Electronic Supplementary Material for PCCP

Physical Chemistry Chemical Physics

Supporting Information for the paper:

Divalent carbon atom as the proton acceptor in hydrogen bonding

by

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1. General information:

Optimized geometries of the H-bonded complexes discussed in the paper are given together with the total energy calculated at the corresponding level of theory (page S7 and subsequent). Note, that optimizations with the use of DFT approximation were done with Opt=Tight option. This concerns both H-bonded complexes as well as monomers. Total energy given in hartrees, geometry in Å.

2. Interaction energy and counterpoise correction:

In the supermolecular approach the interaction energy, ΔE, was calculated as the difference between the total energy of the complex (*AB*) and the sum of total energies of isolated monomers (*A* and *B*):

$$\Delta E = E_{\mathrm{AB}}^{\mathrm{AB}}(\mathrm{AB}) - [E_{\mathrm{A}}^{\mathrm{A}}(\mathrm{A}) + E_{\mathrm{B}}^{\mathrm{B}}(\mathrm{B})]. \quad (1)$$

where the subscripts refer to the basis set, the superscripts correspond to the geometry, and the label in parentheses denotes the system. To take into account the basis set superposition error [S. F. Boys and F. Bernardi, *Mol. Phys.*, 1970, **19**, 553.] the counterpoise correction and corrected interaction energy, ΔE(CP), were also computed according to the equation:

$$\Delta E(\mathrm{CP}) = E_{\mathrm{AB}}^{\mathrm{AB}}(\mathrm{AB}) - [E_{\mathrm{AB}}^{\mathrm{AB}}(\mathrm{A}) + E_{\mathrm{AB}}^{\mathrm{AB}}(\mathrm{B})]. \quad (2)$$

In calculations of ΔE(CP) the total energies of all systems were calculated using the basis set and geometry of the whole system AB. In the case of very strong interactions this may lead to a greater energy penalty caused by geometry distortions of subsystems from their isolated forms than energy gains due to the larger basis set. As a consequence, ΔE(CP) defined by eq. (2) can be obtained as lower (*i.e.* more negative) than ΔE. To take this effect into account, the interaction energy containing the deformation correction was also computed by eq. 3:

$$\Delta E(\mathrm{BSSE}) = \Delta E + [E_{\mathrm{A}}^{\mathrm{AB}}(\mathrm{A}) - E_{\mathrm{AB}}^{\mathrm{AB}}(\mathrm{A})] + [E_{\mathrm{B}}^{\mathrm{AB}}(\mathrm{B}) - E_{\mathrm{AB}}^{\mathrm{AB}}(\mathrm{B})]. \quad (3)$$

Thus, ΔE(BSSE) converges to ΔE as the basis set approaches the complete basis set (CBS) limit. [S. S. Xantheas, *J. Chem. Phys.*, 1996, **104**, 8821.]

For all MP2 calculations the $\Delta E > \Delta E$(CP) relation was always fulfilled (the interaction energy defined as negative value). In the case of DFT calculations $\Delta E < \Delta E$(CP) were found for the strongest interactions. This results from the large energy loss due to the

strong geometry deformation of subsystems upon interaction. Nevertheless, this relation is opposite if the deformation correction is included in energy calculations (see eq. 3). The BSSE-corrected interaction energy obtained on the DFT level of theory was almost the same as the uncorrected counterpart (the difference being less than 0.2 kcal/mol). As shown in Table 1 for MP2/aug-cc-pVTZ the BSSE correction becomes more significant.

3. Interaction energy curves for $C(NH_3)_2$ and $C(PH_3)_2$ interacting with H^+ and the helium atom:

To support conclusion, according to which proton accepting abilities of C(0) are greater in $C(NH_3)_2$ as compared with those of $C(PH_3)_2$ the interaction energy curves were calculated (DFT/aug-cc-pVTZ, C_{2V} symmetry) for $C(NH_3)_2$ and $C(PH_3)_2$ interacting with H^+ and the helium atom (1s function as a contraction of 3 primitive GTOs was used to represent the basis set of H^+ and He). The very small basis set taken for He was meant to obtain mostly the repulsive contribution to the total interaction energy. These calculations showed that for $C(NH_3)_2$ the attractive contribution is more significant than in the case of $C(PH_3)_2$. The two curves for the interaction with He are close to each other, whereas the interaction energy for H^+ is much lower in the case of $[C(NH_3)_2\cdots H]^+$. See Fig. 4(a,b) for graphical representations.

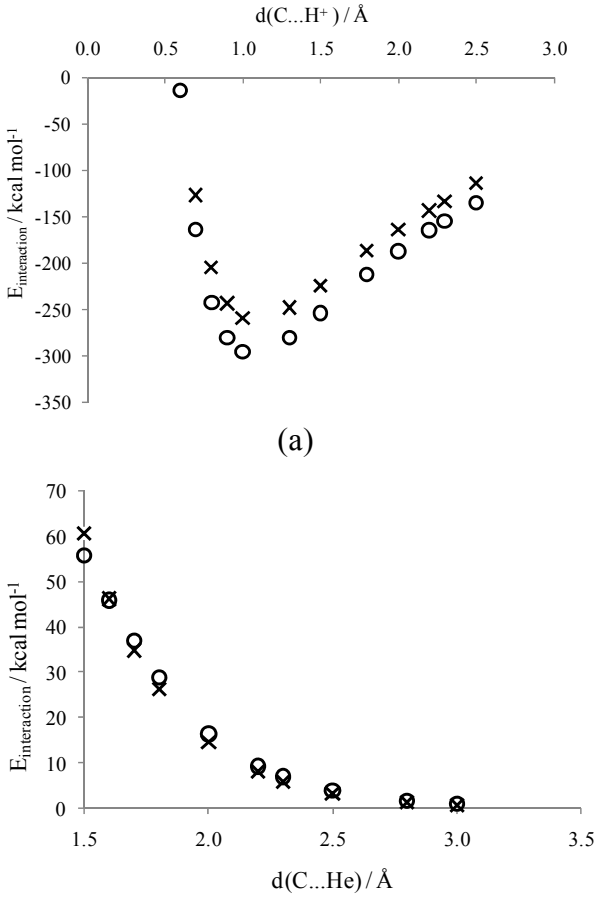

Fig. S1. Interaction energy curves (DFT/aug-cc-pVTZ, C_{2V} symmetry) for $C(NH_3)_2$ (circles) and $C(PH_3)_2$ (crosses) interacting with H^+, (a), and the helium atom, (b). 1s function as a contraction of 3 primitive GTOs has been used to represent the basis set of H^+ and He. Circles and crosses correspond to data obtained for $C(NH_3)_2$ and $C(PH_3)2$, respectively.

4. Optimized geometries and total energies of the H-bonded complexes discussed in the paper:

level: MP2/Aug-cc-pVTZ
complex: $(NH_4)_2C...HCF3$ (with two additional H-bonds)

C	0.034597	-0.018786	-0.049354
N	-0.070083	0.119893	1.461784
N	1.546920	-0.081620	-0.200400
H	0.304591	0.988481	1.897346
H	-1.072447	0.130153	1.630777
H	0.304619	-0.662729	2.030020
H	2.029862	-0.877209	0.257462
H	1.680883	-0.213768	-1.199389
H	2.096034	0.765624	0.054559
H	-0.264627	2.229697	-0.613796
C	0.249220	3.111240	-0.217779
F	1.581436	2.981865	-0.420610
F	0.069753	3.169752	1.122675
F	-0.124627	4.287902	-0.727264

E=-488.5739075

level: MP2/Aug-cc-pVTZ
complex: $(NH_4)_2C...HCF_3$ (with one additional H-bond)

C	0.057330	0.000000	-0.666310
N	-0.244452	0.000000	0.813995
N	1.562858	0.000000	-0.646131
H	1.820020	0.000000	-1.629694
H	2.034359	0.826952	-0.225120
H	2.034359	-0.826952	-0.225120
H	-1.263616	0.000000	0.860912
H	0.068443	-0.826552	1.360638
H	0.068443	0.826552	1.360638
H	-1.838993	0.000000	-1.619114
C	-2.914180	0.000000	-1.419837
F	-3.108471	0.000000	-0.067093
F	-3.540230	1.081679	-1.899308
F	-3.540230	-1.081679	-1.899308

E=-488.5757547

level: B3LYP/Aug-cc-pVTZ
complex: $(NH_4)_2C...HCF_3$

C	0.001073	0.002998	-0.004386
F	-0.017153	0.018421	1.339207
F	1.317452	-0.005028	-0.385597
F	-0.523569	1.162906	-0.436075
N	1.237864	-2.596913	-2.089221
C	-0.193955	-2.638296	-1.647109
N	-0.693154	-3.859441	-2.343179
H	-1.669547	-3.927802	-2.073041
H	-0.686593	-3.863148	-3.396128
H	-0.260130	-4.783366	-2.086583
H	1.626230	-1.770003	-1.638486
H	1.857124	-3.395103	-1.806386
H	1.425648	-2.478693	-3.115291
H	-0.492677	-0.877842	-0.433153

E=-4 89.4598877

level: MP2/Aug-cc-pVTZ
complex: $(NH_4)_2C...HCCH$

C	0.250129	0.353252	-0.058624
N	0.204734	0.235832	1.442242
N	1.606203	-0.226238	-0.343049
H	1.703012	-0.142560	-1.351532
H	2.430505	0.266329	0.070387
H	1.756787	-1.231360	-0.123057
H	-0.681519	0.677781	1.706674
H	0.179409	-0.718544	1.846965
H	0.944872	0.741397	1.976570
H	-1.356023	1.628921	-0.057908
C	-2.129930	1.987119	0.622938
C	-2.918652	2.341447	1.481411
H	-3.633988	2.666457	2.196550

E=-227.8895852

level: B3LYP/Aug-cc-pVTZ
complex: $(NH_4)_2C...HCCH$ (with one additional H-bond)

C	0.249655	0.291686	-0.008646
N	0.247729	0.128910	1.478736
N	1.607377	-0.206585	-0.366220
H	1.673214	-0.077103	-1.371190
H	2.440277	0.301865	0.048227
H	1.825653	-1.217107	-0.196254
H	-0.640678	0.528063	1.786817
H	0.273947	-0.839236	1.868731
H	0.995038	0.643672	2.018527
H	-1.378493	1.646118	0.030511
C	-2.175532	2.050270	0.652620
C	-3.006244	2.472989	1.410760
H	-3.756407	2.856291	2.056947

E=-228.4388617

level: MP2/Aug-cc-pVTZ
complex: $(NH_3)_2C...HCCH$

C	0.129888	0.000000	-0.043037
N	-0.010529	0.000000	1.441083
N	1.610490	0.000000	-0.202242
H	1.765056	0.000000	-1.205947
H	2.145621	0.828547	0.170166
H	2.145621	-0.828547	0.170166
H	-1.012331	0.000000	1.609445
H	0.368588	-0.828437	1.970815
H	0.368588	0.828437	1.970815
H	-1.624919	0.000000	-1.371717
C	-2.551769	0.000000	-1.934365
C	-3.582742	0.000000	-2.549519
H	-4.492240	0.000000	-3.096662

E= =-228.4380736

level: MP2/Aug-cc-pVTZ
complex: $(PH_3)_2C...H2O$

C	-0.120393	0.373629	0.157085
P	0.095716	0.057787	1.772406
P	1.101343	0.118834	-0.941988
H	-1.108395	0.113228	2.486714
H	0.596658	-1.192474	2.221365
H	0.891668	0.901373	2.588569
H	0.633076	0.193256	-2.259627
H	2.209963	0.998377	-1.020220
H	1.808647	-1.110612	-0.985717
H	-1.709503	-0.087486	-0.898750
O	-2.368549	-0.345532	-1.580213
H	-2.913124	0.439490	-1.685359

E= -799.5946051

level: B3LYP/Aug-cc-pVTZ
complex: $(PH_3)_2C...H2O$

C	-0.010060	-0.016717	0.012765
P	0.004543	-0.011142	1.665594
P	1.303888	-0.004964	-0.990360
O	-2.442590	1.189865	-1.234571
H	0.932700	0.021055	-2.347347
H	2.248901	1.065939	-0.975210
H	2.230453	-1.090680	-1.007934
H	-1.294522	0.007071	2.206127
H	0.563994	-1.096912	2.404469
H	0.591493	1.059861	2.406237
H	-1.650031	0.783504	-0.818736
H	-2.991536	0.446297	-1.497676

E= -800.8439337

level: MP2/Aug-cc-pVTZ
complex: $(PH_3)_2C...HCF3$

C	1.228091	-0.142956	-0.000006
P	1.506807	1.496687	0.000003
P	2.503809	-1.206797	-0.000010
C	-2.047723	-0.243656	-0.000012
F	-2.682144	-0.712707	1.083534
F	-2.176841	1.097096	-0.000076
F	-2.682301	-0.712818	-1.083420
H	2.077497	-2.541864	-0.000085
H	3.432222	-1.252721	-1.072954
H	3.432160	-1.252837	1.072984
H	0.311586	2.227865	-0.000132
H	2.184615	2.131036	1.073350
H	2.184859	2.131007	-1.073209
H	-0.992823	-0.515318	-0.000081

E= -1061.1086344

level: B3LYP/Aug-cc-pVTZ
complex: $(PH3)_2C...HCF3$

C	-0.019103	-0.004551	0.034355
P	0.021979	0.008635	1.686329
P	1.295027	-0.013067	-0.968287
C	-2.971808	-0.080338	-1.649430
F	-2.685874	-0.398130	-2.928772
F	-3.827081	-1.007808	-1.177091
F	-3.612090	1.104623	-1.654400
H	0.927790	-0.025522	-2.327625
H	2.230739	1.066196	-0.982372
H	2.232082	-1.091257	-0.963104
H	-1.267409	0.012909	2.252664
H	0.604533	-1.064045	2.428489
H	0.604028	1.093220	2.411422
H	-2.060106	-0.037503	-1.046671

E=-1062.7552015

level: MP2/Aug-cc-pVTZ
complex: $(PH_4)_2C...HCN$

C	-0.072251	0.000001	0.093260
P	0.042305	0.000000	1.750056
P	1.275499	0.000000	-0.878478
C	-2.276073	0.000000	-2.111390
N	-2.960092	-0.000001	-3.059259
H	0.920086	0.000000	-2.236151
H	2.200628	1.074155	-0.862906
H	2.200627	-1.074156	-0.862906
H	-1.217201	0.000000	2.363218
H	0.653671	-1.073756	2.445761
H	0.653672	1.073755	2.445762
H	-1.621489	0.000000	-1.239104

E=-816.5260117

level: B3LYP/Aug-cc-pVTZ
complex: $(PH_4)_2C...HCN$

C	-0.008546	0.000000	0.016393
P	0.009755	0.000000	1.670662
P	1.314337	0.000000	-0.977119
C	-2.851337	0.000000	-1.437426
N	-3.869491	0.000000	-1.968065
H	0.951733	0.000000	-2.337567
H	2.248593	1.079003	-0.972816
H	2.248593	-1.079003	-0.972816
H	-1.289559	0.000000	2.212784
H	0.582698	-1.078918	2.408747
H	0.582698	1.078918	2.408747
H	-1.881815	0.000000	-0.933330

E= -817.8410815

level: MP2/Aug-cc-pVTZ
complex: $(PH_3)_2C...HCCH$

C	0.141900	0.000000	-0.109817
P	0.191549	0.000000	1.550270
P	1.534460	0.000000	-1.011464
H	-1.101038	0.000000	2.097063
H	0.769099	-1.073329	2.277220
H	0.769099	1.073329	2.277220
H	1.271692	0.000000	-2.388212
H	2.462597	1.072659	-0.947063
H	2.462597	-1.072659	-0.947063
H	-2.063214	0.000000	-0.283148
C	-3.102381	0.000000	-0.002072
C	-4.270904	0.000000	0.331859
H	-5.294697	0.000000	0.614883

E= -800.4246538

level: B3LYP/Aug-cc-pVTZ
complex: $(PH_3)_2C...HCCH$

C	-0.019984	0.017495	0.046730
P	0.037480	0.001891	1.695353
P	1.261028	0.003774	-0.992593
C	-3.140896	0.115108	-1.313174
C	-4.242969	0.150450	-1.783340
H	0.855614	0.023144	-2.341480
H	2.217421	1.065418	-1.016854
H	2.178572	-1.090997	-1.036169
H	-1.246273	0.020711	2.274966
H	0.606892	-1.093603	2.415079
H	0.647014	1.062584	2.434073
H	-2.152730	0.083572	-0.890989
H	-5.218817	0.181729	-2.200030

E=-801.736351

level: B3LYP/Aug-cc-pVTZ
complex: $[(P(CH3)]_2C...H2O$

C	-0.012554	-0.010940	0.000262
P	0.000653	0.005075	1.652694
C	1.630682	-0.026169	2.522695
P	0.610858	-1.033571	-1.138006
C	-0.077704	-2.746171	-1.246482
C	0.315255	-0.379525	-2.821095
C	2.430649	-1.355820	-1.129684
C	-0.778834	1.534799	2.285905
C	-0.932096	-1.317917	2.546271
O	-2.664167	0.944328	-0.910290
H	0.696782	-1.055063	-3.586658
H	-0.756155	-0.238688	-2.954483
H	0.804626	0.588831	-2.910950
H	2.734347	-1.966396	-1.980954
H	2.956850	-0.403176	-1.163125
H	2.705100	-1.872015	-0.210322
H	0.328570	-3.295416	-2.096966
H	0.154784	-3.288478	-0.330519
H	-1.160107	-2.677685	-1.343343
H	-0.815545	1.546408	3.375223
H	-0.209641	2.392017	1.930199
H	-1.788104	1.599213	1.882205
H	1.510961	0.078218	3.601768
H	2.136471	-0.968263	2.313994
H	2.247003	0.789210	2.147531
H	-0.942863	-1.150559	3.624230
H	-1.954613	-1.332609	2.172219
H	-0.474926	-2.285733	2.342501
H	-1.765221	0.646665	-0.615164
H	-2.534908	1.842184	-1.227843

E=-1036.8994911

level: B3LYP/Aug-cc-pVTZ
complex: $[(P(CH3)]_2C...HCF3$

C	0.063090	0.039800	0.018625
P	0.039488	0.018009	1.669901
C	1.638460	-0.164641	2.582431
P	0.652927	-1.020859	-1.101282
C	-0.097384	-2.709854	-1.200800
C	0.412515	-0.383518	-2.801035
C	2.459615	-1.417444	-1.075932
C	-0.619727	1.590846	2.338047
C	-1.017364	-1.245798	2.510552
C	-1.780236	2.542751	-1.314812
F	-2.384280	2.121265	-2.446020
F	-2.748992	2.908548	-0.448313
F	-1.068636	3.646061	-1.619742
H	0.805340	-1.075951	-3.545400
H	-0.650300	-0.227890	-2.978287
H	0.921591	0.574412	-2.893831
H	2.746569	-2.048826	-1.917848
H	3.023019	-0.486464	-1.114640
H	2.706241	-1.932956	-0.148456
H	0.303027	-3.283435	-2.037901
H	0.101030	-3.250046	-0.275504
H	-1.175323	-2.607619	-1.316309
H	-0.643264	1.583237	3.427803
H	0.010078	2.410290	1.995349
H	-1.627167	1.748311	1.956680
H	1.500004	-0.076035	3.660705
H	2.072972	-1.139060	2.361934
H	2.327542	0.606972	2.242878
H	-1.041935	-1.102754	3.591656
H	-2.028467	-1.172565	2.113132
H	-0.632945	-2.241982	2.293960
H	-1.145335	1.756882	-0.888601

E= -1298.8086084

level: B3LYP/Aug-cc-pVTZ
complex: $[(P(CH3)]_2C...HCN$

C	-0.07375	0.0882	-0.03427
P	-0.01176	0.00643	1.61865
C	1.64586	-0.03998	2.43539
P	0.4949	-0.93669	-1.20403
C	-0.20929	-2.6439	-1.29521
C	0.14958	-0.27367	-2.87408
C	2.31094	-1.277	-1.27139
C	-0.7897	1.48163	2.37115
C	-0.88478	-1.38727	2.4631
H	-0.75146	1.43683	3.45927
H	-0.26942	2.37446	2.02862
H	-1.82775	1.54374	2.04894
H	-0.85071	-1.28733	3.54879
H	-1.92259	-1.40172	2.13411
H	-0.41995	-2.33134	2.18068
H	1.56208	0.00247	3.52202
H	2.16188	-0.95827	2.15719
H	2.23404	0.80667	2.08513
H	0.52148	-0.94348	-3.64893
H	-0.9248	-0.14523	-2.99432
H	0.62655	0.69923	-2.9793
H	0.16973	-3.19137	-2.15914
H	0.04773	-3.19252	-0.38973
H	-1.29384	-2.57267	-1.36025
H	2.57531	-1.88732	-2.13583
H	2.84436	-0.32913	-1.32246
H	2.61769	-1.79831	-0.36519
H	-0.96063	1.77531	-0.7603
C	-1.44117	2.68872	-1.15481
N	-1.94054	3.63871	-1.56529

E=-1053.8952917

level: B3LYP/Aug-cc-pVTZ
complex: $[(P(CH3)]_2C...HCCH$

C	0.046242	-0.015853	0.001669
P	0.022759	-0.011193	1.649708
C	1.628874	0.096364	2.562869
P	0.629774	1.027377	-1.132949
C	-0.101827	2.725184	-1.232614
C	2.441427	1.405096	-1.138353
C	0.355852	0.382548	-2.824923
C	-0.980155	1.284455	2.510176
C	-0.699715	-1.562837	2.302252
C	-1.591847	-2.681280	-1.326412
C	-2.175271	-3.619376	-1.793428
H	0.745481	1.064878	-3.580359
H	0.847964	-0.583946	-2.918261
H	-0.711807	0.238650	-2.981491
H	0.291153	3.288141	-2.080480
H	-1.182663	2.634539	-1.329230
H	0.118747	3.268902	-0.314471
H	2.722915	2.029730	-1.987252
H	2.706606	1.921497	-0.216391
H	2.994061	0.467823	-1.181093
H	-0.724008	-1.566047	3.392066
H	-1.711620	-1.672780	1.916124
H	-0.106703	-2.404579	1.948759
H	-1.004160	1.130427	3.589926
H	-0.558610	2.267417	2.302261
H	-1.995694	1.254589	2.118369
H	1.488731	-0.000957	3.640251
H	2.286333	-0.697145	2.211241
H	2.100504	1.055854	2.353152
H	-1.068206	-1.836479	-0.906000
H	-2.691105	-4.450039	-2.206839

E= -1037.7883362

level: MP2/Aug-cc-pVTZ
complex: $F_2C...H2O$

C	0.000000	0.000000	0.000000
F	0.000000	0.000000	1.296941
F	1.246671	0.000000	-0.346787
O	-2.159904	0.002337	-2.342060
H	-1.611228	0.000507	-1.546569
H	-3.062270	0.008807	-2.012364

E= -313.7415698

level: B3LYP/Aug-cc-pVTZ
complex: $F_2C...H2O$

C	0.005372	-0.012262	-0.006449
F	-0.009847	-0.015386	1.290328
F	1.261300	0.019432	-0.338960
O	-2.807862	-0.089407	-1.541432
H	-1.905659	-0.062770	-1.193382
H	-2.714400	-0.079018	-2.497939

E= - 314.2685972

level: MP2/Aug-cc-pVTZ
complex: $F_2C...HCF3$

C	0.803294	-0.101972	0.616056
F	0.633934	-1.330383	0.997688
F	1.991486	0.222112	1.023978
H	-0.894170	1.413720	-0.666917
C	-1.616029	2.074038	-1.136587
F	-1.004221	2.950573	-1.941867
F	-2.492328	1.376065	-1.868783
F	-2.298501	2.761912	-0.213214

E= -575.2571609

level: B3LYP/Aug-cc-pVTZ
complex: $F_2C...HCF3$

C	-0.006274	-0.002035	0.009838
F	0.067331	-0.316734	1.269399
F	1.209967	0.298061	-0.338755
C	-3.095649	0.039531	-2.157366
F	-4.008373	-0.840122	-1.712457
F	-3.654022	1.261520	-2.154915
F	-2.788748	-0.279346	-3.425761
H	-2.206152	0.021843	-1.530154

E= -576.1818116

level: MP2/Aug-cc-pVTZ
complex: $Cl_2C...H2O$

C	0.064615	0.042755	-0.073994
Cl	-0.127928	-0.097200	1.605088
Cl	1.713715	0.009665	-0.487836
O	-2.631361	0.295311	-1.543298
H	-1.725681	0.222662	-1.201681
H	-2.524005	0.356532	-2.496139

E= -1033.6721813

level: B3LYP/Aug-cc-pVTZ
complex: $Cl_2C...H2O$

C	-0.001201	0.000481	0.001381
Cl	0.001952	-0.000779	1.721701
Cl	1.602555	0.000844	-0.606835
O	-2.360140	0.005562	-2.059445
H	-1.688825	0.003239	-1.358385
H	-3.205932	0.003825	-1.603122

E= -1034.951641

level: MP2/Aug-cc-pVTZ
complex: $Cl_2C...HCF3$ (linear geometry)

C	-0.017004	-0.220644	0.362533
Cl	0.864464	-0.658797	1.751138
Cl	0.958366	0.710748	-0.676229
C	-3.409225	-1.139391	-0.224035
F	-3.641880	-2.372483	0.244607
F	-3.702420	-1.130138	-1.530944
F	-4.245665	-0.295833	0.394722
H	-2.375257	-0.851003	-0.056951

E= -1295.1872849

level: MP2/Aug-cc-pVTZ
complex: $Cl_2C...HCF3$ (bent geometry)

C	0.475173	-0.232837	0.476882
Cl	0.974658	-1.705332	1.173588
Cl	1.767460	0.874075	0.465395
H	-1.485698	1.011233	-0.584446
C	-1.541043	2.021878	-0.974273
F	-0.657493	2.189275	-1.966773
F	-2.760623	2.297661	-1.450651
F	-1.257754	2.910111	-0.012744

E= -1295.1874047

level: B3LYP/Aug-cc-pVTZ
complex: $Cl_2C...HCF3$

C	0.007780	0.007347	-0.011385
Cl	-0.031529	0.053068	1.709906
Cl	1.635470	-0.075627	-0.567951
C	-3.011370	-0.003821	-2.093330
F	-2.808604	0.543140	-3.304286
F	-3.421829	-1.271598	-2.270338
F	-4.000904	0.675337	-1.488057
H	-2.100383	0.026870	-1.496889

E= -1296.8644691

level: MP2/Aug-cc-pVTZ
complex: imidazol-2-ylidene...H2O

C	-0.000019	-0.004859	-0.006456
N	-0.013139	0.034746	1.369178
C	1.224480	0.048962	1.937197
N	2.016302	0.018244	0.829204
C	1.317571	-0.014728	-0.359773
O	-0.493984	-0.075504	4.188423
H	3.019213	0.017219	0.897953
H	-0.833072	0.046617	1.959771
H	1.787102	-0.041714	-1.326065
H	-0.887747	-0.022668	-0.611753
H	0.383625	-0.018393	3.752942
H	-0.462533	0.579739	4.890506

E= -302.0934286

level: B3LYP/Aug-cc-pVTZ
complex: imidazol-2-ylidene...H2O

C	-0.000474	-0.001341	0.000236
C	0.001065	-0.000555	1.351698
N	1.334478	0.002113	1.726891
C	2.193384	0.005400	0.676498
N	1.336031	0.002066	-0.376204
O	4.157037	0.189808	2.762638
H	1.657801	0.005701	-1.327035
H	1.682008	0.008898	2.672506
H	-0.813553	-0.003961	-0.701817
H	-0.812656	-0.001499	2.053004
H	3.820563	0.118178	1.842022
H	4.869203	-0.451454	2.829911

E=-302.7439202

level: MP2/Aug-cc-pVTZ
complex: imidazol-2-ylidene...HCF3

C	0.089840	-0.200624	-0.201333
N	-0.322665	0.289725	1.020157
C	0.692563	0.559942	1.889734
N	1.769638	0.205605	1.130420
C	1.449903	-0.254897	-0.128693
H	2.706492	0.286614	1.491079
H	-1.283492	0.443862	1.272615
H	2.179306	-0.574034	-0.850476
H	-0.582980	-0.463253	-0.997056
H	1.703241	1.265879	3.911851
C	2.700067	1.365742	4.334015
F	2.864594	0.609459	5.424454
F	3.616608	0.964018	3.420798
F	2.986702	2.631223	4.657570

E= -563.6062225

level: B3LYP/Aug-cc-pVTZ
complex: imidazol-2-ylidene...HCF3

C	-0.014131	0.019108	0.009322
C	0.017113	-0.018818	1.358595
N	1.361948	-0.031740	1.702004
C	2.201376	-0.003748	0.632939
N	1.313439	0.027288	-0.395999
C	5.673782	-0.002037	0.724830
F	6.207556	1.027517	0.037917
F	6.068864	0.113267	2.009488
F	6.202816	-1.140313	0.234280
H	1.611401	0.053723	-1.354408
H	1.704036	-0.058732	2.645627
H	-0.843024	0.040300	-0.673633
H	-0.779335	-0.037147	2.079205
H	4.583643	-0.006313	0.649573

E= -564.6540572