Supporting Information for

Uncommon structural and bonding properties in $Ag_{16}B_4O_{10}$

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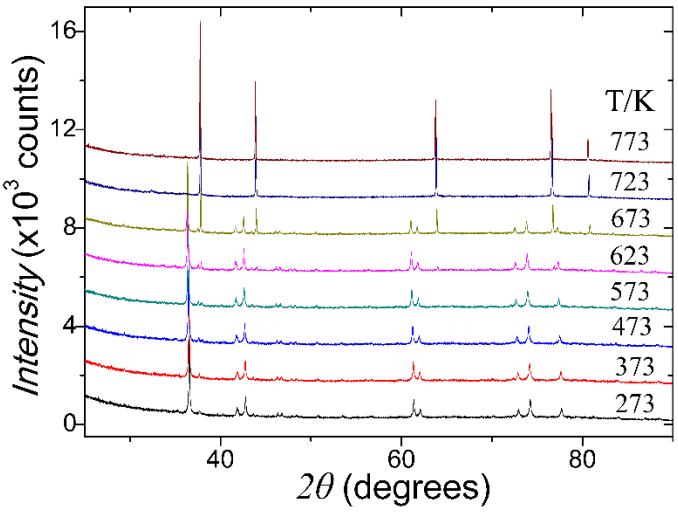

Figure S1. Temperature dependent powder X-ray diffraction indicating $Ag_{16}B_4O_{10}$ start to decompose into elemental Ag at about 623 K

Table S1. Crystal data, data collection and refinement details for $Ag_{16}B_4O_{10}$ at 298 K.

Empirical formula	$Ag_{16}B_4O_{10}$
Formula weight	1929.16
Space group (no.), Z	$I4_1/a$ (88), 4
Lattice parameters /Å,	a = 13.3481(5) c = 8.6228(4)
V /Å^3	1536.3(1)
ρ_{xray} /g×cm^{-3}	8.340
Crystal size /mm^3	0.12 × 0.08 × 0.06
Diffractometer	SMART APEX I, Bruker AXS
X-ray radiation, λ/Å	MoK$_\alpha$, 0.71073
Absorption correction	Multi-scan, SADABS
2θ range /°	$5.62 \leq 2\theta \leq 103.92$
Index ranges	$-29 \leq h \leq 29$, $-27 \leq k \leq 29$, $-19 \leq l \leq 17$
Reflections collected	31920
Data, R_{int}	4280, 0.032
No. of parameters	170
Transmission: t_{min}, t_{max}	0.198, 0.381
Final R indices [I > 2σ(I)]	R1 = 0.033, wR2 = 0.080
R indices (all data)	R1 = 0.037, wR2 = 0.082
Deposition no.	CSD- 1951872

Table S2. Atomic coordinates and displacement parameters U_{eq} /10^{-4} Å^2.

Atom	Site	*x*	*y*	*z*	U_{eq}
Ag1	16*f*	0.16299(2)	0.54868(2)	0.02757(2)	135.8(3)
Ag2	16*f*	0.25826(2)	0.73949(2)	0.01031(2)	136.7(3)
Ag3	16*f*	0.35583(2)	0.45035(2)	0.00220(2)	140.7(3)
Ag4	16*f*	0.10879(2)	0.69713(2)	0.25948(2)	148(3)
O1	8*e*	0	¾	0.0738(2)	102(2)
O2	16*f*	0.1208(1)	0.7899(1)	–0.1258(2)	103(2)
O3	16*f*	0.3371(1)	0.3329(1)	0.1788(2)	123(2)
B	16*f*	0.4160(2)	0.2933(2)	0.2730(3)	108(3)

Table S3. Selected interatomic distances /Å and angles /°.

Atomic contact	Distance /Å	Atomic contact	Angle /°
Ag1 — O2	2.350(2)	O1 — B — O2	106.4(2)
— O3	2.264(2)		107.6(2)
Ag2 — O2	2.280(1)	O1 — B — O3	111.9(2)
— O3	2.307(2)	O2 — B — O2	107.4(2)
Ag3 — O3	2.200(2)	O2 — B — O3	111.3(2)
Ag4 — O1	2.274(1)		111.9(2)
B — O1	1.512(3)		
— O2	1.485(3)		
— O2	1.496(3)		
— O3	1.431(3)		

Table S4. Refined atomic parameters against PXRD in space group I 4_1/a:2. The refined lattice parameters are a = 13.3614(4) Å and c =8.6288(3) Å

Atom	Site	*x*	*y*	*z*
Ag1	16*f*	0.1633(3)	0.5497(2)	0.0265(3)
Ag2	16*f*	0.2578(3)	0.7394(2)	0.0139(4)
Ag3	16*f*	0.3550(2)	0.4506(3)	0.0005(3)
Ag4	16*f*	0.1087(2)	0.6966(3)	0.2607(5)
O1	8*e*	0	¾	0.0738
O2	16*f*	0.1208	0.7899	–0.1258
O3	16*f*	0.3371	0.3329	0.1788
B	16*f*	0.4160	0.2933	0.2730

Computational details

Pseudopotentials (scalar relativistic) and basis sets

	Ag		**B**		**O**	
Pseudopotential core valence ref.	[Ar]3d^{10} 4s^{2}4p^{6}4d^{10}5s^1 [S1]		[He] 2s^{2}2p [S2]		[He] 2s^{2}2p^4 [S2]	
	exponent	coefficient	exponent	coefficient	exponent	coefficient
s-shell	9.088442 7.540731 2.794005 1.480158 0.653851 0.35	-1.9648132 2.7332194 0.1991148 1.0 1.0 1.0	1.690560 0.983666 0.256979	-0.272208 0.201128 0.577763	47.105518 5.911346 0.976483 0.296070	-0.014408 0.129568 -0.563118 1.0
p-shell	4.451240 3.675263 1.291288 0.652578 0.36704	-6.083378 6.4168543 0.7539735 0.2730597 1.0	5.399913 1.271217 0.361909	0.034941 0.186834 0.468463	16.692219 3.900702 1.078253 0.284189	0.044856 0.222613 0.500188 1.0
sp-shell	0.18	1.0 1.0	0.12	1.0 1.0	0.12	1.0 1.0
d-shell	7.99473 2.784773 1.209744 0.505393 0.198851	-0.0163876 0.2814107 0.4863264 0.3867258 1.0	0.5	1.0	1.2	1.0

Tolerance parameters used in the CRYSTAL17 input:

TOLINTEG 12 12 12 12 24

TOLPSEUD 12

TOLDEE 8

BIPOLAR 128 128

Structural parameters used in the calculation

Lattice	
a / Å c / Å	13.3481 8.6228
Site parameter	
Ag1 Ag2 Ag3 Ag4 O1 O2 O3 B	0.16199 0.54868 0.02757 0.25826 0.73949 0.01031 0.35583 0.45035 0.00220 0.10879 0.69713 0.25948 0.00000 0.75000 0.07380 0.12081 0.78993 -0.12579 0.33712 0.33285 0.17879 0.41600 0.29325 0.2730

[S1] Andrae, D.; Haeussermann, U.; Dolg, M.; Stoll, H.; Preuss, H. Energy-adjusted *ab initio* pseudopotentials for the second and third row transition elements. *Theor. Chim. Acta*, **1990**, *77*, 123-141.

[S2] Bergner, A.; Dolg, M.; Küchle, W.; Stoll, H.; Preuss, H. *Ab initio* energy-adjusted pseudopotentials for elements of groups 13–17, *Mol. Phys.* **1993**, *80*, 1431-1441.