

# Supplementary Materials

## [FHF]<sup>-</sup> — The Strongest Hydrogen Bond under the Influence of External Interactions

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**Table S1.** Geometrical parameters (Å, degrees) for the [FHF]<sup>-</sup> anions found in crystal structures through the CSD search; refcodes and R-factors for the crystal structures are included in the table.

Index	Refcode	F-H	H...F	F-F	F-H-F	R-factor (%)
1	BOHSEY	0.947	1.396	2.341	175.6	3.3
2	BOHSIC	1.045	1.274	2.314	172.7	4.2
3	HOPNUX	1.146	1.147	2.292	177.9	4.3
4	HOPNUX	1.153	1.155	2.308	177.9	4.3
5	BEXLUM	1.034	1.244	2.256	164.2	2.5
6	BOCKEK	1.093	1.133	2.224	175.1	2.8
7	BOCKEK01	1.096	1.141	2.237	178.0	3.3
8	BOCKEK02	1.123	1.125	2.248	178.5	3.5
9	BOCKEK03	1.081	1.172	2.252	177.5	3.3
10	BOCKEK04	1.058	1.201	2.258	177.2	3.0
11	BOCKEK05	1.038	1.23	2.268	177.8	3.0
12	BOTRAE	0.915	1.381	2.291	172.4	5.6
13	BOTRAE	1.1	1.192	2.291	176.7	5.6
14	BOTRAE	1.133	1.158	2.287	172.5	5.6
15	BOTRAE	1.063	1.227	2.289	176.5	5.6
16	CIHJOT	1.171	1.227	2.267	141.9	4.6
17	CIHJOT	1.025	1.3	2.3	163.5	4.6
18	CIHJOT	1.156	1.201	2.339	166.0	4.6
19	FAJHAA	1.138	1.138	2.275	178.4	1.9
20	FEDDOH	1.121	1.123	2.238	171.9	3.4
21	GEPYUV	1.131	1.152	2.274	169.8	6.0
22	GIPGOB01	0.89	1.432	2.322	177.9	2.4
23	GIPGOB01	0.892	1.438	2.328	175.2	2.4
24	GIPHAO	1.133	1.133	2.266	180.0	2.4
25	GUHFOE	1.01	1.262	2.249	163.5	3.4
26	GUHFOE	1.05	1.214	2.233	161.0	3.4
27	HEVLEZ	1.017	1.235	2.246	172.6	4.9
28	HEVLEZ	0.953	1.295	2.248	178.1	4.9
29	HITBIW	0.956	1.362	2.315	174.2	2.7
30	HITBIW	1.067	1.319	2.382	173.4	2.7
31	IBOWOL	1.139	1.171	2.293	165.9	4.6
32	KELRIC01	1.129	1.129	2.256	174.9	3.1
33	OCAZUN	0.894	1.513	2.359	156.3	3.3
34	OCAZUN	0.75	1.604	2.354	177.7	3.3
35	PEJQOL	1.01	1.29	2.295	171.6	5.6
36	PEJQUR	0.984	1.249	2.194	158.2	6.2
37	PEJREC	1.041	1.264	2.29	166.9	5.1
38	PEJRIG	0.98	1.258	2.233	172.3	5.9
39	UGOQAI	1.127	1.128	2.25	172.4	3.4
40	XAXPAO	0.95	1.383	2.329	172.8	3.0
41	YAYJIS	1.145	1.145	2.29	180.0	2.6

Table S1. Cont.

Index	Refcode	F-H	H...F	F-F	F-H-F	R-factor (%)
42	YEJRIO	0.976	1.34	2.312	174.1	3.0
43	ZZZMJK02	1.128	1.131	2.249	169.3	2.4
44	LOTCEE	0.97	1.316	2.284	174.4	3.1
45	LOTCEE01	1.04	1.272	2.308	173.2	3.1

Table S2. The names of compounds (index, *i.e.*, the numeration is the same as in the table).

Index	Refcode	Compound Name
1	BOHSEY	(bifluorido)-(1,3-dimethyltetrahydropyrimidin-2(1H)-ylidene)-bis(triphenylphosphine)-rhodium
2	BOHSIC	(bifluorido)-(1,3-diethyltetrahydropyrimidin-2(1H)-ylidene)-bis(triphenylphosphine)-rhodium
3	HOPNUX	2-(pyridin-1-ylamino)pyridinium hydrogen difluoride hemihydrate
4	HOPNUX	2-(pyridin-1-ylamino)pyridinium hydrogen difluoride hemihydrate
5	BEXLUM	bis( $\mu$ 3-Hydroxo)-tris( $\eta$ 4-1,5-cyclooctadiene)-tri-rhodium bifluoride
6	BOCKEK	1-Azonia-4-azabicyclo(2.2.2)octane hydrogen difluoride
7	BOCKEK01	1-Azonia-4-azabicyclo(2.2.2)octane hydrogen difluoride
8	BOCKEK02	1-Azonia-4-azabicyclo(2.2.2)octane hydrogen difluoride
9	BOCKEK03	1-Azonia-4-azabicyclo(2.2.2)octane hydrogen difluoride
10	BOCKEK04	1-Azonia-4-azabicyclo(2.2.2)octane hydrogen difluoride
11	BOCKEK05	1-Azonia-4-azabicyclo(2.2.2)octane hydrogen difluoride
12	BOTRAE	1-(diaminomethylene)thiouron-1-ium hydrogen difluoride
13	BOTRAE	1-(diaminomethylene)thiouron-1-ium hydrogen difluoride
14	BOTRAE	1-(diaminomethylene)thiouron-1-ium hydrogen difluoride
15	BOTRAE	1-(diaminomethylene)thiouron-1-ium hydrogen difluoride
16	CIHJOT	bis( $\eta$ 5-Cyclopentadienyl)-( $\eta$ 6-1,3,5-tri- <i>t</i> -butylbenzene)-iron (hydrogen difluoride) (dihydrogen trifluoride)
17	CIHJOT	bis( $\eta$ 5-Cyclopentadienyl)-( $\eta$ 6-1,3,5-tri- <i>t</i> -butylbenzene)-iron (hydrogen difluoride) (dihydrogen trifluoride)
18	CIHJOT	bis( $\eta$ 5-Cyclopentadienyl)-( $\eta$ 6-1,3,5-tri- <i>t</i> -butylbenzene)-iron (hydrogen difluoride) (dihydrogen trifluoride)
19	FAJHAA	bis(Tetramethylammonium) difluoro-dioxoiodide hydrogen difluoride
20	FEDDOH	tris(Dimethylamino)sulfonium hydrogendifluoride
21	GEPYUV	Trimethylammonium hydrogen-difluoride tris(hydrogen fluoride)
22	GIPGOB01	Tetramethylammonium dihydrogen trifluoride
23	GIPGOB01	Tetramethylammonium dihydrogen trifluoride
24	GIPHAO	Tetramethylammonium hydrogen-difluoride tetraakis(hydrogen fluoride)
25	GUHFOE	L-Argininium fluoride hydrogen fluoride
26	GUHFOE	L-Argininium fluoride hydrogen fluoride
27	HEVLEZ	1,3,5,7-Tetramethyl-8-(propane-1,3-dioxy)-1-azonia-adamantane hydrogen difluoride
28	HEVLEZ	1,3,5,7-Tetramethyl-8-(propane-1,3-dioxy)-1-azonia-adamantane hydrogen difluoride
29	HITBIW	bis(bis(2-Pyridyl)methanediol-N,N',O)-copper(ii) bis(dihydrogen trifluoride)
30	HITBIW	bis(bis(2-Pyridyl)methanediol-N,N',O)-copper(ii) bis(dihydrogen trifluoride)
31	IBOWOL	Diphenylguanidinium hydrogen bifluoride
32	KELRIC01	Tetramethylammonium hydrogen difluoride
33	OCAZUN	(Bifluoride)-phenyl-bis(triphenylphosphine)-palladium
34	OCAZUN	(Bifluoride)-phenyl-bis(triphenylphosphine)-palladium
35	PEJQOL	2-(bis(4-hydroxy-3,5-dimethylphenyl)methyl)pyridinium hydrogen difluoride
36	PEJQUR	(4-Ammoniophenyl)bis(4-hydroxy-3,5-dimethylphenyl)methane hydrogen difluoride
37	PEJREC	4-(bis(4-hydroxy-3,5-dimethylphenyl)methyl)pyridinium hydrogen difluoride monohydrate
38	PEJRIG	4-(bis(4-hydroxy-3,5-dimethylphenyl)methyl)pyridinium hydrogen difluoride
39	UGOQAI	tris(Dimethylamino)-oxo-sulfonium hydrogen bifluoride
40	XAXPAO	trans-(Diphenyl(fluoro)phosphine)-(hydrogen bifluoride)-bis(triphenylphosphine)-rhodium
41	YAYJIS	( $\mu$ 2-Fluoro)-bis( $\mu$ 2-bis(diphenylphosphino)methane)-dimethyl-di-palladium(ii) hydrogen difluoride tetrahydrofuran solvate
42	YEJRIO	Di-isopropylammonium hydrogen difluoride
43	ZZZMJK02	tetrakis(Thiourea-S)-tellurium(ii) bis(hydrogen difluoride)
44	LOTCEE	1-(2-(hydroxymethyl)-1,3-oxathiolan-5-yl)-2-oxo-2,3-dihydropyrimidin-4(1H)-iminium hydrofluoride
45	LOTCEE01	1-(2-(hydroxymethyl)-1,3-oxathiolan-5-yl)-2-oxo-2,3-dihydropyrimidin-4(1H)-iminium hydrofluoride

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