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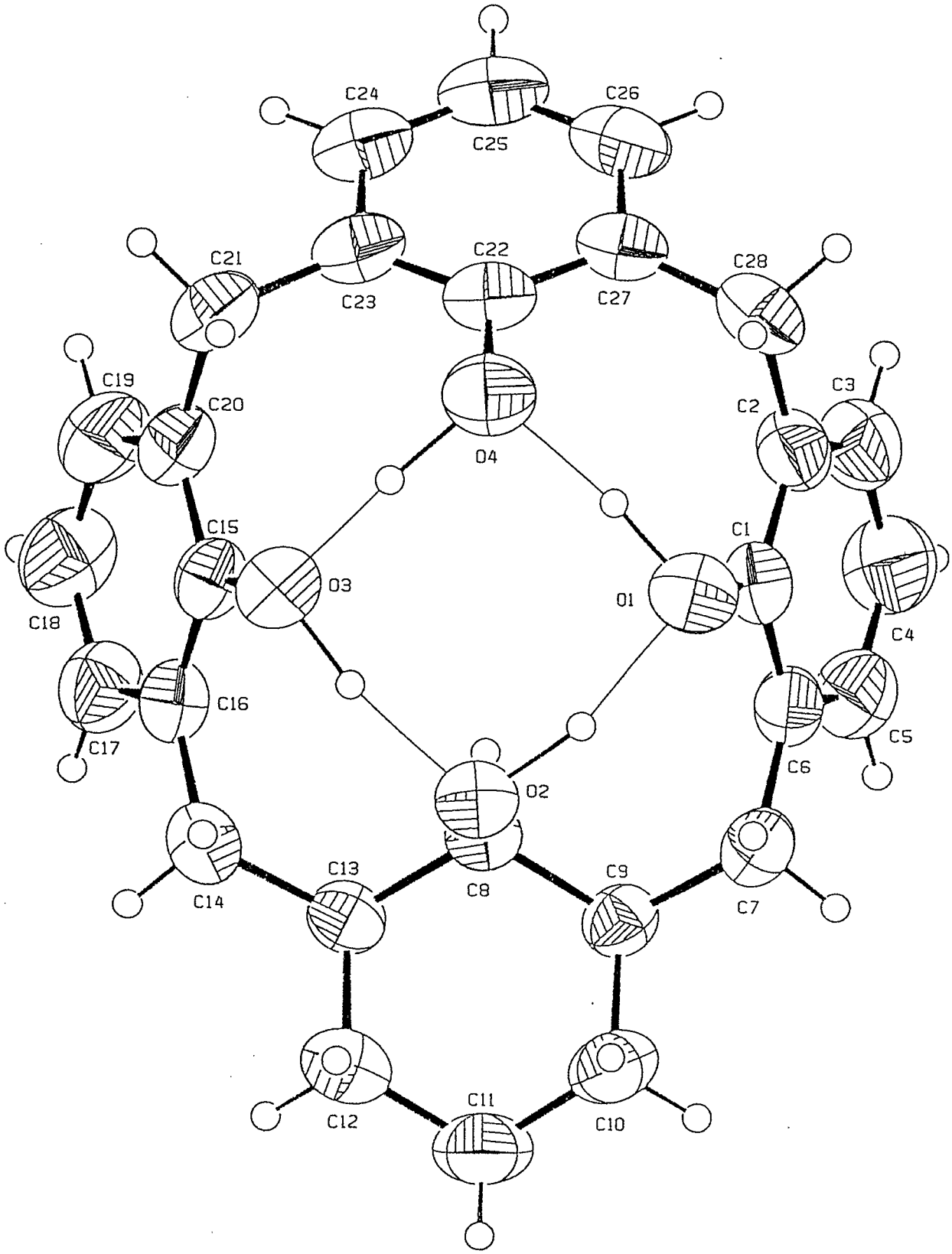


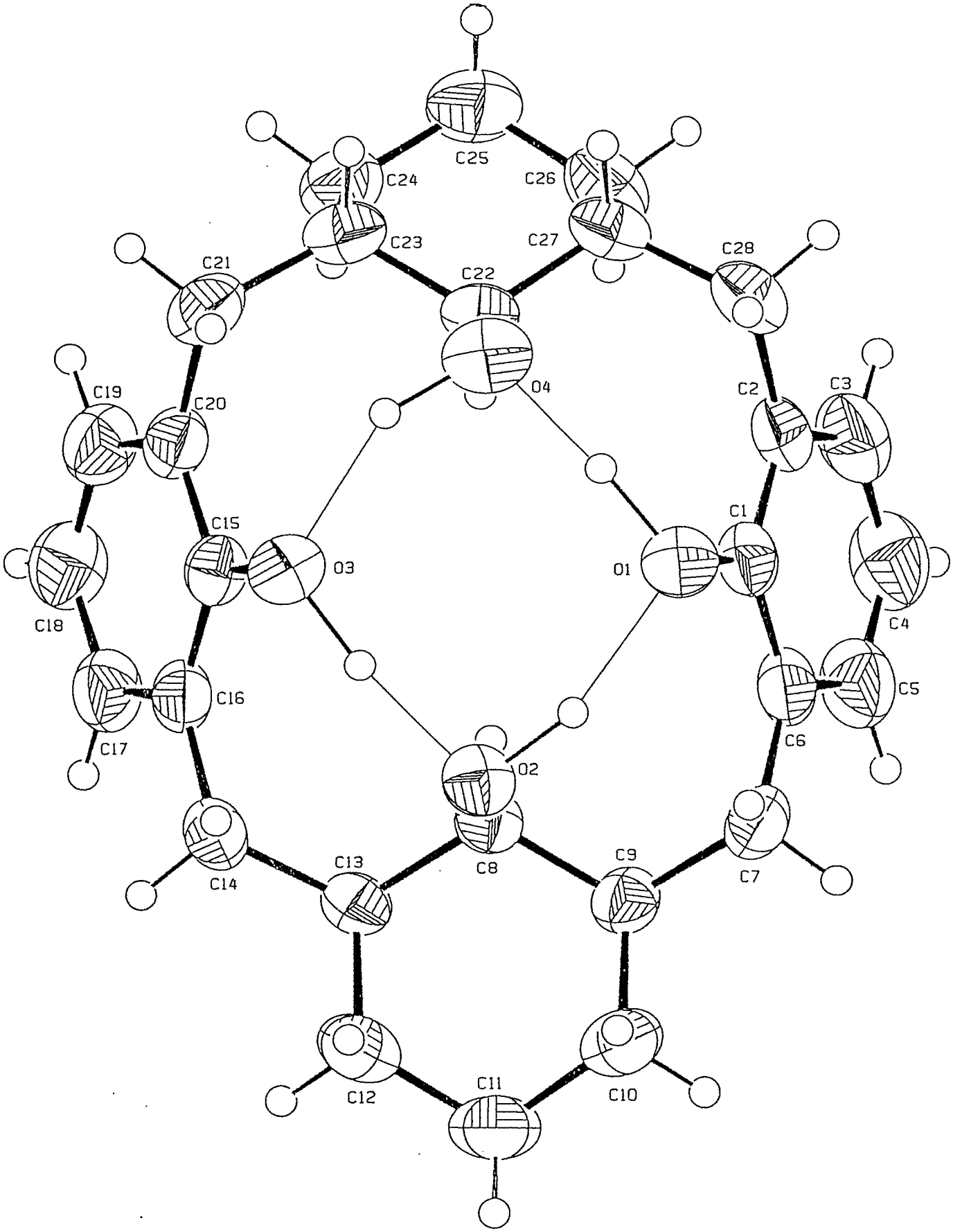
Crystal structure and numbering scheme of **6a**.

Positional parameters and B(eq) for **6a**

atom	x	y	z	B(eq)
O(1)	0.31626(7)	0.4432(1)	0.55878(7)	4.67(6)
O(2)	0.32358(6)	0.2208(1)	0.51827(7)	4.10(5)
O(3)	0.26631(6)	0.2821(1)	0.37621(7)	4.42(6)
O(4)	0.25824(7)	0.4899(1)	0.41800(8)	5.18(6)
C(1)	0.3809(1)	0.4900(2)	0.5710(1)	4.10(8)
C(2)	0.3884(1)	0.5961(2)	0.5467(1)	4.54(9)
C(3)	0.4536(1)	0.6395(2)	0.5611(1)	5.6(1)
C(4)	0.5087(1)	0.5805(2)	0.5979(1)	6.2(1)
C(5)	0.5000(1)	0.4766(2)	0.6224(1)	5.5(1)
C(6)	0.4355(1)	0.4284(2)	0.6100(1)	4.24(8)
C(7)	0.4262(1)	0.3165(2)	0.6395(1)	4.64(8)
C(8)	0.39437(8)	0.2146(1)	0.5161(1)	3.48(7)
C(9)	0.4390(1)	0.2175(2)	0.5945(1)	4.04(8)
C(10)	0.4321(1)	0.1121(2)	0.6363(1)	5.3(1)
C(11)	0.4472(1)	0.0109(2)	0.5964(1)	5.8(1)
C(12)	0.4020(1)	0.0070(2)	0.5192(1)	5.1(1)
C(13)	0.4056(1)	0.1107(2)	0.4745(1)	3.87(7)
C(14)	0.3574(1)	0.0978(2)	0.3980(1)	4.35(8)
C(15)	0.3124(1)	0.2739(2)	0.3319(1)	3.95(7)
C(16)	0.3576(1)	0.1862(2)	0.3414(1)	4.13(8)
C(17)	0.4011(1)	0.1791(2)	0.2938(1)	5.3(1)
C(18)	0.3999(1)	0.2573(2)	0.2402(1)	6.4(1)
C(19)	0.3543(1)	0.3414(2)	0.2314(1)	5.8(1)
C(20)	0.3093(1)	0.3527(2)	0.2776(1)	4.48(8)
C(21)	0.2593(1)	0.4472(2)	0.2670(1)	5.0(1)
C(22)	0.2897(1)	0.5656(2)	0.3823(1)	4.41(8)
C(23)	0.2888(1)	0.5496(2)	0.3076(1)	4.69(9)
C(24)	0.3182(1)	0.6292(2)	0.2726(1)	5.5(1)
C(25)	0.3481(1)	0.7210(2)	0.3097(1)	6.1(1)
C(26)	0.3496(1)	0.7336(2)	0.3833(2)	5.8(1)
C(27)	0.3212(1)	0.6559(2)	0.4217(1)	4.74(9)
C(28)	0.3288(1)	0.6635(2)	0.5041(1)	5.3(1)

Positional parameters and B(eq) for 6a

atom	x	y	z	B(eq)
H(1O1)	0.2884	0.4692	0.5008	5.9
H(1O2)	0.3184	0.3094	0.5450	5.3
H(1O3)	0.2888	0.2463	0.4330	5.7
H(1O4)	0.2612	0.3961	0.3970	6.6
H(3)	0.4602	0.7119	0.5450	6.7
H(4)	0.5529	0.6116	0.6064	7.4
H(5)	0.5384	0.4365	0.6483	6.6
H(71)	0.4562	0.3108	0.6869	5.6
H(72)	0.3805	0.3118	0.6444	5.6
H(8)	0.4050	0.2766	0.4900	4.2
H(9)	0.4849	0.2218	0.5905	4.8
H(101)	0.4629	0.1151	0.6833	6.3
H(102)	0.3869	0.1072	0.6424	6.3
H(111)	0.4935	0.0124	0.5935	6.9
H(112)	0.4393	-0.0525	0.6229	6.9
H(121)	0.4155	-0.0537	0.4939	6.2
H(122)	0.3564	-0.0029	0.5228	6.2
H(13)	0.4505	0.1148	0.4672	4.6
H(141)	0.3687	0.0306	0.3779	5.2
H(142)	0.3125	0.0934	0.4051	5.2
H(17)	0.4322	0.1196	0.2985	6.4
H(18)	0.4309	0.2526	0.2092	7.6
H(19)	0.3531	0.3935	0.1932	7.0
H(211)	0.2456	0.4636	0.2158	6.1
H(212)	0.2208	0.4253	0.2845	6.1
H(24)	0.3179	0.6206	0.2219	6.6
H(25)	0.3676	0.7754	0.2845	7.3
H(26)	0.3705	0.7970	0.4085	6.9
H(281)	0.2883	0.6373	0.5156	6.4
H(282)	0.3356	0.7383	0.5186	6.4



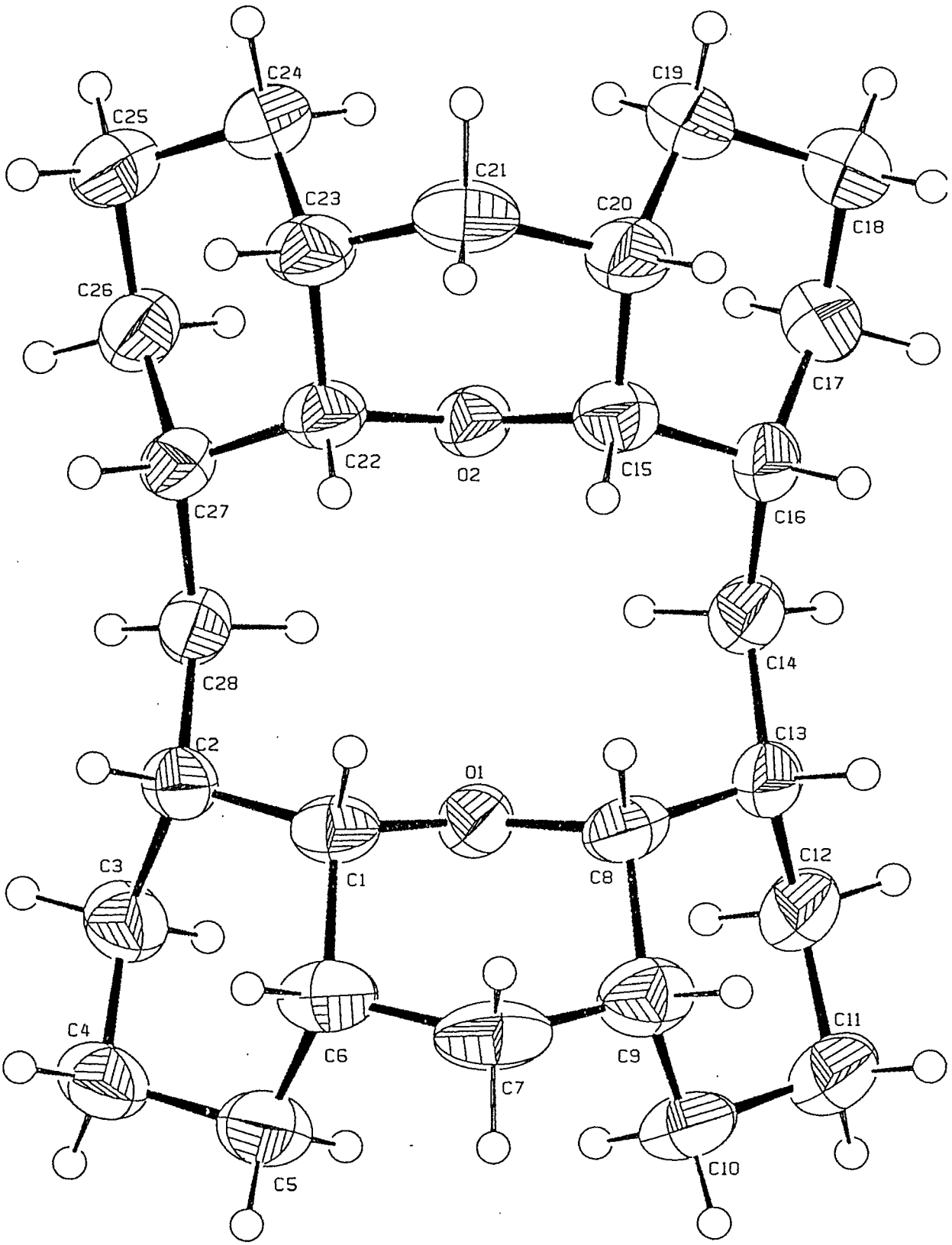
Crystal structure and numbering scheme of **7f**.

Positional parameters and B(eq) for 7f

atom	x	y	z	B(eq)
H(101)	0.2815	0.4654	0.5009	5.0
H(102)	0.3152	0.2885	0.5487	4.4
H(103)	0.2956	0.2448	0.4375	4.7
H(104)	0.2365	0.4171	0.3923	5.6
H(3)	0.4518	0.7100	0.5566	6.3
H(4)	0.5396	0.6085	0.6211	7.1
H(5)	0.5232	0.4328	0.6609	6.4
H(71)	0.4453	0.3025	0.6905	5.0
H(72)	0.3739	0.3016	0.6450	5.0
H(8)	0.4000	0.2739	0.4937	3.8
H(9)	0.4778	0.2214	0.5931	4.4
H(101)	0.4595	0.1071	0.6838	5.8
H(102)	0.3872	0.0944	0.6427	5.8
H(111)	0.4921	0.0139	0.5913	6.4
H(112)	0.4432	-0.0593	0.6200	6.4
H(121)	0.4187	-0.0554	0.4922	5.5
H(122)	0.3613	-0.0114	0.5226	5.5
H(13)	0.4471	0.1179	0.4675	4.1
H(141)	0.3698	0.0313	0.3786	4.6
H(142)	0.3155	0.0904	0.4073	4.6
H(17)	0.4282	0.1257	0.3000	5.4
H(18)	0.4224	0.2581	0.2095	6.2
H(19)	0.3457	0.3967	0.1957	5.9
H(211)	0.2425	0.4581	0.2199	5.4
H(212)	0.2202	0.4160	0.2883	5.4
H(22)	0.3346	0.5016	0.4065	4.2
H(23)	0.2397	0.6011	0.2987	5.0
H(241)	0.3666	0.5622	0.2893	5.8
H(242)	0.3142	0.6202	0.2294	5.8
H(251)	0.3872	0.7454	0.3007	6.6
H(252)	0.3154	0.7705	0.3017	6.6
H(261)	0.4048	0.6657	0.4142	6.0
H(262)	0.3757	0.7817	0.4199	6.0
H(27)	0.2748	0.7036	0.4104	5.1
H(281)	0.2878	0.6328	0.5256	5.5
H(282)	0.3332	0.7338	0.5281	5.5

Positional parameters and B(eq) for 7f

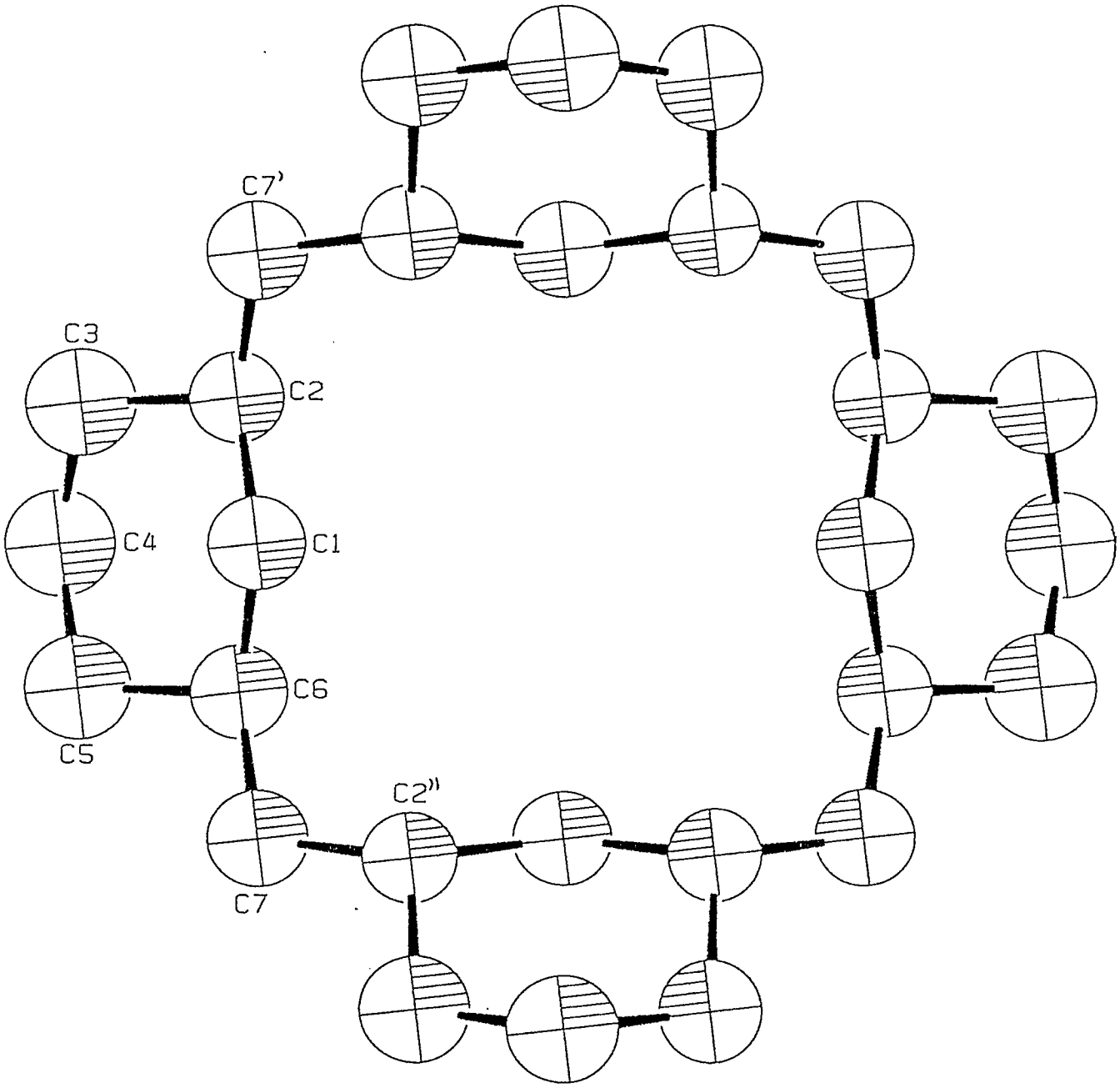
atom	x	y	z	B(eq)
O(1)	0.31383(9)	0.4344(2)	0.5577(1)	4.1(1)
O(2)	0.32311(8)	0.2097(2)	0.5201(1)	3.61(8)
O(3)	0.26887(9)	0.2812(2)	0.3815(1)	3.88(9)
O(4)	0.24597(9)	0.4971(2)	0.4226(1)	4.6(1)
C(1)	0.3752(1)	0.4837(3)	0.5739(2)	3.6(1)
C(2)	0.3828(1)	0.5916(3)	0.5520(2)	3.9(1)
C(3)	0.4452(2)	0.6367(3)	0.5710(2)	5.3(2)
C(4)	0.4973(2)	0.5773(4)	0.6100(2)	5.9(2)
C(5)	0.4873(2)	0.4724(3)	0.6326(2)	5.3(2)
C(6)	0.4267(1)	0.4227(3)	0.6156(2)	3.9(1)
C(7)	0.4181(1)	0.3090(3)	0.6426(2)	4.2(1)
C(8)	0.3913(1)	0.2096(2)	0.5187(1)	3.2(1)
C(9)	0.4340(1)	0.2124(3)	0.5969(2)	3.7(1)
C(10)	0.4303(2)	0.1041(3)	0.6369(2)	4.8(2)
C(11)	0.4481(2)	0.0068(3)	0.5948(2)	5.3(2)
C(12)	0.4045(2)	0.0028(3)	0.5185(2)	4.6(2)
C(13)	0.4046(1)	0.1094(2)	0.4754(2)	3.4(1)
C(14)	0.3583(1)	0.0972(2)	0.3997(2)	3.9(1)
C(15)	0.3120(1)	0.2745(3)	0.3362(1)	3.4(1)
C(16)	0.3565(1)	0.1876(2)	0.3442(2)	3.5(1)
C(17)	0.3972(2)	0.1835(3)	0.2957(2)	4.5(1)
C(18)	0.3937(2)	0.2617(3)	0.2416(2)	5.2(2)
C(19)	0.3485(2)	0.3445(3)	0.2340(2)	4.9(2)
C(20)	0.3066(1)	0.3539(3)	0.2812(2)	3.7(1)
C(21)	0.2560(1)	0.4434(3)	0.2710(2)	4.5(1)
C(22)	0.2967(1)	0.5462(2)	0.3934(2)	3.5(1)
C(23)	0.2766(1)	0.5541(3)	0.3102(2)	4.2(1)
C(24)	0.3297(2)	0.6093(3)	0.2807(2)	4.8(2)
C(25)	0.3502(2)	0.7196(3)	0.3163(2)	5.5(2)
C(26)	0.3670(2)	0.7102(3)	0.3994(2)	5.0(2)
C(27)	0.3122(1)	0.6591(3)	0.4277(2)	4.2(1)
C(28)	0.3256(2)	0.6597(3)	0.5121(2)	4.6(2)



Crystal structure and numbering scheme of **11**.

Positional parameters and B(eq) for 11

atom	x	y	z	B(eq)
H(1)	0.5313	0.3451	0.4918	3.9
H(2)	0.5115	0.2424	0.4442	3.8
H(31)	0.3524	0.1788	0.4562	4.7
H(32)	0.2939	0.2345	0.5070	4.7
H(41)	0.2963	0.2271	0.2467	5.3
H(42)	0.1741	0.2176	0.2786	5.3
H(51)	0.1786	0.3191	0.1993	5.5
H(52)	0.1828	0.3208	0.3465	5.5
H(6)	0.3939	0.3370	0.2758	4.8
H(71)	0.4104	0.4372	0.3254	5.9
H(72)	0.2626	0.4283	0.2524	5.9
H(8)	0.5008	0.4318	0.5868	4.4
H(9)	0.3351	0.4911	0.4547	5.3
H(101)	0.1235	0.4653	0.3763	6.4
H(102)	0.1558	0.3993	0.4423	6.4
H(111)	0.1905	0.5116	0.5874	6.7
H(112)	0.0881	0.4612	0.5788	6.7
H(121)	0.2634	0.4522	0.7857	5.5
H(122)	0.2505	0.3915	0.7009	5.5
H(13)	0.4235	0.4878	0.7187	4.3
H(142)	0.4766	0.4245	0.9162	4.4
H(141)	0.5036	0.3709	0.8322	4.4
H(15)	0.6932	0.4181	0.7319	4.3
H(16)	0.6474	0.4794	0.8768	4.1
H(171)	0.6661	0.4516	1.0908	5.2
H(172)	0.7084	0.3844	1.0705	5.2
H(181)	0.8558	0.4918	1.0864	6.0
H(182)	0.8881	0.4419	1.2008	6.0
H(191)	1.0133	0.4261	1.0740	5.9
H(192)	0.9259	0.3683	1.0628	5.9
H(20)	0.8794	0.4608	0.8668	5.0
H(211)	0.9251	0.3984	0.7285	5.6
H(212)	1.0299	0.3802	0.8684	5.6
H(22)	0.7217	0.3295	0.6446	3.9
H(23)	0.9274	0.2956	0.7198	4.7
H(241)	1.0477	0.2664	0.9388	5.6
H(242)	0.9343	0.2819	0.9822	5.6
H(251)	0.9331	0.1839	0.8079	5.9
H(252)	0.9419	0.1749	0.9557	5.9
H(261)	0.7319	0.1568	0.8015	4.9
H(262)	0.7350	0.2131	0.8950	4.9
H(27)	0.7220	0.2240	0.6293	3.9
H(281)	0.5249	0.2612	0.7056	3.9
H(282)	0.5307	0.1934	0.6553	3.9



Crystal structure of the saturated metacyclophane **13d**.

Positional parameters and B(eq) for 11

atom	x	y	z	B(eq)
O(1)	0.4102(2)	0.3530(1)	0.5811(2)	3.2(1)
O(2)	0.7037(2)	0.3371(1)	0.8194(2)	3.1(1)
C(1)	0.4499(3)	0.3274(2)	0.4790(4)	3.3(2)
C(2)	0.4680(3)	0.2564(2)	0.4998(3)	3.2(2)
C(3)	0.3378(4)	0.2228(2)	0.4502(4)	4.0(2)
C(4)	0.2538(3)	0.2393(2)	0.3046(4)	4.5(2)
C(5)	0.2289(4)	0.3094(2)	0.2918(4)	4.6(2)
C(6)	0.3544(3)	0.3469(2)	0.3376(4)	4.1(2)
C(7)	0.3362(4)	0.4186(2)	0.3317(4)	4.9(2)
C(8)	0.4183(3)	0.4204(2)	0.5843(4)	3.7(2)
C(9)	0.3170(4)	0.4476(2)	0.4550(4)	4.4(2)
C(10)	0.1806(4)	0.4422(2)	0.4518(5)	5.4(2)
C(11)	0.1725(4)	0.4679(2)	0.5814(5)	5.6(2)
C(12)	0.2698(4)	0.4351(2)	0.7061(4)	4.7(2)
C(13)	0.4075(3)	0.4439(2)	0.7140(4)	3.6(2)
C(14)	0.5054(3)	0.4151(2)	0.8454(4)	3.7(2)
C(15)	0.7253(3)	0.4035(2)	0.8232(4)	3.6(2)
C(16)	0.6473(3)	0.4357(2)	0.8949(4)	3.4(2)
C(17)	0.7118(4)	0.4274(2)	1.0491(4)	4.4(2)
C(18)	0.8517(4)	0.4484(2)	1.1051(4)	5.0(2)
C(19)	0.9268(4)	0.4114(2)	1.0399(4)	4.9(2)
C(20)	0.8700(3)	0.4179(2)	0.8860(4)	4.2(2)
C(21)	0.9403(3)	0.3792(2)	0.8137(4)	4.7(2)
C(22)	0.7523(3)	0.3068(2)	0.7279(4)	3.3(2)
C(23)	0.8991(3)	0.3105(2)	0.7877(4)	3.9(2)
C(24)	0.9566(4)	0.2667(2)	0.9104(4)	4.7(2)
C(25)	0.9069(4)	0.2001(2)	0.8763(4)	5.0(2)
C(26)	0.7606(4)	0.1987(2)	0.8247(4)	4.1(2)
C(27)	0.6978(3)	0.2406(2)	0.6988(4)	3.3(2)
C(28)	0.5509(3)	0.2361(2)	0.6470(4)	3.3(2)

Positional parameters and B(eq) for 13d

atom	x	y	z	B(eq)
C(1)	0.5244(5)	0.2906(5)	0.0031(6)	5.5(3)
C(2)	0.6305(5)	0.2888(5)	0.0789(6)	5.2(3)
C(3)	0.6397(6)	0.1806(5)	0.155(1)	7.1(4)
C(4)	0.5402(7)	0.1549(5)	0.2398(8)	7.1(4)
C(5)	0.4363(7)	0.1555(5)	0.1548(7)	6.6(4)
C(6)	0.4202(5)	0.2665(5)	0.0813(7)	5.4(3)
C(7)	0.3146(5)	0.2672(5)	0.0015(9)	5.8(3)
H(2)	0.6248	0.3456	0.1438	6.2
H(6)	0.4136	0.3226	0.1470	6.5
H(11)	0.5167	0.3623	-0.0350	6.6
H(12)	0.5298	0.2369	-0.0656	6.6
H(31)	0.6490	0.1221	0.0928	8.5
H(32)	0.7030	0.1846	0.2109	8.5
H(41)	0.5491	0.0838	0.2791	8.5
H(42)	0.5336	0.2092	0.3076	8.5
H(51)	0.4416	0.0977	0.0910	7.9
H(52)	0.3739	0.1428	0.2103	7.9
H(71)	0.3180	0.2065	-0.0585	7.0
H(72)	0.2550	0.2564	0.0618	7.0
Cl(1)	0.1105(5)	-0.0003(6)	0.0982(7)	18.6(4)
C(8)	0	0	0	10.7(6)