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Redetermination of thermal motion and interatomic distances in urea.*

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A minor error in the program used in a previous three-dimensional least-squares refinement of urea has been corrected. Revised values for the thermal and positional parameters are presented.

The discovery of a keypunch error in our copy of the program (Palenik, 1962) which we used in the refinement (Caron & Donohue, 1964) of the three-dimensional data from urea (Vaughan & Donohue, 1952) has made it necessary that that refinement be repeated with a corrected program. Fortunately, the punching error affected only the values of the derivatives of the imaginary parts of the F_{hkl} with respect to the B_{12} thermal parameters.

The new parameters are presented in Table 1. Except for the B_{12}'s, none of them differ from the previous values by as much as $0{\cdot}3\sigma$. The revised descriptions of the thermal vibration ellipsoids are presented in Table 2, and the revised components of the rigid body tensors are presented in Table 3. The tensors were calculated both with and without the S tensor (Schomaker & Trueblood, 1968). In this particular case, allowance for the additional degree of freedom made little difference to the results on the T and L tensors.

The final values for the interatomic distances and bond angles are depicted in Fig. 1. Values for the bond lengths corrected for thermal motion (Busing & Levy, 1964) are included in Fig. 1. The NH···O hydrogen bond distances have not been corrected as it is not possible to determine the degree of correlation between the thermal vibrations of neighbouring molecules. The changes in the bond distances and angles from the former values are all quite small; accordingly, no modification of the previous discussion of these is required.

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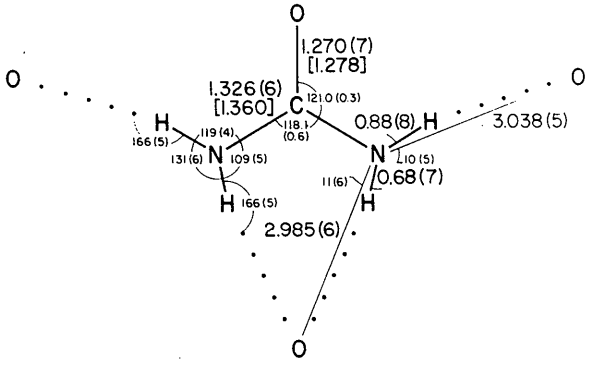

Fig. 1. Bond distances and angles. Standard errors are given in parentheses, and bond distances corrected for libration are given in brackets.

Table 2. *Vibration ellipsoids*

	i	$(\overline{r_i^2})^{1/2}$, Å	q_{ia}	q_{ib}	q_{ic}
O	1	0·241	$-1/2/2$	$-1/2/2$	0
	2	0·219	$-1/2/2$	$1/2/2$	0
	3	0·132	0	0	1
C	1	0·183	$-1/2/2$	$-1/2/2$	0
	2	0·196	$-1/2/2$	$1/2/2$	0
	3	0·154	0	0	1
N	1	0·200	−0·6906	−0·6906	0·2146
	2	0·332	$-1/2/2$	$1/2/2$	0
	3	0·146	0·1517	0·1517	0·9767

Table 3. *Translation and librational root mean sqaure amplitudes*

$T^{1/2}$	$L^{1/2}$	Direction
	(without S tensor)	
0·193 Å	4·4°	$a+b$
0·196	5·1	$a-b$
0·127	13·3	c
$T^{1/2}$	$L^{1/2}$	Direction
	(with S tensor)	
0·193 Å	4·4°	$a+b$
0·196	4·2	$a-b$
0·133	13·3	c

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Table 1. *Thermal parameters and their standard errors* (x10²). *Positional parameters** (x10⁴) *and their standard errors* (x10⁴)

	x (σ)	z (σ)	B_{11} (σ)	B_{33} (σ)	B_{12} (σ)	B_{13} (σ)	B (σ)
O		6000 (8)	4·19 (16)	1·37 (15)	0·79 (49)		
C		3305 (12)	2·84 (14)	1·88 (21)	−0·40 (50)		
N	1421 (7)	1857 (10)	5·90 (17)	1·75 (17)	−5·65 (44)	−0·44 (21)	
H(1)	2378 (100)	2784 (115)					2·48 (1·36)
H(2)	1250 (71)	0451 (145)					0·83 (1·06)

* The temperature factor has the form $\exp[-\{[B_{11}(h^2+k^2)+B_{12}hk]/4a^2+B_{13}(hl+kl)/4ac+B_{33}l^2/4c^2\}]$.