

1:C17 H17 N O7 Pb
#####

Structure consists of molecules (ZD1). The composition of molecule is Sc
Structure consists of molecules (ZE1). The composition of molecule is Pb
Topology for ZD1

Atom ZD1 links by bridge ligands and has
Common vertex with

				R(A-A)	f	Total SA
ZE 1	-0.1601	0.7948	0.0499	(-1 0 0)	7.022A	1 30.06
ZE 1	0.1601	0.2052	0.9501	(1 1 1)	7.022A	1 30.06
ZE 1	-0.1601	0.7052	-0.4501	(-1 1-1)	8.214A	1 19.94
ZE 1	0.1601	0.2948	1.4501	(1-1 1)	8.214A	1 19.94

Topology for ZE1

Atom ZE1 links by bridge ligands and has
Common vertex with

				R(A-A)	f	Total SA
ZD 1	1.0000	0.5000	0.5000	(1 0 0)	7.022A	1 38.04
ZD 1	1.0000	1.0000	1.0000	(1 0 1)	8.214A	1 25.23
ZE 1	0.1601	0.2052	-0.0499	(1 1 0)	14.473A	1 36.73

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZE2ZD

Coordination sequences

ZD1: 1 2 3 4 5 6 7 8 9 10
Num 4 8 20 38 58 88 124 156 204 256
Cum 5 13 33 71 129 217 341 497 701 957

ZE1: 1 2 3 4 5 6 7 8 9 10
Num 3 8 18 35 59 87 119 160 201 250
Cum 4 12 30 65 124 211 330 490 691 941

TD10=946

Vertex symbols for selected sublattice

ZD1 Point (Schlafli) symbol:{8^5;10}
Extended point symbol:[8(2).8(2).8(2).8(2).8(2).10(2)]

ZE1 Point (Schlafli) symbol:{8^3}
Extended point symbol:[8.8(3).8(3)]

Point (Schlafli) symbol for net: {8^3}2{8^5;10}
3,4-c net with stoichiometry (3-c)2(4-c); 2-nodal net

Topological type: fsh-3,4-P21/c (binodal.ttd) {8^3}2{8^5;10} - VS [8.8(3).8(3)] [8(2).8(2).8(2).8(2).8(2).*] (

Non-equivalent circuits

Circuit No 1; Type=8a; Centroid: (0.355,0.787,0.069)

Atom x y z

ZD1 0.0000 0.5000 -0.5000
ZE1 0.1601 0.2052 -0.0499
ZE1 0.8399 0.7948 0.0499
ZD1 1.0000 1.0000 1.0000
ZE1 0.8399 0.7052 0.5499
ZE1 0.1601 1.2948 0.4501
ZD1 0.0000 1.0000 0.0000
ZE1 -0.1601 0.7948 -0.9501

Circuit No 2; Type=8b; Centroid: (0.000,0.000,0.500)

Atom x y z

ZD1 0.0000 -0.5000 0.5000
ZE1 -0.1601 -0.2948 -0.4501
ZD1 0.0000 0.0000 0.0000
ZE1 0.1601 0.2052 0.9501
ZD1 0.0000 0.5000 0.5000
ZE1 0.1601 0.2948 1.4501
ZD1 0.0000 0.0000 1.0000
ZE1 -0.1601 -0.2052 0.0499

Circuit No 3; Type=10; Centroid: (0.500,0.500,0.000)

Atom	x	y	z
ZD1	0.0000	0.5000	-0.5000
ZE1	-0.1601	0.7052	-1.4501
ZD1	0.0000	1.0000	-1.0000
ZE1	0.1601	1.2948	-0.5499
ZE1	0.8399	0.7052	-0.4501
ZD1	1.0000	0.5000	0.5000
ZE1	1.1601	0.2948	1.4501
ZD1	1.0000	0.0000	1.0000
ZE1	0.8399	-0.2948	0.5499
ZE1	0.1601	0.2948	0.4501

Elapsed time: 17.14 sec.