Supplementary material to:

T.A. Ford,

Molecular Complexes of Boron Trifluoride with some Formyl Compounds, HCOX (X = H, CH_3, NH_2, OH, F): Effect of Substitution, and Extension to X = Li, BeH and BH_2,

S. Afr. J. Chem., 2018, **71**, 140–149.

Supplementary Information, South African Journal of Chemistry

Molecular Complexes of Boron Trifluoride with some Formyl Compounds, HCOX (X = H, CH_3, NH_2, OH, F): Effect of Substitution, and Extension to X = Li, Be and BH_2

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Table S1. Optimized Cartesian coordinates of the complex of BF_3 with H_2CO.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.012347	0.615738	0.000000
2	8	0	0.566484	-1.106096	0.000000
3	9	0	-1.336383	0.460956	0.000000
4	9	0	0.566484	1.029933	1.151361
5	9	0	0.566484	1.029933	-1.151361
6	6	0	-0.255723	-2.012885	0.000000
7	1	0	-1.324516	-1.795314	0.000000
8	1	0	0.095991	-3.044697	0.000000

Table S2. Optimized Cartesian coordinates of the complex of BF_3 with CH_3CHO.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.012118	-1.089876	0.000000
2	8	0	-0.530978	0.559929	0.000000
3	9	0	1.371600	-0.965951	0.000000
4	9	0	-0.530978	-1.538417	1.151878
5	9	0	-0.530978	-1.538417	-1.151878
6	6	0	0.277803	1.487100	0.000000
7	1	0	1.344836	1.249599	0.000000
8	6	0	-0.153108	2.901329	0.000000
9	1	0	-1.234846	2.983313	0.000000
10	1	0	0.271144	3.395763	-0.875278
11	1	0	0.271144	3.395763	0.875278

Table S3. Optimized Cartesian coordinates of the complex of BF_3 with $HCONH_2$ (O-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.089630	-1.013187	0.000000
2	8	0	-0.601719	0.502749	0.000000
3	9	0	1.444627	-0.764572	0.000000
4	9	0	-0.378516	-1.560394	1.150766
5	9	0	-0.378516	-1.560394	-1.150766
6	6	0	0.127833	1.509366	0.000000
7	1	0	1.211501	1.416358	0.000000
8	7	0	-0.378516	2.734477	0.000000
9	1	0	-1.377733	2.862597	0.000000
10	1	0	0.226097	3.535696	0.000000

Table S4. Optimized Cartesian coordinates of the complex of BF_3 with $HCONH_2$ (N-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.932273	0.079990	-0.085161
2	7	0	0.513649	-0.389535	0.781731
3	9	0	-1.871676	0.092499	0.902711
4	9	0	-0.612955	1.291502	-0.613686
5	9	0	-1.058236	-0.936916	-0.994077
6	6	0	1.662972	-0.416665	-0.093392
7	8	0	2.551687	0.382657	0.002521
8	1	0	1.592922	-1.202473	-0.851591
9	1	0	0.290698	-1.315069	1.142020
10	1	0	0.677577	0.259306	1.548905

Table S5. Optimized Cartesian coordinates of the complex of BF_3 with HCOOH (OC-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.062909	0.868086	0.000000
2	8	0	0.921892	-0.567684	0.000000
3	9	0	-1.282852	0.464881	0.000000
4	9	0	0.442347	1.452058	1.152318
5	9	0	0.442347	1.452058	-1.152318
6	6	0	0.442347	-1.708381	0.000000
7	8	0	-0.817564	-2.017003	0.000000
8	1	0	-1.327316	-1.166896	0.000000
9	1	0	1.107488	-2.566727	0.000000

Table S6. Optimized Cartesian coordinates of the complex of BF_3 with HCOOH (OH-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.700421	1.110127	0.000000
2	8	0	-0.101079	-1.258118	0.000000
3	9	0	-1.969662	0.726557	0.000000
4	9	0	-0.101079	1.373008	1.143895
5	9	0	-0.101079	1.373008	-1.143895
6	1	0	-0.824328	-1.898968	0.000000
7	6	0	1.099492	-1.901574	0.000000
8	8	0	2.135260	-1.304485	0.000000
9	1	0	1.002404	-2.994563	0.000000

Table S7. Optimized Cartesian coordinates of the complex of BF_3 with HCOF.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.204170	-1.362578	0.000000
2	8	0	-0.715456	0.802376	0.000000
3	9	0	1.445324	-0.884833	0.000000
4	9	0	-0.360728	-1.691950	1.145188
5	9	0	-0.360728	-1.691950	-1.145188
6	6	0	0.049543	1.716192	0.000000
7	1	0	1.137287	1.663291	0.000000
8	9	0	-0.360728	2.983561	0.000000

Table S8. Optimized Cartesian coordinates of the complex of BF_3 with HCOLi (H-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.115008	-0.627999	0.000000
2	8	0	-0.116221	1.026930	0.000000
3	9	0	1.202773	-0.981751	0.000000
4	9	0	-0.790808	-0.919277	1.149884
5	9	0	-0.790808	-0.919277	-1.149884
6	6	0	0.908211	1.802282	0.000000
7	1	0	1.837550	1.213829	0.000000
8	3	0	-0.790808	2.759926	0.000000

Table S9. Optimized Cartesian coordinates of the complex of BF_3 with HCOLi (Li-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.061193	0.529815	0.000000
2	8	0	0.899894	-0.776325	0.000000
3	9	0	-1.337581	0.141633	0.000000
4	9	0	0.351810	1.184669	1.154276
5	9	0	0.351810	1.184669	-1.154276
6	6	0	0.351810	-1.926376	0.000000
7	3	0	-1.690513	-1.601070	0.000000
8	1	0	1.161222	-2.675737	0.000000

Table S10. Optimized Cartesian coordinates of the complex of BF_3 with HCOBeH (H-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.030342	-1.108735	0.000000
2	8	0	-0.201814	1.184953	0.000000
3	9	0	1.295292	-1.030380	0.000000
4	9	0	-0.671949	-1.257459	1.144906
5	9	0	-0.671949	-1.257459	-1.144906
6	6	0	0.805374	1.975529	0.000000
7	1	0	1.786256	1.493052	0.000000
8	4	0	-0.671949	2.764037	0.000000
9	1	0	-1.727025	3.569349	0.000000

Table S11. Optimized Cartesian coordinates of the complex of BF_3 with HCOBeH (Be-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.169045	0.625924	0.000000
2	8	0	1.021751	-0.678924	0.000000
3	9	0	-1.237476	0.084789	0.000000
4	9	0	0.383391	1.272320	1.155090
5	9	0	0.383391	1.272320	-1.155090
6	6	0	0.383391	-1.770237	0.000000
7	4	0	-1.398261	-1.490305	0.000000
8	1	0	-2.554095	-2.154725	0.000000
9	1	0	1.063796	-2.625711	0.000000

Table S12. Optimized Cartesian coordinates of the complex of BF_3 with $HCOBH_2$ (H-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.021961	-0.997504	0.000000
2	8	0	-0.521455	0.659832	0.000000
3	9	0	1.379048	-0.861712	0.000000
4	9	0	-0.521455	-1.443021	1.151810
5	9	0	-0.521455	-1.443021	-1.151810
6	6	0	0.295958	1.591896	0.000000
7	1	0	1.362760	1.332887	0.000000
8	5	0	-0.245350	3.069137	0.000000
9	1	0	-0.437588	3.604357	-1.038356
10	1	0	-0.437588	3.604357	1.038356

Table S13. Optimized Cartesian coordinates of the complex of BF_3 with $HCOBH_2$ (B-bound).

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.158338	0.706174	0.000000
2	8	0	1.225723	-0.008632	0.000000
3	9	0	-1.076486	-0.496823	0.000000
4	9	0	-0.308844	1.372514	1.152761
5	9	0	-0.308844	1.372514	-1.152761
6	6	0	1.139001	-1.264080	0.000000
7	5	0	-0.308844	-1.886182	0.000000
8	1	0	-0.577386	-2.449622	-1.018104
9	1	0	-0.577386	-2.449622	1.018104
10	1	0	2.098450	-1.781019	0.000000