

Supplementary Materials

TOPOS output for Voronoi polyhedra of four non-equivalent antimony atoms. The levels of solid angles (SAng. or Ω) corresponding to different levels of the Sb–O bonding are selected by yellow.

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#####
1:Sb2O3/HP=10GPa
#####
Central atom:Sb1 CN:5 0.234 0.469 0.471 Rsd:1.575
D(CP):0.779 ( 0.2701 0.5405 0.4217 )
D(VDP):0.408 ( 0.2532 0.5130 0.4611 )
Atom:1.881 < r < 3.974 <r>=3.134 Top: 1.758 < R < 2.387 <R>=2.032
CN=9:0:3 NV=20 V=16.378/60.958 S=36.976 Cpac=0.213 Ccov=3.480
G3=0.093452685
Face distribution: {3/1 4/2 5/6 6/2 7/1 }
Vertex distribution: {3/20 }
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	Atom	x	y	z	Dist.	SAng.
	1 O 2	0.154	0.403	0.263	1.881	23.33
	2 O 5	0.248	0.241	0.619	2.054	19.29
	3 O 1	0.090	0.523	0.662	2.240	17.54
	-----> Ω =17.54%					
	4 O 2	0.346	0.597	0.763	2.719	12.86
	-----> Ω =12.77%					
	5 O 1	0.410	0.477	0.162	3.084	7.94
	-----> Ω =5.66%					
	6 O 4	0.504	0.320	0.494	3.345	5.06
	7 O 5	0.252	0.759	0.119	3.438	4.99
	8 O 4	0.004	0.180	0.506	3.463	0.45
*	9 O 6	0.360	0.048	0.301	3.726	1.08
*10	Sb 3	-0.005	0.745	0.258	3.829	1.46
*11	Sb 2	0.488	0.684	0.222	3.860	1.96
	12 Sb 4	0.262	0.990	0.514	3.974	4.04

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Central atom:Sb2 CN:6 0.488 0.684 0.222 Rsd:1.538
D(CP):1.265 ( 0.4508 0.6918 0.3803 )
D(VDP):0.507 ( 0.4777 0.6960 0.2863 )
Atom:1.872 < r < 4.424 <r>=3.314 Top: 1.730 < R < 2.387 <R>=2.109
CN=10:0:4 NV=24 V=15.251/69.424 S=35.302 Cpac=0.225 Ccov=3.738
G3=0.098431982
Face distribution: {3/1 4/3 5/3 6/7 }
Vertex distribution: {3/24 }
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	Atom	x	y	z	Dist.	SAng.
	1 O 1	0.410	0.477	0.162	1.872	21.71
	2 O 4	0.496	0.820	0.006	1.910	20.88
	3 O 6	0.640	0.548	0.199	2.056	19.71
	-----> Ω =17.54%					
	4 O 1	0.590	0.977	0.338	2.656	12.77
	-----> Ω =12.77%					
	5 O 5	0.252	0.759	0.119	2.915	6.75
	6 O 6	0.360	1.048	0.301	3.189	5.66
	-----> Ω =5.66%					
	7 O 4	0.504	0.320	0.494	3.433	3.76
*	8 O 3	0.603	0.474	-0.195	3.745	0.04
* 9	Sb 1	0.234	0.469	0.471	3.860	1.96
	10 Sb 3	0.495	0.755	0.742	3.929	4.82
*11	Sb 4	0.762	0.510	0.486	3.972	0.18
*12	Sb 4	0.262	0.990	0.514	4.136	0.83
	13 O 3	0.397	0.974	0.695	4.296	0.35
	14 O 2	0.346	0.597	0.763	4.424	0.60

Central atom:Sb3 CN:5 0.495 0.755 0.742 Rsd:1.578
 D(CP):1.175 (0.5576 0.7375 0.6201)
 D(VDP):0.482 (0.5172 0.7469 0.6883)
 Atom:2.035 < r < 4.095 <r>=3.166 Top: 1.781 < R < 2.370 <R>=2.111
 CN=9:0:3 NV=20 V=16.469/60.998 S=36.723 Cpac=0.268 Ccov=3.387
 G3=0.094938837
 Face distribution: {3/1 4/2 5/5 6/4 }
 Vertex distribution: {3/20 }

	Atom	x	y	z	Dist.	SAng.
1	O 4	0.496	0.820	1.006	2.035	19.05
2	O 3	0.397	0.974	0.695	2.039	20.00
3	O 2	0.346	0.597	0.763	2.114	19.26
-----> Ω =17.54%						
4	O 3	0.603	0.474	0.805	2.517	14.61
-----> Ω =12.77%						
5	O 5	0.752	0.741	0.881	3.169	5.77
6	O 2	0.654	1.097	0.737	3.179	6.18
-----> Ω =5.66%						
7	O 1	0.590	0.977	0.338	3.631	4.79
* 8	Sb 4	0.262	0.990	0.514	3.667	0.01
9	O 4	0.504	0.320	0.494	3.783	2.07
*10	Sb 1	0.734	1.031	0.529	3.829	1.46
11	Sb 2	0.488	0.684	0.222	3.929	4.82
*12	Sb 4	0.762	0.510	0.486	4.095	1.99

Central atom:Sb4 CN:5 0.762 0.510 0.486 Rsd:1.588
 D(CP):1.187 (0.7173 0.6473 0.5171)
 D(VDP):0.489 (0.7411 0.5638 0.5004)
 Atom:2.004 < r < 4.208 <r>=3.338 Top: 1.687 < R < 2.387 <R>=2.140
 CN=9:0:6 NV=26 V=16.771/79.040 S=37.037 Cpac=0.251 Ccov=3.399
 G3=0.095869772
 Face distribution: {3/2 4/1 5/4 6/8 }
 Vertex distribution: {3/26 }

	Atom	x	y	z	Dist.	SAng.
1	O 6	0.860	0.452	0.699	2.004	21.02
2	O 5	0.748	0.259	0.381	2.055	18.11
3	O 3	0.897	0.526	0.305	2.080	18.66
-----> Ω =17.54%						
4	O 6	0.640	0.548	0.199	2.587	13.38
-----> Ω =12.77%						
5	O 3	0.603	0.474	0.805	3.031	8.84
-----> Ω =5.66%						
6	O 4	0.504	0.320	0.494	3.325	4.16
7	O 5	0.752	0.741	0.881	3.439	4.15
* 8	O 2	0.846	0.903	0.237	3.647	3.05
* 9	Sb 3	0.995	0.745	0.258	3.667	0.01
*10	O 2	0.654	0.097	0.737	3.856	0.23
*11	Sb 2	0.488	0.684	0.222	3.972	0.18
12	Sb 1	0.734	1.031	0.529	3.974	4.04
*13	Sb 3	0.495	0.755	0.742	4.095	1.99
*14	Sb 2	0.988	0.816	0.778	4.136	0.83
15	O 1	0.590	0.977	0.338	4.208	1.34