Supplementary material for:

Synthesis of Heteroboroxines with MB_2O_3 Core (M = Sb, Bi, Sn) - An Influence of the Substitution of Parent Boronic Acids.

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Table S1. Crystallographic Data for 2a, 2b, 3a, 4a and 4b

	2a	2b	3a	4a	4b
empirical formula	$C_{26}H_{27}B_2F_6N_2O_3Sb$	$C_{26}H_{27}B_2BiF_6N_2O_3$	$C_{26}H_{27}B_2F_6N_2O_3Sb$	$C_{24}H_{27}B_2Br_2N_2O_3Sb$	$C_{24}H_{27}B_2BiBr_2N_2O_3$
cryst syst	triclinic	triclinic	monoclinic	orthorhombic	orthorhombic
space group	P-1	P-1	P21/c	Pnma	Pnma
a[Å]	13.1730(10)	13.1011(13)	9.0330(7)	12.6750(10)	12.5821(7)
b[Å]	13.3801(9)	13.2870(8)	16.9461(19)	23.6280(10)	23.4640(6)
c[Å]	17.7910(11)	17.7210(10)	19.9601(9)	9.1971(12)	9.1219(17)
α[deg]	84.722(4)	84.714(5)	90	90	90
β[deg]	68.864(4)	68.641(5)	108.624(5)	90	90
γ[deg]	81.877(5)	81.857(4)	90	90	90
Z	4	4	4	4	4
μ[mm^{-1}]	1.023	6.276	1.027	3.930	9.542
D_x [Mg m^{-3}]	1.545	1.777	1.551	1.675	1.928
cryst size [mm]	0.33x0.31x0.19	0.32x0.26x0.08	0.31x0.25x0.15	0.28x0.26x0.26	0.38x0.35x0.16
θ range, [deg]	1 – 27.5	1 – 27.5	1 – 27.5	1 – 27.5	1 – 27.5
T_{min}, T_{max}	0.812, 0.983	0.348, 0.661	0.801, 0.880	0.432, 0.556	0.145, 0.341
no. of reflections measured	52 706	60 045	24 287	20 386	23 911
no. of unique reflns, R_{int}[a]	13108, 0.051	13002, 0.035	6575, 0.041	3208, 0.033	3453, 0.030
no. of observed reflns [$I>2\sigma(I)$]	9276	10484	4845	2453	3023
no. of parameters	721	721	361	160	160
S[b] all data	1.108	1.102	1.121	1.155	1.126
final R[b] indices [$I>2\sigma(I)$]	0.052	0.031	0.044	0.045	0.026
wR2[b] indices (all data)	0.100	0.060	0.090	0.088	0.049
Δρ, max., min. [e $Å^{-3}$]	1.183, -0.894	1.577, -1.417	1.251, -0.647	0.915, -1.019	1.015, -0.997

[a] $R_{int} = \Sigma \left| F_o^2 - F_{o,mean}^2 \right| / \Sigma F_o^2$, [b] $S = [\Sigma(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$. [b] $R(F) = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$, $wR(F^2) = [\Sigma(w(F_o^2 - F_c^2)^2)/(\Sigma w(F_o^2)^2)]^{½}$

Table S1 (continue). Crystallographic Data for 9a, 9b, 10a and 12c

	9a	9c	10a	12c
empirical formula	$C_{26}H_{27}B_2N_4O_3Sb.(CH_2Cl_2)$	$2(C_{32}H_{32}B_2N_4O_3Sn).3(C_7H_8)$	$C_{24}H_{31}B_2N_4O_3Sb$	$C_{28}H_{32}B_2N_4O_3Sn.1.5(C_6H_6)$
cryst syst	monoclinic	triclinic	orthorhombic	monoclinic
space group	P21/c	P-1	Pbca	C2/c
a[Å]	8.9330(5)	13.521(2)	18.5840(16)	24.2243(6)
b[Å]	18.9640(9)	16.0020(15)	12.1241(18)	9.8101(3)
c[Å]	17.5401(13)	18.2780(19)	22.3840(6)	31.3223(4)
α[deg]	90	87.385(10)	90	90
β[deg]	91.832(6)	88.092(11)	90	103.263(5)
γ[deg]	90	85.368(10)	90	90
Z	4	2	8	8
μ[mm^{-1}]	1.144	0.693	1.127	0.745
D_x [Mg m^{-3}]	1.503	1.349	1.493	1.339
cryst size [mm]	0.36x0.30x0.30	0.60x0.36x0.32	0.36x0.27x0.11	0.44x0.20x0.12
θ range, [deg]	1 – 27.5	1 – 27.5	1 – 27.5	1 – 27.5
T_{min}, T_{max}	0.711, 0.824	0.760, 0.869	0.758, 0.904	0.839, 0.943
no. of reflections measured	33 382	67 690	27 077	34 064
no. of unique reflns, R_{int}[a]	7490, 0.025	17318, 0.047	5750, 0.035	8224, 0.042
no. of observed reflns [$I>2\sigma(I)$]	6534	13784	4396	6884
no. of parameters	352	934	307	397
S[b] all data	1.086	1.214	1.158	1.077
final R[b] indices [$I>2\sigma(I)$]	0.036	0.084	0.034	0.037
wR2[b] indices (all data)	0.083	0.183	0.055	0.064
Δρ, max., min. [e $Å^{-3}$]	2.800, -2.360	2.587, -1.606	0.582, -0.504	0.417, -0.700

[a] $R_{int} = \Sigma \left| F_o^2 - F_{o,mean}^2 \right| / \Sigma F_o^2$, [b] $S = [\Sigma(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{1/2}$. [b] $R(F) = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$, $wR(F^2) = [\Sigma(w(F_o^2 - F_c^2)^2)/(\Sigma w(F_o^2)^2)]^{1/2}$

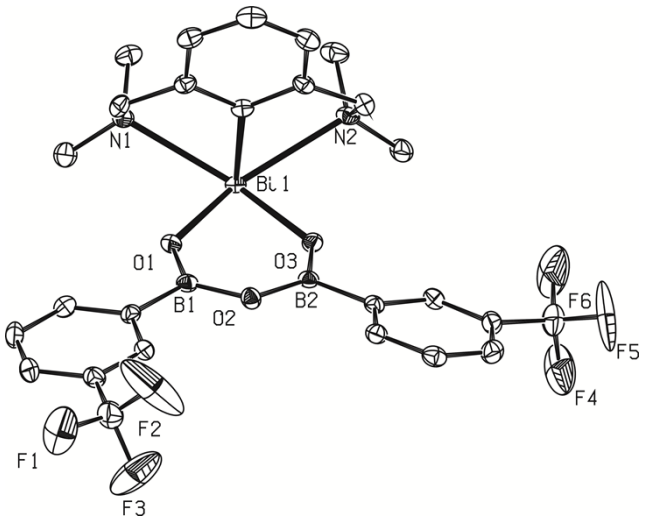

Figure S1 ORTEP plot of a molecule of **2b** showing 30% probability displacement ellipsoid. Hydrogen atoms are omitted for clarity and only one of two independent molecules in the unit cell is presented.

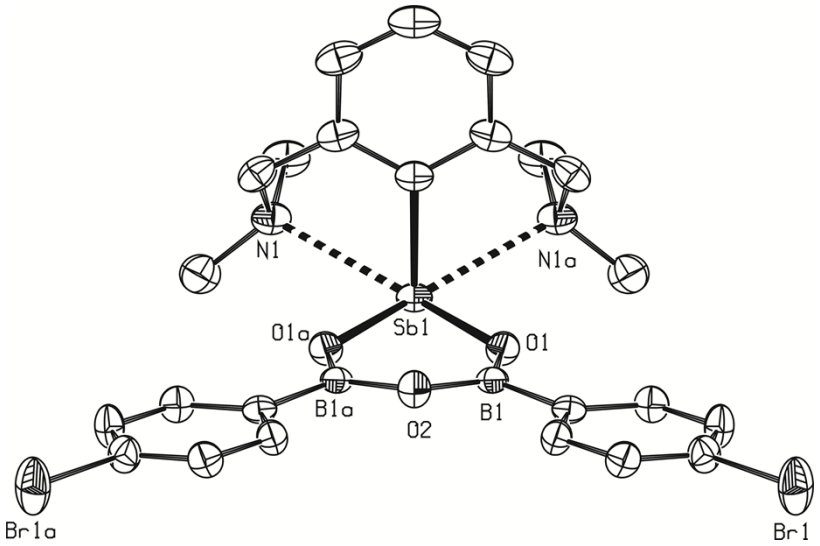

Figure S2 ORTEP plot of a molecule of **4a** showing 30% probability displacement ellipsoid. Symmetry operator a = x, ½-y, z. Hydrogen atoms are omitted for clarity.