$x=0{\cdot}037$ Å $y=0{\cdot}058$ Å $z=0{\cdot}045$ Å

with a possible uncertainty of about $\pm 0{\cdot}002$ Å. It therefore appears that, in spite of the approximation involved in the choice of potential functions, this type of calculation can be used to predict the molecular packing of crystals of unknown structure with satisfactory accuracy, when the molecular shape and size are known. This method will be extended to more general cases where the molecules lie at general positions in the unit cell. In addition, the information about the potential energy minima might be used in order to analyse thermal movements in molecular crystals in terms of rigid-body molecular oscillations.

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X-ray determination of the lattice parameters of potassium dihydrogen phosphate at elevated temperatures.

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A precision determination of the lattice parameters of tetragonal potassium dihydrogen phosphate has been made over the temperature range 25–150°C. The lattice parameters at room temperature are $a=7{\cdot}4528\pm 0{\cdot}0004$, $c=6{\cdot}9683\pm 0{\cdot}0004$ Å. The principal coefficients of thermal expansion have been evaluated and are found to follow the equations

$$\alpha_a=10{\cdot}10\times 10^{-6}+21{\cdot}68\times 10^{-8}t-2{\cdot}62\times 10^{-10}t^2$$
$$\alpha_c=28{\cdot}73\times 10^{-6}+17{\cdot}65\times 10^{-8}t+1{\cdot}83\times 10^{-10}t$$

The results of a systematic study of the temperature variation of the lattice parameters of some phosphates and arsenates isomorphous with potassium dihydrogen phosphate (KDP) at elevated temperatures have been reported from this laboratory (Deshpande & Khan, 1963, 1965*a*, *b*, 1966). Similar results on KDP itself are presented in this communication.

A symmetric focusing camera designed by Sirdeshmukh (1963) was used for obtaining powder photographs with filtered copper radiation. Six Cu $K\alpha_1\alpha_2$ doublets at high angles were used for calculating the lattice parameters by Cohen's analytical procedure. The values of the lattice parameters at five temperatures are given in Table 1.

Table 1. *Lattice parameters of potassium dihydrogen phosphate at various temperatures*

Temperature	a	c
26°C	7·4528 Å	6·9683 Å
64	7·4583	6·9771
86	7·4628	6·9833
121	7·4698	6·9962
151	7·4785	7·0068

The coefficients of thermal expansion, $\alpha_a=(1/a_{25})(da/dt)$ and $\alpha_c=(1/c_{25})(dc/dt)$, were evaluated from the data in Table 1 by the graphical procedure discussed by Deshpande & Mudholker (1961). The values of the coefficients of expansion are given in Table 2. Both the coefficients increase with temperature in an almost linear fashion. However, taking into account the slight non-linearity, the temperature variation of the coefficients of expansion can be represented by the following equations:

$$\alpha_a=10{\cdot}10\times 10^{-6}+21{\cdot}68\times 10^{-8}t-2{\cdot}62\times 10^{-10}t^2$$
$$\alpha_c=28{\cdot}73\times 10^{-6}+17{\cdot}65\times 10^{-8}t+1{\cdot}83\times 10^{-10}t^2$$

where t is the temperature in °C. The mean coefficients of expansion for the range 25–150°C were also calculated and have values $\alpha_a=26{\cdot}9\times 10^{-6}$°C^{-1} and $\alpha_c=46{\cdot}4\times 10^{-6}$°C^{-1}.

Table 2. *Coefficients of thermal expansion of potassium dihydrogen phosphate at various temperatures*

Temperature	$\alpha_a\times 10^6$	$\alpha_c\times 10^6$
40°C	18·8	35·9
60	21·5	40·3
80	25·5	43·8
100	29·5	48·8
120	32·9	51·7
140	34·9	57·4

Values for the lattice parameters of KDP at room temperature have been given by Ubbelohde & Woodward (1947), Klug & Alexander (1954) and recently by Haussühl (1964). The values obtained in this work at 26°C are $a=7{\cdot}4528\pm 0{\cdot}0004$, $c=6{\cdot}9683\pm 0{\cdot}0004$ Å. These values are in reasonable agreement with those given by the workers mentioned above. The density calculated from our values is 2·337 g.cm^{-3} which compares well with the experimental

value 2·338 g.cm^{-3} (*Handbook of Chemistry and Physics*, 1958).

The thermal expansion of KDP has been studied earlier by De Quervain (1944) and Ubbelohde & Woodward (1947) by the X-ray method at low temperatures. At elevated temperatures the thermal expansion has been studied by macroscopic methods by Mason (1946) and by Haussühl (1964). The mean coefficients obtained by Mason (quoted from Megaw, 1957) are $\alpha_a=27$ and $\alpha_c=45$ in units of 10^{-6}°C^{-1}. The values given by Haussühl are $\alpha_a=26{\cdot}5$ and $\alpha_c=44{\cdot}4$ in the same units. The mean coefficients obtained in the present study agree well with these values. A detailed discussion regarding the anisotropy in the thermal expansion of KDP and its isomorphs has been given elsewhere (Deshpande & Khan, 1963; Khan, 1966).

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Refinement of the crystal structure of anthraquinone.

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The crystal structure of anthraquinone has been refined to an R index of 12·5 % by the full-matrix least squares based on the observed structure factors of Murty. From the refinement it is concluded that there is no formal transfer of one electron from the carbon atom to the oxygen atom in the C=O bond as Murty proposed, although there is no significant change in positional atomic parameters. Principal axes of vibration of thermal ellipsoids for the carbon and oxygen atoms are also calculated.

The structure of anthraquinone was first determined by Sen (1948) and was refined by Murty (1960) by three-dimensional Fourier methods, using form factors obtained by an empirical method (Murty, 1957). However, the final R index remained surprisingly high (19·6 % for the observed reflections). It was therefore thought worthwhile to undertake a further refinement of the structure.

* Contribution no. 1420.

Crystal data

Anthraquinone, $C_{14}H_8O_2$.

$a=15{\cdot}810\pm0{\cdot}015$, $b=3{\cdot}942\pm0{\cdot}005$, $c=7{\cdot}865\pm0{\cdot}010$ Å. $\beta=102°43'\pm2'$. Space group $P2_1/a$. $Z=2$.

The refinement was first carried out by three full-matrix least-squares refinements based on the observed structure factors of Murty and beginning with his final atomic coordinates and isotropic temperature factors. In three cycles,

Table 1. *Atomic parameters and standard deviations*

The parameters of carbon and oxygen are multiplied by 10^4. Temperature factors are of the form $\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)$. Hydrogen parameters are multiplied by 10^3.

Hydrogen atoms are assigned arbitrarily an isotropic B value of 3·5 Å^2. Standard deviations (in final significant figure) are given in parenthesis.

	x	y	z	B_{11}	B_{22}	B_{23}	B_{12}	B_{13}	B_{23}
C(1)	1314 (5)	4166 (25)	3985 (10)	50 (4)	640 (69)	162 (14)	30 (26)	−2 (11)	−26 (48)
C(2)	0507 (5)	2707 (25)	3406 (9)	46 (3)	765 (74)	138 (12)	41 (30)	25 (10)	−16 (53)
C(3)	0277 (4)	1390 (19)	1742 (9)	32 (3)	433 (59)	167 (13)	22 (19)	30 (9)	0 (43)
C(4)	0850 (4)	1547 (19)	0616 (9)	26 (2)	488 (59)	166 (11)	33 (19)	41 (8)	32 (42)
C(5)	1662 (5)	2960 (23)	1215 (10)	33 (3)	648 (69)	219 (15)	−19 (24)	53 (10)	46 (54)
C(6)	1894 (5)	4274 (24)	2894 (11)	43 (4)	618 (68)	211 (16)	16 (25)	−32 (11)	−109 (52)
C(7)	0605 (4)	0137 (23)	−1157 (9)	33 (3)	660 (69)	152 (12)	41 (22)	51 (9)	49 (46)
O(8)	1109 (4)	0229 (21)	−2119 (8)	44 (3)	1503 (79)	171 (10)	−111 (24)	81 (8)	−190 (37)
H(1)	145 (5)	514 (22)	519 (11)						
H(2)	007 (5)	245 (23)	416 (11)						
H(5)	207 (5)	323 (23)	036 (10)						
H(6)	246 (5)	565 (22)	337 (11)						