IUCrJ

Volume 7 (2020)

Supporting information for article:

Expression and interactions of stereochemically active lone pairs and their relation to structural distortions and thermal conductivity

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S1. Geometry optimization

The full geometry, i.e. unit cell and fractional coordinates, were optimized starting from the structure from Roelsgaard *et al.* (2016) according to the information given in the manuscript. In Table S1, a comparison of the optimized structure with the 100 K experimental structure is given.

Table S1 Optimized geometry and experimental geometry. The numbers in parentheses are the percentage deviation from experimental values

Parameter	Optimized	Experimental
a (Å)	8.65577671 (-0.40 %)	8.6905
c (Å)	6.01823632 (+0.26 %)	6.0024
Mn	(0,0.5,0.25)	(0,0.5,0.25)
Sb	(0.17886,0.16577,0.5)	(0.17912,0.16801,0.5)
O1	(0.17847,0.32153,0.25)	(0.1795,0.3205,0.25)
O2	(0.40618,0.15253,0.5)	(0.4005,0.1450,0.5)
Mn-O1 (Å)	2.1847 (-0.83 %)	2.203
Mn-O2 (Å)	2.1602 (+0.85 %)	2.142
Sb-O1 (Å)	2.0203 (+0.94 %)	2.002
Sb-O2 (Å)	1.9710 (+1.91 %)	1.934

S2. ICSD search

Table S2 All structures with space group number and ICSD code used in the final analysis of bond angles in SbX_3 (X=O,S,Se) units. There are 77 structures in total with 137 unique connected SbX_3 units and 37 unique isolated SbX_3 units.

Chemical Formula	Space Group number	ICSD code	Connected units	Isolated units
$MgSb_2O_4$	135	4122	1	0
$Ba_3(SbO_3)_2$	2	413764	0	3
$Sr_5Sb_{22}O_{38}$	14	425765	5	0
$Na_3(SbO_3)$	217	23346	0	1
$LiSbO_2$	14	262075	2	0
$K_3(SbO_3)$	198	279579	0	1
$Cs_3(SbO_3)$	198	279580	0	1
KSb_3O_5	14	28493	2	0
$NaSb_5O_8$	2	28494	3	0
$Cs_2SbO_{2.5}$	8	411212	2	0
$Rb_2(Sb_8O_{13})$	11	412329	7	0
$Fe(Sb_2O_4)$	14	155152	2	0
$(Sb_4O_5)(ReO_4)_2$	2	165619	4	0
$Cu(Sb_2O_4)$	106	190731	1	0
Sb_2VO_5	62	203130	1	0
$MnSb_2O_4$	135	243444	1	0
$CoSb_2O_4$	135	262627	1	0
Sb_2VO_5	15	27800	1	0
$ZnSb_2O_4$	135	31996	1	0

$FeO(Sb_2O_3)$	135	4459	1	0
$Sb_2(MoO_6)$	2	59292	8	0
Sb_2WO_6	1	75595	2	0
$NiSb_2O_4$	135	86492	1	0
$Ba_4Sb_4Se_{11}$	58	31500	3	1
$BaSb_2Se_4$	14	32040	2	0
$Ba_3Sb_2Se_7$	15	429279	0	2
$KSbSe_2$	2	100125	1	0
$CsSbSe_2$	14	20773	2	0
$K_2(Sb_4Se_8)$	2	402886	1	0
$Rb_2(Sb_4Se_8)$	2	402887	1	0
Na_3SbSe_3	198	425125	0	1
$CsSb_2Se_4$	2	61220	1	0
$RbSb_3Se_5$	14	64672	3	0
$KSbSe_2$	1	660008	2	0
K_3SbSe_3	198	89607	0	1
Rb_3SbSe_3	198	89608	0	1
Cs_3SbSe_3	198	89609	0	1
$CuSbSe_2$	62	238476	1	0
Cu_3SbSe_3	62	401095	0	1
Ag_5SbSe_4	36	427307	0	1
Ag_3SbSe_3	62	427308	0	3
$SbCrSe_3$	62	84866	1	0
$Ca_2Sb_2S_5$	14	201044	1	1
$Sr_3Sb_4S_9$	33	201400	3	0
$Ba_8(Sb_6S_{17})$	13	26434	2	3
$BaSb_2S_4$	14	38372	2	0
$Ba_3Sb_2S_7$	15	429278	0	2
$Sr_6Sb_6S_{17}$	19	90094	6	0
$RbSbS_2$	1	200263	2	0
$CsSbS_2$	14	200798	1	0
$Cs_4Sb_{14}S_{23}$	2	20866	14	0
$Cs_2Sb_4S_7$	14	2193	3	0
$Rb_2Sb_4S_7$	2	2194	2	0
$K_2Sb_4S_7$	15	25329	1	0
$K(Sb_5S_8)$	7	410178	7	0
Li_3SbS_3	33	424834	0	1
Na_3SbS_3	198	425458	0	1
Cs_3SbS_3	198	426551	0	1
K_3SbS_3	198	426552	0	1
Rb_3SbS_3	198	426554	0	1
$Li_3S_{18}Sb_{11}$	2	433665	10	0
$RbSbS_2$	2	56788	1	0
$Cs_2(S_2)(Sb_4S_6)$	2	67976	1	0
$AgSbS_2$	9	16578	2	0
$CuSbS_2$	62	171051	1	0

$HgSb_4S_8$	15	174377	4	0
Ag_3SbS_3	161	181518	0	1
Ag_5SbS_4	36	290662	0	1
$Ag_3(SbS_3)$	14	33714	0	1
$Cu_3(SbS_3)$	19	403113	0	1
$MnSb_2S_4$	12	411178	2	0
$MnSb_2S_4$	62	56379	2	0
$CrSbS_3$	62	74601	1	0
Cu_3SbS_3	14	74901	0	2
$AgSbS_2$	5	85130	2	0
$FeSb_2S_4$	62	93911	2	0
$AgSbS_2$	15	94647	1	0