Supplementary material to:

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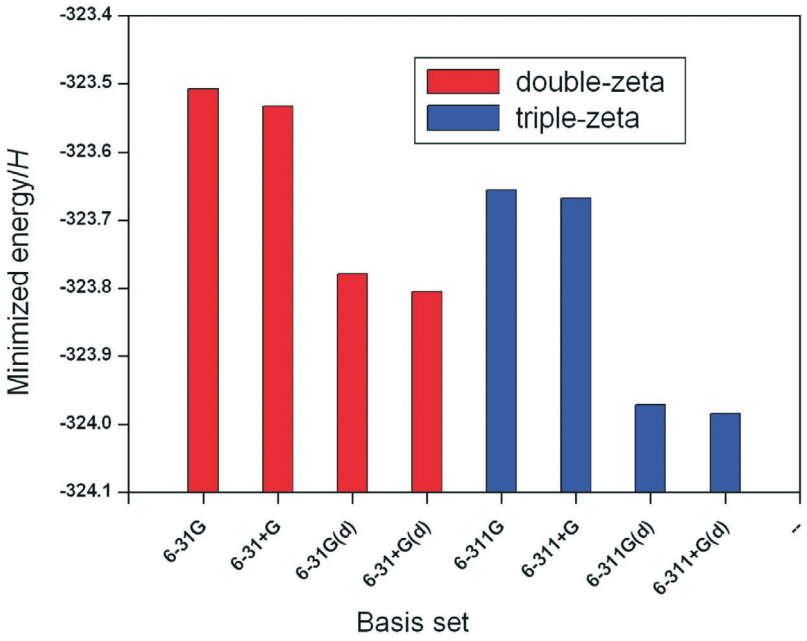

Fig. SM1

Table SM1 Structural parameters of the BF_3, H_2O and H_2S monomers determined using a number of basis sets.

Basis set	BF_3 [a]	H_2O [b]		H_2S [c]	
	r(BF)/pm	r(OH)/pm	HOH/deg	r(SH)/pm	HSH/deg
6-31G	136.32	97.46	109.28	137.48	94.91
6-31++G	136.65	97.65	111.01	137.51	94.93
6-31G(d,p)	132.36	96.14	103.83	133.01	92.87
6-31++G(d,p)	132.78	96.34	105.35	133.04	92.87
6-311G	134.71	96.87	109.99	138.13	94.81
6-311++G	135.00	97.13	111.16	138.13	94.69
6-311G(d,p)	131.62	95.78	102.44	133.37	92.16
6-311++G(d,p)	131.83	95.95	103.47	133.34	92.08
Experimental	130.70	95.7848	104.5424	133.620	92.06

[a] Ref. 18; [b] Ref. 19; [c] Ref. 20.

Table SM2 Minimized energies and Hessian indices of the $BF_3.H_2O$ and $BF_3.H_2S$ complexes, computed with a variety of basis sets.

Complex	Basis set	Eclipsed conformer		Staggered conformer	
		Minimized energy/*H*	Hessian index	Minimized energy/*H*	Hessian index
$BF_3.H_2O$	6-31G	–399.65591133015	1	–399.65591133346	1
	6-31++G	–399.69444761161	1	–399.69444761265	1
	6-31G(d,p)	–400.01921664495	0	–400.01863147338	1
	6-31++G(d,p)	–400.05592989303	0	–400.05569887815	1
	6-311G	–399.84054518903	0	–399.84054518901	0
	6-311++G	–399.86136860813	0	–399.86136860509	0
	6-311G(d,p)	–400.25358687945	0	–400.25339186556	1
	6-311++G(d,p)	–400.27446375737	0	–400.27436430315	1
$BF_3.H_2S$	6-31G	–722.20084121939	1	–722.20119338776	0
	6-31++G	–722.23088721992	0	–722.23072649231	1
	6-31G(d,p)	–722.59428176696	1	–722.59461714872	0
	6-31++G(d,p)	–722.62470448989	0	–722.62465897903	1
	6-311G	–722.38233581410	1	–722.38258021377	0
	6-311++G	–722.39966916545	1	–722.39989338647	0
	6-311G(d,p)	–722.82220533604	1	–722.82246291336	0
	6-311++G(d,p)	–722.83916488261	1	–722.83937270392	0

Table SM3 Computed wavenumbers of the $^{11}BF_3$, H_2O and H_2S monomers determined using the 6-311++G(d,p) basis set.

Monomer	Symmetry species	Mode	Wavenumber/cm^{-1}	
			Computed	Experimental
$^{11}BF_3$ [a]	a_1'	ν_1	873.9	888
	a_2''	ν_2	695.3	691.21479
	e'	ν_3	1434.0	1453.96647
		ν_4	474.8	479.462
H_2O [b]	a_1	ν_1	3884.5	3657.05325
		ν_2	1628.6	1594.74635
	b_2	ν_3	4002.8	3755.9287
H_2S [c]	a_1	ν_1	2816.9	2719.1770
		ν_2	1233.3	1212.840
	b_2	ν_3	2836.1	2735.8241

[a] Refs. 29–32; [b] Ref. 19; [c] Harmonic wavenumbers, ref. 33.