0.0000000
H	2.0632575	1.6533490	0.0000000
I	-0.0042853	4.0827850	0.0000000
F	-0.0100989	6.0641905	0.0000000
F	-0.0261707	-5.2671616	0.0000000
H	-0.0384166	-6.1918435	0.0000000

27.

C	-0.0000012	1.6183899	0.0000000
C	1.2163258	0.9500142	0.0000000
C	1.2164924	-0.4388949	0.0000000
C	-0.0000029	-1.1311036	0.0000000
C	-1.2164973	-0.4388936	0.0000000
C	-1.2163290	0.9500157	0.0000000
H	2.1389996	1.5176031	0.0000000
H	2.1508798	-0.9879656	0.0000000
H	-2.1508854	-0.9879630	0.0000000

H	-2.1390022	1.5176056	0.0000000
C	-0.0000018	-2.5592703	0.0000000
N	0.0000024	-3.7287206	0.0000000
F	0.0000002	2.9567997	0.0000000
F	0.0000071	-6.4700402	0.0000000
H	0.0000049	-5.5295902	0.0000000
F	0.0000041	5.9186959	0.0000000
H	0.0000033	6.8433180	0.0000000

28.

C	0.0000088	1.7577555	0.0000000
C	1.2167642	1.0895749	0.0000000
C	1.2177033	-0.2989640	0.0000000
C	0.0000109	-0.9898444	0.0000000
C	-1.2176825	-0.2989657	0.0000000
C	-1.2167455	1.0895730	0.0000000
H	2.1391919	1.6575671	0.0000000
H	2.1519104	-0.8483799	0.0000000
H	-2.1518887	-0.8483833	0.0000000
H	-2.1391740	1.6575639	0.0000000
C	0.0000089	-2.4154524	0.0000000
N	0.0000021	-3.5849238	0.0000000
F	0.0000064	3.0951136	0.0000000
I	-0.0000181	-6.0612105	0.0000000
F	-0.0000355	-8.0095922	0.0000000
F	-0.0000232	6.0419487	0.0000000
H	-0.0000395	6.9666196	0.0000000

29.

C	0.0000000	0.0000000	-2.4998829
C	1.2156954	0.0000000	-1.8302064
C	1.2151610	0.0000000	-0.4415244
C	0.0000000	0.0000000	0.2600605
C	-1.2151610	0.0000000	-0.4415244
C	-1.2156954	0.0000000	-1.8302064
H	2.1388878	0.0000000	-2.3973125
H	-2.1509558	0.0000000	0.1057794
H	-2.1388878	0.0000000	-2.3973125
F	0.0000000	0.0000000	-3.8392145
H	2.1509558	0.0000000	0.1057794
C	0.0000000	0.0000000	1.6789121
C	0.0000000	0.0000000	2.9042175
C	0.0000000	0.0000000	4.2680339
N	0.0000000	0.0000000	5.4433603
H	0.0000000	0.0000000	7.2651566
F	0.0000000	0.0000000	8.2040092
F	0.0000000	0.0000000	-6.8167666
H	0.0000000	0.0000000	-7.7413582

30.

C	-0.0000142	2.6216318	0.0000000
C	1.2159222	1.9520673	0.0000000
C	1.2157693	0.5635820	0.0000000
C	-0.0000331	-0.1372870	0.0000000
C	-1.2158257	0.5635980	0.0000000

C	-1.2159596	1.9520836	0.0000000
H	2.1389422	2.5194325	0.0000000
H	-2.1515840	0.0162370	0.0000000
H	-2.1389720	2.5194613	0.0000000
F	-0.0000038	3.9603046	0.0000000
H	2.1515199	0.0162080	0.0000000
C	-0.0000377	-1.5550599	0.0000000
C	-0.0000293	-2.7812901	0.0000000
C	-0.0000085	-4.1411735	0.0000000
N	0.0000146	-5.3170524	0.0000000
I	0.0000538	-7.7956584	0.0000000
F	0.0000848	-9.7424275	0.0000000
F	0.0000670	6.9303557	0.0000000
H	0.0000940	7.8549869	0.0000000

31.

C	-0.7422483	0.0198643	0.0000000
C	0.3595669	-0.8241083	0.0000000
C	1.7812250	0.9920836	0.0000000
C	0.7167416	1.8871376	0.0000000
C	-0.5844995	1.3955449	0.0000000
H	0.2352836	-1.9015736	0.0000000
H	2.8093137	1.3366958	0.0000000
H	0.9044320	2.9539558	0.0000000
H	-1.4527967	2.0435245	0.0000000
N	1.6054759	-0.3364530	0.0000000
F	-1.9676827	-0.5113807	0.0000000

H	2.9111023	-1.3637983	0.0000000
F	3.6679328	-1.9558734	0.0000000
F	-4.7041154	-1.6698644	0.0000000
H	-5.5397313	-2.0657547	0.0000000

32.

C	-0.8877999	-0.0823641	0.0000000
C	0.3772071	-0.6517260	0.0000000
C	1.3435023	1.4595064	0.0000000
C	0.0979283	2.0751582	0.0000000
C	-1.0525068	1.2935005	0.0000000
H	0.5194597	-1.7267922	0.0000000
H	2.2693952	2.0231025	0.0000000
H	0.0319871	3.1563054	0.0000000
H	-2.0476339	1.7216620	0.0000000
N	1.4681564	0.1243801	0.0000000
F	-1.9534744	-0.8813151	0.0000000
I	3.6096186	-0.8674261	0.0000000
F	5.4064915	-1.6996617	0.0000000
F	-4.2982431	-2.6144093	0.0000000
H	-4.8840883	-3.3299205	0.0000000

33.

C	1.4331151	-0.0543740	0.0000000
C	1.5914041	-1.4336206	0.0000000
C	0.4547066	-2.2388106	0.0000000
C	-0.8162071	-1.6733738	0.0000000

C	-0.9397103	-0.2794061	0.0000000
C	0.1869325	0.5499761	0.0000000
H	2.5899179	-1.8542156	0.0000000
H	0.5635329	-3.3170721	0.0000000
H	0.1000062	1.6297514	0.0000000
F	2.5221376	0.7224544	0.0000000
C	-2.2407667	0.3124309	0.0000000
N	-3.3072054	0.7925772	0.0000000
H	-1.7044062	-2.2935933	0.0000000
H	-4.9627087	1.5131377	0.0000000
F	-5.8271207	1.8825533	0.0000000
F	4.8516501	2.5435176	0.0000000
H	5.5047221	3.1980676	0.0000000

34.

C	1.5578025	0.1703893	0.0000000
C	1.9611787	-1.1583434	0.0000000
C	0.9884696	-2.1554515	0.0000000
C	-0.3635323	-1.8289461	0.0000000
C	-0.7343889	-0.4791846	0.0000000
C	0.2233238	0.5410220	0.0000000
H	3.0191688	-1.3921351	0.0000000
H	1.2900193	-3.1963634	0.0000000
H	-0.0568238	1.5874851	0.0000000
F	2.4888158	1.1295033	0.0000000
C	-2.1184957	-0.1322872	0.0000000
N	-3.2542118	0.1471275	0.0000000

H	-1.1258382	-2.5986831	0.0000000
I	-5.6671044	0.7241439	0.0000000
F	-7.5618614	1.1744248	0.0000000
F	4.4130259	3.3538998	0.0000000
H	4.9404521	4.1133987	0.0000000

35.

C	-2.2347379	-0.0190394	0.0000000
C	-0.9113589	-0.4255711	0.0000000
C	0.0844741	0.5619602	0.0000000
C	-0.2601631	1.9221827	0.0000000
C	-1.6016701	2.2878580	0.0000000
C	-2.6036961	1.3195136	0.0000000
H	-0.6631184	-1.4803003	0.0000000
H	0.5217041	2.6725178	0.0000000
H	-1.8729004	3.3373063	0.0000000
H	-3.6547748	1.5825788	0.0000000
C	1.4516273	0.1793998	0.0000000
C	2.6338199	-0.1434860	0.0000000
F	-3.1934533	-0.9538891	0.0000000
C	3.9496639	-0.5022204	0.0000000
N	5.0838765	-0.8106660	0.0000000
H	6.8462656	-1.2866491	0.0000000
F	7.7523527	-1.5314444	0.0000000
F	-5.3734370	-2.9954148	0.0000000
H	-5.9544738	-3.7146365	0.0000000

36.

C	-2.3418524	-0.2319163	0.0000000
C	-0.9829367	-0.4963972	0.0000000
C	-0.0975847	0.5914553	0.0000000
C	-0.5833434	1.9080516	0.0000000
C	-1.9560644	2.1294189	0.0000000
C	-2.8499587	1.0604083	0.0000000
H	-0.6245969	-1.5189500	0.0000000
H	0.1148953	2.7367027	0.0000000
H	-2.3369977	3.1442051	0.0000000
H	-3.9229919	1.2108706	0.0000000
C	1.3010623	0.3537991	0.0000000
C	2.5106629	0.1512052	0.0000000
F	-3.1958525	-1.2623624	0.0000000
C	3.8516888	-0.0751883	0.0000000
N	5.0112657	-0.2708419	0.0000000
I	7.4615307	-0.6611765	0.0000000
F	9.3841722	-0.9632155	0.0000000
F	-5.0974336	-3.5307540	0.0000000
H	-5.6456650	-4.2753148	0.0000000

43.

C	0.0000000	0.0000000	-1.0069872
C	1.2029560	0.0000000	-0.3212735
C	-1.1546969	0.0000000	1.0644391
C	-1.2029560	0.0000000	-0.3212735
H	2.1462051	0.0000000	-0.8522415

H	-2.0659837	0.0000000	1.6493471
H	-2.1462051	0.0000000	-0.8522415
F	0.0000000	0.0000000	-2.3372457
N	0.0000000	0.0000000	1.7567898
C	1.1546969	0.0000000	1.0644391
H	2.0659837	0.0000000	1.6493471
Ag	0.0000000	0.0000000	3.8195523
Cl	0.0000000	0.0000000	6.0676258
F	0.0000000	0.0000000	-5.2277240
H	0.0000000	0.0000000	-6.1525534

44.

C	0.0000000	0.0000000	-1.7212161
C	1.2174268	0.0000000	-1.0534462
C	1.2191580	0.0000000	0.3345978
C	0.0000000	0.0000000	1.0233461
C	-1.2191580	0.0000000	0.3345978
C	-1.2174268	0.0000000	-1.0534462
H	2.1394762	0.0000000	-1.6219951
H	2.1531767	0.0000000	0.8843144
H	-2.1531767	0.0000000	0.8843144
H	-2.1394762	0.0000000	-1.6219951
C	0.0000000	0.0000000	2.4467310
N	0.0000000	0.0000000	3.6129358
F	0.0000000	0.0000000	-3.0568295
Ag	0.0000000	0.0000000	5.6221773
Cl	0.0000000	0.0000000	7.8730256

F	0.0000000	0.0000000	-5.9811793
H	0.0000000	0.0000000	-6.9059325

45.

C	1.2163702	0.0000000	-1.9186527
C	1.2166863	0.0000000	-0.5304996
C	0.0000000	0.0000000	0.1691125
C	-1.2166863	0.0000000	-0.5304996
C	-1.2163702	0.0000000	-1.9186527
C	0.0000000	0.0000000	-2.5880036
H	2.1524269	0.0000000	0.0168484
H	-2.1524269	0.0000000	0.0168484
H	-2.1392038	0.0000000	-2.4862979
C	0.0000000	0.0000000	1.5857468
C	0.0000000	0.0000000	2.8126143
C	0.0000000	0.0000000	4.1700798
N	0.0000000	0.0000000	5.3430609
Ag	0.0000000	0.0000000	7.3490894
Cl	0.0000000	0.0000000	9.6005516
H	2.1392038	0.0000000	-2.4862979
F	0.0000000	0.0000000	-3.9254369
F	0.0000000	0.0000000	-6.8774617
H	0.0000000	0.0000000	-7.8021497

46.

C	-0.8644076	-0.1189002	0.0000000
C	0.4136434	-0.6583802	0.0000000

C	1.3294602	1.4685572	0.0000000
C	0.0706460	2.0548846	0.0000000
C	-1.0633841	1.2512810	0.0000000
H	0.5607297	-1.7312779	0.0000000
H	2.2310676	2.0673352	0.0000000
H	-0.0163747	3.1343514	0.0000000
H	-2.0677293	1.6574106	0.0000000
N	1.5006250	0.1325394	0.0000000
F	-1.9066766	-0.9460058	0.0000000
Ag	3.3967762	-0.6806257	0.0000000
Cl	5.4674115	-1.5545572	0.0000000
F	-4.1661425	-2.7473230	0.0000000
H	-4.8856446	-3.3292894	0.0000000

47.

C	1.5102843	0.2080121	0.0000000
C	1.9089775	-1.1225219	0.0000000
C	0.9345787	-2.1178701	0.0000000
C	-0.4167019	-1.7888500	0.0000000
C	-0.7815773	-0.4373991	0.0000000
C	0.1767901	0.5824123	0.0000000
H	2.9663993	-1.3593928	0.0000000
H	1.2339600	-3.1593395	0.0000000
H	-0.1013919	1.6294775	0.0000000
F	2.4428061	1.1624551	0.0000000
C	-2.1631386	-0.0878875	0.0000000
N	-3.2949500	0.1926883	0.0000000

H	-1.1810554	-2.5565120	0.0000000
Cl	-7.4352033	1.1929987	0.0000000
Ag	-5.2470094	0.6673719	0.0000000
F	4.4009461	3.1660443	0.0000000
H	5.0462856	3.8283126	0.0000000

48.

C	-2.3170013	-0.2547903	0.0000000
C	-0.9580010	-0.5190988	0.0000000
C	-0.0741744	0.5701264	0.0000000
C	-0.5588029	1.8872210	0.0000000
C	-1.9315708	2.1076802	0.0000000
C	-2.8245657	1.0380316	0.0000000
H	-0.5992278	-1.5415625	0.0000000
H	0.1390000	2.7162297	0.0000000
H	-2.3130844	3.1221959	0.0000000
H	-3.8976750	1.1887908	0.0000000
C	1.3238529	0.3339887	0.0000000
C	2.5343926	0.1340747	0.0000000
F	-3.1698886	-1.2836885	0.0000000
C	3.8740642	-0.0862653	0.0000000
N	5.0316888	-0.2758793	0.0000000
Ag	7.0116519	-0.5944833	0.0000000
Cl	9.2346348	-0.9490558	0.0000000
F	-4.9578271	-3.4406571	0.0000000
H	-5.5474662	-4.1528581	0.0000000