Oxidation of Germa- and Stanna-*closo*-dodecaborate

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Supporting Information

SI Table 1. Results of the Crystal Structure Determination

Compound	**2**	**3**	**7**·2DMSO
Empirical formula	$C_{26}H_{82}B_{22}Ge_2N_2$	$C_{26}H_{82}B_{22}Ge_2N_2S$	$C_{16}H_{37}B_{11}N_2O_3S_3$ Sn
M_r [g mol^{-1}]	805.94	837.99	639.26
Temperature [K]	173(2)	173(2)	173(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal system	triclinic	triclinic	monoclinic
Space group	*P*–1	*P*-1	$P2_1/c$
Z	3	2	4
a [Å]	12.3369(5)	10.3761(10)	11.8146(10)
b [Å]	16.3463(8)	13.0634(10)	8.6455(4)
c [Å]	19.6863(9)	18.8637(16)	28.438(2)
α [deg]	112.0340(10)	80.125(6)	90
β [deg]	99.0220(10)	74.740(7)	100.542(6)
γ [deg]	96.148(2)	88.692(7)	90
V [Å^3]	3574.3(3)	2429.6(4)	2855.8(3)
Density ρ_{calc} [g/cm^3]	1.123	1.15	1.49
Abs. coeff. μ [mm^{-1}]	1.3	1.3	1.1
F(000)	1278	884	1296
Cryst. size [mm^3]	0.5 × 0.5 × 0.5	0.24 × 0.44 × 0.13	0.30 × 0.24 × 0.22
θ range [deg]	1.70–26.73	2.04–25.35	2.91–28.53
Limiting indices	–15 ≤ h ≤ 14, –20 ≤ k ≤ 20, –24 ≤ l ≤ 24	–12 ≤ h ≤ 12, –15 ≤ k ≤ 15, –22 ≤ l ≤ 22	–14 ≤ h ≤ 15, –11 ≤ k ≤ 10, –36 ≤ l ≤ 38
Reflections collected	15127	31489	7007
Indep reflns/ R_{int}	11736/0.0346	7848/0.0806	5753/0.0177
Completeness [%]	99.5	99.9	96.4
Absorp corr	multi-scan	numerical	numerical
Max./min. transmn	0.827 / 1.00	0.8802 / 0.7216	0.842 / 0.634
Params/ restraints	703/0	478/0	331/0
R_1/wR_2 [$I > 2\sigma(I)$]	0.0356/0.0813	0.0432/0.0906	0.0414/0.0837
R_1/wR_2 all data	0.0544/0.0879	0.0521/0.951	0.0571/0.0940
Goodness-of-fit on F^2	01.034	1.251	1.043
Largest diff. peak/hole [e·A^{-3}]	0.355 and –0.356	0.41 and –0.70	2.94 and –0.79
CCDC	1040057	1040058	1040059