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Crystal Structure of Cyclopentasarcosyl Dihydrate

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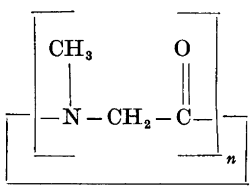
The crystals belong to the monoclinic system with space group $P2_1/c$ and cell dimensions $a=9.31_6$ Å, $b=30.15_4$ Å, $c=7.81_8$ Å, $\beta=113.7_1°$. There are four molecules in the unit cell. The phase problem was solved by direct methods, and the R-value arrived at for 2298 observed reflections was 7.6 %. The conformation is *cis*, *cis*, *cis*, *trans*, *trans*. The water molecules participate in a network of intermolecular hydrogen-bond bridges. Bond distances and angles are compared with those of cyclotetrasarcosyl and cyclooctasarcosyl.

Cyclic oligopeptides of sarcosine of the general formula are studied by Dale and Titlestad, mainly by spectroscopic methods.[1,2] For the pentameric



$n = 2, \cdots, 12$

compound there is strong NMR-evidence for one preferred conformation in solution.[1] From symmetry arguments it could be concluded that the conformation is a mixture of *cis* and *trans* amino acid residues. Whether or not this conformation persists in the solid could not be decided by IR-spectroscopy. However, by dissolving the crystals in chloroform at low temperature ($-50°$C), and slowly heating the solution, no essential changes in the NMR-spectra recorded at different temperatures were observed.[2] In order to obtain detailed information of the molecular geometry, an X-ray crystallographic investigation of cyclopentasarcosyl has been carried out.

The crystals belong to the monoclinic system and the systematic absences lead to the space group $P2_1/c$. The cell parameters measured by means of a four circle diffractometer, and their estimated standard deviations are:

$$a=9.316(2)\text{ Å},\quad b=30.154(8)\text{ Å},\quad c=7.818(1)\text{ Å},\quad \beta=113.71(1)°$$

With four molecules per unit cell the calculated density is $\varrho_c=1.17$ g cm^{-3}.

The observed density, $\varrho_o = 1.28$ g cm^{-3}, corresponds to a difference in molecular weight of 36, which is accounted for by assuming the presence of two water molecules per asymmetric unit.

Whith $2\theta(\max) = 50°$ and Mo$K\alpha$-radiation, about 3800 independent reflections were measured on an automatic four-circle diffractometer. Using an observed-unobserved cutoff at $2.5\sigma(I)$, 2298 were recorded as observed. No corrections have been made for absorption or secondary extinction effects.

The structure was solved by direct methods and refined by full-matrix least squares technique. Methylene hydrogen atom position were calculated. Neither the methyl nor the water hydrogens could be localized in the difference Fourier map, and are not included in the calculations. Anisotropic temperature factors were introduced for O, N, and C-atoms, and weights in least squares were calculated from the standard deviations in intensities, $\sigma(I)$, taken as

$$\sigma(I) = [C_T + (0.02\ C_N)^2]^{\frac{1}{2}}$$

where C_T is the total number of counts and C_N the net count (peak minus background). The conventional R-value arrived at was 7.6 % (weighted value $R_W = 7.9$ %) for 2298 observed reflections. The form factors used were those of Hanson *et al.*[3] except for hydrogen.[4] The final fractional coordinates and thermal vibration parameters are given in Table 1. The expression for anisotropic vibration is:

$$\exp\left[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl)\right]$$

Table 1. Final fractional coordinates and anisotropic thermal vibration parameters with estimated standard deviations (multiplied by 10^5 for non-hydrogens and 10^4 for hydrogens). The symbols CC, CM, and OV are used for carbonyl carbons, methyl carbons, and water oxygens, respectively. Hn1 and Hn2 are bonded to Cn.

ATOM	x	y	z	B	B11	B22	B33	B12	B13	B23
O1	58668(43)	21235(12)	38273(53)		1798(69)	182(6)	2328(97)	-93(32)	1361(139)	-419(38)
O2	134438(41)	19168(12)	54728(49)		1132(57)	169(6)	2629(92)	-86(30)	-327(127)	26(37)
O3	109393(46)	5169(13)	51848(53)		1986(72)	176(6)	3841(122)	676(36)	1344(148)	398(42)
O4	73795(42)	13112(12)	-6463(46)		1965(69)	117(5)	2306(98)	1(32)	1182(127)	155(34)
O5	45592(43)	11314(11)	8956(49)		1963(78)	122(5)	2858(85)	25(38)	716(126)	286(34)
N1	77829(45)	21664(13)	32392(54)		1137(65)	104(5)	2184(102)	-64(32)	128(136)	13(37)
N2	92879(48)	18394(14)	49215(56)		1389(72)	111(6)	2158(102)	266(34)	668(147)	38(39)
N3	89357(54)	6512(13)	8449(56)		1848(85)	121(6)	2846(104)	156(37)	1298(161)	88(40)
N4	43894(52)	11318(14)	-21666(59)		1814(83)	124(6)	1696(99)	-4(36)	141(158)	-113(41)
N5	35051(48)	19589(13)	8879(59)		1198(72)	131(6)	2175(118)	102(34)	55(147)	-87(42)
CC1	49181(68)	20529(15)	22189(78)		1288(89)	84(6)	2325(137)	107(38)	536(195)	-8(47)
CC2	87292(56)	18448(16)	42763(67)		978(79)	122(7)	1921(114)	-19(41)	697(167)	-48(47)
CC3	99383(63)	7619(18)	41568(74)		1388(89)	116(7)	2287(137)	122(44)	794(197)	172(52)
CC4	70372(66)	9280(19)	-4598(69)		1944(107)	119(7)	1853(124)	81(50)	1571(196)	-55(51)
CC5	41179(55)	13153(16)	-7323(78)		1118(82)	107(7)	1878(128)	-148(39)	-174(172)	23(52)
C1	63016(58)	20856(18)	16591(71)		1219(86)	95(7)	1706(128)	-36(39)	257(167)	24(49)
C2	88572(67)	13746(17)	39868(91)		1437(96)	97(7)	2145(149)	175(42)	378(213)	-48(49)
C3	95861(71)	8138(22)	28653(81)		1781(112)	152(9)	2833(153)	142(53)	1413(213)	269(61)
C4	53914(78)	7571(28)	-17262(91)		2312(128)	114(8)	2232(158)	-53(54)	663(238)	-176(58)
C5	34229(78)	17843(18)	-9447(74)		1221(93)	129(8)	1778(131)	19(46)	-323(183)	122(53)
CM1	82944(67)	26487(16)	36136(74)		2121(111)	93(7)	2763(143)	-351(45)	767(289)	-119(48)
CM2	95826(69)	9854(18)	69566(68)		2427(124)	158(8)	1661(124)	23(52)	1232(287)	93(52)
CM3	77119(88)	1788(17)	18415(82)		3285(149)	86(7)	3254(169)	116(54)	1929(264)	284(54)
CM4	39888(79)	13655(21)	-39755(78)		2691(138)	222(10)	1435(124)	181(63)	786(214)	144(57)
CM5	21624(68)	18616(26)	13183(93)		1816(92)	346(15)	3061(198)	-48(61)	1779(231)	-326(86)
OV1	26896(48)	-263(13)	38584(59)		2249(88)	194(6)	3907(128)	69(37)	2635(166)	-42(43)
OV2	49568(59)	4879(16)	33197(71)		3854(186)	254(8)	5983(171)	299(49)	3731(229)	1364(61)
H11	6873(58)	2335(17)	492(69)	5,2(1,3)						
H12	6355(43)	1813(13)	922(51)	2,6(,9)						
H21	7641(59)	1358(16)	2688(74)	4,5(1,3)						
H22	7269(67)	1378(18)	4585(73)	6,4(1,6)						
H31	10614(72)	553(18)	1748(77)	8,4(1,6)						
H32	9655(56)	1125(17)	1728(63)	4,8(1,3)						
H41	5819(67)	529(19)	-1867(77)	6,4(1,7)						
H42	5318(51)	648(14)	-3847(67)	4,1(1,1)						
H51	2242(78)	1837(17)	-1784(73)	6,3(1,3)						
H52	4854(49)	1966(13)	-1413(54)	2,9(1,8)						

A comparison between observed and calculated structure factors is presented in Table 2.

Table 2. Observed and calculated structure factors on 10 times absolute scale.

H=	0,L=12	8	293	276	10	129	127	26	58	29	18	84	77	32	55	41	9	243	244	2	46	51
2	57	5	9	168	180	11	69	55	27	90	88	19	65	55	33	81	77	10	175	176	3	108	95
H=	0,L=11	10	108	115	12	82	89	29	69	59	20	69	57	34	43	32	11	58	74	4	82	87
21	53	10	11	269	269	13	73	68	37	80	63	21	42	36	H=	1,L=	1	12	107	104	5	104	92
H=	0,L=10	12	218	213	14	207	205	H=	0,L=	5	26	68	59	1	1072	1163	13	253	241	7	76	70
4	50	34	13	211	206	15	37	16	1	107	111	H=	1,L=	5	3	1048	1206	14	82	71	9	118	121
21	49	32	16	85	84	16	390	352	2	147	137	1	81	84	4	1473	1599	15	36	34	12	42	42
25	51	10	17	110	120	17	130	108	4	131	127	2	46	44	5	342	270	16	100	98	13	88	77
H=	0,L=	9	18	47	30	18	286	292	5	46	38	3	87	82	6	724	728	17	137	141	14	45	42
5	53	43	19	72	79	19	336	336	9	49	48	4	92	85	7	374	416	18	240	252	16	51	31
6	54	56	20	265	281	20	208	203	10	171	173	5	43	40	8	288	239	20	123	123	H=	1,L=	6
11	51	42	21	38	38	21	223	230	12	46	34	7	110	118	10	261	285	22	223	225	1	44	40
H=	0,L=	8	22	107	108	22	148	140	13	206	207	10	50	50	11	220	187	25	77	71	H=	1,L=	9
3	47	42	23	212	217	23	126	134	14	129	126	16	46	37	12	628	649	26	59	30	3	45	6
4	56	64	24	166	160	25	69	67	15	175	175	17	102	107	13	574	571	28	80	71	H=	1,L=	12
7	53	47	25	116	118	27	136	146	16	50	47	19	179	163	14	325	301	32	59	58	3	51	2
10	71	64	26	149	138	30	53	51	17	157	162	20	124	128	15	127	117	H=	1,L=	3	H=	2,L=	8
15	53	44	28	108	110	32	58	67	18	89	85	22	39	60	16	229	216	1	240	234	0	42	32
H=	0,L=	7	30	45	38	37	79	68	22	54	65	23	112	103	17	47	12	2	156	169	2	54	55
1	162	146	31	102	92	H=	0,L=	2	23	62	65	24	103	97	18	447	468	4	143	127	4	45	43
2	84	87	34	52	50	0	654	701	24	149	137	29	54	49	19	60	35	5	67	61	5	54	33
3	53	59	35	48	15	1	332	367	25	88	85	H=	1,L=	4	20	75	59	6	115	132	6	42	27
4	76	76	39	51	52	2	140	134	30	54	43	0	723	670	21	97	102	7	69	87	12	101	95
5	112	104	H=	0,L=	2	3	69	40	31	47	54	1	116	105	22	116	121	8	257	247	14	80	76
9	89	81	1	332	367	4	412	445	H=	0,L=	6	2	67	66	25	161	161	9	243	234	15	61	56
10	55	57	2	112	134	6	342	296	0	206	226	3	558	531	26	43	36	10	114	108	H=	2,L=	7
11	52	54	3	70	40	7	283	283	1	59	61	4	470	453	27	82	82	12	126	125	2	102	107
13	75	71	4	415	445	9	291	291	3	138	130	5	321	315	30	59	54	13	161	163	3	70	60
15	44	40	6	346	296	10	60	58	4	192	194	7	271	273	31	81	85	14	186	198	4	67	71
16	72	62	7	288	284	11	300	303	5	107	108	8	43	32	33	42	48	15	104	106	5	41	28
19	78	56	9	299	291	13	251	247	6	155	162	9	127	143	H=	1,L=	0	16	177	168	8	157	160
22	47	40	10	63	58	14	197	181	7	60	65	10	201	207	0	526	578	17	66	66	13	43	32
H=	0,L=	6	11	293	304	15	72	78	9	123	124	11	38	39	1	592	640	18	93	82	14	53	56
1	51	61	13	256	247	16	403	404	11	45	44	12	277	294	3	305	349	19	98	99	15	87	74
3	134	130	14	194	192	17	110	116	13	56	51	13	114	109	4	58	36	20	151	153	20	114	107
4	193	195	15	71	78	18	84	92	16	210	213	14	91	109	5	660	532	21	221	220	22	45	41
5	109	108	16	401	404	20	85	75	18	109	109	16	50	32	6	401	340	22	49	39	H=	2,L=	6
6	163	163	17	107	117	21	418	426	20	88	78	18	48	55	7	669	614	23	42	44	0	56	54
7	70	65	18	85	92	22	191	182	21	67	46	19	102	119	8	396	413	25	131	138	2	170	180
8	46	58	20	84	75	24	162	163	H=	0,L=	7	20	166	169	9	266	238	28	124	118	3	49	61
9	121	125	21	415	427	25	131	119	1	155	146	22	110	102	10	95	129	29	94	75	4	58	58
11	49	44	22	185	183	26	63	59	2	97	87	23	109	102	11	43	26	30	66	59	5	126	119
13	68	51	24	164	153	27	68	61	3	58	59	26	46	48	12	860	836	31	54	49	6	53	47
15	208	214	25	134	119	28	80	67	4	80	76	27	61	65	13	101	103	H=	1,L=	4	7	94	95
18	106	109	26	50	59	29	73	55	5	112	103	28	41	25	14	245	250	0	190	180	9	137	136
20	96	79	27	67	61	30	53	44	9	95	81	29	102	104	15	624	598	1	47	39	10	108	120
21	59	46	28	78	67	32	40	40	10	61	57	H=	1,L=	3	16	37	14	3	442	440	11	77	68
33	46	22	29	61	55	34	68	65	11	56	54	1	364	367	17	127	102	4	257	254	12	40	31
H=	0,L=	5	34	74	65	37	59	51	13	79	70	2	325	251	18	158	162	5	176	171	13	79	92
1	107	111	37	57	51	39	47	41	15	50	40	3	80	100	19	130	120	6	35	20	15	152	160
2	144	137	39	57	41	H=	0,L=	3	16	64	62	4	56	55	20	49	45	7	260	266	16	79	98
4	127	127	H=	0,L=	1	1	204	195	19	74	56	5	89	96	21	67	52	8	173	172	17	83	103
5	50	38	2	253	295	2	213	194	22	48	40	6	107	72	22	222	214	9	180	188	19	42	47
9	59	48	3	408	407	3	187	172	H=	0,L=	8	7	127	130	23	89	93	10	78	59	21	54	48
10	172	173	4	391	436	4	240	219	0	96	95	8	329	337	24	244	228	13	300	310	24	60	57
12	39	34	5	315	382	6	192	184	3	49	42	9	634	615	25	109	114	14	89	75	25	45	40
13	204	208	6	1386	1310	7	360	367	4	64	64	10	130	133	26	43	36	15	101	107	H=	2,L=	9
14	128	127	7	49	101	8	298	276	5	58	48	11	282	263	27	138	129	17	83	84	1	46	50
15	171	176	8	205	249	9	170	180	10	59	64	12	208	187	28	69	54	18	187	197	2	69	83
16	53	47	9	215	190	10	112	115	H=	0,L=	9	13	58	69	33	64	45	21	93	82	3	41	38
17	156	162	10	129	127	11	266	269	5	57	43	15	60	66	34	73	67	25	116	116	4	108	112
18	61	65	11	68	55	12	217	213	6	61	56	16	162	161	H=	1,L=	1	27	64	56	5	58	56
22	58	65	12	60	89	13	212	205	11	52	41	17	108	122	1	681	710	28	51	43	6	233	232
23	68	65	14	205	206	16	84	84	H=	0,L=	10	19	88	81	3	404	397	29	95	97	7	149	137
24	147	137	16	387	352	17	117	119	15	48	9	20	174	179	5	311	312	30	56	46	8	57	62
25	86	86	17	123	109	18	42	30	H=	0,L=	11	21	99	99	6	712	676	H=	1,L=	5	9	39	39
30	48	43	18	288	293	19	68	79	24	53	3	22	121	112	8	112	106	1	79	79	11	93	85
31	45	55	19	336	336	20	270	280	H=	1,L=	9	24	259	269	9	173	171	3	93	100	12	76	70
H=	0,L=	4	20	204	204	21	39	38	1	58	35	25	189	202	10	610	551	4	187	182	13	157	161
2	222	215	21	216	230	22	106	107	2	52	49	26	41	38	11	694	700	6	106	120	14	39	33
3	130	118	22	140	141	23	213	217	H=	1,L=	8	28	64	71	12	304	286	7	127	119	15	166	165
4	223	220	23	122	134	24	162	159	0	62	46	32	59	54	13	478	471	8	79	87	16	95	107
5	263	270	25	72	67	25	118	117	2	79	73	H=	1,L=	9	15	41	48	9	229	245	17	68	72
6	257	248	27	132	148	26	156	138	6	55	57	0	947	989	16	59	51	10	184	187	19	98	106
7	128	138	30	56	51	28	106	109	8	50	26	1	47	91	17	198	213	11	115	107	20	98	89
9	60	50	32	62	67	30	41	38	H=	1,L=	7	2	950	781	18	287	308	12	107	115	21	220	223
10	49	22	37	79	68	31	105	92	1	134	134	3	759	759	19	82	83	13	51	47	22	82	84
11	58	61	H=	0,L=	0	32	44	27	3	158	164	4	288	309	20	138	132	14	140	135	23	43	30
13	56	58	4	734	862	34	63	50	4	44	60	5	178	143	21	310	306	16	60	54	24	48	45
14	275	294	6	397	461	39	52	52	5	75	89	6	224	225	22	113	114	17	194	200	H=	2,L=	4
15	153	154	10	1230	1152	H=	0,L=	4	6	60	68	7	45	17	23	115	112	19	234	222	0	264	262
16	163	170	12	768	796	0	505	541	7	70	63	8	477	413	25	166	167	20	74	72	1	112	123
17	94	91	14	359	305	2	222	215	8	76	67	9	144	112	26	180	194	24	73	56	2	159	145
18	44	53	16	519	522	3	128	118	9	49	40	10	144	107	27	54	52	27	91	78	3	155	145
19	154	164	18	67	86	4	218	219	12	48	42	11	62	55	28	199	185	H=	1,L=	6	5	316	332
20	142	153	20	33	56	5	262	270	13	55	56	12	661	641	29	48	21	0	87	98	6	308	326
21	170	183	22	92	112	6	261	248	19	96	87	13	107	112	30	47	48	1	42	46	7	233	213
25	203	194	26	94	92	7	132	137	H=	1,L=	6	14	145	131	31	89	54	2	85	81	9	70	46
27	77	89	28	97	79	9	58	50	0	222	224	16	36	46	33	72	61	3	232	251	10	33	57
28	44	34	32	74	100	10	42	22	1	137	148	17	38	24	34	66	56	4	128	148	11	258	252
29	52	59	34	49	42	11	59	61	3	44	69	18	175	162	H=	1,L=	2	7	42	42	12	243	265
35	52	38	38	87	84	13	46	58	4	88	94	20	105	93	0	182	212	8	157	168	13	151	152
37	80	64	H=	0,L=	1	14	270	293	5	65	71	21	54	43	1	126	109	9	94	89	14	144	140
H=	0,L=	3	1	48	9	15	159	153	7	154	155	22	72	77	2	846	771	11	100	109	15	185	202
1	203	196	2	250	295	16	161	170	8	127	131	23	107	101	3	95	69	12	141	147	16	159	157
2	203	194	3	378	407	17	92	81	10	133	148	25	42	57	4	726	635	14	109	98	17	95	102
3	185	172	5	318	380	19	150	163	11	74	75	26	79	75	5	518	494	15	66	60	18	84	81
4	339	220	6	1386	1309	20	153	153	12	82	87	27	42	48	6	217	178	17	118	106	19	41	44
6	196	184	8	207	249	21	169	183	13	69	58	28	41	9	7	421	421	20	64	48	20	46	30
7	358	368	9	217	190	25	207	193	14	91	96	29	63	58	8	917	486	H=	1,L=	7	22	157	157

Table 2. Continued.

24	74	75	21	38	46	23	95	102	H=	3,L=	4	4	378	352	14	79	73	11	81	98	14	305	309
25	45	50	22	245	248	H=	2,L=	5	0	629	615	5	193	190	15	144	159	12	78	82	15	94	98
H=	2,L=	3	23	81	96	1	109	103	1	55	71	6	290	287	17	65	60	13	115	126	16	94	81
1	579	600	24	99	114	2	144	136	2	46	59	7	91	96	18	127	130	14	84	90	17	136	124
2	308	299	25	166	170	3	143	150	3	428	419	8	85	96	19	116	123	16	37	49	19	42	52
3	99	109	26	201	204	5	177	195	4	128	134	9	771	784	20	41	61	17	44	82	20	47	58
4	159	156	27	67	59	6	60	36	5	408	408	10	479	456	21	54	55	18	285	285	21	50	69
5	270	266	28	58	65	7	340	353	6	285	283	11	344	307	22	103	109	19	85	93	23	60	67
6	175	176	30	65	78	8	184	189	7	141	142	12	396	411	27	63	59	22	53	47	24	105	114
7	225	205	31	70	60	11	73	72	8	123	126	13	519	518	H=	3,L=	5	23	45	71	H=	4,L=	1
8	227	225	32	112	110	12	99	103	9	124	112	14	160	156	1	115	109	25	74	73	1	91	86
9	318	294	33	41	9	14	99	88	10	204	206	15	102	105	2	116	112	26	50	47	2	34	21
10	234	228	H=	2,L=	1	15	74	95	11	217	208	17	109	118	3	102	97	27	66	74	3	213	195
11	347	353	1	458	448	16	69	59	12	71	66	18	277	292	4	55	54	28	48	46	4	79	52
12	214	204	3	681	616	17	56	63	14	56	47	19	153	145	5	220	217	29	52	64	5	448	423
13	121	115	4	76	84	18	51	41	16	62	78	20	52	55	6	198	192	30	79	77	6	305	308
14	74	96	5	238	229	21	78	76	17	190	186	22	153	149	9	39	21	H=	4,L=	3	7	87	99
15	266	248	6	167	156	22	68	59	18	188	198	23	63	77	10	56	48	1	464	473	8	111	92
16	66	69	7	479	468	H=	2,L=	6	19	58	70	24	48	49	11	95	99	2	82	61	9	289	285
18	118	128	8	220	215	1	279	281	20	45	51	25	137	128	13	90	98	3	182	188	10	56	44
19	116	120	9	73	65	2	75	85	21	66	64	26	51	55	14	75	73	4	516	515	12	87	100
20	128	126	10	68	81	7	159	137	22	97	88	28	70	58	16	52	51	5	116	126	14	149	169
22	173	174	11	66	39	9	164	157	23	84	96	29	60	59	18	82	91	7	160	155	16	186	184
23	80	93	13	302	303	11	78	95	24	129	131	H=	3,L=	1	19	46	60	8	127	134	17	183	124
24	111	98	14	220	220	12	118	112	28	49	47	1	43	62	H=	3,L=	6	9	70	62	18	59	51
26	40	24	15	98	104	13	111	100	29	81	73	2	106	107	0	71	62	10	58	35	19	117	110
27	103	98	16	71	68	17	110	103	30	100	85	3	439	446	1	118	110	11	271	293	20	87	108
28	55	39	18	262	260	H=	2,L=	7	H=	3,L=	3	4	347	347	2	60	52	12	292	300	24	80	61
30	58	44	19	80	78	2	57	53	1	216	197	5	294	266	3	103	107	13	207	217	26	68	53
32	51	39	20	100	108	6	123	108	2	819	819	6	663	654	4	68	72	14	189	202	28	43	28
H=	2,L=	2	21	114	131	9	86	85	3	348	382	7	176	162	5	61	63	15	213	227	30	45	61
1	423	431	22	132	129	13	67	48	4	311	309	8	291	299	7	160	151	16	62	66	H=	4,L=	2
2	1046	915	24	49	50	H=	3,L=	9	5	470	455	9	46	27	8	142	131	17	138	131	0	61	71
3	279	274	25	66	59	6	68	47	6	175	172	10	72	48	9	69	94	18	67	74	1	102	105
4	566	505	26	56	49	8	68	53	8	215	237	12	232	211	10	80	43	19	96	97	2	153	166
5	1050	1008	27	156	154	H=	3,L=	8	11	223	215	13	166	164	12	78	70	21	64	85	4	50	33
6	495	497	30	77	72	0	102	98	12	86	84	14	173	170	13	97	97	23	167	170	5	76	57
7	576	495	H=	2,L=	2	1	72	54	13	80	77	15	109	108	H=	3,L=	7	24	56	44	6	73	74
8	85	75	0	499	477	2	62	63	15	219	226	17	61	37	2	68	65	25	89	93	7	298	289
9	34	58	2	90	104	3	42	6	16	144	160	18	212	234	5	44	48	27	109	112	8	202	203
11	265	273	4	57	34	4	51	41	17	98	107	21	123	116	H=	4,L=	9	29	56	57	10	93	95
12	115	114	5	230	223	7	46	29	18	112	123	23	230	225	6	46	25	31	62	61	11	68	51
13	43	54	6	71	84	10	42	51	21	85	101	24	147	158	H=	4,L=	8	32	44	25	12	81	76
14	213	204	7	439	464	13	54	45	22	93	77	25	52	80	1	64	53	H=	4,L=	2	13	307	316
15	147	148	8	88	79	14	64	56	23	280	261	27	78	59	3	62	54	0	657	579	15	273	286
16	57	84	9	253	264	18	57	43	24	181	159	33	63	52	6	80	72	1	234	220	17	100	104
17	47	73	10	54	35	H=	3,L=	7	25	80	67	H=	3,L=	2	10	55	51	2	245	232	18	38	17
18	175	178	11	56	46	2	209	209	26	140	140	0	388	369	H=	4,L=	7	3	53	57	20	48	57
19	91	96	12	71	52	4	39	49	31	64	49	1	554	537	1	52	47	4	103	104	21	57	59
21	110	119	13	32	6	7	51	42	H=	3,L=	2	2	536	545	2	210	199	6	347	354	23	92	85
22	124	124	14	37	45	9	66	61	0	420	392	4	131	137	5	62	43	6	34	30	25	91	81
23	77	77	15	104	104	10	56	79	1	391	424	5	162	167	6	127	127	7	180	182	27	60	59
24	48	53	16	37	29	11	53	46	2	299	275	7	175	168	8	123	121	8	101	88	H=	4,L=	3
25	43	44	17	201	210	12	42	39	3	893	904	8	76	84	10	83	89	9	73	59	3	35	31
27	112	111	18	57	39	14	140	141	4	511	487	9	41	41	11	64	88	10	79	67	4	65	74
28	79	85	19	91	95	16	46	43	6	353	340	10	123	116	12	71	61	11	48	53	6	157	159
29	58	49	21	91	105	18	85	72	8	198	220	11	49	47	15	110	109	13	539	518	7	109	117
30	80	58	22	115	119	19	108	90	9	98	116	12	308	314	16	44	40	14	38	22	8	58	59
H=	2,L=	1	23	79	68	20	61	63	10	233	215	13	374	375	H=	4,L=	6	15	120	125	9	173	177
1	778	744	24	83	88	21	66	58	11	409	404	15	48	79	0	93	99	16	106	117	10	95	94
3	35	56	25	77	59	22	43	29	12	192	183	16	118	113	1	92	84	17	74	73	11	49	56
4	343	294	26	118	119	H=	3,L=	6	13	59	79	17	137	136	2	113	116	18	113	101	12	82	84
5	205	177	28	45	99	0	198	212	14	41	24	18	178	187	3	43	55	19	43	70	13	90	101
6	660	607	31	52	40	1	97	114	16	170	170	19	212	215	4	52	63	20	39	33	14	50	47
7	796	824	H=	2,L=	3	2	70	79	17	222	231	21	68	81	6	110	112	21	86	39	15	234	245
8	146	149	1	35	23	3	254	260	18	52	52	22	122	127	7	81	84	22	97	108	17	169	158
9	524	531	2	103	117	4	62	47	19	116	117	23	65	77	9	196	198	23	132	123	19	227	224
10	60	60	3	118	124	5	156	158	20	79	94	24	112	124	14	84	85	25	83	83	20	150	155
11	279	259	4	186	193	7	81	91	21	89	72	25	143	132	16	63	66	28	102	98	21	58	80
12	250	206	5	39	9	8	102	106	22	92	78	29	69	53	19	96	41	32	61	68	22	70	68
13	110	107	6	582	553	11	102	101	25	94	100	30	58	46	21	78	67	H=	4,L=	1	26	75	66
14	236	256	7	71	60	12	76	77	26	152	149	H=	3,L=	3	22	139	122	1	211	214	27	57	50
15	176	176	8	338	343	13	98	96	29	70	67	1	96	97	24	59	52	2	464	441	H=	4,L=	4
16	176	179	9	77	63	14	50	41	32	52	44	2	149	152	27	62	56	4	41	20	0	196	194
17	176	170	10	128	139	15	56	76	H=	3,L=	1	4	66	52	H=	4,L=	5	5	671	638	1	81	58
18	57	55	11	62	64	17	104	119	1	303	283	5	92	78	1	138	128	7	602	604	2	160	152
19	171	189	12	189	172	18	56	53	2	944	914	6	49	41	2	118	122	8	45	16	3	146	158
21	108	105	13	170	170	19	41	44	3	105	118	7	192	171	4	191	193	9	80	82	4	62	59
22	53	41	14	230	252	20	60	51	4	214	215	8	210	222	5	36	9	10	423	440	5	188	190
23	47	49	15	103	108	22	93	99	5	263	308	10	51	44	6	178	168	11	247	245	7	802	208
24	111	123	16	306	306	24	65	40	6	331	355	11	62	59	7	179	203	12	171	158	8	57	63
25	72	85	17	79	95	25	62	47	7	336	320	12	74	75	9	55	37	13	144	132	12	57	35
26	221	224	18	62	72	H=	3,L=	5	8	121	126	13	128	132	10	123	138	14	167	176	13	39	31
27	44	46	19	74	92	1	43	37	9	217	198	14	144	147	11	106	108	17	88	78	14	159	165
29	78	89	20	50	41	2	52	55	10	373	404	15	53	56	12	114	122	18	138	141	16	69	73
31	63	62	23	170	182	3	382	384	11	248	242	16	169	156	13	123	120	19	88	88	18	51	38
32	60	46	24	42	57	4	72	78	12	504	498	17	67	45	14	69	50	22	180	179	H=	4,L=	5
H=	2,L=	0	28	54	52	6	247	244	13	33	44	18	120	123	15	108	104	24	112	116	2	42	38
0	506	571	29	50	43	8	108	117	14	230	228	19	157	163	16	57	70	25	206	216	4	115	120
1	1115	1061	H=	2,L=	4	9	57	54	15	125	122	21	153	156	19	61	82	26	84	88	5	50	57
2	147	149	0	335	336	10	51	27	17	254	257	22	57	67	20	121	120	27	44	68	6	188	190
3	388	366	1	171	173	12	184	185	19	102	115	23	74	73	22	49	47	31	63	51	7	75	67
4	631	523	3	132	125	13	135	137	20	87	89	24	70	68	24	76	65	32	80	61	10	64	63
5	626	649	4	119	105	14	58	61	22	58	59	26	47	40	25	86	78	H=	4,L=	0	11	55	67
6	1061	971	5	209	218	16	41	59	23	134	128	27	83	82	26	44	36	0	727	735	12	44	37
7	486	416	6	43	51	17	55	51	24	112	140	30	56	46	27	62	47	1	84	78	13	83	84
8	737	680	7	114	106	19	66	63	25	182	195	H=	3,L=	4	H=	4,L=	4	2	252	244	19	48	45
10	249	297	8	91	98	20	80	80	26	124	109	0	96	94	0	134	131	3	604	512	H=	4,L=	6
11	321	329	9	230	240	21	84	72	27	68	72	1	73	86	1	256	239	4	121	138	0	96	78
12	354	352	10	182	193	22	132	129	28	126	121	3	334	348	2	243	253	6	419	433	1	60	65
13	184	196	12	135	138	23	88	83	30	44	36	4	55	59	3	70	75	8	107	126	4	48	35
14	372	344	15	264	265	24	70	53	32	42	45	5	77	79	4	128	148	7	627	621	5	43	44
15	252	232	17	130	127	25	97	95	34	51	37	7	310	313	5	88	69	9	61	71	8	77	70
16	165	180	19	46	46	26	48	38	H=	3,L=	0	8	136	139	6	126	147	10	281	303	11	67	62
17	218	212	20	111	113	27	51	46	0	318	292	9	88	73	7	67	63	11	416	409	H=	5,L=	8
19	76	64	21	110	122	28	72	75	1	439	464	10	218	209	8	218	211	12	69	75	8	53	33
20	153	155	22	105	100	30	43	33	3	522	491	13	72	69	9	94	94	13	265	272	11	61	52

Table 2. Continued.

H=	5,L=	7	15	135	134	17	113	103	16	126	129	8	167	176	2	118	123	0	55	49	6	103	90
1	46	47	16	51	52	19	70	63	17	74	67	9	109	107	3	145	130	5	48	38	H=	9,L=	8
7	98	106	17	45	33	24	43	42	18	65	59	10	121	119	4	106	108	H=	8,L=	5	0	66	59
8	83	81	18	84	95	H=	5,L=	4	19	70	74	11	211	210	5	80	83	1	39	58	H=	9,L=	7
9	56	55	20	164	155	0	174	156	20	43	79	12	113	119	7	70	60	2	54	46	8	52	51
10	74	79	21	125	139	1	102	110	22	75	66	13	58	60	9	139	146	3	38	14	H=	9,L=	8
17	70	81	22	123	116	2	95	101	24	52	60	14	62	61	10	99	127	4	60	50	2	45	31
18	83	79	24	76	89	3	73	89	26	64	42	15	56	52	12	40	35	7	72	76	6	73	64
19	58	40	27	55	46	4	185	188	29	54	53	19	100	97	13	170	163	11	54	64	12	58	42
20	85	80	28	58	58	6	112	108	H=	6,L=	2	22	72	76	14	159	158	14	77	79	14	68	54
H=	5,L=	6	29	46	45	7	124	138	0	212	218	H=	6,L=	3	17	155	161	16	52	44	H=	9,L=	5
0	97	102	H=	5,L=	1	8	117	102	1	216	214	1	150	151	18	99	93	H=	8,L=	4	2	52	57
1	41	29	1	319	322	9	99	105	2	224	216	3	62	66	24	61	64	1	71	83	4	53	50
2	164	164	3	145	156	10	48	61	4	155	156	4	99	91	25	47	46	3	38	33	5	88	84
3	159	169	4	42	21	11	79	83	5	118	114	5	259	259	H=	7,L=	1	5	75	82	10	52	46
4	158	167	5	157	165	14	47	50	6	243	238	6	84	77	2	271	274	8	52	55	11	66	58
6	141	151	6	153	130	19	44	25	7	42	42	7	108	114	4	138	151	9	48	67	H=	9,L=	4
7	164	159	8	231	236	H=	5,L=	5	8	50	44	10	78	66	5	257	260	10	51	44	0	99	88
8	92	90	9	98	88	1	56	50	9	67	72	11	75	69	6	113	119	12	52	57	1	71	60
9	56	41	10	319	322	5	123	108	10	69	67	12	125	132	7	42	36	15	77	64	12	49	53
10	78	87	12	63	47	7	50	37	12	77	74	14	58	60	8	79	78	17	41	32	13	75	85
13	151	145	13	79	89	8	41	15	13	137	126	16	112	121	9	231	228	20	44	48	14	51	59
17	52	24	14	44	48	14	52	46	14	69	66	17	47	54	10	223	225	24	42	24	16	56	50
21	43	39	15	67	44	H=	6,L=	8	15	136	142	19	74	70	11	261	274	H=	8,L=	3	H=	9,L=	3
25	82	72	16	195	214	2	56	46	16	57	49	H=	6,L=	4	14	199	203	1	87	84	2	81	66
H=	5,L=	5	17	168	184	H=	6,L=	7	17	48	66	0	66	61	15	163	159	2	59	69	5	67	67
2	101	105	18	120	137	1	98	88	19	72	72	6	74	69	16	79	81	3	130	140	6	69	74
4	370	375	19	183	189	2	102	104	21	69	85	9	87	70	18	81	79	4	57	57	9	69	70
5	269	279	20	162	162	5	126	123	25	86	63	12	45	21	19	108	110	5	86	54	11	117	126
6	47	38	22	60	60	7	157	150	26	100	104	13	53	55	20	98	102	8	61	56	13	63	50
7	185	181	24	111	107	8	74	60	29	89	84	H=	6,L=	5	23	64	48	10	118	98	18	87	49
9	46	44	25	65	67	10	49	36	H=	6,L=	1	1	60	36	26	44	39	12	90	89	19	47	42
10	52	52	29	77	70	11	50	40	1	192	193	4	54	52	27	81	55	13	99	83	H=	9,L=	2
11	136	129	30	47	41	17	79	77	2	161	157	5	98	91	H=	7,L=	0	14	120	121	0	115	102
12	217	235	H=	5,L=	0	19	52	38	3	156	146	H=	7,L=	8	0	177	172	15	63	72	3	83	73
13	75	67	0	124	138	20	53	32	4	42	30	1	53	46	2	137	143	17	57	66	7	89	87
14	122	121	1	74	78	H=	6,L=	6	5	43	39	4	44	37	3	155	155	H=	8,L=	2	8	144	132
15	115	132	2	247	260	0	225	235	8	37	25	13	50	44	4	154	161	0	87	102	9	105	101
17	52	57	3	172	170	1	245	248	9	114	106	H=	7,L=	7	5	108	123	1	44	30	13	72	82
19	65	67	4	152	154	3	138	132	10	120	112	1	85	69	7	80	76	3	92	86	15	84	71
20	44	31	5	47	33	4	55	65	11	165	169	7	141	133	8	182	184	7	43	31	16	110	97
21	50	60	6	62	55	5	67	66	12	53	40	9	50	38	11	186	194	8	43	44	H=	9,L=	1
26	70	67	8	48	55	6	73	69	13	109	110	10	72	63	12	183	183	9	59	43	1	44	34
28	51	32	9	139	136	8	150	158	14	145	143	11	44	45	13	63	80	10	105	104	6	135	124
H=	5,L=	4	11	49	64	9	44	40	15	266	275	H=	7,L=	6	14	73	68	11	74	58	7	100	103
0	149	135	14	160	147	10	112	121	16	45	50	0	197	195	15	69	86	12	104	112	9	48	38
1	204	245	15	212	214	11	153	150	17	161	155	6	70	53	16	122	120	13	53	52	10	98	87
2	102	106	16	115	117	12	92	86	19	135	135	7	66	66	17	43	37	14	51	60	13	55	47
3	98	95	17	100	108	13	70	81	20	108	110	8	76	61	18	62	65	16	73	65	17	45	32
4	179	173	18	198	188	18	46	48	21	147	144	13	96	84	19	51	29	18	55	46	H=	9,L=	0
5	39	42	20	175	181	19	43	34	23	114	101	15	94	91	22	53	42	20	66	59	0	68	78
6	43	73	23	64	55	20	58	53	24	68	63	18	47	33	26	94	84	H=	8,L=	1	2	52	48
7	91	92	24	57	68	22	51	42	H=	6,L=	0	22	48	45	H=	7,L=	1	1	105	111	6	58	42
8	209	214	25	54	50	25	60	49	0	94	96	H=	7,L=	5	2	101	110	2	161	157	8	135	126
9	175	177	27	39	33	H=	6,L=	5	1	42	44	1	142	147	3	96	104	3	56	67	10	52	50
10	56	50	31	41	6	3	54	59	2	298	304	3	45	35	4	117	109	4	200	198	14	76	69
11	59	63	H=	5,L=	1	4	65	61	3	150	152	4	43	59	5	256	265	8	112	105	16	76	69
12	66	62	1	42	47	5	92	81	4	211	214	11	151	154	6	176	166	7	129	134	H=	9,L=	1
14	147	163	3	184	173	6	96	79	5	163	171	13	79	66	7	154	154	8	199	195	1	42	37
15	61	39	4	218	225	7	102	107	7	201	211	15	66	65	8	161	156	9	86	91	5	47	48
18	125	129	5	40	59	9	62	67	8	427	444	17	70	66	9	81	81	11	136	134	6	69	74
21	71	72	6	130	135	11	121	111	9	55	66	21	58	58	10	60	64	12	141	139	10	51	51
26	48	61	7	132	142	12	48	58	10	91	93	22	90	74	11	175	174	15	65	72	11	53	44
29	47	37	8	203	202	15	100	85	11	73	75	H=	7,L=	4	13	57	50	18	63	59	H=	10,L=	6
H=	5,L=	3	10	48	42	16	84	92	12	74	65	0	120	124	15	72	74	19	91	92	0	44	31
1	193	201	11	188	188	17	87	90	13	124	139	1	71	63	16	84	77	H=	8,L=	0	9	48	49
2	188	185	12	112	116	19	71	54	14	37	41	2	94	88	19	51	63	0	121	117	H=	10,L=	5
3	110	122	14	145	143	20	79	80	15	87	89	3	61	49	23	98	85	1	68	58	1	42	27
4	87	88	15	76	71	21	64	64	17	149	143	4	38	32	H=	7,L=	2	2	148	145	6	43	24
5	352	334	17	130	134	22	44	53	18	156	152	7	42	30	2	82	78	4	140	140	H=	10,L=	4
6	130	138	19	111	111	26	48	64	19	114	125	9	58	56	3	41	40	6	128	121	7	72	74
7	235	247	20	158	164	H=	6,L=	4	21	106	108	10	96	92	5	40	43	7	72	77	8	84	47
8	51	76	23	75	68	0	313	307	22	50	48	11	79	79	6	47	35	8	173	157	12	63	64
9	51	31	H=	5,L=	2	1	74	80	23	68	67	12	45	50	8	124	121	9	90	82	14	73	64
10	56	69	0	98	102	4	114	117	H=	6,L=	1	13	75	74	10	46	28	10	105	94	H=	10,L=	3
11	46	53	1	74	74	5	102	89	1	149	154	15	51	62	13	83	82	12	85	62	2	49	41
17	157	160	4	146	157	6	155	161	2	187	177	16	57	53	17	68	75	13	95	89	5	45	33
19	37	24	5	128	127	7	92	91	3	107	106	17	68	59	H=	7,L=	3	14	78	80	6	42	28
20	52	49	6	138	154	10	106	99	5	40	10	21	88	85	2	45	47	15	94	96	8	46	43
21	44	47	7	175	182	12	80	99	6	41	42	23	44	39	4	81	86	18	76	63	11	42	37
23	85	86	9	197	200	14	129	143	7	129	125	26	47	20	6	48	40	H=	8,L=	2	12	57	39
25	85	81	12	62	76	15	139	154	8	62	54	H=	7,L=	3	10	63	52	1	48	47	H=	10,L=	2
27	80	74	13	71	73	17	114	100	9	45	31	1	62	48	11	44	32	2	44	35	0	60	77
28	68	68	14	71	68	18	145	156	10	69	81	2	56	74	12	52	42	4	70	65	1	57	43
30	42	23	16	108	117	19	69	66	11	43	7	5	103	88	14	62	65	5	76	80	3	44	44
31	48	33	18	211	200	24	92	95	12	67	63	6	113	107	16	71	75	6	94	73	7	77	76
H=	5,L=	2	20	45	37	25	41	26	13	117	114	9	52	35	H=	7,L=	4	7	93	93	8	95	87
0	103	102	28	65	69	27	43	37	14	100	112	10	43	37	0	45	45	10	51	42	12	51	40
1	313	294	28	79	72	29	58	47	15	44	34	11	112	112	2	89	81	12	68	69	H=	10,L=	1
2	247	258	H=	5,L=	3	H=	6,L=	3	16	148	142	12	96	99	5	43	31	13	43	46	1	88	84
3	64	68	1	88	96	1	93	94	18	106	94	13	84	79	6	75	63	17	72	65	3	77	64
4	65	69	3	129	119	2	123	123	19	103	107	14	55	68	H=	8,L=	8	H=	8,L=	2	5	47	25
6	56	58	4	283	300	5	105	106	26	48	47	15	86	79	5	50	40	0	112	110	7	57	44
7	280	289	6	72	86	6	52	44	H=	6,L=	2	16	63	59	6	44	38	4	45	34	H=	10,L=	0
8	217	227	7	75	68	7	240	243	0	73	64	18	71	64	H=	8,L=	7	5	66	60	0	64	61
9	155	144	9	52	45	9	189	197	1	131	148	21	48	43	1	62	51	9	49	37	5	44	38
10	99	110	10	158	166	11	43	24	3	47	50	22	47	51	3	43	50	10	68	74	H=	11,L=	3
11	201	195	11	110	100	12	171	171	4	47	41	26	48	42	5	69	61	11	50	43	2	48	41
12	191	190	13	64	51	13	129	145	5	125	126	H=	7,L=	2	7	54	44	H=	8,L=	3	H=	10,L=	3
13	48	38	14	82	84	14	64	62	6	62	56	0	205	197	11	44	37	5	49	51	12	57	39
14	188	170	16	49	46	15	103	103	7	38	19	1	125	126	H=	8,L=	6						

The principal axes of the thermal vibration ellipsoids for oxygen, nitrogen, and carbon atoms were calculated from the temperature parameters of Table 1. Maximum root mean squares amplitudes range from about 0.28 Å for carbonyl carbons to about 0.40 Å for methyl carbon atoms and water oxygens. Due to the size of the molecule, no rigid-body analysis of translational, librational, and screw motion has been carried out.

Interatomic distances, bond angles and dihedral angles are given in Table 3. The standard deviations, given in parantheses, are estimated from the correlation matrix of the last least squares refinement cycle. Fig. 1 shows the molecule viewed along [0 0 1].

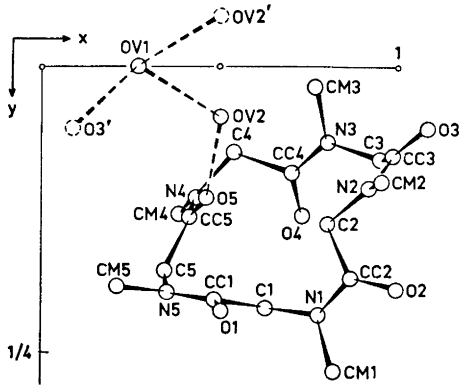


Fig. 1. The molecule viewed along [001].

By averaging bond distances of Table 3, and comparing with the results of the corresponding tetrameric [5] and octameric [6] compounds, no significant differences are observed:

Distance	cycotetrasarcosyl	cyclooctasarcosyl	cyclopentasarcosyl
CC–C	1.531 Å	1.527 Å	1.530 Å
CC–N	1.358	1.344	1.345
CC–O	1.225	1.228	1.232
C–N	1.458	1.456	1.453
CM–N	1.467	1.483	1.487

The somewhat longer CM–N distances of cycloocta- and cyclopentasarcosyl are possibly connected with the fact that methyl hydrogens were localized for the tetrameric compound, but not for the other two.

The geometry of the *cis* and *trans* amide groups, respectively, is also roughly the same:

Angle	cyclotetrasarcosyl	cyclooctasarcosyl	cyclopentasarcosyl
(CM–N–CC)*cis*	119.8°	118.7°	118.6°
(CM–N–CC)*trans*	124.3	123.9	123.5
(C–N–CC)*cis*	123.9	123.8	122.8
(C-N-CC)*trans*	120.1	117.2	117.5

Table 3. Interatomic distances, bond angles and dihedral angles with estimated standard deviations.

DISTANCE	(Å)	DISTANCE	(Å)	DISTANCE	(Å)
O1 - CC1	1,236(6)	O2 - CC2	1,227(5)	O3 - CC3	1,236(6)
O4 - CC4	1,223(6)	O5 - CC5	1,236(6)	N1 - CM1	1,499(6)
N2 - CM2	1,495(6)	N3 - CM3	1,479(6)	N4 - CM4	1,487(6)
N5 - CM5	1,473(7)	CC1 - N5	1,367(6)	CC2 - N1	1,352(6)
CC3 - N2	1,325(6)	CC4 - N3	1,357(6)	CC5 - N4	1,326(6)
CC1 - C1	1,518(7)	CC2 - C2	1,517(7)	CC3 - C3	1,537(7)
CC4 - C4	1,541(8)	CC5 - C5	1,537(7)	N1 - C1	1,456(5)
N2 - C2	1,455(6)	N3 - C3	1,459(7)	N4 - C4	1,468(7)
N5 - C5	1,433(6)	O3 - OV1	2,749(6)	O5 - OV2	2,747(5)
OV1 - OV2	2,735(6)	OV1 - OV2	2,736(6)		

ANGLE	(°)	ANGLE	(°)
N5 - CC1 - O1	122,2(5)	O1 - CC1 - C1	121,7(5)
N1 - CC2 - O2	122,8(4)	O2 - CC2 - C2	121,9(4)
N2 - CC3 - O3	121,1(5)	O3 - CC3 - C3	117,9(5)
N3 - CC4 - O4	122,6(5)	O4 - CC4 - C4	118,6(5)
N4 - CC5 - O5	122,1(5)	O5 - CC5 - C5	118,6(5)
C1 - N1 - CM1	116,4(4)	CM1 - N1 - CC2	119,9(4)
C2 - N2 - CM2	117,5(5)	CM2 - N2 - CC3	118,4(4)
C3 - N3 - CM3	116,5(5)	CM3 - N3 - CC4	124,4(5)
C4 - N4 - CM4	118,7(5)	CM4 - N4 - CC5	122,5(5)
C5 - N5 - CM5	119,8(5)	CM5 - N5 - CC1	117,5(5)
N5 - CC1 - C1	116,1(5)	N1 - CC2 - C2	116,1(4)
N2 - CC3 - C3	121,8(5)	N3 - CC4 - C4	118,8(5)
N4 - CC5 - C5	119,1(5)	CC1 - C1 - N1	113,1(4)
CC2 - C2 - N2	112,5(4)	CC3 - C3 - N3	114,8(5)
CC4 - C4 - N4	107,9(4)	CC5 - C5 - N5	111,2(4)
C1 - N1 - CC2	123,6(4)	C2 - N2 - CC3	124,1(5)
C3 - N3 - CC4	119,8(5)	C4 - N4 - CC5	116,8(5)
C5 - N5 - CC1	120,8(5)	OV1 - OV2 - O5	128,8(2)
OV2 - O5 - CC5	157,7(3)	O3 - OV1 - OV2	118,2(2)
CC3 - O3 - OV1	126,1(4)	O3 - OV1 - OV2	113,1(2)
OV2 - OV1 - OV2	87,7(2)	OV1 - OV2 - O5	139,7(2)

DIHEDRAL ANGLE	(°)	DIHEDRAL ANGLE	(°)
N5 - CC1 - C1 - N1	-176,2(6)	CC1 - C1 - N1 - CC2	89,1(6)
C1 - N1 - CC2 - C2	-9,1(7)	N1 - CC2 - C2 - N2	173,4(5)
CC2 - C2 - N2 - CC3	-102,8(6)	C2 - N2 - CC3 - C3	-1,1(8)
N2 - CC3 - C3 - N3	-78,8(7)	CC3 - C3 - N3 - CC4	122,7(6)
C3 - N3 - CC4 - C4	-179,1(5)	N3 - CC4 - C4 - N4	147,7(5)
CC4 - C4 - N4 - CC5	-83,6(7)	C4 - N4 - CC5 - C5	161,7(5)
N4 - CC5 - C5 - N5	-171,9(5)	CC5 - C5 - N5 - CC1	88,6(6)
C5 - N5 - CC1 - C1	14,1(7)		

Fig. 1 shows that the ring conformation is *cis, cis, cis, trans, trans*. The two water molecules participate in a network of *inter*-molecular hydrogen-bond bridges only. The four OV–O– and OV–OV distances are all about 2.74 Å. The angle OV2–OV1–OV2′ is 87.7°, while other angles of the hydrogen-bond bridges range from 110° to 158°.

Since the shortest CC···N distance across the ring is longer than 3.5 Å, no direct transannular contact can be held responsible for the rigidity of this 15-membered ring. As in the case of cyclooctasarcosyl, the explanation must be sought in the intrinsic conformation of the peptide chain itself.[2]

Apart from the hydrogen bonds, there are no short inter-molecular contacts.

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