ACTA CHEMICA SCANDINAVICA 27 (1973) 3217–3226

Crystal Structure of Cyclooctasarcosyl

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The crystals belong to the orthorhombic system with space group *Pbca* and cell dimensions $a = 18.34_0$ Å, $b = 18.27_9$ Å, $c = 18.87_5$ Å. There are eight molecules in the unit cell. The phase problem was solved by direct methods. The R-value arrived at for 3471 observed reflections was 7.2 %. The ring conformation is surprisingly open with the inner volume filled by a cluster of four water molecules, which participate in a network of inter- and intra-molecular hydrogen bond bridges. Each of the four pairs of diametrically placed amino-acid residues is related by an approximate two-fold axis of symmetry. The conformation is *cis, cis, trans, trans, cis, cis, trans, trans.*

Cyclic oligopeptides of sarcosine of the general formula (I) have been studied by Dale and Titlestad.[1] To account for the relatively high observed

$$\left[CH_3-\underset{|}{N}-CH_2-\overset{\overset{O}{\|}}{C}- \right]_n \qquad n = 2, 3, \cdots, 8 \qquad \text{(I)}$$

resistance to ring inversion, transannular interactions between N and C (carbonyl) were suggested. Such interactions have been reported to exist in certain cyclic aminoketones.[2] In the 10-ring lactone of 6-keto-9-hydroxy-nonanoic acid[3] there is strong evidence for transannular donor-acceptor attraction between the "ether" oxygen of the ester group and the carbonyl carbon atom.

In order to establish whether transannular N···C (carbonyl) attractions actually are stabilising the oligomers (I), and to obtain detailed information of the ring conformations and the geometries of the amino-acid residues, single crystals of some of these compounds are being examined by X-ray methods. Results for the cases $n = 2$ and $n = 4$ have been reported earlier.[4,5] In cyclotetrasarcosyl ($n = 4$) the transannular N···C (carbonyl) distance was 3.08_3 Å, and no conclusion concerning stabilising transannular donor-acceptor attraction could be drawn. In the present paper the results of the crystal structure determination of cyclooctasarcosyl ($n = 8$) are presented.

The crystals belong to the orthorhombic system and the systematic absences lead to the space group *Pbca*. The cell parameters, measured by means of a four circle diffractometer, and their estimated standard deviations are:

$$a = 18.340(3)\text{Å}, \; b = 18.279(3)\text{Å}, \; c = 18.875(2)\text{Å}$$

With eight molecules per unit cell the calculated density is $\varrho_c = 1.20$ g cm^{-3}. The observed density, $\varrho_o = 1.34$ g cm^{-3}, corresponds to a difference in molecular weight of 72 which is accounted for by assuming the presence of four water molecules per asymmetric unit.

With $2\theta(\max) = 50°$ and Mo$K\alpha$-radiation, about 5000 independent reflections were measured on an automatic four-circle diffractometer. Using an observed-unobserved cutoff at $2.5\sigma(I)$, 3471 were recorded as observed. No corrections have been made for absorption or secondary extinction effects.

Table 1. Final fractional coordinates and anisotropic thermal vibration parameters with estimated standard deviations (multiplied by 10^5 for nonhydrogens 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	76027(19)	18723(20)	35265(20)		220(12)	353(15)	383(15)	-152(22)	138(24)	-91(20)
O2	55212(18)	20366(17)	29976(19)		256(13)	217(11)	311(14)	-19(19)	-12(22)	173(21)
O3	43418(20)	26792(18)	41380(19)		415(15)	242(13)	263(13)	141(83)	-213(23)	-126(21)
O4	25152(19)	34098(18)	39854(20)		333(15)	177(11)	396(15)	-141(20)	62(24)	4(24)
O5	24755(17)	57014(19)	35979(19)		280(12)	301(13)	333(14)	-83(20)	-78(22)	140(24)
O6	44802(17)	55267(18)	31185(19)		196(12)	289(13)	307(13)	21(20)	-108(21)	-179(22)
O7	56589(20)	46143(18)	41377(19)		365(15)	278(13)	232(13)	48(23)	110(23)	72(21)
O8	74555(20)	40383(19)	40803(21)		295(14)	170(11)	360(14)	-69(19)	-140(23)	48(23)
OV1	47653(24)	44883(22)	20700(22)		471(18)	412(16)	373(17)	81(29)	-131(29)	-189(27)
OV2	52356(29)	30892(25)	19460(26)		669(23)	479(19)	527(22)	490(36)	114(37)	302(34)
OV3	39965(22)	42211(23)	8128(22)		392(16)	442(17)	372(16)	8(27)	-93(27)	-8(28)
OV4	49236(23)	30748(23)	3794(24)		475(18)	455(17)	388(17)	1(30)	-87(29)	-35(29)
N1	65806(20)	12147(20)	36315(21)		168(13)	168(13)	265(15)	28(21)	7(24)	35(23)
N2	45848(20)	14147(20)	34810(23)		163(13)	178(13)	309(17)	44(21)	-16(24)	-40(24)
N3	37232(23)	31473(21)	31886(22)		264(15)	228(14)	250(15)	158(25)	-78(26)	-144(26)
N4	28332(23)	45016(20)	43437(22)		293(16)	160(13)	266(16)	-43(24)	167(27)	-21(24)
N5	34992(21)	63000(19)	38955(22)		191(14)	147(12)	317(16)	30(20)	64(25)	29(24)
N6	54677(20)	59628(21)	36929(22)		193(13)	185(13)	288(15)	27(22)	-25(25)	-32(24)
N7	62824(22)	42561(21)	31460(22)		244(15)	193(13)	259(15)	114(23)	-12(26)	29(25)
N8	71269(21)	29554(20)	43841(21)		237(15)	171(13)	270(15)	7(23)	-82(25)	35(24)
C1	58284(26)	11303(24)	38679(22)		193(16)	127(14)	282(19)	-38(25)	-7(29)	54(28)
C2	40744(27)	19053(27)	31333(28)		181(17)	235(17)	301(20)	68(29)	-71(31)	-124(33)
C3	36743(27)	38345(27)	35561(28)		250(18)	188(17)	292(19)	59(29)	-48(33)	10(31)
C4	33296(27)	50978(24)	43687(27)		268(18)	139(14)	241(18)	23(28)	-42(31)	-25(27)
C5	42516(27)	62845(24)	41399(29)		208(17)	166(15)	301(20)	-10(27)	-8(31)	-97(29)
C6	59282(25)	65054(26)	32387(27)		155(16)	201(16)	283(19)	22(27)	39(30)	-10(30)
C7	63620(28)	35600(26)	34749(29)		273(19)	163(16)	314(21)	59(28)	-77(34)	17(31)
C8	66769(30)	23279(28)	43298(33)		200(19)	191(18)	271(21)	3(30)	9(34)	80(34)
CM1	68728(30)	6696(29)	31219(31)		263(20)	246(20)	305(22)	86(33)	-11(35)	-222(35)
CM2	42970(31)	8600(30)	39737(32)		257(20)	272(20)	367(23)	-150(34)	155(36)	58(37)
CM3	33320(35)	30825(32)	24836(32)		303(25)	369(23)	252(21)	202(40)	-254(38)	-70(41)
CM4	21360(34)	45811(32)	47466(35)		364(26)	296(23)	459(27)	-18(38)	505(44)	13(42)
CM5	32819(31)	69201(29)	34494(34)		283(20)	186(17)	413(25)	58(32)	108(38)	225(36)
CM6	58018(32)	62977(32)	43483(34)		315(23)	320(23)	391(26)	-58(38)	-234(40)	-279(40)
CM7	66739(32)	43997(30)	24489(30)		320(23)	326(22)	224(20)	114(37)	163(35)	-5(37)
CM8	77972(32)	29054(30)	48336(31)		281(21)	270(21)	344(23)	-40(34)	-292(37)	120(37)
CC1	69905(27)	17906(26)	37865(27)		189(17)	181(16)	218(19)	55(28)	-16(30)	66(29)
CC2	53026(27)	15588(26)	34030(29)		180(17)	148(15)	257(19)	25(27)	19(30)	-60(29)
CC3	40602(26)	26125(29)	35309(28)		198(17)	218(19)	237(19)	59(30)	9(32)	-86(32)
CC4	29560(29)	38951(26)	39039(28)		253(19)	151(16)	216(18)	67(29)	-25(32)	57(30)
CC5	30654(28)	57222(26)	39044(27)		281(18)	186(16)	284(18)	16(29)	56(30)	-13(29)
CC6	47464(26)	58952(26)	36073(28)		168(16)	167(15)	232(18)	8(28)	-31(30)	1(29)
CC7	59450(26)	47547(27)	35485(28)		185(17)	185(17)	284(18)	13(28)	-69(31)	-6(29)
CC8	70287(29)	35365(26)	39767(28)		231(18)	156(16)	223(19)	56(29)	-14(31)	-74(30)
H11	5748(24)	1266(23)	4381(27)	1,82(1,13)						
H12	5712(25)	663(25)	3848(24)	1,04(1,10)						
H21	3562(26)	1703(25)	3170(25)	1,08(1,10)						
H22	4270(25)	1981(23)	2645(27)	2,93(1,08)						
H31	3686(25)	4244(25)	3154(25)	2,77(1,10)						
H32	4105(27)	3914(24)	3877(25)	4,00(1,11)						
H41	3803(26)	4946(24)	4171(24)	4,08(1,13)						
H42	3354(25)	5208(24)	4906(26)	3,42(1,11)						
H51	4362(25)	6065(24)	4595(26)	1,62(1,10)						
H52	4448(24)	6725(26)	4222(24)	2,30(1,11)						
H61	6429(26)	5675(24)	3229(25)	3,18(1,11)						
H62	5714(25)	5469(23)	2653(25)	4,44(1,12)						
H71	6393(25)	3196(25)	3085(25)	3,35(1,11)						
H72	5874(27)	3450(25)	3773(25)	2,39(1,10)						
H81	6227(27)	2468(26)	4244(25)	3,81(1,15)						
H82	6609(25)	2119(25)	4825(27)	2,79(1,19)						

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

H=	0,K=	0
2	766	690
4	5919	6922
6	356	297
8	774	795
10	438	470
12	441	459
16	214	221
18	580	568
20	358	387
H=	0,K=	2
1	1070	1211
2	198	126
3	848	672
4	458	451
5	3419	3302
6	658	621
7	266	194
8	107	98
9	1168	1154
10	364	392
13	855	903
15	108	125
16	162	145
17	183	182
19	214	212
H=	0,K=	4
0	2650	2767
2	334	393
3	240	234
4	3715	3748
5	389	413
6	258	207
7	290	269
8	1739	1844
9	536	509
10	395	375
11	599	584
12	338	344
13	223	220
14	413	432
15	634	661
16	272	251
18	227	191
20	197	188
23	220	187
H=	0,K=	6
0	1138	995
1	849	833
2	245	256
3	1598	1623
4	840	866
5	2164	1990
6	1000	957
7	229	242
8	279	245
9	361	351
10	566	556
11	418	401
12	116	87
13	104	94
15	240	262
16	191	166
17	312	273
18	256	258
22	175	144
H=	0,K=	8
0	2908	2717
1	456	465
2	2132	2061
3	262	281
4	1409	1413
5	319	326
6	1243	1221
7	644	639
8	1165	1145
9	320	317
10	439	456
11	547	556
12	161	84
13	468	504
14	600	607
16	478	492
17	128	122
18	233	225
19	171	167
H=	0,K=	10
0	196	170
1	229	210
2	192	220
3	340	362
4	150	128
5	1151	1254
7	134	118
8	337	382
9	699	686
12	580	591
15	373	381
16	272	264
17	111	116
19	153	159
H=	0,K=	12
0	821	877
2	135	106
3	194	184
4	503	562
6	120	148
7	417	466
8	368	381
9	202	187
13	242	230
H=	0,K=	14
1	508	509
3	278	339
4	171	154
5	739	759
7	291	275
8	237	238
9	490	460
11	245	276
12	144	122
13	286	297
15	173	131
18	123	65
19	200	200
H=	0,K=	16
0	621	655
1	297	299
2	534	499
3	284	286
6	220	232
7	288	324
8	269	291
9	166	153
10	158	170
11	158	99
15	295	292
16	364	349
H=	0,K=	18
0	283	297
1	188	187
2	123	119
3	960	922
4	163	183
5	364	377
6	250	237
7	357	413
9	123	157
10	128	148
11	123	141
H=	0,K=	20
0	227	251
4	178	147
7	213	203
8	176	177
9	181	167
H=	0,K=	22
0	111	65
3	204	209
7	448	388
H=	0,K=	24
1	158	130
2	260	186
3	175	177
H=	1,K=	0
2	234	237
4	255	271
6	411	350
8	138	168
10	140	107
12	202	171
14	136	163
16	220	227
18	129	125
H=	1,K=	1
1	1147	1452
2	1509	1867
3	826	1010
4	1087	1141
5	935	898
6	999	839
7	405	337
9	605	572
10	576	545
11	328	304
13	187	167
14	189	180
15	126	138
16	103	96
19	239	209
21	156	154
22	133	123
H=	1,K=	2
1	348	320
2	434	559
3	146	177
4	2051	1967
5	562	500
6	528	492
7	259	287
8	447	465
9	199	209
10	555	655
11	432	422
12	572	593
14	284	273
15	218	235
16	126	78
18	185	202
19	172	147
20	325	307
H=	1,K=	3
1	934	964
2	1109	1182
3	868	937
4	106	110
5	1321	1268
6	843	803
8	709	678
9	456	452
10	319	319
12	132	143
13	210	202
14	155	173
16	346	297
18	182	174
H=	1,K=	4
1	516	638
2	247	201
3	1777	1773
5	1662	1370
6	94	55
7	292	289
8	224	233
9	618	636
11	219	195
12	213	222
13	122	128
17	197	218
H=	1,K=	5
1	532	526
2	380	440
3	555	615
4	2373	2276
5	1504	1407
6	83	71
8	828	817
10	303	313
11	244	264
13	611	640
14	164	150
15	230	231
16	183	178
19	138	87
20	139	125
H=	1,K=	6
1	154	126
4	95	169
5	148	133
6	1219	1160
7	339	335
8	593	550
10	806	816
11	299	310
12	521	551
15	236	240
16	134	113
18	233	190
21	120	87
H=	1,K=	7
1	635	534
2	236	214
3	797	798
4	237	241
5	81	53
6	579	536
7	1184	1157
9	436	438
10	141	161
12	206	169
13	151	154
14	121	19
15	131	95
18	106	93
H=	1,K=	8
1	652	613
2	129	141
3	498	517
4	199	154
5	260	171
6	120	117
7	189	158
8	234	252
9	138	205
11	114	123
12	117	133
13	204	190
15	116	69
17	136	156
H=	1,K=	9
1	395	405
2	1110	1060
4	370	370
5	473	441
6	925	913
7	122	105
8	759	774
9	108	89
10	305	300
11	423	452
12	779	784
13	352	377
14	368	376
16	349	331
17	248	208
18	244	250
H=	1,K=	10
1	281	281
2	465	475
3	205	167
4	744	694
5	217	230
10	357	381
13	102	96
16	137	127
H=	1,K=	11
1	570	610
3	121	98
4	203	216
5	432	432
7	702	709
8	465	491
9	153	118
10	196	180
11	589	608
14	177	123
15	233	241
H=	1,K=	12
1	93	21
2	147	151
3	683	659
4	114	88
5	101	103
7	668	687
8	123	97
9	423	403
11	160	149
12	136	149
13	271	269
H=	1,K=	13
2	173	148
5	308	334
6	165	181
8	278	297
9	325	330
10	229	195
11	154	135
12	288	273
13	399	373
15	155	145
16	142	114
H=	1,K=	14
1	145	154
3	169	191
4	191	179
6	697	681
7	105	92
8	150	149
10	350	381
11	123	88
12	251	227
14	134	108
H=	1,K=	15
1	220	221
2	127	140
3	280	297
4	431	442
6	420	403
7	108	91
9	101	90
10	209	177
11	136	118
17	252	245
18	171	143
H=	1,K=	16
1	1103	1149
2	367	360
3	291	338
5	650	560
10	143	116
H=	1,K=	17
1	115	89
4	674	653
5	225	231
6	125	90
7	182	207
8	266	273
9	208	188
11	277	280
14	205	188
H=	1,K=	18
1	153	141
2	204	188
4	258	256
8	149	154
10	123	88
H=	1,K=	19
1	169	134
2	107	79
3	190	198
6	167	191
8	168	138
10	188	158
H=	1,K=	20
3	317	300
5	228	209
6	190	152
9	232	222
11	192	149
12	150	158
H=	1,K=	21
3	158	146
H=	1,K=	22
6	339	307
8	170	132
10	126	145
H=	1,K=	23
2	158	147
4	181	143
7	152	99
H=	2,K=	0
2	2139	2215
6	1139	1236
8	1835	1699
10	443	414
12	263	260
14	271	298
16	199	237
18	423	399
22	179	193
H=	2,K=	1
1	515	514
3	1180	1374
4	755	689
5	134	204
7	455	458
8	114	116
9	406	406
10	287	262
11	303	335
12	495	489
13	256	267
15	106	82
18	156	181
22	149	143
H=	2,K=	2
1	1359	1506
2	251	221
3	1696	1684
4	655	592
5	474	381
6	93	42
7	895	825
8	487	464
9	351	417
12	118	103
13	563	567
14	148	167
17	126	133
21	214	202
H=	2,K=	3
0	1468	1534
1	1548	1463
2	1086	953
5	587	612
6	413	406
7	751	736
8	557	593
9	520	519
10	246	242
11	159	113
12	147	140
13	344	388
14	460	473
18	277	261
19	129	157
20	108	92
21	103	91
H=	2,K=	4
0	177	239
1	105	97
2	830	700
3	737	644
4	851	852
5	225	192
6	676	625
7	344	323
8	229	250
9	616	629
10	1160	1152
14	443	450
15	222	240
16	229	243
18	106	81
20	181	169
21	165	146
22	143	130
H=	2,K=	5
2	523	482
3	835	854
4	1307	1238
5	566	561
6	248	279
7	658	599
8	602	583
11	270	303
13	131	162
14	175	174
15	163	170
16	354	368
18	185	173
19	128	105
H=	2,K=	6
0	268	294
1	1575	1486
2	154	172
3	1778	1812
4	727	709
5	1245	1163
6	366	407
7	709	771
8	490	487
10	124	126
14	156	106
15	380	388
17	368	388
19	266	254
H=	2,K=	7
0	881	780
1	472	405
2	440	427
3	257	247
4	662	696
6	106	119
7	245	247
8	189	221
9	182	147
10	158	149
11	158	164
13	95	64
14	383	385
15	368	376
16	329	328
18	173	142
20	147	145
H=	2,K=	8
0	521	517
2	465	505
4	820	847
5	121	103
7	347	391
8	772	758
10	914	925
11	425	435
12	399	397
13	284	294
14	268	267
17	210	171
H=	2,K=	9
0	1004	984
1	938	931
2	448	434
3	867	806
4	558	501
5	135	109
6	531	517
7	358	353
8	292	283
9	149	144
11	129	135
12	294	297
13	136	163
14	107	146
15	186	175
19	106	118
H=	2,K=	10
0	193	199
1	333	320
2	241	202
4	228	198
5	239	214
6	187	181
7	396	372
8	199	158
9	261	276
11	275	241
12	467	473
13	115	120
14	144	171
16	207	176
17	107	23
H=	2,K=	11
0	249	238
2	486	500
3	199	168
4	416	423
6	213	246
7	107	91
9	231	259
11	335	328
13	155	134
14	404	426
16	127	126
H=	2,K=	12
0	394	371
1	140	100
2	454	461
3	132	83
4	212	216
5	133	139
6	192	211
7	516	532
8	322	343
9	197	210
10	608	593
11	276	273
14	196	212
H=	2,K=	13
0	547	570
1	402	403
2	242	271
3	283	283
4	252	283
5	610	629
7	167	150
8	113	125
9	370	383
10	307	318
11	263	235
13	107	90
14	286	259
15	201	175
18	107	110
H=	2,K=	14
0	198	205
1	170	193
3	173	164
5	731	728
6	113	78
7	288	272
9	304	329
11	281	286
12	111	84
16	152	126
17	276	249
H=	2,K=	15
0	348	342
2	258	255
3	98	99
6	330	345
7	178	186
8	314	346
10	190	203
11	256	249
12	134	90
H=	2,K=	16
0	254	216
2	286	287
4	436	439
6	334	348
8	308	282
10	512	488
14	181	165
15	208	191
16	106	102
H=	2,K=	17
0	331	329
1	622	628
3	784	747
4	271	266
5	318	297
7	221	183
12	117	114
13	166	111
H=	2,K=	18
0	222	250
1	761	752
2	140	130
3	669	641
5	266	260
6	133	101
9	146	103
H=	2,K=	19
0	174	189
1	111	77
3	165	170
7	215	209
H=	2,K=	20
1	127	90
2	388	366
4	116	69
6	410	408
9	132	120
12	187	221
H=	2,K=	21
1	109	113
3	173	144
5	217	183
7	134	157
8	134	147
11	231	194
H=	2,K=	22
0	208	185
1	176	161
4	128	121
5	122	123
7	204	174
H=	2,K=	23
0	190	180
H=	3,K=	0
2	366	362
4	804	711
6	113	69
8	218	259
10	211	236
12	337	342
20	146	134
22	148	125
H=	3,K=	1
1	1207	1385
2	1747	1906
3	946	933
5	146	28
6	685	711
7	515	546
8	266	210
9	314	249
10	82	103
11	238	223
14	547	589
15	149	154
18	193	178
19	457	448
20	163	142
23	187	176
H=	3,K=	2
1	547	533
2	3003	3147
3	230	175
4	500	469
5	234	231
6	260	256
7	559	529
8	434	440
9	79	105
10	337	337
11	433	475
12	435	446
13	158	208
14	296	299
15	154	141
16	398	384
17	213	257
18	116	112
H=	3,K=	3
1	1255	1110
2	1023	973
3	1648	1570
4	2009	1882
5	765	695
6	268	259
7	327	321
8	196	177
9	437	424
10	186	169
11	289	269
13	99	117
14	225	230
15	469	468
16	392	413
17	214	214
19	170	161
20	238	227
21	118	132
H=	3,K=	4
1	1240	964
2	335	308
3	820	846
4	382	347
5	1046	1076
7	1864	1899
8	130	97
9	449	430
11	842	844
12	145	126
15	271	263
17	164	179
18	187	157
19	123	94
H=	3,K=	5

Table 2. Continued.

1	799	743
2	84	100
3	796	689
4	1143	1042
5	982	985
6	694	689
7	110	123
8	128	202
9	806	854
10	478	458
11	465	502
12	240	240
14	209	250
15	428	420
19	138	120
21	122	86
H=	3,K=	6
1	534	479
2	287	320
3	148	148
4	673	625
5	369	361
6	136	152
8	354	336
11	173	192
14	354	370
15	181	164
18	371	300
19	105	101
H=	3,K=	7
1	607	637
2	294	333
3	104	136
4	222	237
5	746	673
6	1000	969
7	462	490
8	429	466
10	188	222
12	577	604
13	384	388
14	319	309
16	215	215
H=	3,K=	8
1	1812	1867
2	495	477
3	655	668
4	551	566
5	796	792
6	197	212
7	203	189
8	346	354
9	288	321
12	216	176
14	375	382
15	138	148
16	202	218
17	223	210
18	185	197
H=	3,K=	9
1	215	206
2	511	508
3	300	269
5	162	140
6	437	442
7	127	169
8	175	230
9	129	107
11	112	107
12	204	242
13	174	163
14	200	239
16	106	77
17	162	121
18	173	148
H=	3,K=	10
1	469	488
2	908	878
4	526	481
5	109	114
6	182	120
7	340	341
10	259	282
11	108	138
13	125	115
14	291	232
H=	3,K=	11
1	142	200
2	193	195
3	432	451
4	262	252
5	425	416
6	529	493
7	568	537
8	231	241
9	342	349
10	162	161
11	275	323
12	196	184
14	165	141
16	132	127
19	118	120
H=	3,K=	12
2	153	156
5	286	225
6	140	157
7	337	357

8	199	195
11	144	136
13	295	275
15	122	78
17	163	149
H=	3,K=	13
1	164	148
2	193	202
5	199	188
6	450	505
7	353	347
9	109	109
10	371	398
12	156	150
15	169	155
19	109	28
H=	3,K=	14
1	101	109
2	182	179
4	579	531
5	149	138
7	103	117
8	140	170
11	139	142
14	155	154
H=	3,K=	15
1	622	656
2	410	434
3	235	256
5	226	231
6	186	162
7	103	70
11	109	118
14	156	143
H=	3,K=	16
1	98	28
2	309	314
3	413	431
4	323	343
5	99	69
7	288	317
8	129	135
9	116	107
10	126	109
13	160	118
16	182	125
H=	3,K=	17
1	150	159
2	131	167
3	169	212
4	263	272
6	218	245
8	198	216
9	140	113
12	113	138
H=	3,K=	18
2	341	325
5	105	117
6	146	169
8	113	92
12	118	145
13	138	125
H=	3,K=	19
4	239	241
5	195	166
7	219	217
9	120	69
13	151	131
H=	3,K=	20
1	182	175
3	106	109
7	195	181
H=	3,K=	21
4	139	189
5	117	111
9	116	111
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1	156	149
2	462	490
5	203	198
6	307	364
8	178	162
H=	3,K=	23
1	137	184
3	167	173
7	210	181
H=	4,K=	0
0	513	422
2	1376	1293
6	165	72
8	701	607
10	291	319
12	730	766
16	393	403
20	200	161
H=	4,K=	1
0	2203	2086
1	977	930
2	954	904
3	1772	1649
4	1741	1634
5	723	658
6	460	492
7	420	447
10	418	430
11	225	236
13	129	147

14	154	157
18	110	117
19	158	129
H=	4,K=	2
0	591	536
1	625	674
2	618	639
3	1408	1371
4	158	132
5	2050	2010
7	850	802
8	173	173
9	987	1032
11	1058	1062
12	104	76
13	381	382
14	137	154
15	312	303
17	301	309
19	199	207
H=	4,K=	3
2	1194	1158
3	1334	1280
4	666	725
5	472	583
6	478	515
8	760	724
9	894	877
10	179	202
11	312	341
12	373	362
14	380	379
15	269	278
16	109	142
17	199	198
H=	4,K=	4
1	345	326
3	824	790
4	516	546
5	388	371
6	304	315
8	183	196
10	88	93
11	194	194
12	175	200
16	170	170
17	210	218
19	148	153
21	128	91
H=	4,K=	5
0	741	641
1	148	76
2	218	158
3	472	431
4	646	660
5	379	424
6	501	515
9	176	185
10	127	120
11	406	402
12	223	234
13	207	223
14	136	142
17	216	203
H=	4,K=	6
0	441	443
1	220	209
2	287	233
3	476	390
5	497	493
6	96	120
7	1340	1307
8	273	301
9	102	97
11	122	136
12	134	166
13	225	248
14	112	113
15	185	177
16	119	108
H=	4,K=	7
0	899	929
1	384	381
4	647	660
5	164	240
6	344	353
7	274	265
8	253	252
10	91	55
11	290	278
12	238	233
13	542	540
14	436	443
15	209	172
17	198	198
18	256	288
19	153	134
H=	4,K=	8
0	1873	1833
1	231	226
2	838	800
4	920	870
5	97	29
7	152	169
8	447	442
9	248	221
10	521	512

11	192	176
12	576	581
13	105	104
14	687	701
17	167	158
18	107	62
20	138	110
H=	4,K=	9
1	93	65
2	296	282
3	303	323
4	432	512
6	342	343
7	154	178
8	108	83
9	495	507
10	190	183
12	107	110
14	133	159
H=	4,K=	10
0	178	190
1	755	755
2	216	254
3	482	484
4	105	84
8	181	155
10	114	123
15	224	200
17	284	249
19	127	109
H=	4,K=	11
0	921	926
1	577	586
2	279	284
3	155	179
4	242	232
5	170	125
6	372	387
7	193	216
8	204	205
9	100	118
10	519	562
11	372	372
12	178	177
13	259	278
14	240	250
15	193	185
H=	4,K=	12
0	121	151
1	177	189
2	137	132
3	92	84
4	892	946
7	192	200
8	774	781
13	105	80
16	171	147
H=	4,K=	13
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2	164	200
3	249	229
5	309	343
7	262	280
8	190	195
10	201	251
11	315	312
12	117	87
13	197	228
15	219	205
16	107	110
18	196	177
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1	380	364
3	107	134
4	144	186
5	141	151
6	270	255
7	384	388
8	116	109
9	109	130
10	176	187
13	223	218
14	103	85
H=	4,K=	15
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2	294	315
4	228	252
5	252	282
6	636	677
7	172	175
8	141	155
9	209	206
10	327	342
12	109	131
13	148	129
H=	4,K=	16
0	772	736
1	358	342
4	367	384
5	189	205
6	101	84
10	168	150
12	170	166
14	230	192
16	111	68
H=	4,K=	17

0	543	557
3	146	149
4	368	365
7	166	156
8	134	114
9	128	107
13	176	151
15	186	188
H=	4,K=	18
0	113	124
1	219	230
3	115	117
10	161	142
13	129	144
H=	4,K=	19
1	350	308
3	131	79
4	176	166
5	116	138
6	137	97
8	135	126
H=	4,K=	20
0	568	552
3	120	121
4	190	182
5	120	99
H=	4,K=	21
0	207	190
8	128	113
10	175	164
11	214	192
H=	4,K=	22
8	121	136
9	203	191
H=	4,K=	23
0	368	317
3	123	109
H=	4,K=	24
1	123	99
H=	5,K=	0
4	236	246
6	99	110
8	211	199
10	426	414
16	220	251
18	116	43
20	308	287
H=	5,K=	1
2	678	643
3	878	974
4	1598	1555
5	2244	2070
6	338	329
7	427	412
8	822	844
9	565	566
10	427	439
12	285	293
16	165	167
17	231	214
19	283	264
20	197	192
H=	5,K=	2
1	186	186
2	75	44
4	1720	1736
6	143	244
7	105	113
8	1211	1237
9	142	107
11	107	96
12	148	165
13	215	240
14	281	292
15	126	115
17	203	222
21	190	196
H=	5,K=	3
1	418	386
2	682	601
3	632	586
4	170	188
6	590	578
8	90	64
9	233	272
10	786	787
11	228	247
14	326	316
15	166	151
16	107	114
20	138	144
H=	5,K=	4
1	1198	1143
2	121	121
3	2582	2484
4	538	553
6	158	187
7	170	69
8	348	329
9	403	413
12	240	235
13	98	132
16	219	236
17	486	492
18	111	112
19	100	94
21	242	237

H=	5,K=	5
1	1300	1228
2	931	933
4	416	351
5	853	815
6	736	704
7	343	301
8	352	319
9	729	756
10	490	533
11	164	145
12	132	104
13	265	261
14	254	260
15	269	293
16	146	134
17	120	128
18	284	270
H=	5,K=	6
1	150	177
2	794	840
3	355	362
4	153	217
5	86	49
6	476	435
7	383	403
8	517	551
9	169	140
10	556	564
11	267	237
12	281	281
13	254	260
15	127	111
16	189	227
17	323	301
18	133	106
H=	5,K=	7
1	314	316
2	156	202
3	171	145
5	1172	1150
6	860	874
7	107	95
9	129	148
10	141	98
11	316	312
12	263	241
13	448	453
14	137	134
15	167	160
16	183	150
17	109	68
20	151	131
H=	5,K=	8
1	679	668
2	86	119
3	434	402
4	133	128
5	502	517
7	254	250
8	182	183
11	166	144
12	354	351
13	148	179
14	373	390
15	141	120
16	179	148
17	136	108
18	169	168
19	170	166
H=	5,K=	9
2	441	438
3	567	565
4	520	526
5	434	447
6	186	197
8	100	104
9	120	154
11	142	147
12	449	449
13	402	391
15	110	106
16	244	281
H=	5,K=	10
2	1401	1434
3	185	196
6	96	131
7	214	242
8	234	271
9	212	219
10	139	178
12	104	54
13	219	240
16	167	141
17	110	124
H=	5,K=	11
1	690	728
2	397	413
3	493	478
4	267	269
5	181	170
8	322	318
9	208	184
11	116	110
13	383	389
16	104	108
17	228	220

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1	138	105
2	445	468
3	219	264
5	473	496
7	144	111
8	335	350
9	126	54
11	347	388
12	161	155
15	300	258
H=	5,K=	13
1	127	190
2	609	611
3	253	260
5	165	121
8	115	152
9	220	229
10	378	387
12	268	268
13	122	112
H=	5,K=	14
1	139	162
2	613	623
3	211	211
4	349	339
6	479	479
8	186	197
14	122	104
18	155	124
H=	5,K=	15
1	144	178
4	197	150
5	204	207
6	152	147
11	134	149
H=	5,K=	16
3	197	209
4	118	131
5	255	251
7	228	216
16	156	156
H=	5,K=	17
1	154	169
2	262	272
3	189	175
4	248	244
7	147	134
10	121	163
H=	5,K=	18
3	166	211
4	164	149
5	157	145
7	240	212
8	178	159
11	190	183
H=	5,K=	19
1	258	264
4	121	138
5	292	287
7	180	186
H=	5,K=	20
1	112	117
2	233	228
5	190	168
7	[illegible]	[illegible]
11	220	170
H=	5,K=	[illegible]
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H=	6,K=	0
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2	1554	1608
4	2389	2268
6	668	708
8	178	169
10	665	621
12	890	693
14	274	302
16	366	368
18	173	169
22	197	218
H=	6,K=	1
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1	921	874
2	970	842
3	961	899
4	159	72
5	277	243
6	208	230
7	837	856
8	910	881
9	634	603
10	316	337
11	106	162
14	122	136
15	291	289
16	244	263
17	99	46
H=	6,K=	2
0	658	612
1	758	639
2	419	406
3	1218	1246
4	407	391
5	513	440
7	797	773

9	266	268
10	248	233
11	142	178
13	108	85
14	111	123
15	217	243
17	123	107
H=	6,K=	3
0	177	241
1	815	782
2	860	761
3	154	110
4	204	176
5	540	502
6	191	193
7	343	294
8	237	202
9	204	197
10	210	224
11	192	216
12	421	398
13	271	276
14	161	185
15	235	242
16	255	242
18	195	177
H=	6,K=	4
0	309	247
1	145	137
2	922	932
3	244	247
4	338	346
5	622	601
6	1281	1248
7	300	316
8	493	507
9	295	315
10	333	346
14	224	220
16	199	179
18	241	232
19	154	174
H=	6,K=	5
0	242	223
2	97	61
3	347	354
4	283	307
5	323	289
6	453	442
7	425	410
8	228	205
9	502	477
10	176	152
11	157	217
12	116	55
13	144	126
14	97	99
15	219	219
16	119	69
H=	6,K=	6
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1	899	912
2	481	482
3	1448	1511
4	456	498
5	584	567
6	189	218
7	323	301
9	443	441
10	198	68
11	398	453
12	489	475
14	113	111
16	180	162
H=	6,K=	7
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1	998	1012
2	204	289
3	203	202
4	437	419
5	253	219
6	138	88
7	262	219
8	263	281
9	365	369
10	643	667
11	698	605
14	517	508
15	183	174
16	144	142
H=	6,K=	8
0	140	65
1	129	110
2	172	182
3	83	90
4	798	723
5	138	164
6	447	441
7	133	158
9	193	186
11	172	198
14	323	318
15	108	131
H=	6,K=	9
0	980	845
1	737	710
2	448	453

Table 2. Continued.

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8	371	403
11	174	207
13	367	373
14	168	180
15	229	215
16	147	149
H= 6,K= 10		
0	286	286
1	506	542
2	262	266
3	157	105
5	138	172
8	181	189
9	478	496
10	300	323
11	191	219
12	158	179
13	176	195
14	117	133
15	154	146
17	160	196
18	126	135
19	146	121
H= 6,K= 11		
1	235	279
2	159	174
3	194	212
4	315	302
7	393	356
8	543	544
9	436	442
10	192	164
11	178	173
14	244	228
17	156	144
H= 6,K= 12		
1	121	130
2	94	129
3	197	183
4	376	400
5	223	229
8	536	562
9	191	201
11	172	170
12	175	179
15	118	114
16	139	140
H= 6,K= 13		
1	297	274
5	244	259
6	199	153
7	246	283
8	143	172
9	141	142
10	205	230
11	124	135
H= 6,K= 14		
0	385	385
1	911	931
3	345	340
4	244	239
5	171	214
9	255	265
11	276	244
14	140	105
H= 6,K= 15		
0	249	255
1	103	108
2	274	279
3	275	300
6	517	543
7	175	170
11	288	252
17	119	125
H= 6,K= 16		
0	458	480
3	159	147
6	293	277
8	272	247
10	151	141
14	195	168
15	174	132
H= 6,K= 17		
3	376	417
5	243	272
6	236	249
7	271	263
9	309	317
10	168	189
12	120	98
15	163	153
H= 6,K= 18		
7	127	138
13	161	125
14	196	189
15	132	84
H= 6,K= 19		
1	211	188
2	108	79
6	179	149
7	160	163
9	102	101
10	180	166
H= 6,K= 20		

4	100	70
7	146	126
10	201	208
H= 6,K= 21		
1	119	131
H= 6,K= 22		
1	108	89
3	191	175
5	114	100
H= 6,K= 23		
2	104	61
H= 7,K= 0		
2	399	397
4	417	405
6	232	236
10	396	432
14	357	369
16	151	157
H= 7,K= 1		
1	499	566
2	983	942
4	762	790
5	590	608
6	90	26
7	931	840
8	1005	986
9	100	124
10	205	183
12	262	260
13	248	276
14	159	139
16	217	204
18	187	179
H= 7,K= 2		
2	984	992
3	125	107
4	450	369
6	457	387
7	108	154
8	106	130
9	100	112
10	397	373
12	193	191
14	149	163
15	212	214
16	178	180
18	146	123
19	212	191
H= 7,K= 3		
1	306	280
2	402	406
3	1229	1244
4	715	710
5	547	543
6	578	591
7	310	351
8	607	618
9	178	158
10	254	263
11	207	220
12	181	174
13	103	111
14	117	154
15	102	87
16	213	194
20	206	190
H= 7,K= 4		
1	627	595
2	128	139
3	191	202
4	196	200
5	1160	1134
6	206	187
7	751	754
8	300	308
9	260	272
10	147	130
11	297	316
13	365	363
15	163	213
17	150	156
18	124	67
21	168	170
H= 7,K= 5		
1	438	422
2	703	630
3	124	99
4	310	308
5	481	465
7	86	47
9	314	301
10	521	496
11	197	180
12	792	810
13	150	158
14	223	205
16	448	457
18	131	102
H= 7,K= 6		
2	299	289
3	99	116
4	569	588
7	156	136
8	930	967
9	134	130
10	209	221
12	904	933

14	167	182
15	119	123
16	415	403
H= 7,K= 7		
1	333	267
2	274	280
3	144	122
4	414	427
5	381	363
6	364	401
7	173	186
9	265	258
11	305	314
12	562	608
13	140	175
14	245	239
16	287	259
17	116	106
H= 7,K= 8		
1	1003	968
3	328	310
4	109	114
5	300	313
6	217	233
7	731	750
8	233	221
9	337	360
10	129	131
11	620	650
12	155	148
13	232	211
14	210	187
19	105	65
H= 7,K= 9		
3	137	128
5	205	209
6	437	432
8	234	234
9	97	126
12	180	203
13	106	57
14	114	123
H= 7,K= 10		
1	157	120
2	556	592
3	171	186
4	471	489
6	365	398
7	119	91
8	217	242
12	102	106
14	243	246
18	186	182
H= 7,K= 11		
1	629	626
2	406	397
3	476	481
4	116	88
5	255	294
6	302	288
7	717	702
8	259	265
9	200	174
10	209	225
11	462	442
12	203	222
14	215	189
15	188	185
16	186	161
17	126	77
H= 7,K= 12		
1	112	88
2	142	131
3	275	269
4	194	192
5	103	132
6	289	300
7	103	95
8	282	289
9	498	529
11	165	156
13	305	281
14	109	54
16	170	139
H= 7,K= 13		
1	191	190
2	205	182
6	190	213
7	233	219
9	300	312
11	104	56
14	192	191
H= 7,K= 14		
1	251	269
3	248	262
4	143	103
9	183	172
H= 7,K= 15		
1	206	218
3	369	389
4	176	179
8	141	160
11	209	218
H= 7,K= 16		
2	98	43
3	288	288
5	425	434

11	183	166
H= 7,K= 17		
1	103	124
2	142	101
4	166	174
5	114	147
8	251	248
10	245	235
13	119	130
H= 7,K= 18		
2	283	275
6	220	229
8	218	203
12	254	213
H= 7,K= 19		
2	198	174
3	251	216
11	110	115
13	172	159
H= 7,K= 20		
3	237	232
5	166	169
7	336	307
8	130	117
9	168	151
H= 7,K= 21		
6	210	197
7	133	129
H= 7,K= 22		
2	146	162
3	132	94
4	181	131
7	114	68
8	139	89
H= 7,K= 23		
1	122	67
H= 8,K= 0		
0	1033	1041
2	478	387
4	90	48
6	1594	1603
8	241	251
10	469	495
12	116	94
14	135	177
16	236	220
H= 8,K= 1		
0	1649	1603
1	898	906
2	382	362
3	110	52
4	469	471
5	522	535
6	725	724
7	619	656
8	321	348
9	196	201
10	88	55
12	169	174
13	167	201
14	271	273
18	184	151
H= 8,K= 2		
0	373	348
1	1817	1839
2	175	178
3	759	775
5	515	471
6	225	212
7	380	376
9	607	626
11	450	449
13	159	111
14	328	345
15	221	223
H= 8,K= 3		
1	238	226
2	91	88
3	291	232
4	156	116
5	271	274
6	699	689
7	305	306
8	228	197
10	261	259
11	363	356
12	232	236
13	107	32
14	157	192
15	222	221
16	256	251
H= 8,K= 4		
0	687	673
1	109	90
2	102	82
3	86	87
4	178	158
5	184	187
6	124	92
7	175	207
8	295	287
9	435	428
11	132	159
12	222	227
13	180	195
14	120	102
15	204	189

18	136	152
H= 8,K= 5		
0	501	508
1	768	766
2	159	156
3	397	400
5	478	463
6	433	431
7	108	113
8	287	291
9	220	221
10	194	180
11	416	440
12	318	328
15	142	126
16	240	240
17	107	23
H= 8,K= 6		
0	446	474
1	88	71
2	119	116
3	1025	1050
4	128	109
5	85	61
6	159	139
7	797	820
8	96	70
9	581	581
10	244	256
11	678	669
14	259	268
15	452	440
19	109	174
H= 8,K= 7		
0	116	141
1	122	128
2	474	475
3	578	570
4	176	154
5	136	129
6	370	381
7	467	476
8	508	498
9	193	167
10	246	236
12	168	175
14	153	170
16	115	115
H= 8,K= 8		
0	424	426
1	250	252
2	394	467
3	196	192
4	205	241
5	121	127
6	97	98
7	118	111
8	262	296
9	214	224
10	119	150
11	297	304
12	125	108
14	182	175
H= 8,K= 9		
0	222	246
1	126	96
2	353	332
3	409	365
5	428	449
6	490	494
7	214	212
10	291	322
11	382	371
13	435	407
15	116	93
16	228	226
17	177	178
18	259	236
20	121	110
H= 8,K= 10		
0	288	322
1	342	365
2	136	130
3	298	299
5	129	121
7	205	212
8	273	276
9	632	657
11	495	529
12	252	252
13	476	446
15	263	259
16	120	94
H= 8,K= 11		
0	313	283
4	117	137
8	107	105
9	304	322
10	446	445
11	523	517
12	261	226
14	125	100
15	150	162
H= 8,K= 12		
0	622	657
1	129	103
2	99	89

3	273	268
6	178	155
7	195	191
8	278	283
9	168	164
10	157	148
12	169	152
18	152	137
H= 8,K= 13		
0	177	197
1	422	404
2	130	112
3	206	203
5	205	213
6	112	120
7	286	317
8	180	152
9	226	236
11	120	138
14	156	118
16	191	178
H= 8,K= 14		
1	110	132
2	105	59
3	222	261
4	148	123
7	414	430
8	135	140
9	195	166
H= 8,K= 15		
0	256	259
1	172	174
2	167	164
3	105	122
4	255	269
7	116	108
8	119	141
11	133	133
13	214	171
15	158	156
H= 8,K= 16		
1	145	168
6	197	236
9	252	252
10	102	122
13	125	111
H= 8,K= 17		
0	162	124
1	145	164
3	198	211
7	272	244
12	190	168
H= 8,K= 18		
0	125	111
5	115	136
6	119	107
7	121	117
H= 8,K= 19		
0	152	138
2	108	143
3	176	158
6	175	186
7	216	195
9	182	151
H= 8,K= 20		
2	196	175
4	108	104
6	168	176
H= 8,K= 21		
5	170	149
9	213	191
H= 8,K= 22		
7	129	122
H= 9,K= 0		
2	543	527
6	423	401
14	293	290
18	270	269
H= 9,K= 1		
1	311	300
2	82	5
3	642	628
4	187	240
6	359	398
7	255	286
9	190	157
10	143	153
11	208	203
13	124	146
14	157	157
16	294	276
19	119	93
H= 9,K= 2		
1	195	186
2	445	454
3	161	135
4	461	452
5	99	118
6	329	319
7	130	108
8	593	598
9	97	78
10	262	235
11	231	255
12	505	532
13	209	213
14	303	280

16	339	333
17	106	121
20	220	219
H= 9,K= 3		
1	355	363
2	509	500
3	551	533
6	366	400
7	238	246
8	230	219
9	97	85
12	165	161
14	186	188
15	219	192
H= 9,K= 4		
1	741	753
2	333	355
3	1381	1395
4	103	140
5	967	999
6	118	93
7	118	150
9	377	352
10	194	211
11	300	313
12	103	96
13	279	303
14	174	186
H= 9,K= 5		
1	302	315
2	183	216
3	296	271
4	670	718
7	246	243
8	587	618
10	163	151
11	159	170
12	472	499
14	253	246
15	281	251
H= 9,K= 6		
1	258	281
2	667	668
3	134	146
4	544	571
5	347	359
6	288	299
8	883	875
11	120	120
12	551	568
15	139	57
16	211	197
H= 9,K= 7		
1	112	109
3	179	188
6	163	167
7	640	685
9	210	215
10	472	460
12	254	252
14	111	114
15	152	142
17	309	301
18	202	192
H= 9,K= 8		
1	393	361
2	137	128
3	217	234
5	587	632
9	304	310
10	238	242
11	225	220
15	138	139
16	179	174
17	130	142
20	193	177
H= 9,K= 9		
3	147	149
4	190	167
5	108	98
6	132	150
8	117	143
10	202	171
17	184	143
18	119	135
H= 9,K= 10		
1	213	201
2	353	366
4	210	197
5	257	246
6	282	302
7	214	214
8	394	413
9	99	96
11	290	270
12	377	381
13	111	80
14	137	125
15	278	272
16	140	156
17	122	146
19	262	216
H= 9,K= 11		
4	368	379
5	107	115
6	227	259
7	168	199

9	340	365
10	247	215
11	462	442
12	238	230
13	203	180
15	208	204
17	117	140
H= 9,K= 12		
1	198	176
2	218	231
3	702	732
5	752	761
6	128	93
7	212	204
9	660	668
10	152	176
11	125	114
13	261	260
15	333	324
16	199	186
17	202	156
H= 9,K= 13		
1	142	90
2	258	255
4	324	330
5	191	196
8	220	229
10	155	129
11	143	137
15	144	136
H= 9,K= 14		
2	121	104
4	230	225
5	123	112
9	139	146
13	163	167
15	159	155
17	155	159
H= 9,K= 15		
2	129	122
3	110	111
4	125	104
9	112	77
10	149	132
12	142	135
H= 9,K= 16		
1	240	273
5	237	227
6	108	7
7	197	202
9	217	184
13	204	182
H= 9,K= 17		
3	109	37
7	168	179
H= 9,K= 18		
2	119	37
5	133	109
12	142	103
H= 9,K= 19		
5	170	153
7	211	181
11	142	87
H= 9,K= 20		
2	135	139
7	162	141
10	131	118
H= 9,K= 21		
4	266	248
H= 9,K= 22		
5	133	100
H= 10,K= 0		
0	1160	1115
2	998	924
4	814	815
6	268	270
8	460	475
10	110	44
14	328	331
18	206	220
20	179	144
H= 10,K= 1		
0	417	413
2	293	248
3	169	140
4	210	217
5	270	269
6	310	294
7	129	165
8	224	219
11	188	188
12	130	128
15	136	144
H= 10,K= 2		
1	702	685
2	151	153
3	682	674
5	376	350
7	279	293
8	134	120
9	437	450
10	112	103
12	178	189
13	427	403
15	263	250
16	141	136
19	167	150

Table 2. Continued.

H= 10,K= 3		
0	619	617
1	683	698
2	241	261
3	262	226
4	259	219
6	705	706
7	519	539
11	243	246
13	144	140
15	185	182
18	100	122
19	197	175
H= 10,K= 4		
0	830	868
2	225	217
3	160	186
4	743	740
5	218	220
6	715	689
7	276	273
8	540	546
10	622	623
12	181	190
13	155	135
14	201	207
17	251	226
H= 10,K= 5		
0	167	222
1	136	180
2	107	109
3	124	92
4	359	384
5	231	195
6	348	361
7	140	138
8	281	276
9	251	233
11	419	473
13	315	309
14	116	112
15	155	127
16	164	119
21	159	156
H= 10,K= 6		
1	119	105
2	92	42
5	330	364
7	775	787
8	228	234
11	182	169
12	264	272
13	373	378
15	157	205
16	127	140
18	135	125
H= 10,K= 7		
0	522	507
1	104	73
4	231	216
6	153	103
7	202	208
8	256	267
9	261	249
11	113	111
12	149	134
14	110	124
H= 10,K= 8		
0	259	296
1	179	178
2	568	578
3	146	140
4	186	169
8	106	130
12	129	133
13	155	146
14	121	103
17	115	132
18	164	124
20	187	162
H= 10,K= 9		
0	297	280
1	375	395
3	378	376
4	126	104
5	413	431
6	467	485
7	195	214
8	155	169
9	351	362
10	114	102
11	283	273
18	110	114
H= 10,K= 10		
1	468	479
2	122	100
3	144	118
5	194	195
7	113	112
8	130	133
11	215	241
14	118	105
15	281	265
H= 10,K= 11		
0	440	473
2	99	144
3	208	241

4	479	492
5	208	257
6	314	332
8	140	133
11	101	86
13	108	115
14	116	118
16	178	179
H= 10,K= 12		
2	296	298
4	145	155
6	175	173
8	138	139
H= 10,K= 13		
0	212	208
1	188	165
3	123	181
5	112	141
7	199	209
8	184	171
9	389	370
10	123	111
11	113	89
17	128	90
H= 10,K= 14		
0	220	245
2	147	140
3	185	204
5	131	129
6	259	268
9	126	101
10	131	142
11	286	290
H= 10,K= 15		
0	602	616
1	287	293
2	156	141
4	479	467
5	259	245
H= 10,K= 16		
0	110	82
1	211	226
2	160	132
3	201	224
4	133	111
6	140	139
7	108	128
10	262	226
14	171	138
H= 10,K= 17		
3	272	244
4	154	133
6	194	176
10	112	102
H= 10,K= 18		
3	198	161
7	122	136
11	114	114
H= 10,K= 19		
0	414	406
1	248	213
4	127	169
H= 10,K= 20		
9	143	126
H= 10,K= 22		
0	136	122
3	125	66
H= 11,K= 0		
2	274	309
4	217	200
8	245	277
10	115	114
12	165	184
16	138	115
H= 11,K= 1		
1	468	430
2	312	329
3	479	490
5	118	93
6	410	400
7	290	294
8	96	85
10	452	472
11	218	213
12	112	90
13	299	302
14	196	152
15	148	123
18	165	158
19	161	160
H= 11,K= 2		
2	171	146
3	118	132
4	1076	1118
5	100	98
6	391	382
8	210	196
10	108	132
11	324	359
12	136	164
14	182	196
15	222	202
16	109	76
H= 11,K= 3		
1	435	408
2	327	298
3	151	143

4	281	299
5	267	273
7	286	296
8	111	128
10	357	379
11	193	183
12	329	322
13	133	149
14	311	291
H= 11,K= 4		
1	811	847
2	122	100
3	417	421
4	94	83
5	594	593
7	218	224
8	222	239
9	150	196
10	105	116
11	130	138
12	240	250
14	127	134
15	114	62
17	116	163
H= 11,K= 5		
1	261	278
2	235	262
3	446	429
4	536	514
5	90	46
7	270	271
8	601	629
9	248	261
12	315	318
14	184	153
15	152	141
16	273	271
17	102	116
18	159	122
H= 11,K= 6		
2	418	403
3	163	181
4	538	582
6	518	515
7	316	318
9	166	179
10	217	216
11	148	134
15	115	138
16	196	174
18	114	80
19	164	132
20	222	203
H= 11,K= 7		
1	454	459
2	231	235
3	240	247
4	174	171
7	382	419
9	453	450
11	164	143
15	191	169
16	167	163
H= 11,K= 8		
1	335	366
2	237	254
4	198	188
5	201	195
6	146	141
7	130	111
8	240	257
9	477	462
10	199	214
12	189	178
13	189	149
14	128	131
15	233	216
19	176	184
H= 11,K= 9		
4	135	118
5	357	378
6	199	195
7	253	266
8	153	148
9	199	229
11	135	149
12	152	174
15	191	172
H= 11,K= 10		
2	547	554
3	212	211
4	546	608
5	141	131
6	394	416
7	122	143
8	216	275
9	144	134
11	174	163
12	333	292
15	185	182
18	152	152
H= 11,K= 11		
1	299	291
2	142	117
3	281	285
6	337	353
7	282	300

10	109	104
14	186	150
H= 11,K= 12		
1	370	357
2	331	339
4	101	98
5	394	368
7	425	452
9	307	312
11	333	321
H= 11,K= 13		
1	176	187
2	520	524
3	163	172
5	180	190
6	277	268
7	147	165
8	168	174
12	339	323
H= 11,K= 14		
1	173	157
2	547	588
4	186	157
5	185	195
8	131	111
11	182	205
14	114	100
H= 11,K= 15		
1	103	86
2	150	181
3	116	95
5	251	274
9	175	187
14	116	33
H= 11,K= 16		
1	138	164
4	110	99
13	115	96
H= 11,K= 17		
1	109	131
2	141	145
3	131	148
H= 11,K= 18		
4	202	187
6	110	115
H= 11,K= 19		
5	234	201
H= 12,K= 0		
0	485	482
2	307	329
4	356	342
6	820	793
8	398	431
10	363	363
12	306	326
14	115	125
H= 12,K= 1		
1	267	293
3	347	344
4	198	219
6	121	126
7	245	246
8	293	293
9	94	54
10	102	94
15	120	122
H= 12,K= 2		
1	378	402
3	476	492
5	198	180
7	294	334
9	201	200
10	97	33
H= 12,K= 3		
0	337	333
1	122	91
2	128	173
4	140	75
5	332	339
6	276	261
7	258	260
8	168	227
9	492	516
10	378	416
11	424	436
12	291	317
13	161	182
H= 12,K= 4		
0	228	249
2	311	322
4	195	203
6	484	488
9	154	166
10	456	458
11	164	151
12	153	148
14	229	243
17	99	87
H= 12,K= 5		
0	193	145
1	411	386
2	283	280
4	179	170
6	237	281
8	231	229
9	324	352
11	197	210

13	119	125
H= 12,K= 6		
0	155	123
1	134	102
4	201	232
7	632	681
8	103	122
11	219	243
19	219	186
H= 12,K= 7		
1	284	300
3	547	550
4	310	305
5	105	86
7	511	538
8	326	302
9	112	93
10	250	238
11	110	129
13	112	59
H= 12,K= 8		
0	371	375
1	140	146
2	330	363
5	204	193
6	280	290
8	543	551
10	376	357
12	218	241
16	316	297
H= 12,K= 9		
0	510	508
1	301	313
2	97	82
3	176	184
4	446	461
5	129	141
6	222	215
8	390	388
11	160	159
13	105	25
15	161	132
H= 12,K= 10		
0	216	204
3	591	634
5	496	487
6	116	123
7	516	521
11	108	99
16	158	129
H= 12,K= 11		
0	276	263
1	338	356
3	536	561
4	155	165
5	195	165
6	265	300
7	299	303
10	232	217
14	108	149
H= 12,K= 12		
1	146	146
2	245	287
3	148	133
4	119	122
5	197	209
6	155	173
7	175	167
8	137	124
11	121	97
13	118	113
H= 12,K= 13		
0	489	479
1	416	440
2	203	207
4	318	306
5	341	323
7	164	153
8	103	78
H= 12,K= 14		
0	193	220
1	437	447
3	536	536
4	114	109
5	453	438
6	142	137
H= 12,K= 15		
0	332	311
1	144	132
4	165	141
5	138	122
10	131	117
11	149	123
H= 12,K= 16		
0	295	293
10	335	316
H= 12,K= 17		
1	154	118
3	207	214
11	160	138
H= 12,K= 18		
1	308	301
5	203	197
H= 12,K= 20		
0	195	185
2	138	116
3	160	154

4	112	107
6	121	40
H= 13,K= 0		
2	196	193
4	245	267
6	144	160
8	141	126
10	301	315
12	200	180
14	220	198
16	113	113
H= 13,K= 1		
1	100	72
2	267	246
3	126	94
4	203	226
5	87	17
7	350	367
8	257	256
9	380	387
11	103	118
13	320	293
14	120	108
17	103	122
H= 13,K= 2		
2	446	463
4	406	415
6	283	310
7	126	129
11	304	302
12	236	225
15	211	199
17	144	112
H= 13,K= 3		
1	96	77
2	329	354
3	382	384
5	139	127
6	399	406
7	161	186
10	432	422
13	145	111
14	139	143
H= 13,K= 4		
1	592	594
2	128	144
3	238	236
4	128	151
5	688	707
7	280	286
8	127	109
11	551	556
13	468	439
15	153	144
17	246	223
19	161	152
H= 13,K= 5		
1	297	288
2	835	866
3	631	623
4	358	369
5	433	439
6	338	321
7	324	342
8	223	201
9	228	218
11	235	247
12	116	72
13	115	98
14	151	102
15	172	135
18	131	118
H= 13,K= 6		
1	150	145
2	289	307
3	141	123
4	594	606
6	239	256
8	708	716
10	272	272
12	324	320
16	197	148
H= 13,K= 7		
1	417	437
2	430	447
3	134	134
4	137	136
5	115	102
6	334	356
7	165	182
8	245	252
10	280	276
H= 13,K= 8		
1	284	278
2	235	268
3	576	614
5	352	381
6	290	298
8	108	126
9	216	247
10	183	170
11	266	271
15	196	196
H= 13,K= 9		
1	192	203
2	288	292
3	268	275

4	214	212
5	101	82
6	357	370
7	263	304
8	217	174
11	122	141
16	111	80
H= 13,K= 10		
1	157	200
2	125	132
4	277	292
5	186	171
6	672	648
7	117	89
8	182	193
10	207	175
14	290	293
H= 13,K= 11		
1	293	293
3	197	210
4	281	281
5	144	146
8	165	175
H= 13,K= 12		
1	489	499
2	362	364
3	626	606
4	170	180
6	259	240
7	159	172
8	211	231
9	121	109
10	130	112
11	110	124
14	108	81
H= 13,K= 13		
2	247	264
5	180	154
6	138	92
7	142	140
9	129	98
H= 13,K= 14		
2	309	331
5	146	127
H= 13,K= 15		
4	103	104
6	134	120
H= 13,K= 16		
3	104	114
H= 13,K= 17		
2	238	208
4	110	92
H= 13,K= 18		
2	279	278
4	166	141
H= 13,K= 19		
1	147	124
H= 14,K= 0		
0	96	93
2	831	875
4	345	325
6	610	603
8	207	225
10	372	364
14	161	172
H= 14,K= 1		
0	224	265
1	103	119
2	173	184
3	384	376
4	278	272
5	130	152
6	111	102
7	189	199
8	204	180
9	131	141
10	158	148
13	201	188
15	147	161
H= 14,K= 2		
0	170	176
1	334	336
5	551	553
7	679	700
9	418	415
11	348	313
13	137	181
15	208	200
H= 14,K= 3		
0	263	180
3	148	118
4	288	307
5	190	186
7	165	169
8	771	790
9	460	445
10	384	387
11	187	150
12	189	153
13	118	123
14	219	237
H= 14,K= 4		
4	112	108
6	135	109
7	121	129
11	156	166
13	116	122

17	179	174
H= 14,K= 5		
0	527	544
1	527	533
2	356	364
4	247	239
5	645	673
6	475	453
8	329	301
10	220	221
11	280	243
13	179	162
17	177	158
H= 14,K= 6		
0	107	73
1	315	309
3	745	746
5	395	394
7	115	176
8	106	124
9	322	329
12	121	145
17	142	91
H= 14,K= 7		
0	918	936
1	447	465
4	463	472
5	233	222
8	153	148
9	175	201
10	217	187
11	171	196
12	156	150
13	183	163
15	184	179
H= 14,K= 8		
0	482	483
2	266	306
4	406	397
8	154	193
11	122	99
13	178	188
H= 14,K= 9		
0	420	427
1	340	340
3	125	107
5	210	256
9	203	198
12	142	126
15	213	213
16	120	136
17	196	195
H= 14,K= 10		
1	140	100
2	104	88
5	319	318
6	160	172
9	161	152
H= 14,K= 11		
0	569	579
1	146	183
3	201	220
4	645	616
5	141	159
8	179	166
11	130	126
12	121	83
H= 14,K= 12		
0	796	788
1	178	173
2	336	352
3	112	72
4	346	328
5	132	136
6	169	197
H= 14,K= 13		
0	393	346
1	323	316
5	223	213
7	363	357
8	300	277
9	141	159
10	135	149
11	136	150
H= 14,K= 14		
0	124	74
7	158	158
H= 14,K= 15		
1	139	117
6	123	113
10	171	154
H= 14,K= 16		
1	112	112
4	190	236
5	187	195
7	123	100
9	194	174
H= 14,K= 17		
1	170	124
6	130	117
H= 14,K= 19		
0	180	143
H= 15,K= 0		
2	132	160
8	238	282
12	131	144
H= 15,K= 1		

Table 2. Continued.

1	239	230
2	333	344
3	211	216
6	174	163
7	188	157
8	183	198
11	230	222
12	126	133
H= 15,K= 2		
2	166	109
4	558	593
9	130	143
13	102	88
14	135	147
H= 15,K= 3		
1	320	332
2	265	280
3	260	269
9	328	307
10	117	108
11	125	110
13	159	130
H= 15,K= 4		
1	627	657
3	184	181
7	232	232
8	160	167
11	219	203
12	174	170
13	186	162
H= 15,K= 5		
1	262	282
3	244	236
5	178	186
6	273	267
7	245	263
8	125	137
10	274	269
11	306	300
14	136	133
H= 15,K= 6		
2	327	331
5	161	134
H= 15,K= 7		
1	109	68
2	186	198
3	350	353
7	432	432
11	139	144
15	158	143
17	189	200
H= 15,K= 8		
1	102	91
4	120	110
5	326	314
9	247	234
12	123	103
15	154	141
H= 15,K= 9		
2	427	436
4	290	290
5	175	178
6	114	112
8	251	275
12	225	223
16	118	106
H= 15,K= 10		
2	374	372
4	507	495
6	120	146
12	138	151
H= 15,K= 11		
1	506	485
3	167	132
5	454	437
7	113	59
11	142	134
13	226	195
H= 15,K= 12		
1	129	134
2	144	109
3	241	235
4	131	83
5	185	189
8	178	191
9	249	229
11	149	171
13	149	129
H= 15,K= 13		
1	140	100
2	115	81
4	130	118
6	121	98
H= 15,K= 14		
1	132	100
4	235	214
7	123	131
H= 15,K= 15		
1	104	104
3	202	200
4	217	198
6	120	98
7	200	176
H= 15,K= 16		
1	239	234
H= 15,K= 18		
4	130	132
H= 16,K= 0		
0	197	166
4	187	152
6	162	197
8	126	107
10	533	500
14	353	337
16	131	105
H= 16,K= 1		
0	216	229
1	117	147
3	124	167
4	385	397
5	263	297
7	359	372
8	420	427
9	342	331
10	101	59
H= 16,K= 2		
0	99	57
1	252	272
3	159	176
5	474	455
H= 16,K= 3		
0	209	237
1	113	92
2	134	146
3	300	334
4	326	338
5	203	211
H= 16,K= 4		
0	112	128
1	273	247
3	165	130
H= 16,K= 5		
0	528	543
1	422	431
2	143	160
3	202	217
4	124	161
6	100	33
7	132	170
H= 16,K= 6		
0	228	202
1	498	495
2	144	122
3	235	283
4	127	97
5	260	277
7	110	89
9	400	398
10	142	121
13	215	209
15	115	140
H= 16,K= 7		
1	105	126
2	196	195
3	107	101
6	222	201
7	154	136
9	192	206
H= 16,K= 8		
0	385	404
4	481	470
6	215	199
8	165	176
12	190	147
H= 16,K= 9		
5	217	200
10	169	156
11	144	145
13	145	164
14	144	136
H= 16,K= 10		
0	146	90
1	145	145
3	252	245
6	168	151
7	361	362
H= 16,K= 11		
0	179	140
3	171	161
4	183	179
5	168	166
6	126	140
H= 16,K= 12		
2	120	115
4	126	124
10	159	196
11	135	116
H= 16,K= 13		
2	210	191
3	263	266
6	123	140
7	130	148
9	119	75
12	172	176
H= 16,K= 14		
2	159	134
5	208	203
9	169	130
H= 16,K= 15		
0	170	162
1	114	118
6	130	130
H= 16,K= 16		
6	294	273
7	135	100
H= 16,K= 17		
0	115	115
1	144	113
H= 17,K= 0		
2	172	185
4	194	170
6	291	309
10	133	132
H= 17,K= 1		
2	264	264
5	159	172
6	236	258
8	341	333
12	139	132
H= 17,K= 2		
1	104	109
4	170	171
5	171	189
6	568	571
8	283	277
9	157	163
10	276	247
12	173	156
H= 17,K= 3		
2	183	169
3	406	403
5	150	145
7	364	361
8	133	105
9	146	146
H= 17,K= 4		
1	472	478
3	265	296
5	233	197
6	159	174
7	228	198
10	125	89
H= 17,K= 5		
1	149	156
2	372	372
3	246	229
5	127	123
6	113	89
7	103	87
15	106	84
H= 17,K= 6		
2	323	335
4	220	215
6	295	280
7	112	83
8	110	111
12	202	202
H= 17,K= 7		
2	184	184
5	131	104
8	161	159
9	181	190
11	135	143
12	127	165
H= 17,K= 8		
1	152	132
3	307	294
5	171	169
6	117	103
7	158	121
9	116	78
H= 17,K= 9		
1	145	141
3	178	182
4	214	206
6	136	102
H= 17,K= 10		
2	260	238
4	171	193
7	117	158
11	130	139
H= 17,K= 11		
1	250	226
2	182	166
3	230	231
H= 17,K= 12		
1	120	135
3	123	157
4	131	139
H= 17,K= 13		
1	104	92
2	150	112
3	189	161
H= 17,K= 14		
4	231	208
7	141	124
8	151	140
H= 17,K= 15		
1	161	128
2	145	114
6	157	122
H= 17,K= 16		
3	126	105
H= 17,K= 17		
1	139	89
H= 18,K= 0		
0	374	410
2	137	189
4	770	766
6	189	186
8	259	258
10	133	107
14	138	124
H= 18,K= 1		
0	107	97
3	148	131
5	161	147
7	243	245
12	138	123
H= 18,K= 2		
0	114	106
1	106	78
3	169	132
5	132	88
7	105	80
H= 18,K= 3		
0	244	252
5	190	174
6	160	145
8	262	237
9	268	258
11	127	106
12	206	188
H= 18,K= 4		
0	706	695
1	128	110
2	197	188
3	127	107
4	283	283
6	225	210
7	146	115
H= 18,K= 5		
0	256	250
1	142	135
3	184	153
4	152	159
5	111	103
9	204	196
H= 18,K= 6		
7	150	147
9	290	259
H= 18,K= 7		
0	205	217
4	149	108
H= 18,K= 8		
0	105	67
4	162	129
6	169	167
12	162	136
H= 18,K= 9		
10	128	122
11	136	145
H= 18,K= 10		
0	170	127
1	234	223
5	201	208
9	223	232
H= 18,K= 11		
0	220	213
6	202	192
10	220	205
H= 18,K= 12		
0	278	258
6	101	104
H= 18,K= 13		
6	110	114
7	232	225
H= 18,K= 14		
3	239	229
5	289	263
7	178	140
H= 19,K= 0		
2	127	93
10	132	96
H= 19,K= 1		
4	143	121
7	124	96
8	107	73
12	149	154
13	167	144
H= 19,K= 2		
2	136	129
6	158	138
H= 19,K= 3		
1	179	160
2	277	247
3	243	237
4	206	179
5	146	143
9	172	144
H= 19,K= 4		
1	151	121
5	194	160
7	233	231
11	229	211
H= 19,K= 5		
9	170	169
12	138	134
13	253	200
H= 19,K= 6		
2	120	112
7	136	121
8	161	145
12	130	146
H= 19,K= 7		
6	133	120
H= 19,K= 8		
7	230	224
H= 19,K= 9		
3	108	98
5	176	163
9	181	144
H= 19,K= 10		
2	188	194
6	233	201
10	151	98
H= 19,K= 11		
2	162	150
4	164	154
6	137	112
H= 19,K= 12		
1	246	220
4	108	96
5	246	244
H= 19,K= 13		
4	206	205
H= 19,K= 14		
2	178	148
H= 20,K= 0		
0	271	268
4	414	404
6	243	212
10	149	126
12	254	235
H= 20,K= 1		
0	236	244
1	162	155
4	157	139
5	116	141
6	134	141
7	164	148
10	165	172
11	182	146
H= 20,K= 2		
1	182	202
3	279	250
5	237	218
7	201	195
9	104	69
H= 20,K= 3		
0	135	113
1	135	121
8	124	127
H= 20,K= 4		
0	116	93
2	123	139
6	224	214
8	158	127
10	135	140
H= 20,K= 5		
1	140	114
H= 20,K= 6		
1	290	274
9	328	282
H= 20,K= 7		
10	206	203
H= 20,K= 8		
6	173	154
H= 20,K= 9		
5	130	122
H= 20,K= 10		
4	108	73
H= 20,K= 11		
0	179	176
H= 20,K= 12		
2	142	139
H= 20,K= 13		
1	153	97
H= 21,K= 1		
3	166	174
4	212	202
7	211	182
9	151	128
H= 21,K= 2		
2	157	168
4	215	196
5	141	102
H= 21,K= 3		
5	146	153
H= 21,K= 4		
1	211	179
3	123	155
H= 21,K= 5		
4	122	114
7	113	146
8	140	131
10	249	215
H= 21,K= 6		
9	158	116
H= 21,K= 8		
8	117	116
H= 21,K= 9		
4	110	74
H= 21,K= 10		
2	156	168
4	221	166
H= 22,K= 0		
2	223	240
4	143	134
6	497	434
8	192	165
H= 22,K= 2		
5	143	131
9	215	225
H= 22,K= 4		
0	184	168
4	111	128
H= 22,K= 5		
1	122	95
H= 23,K= 2		
2	204	198
H= 23,K= 4		
3	124	118

The structure was solved by direct methods and refined by full-matrix least squares technique. Methylene hydrogen atom positions were calculated assuming C−H bond lenghts of 1.0 Å. 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

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

were C_T is the total number of counts and C_N the net count (peak minus background). The conventional R-value arrived at was 7.2 % (weighted value $R_w = 7.7$ %) for 3471 observed reflections. The form factors used were those of Hanson *et al.*[6] except for hydrogen.[7] Final fractional coordinates and thermal vibration parameters are given in Table 1. The expression for anisotropic vibration is:

$$\exp - (B11h^2 + B22k^2 + B33l^2 + B12hk + B13hl + B23kl)$$

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

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 square amplitudes range from about 0.20 Å for carbonyl carbons to about 0.30 Å for methyl carbon atoms and water oxygens. Due to the size of the molecule, no rigid-body analysis of translational and librational motion has been carried out.

Interatomic distances, bond angles, and dihedral angles are given in Table 3. The standard deviations, given in parentheses, are estimated from the correlation matrix of the last least squares refinement cycle. Fig. 1 shows the molecule viewed along [001].

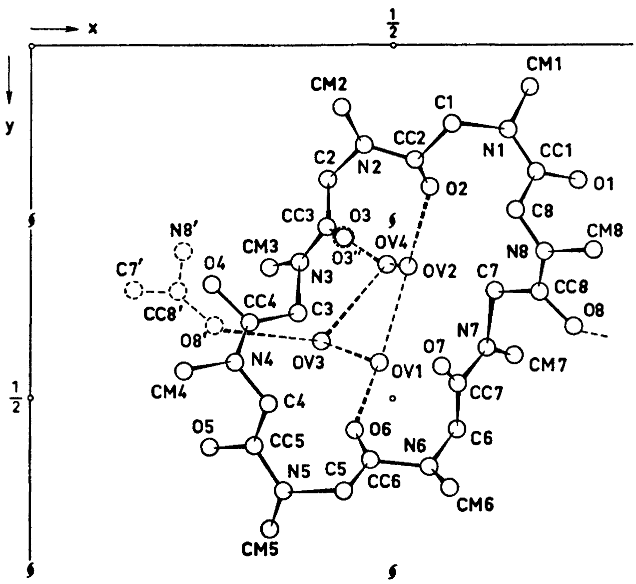

Fig. 1. The molecule viewed along [001].

By averaging bond distances of Table 3, and comparing with the results of the corresponding dimeric [4] and tetrameric [5] compounds, no significant differences are observed:

Distance	Cyclodisarcosyl	Cyclotetrasarcosyl	Cyclooctasarcosyl
CC–CM	1.506 Å	1.531 Å	1.527 Å
CC–N	1.348 Å	1.358 Å	1.344 Å
CC–O	1.234 Å	1.225 Å	1.228 Å
C–N	1.455 Å	1.458 Å	1.456 Å
CM–N	1.475 Å	1.467 Å	1.483 Å

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

DISTANCE	(Å)	DISTANCE	(Å)	DISTANCE	(Å)
O1 - CC1	1,227(5)	O2 - CC2	1,234(5)	O3 - CC3	1,231(5)
O4 - CC4	1,222(5)	O5 - CC5	1,219(5)	O6 - CC6	1,233(5)
O7 - CC7	1,227(5)	O8 - CC8	1,230(5)	N1 - CM1	1,488(6)
N2 - CM2	1,479(6)	N3 - CM3	1,480(6)	N4 - CM4	1,483(6)
N5 - CM5	1,481(6)	N6 - CM6	1,487(6)	N7 - CM7	1,487(6)
N8 - CM8	1,482(6)	N1 - C1	1,454(6)	N2 - C2	1,462(6)
N3 - C3	1,464(6)	N4 - C4	1,448(6)	N5 - C5	1,451(6)
N6 - C6	1,466(6)	N7 - C7	1,452(6)	N8 - C8	1,447(6)
N1 - CC1	1,352(6)	N2 - CC2	1,352(6)	N3 - CC3	1,339(6)
N4 - CC4	1,340(6)	N5 - CC5	1,350(6)	N6 - CC6	1,338(6)
N7 - CC7	1,345(6)	N8 - CC8	1,338(6)	C1 - CC2	1,519(7)
C2 - CC3	1,520(7)	C3 - CC4	1,536(7)	C4 - CC5	1,531(7)
C5 - CC6	1,520(7)	C6 - CC7	1,526(7)	C7 - CC8	1,529(7)
C8 - CC1	1,531(7)	OV1 - OV2,	2,787(6)	OV1 - OV3	2,743(6)
OV2 - O2′	2,814(5)	OV3 - O8′	2,868(6)	OV2 - OV4	2,928(7)
OV4 - O3″	2,883(6)	O6 - OV1	2,791(5)	OV3 - OV4	2,864(6)

ANGLE	(°)	ANGLE	(°)
O1 - CC1 - N1	121,94(46)	O2 - CC2 - N2	121,79(46)
O3 - CC3 - N3	122,55(47)	O4 - CC4 - N4	121,90(48)
O5 - CC5 - N5	122,93(46)	O6 - CC6 - N6	121,99(45)
O7 - CC7 - N7	121,72(47)	O8 - CC8 - N8	121,76(46)
O1 - CC1 - C8	120,64(46)	O2 - CC2 - C1	121,26(43)
O3 - CC3 - C2	120,92(48)	O4 - CC4 - C3	120,86(46)
O5 - CC5 - C4	120,71(45)	O6 - CC6 - C5	120,02(43)
O7 - CC7 - C6	121,16(47)	O8 - CC8 - C7	120,51(45)
CM1 - N1 - C1	116,87(41)	CM2 - N2 - C2	118,99(43)
CM3 - N3 - C3	116,31(43)	CM4 - N4 - C4	116,60(44)
CM5 - N5 - C5	116,20(41)	CM6 - N6 - C6	118,08(41)
CM7 - N7 - C7	118,09(43)	CM8 - N8 - C8	117,33(43)
CM1 - N1 - CC1	119,15(39)	CM2 - N2 - CC2	123,68(43)
CM3 - N3 - CC3	124,64(43)	CM4 - N4 - CC4	118,37(43)
CM5 - N5 - CC5	119,10(42)	CM6 - N6 - CC6	122,83(43)
CM7 - N7 - CC7	124,27(42)	CM8 - N8 - CC8	118,20(42)
C8 - CC1 - N1	117,36(42)	C1 - CC2 - N2	116,88(44)
C2 - CC3 - N3	116,53(44)	C3 - CC4 - N4	117,24(45)
C4 - CC5 - N5	116,23(43)	C5 - CC6 - N6	117,98(44)
C6 - CC7 - N7	117,11(43)	C7 - CC8 - N8	117,73(44)
CC1 - N1 - C1	123,60(42)	CC2 - N2 - C2	116,76(44)
CC3 - N3 - C3	118,82(43)	CC4 - N4 - C4	125,03(45)
CC5 - N5 - C5	122,72(42)	CC6 - N6 - C6	116,57(42)
CC7 - N7 - C7	116,92(44)	CC8 - N8 - C8	123,79(44)
N1 - C1 - CC2	112,19(42)	N2 - C2 - CC3	111,06(43)
N3 - C3 - CC4	110,61(44)	N4 - C4 - CC5	112,44(44)
N5 - C5 - CC6	112,36(44)	N6 - C6 - CC7	110,38(42)
N7 - C7 - CC8	110,80(44)	N8 - C8 - CC1	111,86(44)
CC2 - O2 - OV2	149,97(33)	O2 - OV2 - OV1,	132,15(22)
OV2 - OV1 - OV3	85,23(18)	OV1 - OV3 - O8′	115,40(19)
OV2 - OV4 - O3″	148,08(22)	OV4 - O3 - CC3	144,55(36)
OV4 - OV2 - O2	134,41(22)	OV4 - OV2 - OV1	91,60(17)
O6 - OV1 - OV2,	141,19(20)	O6 - OV1 - OV3,	127,46(19)
OV4 - OV3 - O8′	121,82(19)	OV3 - OV4 - O3″	111,78(18)
OV1 - OV3 - OV4	93,75(17)	OV3 - OV4 - OV2	80,68(16)

DIHEDRAL ANGLE	(°)	DIHEDRAL ANGLE	(°)
CC1 - N1 - C1 - CC2	-77,50(60)	N1 - C1 - CC2 - N2	-167,51(43)
C1 - CC2 - N2 - C2	-169,68(44)	CC2 - N2 - C2 - CC3	70,99(61)
N2 - C2 - CC3 - N3	-167,69(44)	C2 - CC3 - N3 - C3	-178,20(46)
CC3 - N3 - C3 - CC4	93,10(57)	N3 - C3 - CC4 - N4	-179,39(43)
C3 - CC4 - N4 - C4	-1,00(75)	CC4 - N4 - C4 - CC5	-106,89(56)
N4 - C4 - CC5 - N5	179,76(43)	C4 - CC5 - N5 - C5	-15,88(69)
CC5 - N5 - C5 - CC6	-72,30(63)	N5 - C5 - CC6 - N6	-167,04(43)
C5 - CC6 - N6 - C6	-171,72(45)	CC6 - N6 - C6 - CC7	77,63(55)
N6 - C6 - CC7 - N7	-173,03(41)	C6 - CC7 - N7 - C7	-173,94(43)
CC7 - N7 - C7 - CC8	83,07(57)	N7 - C7 - CC8 - N8	-172,52(44)
C7 - CC8 - N8 - C8	-5,60(73)	CC8 - N8 - C8 - CC1	-91,88(58)
N8 - C8 - CC1 - N1	-173,36(42)	C8 - CC1 - N1 - C1	-9,08(67)

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

Angle	Cyclotetrasarcosyl	Cyclooctasarcosyl
(CM – N – CC)*cis*	119.8°	118.7°
(CM – N – CC)*trans*	124.3°	123.9°
(C – N – CC)*cis*	123.9°	123.8°
(C – N – CC)*trans*	120.1°	117.2°

The corresponding angles in cyclodisarcosyl, where the amide group has the *cis* conformation, are 119.7° and 124.6°, respectively.

As may be seen from Fig. 1, the ring has an open conformation with the inner volume filled by a cluster of four water molecules which participate in a network of inter- as well as intra-molecular hydrogen bond bridges. The four water oxygens are situated at the corners of a somewhat distorted square with OV – OV – OV angles of about 81°, 91°, 85°, and 93°, and OV···OV bondlengths ranging from 2.743 Å to 2.920 Å. The two OV···O bond distances of the intramolecular hydrogen-bond bridge are 2.791 Å and 2.814 Å, respectively. The OV···O distances of the two inter-molecular bridges, linking different symmetry related molecules, are somewhat longer: OV3···O8′ = 2.868 Å, OV4···O3″ = 2.883 Å. The OV – OV – O angles are distributed over a wide range (from 112° to 150°).

There are no direct transannular interactions to be held responsible, as originally thought,[1] for the rigity of this rather large ring. Since, from IR-spectra, it can be stated that the same conformation persists in $CHCl_3$ solution, where no water molecules are present to form transannular bridges, the explanation must be sought in the intrinsic conformation of the peptide chain itself.[8]

Fig. 1 clearly shows that the ring conformation is *cis,cis,trans,trans,cis, cis,trans,trans*. It might also be seen that each of the four pairs of diametrically placed amino-acid residues is related by an approximate two fold axis of symmetry.

Apart from the hydrogen bonds, no short intermolecular distances are observed.

Acknowledgment. The author would like to thank cand. real. K. Titlestad for preparing the crystals.

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Received June 5, 1973.