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THE CRYSTAL STRUCTURE OF UREA AND THE MOLECULAR SYMMETRY OF THIOUREA

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The following study of the crystal structure of urea has been undertaken because it is one of the few simple organic compounds having high crystallographic symmetry. Thiourea is of interest since as a simple derivative of urea it offers an opportunity for comparing the molecular symmetry of the two substances.

Urea

Urea, $CO(NH_2)_2$, crystallizes in the tetragonal scalenohedral division of the tetragonal system[1] with the axial ratio, $a:c = 1:0.8333$. H. Mark and K. Weissenberg[2] have previously made a partial determination of the crystal structure of urea. Their results can be summarized as follows. The dimensions of the unit of structure are $d_{001} = 4.70$ Å., $d_{100} = 5.63$ Å., the space group is $4d$–3 with oxygen and carbon at (c)[3] and nitrogen at (e) with $u_N = 0.13$.

Crystals showing development of (111) and (110) were grown from alcohol–water solutions of urea. A Laue photograph made with the incident x-ray beam normal to (110) shows a twofold axis and two planes of symmetry. This observation requires the structure to be isomorphous with one of the point groups $4d$, $4e$, $4D$ or $4Di$. Since point group $4d$ is in agreement with the previously assigned crystallographic symmetry, the assumption is made that the structure is isomorphous with it.

Laue photographs were made with the incident x-ray beam normal to and making small angles with the normals to (110) and (100). Spectrum photographs were made on which (110) and (001) reflected in the equatorial region of the plate. These faces were initially parallel to the x-ray beam and were oscillated through a 20° angle. In the case of (110) the c axis was in the axis of revolution while for (001) the normal to (110) was in the axis. The smallest unit of structure compatible with the data obtained from these photographs (see Tables I–III) has $d_{001} = 4.77$ Å. and $d_{100} = 5.73$ Å. (calculated from the crystallographic axial ratio and the measured value of d_{001}). The density calculated on the basis of such a unit structure containing two $CO(NH_2)_2$ is 1.26 in agreement with the experimentally determined value 1.335.[4]

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[1] P. Groth, "Chemische Kristallographie," Leipzig, **1910**, Vol. III, p. 539.

[2] Mark and Weissenberg, *Z. Physik*, **16**, 4 (1923).

[3] R. W. G. Wyckoff, "The Analytical Expression of the Results of the Theory of Space Groups," Washington, **1922**, p. 74.

[4] G. Mez, *Z. Krist.*, **35**, 246 (1901).

TABLE I

TYPICAL SPECTRUM PHOTOGRAPHIC DATA FROM UREA[a]

Plane	Order	Line	d_{hkl}Å./n	Obs. intensity	Calcd. $\sqrt{S} = \sqrt{A^2 + B^2}$
110	n	Mo Kβ	4.124	m. s.[b]	
		α_1	4.110	v. s.	2.94
	$2n$	β	4.033	m.	
		α_1	4.031	s.	2.01
	$3n$	β	4.023	m.-m. w.	
		α_1	4.019	m. s.	2.82

[a] Mo K radiation. The following wave lengths were used in the calculation: β, λ = 0.6311 Å.; α_1, λ = 0.7078 Å.

[b] The following abbreviations are used throughout this paper: v. s., very strong; s., strong; m. s., medium strong; m., medium; m. w., medium weak; w., weak; v. w., very weak.

TABLE II

SPECTRUM PHOTOGRAPHIC DATA FROM UREA[a]

Plane	d_{hkl}Å.	Obs. intensity	Calcd. $\sqrt{S} = \sqrt{A^2}$
110	4.052	v. s.[b]	2.94
200	2.865	s.	1.88
210	2.565	s.	1.45
220	2.028	s.	2.01
310	1.812	m.	0.95
320	1.589	w.	1.28
400	1.433	abs. or v. w.	0.00
410	1.390	abs. or v. w.	0.17
330	1.351	m. s.	2.82
420	1.282	m.	1.76
510	1.124	w.	0.82

[a] Oscillation through 30° with the normal to ($1\bar{1}0$) in the axis of oscillation, (110) was initially parallel to the x-ray beam, Mo K radiation.

[b] It is to be remembered that the times of exposure are not the same for all of the spectra listed.

Reflections were present in the first order from planes (hkl) having h, k and l odd (Table III). The underlying lattice is therefore the simple tetragonal one necessitating the consideration of only the space groups from $4d$–1, to $4d$–8. The observed presence of reflection from (001) on spectrum photographs and from (113) and (115) in the first order on Laue photographs cannot be explained by space groups $4d$–2, or $4d$–4.[5] The presence of reflections from ($03\bar{4}$), ($10\bar{2}$), ($01\bar{5}$) in the first order on Laue photographs eliminates space groups $4d$–6, $4d$–7 and $4d$–8. The observed absence of reflection in the odd orders from (100) (Table II) cannot be accounted for by space groups $4d$–1, or $4d$–5. In the case of either $4d$–1 or $4d$–5 if a $CO(NH_2)_2$ group is assumed to be present it would be necessary for two (CO) groups of two different urea molecules to be distributed in

[5] R. W. G. Wyckoff and S. B. Hendricks, *Z. Krist.*, **66**, 86 (1927).

TABLE III

TYPICAL LAUE PHOTOGRAPHIC DATA FROM UREA[a]

Plane	d_{hkl} Å.	$n\lambda$	Obs. intensity	Calcd.[b] $S = A^2 + B^2$
$10\bar{2}$[c]	2.204	0.41	v. s.	0.67
221	1.865	.39	v. s.	5.38
$12\bar{2}$	1.747	.38	m. w.	1.37
$\bar{3}\bar{2}0$	1.590	.47	m. w.	1.64
$\bar{1}\bar{1}3$	1.482	.45	w.	0.41
$13\bar{3}$	1.197	.42	m.-m. s.	2.71
114	1.145	.41	w.-m. w.	1.03
341	1.114	.47	w.	0.96
$\bar{3}0\bar{4}$	1.012	.42	m. s.	11.70
$03\bar{4}$	1.012	.47	m. s.	11.70
$\bar{3}\bar{2}4$	0.954	.44	w.	4.35
$\bar{5}\bar{3}0$	0.982	.39	m. w.	8.58
343	0.930	.45	w.	4.59
$14\bar{4}$	0.906	.39	w.	10.58
$\bar{4}1\bar{1}$[d]	1.334	.44	s.	3.42
$\bar{4}1\bar{2}$	1.202	.46	m.	0.70
412	1.202	.43	m.	0.70
313	1.195	.43	m. s.	2.71
114	1.145	.41	w.	1.03
510	1.123	.40	w.	1.42
$51\bar{1}$	1.093	.41	m.	3.74
413	1.047	.31	v. v. w.	0.18
$51\bar{2}$	1.017	.39	w.-v. w.	1.00
$\bar{3}1\bar{4}$	0.996	.41	w.-v. w.	1.26
$01\bar{5}$	0.942	.47	w.-m. w.	1.96
$\bar{1}1\bar{5}$	0.929	.45	v. w.	0.50
$11\bar{5}$	0.929	.47	v. w.	0.50
$41\bar{4}$	0.905	.38	w.-m. w.	10.58
325	0.819	.43	v. w.	3.60

[a] Tungsten general radiation, 54,000 *V* peak.

[b] The structure factor calculations given in this paper are for $u_N = 0.13$; $v_N = 0.20$; $v_C = 0.32$; $v_O = 0.57$. The relative reflecting powers of N, O and C are assumed to be the same.

[c] The incident x-ray beam made an angle of about 8° with the normal to (110).

[d] A second photograph. The incident x-ray beam made an angle of about 2° with the normal to (010).

a linear distance of 4.77 Å., an unlikely distribution. Space group 4*d*–3 is in agreement with the x-ray data.

If it is assumed that there are two $CO(NH_2)_2$ groups present in the unit of structure, then the C and O atoms of such a group must be at:[3] (*c*) $0\frac{1}{2}v$; $\frac{1}{2}0\bar{v}$, and the N atoms at (*e*) $u, \frac{1}{2} - u, v$; $\frac{1}{2} - u, \bar{u}, \bar{v}$; $\bar{u}, u + \frac{1}{2}, v$; $u + \frac{1}{2}, u, \bar{v}$. To determine the structure completely it is necessary to evaluate four parameters, three of which are in the *c* direction.

Without assumptions concerning the relative reflecting powers, the comparisons (see Table II) (420) > (310), and (320) > (410) restrict the value of u_N to 0.10 to 0.14. If one assumes that C, O and N have approximately the same relative reflecting power (within 25%), the comparison (510) > (320) restricts the value of u_N to 0.12 to 0.14; the value of u_N is therefore taken as 0.13 ± 0.01.

If one assumes that the C–O distance is between 1.0 – 1.7 Å., that the C–N distance is between 1.0–1.5 Å and that C, O and N have approximately the same relative reflecting powers (within 25%), the comparisons, using the value of u_N given above, (002) > (001), $(13\bar{3}) > (\bar{1}\bar{1}3)$ and $(\bar{3}0\bar{4}) > (\bar{5}\bar{3}0)$ restrict the values of v_N, v_C and v_O to the regions shown in Fig. 1. The intensity differences in these cases are quite large. A further limitation of parameter values can be made by the utilization of planes having less pronounced intensity differences. The restrictions necessitated by the comparisons $(12\bar{2}) > (\bar{3}\bar{2}0)$, $(\bar{4}1\bar{1}) > (412)$, $(510) > (51\bar{2})$, $(0\bar{1}\bar{5}) > (1\bar{1}\bar{5})$ are shown in Fig. 1. The probable parameter values determined in this manner are $v_N = 0.20 \pm 0.02$; $v_C = 0.32 \pm 0.02$; $v_O = 0.57 \pm 0.03$. It must be emphasized that these narrower limits depend upon comparisons between planes the reflections from which do not differ greatly in intensity.

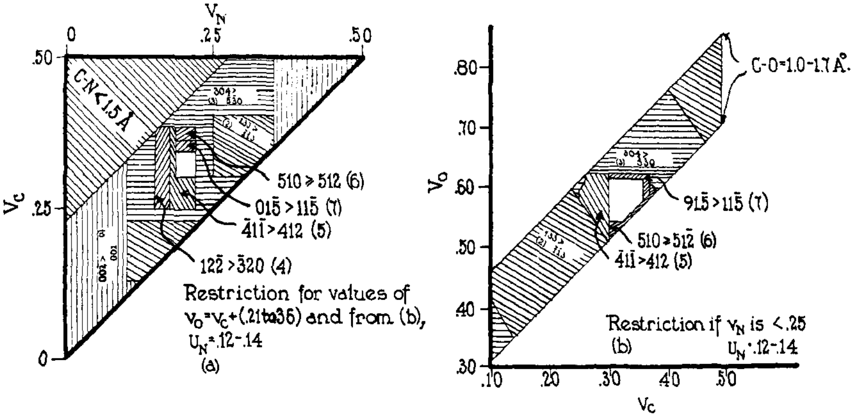

Fig. 1.—Intensity comparisons leading to a restriction of the values of the parameters for urea.

Structure factors, $S = A^2 + B^2$, calculated for reflections from the various planes, are listed in Tables I–III. In these calculations it was assumed that the relative reflecting powers of C, O and N are equal and that the values of the parameters are, $u_N = 0.13$, $v_N = 0.20$, $v_C = 0.32$ and $v_O = 0.57$. The structure factors calculated for $(14\bar{4})$ and $(10\bar{2})$ change rapidly with small changes in the parameter values. The observed intensities and the calculated structure factors, Tables I–III, are concomitant.

Thiourea

Thiourea, $CS(NH_2)_2$, crystallizes in the rhombic bipyramidal division of the rhombic system with the axial ratio $a:b:c = 0.7163:1:1.1155$.[6] Crystals, tabular parallel to $(100)_{\text{crys.}}$ and $(010)_{\text{crys.}}$, were obtained from alcohol and alcohol–water solutions of thiourea.

Spectrum photographs, with 20° oscillation, were made with the crystallographic axes in the axis of rotation. In these photographs the various pinacoids were initially parallel to the x-ray beam. Partial reproductions (Mo $K\alpha_1$ reflections) of some of these photographs are given in Fig. 4. The smallest unit of structure compatible with these data and with the spectrum and Laue data listed in Tables IV and V has $d_{(001)\text{crys.}} = 8.57$ Å.

TABLE IV

TYPICAL SPECTRUM PHOTOGRAPHIC DATA FROM $(001)_{\text{crys.}}$ OF THIOUREA

Order	Line	d_{hkl}, Å. n	Obs. intensity
n	Mo $K\beta$	8.92	m. s.
	α_1	8.87	v. s.
$2n$	β	8.67	w.
	α_1	8.57	m. s.-m.
$3n$	β	8.57	m. w.
	α_1	8.57	s.
	α_2	8.56	w.
$4n$	β	8.59	w.
	α_1	8.58	m.

TABLE V

LAUE PHOTOGRAPHIC DATA FROM THIOUREA[a]

Plane	d_{hkl}, Å.	n	Obs. intensity	Plane	d_{hkl}. Å.	n	Obs. intensity
$(1\bar{4}2)_{\text{s.g.}}$[b]	1.547	0.41	ab.	163	1.032	0.35	m.-m. w.
$1\bar{3}3$	1.468	.43	ab.	$2\bar{6}3$	1.018	.37	ab.
$10\bar{4}$	1.358	.45	ab.	172	1.012	.37	m.-m. w.
$11\bar{4}$	1.338	.47	m. s.	$2\bar{5}4$	0.996	.39	ab.
$1\bar{1}\bar{4}$	1.338	.40	m. s.	$2\bar{7}2$	0.991	.34	ab.
143	1.310	.38	s.	$2\bar{3}5$	0.984	.38	m.-m. w.
$12\bar{4}$	1.281	.47	w.	173	0.935	.31	ab.
$13\bar{4}$	1.200	.43	m.-m. s.	255	0.876	.42	w.
$15\bar{3}$	1.166	.45	ab.	$30\bar{7}$	0.758	.41	w.
$16\bar{2}$	1.148	.45	ab.	114[c]	1.338	.42	w.
$2\bar{5}3$	1.135	.47	w.	152	1.324	.40	m. s.
$14\bar{4}$	1.108	.38	ab.	143	1.310	.39	m.
170	1.088	.43	ab.	160	1.264	.37	w.
$17\bar{1}$	1.077	.41	ab.	161	1.233	.36	m. w.
$2\bar{1}5$	1.056	.48	s.	235	0.984	.46	m.

[a] Tungsten general radiation, 54,000 V peak.

[b] The incident x-ray beam made an angle of about 3° with the normal to $(100)_{\text{sp. g.}}$. All of the indices in this table are referred to the space group axes.

[c] A second photograph. The incident x-ray beam was normal to $(100)_{\text{sp. g.}}$.

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[6] Ref. 1, p. 555.

(Table IV), $d_{(010)\text{crys.}} = 7.68$ Å. and $d_{(100)\text{crys.}} = 5.50$ Å. The values of $d_{(010)\text{crys.}}$ and $d_{(100)\text{crys.}}$ were calculated from the crystallographic axial ratio and the measured value of $d_{(001)\text{crys.}}$. The density calculated on the basis of such a unit containing $4CS(NH_2)_2$ is 1.371 in agreement with the experimentally determined value 1.406.[6]

The presence of reflections in the first order from $(120)_{\text{crys.}}$ and $(021)_{\text{crys.}}$ requires the lattice to be the simple orthorhombic one. The observed presence of reflections in the first order from $(120)_{\text{crys.}}$, $(021)_{\text{crys.}}$, $(101)_{\text{crys.}}$ and $(110)_{\text{crys.}}$ can be accounted for only by space groups $2Di-1$, $2Di-5$, $2Di-13$, and $2Di-16$. The characteristic absences of reflections required by the general positions of these space groups are:[7] $2Di-1$, none; $2Di-5$, $(h0l)$ in odd orders when l is odd; $2Di-13$, $(hk0)$ in odd orders when $(h+k)$ is odd; $2Di-16$, $(h0l)$ in odd orders when $(h+l)$ is odd; $(hk0)$ in odd orders when k is odd. Reflections were absent on the spectrum photographs from the following planes having one index zero which were in position to reflect (crystallographic axes): (012), (014), (016), (034), (102), (203), (104), (205), (106), (201), (401), (302), (410), (210), (220), (001), (003), (010), (030), (100), (300), (160), (025), (023), (520), (220). The only one of the above space groups explaining these absences of reflections is $2Di-16$. This space group, in the general case, does not account for absence of reflections from (410), (210), (160), (025), (023), (220). The relationships between the crystallographic indices and the space group indices are: $h_{\text{sp. g.}} = l_{\text{crys.}}$; $k_{\text{sp. g.}} = k_{\text{crys.}}$; $l_{\text{sp. g.}} = h_{\text{crys.}}$.

Inspection of the Laue data listed in Table V shows that first order reflections are present from only two planes having $(h+k+l)$ odd, namely, $(160)_{\text{sp. g.}}$ and $(12\bar{4})_{\text{sp. g.}}$. The listed planes from which reflections were not obtained represent all planes having interplanar spacings between 0.935 Å and 1.547 Å which were in position to reflect in the first order between $\lambda = 0.24$–0.48 Å. All of these planes have $(h+k+l)$ odd with $h_{\text{sp. g.}}$ either equal to one or two. Inspections of the spectrum data (Fig. 4) shows that first order reflections are present from a number of planes having $(h+k+l)$ odd, in particular (space group axes) (160), (320), (120), (021) and (041). With the exception of $(220)_{\text{crys.}}$ all of the previously listed planes, the absence of reflections from which are not accounted for by the general space group criteria, have $(h+k+l)$ odd.

In order to have a $CS(NH_2)_2$ group in the unit of structure the C and S atoms of such a molecule must be at $2Di-16$,[8] (c) $0uv$; $\frac{1}{2}, \frac{1}{2}-u, \bar{v}$; $0, u+\frac{1}{2}, \frac{1}{2}-v$; $\frac{1}{2}, \bar{u}, v+\frac{1}{2}$, with the nitrogen atoms in the general positions (d) $x\,y\,z$; $x+\frac{1}{2}, \frac{1}{2}-y, \bar{z}$; $\bar{x}, y+\frac{1}{2}, \frac{1}{2}-z$; $\frac{1}{2}-x, \bar{y}, z+\frac{1}{2}$; $\frac{1}{2}-x, \frac{1}{2}-y, \bar{z}$; $\bar{x}yz$; $x+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$; $x, y+\frac{1}{2}, \frac{1}{2}-z$, or in two crystallographi-

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[7] R. W. G. Wyckoff, *Z. Krist.*, 61, 425 (1925).

[8] Ref. 3, p. 64.

cally non-equivalent sets at (*c*). The observation that the 6th order reflection from $(100)_{\text{sp. g.}}$ is stronger than the 4th order can be explained only if the nitrogen atoms are at (*d*).

Examination of the special types of reflections required by the above arrangement shows that in the case of (*c*) if the value of u is $\frac{1}{4}$ or $\frac{3}{4}$ then reflections will be absent in the odd orders from planes having $(h + k + l)$ odd. It must be remembered that the sulfur atom is much heavier than the carbon, nitrogen or hydrogen atom and thus at a particular wave length probably has a relative increasingly greater effective scattering power for x-rays, with decreasing interplanar spacings. Thus if the sulfur atom is at (*c*) with the value of u_S equal, or approximately equal, to $\frac{1}{4}$ or $\frac{3}{4}$, then reflections from planes having $(h + k + l)$ odd would be due to the carbon and nitrogen atoms alone. One would thus expect the relative intensity of the reflections from such planes to decrease rapidly with decreasing interplanar spacings. Such an explanation would be in accord with the experimental observation.

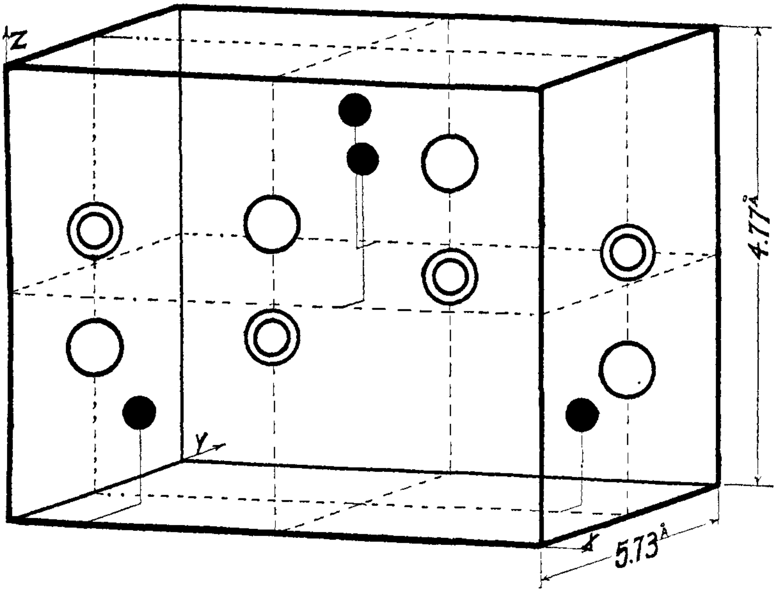

Fig. 2.—A representation of the unit of structure containing two $CO(NH_2)_2$. The nitrogen atoms are represented by the small black circles, the oxygen atoms by the ringed circles and the carbon atoms by the large circles.

The intensity observations, $(600)_{\text{sp. g.}} > (400)_{\text{sp. g.}}$, and $(800)_{\text{sp. g.}} \geqslant (400)_{\text{sp. g.}}$, can be explained only if $x_N = 0.10-0.16$. The intensity distribution for these planes shows that x_N is probably equal to 0.14 ± 0.02. The observed low intensity of reflection of (040), (060) >> (040) cannot be explained if $y_N = 0.22-0.28$, under the assumption that $u_S = \frac{1}{4}$ or

$\frac{3}{4}$. In fact the data could best be explained by a value of y_N not differing greatly from 0.15 or 0.35. The presence of seven parameters prevents a more complete analysis of the structure at the present time.

Discussion

A representation of the unit of structure containing two $CO(NH_2)_2$ is shown as Fig. 2. Within the probable limits of the parameter values the interatomic distances within a particular molecule are: C–O, 1.05 to 1.42 Å; $C-NH_2$, 1.07 to 1.30 Å. Even though the limits are broad these distances are much less than the C–C distance in the diamond. They are in agreement with the values found for $C-N(CH_2-NH_3)$ and $C-C(CH_2-CH_2)$ distances in the mono-alkyl ammonium halide series which are being studied in this Laboratory.[9] The value as a rule is between 1.20 to 1.30 Å. with no particular distinction between carbon and nitrogen.

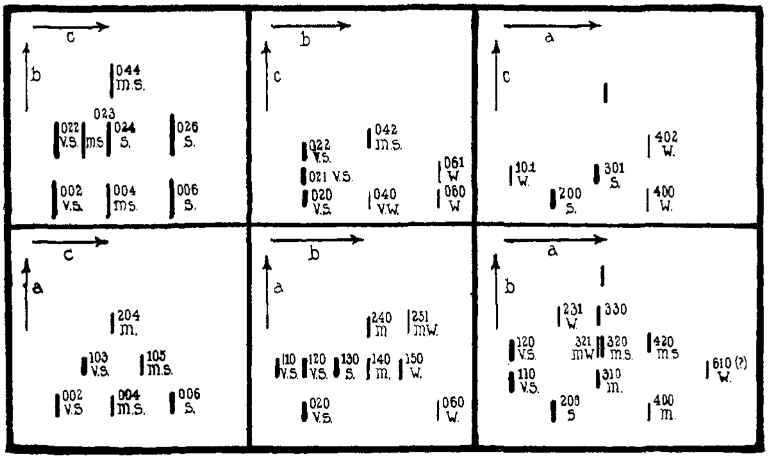

Fig. 3.—A partial reproduction of spectrum photographic data (Mo $K\alpha_1$ lines only) from thiourea. 20° oscillation. Crystallographic indices.

The $CO(NH_2)_2$ molecule has a twofold axis and two planes of symmetry (point group 2*e*). The angle between the axis of a (CO) group and a line connecting (NH_2) with the carbon atom of a $CO(NH_2)_2$ group is 52–73.5°. The resulting configuration of a $CO(NH_2)_2$ molecule is shown as Figure 4a.

The results of crystal structure investigations of inorganic compounds have led many authors to a concept of space filling with spherical or approximately spherical atoms in crystals of inorganic compounds. The expression of ionic radii on such a basis has been of great assistance in investigations of the structures of complex inorganic substances. An examination of the very limited results obtained with molecular compounds,

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[9] S. B. Hendricks, *Z. Krist.* (in press).

the crystal structure of which have been completely determined, indicates that the only structural similarity is the approximate constancy of certain interatomic distances. The closest distances between atoms of separate molecules are usually much greater than the interatomic distances within the molecules, and greater than the values calculated from the inorganic "ionic radii." Such a result is of course not an unexpected one.

In the case of urea the closest possible distance of approach between two atoms not of the same molecule is ($O–NH_2$) about 3.0 Å., with a probable value of approximately 3.15 Å. In the previously determined structure of carbon dioxide[10] the C–O distance within a CO_2 molecule is about 1.05 Å., while the closest distance of approach O–O is about 3.23 Å. In the structure of hexamethylenetetramine[11] the closest approach between two atoms not of the same molecule is (C–C) about 3.72 Å. with a corresponding distance (C–N) of about 1.33 Å. within the molecule. In the determined structure of benzene hexahydrobromide and chloride[12] the closest distances of approach between halogen atoms are Br–Br about 3.40 Å. and 3.74 Å. with the smaller distance probably that within the $C_6H_6Br_6$ molecule.

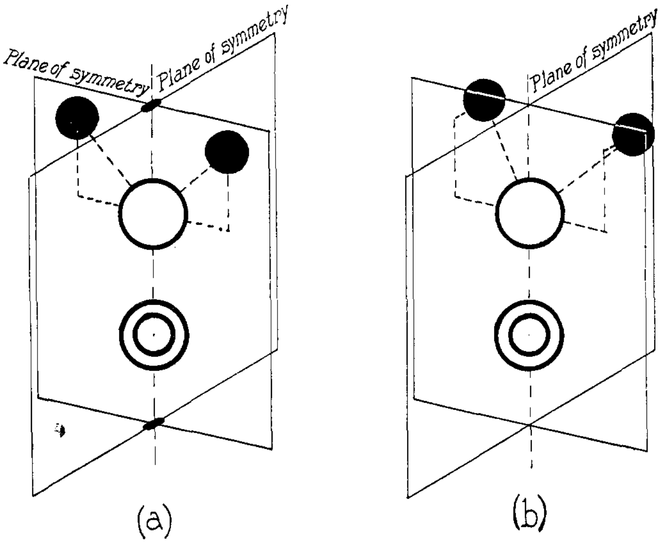


Fig. 4.—Possible configurations of the (a) urea and ((a) and (b)) of the thiourea molecule. The nitrogen atoms are represented by the small black circles, the oxygen atoms by the ringed circles and the carbon atoms by the large circles.

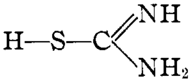
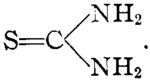
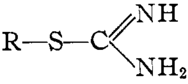
[10] W. H. Keesom and J. De Smedt, *Verslag. Akad. Wetenschappen. Amsterdam*, **33**, 888 (1924). The results of the above authors were checked by L. Thomassen and S. B. Hendricks (unpublished work), $a_0 = 5.60$, $u_0 = 0.11$.

[11] R. G. Dickinson and A. L. Raymond, THIS JOURNAL, **45**, 22 (1923).

[12] R. G. Dickinson and C. Bilicke, *ibid.*, **50**, 764 (1928).

The presence of the hydrogen atoms undetermined in positions vitiates the above analysis except in the discussion of carbon dioxide. Only in the case of the hexahydrohalides of benzene are the distances of closest approach near the values suggested by the inorganic "atomic radii."

The analysis of the structure of thiourea is not complete enough to allow close comparison with that of urea. The geometrical relationships between the molecules cannot be similar for the two compounds. The minimum molecular symmetry of thiourea is that of the point group 2c, which has a plane of symmetry. It is possible, as is shown in Fig. 4a, that all of the atoms of a thiourea molecule might be coplanar.

It has been suggested that thiourea has the formula  $H—S—C\begin{matrix}\nearrow NH \\ \searrow NH_2\end{matrix}$ rather than  $S=C\begin{matrix}\nearrow NH_2 \\ \searrow NH_2\end{matrix}$. The existence of salts of the general formula  $R—S—C\begin{matrix}\nearrow NH \\ \searrow NH_2\end{matrix}$ ·HI, the behavior of thiourea on oxidation in acid solutions and other chemical properties are said to be evidence in favor of the first formula. The observed crystallographic equivalence of the nitrogen atoms shows that in the solid state the symmetrical formula is correct.

Summary

The crystal structure of urea $CO(NH_2)_2$ has been determined by the use of Laue and spectrum photographs. The unit of structure containing two $CO(NH_2)_2$ has $d_{100} = 5.73$ Å. and $d_{001} = 4.77$ Å. The space group is $4d-3$ (V_d^3) with O and C at (c) $0\frac{1}{2}v$, $\frac{1}{2}0\bar{v}$; and N at (e) $u, \frac{1}{2}-u, v$; $\frac{1}{2}-u, \bar{u}, \bar{v}$; $\bar{u}, u+\frac{1}{2}, v$; $u+\frac{1}{2}, u, \bar{v}$. The probable parameter values are $u_N = 0.13 \pm 0.01$, $v_N = 0.20 \pm 0.02$, $v_C = 0.32 \pm 0.02$ and $v_O = 0.57 \pm 0.03$.

Laue and spectrum photographs were made from crystals of thiourea. The unit of structure containing four $CS(NH_2)_2$ has $a_0 = 5.50$ Å., $b_0 = 7.68$ Å. and $c_0 = 8.57$ Å. The space group is $2Di-16$ (V_h^{16}) with S and C at (c) $0uv$; $\frac{1}{2}, \frac{1}{2}-u, \bar{v}$; $0, u+\frac{1}{2}, \frac{1}{2}-v$; $\frac{1}{2}, \bar{u}, v+\frac{1}{2}$ and with N in the general positions. The molecular symmetry is that of the point group $2c$ (C_S) which has a plane of symmetry.

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