Supplementary Information

Hydrogen bonds in complexes of noble gases with the $H(HCB_{11}F_{11})$ carborane acid – DFT calculations

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Abstract. The noble gases when interact with the $H(HCB_{11}F_{11})$ carborane acid, that is classified in several studies as the strongest acid, lose the part of their electron charge. Hence the noble gases act as Lewis base units in complexes formed. These complexes are linked by interactions which possess numerous characteristics of the hydrogen bond.

Theoretical methods. The ωB97XD/aug-cc-pVTZ calculations on complexes of the $H(HCB_{11}F_{11})$ carborane acid with noble gas centres have been performed with the use of Gaussian16 set of codes.[1] The ωB97XD functional [2] with the aug-cc-pVTZ basis sets (aug-cc-pVTZ-PP for Xe and Rn) [3-6] were used. In earlier studies it has been proven that in analyses of interactions, the ωB97XD functional in conjunction with the Dunning-style basis sets offers results more reliable than other functionals.[7] Frequency calculations have been performed at the same ωB97XD/aug-cc-pVTZ level for complexes analysed in this study to justify that they correspond to energetic minima (there are not imaginary frequencies). Interaction energies were calculated as differences between the energy of the complex and the sum of energies of monomers. The monomers´ geometries in the above calculations come from geometries of complexes. The interaction energies contain BSSE corrections.[8]

The calculations with other functionals and basis sets were not performed for complexes analysed here. However, the aim of this study was to analyse how hydrogen bond properties change with the change of the atomic number of the noble gas centre and not to obtain precise geometric and energetic values.

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Geometries of complexes analysed

Atoms´ coordinates related to Å.

H($HCB_{11}F_{11}$)-He

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.198487	0.000044	1.232147

2	5	-0.223404	0.915509	1.529650
3	5	-1.411715	-0.000151	0.605357
4	5	-0.223254	-0.915687	1.529576
5	5	-0.653611	-1.487991	-0.104820
6	5	-0.863542	-0.000036	-1.046115
7	5	-0.653853	1.487879	-0.104694
8	5	1.048197	1.467771	0.350785
9	5	0.604895	0.928934	-1.312994
10	5	0.605050	-0.928735	-1.313073
11	5	1.048438	-1.467628	0.350664
12	5	1.814961	0.000163	-0.378283
13	9	-2.818040	-0.000253	0.570186
14	9	-0.380504	1.573334	2.687667
15	9	-0.380236	-1.573637	2.687537
16	9	-1.441752	2.563166	-0.348371
17	9	-2.208268	-0.000094	-1.804898
18	9	-1.441310	-2.563404	-0.348579
19	1	1.934973	0.000070	2.026292
20	9	1.822356	2.518387	0.662744
21	9	3.141276	0.000277	-0.583361
22	9	1.822771	-2.518149	0.662529
23	9	0.890254	1.638072	-2.423327
24	9	0.890539	-1.637734	-2.423459
25	1	-2.835708	-0.000080	-1.042766
26	2	-5.412382	-0.000035	-1.477345

$H(HCB_{11}F_{11})$-Ne

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.666019	0.000014	1.009511
2	5	-0.323244	-0.915478	1.563533
3	5	1.015718	-0.000049	0.874416
4	5	-0.323199	0.915420	1.563567
5	5	0.401256	1.487775	0.036567
6	5	0.780455	-0.000010	-0.849823
7	5	0.401182	-1.487811	0.036512
8	5	-1.355821	-1.467856	0.170631
9	5	-0.613810	-0.928662	-1.382647
10	5	-0.613765	0.928726	-1.382613
11	5	-1.355749	1.467898	0.170686
12	5	-1.975192	0.000052	-0.686341
13	9	2.402743	-0.000092	1.101733
14	9	-0.382031	-1.573433	2.730654
15	9	-0.381955	1.573335	2.730712
16	9	1.220145	-2.563392	-0.057920
17	9	2.240666	-0.000041	-1.351928
18	9	1.220265	2.563324	-0.057824
19	1	-2.536115	0.000023	1.654451
20	9	-2.174227	-2.518446	0.334781

21	**9**	**-3.240949**	**0.000092**	**-1.132675**
22	**9**	**-2.174103**	**2.518523**	**0.334873**
23	**9**	**-0.689988**	**-1.637157**	**-2.527020**
24	**9**	**-0.689912**	**1.637267**	**-2.526960**
25	**1**	**2.722457**	**-0.000013**	**-0.491839**
26	**10**	**5.346471**	**0.000006**	**-0.399796**

$H(HCB_{11}F_{11})$-Ar

Center	**Atomic**	**Coordinates (Angstroms)**		
Number	**Number**	**X**	**Y**	**Z**

1	**6**	**1.856420**	**0.000075**	**0.990186**
2	**5**	**0.966463**	**1.466395**	**0.934301**
3	**5**	**-0.704902**	**0.914672**	**0.691920**
4	**5**	**0.345357**	**0.000011**	**1.799395**
5	**5**	**-0.704820**	**-0.914772**	**0.691943**
6	**5**	**-0.643121**	**-0.000061**	**-0.812269**
7	**5**	**0.303169**	**1.488444**	**-0.723594**
8	**5**	**1.965958**	**0.905168**	**-0.465689**
9	**5**	**0.929024**	**0.000005**	**-1.605995**
10	**5**	**0.303309**	**-1.488476**	**-0.723555**
11	**5**	**0.966598**	**-1.466338**	**0.934341**
12	**5**	**1.966040**	**-0.905031**	**-0.465661**
13	**9**	**-1.840451**	**1.579161**	**1.044444**

14	**9**	**1.368062**	**2.530136**	**1.649808**
15	**9**	**0.290139**	**0.000041**	**3.142116**
16	**9**	**-0.038839**	**2.608807**	**-1.401312**
17	**9**	**-1.937393**	**-0.000153**	**-1.661546**
18	**9**	**-1.840314**	**-1.579343**	**1.044479**
19	**1**	**2.737317**	**0.000127**	**1.619739**
20	**9**	**3.099913**	**1.558912**	**-0.767695**
21	**9**	**3.100053**	**-1.558678**	**-0.767668**
22	**9**	**1.368312**	**-2.530022**	**1.649865**
23	**9**	**1.083222**	**-0.000018**	**-2.948981**
24	**9**	**-0.038587**	**-2.608876**	**-1.401267**
25	**1**	**-2.744263**	**-0.000158**	**-1.137227**
26	**18**	**-4.506888**	**-0.000012**	**-0.218860**

$H(HCB_{11}F_{11})$-Kr

Center	**Atomic**	**Coordinates (Angstroms)**		
Number	**Number**	**X**	**Y**	**Z**

1	**6**	**2.303284**	**0.000011**	**0.965868**
2	**5**	**1.412238**	**1.466005**	**0.924857**
3	**5**	**-0.263914**	**0.915098**	**0.712308**
4	**5**	**0.806307**	**0.000437**	**1.800608**
5	**5**	**-0.264192**	**-0.914401**	**0.712740**
6	**5**	**-0.230714**	**-0.000014**	**-0.793548**

7	**5**	**0.719454**	**1.487616**	**-0.720492**
8	**5**	**2.386811**	**0.904654**	**-0.491903**
9	**5**	**1.329370**	**-0.000445**	**-1.612505**
10	**5**	**0.719002**	**-1.487900**	**-0.719787**
11	**5**	**1.411792**	**-1.465733**	**0.925551**
12	**5**	**2.386540**	**-0.905341**	**-0.491484**
13	**9**	**-1.388293**	**1.584516**	**1.090334**
14	**9**	**1.825608**	**2.530157**	**1.633393**
15	**9**	**0.773864**	**0.000766**	**3.144324**
16	**9**	**0.366541**	**2.608286**	**-1.392527**
17	**9**	**-1.527266**	**-0.000050**	**-1.630616**
18	**9**	**-1.388780**	**-1.583289**	**1.091068**
19	**1**	**3.195069**	**0.000024**	**1.579847**
20	**9**	**3.515352**	**1.558382**	**-0.814291**
21	**9**	**3.514886**	**-1.559553**	**-0.813571**
22	**9**	**1.824832**	**-2.529673**	**1.634594**
23	**9**	**1.459394**	**-0.000782**	**-2.958334**
24	**9**	**0.365718**	**-2.608766**	**-1.391296**
25	**1**	**-2.339172**	**0.000109**	**-1.103216**
26	**36**	**-4.189327**	**-0.000001**	**-0.106702**

$H(HCB_{11}F_{11})$-Xe

Center	**Atomic**	**Coordinates (Angstroms)**

Number	Number	X	Y	Z
1	6	2.691948	0.000093	0.960304
2	5	1.799876	1.465130	0.922303
3	5	0.122045	0.914786	0.716247
4	5	1.197568	0.000088	1.799408
5	5	0.122122	-0.914784	0.716344
6	5	0.147165	-0.000078	-0.791473
7	5	1.100358	1.486770	-0.719595
8	5	2.769295	0.904911	-0.497549
9	5	1.707338	-0.000073	-1.613006
10	5	1.100476	-1.486854	-0.719425
11	5	1.799981	-1.465020	0.922468
12	5	2.769364	-0.904864	-0.497446
13	9	-0.994440	1.590341	1.106851
14	9	2.214321	2.529719	1.630131
15	9	1.169114	0.000169	3.143573
16	9	0.745851	2.608141	-1.390208
17	9	-1.135481	-0.000248	-1.638076
18	9	-0.994331	-1.590394	1.106945
19	1	3.585899	0.000167	1.571052
20	9	3.896369	1.559481	-0.824241
21	9	3.896494	-1.559366	-0.824092
22	9	2.214502	-2.529498	1.630412
23	9	1.831544	-0.000154	-2.959758
24	9	0.745972	-2.608284	-1.389944

25	**1**	**-1.966881**	**-0.000052**	**-1.123502**
26	**54**	**-3.949220**	**0.000002**	**-0.068983**

$H(HCB_{11}F_{11})$-Rn

Center Number	**Atomic Number**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	**6**	**3.219749**	**0.000149**	**0.960616**
2	**5**	**2.327662**	**1.464933**	**0.921645**
3	**5**	**0.649521**	**0.915074**	**0.715213**
4	**5**	**1.724810**	**0.000605**	**1.798648**
5	**5**	**0.649309**	**-0.914318**	**0.715824**
6	**5**	**0.673377**	**-0.000124**	**-0.793161**
7	**5**	**1.628378**	**1.486043**	**-0.720050**
8	**5**	**3.297435**	**0.904468**	**-0.497419**
9	**5**	**2.235437**	**-0.000586**	**-1.612306**
10	**5**	**1.628037**	**-1.486472**	**-0.719050**
11	**5**	**2.327313**	**-1.464462**	**0.922633**
12	**5**	**3.297226**	**-0.905159**	**-0.496816**
13	**9**	**-0.463676**	**1.594202**	**1.109488**
14	**9**	**2.741385**	**2.529918**	**1.629538**
15	**9**	**1.695176**	**0.001077**	**3.142939**
16	**9**	**1.274732**	**2.607671**	**-1.391000**
17	**9**	**-0.601209**	**-0.000374**	**-1.646562**

18	**9**	**-0.464077**	**-1.592912**	**1.110480**
19	**1**	**4.113481**	**0.000253**	**1.571651**
20	**9**	**4.424624**	**1.559034**	**-0.824118**
21	**9**	**4.424274**	**-1.560180**	**-0.823091**
22	**9**	**2.740790**	**-2.529063**	**1.631242**
23	**9**	**2.360020**	**-0.001058**	**-2.959197**
24	**9**	**1.274052**	**-2.608422**	**-1.389283**
25	**1**	**-1.440859**	**-0.000295**	**-1.136306**
26	**86**	**-3.474866**	**0.000001**	**-0.042893**

$H(HCB_{11}F_{11})$ not involved in interactions

Center Number	**Atomic Number**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	**6**	**-0.682392**	**0.003005**	**-1.513202**
2	**5**	**-0.816647**	**1.471468**	**-0.629446**
3	**5**	**0.649063**	**1.485274**	**0.348103**
4	**5**	**0.763438**	**0.912180**	**-1.338131**
5	**5**	**1.587848**	**-0.007170**	**-0.081545**
6	**5**	**0.539417**	**-0.002425**	**1.307434**
7	**5**	**-0.933117**	**0.932879**	**1.088600**
8	**5**	**-1.782422**	**0.007699**	**-0.185640**
9	**5**	**-0.941182**	**-0.924805**	**1.088299**
10	**5**	**0.636136**	**-1.490945**	**0.347861**

11	**5**	**0.755622**	**-0.919105**	**-1.338365**
12	**5**	**-0.829367**	**-1.464593**	**-0.629773**
13	**9**	**1.322615**	**2.557510**	**0.830744**
14	**9**	**-1.445042**	**2.524863**	**-1.173232**
15	**9**	**1.286952**	**1.568173**	**-2.383992**
16	**9**	**-1.558121**	**1.644232**	**2.047900**
17	**9**	**1.573847**	**-0.006853**	**2.453993**
18	**9**	**2.908495**	**-0.012310**	**0.405894**
19	**1**	**-1.124917**	**0.004790**	**-2.501729**
20	**9**	**-3.104501**	**0.013265**	**-0.416537**
21	**9**	**-1.467542**	**-2.511903**	**-1.173780**
22	**9**	**1.273603**	**-1.578628**	**-2.384720**
23	**9**	**-1.571690**	**-1.630960**	**2.047916**
24	**9**	**1.299785**	**-2.569028**	**0.831117**
25	**1**	**2.409706**	**-0.010342**	**1.926201**
