

A fragment of the TOPOS output for the FORXAM crystal structure showing the table of symmetry independent bonds with the size (N) of the minimum (shortest) circuits to which each of them belong shown in the last column. The bonds of groups (i)-(iv) are selected by green, yellow, cyan, and grey, respectively.

(i) grey N=0 are dangling bonds: typically C-H, and here also Zn-O(water).

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1;RefCode:FORXAM:C38 H32 N2 O18 Zn4

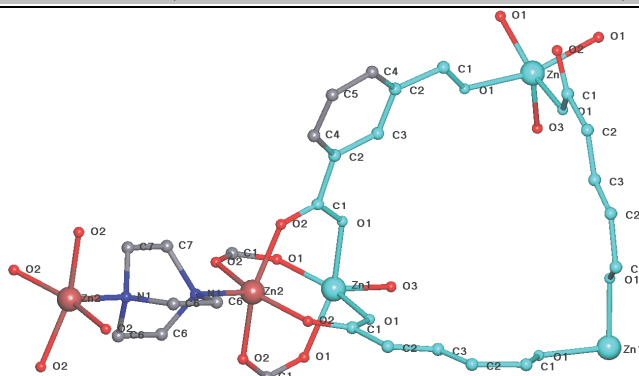
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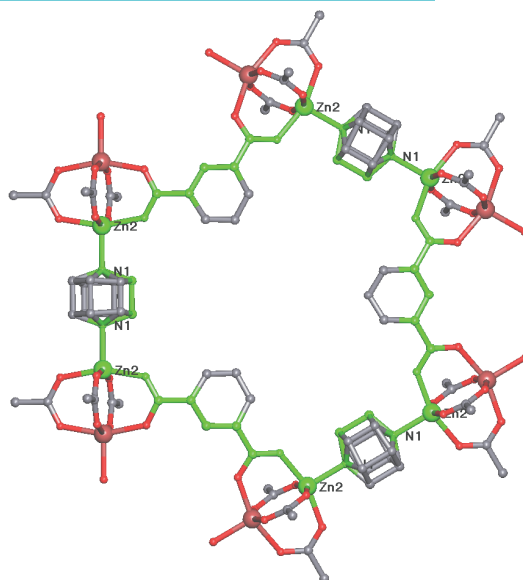
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Minimum circuits for independent edges (bonds)

No	Atom	x	y	z	Atom	x	y	z	Dist.	N
1	H1	0.9182	0.1791	0.4182	C3	0.9100	0.1998	0.4099	0.948	0
2	H2	0.8478	0.2507	0.4176	C4	0.8677	0.2414	0.4084	0.951	0
3	H3	0.8689	0.2728	0.3689	C5	0.8799	0.2548	0.3799	0.950	0
4	H4	0.7734	0.2337	0.4499	C6	0.7758	0.2480	0.4701	0.992	0
5	H5	0.7982	0.2585	0.4696	C6	0.7758	0.2480	0.4701	0.988	0
6	H6	0.8014	0.2650	0.4800	C7	0.7871	0.2622	0.5000	0.988	0
7	C1	0.8656	0.1972	0.4536	O2	0.8393	0.2097	0.4648	1.245	8
8	C1	0.8656	0.1972	0.4536	O1	0.8789	0.1708	0.4645	1.260	8
9	C1	0.8656	0.1972	0.4536	C2	0.8828	0.2143	0.4254	1.485	24
10	C2	0.8828	0.2143	0.4254	C3	0.9100	0.1998	0.4099	1.375	6
11	C2	0.8828	0.2143	0.4254	C4	0.8677	0.2414	0.4084	1.414	6
12	C4	0.8677	0.2414	0.4084	C5	0.8799	0.2548	0.3799	1.349	6
13	C6	0.7758	0.2480	0.4701	C6	0.7520	0.2242	0.4701	1.344	3
14	C6	0.7758	0.2480	0.4701	C7	0.7871	0.2622	0.5000	1.397	3
15	C6	0.7758	0.2480	0.4701	N1	0.7724	0.2276	0.5000	1.452	3
16	C6	0.7758	0.2480	0.4701	C6	0.7480	0.2758	0.4701	1.570	4
17	C7	0.7871	0.2622	0.5000	C7	0.7622	0.2871	0.5000	1.406	4
18	C7	0.7871	0.2622	0.5000	N1	0.7724	0.2276	0.5000	1.501	3
19	N1	0.7724	0.2276	0.5000	Zn2	0.8087	0.1913	0.5000	2.051	39
20	O1	0.8789	0.1708	0.4645	Zn1	0.8608	0.1392	0.5000	2.028	8
21	O2	0.8393	0.2097	0.4648	Zn2	0.8087	0.1913	0.5000	2.004	8
22	O3	0.8976	0.1024	0.5000	Zn1	0.8608	0.1392	0.5000	2.079	0



24-circuit for C1-C2 (C-H removed)



39-circuit for Zn2-N1 (C-H removed and disordered ligand)