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Studies on Benzodiazepinooxazoles. II.[1] Crystal and Molecular Structure of 10-Bromo-2,3,5,6,7,11b-hexahydro-2-methyl-11b-phenylbenzo[6,7]-1,4-diazepino[5,4-*b*]oxazol-6-one, $C_{18}H_{17}O_2N_2Br \cdot C_2H_5OH$

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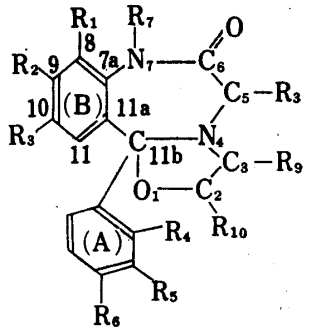
The crystal structure of 10-bromo-2,3,5,6,7,11b-hexahydro-2-methyl-11b-phenylbenzo-[6,7]-1,4-diazepino[5,4-*b*]oxazol-6-one, $C_{18}H_{17}O_2N_2Br \cdot C_2H_5OH$, has been determined by the three dimensional Patterson method. This substance occurs as monoclinic crystals, space group $P2_1/c$, with $Z=4$ in the unit cell dimensions $a=16.34$, $b=8.88$, $c=13.89$ Å, and $\beta=102°$. The block-diagonal least-squares refinements using 2780 reflections gave the final $R=11.3\%$. The methyl and phenyl ring substituents are trans with respect to the plane of the oxazole ring.

Introduction

In the preceding paper,[1] the authors reported the synthesis and the pharmacology activity of benzo[6,7]-1,4-diazepino [5,4-*b*]oxazole derivatives and their analogues.

In these derivatives, compounds having substituents at 2- or 3-position can exist as two configurational isomers. The nuclear magnetic resonance (NMR) spectrum of 10-bromo-2,3,5,6,7,11b-hexahydro-2-methyl-11b-phenylbenzo-[6,7]-1,4-diazepino[5,4-*b*]oxazol-6-one ($R_1=R_2=R_4=R_5=R_6=R_7=R_8=R_9=H$, $R_3=Br$ and $R_{10}=CH_3$) in deuteriochloroform showed two pairs of methyl protons at 1.25 ($J=6.5$ Hz) and 1.38 ppm ($J=6.5$ Hz) and two kinds of amino-protons at 8.32 and 8.53 ppm suggesting the existence of such isomers. After the compound was recrystallized from aqueous ethanol, the NMR spectrum of the crystals showed that the only one of the crystalline isomers had separated. Such crystals would be suitable for determining its structure and stereochemistry. The compound was labile in solution and a peak assigned to amino-proton splitted to the above values within a few minutes.



Experimental

We have succeeded in obtaining crystals which belong to the monoclinic system by slow evaporation from 70% aqueous ethanol in the form of needles elongated along the c-axis. The crystals consisted of only one component isomer at the NMR level. The cell constants are determined by Weissenberg and oscillation photographs: $a=16.34$, $b=8.88$, $c=13.89$ Å, and $\beta=102.0°$. From the systematic absence of reflection, the space group was determined to be $P2_1/c$. Intensity data are collected by an equi-inclination Weissenberg technique for the reflections of hk0 to hk11. After several days under the X-ray beam the crystal turned opaque so that two crystals were used to take a total of 2780 independent reflections. They

1) This paper forms part II of a Series entitled "Anxiolytic Sedative". For previous paper, see Ref. 1. Part I: T. Miyadera, A. Terada, M. Fukunaga, Y. Kawano, T. Kamioka, C. Tamura, H. Takagi and R. Tachikawa, *J. Med. Chem.*, **14**, 520 (1791).

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were estimated by visual comparison of the calibrated standard film. Two sets of five multiple film were exposed until $l=4$, and one set of five for over $l=5$. The observed density was 1.452 g cm^{-3} measured by floatation method while the calculated value was 1.451 g cm^{-3} which was obtained by taking into account that four molecules of $C_{18}H_{17}O_2N_2Br \cdot C_2H_5OH$ are contained in the unit cell dimensions. Lorentz and Polarization corrections were calculated but no absorption correction was made because of the small size of the crystals.

Structure Analysis

The structure was determined by the three dimensional heavy atom method, using Sim's weighting scheme.[3] The position of the bromine atom was readily obtained on the basis of the $P2_1/c$ vector sets in the crystal. The first Fourier synthesis were calculated with phases derived from the contribution of the bromine atom alone (R=46.9%). The 22 peaks in the electron density map were corresponded to the proposed structure. The values of the temperature parameters in the early stages of structure factor calculation were used 3.5 for bromine and 4.0 for all light atoms. The whole atomic coordinates of the molecule were determined in the next cycle of Fourier calculation and refined by means of block diagonal least squares procedures. After 6 cycles of refinements with isotropic temperature parameters for whole atoms the R-factor reduced to 15%. At this stage the molecule of ethanol which is contained as the solvent of crystallization came out in the vacant areas of the molecular packing in the electron density map. In order to find out the positions of hydrogen atoms, the difference Fourier synthesis was computed. All hydrogen atoms were obtained around the expected positions.

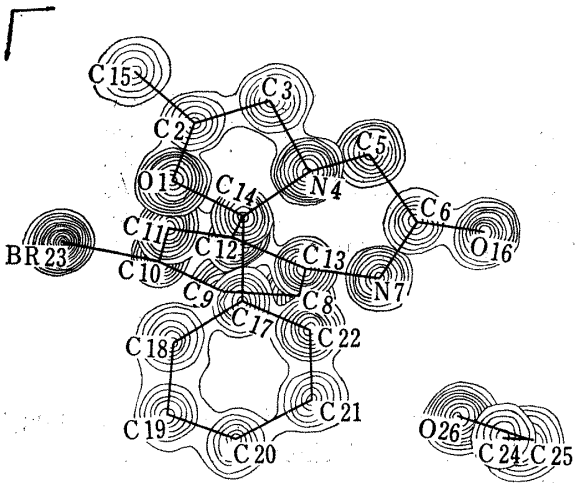


Fig. 1. The Final Electron Density Map Projected on the (010) Plane, Contours are Arbitary in Equal Intervals except Bromine Atom

By two more cycles of the block diagonal least squares refinements with anisotropic thermal parameters for bromine the R-factor decreased to 12.4%, further refinements with anisotropic thermal parameters for all atoms except hydrogen reduced the R to 11.3%. The final Fourier map and the molecular packing diagram viewed along the b-axis are shown in Fig. 1 and 3, and the bond distances and angles are shown in Fig. 2. The least squares planes for two benzene, oxazole, and diazepine ring systems are calculated as Fig. 4 which show the deviations of atomic coordinates from these planes. The final parameters of the atomic positions and the temperature factors are listed in Table I, and their standard deviations in Table II. The final values of Fo-Fc are shown in Table III.

All computations have been carried out with the CDC 3600 system at C. Itoh Electornic Computing Service Co., Ltd. using the set of programs registered as UNICS.

Result and Discussion

The C15 methyl and C17 phenyl groups which are attached to the oxazole ring deviate 0.30 and −1.44 Å respectively from the five membered ring least squares plane. Therefore, the stereo-chemistry of the substituents on the oxazole ring is determined as *trans* for the methyl group and the benzene ring B. The planarity calculation of the C3, N4, C5 and C14, shows that the lone pair of the N4 atom is directed towards the same side of the C17 phenyl group that is the lone pair of nitrogen and phenyl group are *cis*. The least squares plane in the seven membered ring is constructed with four atoms of C14, N4, C6 and N7. The C12, C13 and C5 atoms in this ring deviate +0.88, +0.81 and +0.75 Å from this least squares plane respectively. The deviations of all plus sings indicate that the ring system takes a boat form, this is a common feature found in the compounds containing unsaturated seven membered rings, *e.g.*, fulvane,[4]

3) G.A. Sim, *Acta Cryst.*, **11**, 123 (1958).
4) R.E. Davio and A. Tulinsky, *J. Am. Chem. Soc.*, **88**, 4583 (1966); H. Shimanouchi, T. Hata and Y. Sasada, *Tetrahedron Letters*, **1968**, 3573.

TABLE I. Fractional Atomic Coordinates and Anisotropic Thermal Parameter. Anisotropic Temperature Factor: $T=\exp[-(B11h^2+B22k^2+B33l^2+B12hk+B13hl+B23kl)]$ Each Thermal Parameter is multiplied by 10^4

Atom	X	Y	Z	B11	B22	B33	B12	B13	B23
O 1	.1412	.8894	.0525	19	55	15	0	0	14
C 2	.1561	1.0118	-.0110	34	86	36	3	-3	22
C 3	.2347	.9687	-.0411	26	81	21	0	2	12
N 4	.2830	.8990	.0529	20	52	8	-4	4	2
C 5	.3432	.7885	.0308	24	70	18	0	7	1
C 6	.4033	.7513	.1296	14	55	18	1	6	0
N 7	.3723	.6662	.1964	19	55	18	0	2	3
C 8	.2877	.4474	.2075	23	52	21	0	5	2
C 9	.2118	.3732	.1898	21	57	31	-2	3	-2
C10	.1422	.4504	.1427	18	65	17	-12	3	2
C11	.1442	.6033	.1152	16	58	11	-5	1	1
C12	.2202	.6792	.1326	21	44	12	-4	3	0
C13	.2926	.5986	.1776	15	57	7	-2	3	-4
C14	.2208	.8501	.1118	17	50	14	2	6	4
C15	.0811	1.0371	-.0956	30	142	42	3	0	25
O16	.4765	.7941	.1473	19	75	41	-3	4	10
C17	.2331	.9337	.2139	23	44	13	2	2	2
C18	.1675	.9422	.2659	31	74	31	-4	11	-2
C19	.1765	1.0170	.3570	37	102	36	2	15	-5
C20	.2526	1.0824	.3990	48	88	21	9	3	-7
C21	.3190	1.0764	.3487	35	60	26	4	-2	-2
C22	.3091	1.0031	.2571	24	69	18	3	1	-3
BR23	.0376	.3457	.1163	26	91	51	-29	-3	5
C24	.5253	.8476	.4091	36	108	45	-2	12	5
C25	.5509	.6844	.4192	28	99	48	4	7	-12
O26	.4806	.5906	.3836	22	69	32	3	1	0

TABLE II. Estimated Standard Deviations of the Fractional (Å) and Thermal Parameters. Each Thermal Parameter is multiplied by 10^4

Atom	X	Y	Z	B11	B22	B33	B12	B13	B23
O 1	.0061	.0057	.0065	2	7	4	3	2	3
O 2	.0111	.0104	.0119	4	13	8	6	4	7
O 3	.0100	.0095	.0105	3	11	7	5	3	6
N 4	.0073	.0068	.0076	2	8	5	3	2	4
O 5	.0095	.0090	.0102	3	11	6	4	3	6
O 6	.0083	.0080	.0098	3	9	6	4	3	5
N 7	.0074	.0070	.0081	2	8	5	3	2	5
O 8	.0092	.0084	.0101	3	10	6	4	3	5
O 9	.0094	.0086	.0107	3	10	7	4	3	6
O10	.0086	.0084	.0096	3	10	6	4	3	5
O11	.0084	.0081	.0092	3	9	6	4	3	5
O12	.0086	.0079	.0092	3	9	6	4	3	5
O13	.0082	.0079	.0090	3	9	5	4	3	5
O14	.0082	.0080	.0091	3	9	6	4	3	5
O15	.0119	.0125	.0132	4	17	9	7	4	9
O16	.0066	.0066	.0076	2	8	5	3	2	4
O17	.0090	.0079	.0094	3	9	6	4	3	5
O18	.0106	.0097	.0114	4	11	7	5	4	6
O19	.0119	.0111	.0125	4	14	7	5	4	8
O20	.0125	.0108	.0118	5	13	7	6	4	7
O21	.0109	.0093	.0110	4	11	7	5	4	6
O22	.0094	.0089	.0101	3	10	6	4	3	6
BR23	.0011	.0011	.0013	0	1	0	0	0	0
O24	.0125	.0117	.0134	5	15	9	6	4	8
O25	.0114	.0111	.0130	4	14	8	6	4	8
O26	.0066	.0066	.0073	2	8	5	3	2	4

TABLE III. Observed and Calculated Structure Factors (×10)

H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC
K=L= 1 0			0	381	401	-14	240	187	13	305	309	-8	392	39	1	597	-692	2	209	-199	-2	897	-889
1	602	667	1	521	538	15	347	322	14	250	224	-9	321	3 1	2	1110	-1428	3	378	-351	-3	267	219
2	608	-720	2	575	590	17	88	60	15	71	75	-10	201	191	3	749	-801	4	173	149	-4	349	-343
3	503	-603	3	362	351	19	130	-139	K=L= 8 1			-11	391	361	4	521	-526	5	178	162	-5	334	-348
1	602	667	4	214	239	20	145	-178	1	206	209	-12	208	189	5	601	-544	6	68	61	-6	82	-22
2	608	-720	5	387	425	K=L= 2 1			2	423	434	-13	288	295	6	453	-344	7	394	4365	-7	264	269
3	503	-606	7	405	-394	2	720	773	3	278	285	-14	108	119	8	422	366	8	112	90	-8	298	-291
4	809	-905	8	276	-286	3	171	138	4	389	361	-16	88	-72	9	215	169	9	192	191	-10	129	-124
5	908	-1164	9	77	-75	4	1041	1113	5	273	248	-17	141	-145	10	625	585	10	343	345	-12	141	145
6	704	-847	10	315	-436	5	1040	1164	6	378	393	-19	209	-219	11	195	174	11	309	285	-13	318	337
1	602	667	11	249	-253	6	503	453	7	298	272	K=L= 5 1			12	488	397	12	269	225	-14	244	258
2	608	-720	12	401	-422	7	642	606	8	157	139	-1	149	-167	13	443	421	13	221	185	-15	73	-54
3	503	-606	13	224	-232	8	275	246	10	164	130	-2	198	-178	14	285	310	14	74	64	-16	130	133
4	809	-903	14	296	-285	9	653	567	11	109	-112	-3	123	79	15	379	426	K=L= 8 2			-18	204	148
5	908	-1164	15	292	-315	12	410	-345	12	201	-192	-4	171	-174	16	227	194	1	69	51	K=L= 4 2		
6	704	-847	16	77	-74	13	257	-194	13	194	-178	-6	268	-261	17	174	149	2	69	-45	0	197	-211
7	801	-981	17	116	-138	14	302	-393	K=L= 9 1			-7	382	3 9	18	139	111	3	124	-113	-1	668	-634
8	707	-873	K=L= 7 0			15	137	-119	2	102	149	-8	53	-2	K=L= 2 2			4	71	-83	-2	781	-814
9	202	-234	1	223	-224	16	555	-473	3	111	-78	-9	216	2 8	1	746	937	5	51	43	-3	162	-159
10	559	-456	2	237	-226	17	273	-222	4	226	-196	-10	134	-12	2	212	136	6	129	26	-4	482	-442
11	84	-56	3	387	-446	18	254	-213	5	187	-155	-11	298	325	3	219	199	7	136	108	-5	164	-127
12	517	-402	4	246	-277	19	204	-178	7	208	-164	-12	206	184	4	108	-89	9	127	-110	-6	670	-617
15	444	407	5	146	-128	K=L= 3 1			8	195	177	-13	230	214	5	982	891	10	229	-221	-7	755	-814
16	84	63	6	263	270	1	196	341	9	299	-296	-15	183	144	6	331	298	11	172	-133	-8	482	-489
17	196	158	7	286	-315	2	224	414	10	184	-172	K=L= 6 1			7	390	364	12	87	-71	-9	254	-265
18	248	244	8	416	-524	3	283	264	11	238	-242	0	50	-14	8	132	136	13	133	-119	-10	445	-393
19	283	231	9	102	-86	4	126	34	12	119	-140	-1	180	-179	9	144	101	K=L= 9 2			-11	285	-191
20	87	103	10	104	99	5	82	28	K=L= 10 1			-2	88	83	10	117	-73	1	175	-155	-12	82	-76
K=L= 2 0			12	139	132	6	903	-910	1	102	-62	-3	73	-51	11	185	151	3	298	-305	-13	199	200
0	619	600	13	206	176	7	858	-749	2	181	-63	-4	193	-13	12	132	-98	4	314	-315	-14	184	-172
1	602	659	14	213	215	8	492	-417	3	123	-57	-5	117	-115	13	262	263	5	181	49	-15	74	-99
2	1114	-1441	K=L= 8 0			9	582	-572	4	148	-128	-6	147	134	14	71	-71	6	119	-103	-17	195	169
3	509	-545	0	85	-45	10	551	-533	5	74	-51	-7	213	219	15	52	-59	7	147	-131	-18	238	209
4	179	-203	1	128	131	11	621	-651	6	70	44	-8	253	257	16	181	-168	8	143	-125	K=L= 5 2		
5	506	-584	2	76	47	12	423	-344	7	100	-61	-9	58	-71	17	210	-176	9	146	-46	0	757	787
6	239	282	3	79	49	13	275	-225	9	118	131	-10	137	122	18	147	-121	10	93	127	-1	454	507
7	713	576	4	98	-81	14	870	-329	K=L= 11 1			-11	248	29	K=L= 3 2			11	148	135	-2	971	1176
9	113	-67	5	143	134	15	197	-122	2	148	125	-12	280	253	1	504	403	K=L= 10 2			-3	494	507
10	141	130	6	159	128	18	154	121	K=L= 1 1			-13	139	147	2	856	-929	1	117	76	-4	238	206
11	120	140	7	188	219	19	195	145	-1	359	-350	-14	228	234	3	168	195	3	90	91	-5	148	104
12	415	349	8	92	60	K=L= 4 1			-2	444	-464	-15	168	173	4	346	-324	5	254	236	-6	72	31
13	398	370	10	185	178	1	173	134	-3	1043	-1359	-16	150	143	5	339	-284	6	257	333	-7	126	-124
14	247	200	13	76	-51	2	850	-924	-4	602	-592	-17	112	124	6	581	-529	7	206	230	-8	488	-353
15	90	-85	K=L= 9 0			3	686	-741	-5	762	-857	K=L= 7 1			7	323	237	8	179	233	-9	413	-369
16	106	151	1	168	-138	4	878	-949	-6	509	-508	0	382	-382	8	78	-48	9	94	129	-10	220	-209
18	82	-56	2	204	-177	6	742	-663	-7	253	-260	-1	248	-249	9	111	59	K=L= 11 2			-11	431	-405
19	87	-84	3	106	-99	7	332	-273	-8	95	-73	-2	506	-595	10	141	-113	1	268	327	-12	274	-278
K=L= 3 0			4	117	-104	9	92	21	-9	217	-219	-3	436	-429	11	259	242	2	184	236	-13	345	-366
2	440	361	5	131	-131	10	96	57	-10	97	52	-4	390	-374	14	134	101	3	54	37	-14	493	-494
3	368	-333	6	91	-75	11	244	237	-11	242	-184	-5	394	-373	15	101	80	4	42	47	-15	168	-157
4	493	-391	7	327	-337	12	144	116	-12	208	192	-6	458	-517	16	333	291	K=L= 3 2			-16	187	-189
5	195	-138	8	137	-147	14	244	260	-13	435	492	-7	101	-1 5	K=L= 4 2			-2	746	871	-17	131	-142
6	489	-444	9	236	-249	14	381	459	-14	347	364	-9	214	-237	1	590	555	-3	656	591	-18	144	-133
7	212	-175	12	168	-108	15	89	56	-17	178	180	-12	137	1 5	2	635	606	-4	141	106	K=L= 6 2		
9	85	36	K=L= 10 0			16	246	219	-18	284	215	-13	130	127	3	197	166	-5	957	846	0	115	79
10	243	-211	0	181	-164	17	192	161	-19	195	119	-14	217	219	4	361	288	-6	659	608	-1	274	240
11	193	-120	1	284	-283	18	204	203	K=L= 7 1			-15	174	175	5	690	619	-7	993	975	-2	168	128
12	241	-193	2	235	-215	K=L= 5 1			-1	183	193	-16	179	225	6	475	439	-8	1083	1072	-3	203	202
14	80	74	3	178	-197	1	221	-184	-2	196	210	K=L= 8 1			7	251	251	-9	1064	989	-4	475	495
16	101	-143	4	145	-124	2	156	89	-3	85	-79	0	357	359	8	556	515	-10	201	204	-5	698	784
19	81	84	5	297	-300	3	45	15	-4	145	172	-1	289	284	9	526	481	-11	596	586	-6	477	552
K=L= 4 0			6	118	98	4	171	123	-5	458	-479	-4	85	63	10	322	351	-12	62	-45	-7	459	534
0	1134	-1103	7	137	101	5	115	85	-6	258	-320	-5	309	-329	11	285	309	-13	548	-595	-8	138	-123
1	596	-583	9	46	52	6	420	394	-7	717	-778	-6	287	-304	12	256	233	-15	344	346	-9	415	468
2	469	-420	K=L= 11 0			7	275	-220	-8	478	-609	-7	156	-157	13	140	-120	K=L= 1 2			-10	147	142
3	290	-300	2	75	76	8	198	82	-9	801	-860	-8	367	-370	14	222	234	-1	848	-1079	-11	148	145
4	684	-672	3	132	122	9	279	247	-10	503	-578	-9	248	-284	16	82	-55	-2	1082	-1710	-14	150	-143
5	103	-143	4	234	275	10	81	58	-13	302	-408	-10	367	-377	17	124	-115	-3	82	-61	-15	262	-260
6	171	-135	K=L= 3 0			11	101	-115	-15	245	-230	-11	297	-343	K=L= 5 2			-4	969	-930	-16	251	-293
8	192	-164	2	422	-382	12	188	166	-16	178	-160	-12	164	-163	1	590	519	-5	239	188	-17	97	-100
9	196	131	3	407	-347	14	89	-59	-18	127	135	-13	93	-102	2	599	537	-6	156	-140	K=L= 7 2		
10	247	256	4	975	1023	15	185	-157	-19	85	58	-14	100	-125	3	666	671	-8	545	494	0	375	-388
11	297	330	5	185	-75	16	76	-66	K=L= 3 1			K=L= 9 1			4	685	645	-9	286	414	-1	108	-128
12	578	610	6	615	678	17	171	-163	0	642	735	0	330	359	5	280	291	-10	363	310	-3	81	-42
13	294	284	7	77	-36	18	104	-111	-1	1178	1306	-1	236	219	6	100	42	-11	414	330	-5	67	36
14	63	50	8	53	29	K=L= 6 1			-2	693	809	-2	170	131	8	280	-264	-12	439	409	-6	112	88
15	245	222	9	608	-580	1	293	-273	-3	692	819	-3	258	284	9	246	-190	-13	559	597	-7	247	-266
16	283	269	10	657	-608	2	296	-285	-4	748	914	-4	258	264	10	267	-241	-14	528	543	-8	150	161
17	253	277	11	856	-879	3	380	-332	-5	544	594	-5	89	58	11	232	-191	-15	198	173	-9	373	407
18	114	130	12	794	-718	4	256	-239	-6	728	758	-6	142	154	12	207	-159	K=L= 2 2			-10	223	244
K=L= 5 0			14	197	-184	5	556	-548	-7	245	292	-7	135	131	13	511	-447	0	376	-344	-11	224	278
1	91	-76	15	407	-389	6	195	-144	-8	340	345	-8	151	122	14	571	-514	-1	524	-540	-12	168	186
2	109	163	16	638	-588	7	80	-84	-9	85	-45	-9	78	-75	15	264	-242	-2	297	297	-13	86	67
3	502	504	17	161	-153	8	283	-171	-11	148	-143	-10	192	-199	16	253	-238	-3	846	-1033	-14	62	59
4	294	252	18	211	-178	9	247	-256	-12	247	-220	-11	78	-85	17	120	-119	-4	120	65	-16	77	89
5	803	914	19	104	-83	10	191	-135	-13	244	-210	-12	153	-169	K=L= 6 2			-5	307	-332	K=L= 8 2		
6	615	668	20	63	-54	11	88	-94	-14	241	-230	K=L= 10 1			2	94	-52	-6	719	-785	0	120	145
7	603	677	K=L= 1 1			13	156	118	-15	457	-507	0	83	62	3	411	-439	-7	589	-575	-1	102	81
8	411	417	1	479	-522	17	179	198	-16	382	-383	-1	128	-149	4	234	-220	-8	592	588	-2	127	-105
9	475	496	3	72	-55	K=L= 7 1			-17	255	-243	-3	88	78	5	600	-613	-9	277	-279	-3	135	-104
10	314	353	4	379	297	2	404	-413	-18	313	-308	-4	122	130	6	524	-577	-11	162	-124	-6	90	77
11	234	250	5	276	187	4	286	-166	-19	77	-90	-5	94	90	7	493	-528	-12	228	177	-7	90	78
12	143	122	6	89	109	5	243	224	K=L= 4 1			-6	72	54	9	335	-414	-13	201	-182	-8	254	258
13	267	280	7	97	92	6	241	215	0	277	-249	-7	178	37	10	282	-298	-14	206	173	-9	101	-81
14	183	-147	8	554	496	7	334	340	-1	353	-300	-8	122	151	11	271	-270	-15	183	148	-10	102	84
15	174	-142	9	549	503	8	142	148	-2	384	-361	K=L= 11 1			12	74	29	-16	187	178	-11	139	131
16	243	-246	10	134	148	9	367	409	-3	368	312	0	57	38	15	134	129	-17	98	73	-12	158	189
17	245	-245	11	615	529	10	289	268	-5	435	414	-2	106	116	16	134	121	K=L= 3 2			-13	195	232
18	94	-102	12	438	418	11	178	166	-6	282	268	-4	99	127	K=L= 7 2			0	158	-91	-14	82	108
K=L= 6 0			13	178	89	12	321	273	-7	546	614	K=L= 1 2			1	365	-359	-1	295	257	K=L= 9 2		

TABLE III. (Continued)

H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC
0	267	-299	2	201	178	-2	88	-14	-6	100	97	12	279	-274	-16	154	-143	-4	78	-69	2	81	-73
-1	201	-283	3	322	-284	-3	373	-354	-8	74	94	13	184	-182	-17	153	155	-5	238	-206	3	326	309
-3	122	-115	4	331	267	-4	407	399	-10	53	21	14	102	105	K,L=	3	4	-6	189	-181	4	362	383
-4	104	-165	5	383	336	-5	298	328	K,L=	11	3	16	88	105	-1	233	-207	-7	303	-284	5	522	578
-5	129	-120	7	408	-363	-6	627	719	-2	98	-84	K,L=	6	4	-2	266	-221	-8	177	-169	6	169	149
-6	193	-156	8	202	164	-7	765	874	K,L=	0	4	0	317	-321	-3	426	-398	-9	166	-194	8	98	-68
-11	143	108	9	146	-150	-8	505	628	8	322	-299	1	617	-668	-4	93	-100	-11	215	-229	9	231	198
-12	197	214	10	84	-100	-9	497	459	9	237	218	2	383	-379	-5	375	-342	-12	117	-137	10	205	162
K,L=	10	2	11	88	-75	-10	418	437	10	95	108	3	211	-210	-6	326	-340	K,L=	10	4	11	215	289
0	95	101	13	226	-229	-11	438	491	11	646	738	4	388	-405	-7	309	307	-1	349	334	12	201	159
-1	106	-62	14	125	-128	-12	475	597	12	343	368	5	583	-622	-8	236	-190	-2	118	146	15	44	-49
-2	172	-153	15	185	-168	-13	358	396	13	308	327	6	72	48	-9	313	-288	-3	202	226	K,L=	7	5
-3	208	-207	K,L=	6	3	-14	121	-141	14	435	499	7	176	108	-10	230	-228	-6	105	-59	0	317	285
-4	177	-189	0	413	-418	-16	91	174	15	219	204	8	279	195	-11	119	4	K,L=	1	5	1	286	299
-5	193	-221	1	330	-381	K,L=	4	3	16	209	244	10	251	215	-13	222	-234	0	262	235	2	473	529
-6	267	-290	3	109	-116	-1	82	37	17	204	304	11	138	132	-14	75	66	1	222	255	4	87	-83
-7	87	-99	4	240	-205	-2	391	-475	18	192	235	12	367	353	-15	153	174	2	81	-29	5	247	-225
-8	91	-120	6	451	422	-3	394	-439	K,L=	1	4	13	259	259	-16	79	-91	3	157	-92	6	158	119
-9	109	-234	7	144	-131	-4	612	-628	0	298	-278	14	189	185	-17	110	-84	4	139	-87	8	262	-215
-10	147	-245	8	147	-147	-5	608	-648	1	621	637	16	92	262	K,L=	4	4	5	408	362	9	322	-303
K,L=	11	2	10	285	302	-6	284	-284	2	381	-368	K,L=	7	4	-1	387	403	6	274	234	10	267	-232
0	108	192	11	129	139	-8	318	-285	3	482	428	0	292	-298	-2	52	6	7	98	-118	11	252	-262
-2	176	199	12	330	322	-9	287	188	4	733	709	1	125	100	-3	238	211	8	308	-287	12	184	-173
-3	53	55	13	149	157	-10	284	296	5	347	314	2	141	165	-4	475	505	9	338	-316	13	249	-257
-4	65	84	14	134	160	-11	264	194	6	507	590	3	409	468	-5	56	-50	10	541	-598	K,L=	8	5
-5	85	-80	15	192	205	-12	144	148	7	702	792	4	73	71	-6	485	548	11	416	-477	0	376	-377
K,L=	1	3	16	127	150	-13	147	192	8	630	637	6	191	168	-7	135	-79	14	232	-269	1	253	-274
0*	2326	1812	K,L=	7	3	-14	398	394	9	543	525	7	248	219	-8	284	-263	15	228	-235	2	184	-148
1	831	838	0	336	304	-15	278	274	10	341	348	8	138	118	-9	244	-235	16	116	-109	3	467	-443
3	860	785	1	260	271	-16	274	244	12	414	451	9	138	125	-10	347	-390	17	69	-79	4	232	-213
5	668	539	2	301	296	-18	101	78	14	244	209	10	156	13.	-11	338	-364	K,L=	2	5	6	437	-407
6	869	799	3	161	140	K,L=	5	3	15	139	-129	14	110	-137	-12	200	-198	0	397	250	7	391	-341
7	959	980	4	613	663	-1	274	-280	16	179	-158	K,L=	8	4	-13	196	-166	1	959	-589	8	223	-202
10	75	11	5	462	503	-2	94	-88	17	136	-168	1	150	-135	-14	184	-170	2	718	-758	9	249	-226
11	158	-119	6	171	181	-3	289	284	18	93	-121	2	110	-87	-15	154	-397	3	613	-707	10	99	-69
12	411	-415	7	252	257	-4	487	-458	K,L=	2	4	3	198	-194	-16	386	-259	4	712	-814	11	149	131
13	238	207	8	365	356	-5	177	164	0	704	698	8	202	-168	-17	220	-178	5	769	-959	K,L=	9	5
14	145	91	9	91	95	-6	186	-78	1	344	334	9	122	-105	-18	147	-110	6	383	-373	0	129	-130
15	182	-176	14	177	-198	-7	264	-218	2	263	224	10	86	-65	K,L=	5	4	7	407	-393	1	228	-212
16	274	-276	K,L=	8	3	-8	248	-246	3	45	41	11	114	-117	-1	157	-143	8	423	-410	4	351	-314
17	143	-131	0	370	365	-9	210	167	4	693	633	K,L=	9	4	-2	284	239	9	494	-563	5	251	102
18	173	-173	1	122	104	-10	243	-251	5	641	648	1	79	-78	-3	831	883	10	117	89	6	291	258
19	134	-167	2	154	164	-12	214	211	6	145	-91	2	136	141	-4	459	448	11	234	-208	7	124	178
K,L=	2	3	7	398	-372	-13	155	154	7	83	-42	3	110	79	-5	459	489	14	297	320	8	161	125
0	639	698	8	360	-382	-16	119	106	8	226	-207	4	109	75	-6	467	485	15	224	233	9	160	154
1	699	745	9	239	-218	-17	127	144	9	93	-89	5	129	122	-7	679	627	16	260	289	K,L=	10	5
2	706	542	10	333	-311	K,L=	6	3	11	403	-409	7	204	190	-8	814	891	17	115	167	1	125	108
3	652	558	11	268	-266	-1	186	-184	12	239	-231	9	241	289	-9	166	-153	18	134	250	2	121	89
5	759	-660	12	218	-259	-2	75	50	14	138	-114	10	105	128	-11	477	526	K,L=	3	5	3	116	76
6	331	-262	13	103	-14	-3	76	-103	15	137	-124	K,L=	10	4	-14	243	-227	0	420	-448	7	70	77
7	653	-605	K,L=	9	3	-4	389	-392	16	193	-184	0	214	215	-15	152	-164	1	331	-361	K,L=	1	5
8	197	-158	0	129	-99	-5	583	-618	18	123	121	1	115	121	-16	171	-168	2	491	-484	-1	946	1143
9	930	-656	1	214	-161	-6	445	-532	K,L=	3	4	2	178	177	-17	194	-187	3	479	-477	-2	527	550
10	567	-542	2	409	-433	-7	256	-255	0	327	338	3	291	273	-18	209	-205	4	266	-212	-3	269	253
11	518	-545	3	225	-225	-8	116	96	1	642	577	5	203	213	K,L=	6	4	5	416	363	-4	424	362
12	465	-435	4	174	-167	-10	211	-203	2	140	69	6	70	78	-1	611	-624	6	376	318	-5	489	431
13	546	-560	5	232	-204	-15	225	231	3	239	-238	8	40	-77	-2	298	-296	7	218	226	-6	208	-156
14	89	-79	6	201	-170	-16	124	126	4	92	-110	K,L=	0	4	-3	244	-217	8	531	523	-7	376	389
15	158	-126	8	107	-102	-17	101	118	5	177	94	-2	1629	-1482	-4	352	-352	9	528	527	-8	651	655
16	154	-144	K,L=	10	3	K,L=	7	3	6	237	182	-3	731	703	-6	122	104	10	447	455	-9	303	277
K,L=	3	3	0	80	69	-1	115	119	7	274	248	-4	840	-935	-7	395	398	11	329	327	-10	449	-405
0	517	-518	1	79	-58	-2	408	435	8	303	297	-5	538	-565	-8	265	241	12	384	362	-11	237	-217
2	805	-818	2	78	-71	-3	253	-252	9	119	-60	-6	409	-359	-9	126	96	13	298	289	-12	113	-87
3	1073	-1153	3	107	-30	-4	262	-222	10	150	130	-7	732	989	-10	356	362	14	343	308	-13	387	-418
4	1005	-676	4	191	177	-7	432	-459	11	193	121	-8	470	453	-11	246	238	15	120	127	-14	287	-293
5	953	-905	7	98	101	-8	238	-254	13	246	218	-9	404	473	-12	353	369	16	129	134	K,L=	2	5
6	556	-497	8	68	85	-9	288	-328	14	219	247	-10	478	493	-13	353	359	17	80	-82	-1	177	-144
7	369	-327	K,L=	1	3	-10	272	-271	15	109	95	-11	474	497	-14	193	146	K,L=	4	5	-2	599	-737
8	546	-501	-1	584	584	-11	281	-292	17	82	-93	-12	584	675	-15	208	213	0	657	618	-3	273	307
9	333	-314	-2	1196	-1458	-12	277	-311	K,L=	4	4	-13	340	384	-16	87	87	1	209	212	-4	198	183
10	80	-29	-3	448	-504	-13	165	-186	0	801	837	-14	254	242	K,L=	7	4	2	482	451	-5	169	152
11	82	-32	-4	455	-481	-14	134	-150	1	641	681	K,L=	1	4	-1	179	-150	3	348	313	-6	591	677
12	219	216	-5	383	-340	-15	47	-82	2	542	525	-1	305	309	-2	169	-140	4	746	686	-7	1273	942
13	219	188	-8	202	-222	K,L=	8	3	3	572	562	-2	847	-1023	-3	312	-285	5	196	175	-8	487	608
14	348	314	-9	513	-658	-1	395	424	4	603	569	-3	690	-691	-4	171	-126	6	680	624	-9	511	592
15	310	280	-10	459	-479	-2	483	594	5	107	152	-4	1148	-13	-5	314	-243	7	301	258	-11	477	523
16	338	296	-11	296	-299	-3	239	240	6	130	117	-5	412	-459	-6	172	-117	8	82	51	-10	240	220
17	317	322	-12	134	-103	-4	366	406	8	101	143	-6	542	-681	-7	129	-129	9	84	-76	-12	214	239
18	177	206	-13	282	-303	-5	172	170	9	107	172	-7	458	-482	-8	331	-324	10	86	76	-13	355	366
K,L=	4	3	-15	148	-143	-6	127	123	10	242	-202	-8	582	-621	-9	157	-146	11	128	78	-14	213	219
0	904	-913	K,L=	2	3	-8	326	332	11	354	-365	-9	376	-37.	-10	218	198	12	232	-179	-16	219	-216
1	535	-439	-1	753	808	-11	221	-211	12	353	-368	-10	286	-287	-11	112	114	13	218	-190	K,L=	3	5
2	60	43	-2	981	1252	-12	109	-94	13	112	-144	-12	222	-214	-12	238	251	14	175	-157	-1	1058	-1093
3	82	47	-3	888	1128	-13	217	-258	14	238	-204	-14	238	228	-14	196	151	15	193	-176	-2	924	-1123
4	363	-233	-4	305	324	-14	141	-225	15	228	-239	-15	416	467	-15	175	128	16	195	-201	-3	587	-682
5	372	341	-5	740	909	K,L=	9	3	16	195	-169	K,L=	2	4	-16	105	110	17	57	-104	-4	558	-610
6	162	-64	-6	548	599	-1	91	84	17	148	-202	-1	277	-234	K,L=	8	4	K,L=	5	5	-5	143	-141
7	603	549	-7	669	758	-5	175	166	K,L=	5	4	-2	74	7	-3	189	-113	0	181	170	-6	471	-556
8	238	210	-8	126	-77	-6	222	211	0	259	233	-3	148	153	-5	240	-218	1	224	210	-7	265	-244
9	400	394	-9	115	-39	-7	247	260	1	107	151	-4	245	24	-6	186	-98	2	324	249	-8	70	-11
10	300	303	-10	100	54	-8	147	167	2	352	345	-5	112	-112	-7	159	-173	3	191	-76	-9	144	92
11	431	422	-11	106	-66	-9	287	272	3	403	-434	-6	178	-145	-8	79	-43	4	152	-157	-11	336	343
12	265	177	-12	490	-538	-10	125	141	4	502	-575	-7	80	85	-9	186	124	5	113	-87	-12	83	82
13	213	176	-13	144	-119	-12	93	98	5	612	-612	-8	95	-78	-10	173	-114	6	164	-154	-13	472	518
14	100	164	-14	285	-315	K,L=	18	3	6	608	-527	-9	295	-254	-12	156	-115	7	145	-143	-14	305	308
15	134	137	-15	276	-269	-1	80	-80	7	506	-479	-10	263	-208	-13	83	76	10	215	-170	-15	204	175
17	192	-160	-16	361	-359	-2	80	-59	8	625	-615	-11	256	-238	-14	94	116	12	138	-127	-16	273	281
K,L=	5	3	-17	266	-254	-3	119	-88	9	602	-576	-12	268	-245	K,L=	9	4	15	178	198	-17	265	268
0	117	-71	K,L=	3	3	-4	189	-93	10	295	-232	-14	231	-218	-2	233	-183	K,L=	6	5	-18	176	158
1	408	341	-1	721	-804	-5	185	-77	11	244	-229	-15	211	-2 5	-3	242	-199	1	355	309	K,L=	4	5

TABLE III. (Continued)

H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC	H	FO	FC
-1	150	-109	4	308	285	K=L= 8 6			-10	105	190	9	373	367	-2	303	-262
-2	110	84	5	332	331	2	240	-194	-11	246	185	10	190	145	-3	82	-65
-3	264	-279	6	360	349	3	114	-95	-12	295	239	12	195	-162	-4	335	-323
-4	292	-231	7	334	256	4	80	94	-13	305	334	14	167	-13	-5	346	-341
-5	594	-586	9	138	-134	5	156	141	-14	358	402	15	186	-195	-6	262	-245
-6	365	-349	10	395	-471	6	77	-54	-15	185	158	16	190	-269	-7	381	-381
-8	421	-451	12	285	-267	K=L= 9 6			K=L= 6 6			K=L= 4 7			-8	788	-709
-9	457	-486	13	305	-316	1	181	151	-1	347	-332	0	410	4.5	-9	473	-549
-10	204	-190	14	247	-250	2	198	189	-2	459	-498	1	170	151	-10	425	-445
-11	198	-177	15	282	-305	3	216	197	-3	197	-209	2	455	475	-11	388	-273
-12	120	-95	16	143	-164	4	166	159	-4	592	-519	3	139	112	-12	137	-125
-14	159	-167	17	126	-147	6	162	162	-5	568	-515	4	185	114	-13	246	-235
-16	91	93	K=L= 7 6			7	146	135	-6	299	-220	5	200	-213	-14	121	84
-17	117	141	0	163	-107	9	44	4	-7	373	-380	9	477	-469	-16	121	79
-18	125	126	1	103	-65	K=L= 10 6			-8	168	107	10	195	-179	K=L= 4 7		
K=L= 5 5			2	49	19	0	83	81	-9	340	-339	11	278	-29	-1	406	394
-1	100	-137	3	218	-194	1	81	-65	-10	351	-312	12	343	-319	-2	263	230
-2	318	-230	4	191	-174	3	89	-105	-12	249	248	13	109	-1.9	-3	265	214
-4	410	385	5	420	-411	K=L= 0 6			-13	178	124	14	149	-123	-4	376	383
-5	106	-91	6	88	-83	-3	726	-704	-14	179	155	K=L= 5 7			-5	384	374
-6	408	398	7	66	-44	-4	385	-378	-16	208	248	0	217	189	-7	102	-24
-7	177	-151	8	212	-235	-5	705	-661	-17	103	195	3	108	85	-8	187	162
-8	368	-370	10	127	-128	-6	624	-631	K=L= 7 6			4	240	-223	-9	108	-93
-9	357	-364	11	287	-274	-7	672	-612	-1	101	101	5	333	-335	-10	241	-264
-10	259	230	13	115	-94	-8	545	-569	-2	296	267	6	112	-114	-11	168	-154
-11	201	-252	14	112	114	-9	507	-421	-4	254	-242	7	198	154	-12	291	-274
-13	159	-135	16	106	109	-10	475	-438	-6	185	-95	8	216	2.4	-13	302	-304
-15	214	-221	17	64	81	-11	115	-65	-7	108	-178	13	150	135	-14	151	-129
-16	83	-72	K=L= 3 6			-12	289	227	-9	246	-229	14	120	147	-15	149	-108
K=L= 6 5			0	353	364	-13	103	-94	-10	208	-215	K=L= 6 7			-16	182	-167
-1	79	47	1	318	-285	-14	205	177	-11	243	-227	2	259	252	-17	162	-162
-2	112	97	2	324	336	-15	248	219	-14	109	-106	5	118	-79	K=L= 5 7		
-3	245	228	3	163	-142	K=L= 1 6			-15	74	48	6	121	-102	-1	125	-94
-4	262	-212	4	584	477	-1	604	528	K=L= 8 6			8	123	-80	-4	104	78
-6	117	-61	5	247	197	-2	923	980	-1	80	25	10	141	-125	-6	399	436
-7	361	-316	6	201	158	-3	448	423	-2	202	185	12	176	118	-7	183	161
-8	250	-213	8	224	225	-4	120	-45	-3	114	-107	13	151	-179	-9	189	-189
-9	85	-67	9	223	-202	-5	580	-563	-4	81	-80	K=L= 7 7			-11	146	-131
-11	169	-135	11	111	-91	-6	244	235	-6	114	-128	2	436	-401	-14	122	-86
-13	243	-233	15	95	-73	-7	227	-217	-8	141	-132	3	273	-251	-16	182	-166
-14	234	-257	16	152	-166	-9	624	-628	-9	105	-104	4	311	-305	-17	162	-175
-15	212	-231	K=L= 4 6			-10	373	-416	-10	104	-157	5	305	-296	K=L= 6 7		
K=L= 7 5			0	322	320	-11	294	-278	-13	135	-193	6	230	-235	-2	174	144
-1	283	214	1	354	286	-12	350	-402	-14	91	-124	7	227	-193	-3	240	194
-2	440	434	2	86	-70	-13	381	-462	K=L= 9 6			8	350	-321	-4	336	343
-3	298	302	3	471	-451	-14	196	-181	-1	296	259	11	113	-125	-5	242	270
-4	419	456	4	348	-304	-15	207	-203	-2	216	222	K=L= 8 7			-7	344	-79
-5	180	176	5	228	-193	K=L= 2 6			-4	108	-51	0	500	-545	-10	122	148
-6	274	300	6	396	-381	-1	455	444	-6	146	122	1	151	-144	-13	169	-126
-7	375	395	7	383	-351	-2	119	105	-10	139	-149	2	123	-74	-15	98	-134
-9	230	-201	8	104	-81	-4	90	102	-11	47	-79	4	120	-8.	-16	101	-194
-11	130	134	9	326	-333	-5	841	828	K=L= 10 6			5	116	-75	-17	121	-90
-12	191	-170	10	453	-497	-6	203	199	-1	104	170	6	109	75	K=L= 7 7		
-13	177	-151	11	180	-151	-7	318	396	-2	141	131	7	125	128	-1	117	-133
-14	231	-229	12	261	-260	-8	83	60	-3	139	127	8	113	125	-3	187	133
-15	198	-228	13	185	-157	-9	88	-64	-4	109	198	9	189	193	-4	84	68
-16	168	-168	14	121	-116	-10	182	-189	-5	177	189	10	191	295	-5	262	269
K=L= 8 5			16	62	-73	-11	274	239	-6	170	192	K=L= 9 7			-6	85	86
-1	91	-79	K=L= 5 6			-12	213	-211	-7	95	90	0	110	80	-7	206	167
-2	177	177	0	597	-644	-14	180	-168	K=L= 1 7			2	105	125	-8	427	424
-3	91	68	1	539	-495	-16	162	-162	0	465	-471	4	283	280	-9	369	367
-4	91	62	2	556	-569	-17	210	-179	1	209	-230	5	268	275	-10	86	113
-5	160	152	3	626	-707	K=L= 3 6			2	232	-210	6	98	124	-12	209	225
-6	308	359	4	176	-171	-1	248	201	3	675	-681	K=L= 10 7			-13	251	265
-7	219	187	5	124	-142	-2	608	554	4	200	-280	0	77	85	-14	124	132
-8	294	216	6	146	-117	-4	74	-59	5	329	-301	2	48	34	K=L= 8 7		
-9	321	329	7	382	-385	-5	292	-287	6	118	-64	K=L= 1 7			-1	297	-314
-10	316	361	8	108	-78	-6	156	-85	7	490	-445	-1	751	-660	-2	333	-347
-11	226	253	9	199	204	-7	303	357	8	265	-214	-2	430	395	-3	208	-172
-12	197	185	10	192	150	-8	89	178	9	412	-435	-3	593	633	-4	269	-235
K=L= 9 5			11	114	113	-9	93	-65	11	146	92	-4	350	365	-5	123	-99
-1	149	-103	12	248	222	-10	204	85	14	196	197	-5	159	135	-6	194	-167
-2	357	-309	13	270	249	-11	241	-214	15	72	-37	-6	160	127	-7	148	119
-3	292	-199	14	272	306	-12	217	-319	K=L= 2 7			-7	322	315	-8	259	-278
-4	128	-144	15	207	282	-14	166	-121	0	351	-360	-8	259	269	-10	224	211
-5	127	-139	K=L= 6 6			-15	203	49	1	695	-695	-9	292	3.4	-11	192	210
-6	151	-143	0	126	-112	-18	149	-183	2	603	-572	-10	297	275	-12	87	87
-7	146	35	1	321	316	K=L= 4 6			3	228	-195	-11	331	344	-13	217	235
-8	80	86	3	364	-329	-18	183	-124	5	240	-208	-12	133	93	K=L= 9 7		
-11	249	268	4	227	244	-2	594	564	6	226	218	-13	136	97	-1	111	80
-12	118	150	5	376	662	-4	438	467	7	406	388	-14	207	-201	-3	140	-97
K=L= 10 5			6	227	212	-5	390	404	8	350	327	-15	121	122	-4	110	-103
-2	74	63	7	351	369	-6	656	684	9	359	343	-16	123	77	-5	226	-215
-3	103	-86	8	338	343	-7	554	536	10	103	154	K=L= 2 7			-6	219	-198
-4	246	-204	9	249	231	-8	370	385	11	271	268	-1	495	-453	-7	301	-306
-5	97	-70	10	221	204	-9	121	94	12	375	375	-2	491	-467	-8	129	-128
-6	92	-81	11	329	292	-10	72	64	13	341	354	-3	1112	-1249	-9	144	135
K=L= 0 6			12	67	74	-12	244	297	14	330	317	-4	511	-5.1	-10	141	-160
8	597	584	K=L= 7 6			-16	196	-198	15	205	217	-5	478	-442	-11	150	-241
9	428	484	0	74	23	-17	140	-145	16	93	84	-6	328	-25	K=L= 10 7		
10	708	751	1	178	174	K=L= 5 6			K=L= 3 7			-7	260	-21.	-1	56	60
13	213	201	2	239	259	-1	240	-279	0	148	141	-8	218	214	-4	149	-70
14	159	118	3	326	331	-2	390	-446	1	672	641	-10	214	159	-5	72	-82
16	93	-85	4	112	-124	-3	349	-384	2	374	360	-11	169	139	-6	65	14
17	130	-165	5	330	284	-4	129	-121	3	496	524	-12	232	215	K=L= 8 8		
K=L= 1 6			8	156	-150	-5	142	-114	4	595	584	-14	354	367	6	646	685
0	528	560	9	76	-69	-6	172	-24	5	430	420	-15	489	572	11	408	-418
1	576	650	10	208	-177	-7	321	166	6	246	238	-16	171	171	13	226	-227
2	463	417	11	122	-143	-8	143	342	7	779	774	K=L= 3 7			14	201	-232
3	1004	1034	12	93	-122	-9	659	687	8	392	417	-1	57	73	15	265	-309

TABLE III. (Continued)

H FO FC	H FO FC	H FO FC	H FO FC	H FO FC	H FO FC	H FO FC	H FO FC
-12 103 -169	7 230 230	-10 250 -241	K=L= 0 10	8 147 -141	-10 252 -239	8 441 -426	-5 173 186
-14 228 -225	8 179 172	-11 282 -285	6 587 -715	9 197 -214	-11 124 145	10 73 -87	-6 244 -240
K=L= 8 8	9 144 -114	-12 124 -134	7 308 -366	10 134 -165	-13 175 175	11 227 -237	-7 66 -91
-3 129 126	11 66 79	-13 187 -218	8 187 -205	K=L= 7 10	K=L= 5 10	12 142 -172	-8 69 -82
-4 129 105	12 54 51	-14 122 -122	9 297 -356	1 130 -97	-1 263 234	K=L= 3 11	-9 209 182
-5 128 125	K=L= 6 9	-15 208 -223	10 308 -305	2 179 -137	-2 213 173	0 213 199	-10 94 -86
-8 96 90	1 194 -155	-16 154 -169	12 179 -173	3 145 -109	-3 275 248	2 168 -178	-11 185 -188
-9 91 -82	3 272 -236	-17 198 -225	13 93 -108	4 63 23	-5 66 58	3 398 -433	-12 198 -212
-10 85 96	4 163 -146	K=L= 4 9	K=L= 1 10	5 211 -229	-6 67 -64	4 351 -351	-13 301 -306
K=L= 9 8	5 147 -169	-1 257 246	0 108 -126	7 142 -112	-7 257 -275	5 416 -441	-14 195 -130
-2 89 152	6 90 -82	-2 217 170	1 493 -561	8 56 64	-8 141 -146	6 148 -127	-15 158 -169
-3 167 136	7 224 -208	-3 130 69	2 434 -467	K=L= 8 10	-9 295 -300	7 149 -136	-16 168 -175
-4 148 48	9 58 -57	-4 157 170	3 322 -416	1 152 125	-10 315 -312	8 243 -233	K=L= 3 11
-5 145 161	10 150 -139	-5 150 130	4 208 -274	2 103 81	-11 259 -238	9 391 -453	-1 189 -63
-7 249 265	11 73 -91	-6 233 230	5 214 -237	3 214 -207	-12 70 -65	10 68 -74	-2 118 103
-8 169 110	K=L= 7 9	-7 453 429	6 125 -134	5 82 74	-13 252 -244	11 71 -57	-3 243 253
-9 115 143	0 164 -184	-8 427 384	7 274 -286	6 72 86	-14 149 -163	12 41 -33	-5 150 154
K=L= 1 9	1 220 -185	-9 141 115	8 70 -47	K=L= 9 10	-15 53 -58	K=L= 4 11	-6 335 336
0 401 -393	2 297 -289	-10 214 219	9 159 136	1 119 -150	-16 83 -85	0 268 -245	-7 311 334
1 501 -530	3 187 -165	-11 112 -114	10 71 77	2 65 -85	K=L= 6 10	1 398 -445	-8 201 222
2 169 99	7 110 117	-14 70 71	12 140 167	K=L= 0 10	-1 177 140	2 325 -329	-9 184 204
3 191 -187	8 115 104	-18 118 -126	13 62 170	-4 677 635	-2 329 304	3 188 130	-10 165 151
4 257 -231	9 53 67	K=L= 5 9	14 171 261	-5 521 532	-3 177 168	4 101 -77	-11 293 270
5 101 82	10 57 92	-1 198 155	K=L= 2 10	-6 368 359	-4 160 139	5 136 -85	-12 116 85
6 99 83	K=L= 8 9	-2 268 -242	0 171 -132	-7 238 -230	-5 300 313	7 81 66	K=L= 4 11
7 323 -331	0 66 -35	-4 158 -175	1 157 94	-8 307 288	-6 276 259	8 76 63	-1 98 -86
9 510 458	1 198 186	-7 404 389	2 90 80	-9 275 220	-7 241 229	9 135 150	-2 119 -127
10 442 401	2 224 225	-8 144 109	3 58 -31	-10 452 370	-8 115 68	10 141 151	-3 168 -165
12 181 157	3 190 191	-10 201 -194	4 112 106	-12 259 -232	-11 81 82	11 93 130	-4 97 -83
13 181 180	4 70 92	-11 115 103	6 66 84	-13 122 -120	-12 109 -107	K=L= 5 11	-6 143 -124
14 82 83	5 101 194	-12 112 97	7 98 106	K=L= 1 10	-13 158 -159	0 280 233	-7 96 -76
15 57 76	6 179 185	-13 206 187	8 106 187	-1 225 -242	-14 60 -73	1 119 89	-10 326 359
K=L= 2 9	7 204 229	-14 65 59	10 150 106	-2 234 -206	-15 37 -31	2 226 -202	-11 234 241
0 104 132	K=L= 9 9	-15 58 65	11 142 131	-3 229 -213	K=L= 7 10	3 102 -76	-14 137 129
1 122 70	0 87 76	-16 50 -71	13 66 70	-4 127 -102	-1 223 -184	4 102 86	-15 127 136
2 239 225	2 146 126	K=L= 6 9	K=L= 3 10	-5 402 448	-2 71 -42	5 147 110	-16 120 109
3 386 344	3 155 160	-1 160 -133	0 412 -454	-6 143 -119	-4 223 181	6 78 58	K=L= 5 11
4 263 252	4 75 95	-2 122 93	1 82 -34	-7 158 143	-5 124 100	7 104 112	-1 81 44
5 614 702	K=L= 1 9	-3 139 -96	2 270 -231	-8 250 242	-6 130 96	8 66 -50	-2 246 -206
6 536 572	-1 264 -215	-4 96 -64	3 61 -33	-9 540 512	-7 160 135	9 124 -92	-3 131 -70
7 436 469	-2 358 -287	-5 147 140	4 157 -143	-10 167 145	-8 66 -44	K=L= 6 11	-5 243 -225
8 206 194	-3 363 -289	-6 333 337	8 157 -139	-11 206 163	-9 173 156	1 228 -169	-6 182 -163
9 114 85	-4 70 76	-7 161 149	9 161 106	-12 224 207	-10 135 124	2 198 -137	-7 162 151
11 310 294	-5 301 -248	-9 164 146	12 91 -99	-13 272 243	-11 96 111	5 209 -173	-10 117 99
14 85 -82	-6 228 -197	-11 98 117	13 88 120	K=L= 2 10	-12 69 -45	7 61 55	-13 70 67
15 85 -166	-7 162 -139	-12 93 103	K=L= 4 10	-1 406 -362	-13 125 125	8 143 139	-14 63 64
K=L= 3 9	-8 66 -70	-13 170 184	0 269 -305	-2 77 56	K=L= 8 10	K=L= 7 11	-15 120 139
0 592 574	-9 157 -121	-14 94 122	1 62 34	-3 185 -178	-1 94 -72	0 93 73	K=L= 6 11
1 475 510	-11 259 -248	-15 150 154	2 253 192	-4 79 32	-4 61 -38	1 139 96	-1 83 -68
2 411 376	-12 266 263	K=L= 7 9	4 83 -61	-5 150 -143	-5 60 51	2 72 68	-2 171 -149
3 220 211	-13 206 200	-1 147 -153	5 85 -22	-6 380 -329	-6 72 91	3 167 168	-4 250 -234
4 80 -51	-14 121 116	-2 293 -262	6 224 198	-7 254 -249	-8 123 127	4 243 248	-5 166 -133
5 129 -93	K=L= 2 9	-3 342 -317	7 344 363	-11 66 60	-9 113 138	5 108 81	-8 225 -211
6 78 67	-1 109 77	-4 314 -303	8 193 186	-12 206 183	K=L= 9 10	6 188 209	-13 69 81
7 163 -148	-2 298 209	-5 87 -68	9 180 174	-13 87 -91	-1 106 -122	7 62 109	-14 54 81
8 240 -218	-3 119 67	-6 100 -93	10 223 230	-14 167 161	-2 43 -47	K=L= 8 11	K=L= 7 11
9 87 -97	-4 517 -528	-7 128 -126	11 122 125	-15 86 77	-3 52 -50	0 249 275	-1 112 -76
10 460 -421	-5 835 -754	-11 160 173	12 135 139	K=L= 3 10	-5 49 -55	1 206 223	-2 113 -77
11 254 -252	-6 432 -441	-12 68 70	K=L= 5 10	-1 205 179	-6 36 25	2 52 70	-4 78 -68
12 274 -284	-7 185 -182	-13 59 58	0 169 165	-3 306 -263	-7 36 49	3 90 -61	-5 144 -114
13 203 -229	-8 56 -61	-14 208 234	1 185 208	-4 68 53	K=L= 1 11	4 107 105	-6 259 -257
14 174 -223	-9 497 -447	K=L= 8 9	2 496 466	-5 188 172	1 361 441	K=L= 1 11	-7 186 -117
K=L= 4 9	-10 451 -431	-3 128 -96	5 230 232	-6 148 -118	2 226 226	-1 110 -87	-8 136 -156
0 269 -269	-11 439 -222	-4 321 -277	4 150 140	-7 206 -227	3 195 165	-2 156 46	-9 157 -179
2 449 -451	-12 218 -199	-5 65 -58	5 244 232	-8 263 245	5 125 118	-3 278 -261	-10 177 -177
3 457 -451	-13 228 -222	-6 122 -126	6 88 70	-9 164 135	6 131 146	-4 414 -423	-12 93 -87
4 177 -221	-14 86 -83	-7 146 -183	7 254 239	-10 149 -133	7 360 385	-5 99 30	K=L= 8 11
6 252 -262	-16 233 269	-8 183 -195	8 81 77	-12 165 199	8 102 100	-6 227 211	-1 167 168
7 161 -146	-17 88 82	-9 214 -218	10 65 57	-14 109 100	9 101 94	-7 430 -370	-2 249 238
8 238 -244	K=L= 3 9	-10 213 -241	11 52 -83	-15 95 74	11 133 137	-8 546 -517	-4 151 167
9 129 -109	-1 478 484	-12 80 -101	K=L= 6 10	-16 178 164	K=L= 2 11	-9 206 -188	-6 134 152
10 118 -92	-2 720 651	K=L= 9 9	0 245 205	K=L= 4 10	0 247 251	-11 186 -163	-9 78 -86
13 76 95	-3 257 221	-2 216 207	1 152 95	-2 462 -402	1 150 171	-12 173 144	
K=L= 5 9	-4 284 265	-1 183 171	2 72 32	-3 143 -107	2 187 190	-14 130 -106	
1 244 192	-5 291 267	-3 64 78	3 88 92	-4 330 -343	3 253 312	K=L= 2 11	
2 84 -30	-6 247 215	-4 98 106	4 301 -290	-5 333 -319	4 109 109	-1 588 582	
3 295 -280	-7 251 237	-5 90 108	5 186 -185	-6 319 -332	5 241 220	-2 173 126	
4 282 -248	-8 160 137	-8 153 -176	6 142 -132	-8 220 -214	6 118 106	-3 580 549	
5 155 121	-9 476 -485	-9 88 -135	7 219 -214	-9 253 -250	7 191 -169	-4 608 537	

tropone derivatives[5] or the homotropone series.[6] The maximum deviation of the atoms in the least squares plane is 0.02 Å at C6. It means that the conformation is a less skewed boat than Karle determined[7] in which the maximum deviation of the corresponding least squares plane is 0.16 Å. The least squares plane of five atoms of lactam and its neighbors, C5, C6, C13, O16 and N7, is almost planar within the deviation of 0.05 Å. The two nitrogen atoms in the seven-membered ring have different bond character. The N4 atom is bonded to three

5) H. Shimanouchi, T. Hata and Y. Sasada, *Abstracts of Papers of ISNA in Japan*, 1970, 31.
6) C. Tamura, N. Sakurai, S. Sato, Y. Sugimura and N. Soma, *Abstracts of Papers of ISNA in Japan*, 1970, 110.
7) J. Karle and I.L. Karle, *J. Am. Chem. Soc.*, 89, 804 (1967).

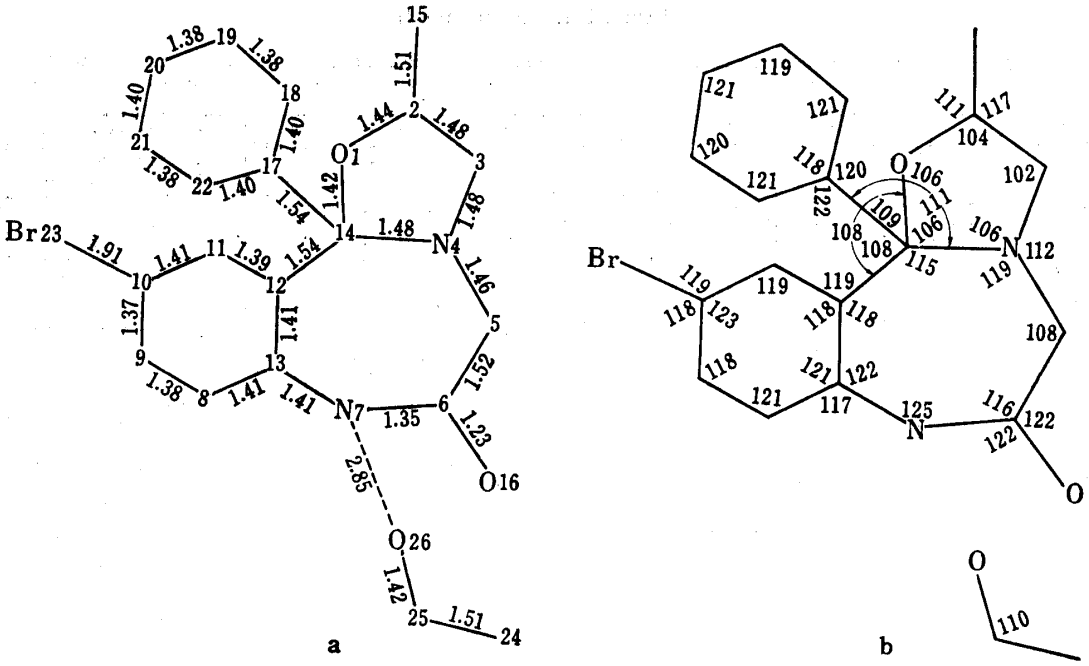


Fig. 2. (a) Bond Distances (b) Bond Angles

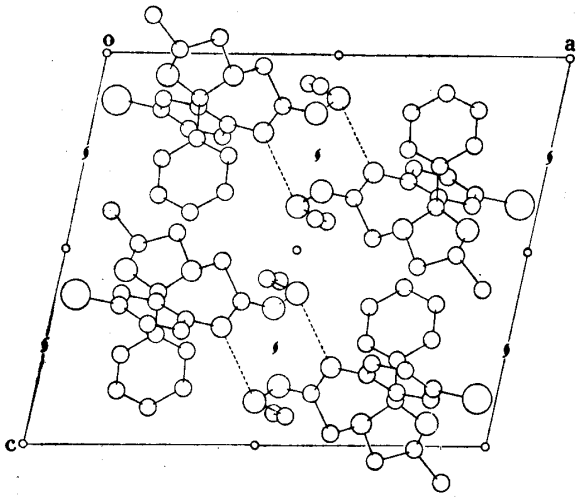


Fig. 3. The Crystal Structure as Viewed along the b Axis

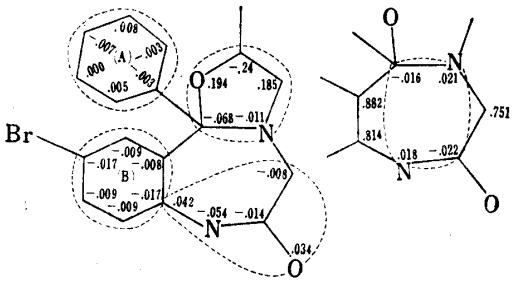
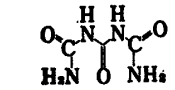
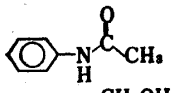
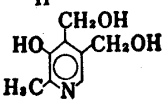
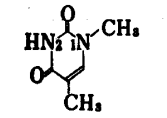


Fig. 4. Deviation in Ångstrom Units from Least-Sqauares Planes

saturated carbon atoms in a pyramidal form. The bond lengths of C3-N4, C5-N4 and C14-N4 are normal, and their values are 1.48, 1.46 and 1.48 Å. The angles of C3-N4-C14, C3-N4-C5 and C5-N4-C14 are 106.2, 111.5 and 118.6° respectively. On the other hand, the N7 atom is bonded to a carbonyl group and a benzene ring; the bond lengths of C6-N7 and C13-N7, 1.35 and 1.41 Å respectively are shorter than the normal C-N single bond of 1.47 Å. Shorter carbon-nitrogen bond lengths have been pointed out by Karle[5] such that nitrogen atoms adjacent to C=S, C=O, and C=C bonds, tend to be in a planar configuration with short C-N bond lengths of in the range 1.34—1.40 Å. The bond angle for C6-N7-C13 is 125.3°. Several molecules containing such systems have usually larger bond angles, some examples of these compounds are shown in Table IV. The value of the mean bond lengths of the benzene rings is 1.39 Å which is normal. The deviations of the atoms from the benzene least squares planes are within 0.01 Å for benzene ring A and 0.02 Å for ring B. The intermolecular contacts within 3.7 Å are given in Table V. They are

within the range of normal van der Waals radii. Intermolecular hydrogen bonds are observed in N7···026=2.85 Å and 026···016=2.78 Å.

TABLE IV. Comparison of Csp^2-N-Csp^2 Bond Angles

Compound	Angle	Reference
	125.3	This work
	128.4 127.5	H. Ringertz (1966)[a]
	127.6	B.F. Pedersen (1967)[b]
	124.5	F. Hanic (1966)[c]
	1; 120.6 2; 126.3	K.Hoogsteen (1963)[d]

a) H. Ringertz, *Acta Cryst.*, **20**, 932 (1966) b) B.F. Pederson, *Acta Chem. Scand.*, **21**, 1415 (1967)
c) F. Hanic, *Acta Cryst.*, **21**, 332 (1966) d) K. Hoogsteen, *Acta Cryst.*, **16**, 28 (1963)

TABLE V. Intermolecular Contacts within 3.7 Å

O26···O26(I)	3.47	C21···C 9(III)	3.61
N 4···C25(II)	3.67	C22···C 9(III)	3.68
C 6···O26(II)	3.58	C25···O16(IV)	3.54
O16···C25(II)	3.58	O26···C 5(IV)	3.46

I: 1−x, 1−y, 1−z
II: 1−x, 1/2+y, 1/2−z
III: x, 3/1+y, z
IV: x, 3/2−y, 1/2+z