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The crystal structure of calcium 4*H*-pyran-2,6-dicarboxylate trihydrate, $Ca.C_7O_5H_4.3H_2O$.

By K. J. Palmer and Kay Sue Lee, *Western Regional Research Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Albany, California* 94710, *U.S.A.*

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Crystals of calcium 4*H*-pyran-2,6-dicarboxylate trihydrate ($Ca.C_7O_5H_4.3H_2O$) are isostructural with calcium dipicolinate trihydrate ($Ca.C_7O_4NH_3.3H_2O$).

Calcium dipicolinate is believed to play an important role in the heat resistance and metabolic inertness of bacterial spores (Murrell & Warth, 1965). The discovery by Strahs & Dickerson (1968) of a strong dimeric linkage in the crystal structure of calcium dipicolinate (Ca.DPA) trihydrate has encouraged speculation as to the role of Ca.DPA in bacterial spores. Investigation of analogues of dipicolinic acid has shown that 4*H*-pyran-2,6-dicarboxylic acid (PDC) substitutes very effectively for DPA in the germination of bacterial spores induced by 0·04 *M* Ca.DPA (Lewis, 1967; Riemann & Ordal, 1961) and in the formation of spores by a DPA-requiring mutant of *Bacillus megaterium* (Fukuda & Gilvarg, 1968; Fukuda *et al.*, 1969). Because of the interest in determining the structural features responsible for the observed spore properties (Murrell, 1969), we have undertaken the determination of the crystal structure of several salts of DPA and of a few compounds which have a close chemical relationship to DPA.

One of these latter is Ca.PDC, synthesized by Richard M. Seifert of this Laboratory. The molecular structures of Ca.DPA and Ca.PDC are shown in Fig. 1.

Ca.PDC, like Ca.DPA, crystallizes from water as the trihydrate. The unit-cell dimensions, density, and space group for Ca.PDC indicate that it is isostructural with Ca.DPA. Preliminary crystallographic data for Ca.PDC.$3H_2O$ were obtained from Weissenberg and precession photographs. The unit-cell dimensions were refined from high angle 2θ scans with an automatic diffractometer at a take-off angle of 1°. The final values are listed in Table 1, along with the published values for Ca.DPA.$3H_2O$ (Strahs & Dickerson, 1968).

Table 1. *Crystallographic data*

Ca . DPA . $3H_2O$	Ca . PDC . $3H_2O$
$a = 9{\cdot}94$ Å	$a = 9{\cdot}992 \pm 0{\cdot}005$ Å
$b = 17{\cdot}65$	$b = 17{\cdot}68 \pm 0{\cdot}01$
$c = 5{\cdot}87$	$c = 5{\cdot}88 \pm 0{\cdot}003$
$\beta = 99{\cdot}45°$	$\beta = 99{\cdot}44 \pm 0{\cdot}02°$
ϱ (obs.) $= 1{\cdot}675 \pm 0{\cdot}015$	ϱ (obs.) $= 1{\cdot}709 \pm 0{\cdot}01$
ϱ (calc.) $= 1{\cdot}699$	ϱ (calc.) $= 1{\cdot}716$
Space group: $P2_1/n$	Space group: $P2_1/n$

The intensities of 288 randomly selected reflections were obtained for Ca.PDC.$3H_2O$ with an automatic diffractometer. Ni filtered Cu $K\alpha$ radiation was used. After Lorentz and polarization corrections were applied a scale factor, k, was obtained from the expression $k = \Sigma |F_{DPA}| / \Sigma |F_{PDC}|$,

The average discrepancy $\dfrac{\Sigma \left| k|F_{PDC}| - |F_{DPA}| \right|}{\Sigma k|F_{PDC}|}$

between the two sets of data was 0·115.

The fact that crystals of Ca.DPA.$3H_2O$ and Ca.PDC.$3H_2O$ have the same space group and unit-cell dimensions, and that the relative F values of 288 reflections are in good agreement, leads us to conclude that the two crystals are indeed isostructural.

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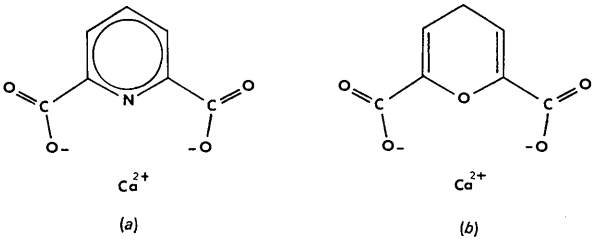

Fig. 1. The molecular structure of (*a*) calcium dipicolinate and calcium pyran-2,6-dicarboxylate (*b*).

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