Title
THE CRYSTAL AND MOLECULAR STRUCTURE OP 2-(N-NITROSOMETHYL-AMINO) ACETAMIDE

Author
Templeton, Lieselotte K.

Publication Date
1972-05-01

Submitted to Journal of American
Chemical Society

LBL-669
Preprint

THE CRYSTAL AND MOLECULAR STRUCTURE OF 2-(N-NITROSOMETHYL-AMINO) ACETAMIDE

Lieselotte K. Templeton, David H. Templeton,
and Allan Zalkin

May 1972

AEC Contract No. W-7405-eng-48

LBL-669

DISCLAIMER

The Crystal and Molecular Structure of 2-(N-nitrosomethylamino)Acetamide.[1]

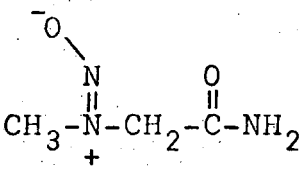
Lieselotte K. Templeton, David H. Templeton and Allan Zalkin.

Contribution from the Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720.

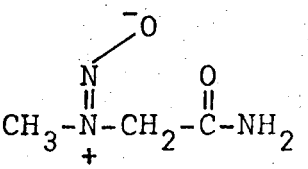
Received

Abstract: Crystals of 2-(N-nitrosomethylamino) acetamide are monoclinic, space group $P2_1/n$, with a = 16.681(30), b = 4.774(5), c = 14.318(15) Å and β = 92.95(0.2)°. Each unit cell contains four molecules of the E isomer and four of the Z isomer. The structural model was refined to R = 0.044 for 1184 independent reflections measured with an automatic diffractometer. Hydrogen bonds from amide groups to carbonyl or nitroso oxygen atoms connect the molecules in sheets parallel to (100).

Kenyon and Rowley[2] found 2-(N-nitrosomethylamino) acetamide as the hydrolysis product of a secondary N-nitrosoamine. It crystallized as a mixture of needles and plates. On the basis of nmr spectra they concluded that the needles contained a mixture of the E and Z isomers:



E



Z

In this paper we report a crystal structure determination which confirms this result. We found a 50:50 mixture of the isomers with conformations as shown in Fig. 1.

EXPERIMENTAL.

Colorless, needlelike crystals, synthesized by the reaction of sarcosinamide with nitrous acid,[2] were provided by Professor Kenyon of the University of California, Berkeley. A crystal of dimensions 0.066 x 0.042 x 0.111 mm was glued to the tip of a glass fiber in air with the b axis parallel to the axis of the fiber. Preliminary X-ray diffraction data were obtained from oscillation and Weissenberg photographs taken with copper radiation. Accurate unit cell dimensions were determined from measurement of h 0 0, 0 k 0, 0 0 ℓ reflections using a Picker automatic diffractometer equipped with a full circle goniostat, graphite monochromator and PDP-8I computer. Intensity data were collected

with the same instrument. The integrated intensity of each reflection was measured by a θ-2θ scan technique, using a scanning rate of 1°/min., from 1° below the 2θ angle at which $K_{\alpha 1}$ was diffracted to 1° above the 2θ angle at which $K_{\alpha 2}$ was diffracted. Two 10-second background counts with the apparatus stationary were taken 0.5° below and 0.5° above the 2θ angle at which the scanning was begun and ended. Three strong reflections (600, 004, 020) were checked periodically (every 100 reflections) for crystal decomposition and/or machine malfunction. The crystal had to be slightly realigned several times during the data taking which lasted 9 days.

From the above three "standard" reflections it was found that there was a 30% decay in the intensities during the experiment. Scale factors were adjusted on the assumption that all reflections decreased at the same rate.

All calculations were made on the CDC 6600. Recorded counts were treated as follows: (recorded counts) x 10 + 4.5 = actual counts. When the background was recorded as zero, it was set equal to 6 (because we do not have a counter for the last digit). The actual counts were converted into structure factors and standard deviations σ(F) using the formula given elsewhere,[3] except that the additional term in $\sigma^2(I)$ was $(0.06I)^2$.

The absorption coefficient for this compound is μ = 9.9 cm^{-1}. No correction for absorption was made, because it was considered to be negligible (at most 7%).

The hemisphere ± h, k, ± ℓ was measured. Excluding systematic space group absences, there were 2444 data of which 576 had intensities less than the standard deviations and included 168 reflections measured to be zero. When a reflection was measured more than once, the intensities were averaged and its standard deviation was treated as set forth elsewhere.[3] These 2444 reflections represent 1417 unique reflections of which 1184 are greater than one standard deviation.

The two figures were prepared with Johnson's ORTEP program.[4]

The ratios of observed and calculated structure factors for the strongest reflections range from 0.95 to 1.05 and give no indication of any significant extinction effect.

CRYSTAL DATA.

The crystals are monoclinic with unit cell dimensions measured at room temperature (~24°C): a = 16.681 ± 0.030, b = 4.774 ± 0.005, c = 14.318 ± 0.015 Å, β = 92.95 ± 0.2°. There are eight molecules of $C_3H_7N_3O_2$ (four of each isomer) in the unit cell. The calculated density ρ = 1.367 g/cc agrees well with the observed density ρ = 1.36 ± 0.02 g/cc measured by flotation in solutions of chloroform and hexane.

The extinction rules (h0ℓ absent if h + ℓ = 2n + 1 and 0k0 absent if k = 2n + 1) are characteristic of space group $P2_1/n$. All atoms are in general positions.

DETERMINATION OF THE STRUCTURE.

The structure was solved from statistics. The phases of normalized structure factors E were calculated with Long's program[5] which uses Sayre's equation. The 16 possible combinations of signs of four reflections (in addition to 3 origin determining reflections) were used to calculate probable phases for the 165 reflections whose |E| values were $\geq$ 1.50. One combination of signs was better than the rest. This solution had a consistency index of 0.80 compared to the next best value of 0.77, and also took the fewest cycles (6) to determine all the signs. The Fourier synthesis of this best E set showed both the E and Z isomers and yielded the coordinates of the 16 non hydrogen atoms (carbon, nitrogen and oxygen) in the asymmetric unit.

With anisotropic thermal parameters (for the 16 atoms) the full matrix least squares refinement reduced $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$ to 0.089 for 1184 non zero reflections. The scattering factors of Cromer and Waber[6] were used for all atoms except hydrogen whose scattering factors are those of Stewart, Davidson, and Simpson.[7] All 14 hydrogens except for one in the methyl group of the E isomer showed well defined peaks in a ΔF Fourier. When in addition to the 16 non hydrogen atoms with anisotropic temperature factors, three positional parameters and an isotropic thermal temperature factor were included for each of the 14 hydrogens, refinement gave $R_1 = 0.0477$ after 4 cycles. Further

refinements were made with a variation of our least squares program (written by Arthur Olson)[8] which uses the scattering factors of Stewart et al.[7] for polarized H atoms. The R hardly changed (R = 0.0476), but the hydrogen distances lengthened by about 0.1 Å. Final refinement, using for C, N, and O the scattering factors of Doyle and Turner[9] and anomalous dispersion of Cromer and Liberman[10] brought R_1 down to 0.044 and $R_2 = [\Sigma w(\Delta F)^2/\Sigma w(F_o)^2]^{1/2}$ to 0.052. No parameter shifted more than 2.7% of its estimated standard deviation in the final refinement.[11]

RESULTS AND DISCUSSION.

Final values for atomic coordinates and thermal parameters are given in Tables I, II and III. Bond distances and angles are listed in Tables IV and V. Corresponding bond distances in the two isomers (Figure 1) are equal within the experimental accuracy except perhaps the N-N and N-O distances; the latter differ respectively by three and two times the sums of the standard deviation.

The dimensions of the amide groups (corrected for thermal motion) are in excellent agreement with the corresponding bond lengths C-N = 1.338(7) and C-O = 1.258(6) Å reported by Denne and Small[12] for acetamide, and C-N = 1.334(7), 1.333(7) and C-O = 1.255(7), 1.254(7) Å reported by Chieh, Subramanian, and Trotter[13] for malonamide. For the amide-methylene bond (uncorrected for thermal motion)

our values C-C = 1.513(4), 1.518(4) Å are almost identical with C-C = 1.503(8), 1.513(8) Å in malonamide.[13] The C-N bond lengths exhibit the partial double-bond character typical of amides. The bond lengths in the vicinity of the nitroso groups agree within 0.03 Å or better with corresponding bonds in gaseous nitrosodimethylamine as determined by Rademacher, Stølevik and Lüttke[14] by electron diffraction: N-O = 1.235(2), N-N = 1.344(2), and N-C = 1.461(2) Å. We have failed to find reports of accurate determinations in the solid phase of structures of strictly analogous molecules. Boer and Turley[15] have reviewed the rather discordant results for several nitroso monomers and dimers. In dimethylnitrosamine copper(II) chloride, Klement[16] found N-O = 1.22(2), N-N = 1.29(2), and N-C = 1.46(3) and 1.47(3) Å.

Each amide hydrogen atom is pointed toward an oxygen atom at a reasonable distance for an N-H···O hydrogen bond. These bond lengths are listed in Table IV. These bonds, as shown in Figure 2, connect the amide of the Z molecule to nitroso oxygen atoms of each kind of molecule. The amide of the E molecule is connected to carbonyl oxygen atoms of each kind of molecule. These bonds connect the molecules in infinite layers parallel to b and c.

We thank Professor George Kenyon and Mr. George Rowley for providing the crystals for this study.

REFERENCES

(1) Work performed under the auspices of the U.S. Atomic Energy Commission.

(2) G. L. Kenyon, G. L. Rowley, J. Amer. Chem. Soc., 93, 5522 (1971).

(3) D. St. Clair, A. Zalkin and D. H. Templeton, Inorg. Chem., 10, 2587 (1971).

(4) C. K. Johnson, "ORTEP: A Fortran Thermal-Ellipsoid Program for Crystal Structure Illustration." Report ORNL - 3794 Oak Ridge National Laboratory, Oak Ridge, Tenn., (1965).

(5) R. E. Long, thesis, University of California, Los Angeles (1965).

(6) D. T. Cromer and J. T. Waber, Acta Cryst., 18, 104 (1965).

(7) R. F. Stewart, E. R. Davidson and W. T. Simpson, J. Chem. Phys., 42, 3175 (1965).

(8) This unpublished program uses a complex form factor to represent a noncentric distribution of electron density in the hydrogen atom, with the proton taken as the point of reference. The coordinates which result are therefore an estimate of the proton position, rather than the estimate of some kind of average position of the electron cloud which is given by the traditional X-ray method.

(9) P. A. Doyle and P. S. Turner, Acta Cryst., A24, 390 (1968).

(10) D. T. Cromer and D. Liberman, J. Chem. Phys., 53, 1895 (1970).

(11) A table of observed and calculated structure factors will appear following these pages in the microfilm edition of this volume of this journal. Single copies may be obtained

(12) W. A. Denne and R. W. H. Small, Acta Cryst. B27, 1094 (1971).

(13) P. C. Chieh, E. Subramanian, and J. Trotter, J. Chem. Soc.(A), 179 (1970).

(14) P. Rademacher, R. Stølevik and W. Lüttke, Angew. Chem., 80, 842 (1968).

(15) F. P. Boer and J. W. Turley, J. Amer. Chem. Soc., 91, 1371 (1969).

(16) U. Klement, Acta Cryst., B25, 2460 (1969).

Table I. Coordinates for Nonhydrogen Atoms.

Atom	x	y	z
N(1)	.2044(2)	.6926(6)	.3999(2)
C(2)	.2823(2)	.6506(5)	.4120(2)
O(3)	.3267(1)	.7901(4)	.4652(1)
C(4)	.3160(2)	.4141(6)	.3557(2)
N(5)	.3997(1)	.4585(5)	.3391(2)
C(6)	.4625(3)	.306(1)	.3905(3)
N(7)	.4219(2)	.6529(6)	.2816(2)
O(8)	.3648(1)	.7866(5)	.2456(1)
N(9)	.8394(2)	.4168(6)	.1479(2)
C(10)	.8483(1)	.5837(5)	.2205(2)
O(11)	.8485(1)	.8405(4)	.2149(1)
C(12)	.8573(2)	.4421(6)	.3154(2)
N(13)	.9008(1)	.6173(5)	.3823(1)
C(14)	.9856(2)	.665(1)	.3783(3)
N(15)	.3540(2)	.7544(6)	.4391(2)
O(16)	.8910(1)	.9194(5)	.4903(1)

Table II. Anisotropic Thermal Parameters.[a]

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
N(1)	5.3(2)	4.1(1)	4.5(1)	.1(1)	1.0(1)	-.9(1)
C(2)	5.5(2)	2.2(1)	2.7(1)	-.2(1)	.6(1)	.1(1)
O(3)	6.8(1)	3.9(1)	3.99(9)	-.48(9)	.12(8)	-1.26(8)
C(4)	5.2(2)	2.5(1)	4.1(1)	-.2(1)	.3(1)	-.3(1)
N(5)	5.0(1)	2.7(1)	4.3(1)	-.11(9)	.53(9)	-.4(1)
C(6)	5.7(2)	5.4(2)	7.1(2)	.5(2)	-1.0(2)	-.9(2)
N(7)	5.8(1)	4.2(1)	5.3(1)	.1(1)	1.1(1)	-.7(1)
O(8)	7.1(1)	5.4(1)	5.3(1)	.4(1)	.8(1)	.9(1)
N(9)	6.8(1)	2.1(1)	3.3(1)	-.2(1)	-.7(1)	.2(1)
C(10)	4.0(1)	2.1(1)	3.5(1)	.02(9)	-.33(9)	.3(1)
O(11)	7.5(1)	1.87(9)	4.4(1)	.07(8)	-.58(8)	.31(7)
C(12)	5.8(2)	2.5(1)	3.4(1)	-.4(1)	-.6(1)	.0(1)
N(13)	4.5(1)	2.5(1)	2.90(9)	.39(8)	.34(8)	-.61(8)
C(14)	4.0(2)	7.7(3)	4.5(2)	.1(2)	.0(1)	-.5(2)
N(15)	6.7(1)	4.1(1)	3.6(1)	-.6(1)	-.5(1)	-.1(1)
O(16)	7.2(1)	6.6(1)	5.7(1)	.4(1)	.3(1)	-2.1(1)

[a]The temperature factor is $\exp(-\Sigma_i \Sigma_j B_{ij} h_i h_j b_i b_j/4)$, where b_i is the length of the ith reciprocal cell dimension.

Table III. Parameters for Hydrogen Atoms.

Atom	x	y	z	B
H(1)	.180(2)	.825(8)	.439(2)	6.5(10)
H(2)	.171(2)	.583(8)	.361(2)	5.1(9)
H(3)	.280(2)	.395(7)	.291(2)	5.1(7)
H(4)	.312(1)	.253(6)	.395(2)	3.2(6)
H(5)	.459(2)	.10(1)	.370(3)	9.2(12)
H(6)	.516(2)	.381(8)	.375(2)	6.0(10)
H(7)	.459(2)	.326(9)	.462(3)	8.3(11)
H(8)	.326(2)	.485(7)	.089(2)	4.8(8)
H(9)	.839(2)	.224(8)	.156(2)	4.6(8)
H(10)	.795(2)	.397(8)	.335(2)	6.7(9)
H(11)	.392(2)	.268(7)	.307(2)	4.5(7)
H(12)	1.010(2)	.723(9)	.441(3)	7.9(10)
H(13)	.996(3)	.79(2)	.323(4)	15.4(22)
H(14)	1.010(3)	.48(1)	.362(4)	11.4(17)

Table IV. Bond distances (Å). Distances after correction for thermal motion by the riding model are given in parentheses.

Z Molecule		E Molecule	
N(1)-C(2)	1.318(4)	N(9)-C(10)	1.312(4)
	(1.335)		(1.326)
C(2)-O(3)	1.230(4)	C(10)-O(11)	1.229(3)
	(1.252)		(1.252)
C(2)-C(4)	1.513(4)	C(10)-C(12)	1.518(4)
C(4)-N(5)	1.444(4)	C(12)-N(13)	1.439(4)
N(5)-C(6)	1.445(5)	N(13)-C(14)	1.438(5)
	(1.471)		(1.467)
N(5)-N(7)	1.308(3)	N(13)-N(15)	1.328(4)
N(7)-O(8)	1.237(4)	N(15)-O(16)	1.223(3)
	(1.250)		(1.241)
N(1)-H(1)	0.96(4)	N(9)-H(8)	0.92(3)
N(1)-H(2)	0.93(4)	N(9)-H(9)	0.93(4)
C(4)-H(3)	1.08(3)	C(12)-H(10)	1.12(3)
C(4)-H(4)	0.95(3)	C(12)-H(11)	1.02(3)
C(6)-H(5)	1.04(5)	C(14)-H(12)	1.01(4)
C(6)-H(6)	1.00(4)	C(14)-H(13)	1.02(7)
C(6)-H(7)	1.04(4)	C(14)-H(14)	0.99(6)
N(1)···O(16)	2.948(5)	N(9)···O(3)	2.965(4)
N(1)···O(8)	3.030(5)	N(9)···O(11)	2.915(4)

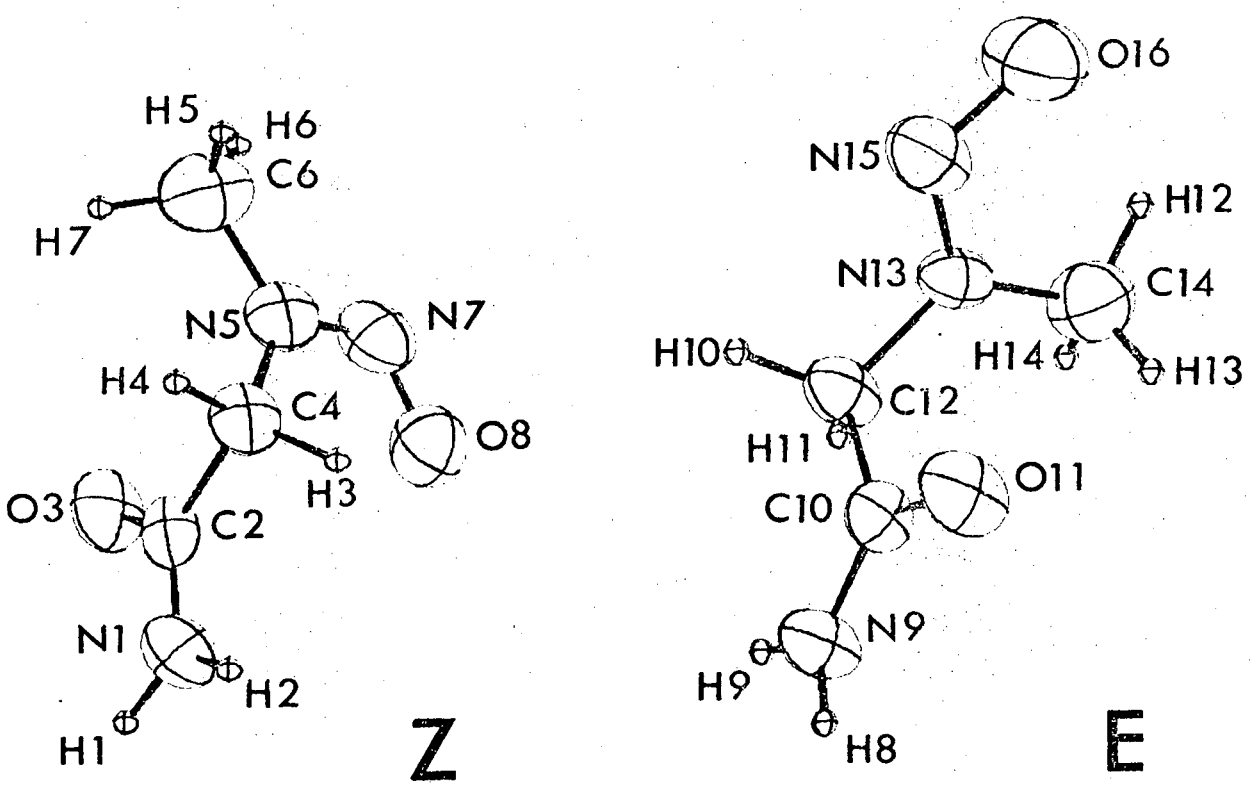
Table V. Bond Angles.

Z Molecule		E Molecule	
N(1)-C(2)-O(3)	123.9(3)°	N(9)-C(10)-O(11)	123.7(3)°
N(1)-C(2)-C(4)	115.8(3)	N(9)-C(10)-C(12)	116.2(3)
O(3)-C(2)-C(4)	120.3(3)	O(11)-C(10)-C(12)	120.2(2)
C(2)-C(4)-N(5)	111.6(3)	C(10)-C(12)-N(13)	111.1(2)
C(4)-N(5)-C(6)	121.6(4)	C(12)-N(13)-C(14)	121.9(3)
C(6)-N(5)-N(7)	117.2(4)	C(14)-N(13)-N(15)	123.8(4)
C(4)-N(5)-N(7)	121.1(3)	C(12)-N(13)-N(15)	113.7(3)
N(5)-N(7)-O(8)	113.0(3)	N(13)-N(15)-O(16)	113.0(2)
C(2)-N(1)-O(16)	125.6(2)	C(10)-N(9)-O(3)	114.4(2)
C(2)-N(1)-O(8)	109.3(2)	C(10)-N(9)-O(11)	108.1(2)
C(2)-N(1)-H(1)	119(2)	C(10)-N(9)-H(8)	121(2)
C(2)-N(1)-H(2)	123(2)	C(10)-N(9)-H(9)	120(2)
H(1)-N(1)-H(2)	118(4)	H(8)-N(9)-H(9)	118(3)
H(5)-C(6)-H(6)	109(4)	H(12)-C(14)-H(13)	118(5)
H(5)-C(6)-H(7)	111(5)	H(12)-C(14)-H(14)	107(4)
H(6)-C(6)-H(7)	107(4)	H(13)-C(14)-H(14)	104(7)

Figure Captions

Figure 1. Perspective drawing of the E and Z isomers. Thermal boundaries are at the 50% probability level. For this drawing the hydrogen atoms were given artificial thermal parameters of B = 0.5.

Figure 2. Projection of the unit cell looking down the b axis. Hydrogens are represented by the small circles. The dotted lines are hydrogen bonds. When the line is broken the bond is to the molecule above or below. The numbers identify the different oxygen atoms.



XBL 719-1339

Fig. 1

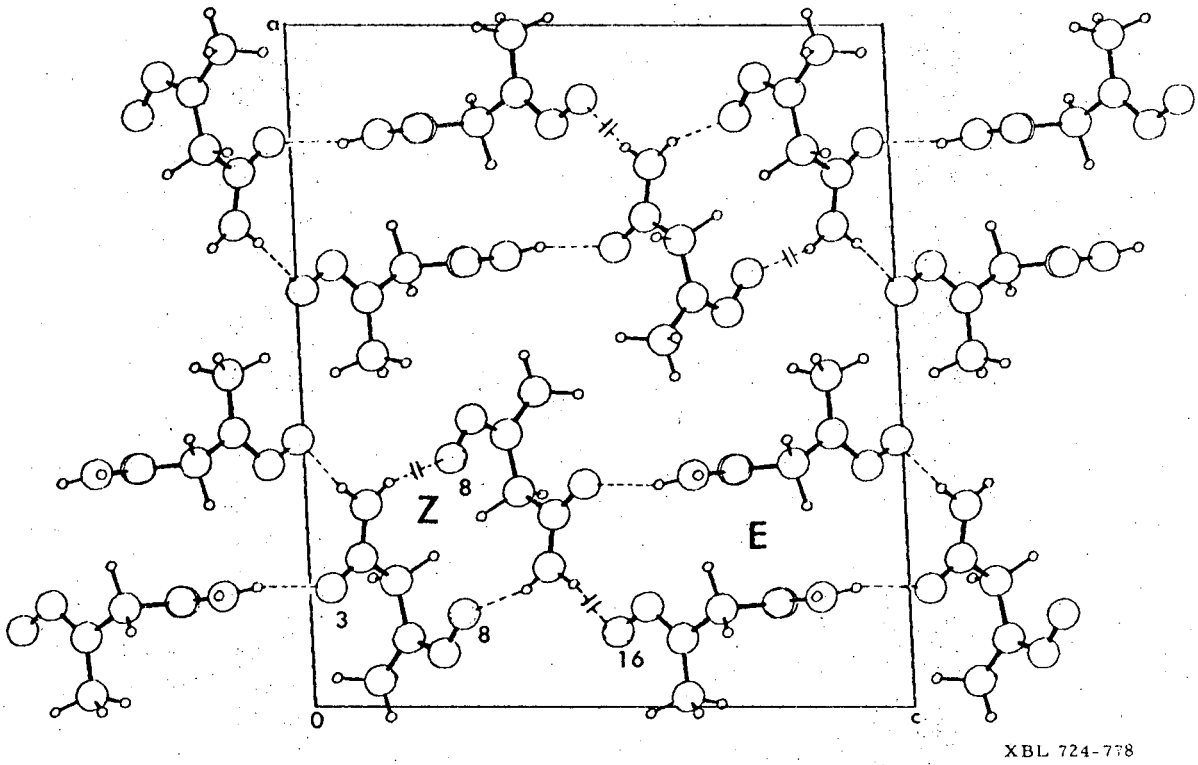


Fig. 2

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 8.0) FOR
2-(3-NITROSOMETHYLAMINO) ACETAMIDE F(0,0,0) = 3983

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	0,	0		1	47	7	-5	-13	29	6	1	H,K=	1,	4		-4	939	31	9
2	305	9	-19	2	71	3	-7	-12	62	6	5	-9	49	11	-10	-3	0	9	-3*
4	252	8	-29	3	109	4	3	-11	103	6	-2	-8	48	3	6	-2	128	5	6
6	94	3	0	4	51	6	-2	-10	180	7	2	-7	66	3	-0	-1	514	19	-4
8	206	6	-14	5	175	6	2	-9	125	4	2	-6	16	22	4*	0	698	21	29
10	13	7	3	H,K=	1,	0		-8	9	14	0*	-5	61	4	-0	1	523	16	-18
12	48	2	-2	-13	34	6	-2	-7	89	3	1	-4	13	24	-7*	2	239	7	-5
14	12	15	-8*	-13	204	7	-4	-6	239	9	6	-3	32	12	-8	3	156	6	-5
H,K=	0,	1		-11	154	5	1	-5	213	7	4	-2	48	5	-5	4	257	8	5
1	275	8	-1	-9	46	2	-2	-4	58	2	1	-1	68	3	-3	5	381	12	9
2	437	13	-4	-7	234	9	-4	-3	159	6	1	0	49	4	-3	6	235	8	13
3	693	22	-0	-5	349	11	4	-2	321	13	11	1	39	4	-8	7	23	8	2
4	605	19	19	-3	76	2	2	-1	189	6	10	2	76	3	4	8	24	9	1
5	165	5	-8	-1	55	2	5	0	193	8	17	3	94	4	4	9	0	19	-12*
6	47	2	1	1	110	4	-8	1	174	6	8	4	60	3	-0	10	53	2	-4
7	74	2	2	3	647	20	-36	2	315	12	5	5	37	7	6	11	22	7	-1
8	76	3	5	5	74	3	4	3	99	4	0	6	127	5	-1	12	117	4	4
9	29	3	1	7	64	3	8	4	26	5	-8	7	89	4	-1	13	11	12	6*
10	15	6	-1	9	90	3	-5	5	50	4	4	8	44	4	-2	14	27	5	2
11	40	3	-1	11	67	3	2	6	231	7	5	9	40	6	-8	H,K=	2,	2	
12	38	6	1	13	36	2	-1	7	46	2	1	H,K=	1,	5	-13	57	3	-0	
13	48	3	-2	15	58	3	-4	8	116	4	6	-2	54	3	-1	-12	63	4	-2
14	14	10	1	H,K=	1,	1		9	24	13	-5	-1	66	3	-0	-11	79	4	3
H,K=	0,	2	-14	126	4	2	10	52	3	-1	0	29	31	-8*	-10	18	11	-1	
0	325	10	7	-13	83	4	-2	11	31	5	-1	1	34	9	-13	-9	13	16	-1*
1	151	5	7	-12	22	7	-3	12	61	6	-4	2	5	15	-5*	-8	36	5	5
2	143	4	5	-11	114	5	5	13	117	4	-6	H,K=	2,	0	-7	157	5	2	
3	137	4	-3	-10	17	13	-2	H,K=	1,	3	-14	54	3	-3	-6	107	6	2	
4	156	5	11	-9	75	4	5	-12	12	18	-7*	-12	42	2	-2	-5	50	2	1
5	83	3	2	-8	27	3	-0	-11	43	4	-7	-10	0	16	-4*	-4	180	6	10
6	368	11	-4	-7	379	12	3	-10	14	16	8*	-8	372	11	1	-3	71	3	-0
7	278	8	8	-6	7	15	7*	-9	80	5	-5	-6	137	5	-4	-2	152	5	8
8	10	12	-8*	-5	50	3	-4	-8	137	5	3	-4	202	7	10	-1	250	8	12
9	138	4	5	-4	177	6	3	-7	252	8	0	-2	500	15	-41	0	82	4	12
10	0	18	-6*	-3	509	19	6	-6	114	4	4	0	285	9	-1	1	40	4	1
11	94	3	2	-2	412	15	-8	-5	61	3	3	2	650	21	-2	2	117	7	11
12	54	3	6	-1	272	10	-6	-4	152	5	5	4	353	11	19	3	285	9	14
13	8	16	-4*	0	32	6	8	-3	27	5	-7	6	23	6	-11	4	320	11	12
H,K=	0,	3		1	101	3	4	-2	63	3	1	8	125	5	9	5	180	7	9
1	135	4	-2	2	253	10	5	-1	56	3	-4	10	76	3	-0	6	17	4	-2
2	75	4	-2	3	470	16	6	0	14	8	13	12	147	6	-0	7	11	9	-11
3	159	5	0	4	229	7	-4	1	213	7	15	14	25	8	-3	8	32	4	0
4	36	3	-3	5	295	9	5	2	95	3	0	H,K=	2,	1	9	185	6	5	
5	110	4	3	6	221	7	-5	3	67	3	-0	-14	58	8	5	10	32	4	-2
6	148	5	-5	7	141	4	1	4	11	14	1*	-13	50	3	3	11	36	7	-6
7	119	4	0	8	67	3	-4	5	29	7	5	-12	4	18	-5*	12	24	8	-10
8	41	4	-3	9	151	5	4	6	53	3	-1	-11	112	4	3	13	71	2	-0
9	205	7	8	10	11	14	9*	7	188	6	4	-10	87	3	0	H,K=	2,	3	
10	30	5	-1	11	28	6	-5	8	29	10	-5	-9	15	18	6*	-12	52	3	-5
11	12	16	6*	12	122	4	-1	9	71	3	0	-8	68	2	1	-11	23	7	-7
12	27	7	-3	13	19	4	2	10	121	4	-4	-7	47	3	-6	-10	112	4	-4
H,K=	0,	4	14	38	5	-4	11	18	10	8	-6	268	9	-7	-9	17	20	9*	
0	117	4	-1	H,K=	1,	2	12	22	9	-11	-5	397	13	-4	-8	94	3	2	

OBSERVED STRUCTURES FACTORS (CONT) FOR
2-(N-NITROSOMETHYLAMINO) ACETAMIDE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	25	7	7	7	123	4	5	9	62	2	3	-4	811	24	-13	3	55	3	0
-6	117	4	-3	9	91	4	1	10	44	8	1	-2	752	25	-45	4	110	4	-2
-5	12	8	-1	11	291	9	-1	11	62	3	-4	0	958	33	-43	5	10	13	-3*
-4	48	7	4	13	60	4	-1	12	72	6	-2	2	0	13	-14*	6	243	8	4
-3	103	4	-3	H,K=		3,	1	13	53	3	-9	4	176	6	-7	7	39	8	7
-2	25	5	-2	-14	5	16	-5*	H,K=		3,	3	6	18	4	-2	8	148	6	3
-1	120	4	10	-13	94	3	-1	-12	31	5	11	8	221	7	1	9	39	3	1
0	138	5	1	-12	60	2	3	-11	68	4	-2	10	46	3	2	10	65	3	1
1	140	5	12	-11	75	4	3	-10	34	7	-4	12	23	6	-6	11	95	3	3
2	125	8	7	-10	5	15	-2*	-9	99	6	-1	14	58	4	-3	12	8	15	8*
3	79	6	4	-9	115	5	-4	-8	39	5	-4	H,K=		4,	1	13	22	9	4
4	84	3	-3	-8	85	3	3	-7	71	3	4	-14	16	16	-7*	H,K=		4,	3
5	78	4	4	-7	33	6	-9	-6	48	5	-10	-13	41	5	-3	-11	125	4	-4
6	54	3	-2	-6	115	4	-0	-5	62	3	0	-12	10	12	1*	-10	0	21	-4*
7	112	7	0	-5	233	9	-13	-4	50	3	2	-11	53	3	8	-9	19	8	-8
8	62	3	0	-4	157	6	10	-3	89	4	3	-10	49	4	-2	-8	40	3	2
9	9	16	4*	-3	14	11	6	-2	35	8	-3	-9	52	5	1	-7	13	18	-4*
10	197	9	-2	-2	205	6	-14	-1	125	4	2	-8	264	8	-2	-6	29	5	-4
11	93	4	6	-1	397	13	8	0	14	17	12*	-7	15	6	7	-5	18	21	2*
12	6	15	-14*	0	147	5	-4	1	8	11	0*	-6	61	2	0	-4	15	11	-3
H,K=		2,	4	1	492	15	-10	2	214	7	3	-5	37	2	0	-3	18	3	10
-9	9	15	3*	2	89	3	-5	3	128	5	6	-4	56	2	-2	-2	28	5	-4
-8	7	15	-12*	3	143	4	2	4	24	9	-4	-3	245	8	4	-1	258	8	12
-7	86	3	-3	4	79	6	-7	5	99	4	3	-2	183	6	19	0	194	11	-3
-6	86	3	2	5	354	12	14	6	77	3	1	-1	155	6	0	1	76	3	4
-5	83	4	5	6	157	6	1	7	136	4	2	0	53	10	22	2	93	4	2
-4	28	5	-7	7	115	4	5	8	35	5	-2	1	158	6	-3	3	13	16	10*
-3	7	14	-7*	8	145	4	1	9	67	3	0	2	137	4	4	4	55	3	-0
-2	11	14	4*	9	137	6	4	10	58	7	-10	3	258	8	-3	5	159	7	3
-1	29	4	-2	10	25	3	-5	11	22	12	-4	4	500	15	17	6	185	6	-1
0	19	6	6	11	47	4	-3	H,K=		3,	4	5	162	7	8	7	65	10	1
1	13	13	12*	12	30	3	1	-9	16	19	0*	6	130	4	10	8	13	17	-3*
2	26	4	-7	13	58	3	-0	-8	32	8	-11	7	97	3	-10	9	64	4	2
3	177	7	1	14	74	3	4	-7	100	3	-6	8	31	4	2	10	93	8	-6
4	12	15	2*	H,K=		3,	2	-6	132	4	3	9	91	4	-2	11	30	2	13
5	200	7	4	-13	65	4	-6	-5	43	3	1	10	37	4	-3	H,K=		4,	4
6	99	3	-1	-12	45	2	5	-4	47	2	5	11	68	3	0	-8	70	3	4
7	0	24	-7*	-11	11	16	8*	-3	36	7	7	12	19	14	-5	-7	118	4	-2
8	53	3	4	-10	44	3	-4	-2	26	6	-4	13	39	4	-2	-6	32	4	2
9	63	7	6	-9	32	3	-2	-1	103	4	-3	14	52	2	3	-5	111	4	1
H,K=		2,	5	-8	140	4	7	0	35	10	4	H,K=		4,	2	-4	31	3	12
-2	78	4	-3	-7	55	5	2	1	10	16	-8*	-13	85	4	-3	-3	64	3	-5
-1	93	6	-2	-6	176	6	6	2	87	3	2	-12	35	4	-0	-2	70	4	-3
0	100	4	-2	-5	72	5	1	3	120	4	1	-11	0	18	-16*	-1	0	30	-12*
1	114	6	0	-4	378	12	7	4	16	19	12*	-10	80	5	3	0	19	5	7
H,K=		3,	0	-3	234	10	8	5	38	7	2	-9	50	3	4	1	63	4	0
-15	21	7	-6	-2	138	6	7	6	176	6	-1	-8	110	4	-1	2	22	14	4
-13	62	3	-2	-1	50	2	2	7	22	5	6	-7	90	3	6	3	0	15	-12*
-11	62	3	2	0	71	2	-1	8	90	4	5	-6	66	3	0	4	22	5	8
-9	45	3	-5	1	31	3	3	H,K=		3,	5	-5	22	3	6	5	89	3	-1
-7	34	3	3	2	80	4	1	0	0	14	-3*	-4	329	10	8	6	65	3	-2
-5	179	6	-4	3	19	4	2	H,K=		4,	0	-3	99	3	-1	7	34	7	-1
-3	171	6	-2	4	214	7	-2	-14	13	16	3*	-2	33	5	-8	8	28	8	-8
-1	188	7	-14	5	263	7	7	-12	19	9	4	-1	122	6	8	H,K=		5,	0
1	76	3	2	6	129	4	-2	-10	237	8	-1	0	80	4	-7	-13	79	4	-3
3	829	26	-30	7	18	20	-2*	-8	256	8	2	1	263	8	13	-11	19	20	-10*
5	194	6	6	8	31	5	-1	-6	297	10	-1	2	29	3	-1	-9	155	5	1

OBSERVED STRUCTURES FACTORS (CONT) FOR
2-(N-NITROSOMETHYLAMINO) ACETAMIDE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	161	5	-3	2	55	3	-2	-10	32	3	2	1	239	7	2	-5	68	3	-1
-5	19	3	6	3	123	4	-0	-8	130	4	2	2	89	3	2	-3	346	11	-7
-3	260	8	-19	4	133	4	1	-6	13	14	-7*	3	40	4	-11	-1	183	6	-2
-1	830	25	-43	5	52	3	9	-4	126	4	-1	4	140	4	3	1	41	2	2
1	226	7	19	6	177	6	8	-2	32	2	-1	5	105	4	-0	3	338	10	-17
3	207	6	-7	7	26	3	1	0	580	18	17	6	36	5	-0	5	33	2	-0
5	46	7	-7	8	28	8	2	2	107	3	2	7	4	14	-13*	7	60	2	1
7	54	3	-2	9	16	6	7	4	54	2	1	8	20	15	-1	9	40	3	-4
9	236	7	6	10	80	3	2	6	31	2	0	9	45	5	3	11	173	5	1
11	26	5	-6	11	11	13	6*	8	66	3	-3	10	41	3	-4	13	12	20	-6*
13	58	3	0	12	24	11	-2	10	214	7	9	11	41	6	0	H,K=		7,	1
H,K=		5,	1	13	43	5	-2	12	0	15	-14*	12	52	4	-4	-13	101	3	-1
-14	34	3	3	H,K=		5,	3	14	0	19	-3*	H,K=		6,	3	-12	33	3	-3
-13	62	4	4	-11	13	20	6*	H,K=		6,	1	-11	20	17	7	-11	0	15	-22*
-12	31	3	-2	-10	25	11	2	-14	23	11	-1	-10	25	5	-13	-10	50	4	-2
-11	29	3	4	-9	8	21	-6*	-13	31	3	6	-9	23	4	4	-9	68	4	6
-10	37	6	1	-8	53	4	-4	-12	13	13	8*	-8	93	4	1	-8	27	4	-5
-9	101	3	-1	-7	205	6	-0	-11	55	4	1	-7	12	20	4*	-7	27	6	-6
-8	80	3	-3	-6	101	4	4	-10	49	3	-2	-6	29	8	1	-6	178	6	-4
-7	139	4	-5	-5	0	14	-15*	-9	44	9	1	-5	12	14	-4*	-5	197	6	-10
-6	4	16	-6*	-4	56	2	-3	-8	321	10	-1	-4	9	19	7*	-4	24	2	0
-5	141	5	7	-3	35	5	-4	-7	21	3	12	-3	118	4	1	-3	142	4	-18
-4	127	4	-5	-2	65	3	2	-6	179	6	-1	-2	40	5	-1	-2	240	7	-4
-3	73	3	-4	-1	33	2	-1	-5	136	4	-2	-1	88	3	2	-1	159	5	2
-2	80	3	-8	0	30	6	0	-4	296	9	-2	0	53	2	2	0	272	8	-11
-1	220	7	2	1	102	3	-4	-3	129	4	-11	1	154	5	4	1	38	2	-4
0	192	6	-8	2	104	4	1	-2	11	6	9	2	104	3	-3	2	57	2	-1
1	242	7	5	3	76	3	0	-1	100	3	3	3	15	19	4*	3	148	5	-5
2	32	2	-1	4	59	2	1	0	408	12	-8	4	87	3	2	4	21	6	-3
3	150	5	1	5	91	3	3	1	11	6	6	5	9	20	9*	5	5	11	-5*
4	110	3	-3	6	72	3	-0	2	86	3	5	6	142	5	-2	6	93	3	-3
5	100	3	3	7	75	3	-6	3	111	4	-2	7	40	6	2	7	47	2	0
6	287	9	2	8	71	4	-2	4	193	6	8	8	19	5	4	8	58	4	-0
7	167	5	-3	9	18	6	8	5	63	3	-3	9	35	4	-4	9	103	4	-2
8	84	3	4	10	47	5	-9	6	129	4	4	10	65	3	-1	10	16	6	8
9	76	3	1	11	0	14	-4*	7	68	2	2	H,K=		6,	4	11	25	4	0
10	64	3	3	H,K=		5,	4	8	110	4	3	-8	12	19	-1*	12	12	13	2*
11	13	11	8	-8	35	3	-0	9	0	14	-10*	-7	31	7	-2	13	52	4	-1
12	96	3	-4	-7	10	22	-17*	10	58	3	-1	-6	63	3	1	H,K=		7,	2
13	78	3	-4	-6	25	11	-6	11	40	6	-4	-5	59	3	3	-12	19	7	-8
14	14	7	5	-5	0	15	-23*	12	0	21	-11*	-4	20	5	1	-11	44	5	-7
H,K=		5,	2	-4	13	6	17	13	24	11	-4	-3	30	8	-1	-10	11	20	-2*
-13	34	7	2	-3	125	4	-3	H,K=		6,	2	-2	0	21	-8*	-9	0	20	-1*
-12	10	13	5*	-2	71	3	0	-13	9	20	6*	-1	0	21	-3*	-8	38	3	-0
-11	21	5	2	-1	127	4	-11	-12	29	3	5	0	18	6	-3	-7	99	3	0
-10	30	8	-5	0	30	3	-0	-11	74	3	-0	1	82	3	-9	-6	0	19	-4*
-9	173	5	3	1	21	18	2	-10	0	15	-12*	2	121	4	2	-5	0	12	-2*
-8	20	13	-6	2	17	6	10	-9	6	20	-3*	3	76	3	-0	-4	129	4	-2*
-7	46	4	5	3	16	13	-7	-8	24	10	5	4	8	21	-2*	-3	48	4	0
-6	57	3	-2	4	13	21	-4*	-7	22	5	-3	5	154	5	-2	-2	57	3	-1
-5	38	2	-3	5	80	4	2	-6	19	11	6	6	12	20	9*	-1	41	3	5
-4	58	2	-2	6	32	4	-4	-5	94	3	-1	7	19	20	2*	0	26	3	-7
-3	123	4	-5	7	56	4	-4	-4	16	13	9	H,K=		7,	0	1	86	3	-2
-2	79	3	-4	8	8	19	3*	-3	115	4	12	-13	10	13	-1*	2	163	5	2
-1	86	3	-5	H,K=		6,	0	-2	191	6	-1	-11	76	3	-7	3	124	4	-5
0	56	3	-1	-14	34	7	-11	-1	232	7	-4	-9	144	5	-3	4	99	3	2
1	60	3	5	-12	135	4	-1	0	174	5	-8	-7	40	4	-7	5	68	3	-3

OBSERVED STRUCTURE FACTORS (CONT) FOR
2-(N-NITROSOMETHYLAMINO) ACETAMIDE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	38	5	-2	10	93	3	-0	-8	51	5	0	-3	54	5	0	6	16	18	-1*
7	0	19	-2*	12	51	2	-1	-7	10	13	-1*	-2	63	2	2	7	28	6	3
8	15	10	-10	H,K=		8,	1	-6	21	8	-0	-1	129	7	-7	8	89	4	3
9	0	20	-5*	-13	44	3	2	-5	91	5	1	0	123	4	-1	9	18	4	15
10	41	3	2	-12	0	20	-13*	-4	8	13	-2*	1	151	6	3	H,K=		9,	4
11	49	3	0	-11	20	5	2	-3	95	4	4	2	135	6	-1	-5	35	4	-4
12	38	6	2	-10	21	16	-4	-2	91	3	1	3	139	4	2	-4	64	11	-8
H,K=		7,	3	-9	18	7	-6	-1	75	3	-1	4	40	2	1	-3	108	6	-5
-11	71	3	0	-8	82	3	-6	0	140	7	-2	5	174	7	10	-2	0	30	-7*
-10	18	20	7*	-7	0	13	-14*	1	84	4	-0	6	120	4	4	-1	58	3	-4
-9	57	3	8	-6	62	2	-2	2	75	3	1	7	7	16	3*	0	79	3	1
-8	19	5	6	-5	34	2	-9	3	20	15	5	8	0	18	-10*	1	0	22	-18*
-7	86	3	-7	-4	120	4	7	4	69	4	3	9	79	5	4	2	24	5	-8
-6	25	10	2	-3	60	2	-1	5	84	4	1	10	51	4	-5	3	8	16	6*
-5	94	4	-1	-2	49	3	2	6	50	4	3	11	24	18	-3	4	66	3	5
-4	37	3	3	-1	55	2	1	7	12	18	-7*	12	61	3	2	H,K=		10,	0
-3	81	3	-0	0	88	4	-1	8	9	11	-5*	H,K=		9,	2	-12	50	3	0
-2	35	6	-6	1	18	3	6	9	31	2	1	-12	4	16	3*	-10	12	8	10
-1	38	3	-0	2	43	2	-2	H,K=		8,	4	-11	32	4	-4	-8	75	5	-2
0	0	14	-6*	3	53	3	-2	-6	15	17	2*	-10	12	17	-1*	-6	27	14	-1
1	18	5	10	4	200	6	1	-5	20	8	-3	-9	43	2	5	-4	194	6	3
2	68	4	-2	5	0	17	-6*	-4	0	37	-13*	-8	74	4	7	-2	254	9	-2
3	90	3	-1	6	131	6	0	-3	49	3	1	-7	9	15	7*	0	42	5	18
4	21	4	12	7	45	2	3	-2	57	3	1	-6	73	3	1	2	95	3	5
5	80	4	-7	8	35	6	0	-1	0	15	-4*	-5	74	3	-2	4	198	8	1
6	114	4	-8	9	53	4	4	0	8	20	-8*	-4	95	7	4	6	160	9	13
7	61	4	1	10	57	3	-4	1	72	3	-3	-3	76	3	8	8	133	6	-2
8	38	3	1	11	10	13	6*	2	93	3	-10	-2	6	15	2*	10	77	4	-1
9	48	5	0	12	54	2	3	3	10	20	8*	-1	23	9	0	12	14	15	6*
10	30	8	-4	H,K=		8,	2	4	0	15	-19*	0	0	14	-3*	H,K=		10,	1
H,K=		7,	4	-12	0	16	-10*	5	35	5	-6	1	97	3	1	-12	18	5	17
-7	30	4	2	-11	9	11	5*	6	21	21	-6*	2	21	6	0	-11	20	23	-9*
-6	63	3	4	-10	37	7	5	H,K=		9,	0	3	133	6	-1	-10	100	4	2
-5	25	4	0	-9	98	4	4	-13	89	5	7	4	30	4	-0	-9	34	6	-6
-4	3	20	-11*	-8	37	4	3	-11	65	5	-2	5	50	3	2	-8	194	7	3
-3	0	21	-2*	-7	32	4	-1	-9	87	5	-7	6	128	4	-0	-7	26	5	-14
-2	21	21	-4*	-6	83	6	8	-7	173	8	-2	7	11	16	10*	-6	6	16	4*
-1	25	11	-3	-5	130	4	-3	-5	31	2	-3	8	0	18	-10*	-5	85	4	-0
0	31	8	-3	-4	83	7	-9	-3	15	18	-1*	9	15	17	-5*	-4	45	3	0
1	13	13	12*	-3	105	6	-2	-1	584	18	-1	10	44	4	-2	-3	127	4	5
2	64	3	1	-2	84	3	4	1	10	13	8*	11	24	11	6	-2	143	4	5
3	54	5	0	-1	19	5	6	3	93	5	-3	H,K=		9,	3	-1	40	3	1
4	117	4	-2	0	43	3	3	5	73	2	1	-9	20	10	-0	0	19	3	1
5	74	4	2	1	46	3	-4	7	29	5	-1	-8	41	4	-6	1	126	4	4
6	84	4	-9	2	237	10	7	9	195	7	6	-7	8	18	-2*	2	92	4	6
H,K=		8,	0	3	107	5	1	11	92	5	1	-6	41	5	0	3	204	9	8
-12	108	4	2	4	96	3	2	H,K=		9,	1	-5	47	6	0	4	87	4	-0
-10	66	3	-0	5	0	15	-4*	-13	16	14	8	-4	48	4	2	5	115	4	1
-8	108	4	-2	6	24	3	3	-12	49	3	-3	-3	24	8	-6	6	31	4	-8
-6	43	3	2	7	84	3	3	-11	51	3	1	-2	69	2	2	7	39	4	-1
-4	410	13	-21	8	38	3	-1	-10	12	15	3*	-1	130	12	3	8	84	4	-2
-2	244	7	5	9	17	14	-2	-9	60	3	-4	0	82	4	-6	9	49	3	-1
0	69	2	0	10	75	3	3	-8	36	7	-0	1	71	3	2	10	46	5	-1
2	38	3	-5	11	11	15	4*	-7	98	5	7	2	82	9	5	11	71	3	2
4	175	5	3	H,K=		8,	3	-6	76	3	-2	3	96	4	-1	H,K=		10,	2
6	37	2	3	-10	39	7	-5	-5	36	5	2	4	14	15	1*	-11	46	5	-0
8	54	4	-0	-9	13	7	8	-4	144	5	-1	5	81	3	5	-10	15	17	-8*

OBSERVED STRUCTURES FACTORS (CONT) FOR
2-(N-NITROSOMETHYLAMINO) ACETAMIDE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	7	17	5*	5	123	5	1	-2	20	12	-2	2	68	4	0	-7	37	6	2
-3	18	8	-1	7	28	3	4	-1	16	5	12	3	71	4	2	-6	18	12	10
-7	100	5	4	9	73	4	-1	0	85	5	-2	4	70	3	0	-5	54	5	-3
-6	75	3	0	11	28	5	-5	1	77	6	-1	5	14	17	-1*	-4	104	5	4
-5	64	4	-3	H,K= 11,				1	2	36	3	3	6	26	5	-0	-3	10	15	3*
-4	31	5	-7	-12	54	3	-2	3	80	5	7	7	33	5	-6	-2	66	3	-1
-3	58	3	-4	-11	24	14	-4	4	24	3	2	8	0	13	-5*	-1	81	5	-0
-2	24	6	-0	-10	79	3	-3	5	11	15	-5*	H,K= 12,				3	0	95	4	-6
-1	80	4	-4	-9	38	5	-3	6	16	20	-4*	-7	18	9	3	1	34	5	-4
0	71	4	0	-8	0	18	-4*	7	0	15	-0*	-6	19	4	7	2	20	21	-8*
1	120	4	-5	-7	94	3	4	H,K= 12,				0	-5	40	5	-2	3	55	7	3
2	18	21	-4*	-6	108	5	-0	-10	60	3	5	-4	17	18	2*	4	80	3	-2
3	84	3	-4	-5	139	8	5	-8	44	2	3	-3	35	4	-3	5	25	8	3
4	38	4	-1	-4	76	3	5	-6	32	4	9	-2	37	2	6	6	13	17	-2*
5	91	5	4	-3	25	6	2	-4	73	6	2	-1	10	12	-0*	7	31	4	5
6	55	4	-2	-2	33	4	-6	-2	78	5	-6	0	19	15	-4	H,K= 13,			
7	59	2	3	-1	19	3	7	0	55	6	-2	1	63	4	-0	-5	13	16	-11*
8	29	4	0	0	55	3	0	2	181	6	5	2	52	6	8	-4	0	16	-3*
9	35	2	-3	1	72	2	2	4	99	5	-0	3	12	17	10*	-3	13	21	13*
10	56	3	-4	2	72	5	-1	6	119	6	-5	4	15	18	-7*	-2	108	4	-1
H,K= 10,				3	3	29	3	1	8	23	21	3	5	40	3	-5	-1	91	8	7
-9	26	7	5	4	19	6	5	10	163	6	-2	6	37	5	-2	0	52	7	-4
-8	82	3	1	5	12	15	-2*	H,K= 12,				1	H,K= 13,			0	1	56	4	3
-7	18	4	7	6	37	5	-5	-11	33	5	3	-9	98	7	7	2	38	2	-0
-6	30	5	-2	7	63	4	0	-10	27	5	-2	-7	105	4	5	3	69	3	-3
-5	75	6	1	8	45	2	3	-9	50	8	-6	-5	77	3	2	4	41	4	2
-4	70	3	4	9	92	6	4	-8	0	18	-4*	-3	49	5	-8	H,K= 14,			
-3	95	4	-1	10	1	13	-14*	-7	24	3	11	-1	13	16	-4*	-8	81	5	12
-2	53	6	-2	11	55	3	2	-6	58	3	2	1	49	4	2	-6	145	6	6
-1	30	3	2	H,K= 11,				2	-5	44	4	-5	3	37	3	2	-4	99	5	-11
0	52	3	-2	-10	26	7	-9	-4	18	20	-9*	5	72	3	-1	-2	52	6	3
1	38	5	-5	-9	20	4	5	-3	45	3	-2	7	172	8	-6	0	21	6	-3
2	54	3	-6	-8	6	15	-1*	-2	46	6	3	9	88	6	10	2	135	5	-3
3	76	3	2	-7	83	3	4	-1	4	16	-5*	H,K= 13,				1	4	15	5	9
4	22	4	5	-6	89	3	0	0	75	6	-6	-10	4	18	-1*	6	49	6	-0
5	63	3	-2	-5	62	5	1	1	41	2	-4	-9	56	3	3	8	50	4	0
6	112	4	-2	-4	74	4	4	2	116	4	3	-8	44	4	-3	H,K= 14,			
7	8	17	3*	-3	149	6	-2	3	29	5	-9	-7	12	8	11	-9	25	8	5
8	16	16	-9*	-2	208	9	-0	4	52	3	2	-6	45	2	5	-8	38	4	-4
H,K= 10,				4	-1	25	7	-4	5	95	4	4	-5	114	6	2	-7	59	6	-4
-4	12	15	7*	0	57	3	-4	6	79	5	0	-4	61	3	-1	-6	9	12	4*
-3	26	3	5	1	30	5	2	7	45	5	-4	-3	50	4	1	-5	9	18	-3*
-2	53	8	-4	2	20	6	-6	8	74	4	-2	-2	11	16	2*	-4	67	3	-0
-1	42	3	-1	3	53	4	2	9	16	18	-7*	-1	75	3	-6	-3	64	3	0
0	26	7	0	4	65	3	4	10	45	3	-3	0	73	4	4	-2	47	3	6
1	92	3	-0	5	22	3	-2	H,K= 12,				2	1	16	9	-4	-1	73	4	-4
2	42	4	3	6	23	6	1	-9	13	16	2*	2	16	9	11	0	88	3	-4
3	9	18	-3*	7	13	7	12	-8	36	4	-2	3	138	6	0	1	46	4	-4
H,K= 11,				0	8	40	5	-4	-7	10	12	5*	4	82	3	-5	2	52	4	-6
-11	98	6	8	9	30	5	-3	-6	38	3	-2	5	14	8	1	3	30	6	-0
-9	188	6	3	H,K= 11,				3	-5	53	4	6	6	76	3	1	4	3	18	-4*
-7	0	13	-7*	-8	30	2	-2	-4	29	11	-7	7	63	4	4	5	53	4	1
-5	92	4	1	-7	56	2	1	-3	58	6	5	8	72	3	1	6	71	9	-1
-3	14	4	8	-6	8	15	3*	-2	15	18	3*	9	34	9	-1	7	13	15	3*
-1	149	5	-3	-5	72	3	-3	-1	62	11	6	H,K= 13,				2	8	5	16	-3*
1	143	4	6	-4	98	3	1	0	40	6	0	-9	0	20	-2*	H,K= 14,			
3	9	11	-3*	-3	110	9	-0	1	27	7	3	-8	39	5	10	-7	10	18	-10*

OBSERVED STRUCTURES FACTORS (CONT) FOR
2-(N-NITROSOMETHYLAMINO) ACETAMIDE

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	13	17	-6*	-6	31	5	8												
-5	47	2	-2	-4	12	10	4												
-4	9	17	6*	-2	7	13	5*												
-3	77	5	1	0	89	3	-3												
-2	30	3	6	2	30	6	-3												
-1	18	8	2	4	37	9	-5												
0	49	4	2	H,K= 16,			1												
1	80	4	-2	-6	47	3	1												
2	31	6	-2	-5	43	4	1												
3	2	18	-11*	-4	24	26	-3*												
4	18	12	-6	-3	11	18	-7*												
5	14	15	-8*	-2	19	22	-8*												
6	0	17	-13*	-1	0	18	-11*												
H,K= 14,			3	0	28	13	-5												
-3	17	12	2	1	8	23	-9*												
-2	9	17	-1*	2	65	3	2												
-1	41	5	1	3	17	23	-2*												
0	4	15	2*	4	20	22	-5*												
1	6	15	-2*	5	0	16	-3*												
H,K= 15,			0	H,K= 16,			2												
-7	7	18	-9*	-3	22	22	1*												
-5	37	2	-1	-2	7	22	-16*												
-3	21	4	-9	-1	36	8	3												
-1	119	4	-6	0	0	16	-9*												
1	21	9	-2	1	0	22	-1*												
3	58	3	3	H,K= 17,			0												
5	10	16	-9*	-3	26	13	-9												
7	21	11	4	-1	47	4	0												
H,K= 15,			1	1	0	16	-1*												
-8	27	6	7	3	49	3	2												
-7	11	16	3*	H,K= 17,			1												
-6	10	15	4*	-3	41	7	7												
-5	25	8	0	-2	18	22	-12*												
-4	8	12	7*	-1	10	22	-10*												
-3	12	17	-2*	0	0	16	-26*												
-2	0	15	-10*	1	10	16	-11*												
-1	14	23	-13*	2	6	22	-6*												
0	25	3	5																
1	26	8	-9																
2	15	6	1																
3	63	6	-1																
4	22	6	2																
5	17	20	-0*																
6	32	4	-7																
H,K= 15,			2																
-6	4	17	-0*																
-5	11	14	-0*																
-4	4	18	0*																
-3	68	3	6																
-2	62	3	8																
-1	18	10	10																
0	42	2	1																
1	47	3	2																
2	23	7	-12																
3	0	18	-4*																
4	42	5	2																
H,K= 16,			0																

TECHNICAL INFORMATION DIVISION
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720