

#####  
1:C26 H18 Cd N2 O6  
#####

Structure consists of molecules (ZD1). The composition of molecule is Ti  
Structure consists of molecules (ZE1). The composition of molecule is Cd  
Topology for ZD1

-----  
Atom ZD1 links by bridge ligands and has  
Common vertex with

				R(A-A)	f	Total SA
ZE 1	1.0000	0.3998	0.2500	( 1 1 1)	7.601A	1 25.43
ZE 1	0.5000	1.1002	-0.2500	( 0 0 0)	7.601A	1 25.43
ZE 1	1.0000	0.6002	0.7500	( 1 0 0)	8.044A	1 24.57
ZE 1	0.5000	0.8998	-0.7500	( 0 1-2)	8.044A	1 24.57

Topology for ZE1

-----  
Atom ZE1 links by bridge ligands and has  
Common vertex with

				R(A-A)	f	Total SA
ZD 1	0.2500	0.2500	1.0000	( 1 1 1)	7.601A	1 25.43
ZD 1	-0.2500	0.2500	0.5000	(-1 1 0)	7.601A	1 25.43
ZD 1	-0.2500	0.7500	0.0000	(-1 0 0)	8.044A	1 24.57
ZD 1	0.2500	0.7500	1.5000	( 1 0 1)	8.044A	1 24.57

-----  
Structural group analysis  
-----

-----  
Structural group No 1  
-----

Structure consists of 3D framework with ZE1D

-----  
Coordination sequences  
-----

ZD1: 1 2 3 4 5 6 7 8 9 10  
Num 4 10 24 42 64 92 124 162 204 252  
Cum 5 15 39 81 145 237 361 523 727 979

ZE1: 1 2 3 4 5 6 7 8 9 10  
Num 4 10 24 42 64 90 124 162 204 250  
Cum 5 15 39 81 145 235 359 521 725 975

-----  
TD10=977

-----  
Vertex symbols for selected sublattice  
-----

ZD1 Point (Schlafli) symbol: {4<sup>2</sup>;8<sup>4</sup>}  
Extended point symbol: [4.4.8(2).8(2).8(8).8(8)]

ZE1 Point (Schlafli) symbol: {4<sup>2</sup>;8<sup>4</sup>}  
Extended point symbol: [4.4.8(7).8(7).8(7).8(7)]

-----  
Point (Schlafli) symbol for net: {4<sup>2</sup>;8<sup>4</sup>}  
4-c net; 2-nodal net

-----  
Topological type: pts PtS, Cooperite; sqc183 (topos&RCSR.ttd) {4<sup>2</sup>;8<sup>4</sup>} - VS [4.4.8(7).8(7).8(7).8(7)] [4.4.8(

-----  
Non-equivalent circuits  
-----

Circuit No 1; Type=4; Centroid: (0.000,0.500,0.500)

-----  
Atom x y z  
-----  
ZD1 -0.2500 0.7500 0.0000  
ZE1 0.0000 0.6002 0.7500  
ZD1 0.2500 0.2500 1.0000  
ZE1 0.0000 0.3998 0.2500

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

-----  
Atom x y z  
-----  
ZD1 -0.2500 -0.2500 -0.0000  
ZE1 -0.5000 0.1002 -0.2500  
ZD1 -0.2500 0.2500 0.5000  
ZE1 0.0000 0.6002 0.7500  
ZD1 0.2500 0.2500 1.0000  
ZE1 0.5000 -0.1002 1.2500  
ZD1 0.2500 -0.2500 0.5000  
ZE1 0.0000 -0.6002 0.2500

Circuit No 3; Type=8b; Centroid: (0.000,0.950,0.250)

-----  
Atom x y z  
-----

ZD1	-0.2500	0.7500	0.0000
ZE1	-0.5000	0.8998	-0.7500
ZD1	-0.2500	1.2500	-0.5000
ZE1	0.0000	1.3998	0.2500
ZD1	0.2500	1.2500	1.0000
ZE1	0.5000	0.8998	1.2500
ZD1	0.2500	0.7500	0.5000
ZE1	0.0000	0.3998	0.2500

Circuit No 4; Type=8c; Centroid: (0.500,0.500,0.000)

Atom	x	y	z
ZD1	0.7500	0.7500	1.0000
ZE1	0.5000	0.8998	0.2500
ZD1	0.2500	0.7500	-0.5000
ZE1	0.0000	0.6002	-1.2500
ZD1	0.2500	0.2500	-1.0000
ZE1	0.5000	0.1002	-0.2500
ZD1	0.7500	0.2500	0.5000
ZE1	1.0000	0.3998	1.2500

Circuit No 5; Type=8d; Centroid: (0.688,0.688,0.375)

Atom	x	y	z
ZD1	0.7500	0.7500	1.0000
ZE1	0.5000	0.8998	0.2500
ZD1	0.2500	0.7500	-0.5000
ZE1	0.5000	1.1002	-0.2500
ZD1	0.7500	0.7500	-0.0000
ZE1	1.0000	0.6002	0.7500
ZD1	0.7500	0.2500	0.5000
ZE1	1.0000	0.3998	1.2500

Circuit No 6; Type=8e; Centroid: (0.750,0.750,0.500)

Atom	x	y	z
ZD1	0.7500	0.7500	1.0000
ZE1	0.5000	0.8998	0.2500
ZD1	0.7500	1.2500	0.5000
ZE1	0.5000	1.1002	-0.2500
ZD1	0.7500	0.7500	-0.0000
ZE1	1.0000	0.6002	0.7500
ZD1	0.7500	0.2500	0.5000
ZE1	1.0000	0.3998	1.2500

Circuit No 7; Type=8f; Centroid: (0.750,0.750,0.500)

Atom	x	y	z
ZD1	0.7500	0.7500	1.0000
ZE1	0.5000	0.8998	0.2500
ZD1	0.2500	0.7500	-0.5000
ZE1	0.5000	1.1002	-0.2500
ZD1	0.7500	0.7500	-0.0000
ZE1	1.0000	0.6002	0.7500
ZD1	1.2500	0.7500	1.5000
ZE1	1.0000	0.3998	1.2500

Elapsed time: 13.44 sec.