One hydrogen atom attached to the amino nitrogen is in the plane of the ring, and the N–H bond points towards the carbonyl oxygen (O_6) of the next molecule along the c axis. In contrast, the other hydrogen atom of the amino-group is situated in a position such that the N–H bond makes an angle of about 30° with the plane of the molecule. However, this N–H bond points to within a few degrees of the ring nitrogen (N_3) 3·04 Å away in a neighbouring molecule. Thus the proton is in a normal position for forming a hydrogen bond between the two nitrogen atoms. Although the amino-group is not in a planar trigonal configuration, the bond length C_4–N_4 is none the less shortened to 1·35 Å ± 0·005 Å, as had been predicted for cytosine in the nucleic acids[11] and found in N_1-methyl cytosine hydrobromide[12].

The molecules are closely packed in this crystal, and there are van der Waals contacts between methyl groups which can be seen in Fig. 2. It is quite likely that this arrangement arises from optimizing the stabilizing energy obtained from the packing of molecules even if it does not minimize the energy associated with the configuration of the amino-group.

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1. Green, D. W., Mathews, F. S., and Rich, A., J. Biol. Chem., 237, 3573 (1962).
2. Hoogsteen, K., Acta Cryst., 16, 28 (1963).
3. Parry, G. S., Acta Cryst., 7, 313 (1964).
4. Marsh, R. E., Bierstedt, R., and Eichhorn, E. L., Acta Cryst., 15, 310 (1962).
5. Cochran, W., Acta Cryst., 4, 81 (1951).
6. Iball, J., and Wilson, H. R., Nature, 198, 1193 (1963).
7. Hoogsteen, K., Acta Cryst., 12, 822 (1959).
8. Mathews, F. S., and Rich, A., J. Mol. Biol. (in the press).
9. Sobell, H. M., Tomita, K., and Rich, A., Proc. U.S. Nat. Acad. Sci., 49, 885 (1963).
10. O'Brien, E. J., J. Mol. Biol., 7, 107 (1963).
11. Pauling, L., and Corey, R. B., Arch. Biochem. Biophys., 65, 164 (1956).
12. Bryan, R. F., and Tomita, K., Acta Cryst., 15, 1174 (1962).

Unit Cell and Space Group of Seleno-urea

A PRELIMINARY X-ray investigation of the crystal structure of seleno-urea has been made. The crystals are hexagonal white needles, elongated along the c axis. The values found for the unit cell dimensions are: $a = 15\cdot34 \pm 0\cdot02$ Å; $c = 12\cdot99 \pm 0\cdot02$ Å. The number of molecules per unit cell is $N = 27$; calculated value 27·08, for a density of 2·1 g/c.c.

The lattice constants were determined from Weissenberg photographs, on which the diffraction pattern of a copper wire was superimposed for calibration. While the reflexions give an apparent D_{3d} symmetry, careful examination of the intensities showed the symmetry to be consistent with the space group $C_3^2 - P_{3_1}$.

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CHEMISTRY

Chemiluminescence from Dissolved Oxygen

RED chemiluminescence corresponding to about 40 kcal mol., and attributable to the forbidden transition $^1\Sigma_g^+ \to {}^3\Sigma_g^-$ of the oxygen molecule, has been observed in three recent investigations[1-3], but no explanation of the effect has been presented. These involve organic hydroperoxides or oxidations with hydrogen peroxide and also the reaction of hydrogen peroxide with HClO. In contrast with this, decompositions of hydrogen peroxide catalysed by copper ions or by platinum show no trace of the effect, and in the photochemical decomposition of ozone ground state oxygen molecules are formed with vibrational energies up to 70 kcal/mol. (ref. 4). The state of newly formed oxygen molecules is evidently not determined solely by energy factors. Since in the thermal decomposition of an organic peroxide to a ketone (or quinone)
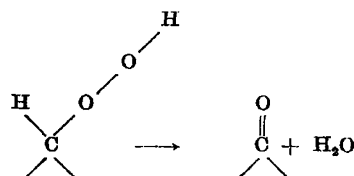
about 70 kcal/mol. is liberated it is very possible that the ketone (K) is formed in its triplet state. The spin-allowed reaction $^3K + {}^3O_2 \to {}^1K + {}^1O_2$ would then account for the formation of singlet excited oxygen molecule.

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1. Khan, A. u., and Kasha, M., J. Chem. Phys., 39, 2105 (1963).
2. Bowen, E. J., and Lloyd, R. A., Proc. Roy. Soc., A, 275, 465 (1963).
3. Bowen, E. J., and Lloyd, R. A., Proc. Chem. Soc., 305 (1963).
4. McGrath, W. D., and Norrish, R. G. W., Proc. Roy. Soc., A, 254, 317 (1960).

A Lithium–Scandium–Molybdenum(IV) Oxide

THE structure of compounds $A_2^{II}Mo_3^{IV}O_8$, where A^{II} may be Mg, Mn, Fe, Co, Ni, Zn, and Cd, has been reported[1]. In this structure the divalent cations occupy both tetrahedral and octahedral holes. The arrangement leads to fairly large deviations from Pauling's electrostatic valence rule. Sums of strengths of the electrostatic bonds to oxygens range from as low as $1\frac{5}{8}$ to as high as $2\frac{1}{2}$, though the high figure applies to only two of the sixteen oxygens in the unit cell.

The two different kinds of sites for the divalent ions suggest the possibility of testing for site preference on the basis of cation charge and/or size. The charge distribution could be changed by using a monovalent ion and a trivalent ion rather than two divalent ions. If the tetrahedral holes were occupied by the monovalent ions and the octahedral holes by the trivalent ions, the charge distribution would be improved: the electrostatic bond strength sums would then range from a low of $1\frac{3}{8}$ to a high of $2\frac{1}{4}$ (If the monovalent ion were the smaller ion, the relative sizes should also favour the occupancy of the tetrahedral sites by the monovalent ions and the octahedral sites by the trivalent ions.)

Although several combinations of mono- and tri-valent ions were tried unsuccessfully, a product was obtained with the reagents Li_2O, Sc_2O_3, and MoO_2 in the mole ratios of 1 : 1 : 6. The $\sin^2\theta$ values for the low-angle powder diffraction lines of the compound are listed in Table 1. Interestingly, the lines of this pattern can almost be indexed on the basis of a simple cubic cell with $a = 4\cdot9$ Å. However, the cubic 211 line is rather abruptly missing, and a line corresponding to the forbidden value 7 for $h^2 + k^2 + l^2$ ($= N$) is present. Doubling the values of $h^2 + k^2 + l^2$ in order to avoid the number 7, by using a