(c) *Intermolecular distances*

All the intermolecular distances are greater than 3·4 Å, and the arrangement of the molecules with some of these distances is shown in Figs. 7 and 8.

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References

BAEYER, A. (1882). *Ber. dtsch. chem. Ges.* **15**, 50.

BUSING, W. R. & LEVY, H. A. (1959). *A Crystallographic Least-Squares Refinement Program for the IBM* 704. Oak Ridge National Lab., Oak Ridge, Tennessee.

COHEN, T. & PINKUS, J. (1959). Private communication.

COULSON, C. A. (1948). *Victor Henri Memorial Volume.* Liege: Desoer.

DAUDEL, R., LEFEBVRE, R. & MOSER, C. (1959). *Quantum Chemistry.* London: Interscience Publication Ltd.

DEWAR, M. J. S. & SCHMEISING, H. N. (1959). Tetrahedron, **5**, 166.

HUGHES, E. W. (1941). *J. Amer. Chem. Soc.* **63**, 1737.

MAXWELL, L. R. & MOSLEY, W. M. (1940). *J. Chem. Phys.* **8**, 738.

PAULING, L. (1960). *The Nature of the Chemical Bond.* Ithaca: Cornell Press.

PINKUS, J. L., COHEN, T., SUNDARALINGAM, M. & JEFFREY, G. A. (1960). *Proc. Chem. Soc.* p. 70.

RUGGLI, P. (1919). *Ber. dtsch. chem. Ges.* **1**, 52.

RUGGLI, P., CASPAR, E. & HEGEDUS, B. (1939). *Ber. dtsch. chem. Ges.* **22**, 140.

SHIONO, R. (1960). *Technical Report No.* 16, *Computation and Data Processing Center and The Crystallography Lab.*, University of Pittsburgh.

TROTTER, J. (1960). Tetrahedron, **8**, 13.

WOOLFSON, M. M. (1961). *Direct methods in Crystallography*, p. 64. Oxford: University Press.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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The unit cell and space group of Li_2C_2.

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A review of the literature has indicated that no work has been reported on the unit cell or structure of the various alkali carbides.

As part of a study of the ternary system, lithium–boron–carbon, a brief examination of the lithium–carbon system was conducted. A single crystal of lithium carbide was synthesized and isolated for study. The crystal was formed by reacting lithium and graphite at 700 °C. for two days and slow-cooling. The elements were contained in an iron capsule with an argon atmosphere.

The crystal was identified as monoclinic. Weissenberg and rotation photographs were recorded about the b_0 axis. The Bradley–Jay (1932) extrapolation method was used to refine the a_0 and c_0 lattice constants computed from the zero-level Weissenberg photograph. The identity period along the b_0 axis was obtained from the rotation photograph. The angle β was measured directly on the zero-level Weissenberg photograph.

Debye–Scherrer X-ray powder patterns were made using nickel-filtered Cu $K\alpha$ radiation. Line intensities were visually estimated. The (*hkl*) combinations satisfying the powder pattern data were supplied by a computer. The observed and calculated $\sin^2\theta$ values are compared in Table 1. Since the identity period along the b_0 axis could only be measured to $\pm 0{\cdot}1$ Å, the b_0 value for each (*hkl*) reflection was recalculated using the a_0, c_0, and β measurements from the Weissenberg photograph and the corresponding observed $\sin^2\theta$ value from the powder pattern. In this manner, b_0 was refined to $\pm 0{\cdot}005$ Å. The resulting cell dimensions are:

$$a_0 = 7{\cdot}801 \pm 0{\cdot}002,\ b_0 = 8{\cdot}815 \pm 0{\cdot}005 \text{ Å},$$
$$c_0 = 10{\cdot}865 \pm 0{\cdot}005 \text{ Å};\ \beta = 76{\cdot}8 \pm 0{\cdot}1°.$$

The adjacent layer levels were similar and contained no systematic extinctions. The unit cell is, therefore, primitive and the space group is either $P2$, Pm, or $P2/m$. Since the crystal exhibited prismatic habit (elongated development along the c_0 axis), the space group $P2/m$ is suggested. The density of lithium carbide has been reported in the literature as 1·65 g.cm.$^{-3}$ (*International Critical Tables*, 1926). If the value is correct within 5%, the unit cell would contain 18 to 20 molecules. A chemical analysis of the carbide confirmed the 50–50 at.% combination. The formula ratio Li_2C_2 is discussed by Thorne & Roberts (1948), based on the production of acetylene when the alkali carbides react with water.

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References

BRADLEY, A. J. & JAY, A. H. (1932). *Proc. Phys. Soc.* **44**, 563.

International Critical Tables (1926), Vol. 1, p. 149. New York: McGraw-Hill.

THORNE, P. L. & ROBERTS, E. R. (1948). *Inorganic Chemistry*, 5th Ed., p. 865. New York: Interscience Publishers.

Table 1. *Interplanar spacings for* Li_2C_2

$\sin^2\theta$ Observed	$\sin^2\theta$ Calculated	*hkl*	I/I_o*	d_o
0·0311	0·0306	020	60	4·37 Å
0·0345	0·0351	201		4·15
	0·0359	021	5	
0·0475	0·0473	212		3·54
	0·0478	003	30	
0·0490	0·0487	113		3·49
	0·0489	210	15	
0·0661	0·0655	$\bar{2}11$	50	3·00
	0·0657	221		
0·0755	0·0742	031	20	2·80
	0·0752	$\bar{1}03$		
0·0789	0·0784	023		2·75
	0·0788	131	100	
0·0831	0·0828	$\bar{1}13$	70	2·67
0·0898	0·0890	132	25	2·57
	0·0894	303		
	0·0901	032		
0·0936	0·0926	014		2·52
	0·0927	300	40	
	0·0928	$\bar{2}12$		
0·1003	0·1004	310	30	2·44
0·1107	0·1101	230	10	2·32
	0·1105	322		
	0·1113	224		
	0·1115	321		
0·1177	0·1167	033	20	2·24
	0·1180	$\bar{1}04$		
0·1259	0·1248	$\bar{2}15$	20	2·17
	0·1257	$\bar{1}14$		
	0·1267	$\bar{2}31$		
0·1543	0·1537	$\bar{2}23$	25	1·96
	0·1538	034		
	0·1540	$\bar{2}32$		
	0·1550	411		
0·1588	0·1582	333		1·93
	0·1589	404	1	
0·1748	0·1750	116		1·84
	0·1750	423	20	
0·1876	0·1860	$\bar{2}35$		1·78
	0·1868	$\bar{1}34$	50	
0·1952	0·1948	226		1·75
	0·1949	144		
	0·1954	420	40	
0·2137	0·2133	433	5	1·67
	0·2145	425		
0·2192	0·2196	406	40	1·65
	0·2201	503		
0·2274	0·2264	251		1·62
	0·2272	416		
	0·2277	434		
	0·2277	513	10	
0·2348	0·2337	430	5	1·59
	0·2342	$\bar{1}52$		
	0·2344	501		
0·2452	0·2455	$\bar{2}43$	5	1·56
	0·2459	$\bar{3}04$		
0·2647	0·2642	327		1·50
	0·2650	521	40	
	0·2652	510		
0·2735	0·2735	417	10	1·47
0·2832	0·2840	350	5	1·45
0·2911	0·2902	208	10	1·43 Å
	0·2907	237		
	0·2908	532		
	0·2908	027		
	0·2913	$\bar{5}01$		
0·2974	0·2977	534	2	1·41
	0·2978	218		
0·3138	0·3136	046	15	1·38
	0·3141	$\bar{3}43$		
	0·3144	$\bar{2}53$		
0·3249	0·3239	602	5	1·35
	0·3240	613		
	0·3240	055		
0·3383	0·3386	451	5	1·32
	0·3393	$\bar{3}52$		
0·3751	0·3748	070	30	1·26
	0·3751	455		
0·3844	0·3841	$\bar{4}51$	10	1·24
	0·3848	171		
	0·3849	364		
	0·3852	170		
	0·3852	633		
0·4075	0·4082	065	5	1·21
0·4255	0·4248	357	20	1·18
	0·4257	551		
	0·4262	636		
0·4330	0·4332	$\bar{3}45$	10	1·17
0·4517	0·4515	057	5	1·15
0·4721	0·4721	$\bar{2}08$	20	1·12
	0·4721	$\bar{4}53$		
0·4899	0·4899	$\bar{3}71$	10	1·10
0·5052	0·5048	700	1	1·09
0·5296	0·5292	$\bar{6}32$	10	1·06
	0·5293	282		
0·5388	0·5390	276	1	1·05
	0·5392	731		
0·5562	0·5563	$\bar{4}63$	3	1·03
	0·5564	376		
0·6082	0·6082	826	5	0·988
	0·6084	377		
0·6159	0·6162	$\bar{4}64$	3	0·982
0·6492	0·6487	748	1	0·957
	0·6498	821		
0·6578	0·6585	832	5	0·950
0·6864	0·6867	$\bar{4}08$	1	0·930
	0·6867	465		
0·6954	0·6961	750	?	0·924
0·7286	0·7288	903	2	0·903
0·7449	0·7449	578	2	0·893
0·7618	0·7619	767	1	0·883
	0·7619	853		
0·7937	0·7943	188	1	0·865
	0·7943	$\bar{7}43$		
0·8324	0·8325	$\bar{5}18$	1	0·845
	0·8325	$\bar{8}41$		
0·8795	0·8797	770	1	0·822
0·9122	0·9124	$\bar{8}33$	1	0·807
0·9346	0·9347	860	1	0·797
	0·9347	$\bar{7}06$		
0·9412	0·9402	$\bar{7}54$	?	0·795
0·9771	0·9771	696	1	0·780

* The I/I_0 value corresponds to the Debye–Scherrer line intensity, and has been placed next to the most probable (*hkl*) value, as determined from the Weissenberg photographs.