

Influence of ring size on the strength of carbon bonding complexes between anions and perfluorocycloalkanes

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Supplementary Information

Table of Contents:

Cartesian coordinates	Pages 2-12
CSD reference codes	Page 13

Optimized geometries:

1. D_{3d}

C	1.2865712	-0.7428022	-0.2129976
C	1.2865712	0.7428022	0.2129976
C	0.0000000	1.4856045	-0.2129976
C	-1.2865712	0.7428022	0.2129976
C	-1.2865712	-0.7428022	-0.2129976
C	0.0000000	-1.4856045	0.2129976
F	-1.4000273	0.8083061	1.5489905
F	-2.3412547	1.3517241	-0.3440521
F	0.0000000	-1.6166123	1.5489905
F	-2.3412547	-1.3517241	0.3440521
F	-1.4000273	-0.8083061	-1.5489905
F	0.0000000	-2.7034481	-0.3440521
F	1.4000273	-0.8083061	-1.5489905
F	2.3412547	-1.3517241	0.3440521
F	1.4000273	0.8083061	1.5489905
F	2.3412547	1.3517241	-0.3440521
F	0.0000000	1.6166123	-1.5489905
F	0.0000000	2.7034481	0.3440521

1. D_{6h}

C	1.3712479	-0.7916903	0.0000000
C	1.3712479	0.7916903	0.0000000
C	0.0000000	1.5833807	0.0000000
C	-1.3712479	0.7916903	0.0000000
C	-1.3712479	-0.7916903	0.0000000
C	0.0000000	-1.5833807	0.0000000
F	2.0539941	-1.1858740	1.0823355
F	2.0539941	-1.1858740	-1.0823355
F	0.0000000	-2.3717481	-1.0823355
F	0.0000000	-2.3717481	1.0823355
F	-2.0539941	-1.1858740	1.0823355
F	-2.0539941	1.1858740	1.0823355
F	0.0000000	2.3717481	1.0823355
F	0.0000000	2.3717481	-1.0823355
F	2.0539941	1.1858740	1.0823355
F	2.0539941	1.1858740	-1.0823355
F	-2.0539941	1.1858740	-1.0823355
F	-2.0539941	-1.1858740	-1.0823355

2. C₁

C	0.4237364	1.1854399	0.3257629
C	1.3057287	-0.0262530	-0.0857473
C	0.3282853	-1.2564442	-0.1696370
C	-1.0972466	-0.6935096	0.1212223

C	-0.9834741	0.8144495	-0.1789598
F	-1.9488097	1.5340696	0.3905176
F	-1.0152864	0.9858165	-1.5140990
F	0.8632903	2.3337508	-0.1898659
F	0.3974707	1.2784260	1.6651866
F	1.8460650	0.2078514	-1.2874900
F	2.2800823	-0.2392652	0.8011352
F	0.3602731	-1.7835077	-1.3982513
F	0.6616382	-2.1936480	0.7208536
F	-1.3876627	-0.8616483	1.4201604
F	-2.0340904	-1.2855277	-0.6207883

2. D₅H

C	-1.0782543	0.7833976	0.0000000
C	-1.0782543	-0.7833976	0.0000000
C	0.4118565	-1.2675640	0.0000000
C	1.3327956	0.0000000	0.0000000
C	0.4118565	1.2675640	0.0000000
F	0.6517879	2.0059968	-1.0881205
F	0.6517879	2.0059968	1.0881205
F	-1.7064028	1.2397742	1.0881205
F	-1.7064028	1.2397742	-1.0881205
F	-1.7064028	-1.2397742	1.0881205
F	-1.7064028	-1.2397742	-1.0881205
F	0.6517879	-2.0059968	1.0881205
F	0.6517879	-2.0059968	-1.0881205
F	2.1092299	0.0000000	-1.0881205
F	2.1092299	0.0000000	1.0881205

3. D₄H

C	0.7834219	-0.7834219	0.0000000
C	0.7834219	0.7834219	0.0000000
C	-0.7834219	0.7834219	0.0000000
C	-0.7834219	-0.7834219	0.0000000
F	1.3222770	1.3222770	1.0933658
F	-1.3222770	1.3222770	1.0933658
F	-1.3222770	-1.3222770	1.0933658
F	1.3222770	-1.3222770	1.0933658
F	-1.3222770	-1.3222770	-1.0933658
F	1.3222770	-1.3222770	-1.0933658
F	1.3222770	1.3222770	-1.0933658
F	-1.3222770	1.3222770	-1.0933658

3. C₁

C	0.7808822	0.7731926	0.0275410
C	-0.7801158	0.7740679	-0.0245276
C	0.7440850	-0.7744772	0.2343101
C	-0.7448514	-0.7728211	-0.2373216

F	-1.3097764	1.0935911	1.1617407
F	-1.3418514	1.4937601	-0.9897578
F	1.3433318	1.4885652	0.9955622
F	1.3108586	1.0968052	-1.1574773
F	-1.5975777	-1.4914701	0.4848532
F	-0.8488585	-1.0916303	-1.5324928
F	0.8477738	-1.0984304	1.5282298
F	1.5960998	-1.4911529	-0.4906599

4.

C	-0.4391535	0.7606362	0.0000000
C	-0.4391535	-0.7606362	0.0000000
C	0.8783070	0.0000000	0.0000000
F	-0.8087665	1.4008247	1.1036956
F	-0.8087665	1.4008247	-1.1036956
F	-0.8087665	-1.4008247	1.1036956
F	-0.8087665	-1.4008247	-1.1036956
F	1.6175330	0.0000000	1.1036956
F	1.6175330	0.0000000	-1.1036956

5.

C	-0.7862900	-0.7862900	0.7862900
C	-0.7862900	-0.7862900	-0.7862900
C	0.7862900	-0.7862900	-0.7862900
C	0.7862900	-0.7862900	0.7862900
C	-0.7862900	0.7862900	0.7862900
C	-0.7862900	0.7862900	-0.7862900
C	0.7862900	0.7862900	-0.7862900
C	0.7862900	0.7862900	0.7862900
F	1.5566523	-1.5566523	-1.5566523
F	1.5566523	1.5566523	-1.5566523
F	-1.5566523	-1.5566523	-1.5566523
F	-1.5566523	1.5566523	-1.5566523
F	-1.5566523	1.5566523	1.5566523
F	1.5566523	1.5566523	1.5566523
F	1.5566523	-1.5566523	1.5566523
F	-1.5566523	-1.5566523	1.5566523

6.

C	0.7792267	-1.3496602	-0.2098546
C	1.5781048	0.0000000	-0.1165310
C	0.7792267	1.3496602	-0.2098546
C	-0.7890524	1.3666788	-0.1165310
C	-1.5584534	0.0000000	-0.2098546
C	-0.7890524	-1.3666788	-0.1165310
F	-1.2081119	2.0925111	0.9299168
F	-1.2217677	2.1161638	-1.1906010
F	-1.2081119	-2.0925111	0.9299168

F	-2.5626557	0.0000000	0.6838270
F	-2.1823293	0.0000000	-1.4316270
F	-1.2217677	-2.1161638	-1.1906010
F	1.0911647	-1.8899526	-1.4316270
F	1.2813279	-2.2193250	0.6838270
F	2.4162237	0.0000000	0.9299168
F	2.4435355	0.0000000	-1.1906010
F	1.0911647	1.8899526	-1.4316270
F	1.2813279	2.2193250	0.6838270
O	0.0000000	0.0000000	1.5222723
H	0.0000000	0.0000000	2.4823369

7.

C	0.7604203	-1.3170867	-0.3539768
C	1.5765382	0.0000000	-0.1080421
C	0.7604203	1.3170867	-0.3539768
C	-0.7882691	1.3653221	-0.1080421
C	-1.5208407	0.0000000	-0.3539768
C	-0.7882691	-1.3653221	-0.1080421
F	-1.1138991	1.9293298	1.0425323
F	-1.2842136	2.2243231	-1.0507027
F	-1.1138991	-1.9293298	1.0425323
F	-2.6740908	0.0000000	0.3260802
F	-1.8231133	0.0000000	-1.6804524
F	-1.2842136	-2.2243231	-1.0507027
F	0.9115566	-1.5788624	-1.6804524
F	1.3370454	-2.3158306	0.3260802
F	2.2277981	0.0000000	1.0425323
F	2.5684271	0.0000000	-1.0507027
F	0.9115566	1.5788624	-1.6804524
F	1.3370454	2.3158306	0.3260802
C	0.0000000	0.0000000	3.3303133
N	0.0000000	0.0000000	2.1433710

8.

C	-0.7620459	1.3199023	-0.3490603
C	-1.5769801	0.0000000	-0.1192870
C	-0.7620459	-1.3199023	-0.3490603
C	0.7884900	-1.3657048	-0.1192870
C	1.5240919	0.0000000	-0.3490603
C	0.7884900	1.3657048	-0.1192870
F	1.1295073	-1.9563640	1.0188506
F	1.2785078	-2.2144404	-1.0772370
F	1.1295073	1.9563640	1.0188506
F	2.6648469	0.0000000	0.3543679
F	1.8624477	0.0000000	-1.6686326
F	1.2785078	2.2144404	-1.0772370
F	-0.9312238	1.6129270	-1.6686326
F	-1.3324235	2.3078251	0.3543679
F	-2.2590146	0.0000000	1.0188506
F	-2.5570155	0.0000000	-1.0772370
F	-0.9312238	-1.6129270	-1.6686326

F	-1.3324235	-2.3078251	0.3543679
C	0.0000000	0.0000000	2.1699991
N	0.0000000	0.0000000	3.3529963

9.

C	-1.0276906	0.3813279	0.7843165
C	0.2602309	-0.3715493	1.2689880
C	1.0562053	-0.8367696	0.0000000
C	0.2602309	-0.3715493	-1.2689880
C	-1.0276906	0.3813279	-0.7843165
F	-0.1600975	-1.5104454	-1.9211628
F	0.9815469	0.2634830	-2.1992696
F	-2.1098943	-0.3705541	-1.1874412
F	-1.2502810	1.5683047	-1.3591801
F	-1.2502810	1.5683047	1.3591801
F	-2.1098943	-0.3705541	1.1874412
F	0.9815469	0.2634830	2.1992696
F	-0.1600975	-1.5104454	1.9211628
F	1.0451081	-2.2147856	0.0000000
F	2.3610417	-0.5427504	0.0000000
H	1.3180451	2.2496711	0.0000000
O	0.8319710	1.4235007	0.0000000

10.

C	-1.0776988	0.2981688	0.7852830
C	0.2116626	-0.4558533	1.2705756
C	1.0085834	-0.9217951	0.0000000
C	0.2116626	-0.4558533	-1.2705756
C	-1.0776988	0.2981688	-0.7852830
F	-0.1905565	-1.5732352	-1.9377245
F	0.9428868	0.2375810	-2.1358182
F	-2.1570504	-0.4231888	-1.1976354
F	-1.2244990	1.5050829	-1.3200480
F	-1.2244990	1.5050829	1.3200480
F	-2.1570504	-0.4231888	1.1976354
F	0.9428868	0.2375810	2.1358182
F	-0.1905565	-1.5732352	1.9377245
F	1.0250531	-2.2837694	0.0000000
F	2.2823647	-0.5453767	0.0000000
C	1.6369032	2.7989734	0.0000000
N	1.0376063	1.7748570	0.0000000

11.

C	-1.0791595	-0.2865535	-0.7840161
C	0.4121319	-0.2867398	-1.2685736
C	1.3338119	-0.2868110	0.0000000
C	0.4121319	-0.2867398	1.2685736
C	-1.0791595	-0.2865535	0.7840161
F	0.6282821	-1.4591447	1.9341463
F	0.6989517	0.6692190	2.1510280
F	-1.6455056	-1.4588729	1.1954038
F	-1.8296931	0.6695266	1.3293844
F	-1.8296931	0.6695266	-1.3293844

F	-1.6455056	-1.4588729	-1.1954038
F	0.6989517	0.6692190	-2.1510280
F	0.6282821	-1.4591447	-1.9341463
F	2.0335655	-1.4592327	0.0000000
F	2.2617437	0.6691170	0.0000000
C	0.0002362	2.0998036	0.0000000
N	0.0006276	3.2822538	0.0000000

12.

C	-0.7904483	0.7904483	-0.2401012
C	-0.7904483	-0.7904483	-0.2401012
C	0.7904483	-0.7904483	-0.2401012
C	0.7904483	0.7904483	-0.2401012
F	-1.5214223	-1.5214223	0.5932917
F	1.5214223	-1.5214223	0.5932917
F	1.5214223	1.5214223	0.5932917
F	-1.5214223	1.5214223	0.5932917
F	1.2147302	1.2147302	-1.4827769
F	-1.2147302	1.2147302	-1.4827769
F	-1.2147302	-1.2147302	-1.4827769
F	1.2147302	-1.2147302	-1.4827769
O	0.0000000	0.0000000	1.7800390
H	0.0000000	0.0000000	2.7383067

13.

C	-0.7868262	0.7868262	-0.4527141
C	-0.7868262	-0.7868262	-0.4527141
C	0.7868262	-0.7868262	-0.4527141
C	0.7868262	0.7868262	-0.4527141
F	-1.4073852	-1.4073852	0.5303087
F	1.4073852	-1.4073852	0.5303087
F	1.4073852	1.4073852	0.5303087
F	-1.4073852	1.4073852	0.5303087
F	1.2674463	1.2674463	-1.6248716
F	-1.2674463	1.2674463	-1.6248716
F	-1.2674463	-1.2674463	-1.6248716
F	1.2674463	-1.2674463	-1.6248716
N	0.0000000	0.0000000	2.5007951
C	0.0000000	0.0000000	3.6883128

14.

C	-0.7856343	0.7856343	-0.5247418
C	-0.7856343	-0.7856343	-0.5247418
C	0.7856343	-0.7856343	-0.5247418
C	0.7856343	0.7856343	-0.5247418
F	-1.3876886	-1.3876886	0.4817350
F	1.3876886	-1.3876886	0.4817350
F	1.3876886	1.3876886	0.4817350
F	-1.3876886	1.3876886	0.4817350
F	1.2788848	1.2788848	-1.6834476
F	-1.2788848	1.2788848	-1.6834476

F	-1.2788848	-1.2788848	-1.6834476
F	1.2788848	-1.2788848	-1.6834476
C	0.0000000	0.0000000	2.8595902
N	0.0000000	0.0000000	4.0462273

15.

C	-0.4418939	0.7653827	-0.5824617
C	-0.4418939	-0.7653827	-0.5824617
C	0.8837878	0.0000000	-0.5824617
F	-0.8779348	1.5206276	0.3898603
F	-0.7618639	1.3195870	-1.7803353
F	-0.8779348	-1.5206276	0.3898603
F	-0.7618639	-1.3195870	-1.7803353
F	1.7558695	0.0000000	0.3898603
F	1.5237279	0.0000000	-1.7803353
O	0.0000000	0.0000000	2.4767045
H	0.0000000	0.0000000	3.4421058

16.

C	-0.4400414	0.7621741	-0.7409583
C	-0.4400414	-0.7621741	-0.7409583
C	0.8800828	0.0000000	-0.7409583
F	-0.8393765	1.4538428	0.3024207
F	-0.7862881	1.3618910	-1.8942679
F	-0.8393765	-1.4538428	0.3024207
F	-0.7862881	-1.3618910	-1.8942679
F	1.6787531	0.0000000	0.3024207
F	1.5725762	0.0000000	-1.8942679
N	0.0000000	0.0000000	2.9052139
C	0.0000000	0.0000000	4.0932028

17.

C	-0.4398693	0.7618760	-0.8059054
C	-0.4398693	-0.7618760	-0.8059054
C	0.8797386	0.0000000	-0.8059054
F	-0.8356703	1.4474234	0.2438171
F	-0.7887025	1.3660727	-1.9548977
F	-0.8356703	-1.4474234	0.2438171
F	-0.7887025	-1.3660727	-1.9548977
F	1.6713406	0.0000000	0.2438171
F	1.5774049	0.0000000	-1.9548977
C	0.0000000	0.0000000	3.1818157
N	0.0000000	0.0000000	4.3691423

18.

C	-0.7842289	0.7842289	0.4518215
C	-0.7808650	0.7808650	-1.1313468
C	-0.7808650	-0.7808650	-1.1313468
C	-0.7842289	-0.7842289	0.4518215
C	0.7842289	0.7842289	0.4518215

C	0.7808650	0.7808650	-1.1313468
C	0.7808650	-0.7808650	-1.1313468
C	0.7842289	-0.7842289	0.4518215
F	-1.5530780	-1.5530780	-1.9296837
F	1.5530780	-1.5530780	-1.9296837
F	-1.5530780	1.5530780	-1.9296837
F	1.5530780	1.5530780	-1.9296837
F	1.6133066	1.6133066	1.0910405
F	1.6133066	-1.6133066	1.0910405
F	-1.6133066	-1.6133066	1.0910405
F	-1.6133066	1.6133066	1.0910405
O	0.0000000	0.0000000	2.5554004
H	0.0000000	0.0000000	3.5172735

19.

C	-0.7852738	0.7852738	0.3942206
C	-0.7820543	0.7820543	-1.1844970
C	-0.7820543	-0.7820543	-1.1844970
C	-0.7852738	-0.7852738	0.3942206
C	0.7852738	0.7852738	0.3942206
C	0.7820543	0.7820543	-1.1844970
C	0.7820543	-0.7820543	-1.1844970
C	0.7852738	-0.7852738	0.3942206
F	-1.5548901	-1.5548901	-1.9720455
F	1.5548901	-1.5548901	-1.9720455
F	-1.5548901	1.5548901	-1.9720455
F	1.5548901	1.5548901	-1.9720455
F	1.5966123	1.5966123	1.0711199
F	1.5966123	-1.5966123	1.0711199
F	-1.5966123	-1.5966123	1.0711199
F	-1.5966123	1.5966123	1.0711199
N	0.0000000	0.0000000	2.7885382
C	0.0000000	0.0000000	3.9762694

20.

C	-0.7840703	0.7840703	0.3906421
C	-0.7817538	0.7817538	-1.1899200
C	-0.7817538	-0.7817538	-1.1899200
C	-0.7840703	-0.7840703	0.3906421
C	0.7840703	0.7840703	0.3906421
C	0.7817538	0.7817538	-1.1899200
C	0.7817538	-0.7817538	-1.1899200
C	0.7840703	-0.7840703	0.3906421
F	-1.5544099	-1.5544099	-1.9794192
F	1.5544099	-1.5544099	-1.9794192
F	-1.5544099	1.5544099	-1.9794192
F	1.5544099	1.5544099	-1.9794192
F	1.6038642	1.6038642	1.0531921
F	1.6038642	-1.6038642	1.0531921

F	-1.6038642	-1.6038642	1.0531921
F	-1.6038642	1.6038642	1.0531921
C	0.0000000	0.0000000	2.8591190
N	0.0000000	0.0000000	4.0429009

21.

C	0.0000000	-1.1089836	0.7806461
C	-1.1067269	0.0000000	0.7920503
C	-1.1090040	0.0000000	-0.7807229
C	0.0000000	-1.1067065	-0.7921113
C	1.1090040	0.0000000	-0.7807229
C	0.0000000	1.1067065	-0.7921113
C	1.1067269	0.0000000	0.7920503
C	0.0000000	1.1089836	0.7806461
F	0.0000000	2.2021971	1.5210763
F	-2.2021260	0.0000000	-1.5212342
F	2.2021260	0.0000000	-1.5212342
F	0.0000000	-2.2021971	1.5210763
N	0.0000000	-2.3373831	-1.5675201
O	1.1018208	-2.8073608	-1.8332193
O	-1.1018208	-2.8073608	-1.8332193
N	2.3373321	0.0000000	1.5675829
O	2.8072797	-1.1018207	1.8333356
O	2.8072797	1.1018207	1.8333356
N	-2.3373321	0.0000000	1.5675829
O	-2.8072797	-1.1018207	1.8333356
O	-2.8072797	1.1018207	1.8333356
N	0.0000000	2.3373831	-1.5675201
O	1.1018208	2.8073608	-1.8332193
O	-1.1018208	2.8073608	-1.8332193

22.

C	-0.8986504	0.6304311	0.5585440
C	0.6310497	0.8994029	0.5664382
C	0.6394867	0.9113832	-1.0202250
C	-0.8948212	0.6280002	-1.0393611
C	-0.6394867	-0.9113832	-1.0202250
C	0.8948212	-0.6280002	-1.0393611
C	-0.6310497	-0.8994029	0.5664382
C	0.8986504	-0.6304311	0.5585440

F	1.8540981	-1.3009021	1.1731459
F	1.2614547	1.7965067	-1.8011444
F	-1.2614547	-1.7965067	-1.8011444
F	-1.8540981	1.3009021	1.1731459
N	-1.8946600	1.3275812	-1.8072174
O	-2.9247822	0.7088543	-2.0741372
O	-1.6594311	2.5022409	-2.0902530
N	-1.3378118	-1.9077261	1.3200893
O	-2.5206710	-1.6857526	1.5619642
O	-0.7262094	-2.9448648	1.5595226
N	1.3378118	1.9077261	1.3200893
O	0.7262094	2.9448648	1.5595226
O	2.5206710	1.6857526	1.5619642
N	1.8946600	-1.3275812	-1.8072174
O	1.6594311	-2.5022409	-2.0902530
O	2.9247822	-0.7088543	-2.0741372
O	0.0000000	0.0000000	2.6112125
H	0.0000000	0.0000000	3.5740552

23.

C	-0.9006368	0.6385142	0.5395985
C	0.6380373	0.8953354	0.5486201
C	0.6435364	0.9022554	-1.0327074
C	-0.8922988	0.6415239	-1.0496820
C	-0.6435364	-0.9022554	-1.0327074
C	0.8922988	-0.6415239	-1.0496820
C	-0.6380373	-0.8953354	0.5486201
C	0.9006368	-0.6385142	0.5395985
F	1.8285025	-1.3054182	1.1939777
F	1.2976093	1.7744780	-1.7959384
F	-1.2976093	-1.7744780	-1.7959384
F	-1.8285025	1.3054182	1.1939777
N	-1.9103077	1.2976427	-1.8391598
O	-3.0166360	0.7612285	-1.8311366
O	-1.6042540	2.3371559	-2.4210301
N	-1.3492775	-1.9329010	1.2656915
O	-2.5165176	-1.7009249	1.5583892
O	-0.7382519	-2.9849441	1.4295383
N	1.3492775	1.9329010	1.2656915
O	0.7382519	2.9849441	1.4295383
O	2.5165176	1.7009249	1.5583892
N	1.9103077	-1.2976427	-1.8391598
O	1.6042540	-2.3371559	-2.4210301

O	3.0166360	-0.7612285	-1.8311366
N	0.0000000	0.0000000	2.8397211
C	0.0000000	0.0000000	4.0279568

24.

C	-0.8984193	0.6343715	0.5412675
C	0.6350095	0.8967941	0.5526582
C	0.6411908	0.9049337	-1.0380948
C	-0.8925678	0.6350504	-1.0533697
C	-0.6411908	-0.9049337	-1.0380948
C	0.8925678	-0.6350504	-1.0533697
C	-0.6350095	-0.8967941	0.5526582
C	0.8984193	-0.6343715	0.5412675
F	1.8424312	-1.3055653	1.1750278
F	1.2810559	1.7838162	-1.8069071
F	-1.2810559	-1.7838162	-1.8069071
F	-1.8424312	1.3055653	1.1750278
N	-1.9056392	1.3140793	-1.8281186
O	-2.9804657	0.7277275	-1.9456423
O	-1.6298121	2.4298352	-2.2667890
N	-1.3596652	-1.9422897	1.2464547
O	-2.5377828	-1.7175568	1.5040057
O	-0.7503828	-2.9927419	1.4275575
N	1.3596652	1.9422897	1.2464547
O	0.7503828	2.9927419	1.4275575
O	2.5377828	1.7175568	1.5040057
N	1.9056392	-1.3140793	-1.8281186
O	1.6298121	-2.4298352	-2.2667890
O	2.9804657	-0.7277275	-1.9456423
C	0.0000000	0.0000000	2.9003261
N	0.0000000	0.0000000	4.0835739

2. CSD reference codes of nitrocubanes exhibiting carbon bonds:

HASHAK

NACXEU

WASMAE

NEFLIT

NURPAR