Supporting Information

Chalcogen and Pnicogen Bonds in Complexes of Neutral Icosahedral and Bicapped Square-Antiprismatic Heteroboranes

Adam Pecina,[1] Martin Lepšík,[1] Drahomír Hnyk,[2] Pavel Hobza,[1,3] and Jindřich Fanfrlík*[1]*

[1]Gilead Sciences and IOCB Research Center and Institute of Organic Chemistry and Biochemistry (IOCB), Academy of Sciences of the Czech Republic, v.v.i.; Flemingovo nám. 2, 16610 Prague 6 (Czech Republic)

[2]Institute of Inorganic Chemistry, Academy of Sciences of the Czech Republic, v.v.i.; 250 68 Řež (Czech Republic)

[3] Regional Center of Advanced Technologies and Materials Department of Physical Chemistry, Palacký University, 77146 Olomouc (Czech Republic)

Table S1. The structural and energetic characteristics of **Cl-SB$_{11}$** and **SB$_9$** complexes. The B12-chalcogen-chalcogen-bond acceptor angle (α) in degrees. The chalcogen...chalcogen-bond acceptor distance (d) in Å. The interaction energy (ΔE) and its decomposition into electrostatic (E_1^{Pol}), exchange-repulsion (E_1^{Ex}), dispersion (E_2^{D}) and induction (E^{Ind}) terms; energy in kcal mol^{-1}.

Complex	α	d	DFD-D3	DFT-SAPT				
			ΔE	E_1^{Pol}	E_1^{Ex}	E_2^{D}	E^{Ind}[a]	ΔE
Cl-SB$_{11}$								
Cl-SB$_{11}$...BEN	180	3.11	–6.2	–5.4	9.2	–8.4	–2.1	–6.7
	165	3.13	–6.3	–5.4	9.3	–8.6	–2.0	–6.7
Cl-SB$_{11}$...TMA	180	3.24	–4.2	–4.0	5.6	–4.8	–1.1	–4.3
	140	3.03	–6.3	–7.5	11.5	–7.8	–2.2	–6.1
Cl-SB$_{11}$...DME	180	3.18	–3.2	–2.8	3.7	–3.4	–0.7	–3.2
	135	3.07	–4.9	–4.5	5.8	–5.2	–1.1	–5.0
Cl-SB$_{11}$...DMK	180	3.21	–3.7	–3.4	3.7	–3.2	–0.9	–3.9
	135	3.04	–5.4	–5.8	7.1	–5.5	–1.6	–5.9
Cl-SB$_{11}$...FA	180	3.15	–3.7	–3.8	3.8	–2.8	–1.0	–3.8
	130	3.01	–5.9	–6.6	7.6	–5.3	–1.8	–6.1
SB$_9$								
SB$_9$...BEN	180	3.13	–5.0	–4.8	8.4	–7.2	–1.8	–5.5
	150	3.19	–5.3	–4.6	8.2	–7.8	–1.6	–5.8
SB$_9$...TMA	180	3.19	–3.6	–4.2	6.0	–4.4	–1.1	–3.7
	125	2.98	–6.1	–8.3	13.1	–8.4	–2.4	–6.0
SB$_9$...DME	180	3.23	–2.8	–2.2	3.3	–3.4	–0.6	–2.8
	125	3.08	–4.5	–4.3	6.0	–5.3	–1.1	–4.6
SB$_9$...DMK	180	3.20	–3.1	–3.2	4.2	–3.3	–0.9	–3.3
	120	3.11	–5.7	–5.2	6.6	–5.6	–1.4	–5.6
SB$_9$...FA	180	3.17	–3.2	–3.3	3.4	–2.4	–1.0	–3.4
	115	3.14	–5.3	–3.3	3.4	–2.4	–1.1	–3.6

[a] $E^{Ind} = E_2^{Ind} + E_2^{Ex\text{-}Ind} + \delta HF$

Figure S1. Interaction energy (ΔE) plotted against B12-S-chalcogen bond acceptor angle. Structures of complexes at an optimal angle (right) and at 180 degrees (left) are shown. Energy in kcal mol^{-1}, angle in degrees and Color coding as follows: black, C; light-pink, B; yellow, S; white, H.

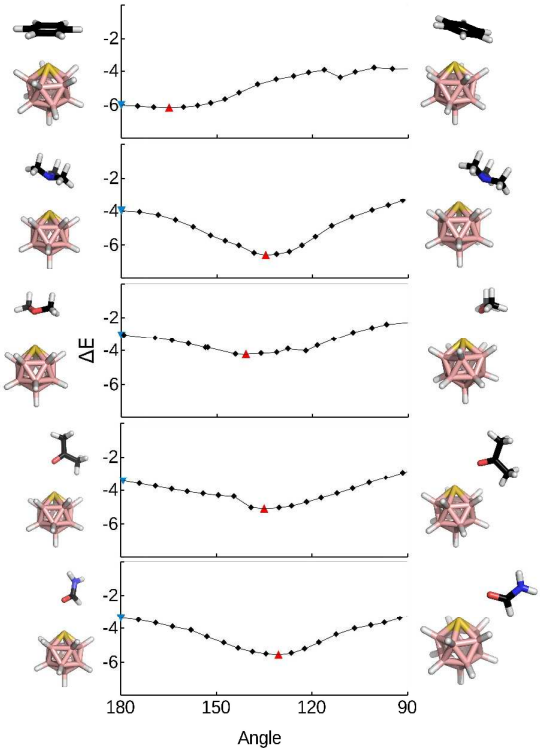

Figure S2. Interaction energy (ΔE) plotted against the centre of B9 and B12 -the centre of P1 and P2 -pnictogen-bond acceptor angle. Energy in kcal mol^{-1}, angle in degrees