How short can the H…H intermolecular contact be? New findings that reveal the covalent nature of extremely strong interactions.

Supporting Material

Sławomir J. Grabowski,[a,b]* W. Andrzej Sokalski,[c] and Jerzy Leszczynski [b]

[a] Department of Crystallography and Crystal Chemistry, University of Łódź, 90-236 Łódź, ul.Pomorska 149/153, Poland

[b] Computational Center for Molecular Structure and Interactions, Department of Chemistry, Jackson State University, Jackson, MS 39217, USA

[c] Institute of Physical and Theoretical Chemistry, Wrocław University of Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

* Address correspondence to this author. Address: Department of Crystallography and Crystal Chemistry, University of Łódź, 90-236 Łódź, ul.Pomorska 149/153, Poland.
E-mail: slagra@uni.lodz.pl

The coordinates of the optimized systems investigated (level of approximation is given in parentheses), order number, atomic number and x,y,z coordinates allowing to obtain distances in Å are given.

H_2OH^+…HBeF (MP2/aug-cc-pVDZ)

			X	y	z
1	4	0	1.144807	0.007279	0.144261
2	1	0	-0.197907	0.017061	0.335325
3	1	0	-1.453384	0.001349	0.080634
4	8	0	-2.471623	-0.002616	-0.116804
5	1	0	-2.905144	-0.799400	0.252505
6	1	0	-2.906899	0.801494	0.234113
7	9	0	2.517454	-0.003188	-0.060577

H_2OH^+…HBeH (MP2/aug-cc-pVDZ)

1	4	0	2.328145	0.001031	0.031416
2	1	0	0.971262	0.009539	0.225563
3	1	0	-0.240625	-0.000406	0.053699
4	8	0	-1.283480	-0.000921	-0.100403
5	1	0	-1.703640	-0.797824	0.281828
6	1	0	-1.702509	0.799313	0.276078
7	1	0	3.630777	-0.007377	-0.159605

HClOH+…HBeH (MP2/aug-cc-pVDZ)

1	4	0	-3.210557	-0.361390	0.053216
2	1	0	-1.977335	0.167783	0.378240
3	1	0	-0.953365	0.564798	0.098345
4	8	0	0.052007	0.932307	-0.142244
5	1	0	0.338768	1.581949	0.543147
6	17	0	1.141005	-0.438623	0.010505
7	1	0	-4.378970	-0.870837	-0.273234

Cl_2OH^+…HBeF (MP2/aug-cc-pVDZ)

1	4	0	2.779346	-0.001936	-0.177618
2	1	0	1.416506	-0.003160	-0.341749
3	1	0	0.428592	-0.001464	0.155908
4	8	0	-0.608640	-0.000233	0.567028
5	17	0	-1.335354	1.460828	-0.108564
6	17	0	-1.338812	-1.459548	-0.108613
7	9	0	4.151941	-0.000836	0.005789

Cl_2OH^+…HBeH (MP2/aug-cc-pVDZ)

1	4	0	3.439266	-0.016808	-0.171420
2	1	0	2.079293	-0.013409	-0.488691
3	1	0	1.161863	-0.007656	0.019925
4	8	0	0.113068	-0.001289	0.525857
5	17	0	-0.656237	1.460603	-0.094363
6	17	0	-0.674064	-1.453634	-0.094436
7	1	0	4.712361	-0.019867	0.157180

H_2OH^+…HBeBeH (MP2/aug-cc-pVDZ)

1	4	0	1.353270	0.002014	0.198323
2	1	0	-0.035126	0.004104	0.403805
3	1	0	-1.118413	0.001372	0.126395
4	8	0	-2.189361	-0.000951	-0.141177
5	1	0	-2.648777	-0.793770	0.198564
6	1	0	-2.650379	0.793875	0.191644
7	4	0	3.447135	-0.000834	-0.081103
8	1	0	4.765968	-0.002692	-0.259866

H_2OH^+…HBeBeH (MP2/6-311++G(d,p))

1	4	0	1.337714	0.000029	0.240003
2	1	0	-0.034659	0.000046	0.481359
3	1	0	-1.112472	0.000014	0.153617
4	8	0	-2.159167	-0.000012	-0.146175
5	1	0	-2.638469	-0.793995	0.145395
6	1	0	-2.638481	0.794000	0.145297
7	4	0	3.408575	-0.000020	-0.099850
8	1	0	4.712260	-0.000010	-0.316878

Cl_2OH^+…HBeH (MP2/6-311++G(d,p))

1	4	0	-3.450666	-0.003802	-0.144358
2	1	0	-2.113739	-0.003241	-0.513436
3	1	0	-1.169410	-0.001718	-0.038436
4	8	0	-0.133623	-0.000305	0.410890
5	17	0	0.674337	-1.468168	-0.070207
6	17	0	0.670342	1.469748	-0.070209
7	1	0	-4.704746	-0.004258	0.229256

Cl_2OH^+…HBeF (MP2/6-311++G(d,p))

1	4	0	-2.862361	-0.005873	0.046074
2	1	0	-1.512305	-0.013589	0.165226
3	1	0	-0.387281	-0.006961	0.299145
4	8	0	0.666476	-0.001113	0.521147
5	17	0	1.360190	-1.470060	-0.117605
6	17	0	1.343382	1.475972	-0.116909
7	9	0	-4.215944	-0.005284	-0.092345

H_2OH^+…HBeF (MP2/6-311++G(d,p))

1	4	0	-1.160653	-0.001473	0.028017
2	1	0	0.185006	-0.003792	0.077994
3	1	0	1.463581	-0.000996	0.008852
4	8	0	2.488360	0.000380	-0.086860
5	1	0	2.898833	0.802026	0.284472
6	1	0	2.900839	-0.800432	0.284061
7	9	0	-2.523615	0.000672	-0.008063

H_2OH^+…HBeH (MP2/6-311++G(d,p))

1	4	0	2.310908	-0.000184	0.037701
2	1	0	0.970669	-0.006424	0.292071
3	1	0	-0.239182	-0.001579	0.075759
4	8	0	-1.269482	0.000557	-0.098774
5	1	0	-1.709026	-0.798395	0.242584
6	1	0	-1.706651	0.799164	0.246389
7	1	0	3.596413	0.003512	-0.217419

ClHOH+…HBeH (MP2/6-311++G(d,p))

1	4	0	3.299672	-0.364873	0.049443
2	1	0	2.035969	0.069104	0.358843
3	1	0	0.979855	0.464810	0.099199
4	8	0	0.005394	0.847153	-0.130370
5	17	0	-1.208293	-0.391518	0.010086
6	1	0	-0.220178	1.583627	0.473979
7	1	0	4.503498	-0.779470	-0.258290