son, 1957, for semiconductivity, and is seemingly isostructural with Li_2MgSn investigated by Laves (cited in Mooser & Pearson, 1957). The only other work on the Li–Mg–Pb system of which we are aware is that of Brauer & Tiesler (1950*b*) who showed that Mg_2Pb can take as much as 9·8 mole per cent Li_4Pb into solid solution.

We are indebted to Mr D. H. Wood for preparing one of the samples of the compound, to Mr V. G. Silveira for the powder photography, and to the Analytical group for chemical analysis.

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The variation of apparent bond lengths with temperature in molecular crystals.

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(*Received* 30 *May* 1961)

Atomic coordinates obtained from Fourier or least-squares calculations, in which the structure factors are calculated for atoms assumed to be undergoing *linear* anisotropic vibrations, will be in error if a molecule is undergoing *angular* oscillations (Cox, Cruickshank & Smith, 1955; Cruickshank, 1956*a*, 1961). In the simplest case an atom will appear too close to the axis of angular oscillation by roughly $\frac{1}{2}r\theta^2$, where r is its distance from the axis and θ^2 is the m.s. amplitude of angular oscillation. At temperatures above the characteristic temperature Θ_E, which is often about 50–100 °K. for the librations in molecular crystals (Cruickshank, 1956*b*), θ^2 will be roughly proportional to the absolute temperature. Thus, as the temperature falls below room temperature, the apparent displacement $\frac{1}{2}r\theta^2$ should decrease appreciably. Consequently the uncorrected bond lengths in a molecule such as benzene ought actually to *increase* as the temperature *falls*, provided that the intermolecular forces are too small to cause any appreciable change in the 'true' bond lengths.

Table 1. *The* CN *bond length in* $(CH_2)_6N_4$

Temperature (°K.)	Cell dimension (Å)	Radiation used	Uncorrected length (Å)	Rotational correction (Å)	Corrected length (Å)
298	$7{\cdot}021 \pm 9$	Cu	$1{\cdot}464 \pm 5$	0·014	1·478
		Mo	$1{\cdot}465 \pm 2$		1·479
100	$6{\cdot}931 \pm 8$	Cu	$1{\cdot}474 \pm 7$	0·005	1·479
		Mo	$1{\cdot}467 \pm 2$		1·472
34	$6{\cdot}910 \pm 8$	Cu	$1{\cdot}474 \pm 4$	0·002	1·476
		Mo	$1{\cdot}475 \pm 1_2$		1·477

We have recently undertaken single crystal X-ray studies of $(CH_2)_6N_4$ at 298, 100 and 34 °K. in order to investigate the variation of vibration amplitudes with temperature and to interpret them by a lattice-vibration spectrum. The main results will be reported elsewhere, but the values found for the CN bond lengths at different temperatures are relevant here. The bond lengths and their e.s.d.'s derived from full-matrix least-squares calculations for the three temperatures and from the independent observations made with Cu and Mo radiation are shown in Table 1. These show fairly clearly that the uncorrected CN bond length does increase as the temperature decreases.

At 298 °K. the angular oscillation θ^2 about any molecular axis is found to be $43{\cdot}1 \pm 2{\cdot}0$ deg.^{2}, which corresponds to a characteristic temperature $\Theta_E = 64{\cdot}5$ °K. The angular oscillations at the lower temperatures are $11{\cdot}2 \pm 1{\cdot}1$ deg.^{2} at 100 °K. and $6{\cdot}0 \pm 0{\cdot}8$ deg.^{2} at 34 °K.; these are close to those predicted with the above Θ_E. After application of the rotational corrections (Cruickshank, 1956*a*), the CN lengths given in the last column of Table 1 are obtained.[†] The results show that the corrected CN length is the same at all temperatures within experimental error and so provide direct evidence for the validity of this type of correction. Similar evidence from other crystals is of course desirable for further confirmation.

It may be added that the uncorrected C–N lengths obtained in the present work for 298 °K. are in satisfactory agreement with those obtained from new least-squares refinements of the previous X-ray (Brill *et al.*, 1939) and neutron data (Andreson, 1957), which are $1{\cdot}457 \pm 5$ Å and $1{\cdot}457 \pm 4$ Å. The weighted mean estimate of the corrected CN length derived from the various crystal-diffraction results is $1{\cdot}476 \pm 0{\cdot}002$ Å, where the e.s.d. has been set rather conservatively. This is in satisfactory agreement with the gas-phase electron-diffraction value of $1{\cdot}48 \pm 0{\cdot}01$ Å (Schomaker & Schaffer, 1947).

We are indebted to Prof. Dame Kathleen Lonsdale for some stimulating correspondence on this topic.

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[†] The proper e.s.d.'s for the corrected lengths will be a little greater than those assigned to the uncorrected lengths, because these did not allow for the e.s.d.'s of the cell dimensions or for any error in the rotational corrections.