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2, 4, 4-TRIPHENYL-1, 2-DIAZETIDINE-3-ONE-1-CARBOXYLIC ACID, ETHYL ESTER

Helena Ruben, Hans Bates, Allan Zalkin and David H. Templeton

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2,4,4-Triphenyl-1,2-diazetidine-3-one-1-Carboxylic acid, Ethyl ester*

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Abstract. $C_6H_5NN(COOC_2H_5)C(C_6H_5)_2CO$ crystallizes in the triclinic space group $P\bar{1}$ with cell dimensions a = 9.877(5), b = 14.037(5), c = 8.420(5) Å, α = 94.45(3)°, β = 108.97(3)°, and γ = 112.67(3)°; Z = 2, and D_x = 1.24 g cm^{-3}. Bond distances in the slightly puckered nearly-planar four-membered diazetidine ring are N-N 1.450(2) Å, C-C 1.535(2) Å, N-C(ketone) 1.362(2) Å, and N-C 1.511(2) Å.

* Research performed under the auspices of the U.S. Atomic Energy Commission.

† Summer student at Lawrence Berkeley Laboratory, 1969.

Experimental. The title compound was given to us by Dr. Robert Kerber (1970) and recrystallized from ethanol. A yellow crystal with approximate dimensions 0.1x0.2x0.4 mm was glued to a pyrex fiber and used for the measurement of 6599 data, including standards, with a Picker FACS-I automatic diffractometer system. Graphite monochromated Cu$K\alpha$ (λ=1.54051 Å for $K\alpha_1$) X-rays were used in the collection of data by a θ-2θ scan technique using a scintillation counter. No absorption correction was deemed necessary, μ=6.8 cm^{-1}. All of the reflections within the sphere of reflection out to a 2θ angle of 106° were collected, yielding 3279 unique reflections of which 2688 were greater than their standard deviation. Standard deviations were estimated as described by St. Clair, Zalkin and Templeton(1971), with $(0.04I)^2$ as the additional term in$(\sigma(I))^2$. The positions of all the non-hydrogen atoms were obtained from an E map phased by the application of "direct" methods. Hydrogen positions were obtained from a difference Fourier map calculated after a least-squares refinement of the heavy atoms with anisotropic thermal parameters was perfromed. Full-matrix least-squares refinements were then performed on all of the positional, anisotropic thermal (for the heavy atoms), and isotropic thermal (hydrogen atoms) parameters. The maximum final shift was less than 28% of its standard deviation. The weights were $1/\sigma^2(F)$, or zero if $F<\sigma(F)$.

An empirical correction for extinction was applied, $F_0' = F_0(1 + 4\times10^{-8} I)$, which increased F_0 about 15% for the strongest reflection $(\bar{2},2,1)$. The final R factor, $R = \Sigma|\Delta F|/\Sigma|F_0|$, for all of the reflections was 0.045, and for the 2688 non-zero weighted reflections was 0.036. The weighted R factor, $R_w = [\Sigma w(\Delta F)^2/\Sigma w F_0^2]^{\frac{1}{2}}$, was 0.046. The goodness-of-fit was 1.68. Atomic form factors for spherical hydrogen were those of Stewart, Davidson and Simpson(1965) and for the other atoms those of Cromer and Waber(1965).

The final atomic parameters are given in Tables 1, 2 and 3. A table of calculated and observed structure factors has been deposited with the National Lending Library as Supplementary Publication No. SUP 00000*

* Copies may be obtained from the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Discussion. The structure determination of this material was undertaken to verify the postulated structure of the four membered ring, the dimensions of which is shown in Fig. 1. A least-squares plane calculated through the four atoms of the ring show deviations of 0.028, -0.025, -0.026 and 0.023 for atoms N(1), N(2), C(1) and C(2) respectively. The above results indicate a slight puckering of the ring from planarity. With the exception of two bonds in the ring, the interatomic distances listed in Table 4 are similar to those tabulated for bonds with comparable chemical arrangements (Sutton, 1965). The N(1)-C(1) bond is 1.362 Å versus 1.333 Å in amides and the N(2)-C(2) bond is 1.511 Å versus 1.472 Å for an N-C bond in paraffinic and saturated heterocyclic compounds. The C-C and N-N bonds are both within 0.002 Å of the average values reported for C-C and N-N single bonds. A list of bond angles is given in Table 5.

The relative orientation to the ring of the three phenyl rings, the ethyl ester and the oxygen, O(1), can be seen in the stereogram shown in Fig. 2. The oxygen, O(1), is -0.12 Å from the mean plane of the ring, and C(15), the bonding carbon atom of the phenyl group to the four-membered ring at N(1) is -0.55 Å from this plane. The remaining atoms are all more than 1.0 Å away from the plane of the ring. It can be noted that the three bonds about N(1) are somewhat more planar than those about N(2).

A stereoscopic view of the packing is shown in Fig. 3.

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Table 1. *Positional Parameters*

ATOM	X	Y	Z
N(1)	-.0929(1)	.77498(9)	.1585(2)
N(2)	-.0380(1)	.7C741(9)	.2566(1)
O(1)	.1023(1)	.94418(8)	.1858(1)
O(2)	-.2555(1)	.6538(1)	.3334(2)
O(3)	-.0452(1)	.62293(9)	.4667(2)
C(1)	.0530(2)	.8595(1)	.2205(2)
C(2)	.1246(2)	.8C01(1)	.3421(2)
C(3)	.1713(2)	.8438(1)	.5315(2)
C(4)	.0861(2)	.8901(1)	.5837(2)
C(5)	.1250(2)	.9280(2)	.7564(2)
C(6)	.2488(2)	.9203(2)	.8766(2)
C(7)	.3332(2)	.8747(2)	.8266(2)
C(8)	.2953(2)	.8362(1)	.6543(2)
C(9)	.2495(2)	.7814(1)	.2944(2)
C(10)	.3887(2)	.8681(2)	.3188(2)
C(11)	.5068(2)	.8545(2)	.2801(3)
C(12)	.4870(3)	.7558(2)	.2152(3)
C(13)	.3491(3)	.670C(2)	.1892(3)
C(14)	.2290(3)	.6825(2)	.2278(2)
C(15)	-.2137(2)	.7378(1)	-.0062(2)
C(16)	-.3165(2)	.6321(1)	-.0648(2)
C(17)	-.4310(2)	.5987(2)	-.2284(3)
C(18)	-.4411(3)	.6693(2)	-.3305(3)
C(19)	-.3397(2)	.774C(2)	-.2697(3)
C(20)	-.2256(2)	.8C99(2)	-.1072(2)
C(21)	-.1263(2)	.6617(1)	.3556(2)
C(22)	-.1151(3)	.5748(3)	.5874(4)
C(23)	.0020(5)	.6C80(3)	.7567(4)
H(1)	-.005(2)	.894(1)	.499(2)
H(2)	.C62(2)	.960(1)	.791(2)
H(3)	.281(2)	.948(2)	1.001(3)
H(4)	.426(3)	.867(2)	.917(3)
H(5)	.356(2)	.8C2(1)	.622(2)
H(6)	.399(2)	.942(2)	.366(2)
H(7)	.607(3)	.923(2)	.299(3)
H(8)	.568(3)	.745(2)	.184(3)
H(9)	.322(3)	.6C1(2)	.138(3)
H(10)	.135(2)	.622(1)	.206(2)
H(11)	-.31C(2)	.583(1)	.013(2)
H(12)	-.502(2)	.524(2)	-.263(3)
H(13)	-.523(3)	.643(2)	-.442(3)
H(14)	-.344(2)	.827(2)	-.341(3)
H(15)	-.151(2)	.885(2)	-.065(2)
H(16)	-.196(5)	.516(4)	.546(6)
H(17)	-.180(5)	.610(3)	.604(5)
H(18)	.085(5)	.581(4)	.728(6)
H(19)	.C71(4)	.691(3)	.799(5)
H(20)	-.04C(3)	.575(2)	.84C(3)

Table 2. *Anisotropic thermal parameters, Å*
Anisotropic temperature factors have the form: $\exp\{-\frac{1}{4}\Sigma_i\Sigma_j(a_i^* a_j^* h_i h_j B_{ij})\}$ where a_i^* is a reciprocal cell edge and h_i is one of the Miller indices.

ATOM	B11	B22	B33	B12	B13	B23
N(1)	3.39(5)	3.52(5)	3.39(5)	1.46(4)	.73(4)	1.34(4)
N(2)	3.27(5)	3.41(5)	3.47(5)	1.45(4)	1.06(4)	1.40(4)
C(1)	4.43(5)	3.50(5)	4.54(5)	1.68(4)	1.69(4)	1.61(4)
C(2)	3.86(5)	7.00(7)	6.08(7)	2.47(5)	2.27(5)	2.89(5)
C(3)	4.93(6)	6.15(6)	5.86(6)	2.76(5)	2.47(5)	3.96(5)
C(1)	3.39(6)	3.33(6)	3.21(6)	1.63(5)	1.33(5)	.88(5)
C(2)	3.06(6)	3.33(6)	3.00(6)	1.44(5)	1.16(5)	.98(5)
C(3)	3.38(6)	3.95(6)	2.98(6)	1.56(5)	1.39(5)	.95(5)
C(4)	4.17(7)	4.97(8)	3.97(8)	2.16(6)	1.77(6)	.81(6)
C(5)	5.51(9)	5.80(9)	4.77(9)	2.29(8)	2.94(8)	.49(7)
C(6)	6.0(1)	6.6(1)	3.31(8)	1.63(8)	2.14(7)	.53(7)
C(7)	5.13(9)	7.1(1)	3.10(8)	2.21(8)	1.13(7)	1.25(7)
C(8)	4.24(7)	5.80(9)	3.31(7)	2.52(7)	1.39(6)	1.34(6)
C(9)	3.82(6)	4.60(7)	2.75(6)	2.45(6)	1.38(5)	1.37(5)
C(10)	3.66(7)	5.83(9)	4.25(8)	1.99(7)	1.77(6)	1.49(7)
C(11)	4.52(9)	9.0(1)	5.6(1)	3.6(1)	2.75(8)	3.35(9)
C(12)	7.0(1)	11.5(2)	6.5(1)	6.8(1)	4.3(1)	4.6(1)
C(13)	9.1(2)	7.6(1)	7.5(1)	6.1(1)	4.5(1)	2.5(1)
C(14)	6.0(1)	5.01(9)	5.39(9)	3.37(8)	2.78(8)	1.71(7)
C(15)	3.06(6)	4.30(7)	3.30(6)	1.72(5)	.95(5)	.98(5)
C(16)	4.28(7)	4.41(8)	4.33(8)	1.33(7)	.76(6)	.94(6)
C(17)	4.84(9)	5.8(1)	5.0(1)	.89(8)	.15(7)	.29(8)
C(18)	5.0(1)	8.4(1)	4.6(1)	2.3(1)	-.34(8)	1.26(9)
C(19)	4.93(9)	7.3(1)	4.73(9)	2.63(9)	.54(7)	2.49(9)
C(20)	4.14(7)	5.12(9)	4.23(8)	2.16(7)	1.04(6)	1.85(7)
C(21)	3.87(7)	3.91(7)	4.09(7)	1.66(6)	1.46(6)	1.62(6)
C(22)	6.6(1)	11.1(2)	8.1(2)	3.2(1)	3.6(1)	7.3(2)
C(23)	12.4(2)	8.5(2)	5.1(1)	.1(2)	3.6(1)	2.2(1)

Table 3. *Isotropic thermal parameters,* $\mathring{A}^2$
Temperature factor has the form: $\exp(-B\sin^2\theta/\lambda^2)$

ATOM	B
H(1)	4.7(4)
H(2)	5.7(4)
H(3)	6.1(5)
H(4)	7.7(5)
H(5)	4.4(4)
H(6)	6.4(5)
H(7)	8.4(6)
H(8)	7.1(5)
H(9)	8.3(6)
H(10)	4.7(4)
H(11)	4.9(4)
H(12)	6.1(5)
H(13)	8.4(6)
H(14)	6.8(5)
H(15)	5.4(4)
H(16)	16.0(15)
H(17)	13.5(12)
H(18)	17.4(16)
H(19)	14.2(11)
H(20)	9.3(7)

Table 4. *Interatomic distances, Å*

Atoms	Dist.	Atoms	Dist.	Atoms	Dist.
N(1) - C(1)	1.362(2)	C(5) - H(2)	1.00(2)	C(15) - C(16)	1.370(2)
N(1) - C(15)	1.396(2)	C(6) - C(7)	1.372(3)	C(15) - C(20)	1.386(2)
N(1) - N(2)	1.450(2)	C(6) - H(3)	.98(2)	C(16) - C(17)	1.369(3)
N(2) - C(21)	1.411(2)	C(7) - C(8)	1.380(2)	C(16) - H(11)	.99(2)
N(2) - C(2)	1.511(2)	C(7) - H(4)	1.03(2)	C(17) - C(18)	1.372(3)
O(1) - C(1)	1.198(2)	C(8) - H(5)	.99(2)	C(17) - H(12)	.97(2)
O(2) - C(21)	1.187(2)	C(9) - C(14)	1.368(2)	C(18) - C(19)	1.357(3)
O(3) - C(21)	1.319(2)	C(9) - C(10)	1.379(2)	C(18) - H(13)	.95(3)
O(3) - C(22)	1.474(3)	C(10) - C(11)	1.382(3)	C(19) - C(20)	1.360(3)
C(1) - C(2)	1.535(2)	C(10) - H(6)	1.03(2)	C(19) - H(14)	1.00(2)
C(2) - C(3)	1.511(2)	C(11) - C(12)	1.364(3)	C(20) - H(15)	.98(2)
C(2) - C(9)	1.520(2)	C(11) - H(7)	1.04(3)	C(22) - C(23)	1.413(4)
C(3) - C(8)	1.369(2)	C(12) - C(13)	1.362(3)	C(22) - H(16)	.84(5)
C(3) - C(4)	1.394(2)	C(12) - H(8)	.97(2)	C(22) - H(17)	.99(4)
C(4) - C(5)	1.380(3)	C(13) - C(14)	1.394(3)	C(23) - H(18)	1.11(5)
C(4) - H(1)	.97(2)	C(13) - H(9)	.92(2)	C(23) - H(19)	1.06(4)
C(5) - C(6)	1.358(3)	C(14) - H(10)	.93(2)	C(23) - H(20)	.99(3)

Table 5. *Selected Bond Angles, deg.*

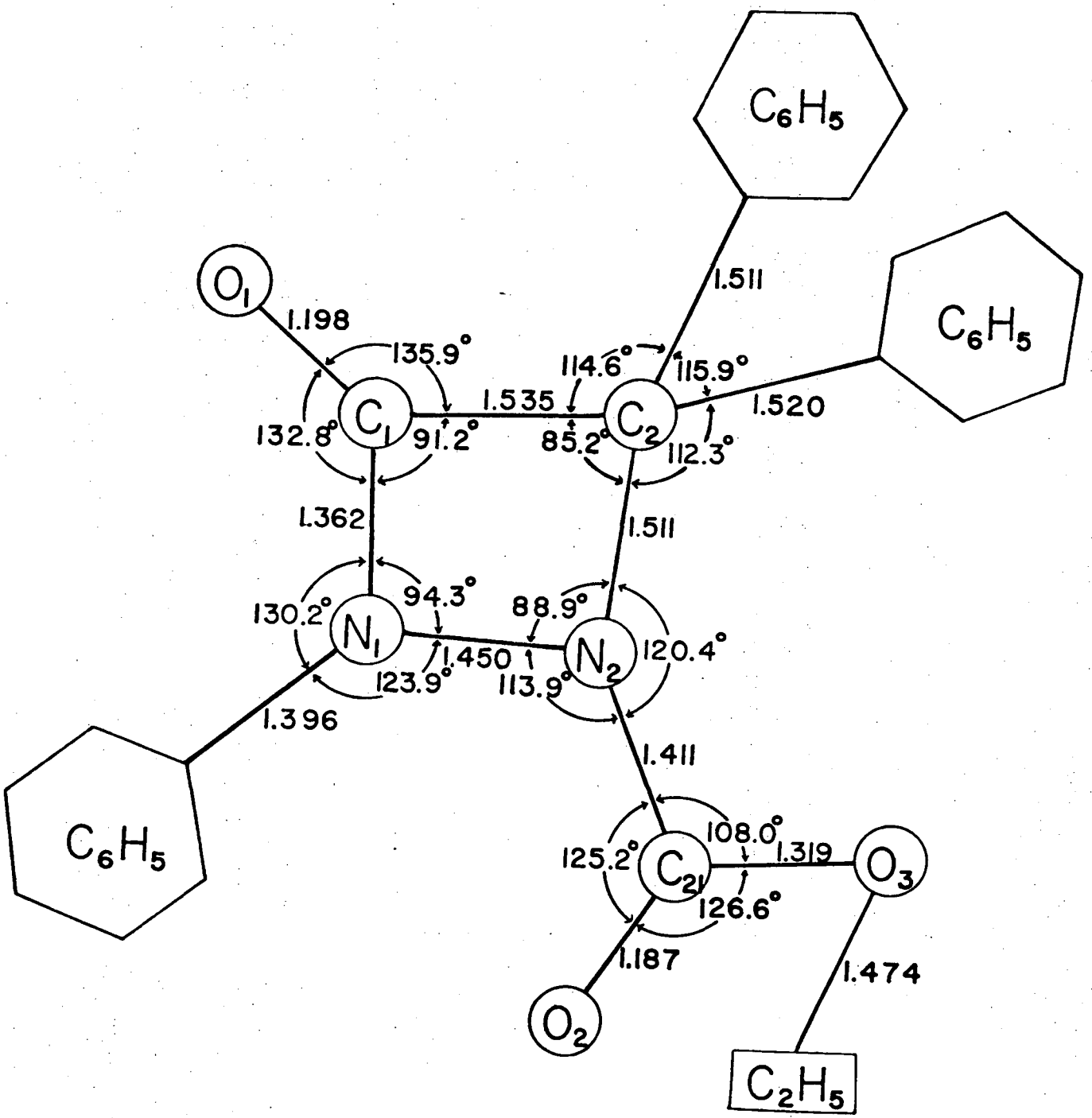
N(2) -N(1) -C(1)	94.3(1)	O(3) -C(22)-C(23)	110.7(1)
N(2) -N(1) -C(15)	123.9(1)	C(4) -C(3) -C(8)	119.0(2)
C(1) -N(1) -C(15)	130.2(1)	C(3) -C(4) -C(5)	121.0(2)
N(1) -N(2) -C(2)	88.9(1)	C(4) -C(5) -C(6)	119.3(2)
N(1) -N(2) -C(21)	113.9(1)	C(5) -C(6) -C(7)	120.2(2)
C(2) -N(2) -C(21)	120.4(1)	C(6) -C(7) -C(8)	121.1(2)
N(1) -C(1) -C(2)	91.2(1)	C(7) -C(8) -C(3)	119.4(2)
N(1) -C(1) -O(1)	132.8(1)	C(10)-C(9) -C(14)	119.0(2)
C(2) -C(1) -O(1)	135.9(1)	C(9) -C(10)-C(11)	120.3(2)
C(1) -C(2) -C(3)	114.6(1)	C(10)-C(11)-C(12)	120.8(2)
C(1) -C(2) -C(9)	110.7(1)	C(11)-C(12)-C(13)	119.2(2)
N(2) -C(2) -C(9)	112.3(1)	C(12)-C(13)-C(14)	120.7(2)
N(2) -C(2) -C(3)	114.3(1)	C(13)-C(14)-C(9)	120.1(2)
C(3) -C(2) -C(9)	115.9(1)	C(16)-C(15)-C(20)	121.5(2)
N(2) -C(2) -C(1)	85.2(1)	C(15)-C(16)-C(17)	118.0(2)
N(2) -C(21)-O(2)	125.2(1)	C(16)-C(17)-C(18)	120.8(2)
N(2) -C(21)-O(3)	108.0(1)	C(17)-C(18)-C(19)	120.5(2)
O(2) -C(21)-O(3)	126.6(1)	C(18)-C(19)-C(20)	120.1(2)
C(21)-O(3) -C(22)	116.5(1)	C(19)-C(20)-C(15)	119.0(2)

Figure Captions

Fig. 1 Schematic drawing showing distances in Å and angles in the ring.

Fig. 2 Stereoscopic view of the molecule.

Fig. 3 Stereoscopic view of a unit cell showing the packing.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C1
C2
132.8°
91.2°
85.2°
112.3°
1.362
1.511
130.2°
94.3°
88.9°
N1
N2
1.450
120.4°
123.9°
113.9°
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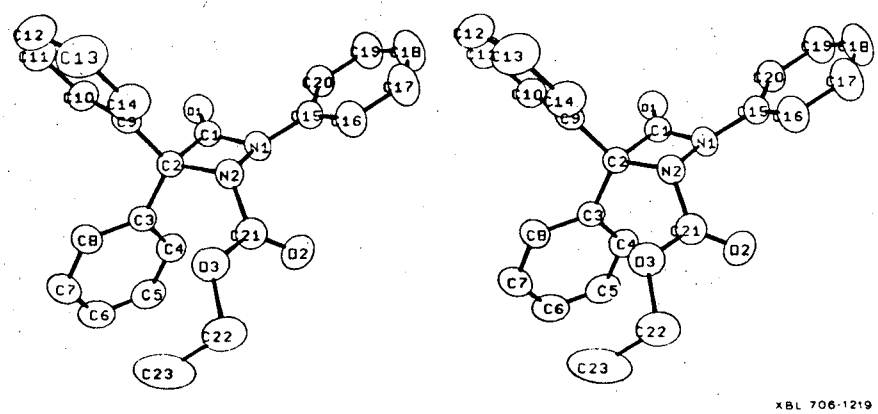
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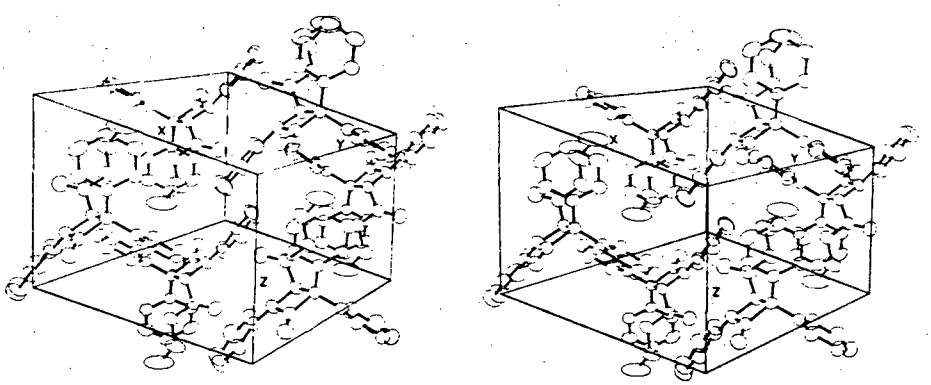

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Table 6. *Table of Observed and Calculated Structure Factors for 2,4,4-Triphenyl-1,2-Diazetidine-3-one-1-Carboxylic Acid, Ethyl Ester*[a]

L	FOB	FCA
H,K=	0,	0
1	159	155
2	729	723
3	18	16
4	119	110
5	16	18
6	55	55
7	24	25
8	8	4*
H,K=	0,	1
-9	4	5*
-8	8	8*
-7	14	13
-6	23	23
-5	59	57
-4	41	39
-3	213	204
-2	57	54
-1	224	217
0	110	128
1	435	458
2	189	188
3	368	365
4	86	86
5	57	55
6	46	47
7	60	61
8	8	8*
H,K=	0,	2
-9	28	28
-8	41	40
-7	8	7*
-6	112	114
-5	29	30
-4	155	153
-3	39	38
-2	255	245
-1	4	3*
0	560	624
1	34	30
2	227	231
3	340	334
4	57	51
5	73	70
6	4	3*
7	6	0*
8	2	1*
H,K=	0,	3
-9	8	10*
-8	32	32
-7	102	104
-6	11	10*
-5	114	114
-4	9	11
-3	31	29
-2	42	44
-1	438	456
0	42	39
1	257	276
2	124	124
3	40	38
4	103	102
5	21	19
6	10	17
7	4	6*
8	2	1*
H,K=	0,	4
-9	35	35
-8	61	63
-7	91	89
-6	52	52
-5	10	8*
-4	143	134
-3	49	47
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-1	30	29
0	483	509
1	386	411
2	3	10*
3	11	16
4	43	41
5	40	38
6	44	44
7	41	44
8	3	2*
H,K=	0,	5
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-8	21	18
-7	57	57
-6	14	14
-5	19	21
-4	38	41
-3	87	86
-2	102	101
-1	3	7*
0	55	50
1	69	74
2	157	161
3	82	80
4	57	57
5	69	67
6	10	6*
7	22	22
H,K=	0,	6
-9	35	37
-8	30	30
-7	222	218
-6	97	94
-5	29	30
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-3	33	33
-2	50	53
-1	143	143
0	14	12
1	149	152
2	63	57
3	185	185
4	113	111
5	126	124
6	17	17
7	10	8
H,K=	0,	7
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-7	47	49
-6	146	150
-5	50	50
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-2	17	19
-1	159	161
0	139	137
1	78	81
2	46	43
3	39	40
4	41	42
5	49	47
6	18	21
H,K=	0,	8
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-7	82	79
-6	32	35
-5	107	106
-4	85	89
-3	34	32
-2	29	28
-1	37	39
0	6	2*
1	45	47
2	113	114
3	11	13*
4	27	28
5	47	48
6	4	3*
H,K=	0,	9
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-7	46	48
-6	50	49
-5	0	4*
-4	77	75
-3	65	64
-2	50	51
-1	82	84
0	0	0*
1	18	13
2	19	19
3	24	24
4	64	63
5	10	13*
H,K=	0,	10
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-7	28	24
-6	88	88
-5	18	11
-4	64	60
-3	18	17
-2	47	45
-1	81	86
0	39	39
1	66	64
2	11	11*
3	0	0*
4	19	14
5	14	16
H,K=	0,	11
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-5	78	78
-4	47	45
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0	61	61
1	3	3*
2	53	53
3	23	22
4	3	3*
H,K=	0,	12
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-3	31	30
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0	26	25
1	34	36
2	14	16
3	6	3*
H,K=	0,	13
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-5	20	20
-4	49	47
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0	15	16
1	48	47
2	5	10*
H,K=	0,	14
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-3	12	9
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0	28	28
1	13	11
H,K=	1,	-15
0	3	3*
1	21	19
2	26	25
3	23	21
H,K=	1,	-14
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0	21	20
1	25	29
2	36	37
3	51	53
4	1	0*
5	5	2*
H,K=	1,	-13
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2	32	29
3	14	12
4	32	32
5	15	14
6	25	24
H,K=	1,	-12
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-2	9	14
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0	28	20
1	95	96
2	25	32
3	52	48
4	13	16
5	35	31
6	9	9
7	18	13
H,K=	1,	-11
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-4	24	25
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-2	29	32
-1	39	37
0	9	7*
1	17	15
2	23	21
3	90	87
4	60	58
5	81	86
6	0	2*
7	0	5*
H,K=	1,	-10
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-3	16	16
-2	31	32
-1	9	8*
0	4	1*

[a]Asterisk indicates a zero weighted datum.

1	108	109
2	8	1*
3	67	70
4	102	102
5	43	40
6	17	17
7	15	17
H,K=	1,	-9
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-5	36	36
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-3	43	43
-2	28	27
-1	18	14
0	1	0*
1	28	27
2	54	56
3	100	101
4	61	56
5	67	62
6	54	57
7	4	9*
8	18	19
H,K=	1,	-8
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-5	78	77
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-2	91	86
-1	39	39
0	107	109
1	58	57
2	111	111
3	27	25
4	18	19
5	68	72
6	75	72
7	86	85
8	26	25
H,K=	1,	-7
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-1	25	26
0	162	157
1	92	96
2	143	142
3	71	68
4	62	62
5	34	38
6	170	170
7	47	48
8	24	24
H,K=	1,	-6
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0	26	26
1	58	58
2	118	122
3	206	196
4	87	88
5	12	9
6	24	22
7	90	92
8	4	0*
H,K=	1,	-5
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-6	22	26
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0	54	53
1	220	216
2	29	27
3	93	89
4	84	80
5	55	53
6	190	187
7	65	64
8	70	71
H,K=	1,	-4
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-7	19	19
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-2	200	206
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0	142	150
1	231	234
2	165	169
3	404	394
4	122	122
5	119	112
6	205	199
7	23	23
8	32	33
H,K=	1,	-3
-8	33	35
-7	37	39
-6	50	48
-5	38	36
-4	152	154
-3	180	180
-2	265	281
-1	376	403

0	131	139
1	115	110
2	456	446
3	151	150
4	338	339
5	109	107
6	139	137
7	93	94
8	23	23
H,K=	1,	-2
-8	0	4*
-7	43	45
-6	17	18
-5	81	80
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-3	162	163
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0	620	639
1	436	443
2	249	251
3	217	216
4	271	264
5	186	183
6	188	180
7	4	11*
8	3	8*
H,K=	1,	-1
-9	14	13
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-7	33	36
-6	0	4*
-5	46	45
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-3	41	32
-2	13	15
-1	383	387
0	12	14
1	252	247
2	238	239
3	115	105
4	100	99
5	133	130
6	34	35
7	43	40
8	32	34
H,K=	1,	0
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-8	43	43
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-6	8	9*
-5	187	183
-4	135	119
-3	374	375
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0	355	364
1	330	323
2	22	21

3	86	84
4	36	30
5	10	11*
6	43	46
7	6	12*
8	19	21
H,K=	1,	1
-9	19	23
-8	35	34
-7	52	50
-6	9	7*
-5	105	106
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-3	347	339
-2	385	390
-1	295	309
0	64	66
1	251	257
2	128	128
3	147	150
4	44	42
5	62	60
6	24	26
7	29	30
8	39	41
H,K=	1,	2
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-8	64	63
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-6	13	13
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-3	265	268
-2	405	420
-1	319	327
0	691	724
1	174	174
2	170	166
3	17	17
4	22	25
5	24	23
6	55	54
7	40	41
8	18	19
H,K=	1,	3
-9	0	7*
-8	107	104
-7	41	41
-6	17	19
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-3	106	104
-2	195	200
-1	255	266
0	286	297
1	45	43
2	130	124
3	74	77
4	88	86

5	10	8*
6	14	16
7	35	39
H,K=	1,	4
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-8	14	13
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0	59	55
1	251	264
2	32	33
3	138	135
4	21	20
5	39	38
6	5	3*
7	17	18
H,K=	1,	5
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-8	72	71
-7	77	78
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-5	91	86
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-3	148	148
-2	51	51
-1	98	109
0	8	7
1	122	125
2	48	48
3	16	17
4	140	140
5	72	67
6	22	20
7	14	14
H,K=	1,	6
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-8	24	26
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-5	82	80
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0	172	174
1	36	37
2	137	141
3	103	101
4	43	41
5	26	24
6	2	1*
H,K=	1,	7
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-7	18	18
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-5	78	78
-4	84	83
-3	49	50
-2	71	69
-1	54	54
0	18	15
1	86	88
2	34	30
3	3	6*
4	114	109
5	21	19
6	17	16
H,K=	1,	8
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-7	31	29
-6	20	24
-5	63	62
-4	101	103
-3	22	18
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-1	116	116
0	10	8
1	34	36
2	86	87
3	39	40
4	72	71
5	12	12
H,K=	1,	9
-8	16	17
-7	15	13
-6	66	72
-5	57	55
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-1	3	4*
0	84	80
1	29	33
2	82	77
3	18	20
4	65	64
5	7	5*
H,K=	1,	10
-8	40	44
-7	38	35
-6	68	66
-5	31	32
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-3	93	94
-2	79	76
-1	22	18
0	21	25
1	6	3*
2	50	52
3	23	20
4	12	11
H,K=	1,	11

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-6	47	46
-5	79	79
-4	13	14*
-3	170	171
-2	36	35
-1	97	98
0	0	6*
1	3	10*
2	12	10
3	14	14
H,K=	1,	12
-6	4	9*
-5	17	18
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-3	5	5*
-2	75	79
-1	15	12
0	74	76
1	0	3*
2	13	13
H,K=	1,	13
-5	8	9
-4	0	5*
-3	83	83
-2	14	18
-1	31	33
0	6	5*
1	15	12
H,K=	1,	14
-4	12	18
-3	2	3*
-2	29	29
-1	0	1*
H,K=	2,	-15
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0	0	6*
1	24	24
2	50	46
3	13	15
4	4	3*
H,K=	2,	-14
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-2	49	50
-1	24	24
0	17	18
1	7	2*
2	9	11*
3	48	47
4	29	27
5	21	21
H,K=	2,	-13
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-3	24	23
-2	42	37
-1	24	25
0	40	40
1	105	103
2	24	24

3	22	21
4	41	41
5	63	62
6	5	6*
H,K=	2,	-12
-5	19	19
-4	50	51
-3	0	3*
-2	10	4
-1	13	13
0	27	29
1	67	68
2	42	42
3	25	25
4	15	17
5	32	32
6	1	2*
7	25	25
H,K=	2,	-11
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-2	30	32
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0	41	34
1	46	49
2	14	15
3	89	88
4	41	41
5	3	1*
6	32	32
7	17	14
H,K=	2,	-10
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-5	18	18
-4	18	16
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-2	28	30
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0	89	87
1	77	81
2	27	28
3	0	4*
4	72	72
5	77	81
6	29	29
7	3	1*
H,K=	2,	-9
-6	52	53
-5	85	84
-4	62	61
-3	2	6*
-2	50	55
-1	38	40
0	19	17
1	51	53
2	96	98
3	90	87
4	45	42

5	118	119
6	79	81
7	25	28
8	27	26
H,K=	2,	-8
-7	0	0*
-6	37	37
-5	4	0*
-4	19	17
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-1	14	11
0	88	83
1	147	148
2	75	76
3	158	161
4	45	42
5	58	60
6	64	63
7	11	8
8	17	17
H,K=	2,	-7
-7	26	28
-6	83	80
-5	19	18
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-3	101	96
-2	112	110
-1	50	50
0	97	103
1	12	13
2	218	210
3	91	90
4	11	9
5	78	75
6	137	134
7	58	60
8	0	4*
H,K=	2,	-6
-8	22	21
-7	20	20
-6	7	10*
-5	2	3*
-4	47	46
-3	71	71
-2	291	300
-1	69	73
0	281	290
1	71	75
2	106	104
3	106	101
4	60	56
5	44	45
6	9	3
7	100	97
8	32	35
H,K=	2,	-5
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-7	20	20

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1	85	88
2	382	382
3	129	123
4	16	15
5	163	162
6	51	53
7	34	34
8	21	23
H,K=	2,	-4
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-7	48	52
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-4	53	52
-3	102	103
-2	71	78
-1	31	32
0	148	149
1	153	153
2	33	34
3	8	9
4	91	90
5	105	101
6	45	43
7	54	56
8	9	10*
H,K=	2,	-3
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-8	23	23
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-5	141	142
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3	8	0*
4	26	27
5	136	133
6	116	114
7	25	27
8	29	27
H,K=	2,	-2
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2	96	97
3	324	320
4	21	17
5	13	17
6	49	51
7	11	10
8	7	13*
H,K=	2,	-1
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-1	396	406
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1	154	166
2	303	292
3	19	14
4	24	20
5	59	58
6	15	20
7	5	2*
8	11	13
H,K=	2,	0
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-7	13	8
-6	21	21
-5	21	18
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-2	155	151
-1	450	472
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1	0	9*
2	254	252
3	178	168
4	143	143
5	121	126
6	91	94
7	20	24
8	2	4*
H,K=	2,	1
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-6	13	14*
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0	122	118
1	55	55
2	42	45
3	163	157
4	40	38
5	80	79
6	93	94
7	54	56
8	15	13
H,K=	2,	2
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-3	143	138
-2	116	116
-1	536	557
0	292	293
1	35	35
2	9	14
3	58	58
4	101	99
5	4	5*
6	14	14
7	10	6
H,K=	2,	3
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-3	320	318
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-1	5	13*
0	175	172
1	125	125
2	48	52
3	50	46
4	84	85
5	32	31
6	4	5*
7	17	20
H,K=	2,	4
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-5	57	51
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-3	23	24
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0	11	4
1	39	39
2	112	112
3	156	157
4	124	125
5	8	5*
6	2	4*
7	22	21
H,K=	2,	5
-9	6	4*
-8	14	13
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-6	53	51
-5	92	96
-4	86	86
-3	43	42
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0	38	45
1	11	11
2	48	45
3	81	82
4	48	48
5	29	28
6	25	26
H,K=	2,	6
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-8	17	15
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-1	198	204
0	22	20
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2	27	30
3	167	168
4	15	16
5	30	32
6	14	11
H,K=	2,	7
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-8	1	5*
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-6	33	31
-5	55	54
-4	27	26
-3	51	52
-2	67	70
-1	73	73
0	102	103
1	6	1*
2	93	94
3	4	1*
4	15	11
5	19	20
H,K=	2,	8
-8	27	23
-7	101	101
-6	41	44
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-2	93	91
-1	112	115
0	55	58
1	69	70
2	81	81
3	61	65
4	12	12
5	10	3*
H,K=	2,	9
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-7	35	37
-6	82	82
-5	47	49
-4	8	5
-3	8	10*
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0	57	55
1	72	73
2	62	64
3	21	18
4	27	28
H,K=	2,	10
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-5	22	26
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-1	18	17
0	13	11
1	43	45
2	44	49
3	6	4*
H,K=	2,	11
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-6	16	15
-5	21	21
-4	6	9*
-3	45	43
-2	7	2*
-1	34	33
0	35	34
1	42	43
2	23	19
H,K=	2,	12
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-4	56	57
-3	34	34
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H,K=	3,	-15
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H,K=	3,	11
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H,K=	4,-16	
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H,K=	4,-15	
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H,K=	4,-12	
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4	48	50
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3	17	16

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H,K=	5,	-15
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3	30	29
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4	66	65

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2	141	138
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4	45	41
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6	12	6
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H,K=	5,	-6
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3	208	205
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3	73	73
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0	43	40
1	74	75
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H,K=	8, 3	
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H,K=	8, 4	
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0	28	30
H,K=	8, 5	
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-2	8	6*
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H,K=	8, 6	
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H,K=	9,-14	
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0	25	26
H,K=	9,-13	
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0	38	38
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H,K=	9,-12	
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0	33	34
1	13	14
2	11	11
H,K=	9,-11	
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0	5	4*
1	55	56
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H,K=	9,-10	
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0	12	11
1	20	18
2	5	7*
3	16	18
H,K=	9,	-9
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0	55	55
1	68	66
2	45	46
3	0	2*
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-5	2	4*
-4	20	23
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-2	17	18
-1	24	24
0	30	28
1	42	40
2	3	3*
3	0	1*
H,K=	9,	-7
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0	47	47
1	0	4*
2	49	49
3	15	16
H,K=	9,	-6
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0	80	79
1	14	17*
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H,K=	9,	-5
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H,K=	9,	-3
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-3	6	7*
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2	23	27
H,K=	9,	-1
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-6	7	12*
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1	0	7*
2	25	27
H,K=	9,	0
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0	29	29
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H,K=	10,	-11
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0	9	9
1	23	23
H,K=	10,	-10
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H,K=	10,	-9

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0	0	1*
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H,K=	10,	-6
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H,K=	10,	-4
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0	8	12*
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H,K=	10,	-3
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H,K=	10,	-2
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H,K=	10,	-1
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H,K=	10,	0
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H,K=	10,	1
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H,K=	11,	-10
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H,K=	11,	-9
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H,K=	11,	-8
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H,K=	11,	-7
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H,K=	11,	-6
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