THE UNIT CELL DIMENSIONS OF CALCIUM SUCCINATE TRIHYDRATE

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Bone maintains an active citrate metabolism, as indicated by the occurrence of 1% of citrate in bone (1), with a potential role of citrate in the solubilization of the calcium in bone as the citrate complex. In a recent publication (2), one of the authors determined the unit cell of tricalcium citrate tetrahydrate in an effort to demonstrate a possible isomorphism with hydroxyapatite or collagen as the basis for retention of calcium citrate in bone, but this did not yield definite potentiality for isomorphism; although there was a close correspondence of the 30.8 A *a* axis of calcium citrate with the 30.0 A *c* axis of collagen. The present work is designed to compare another member of the tricarboxylic acid cycle, succinate in the form of calcium succinate trihydrate, with hydroxyapatite and collagen.

When rotating crystal runs were made on calcium succinate trihydrate, good layer lines were obtained on three axes for the monoclinic crystals with the angle beta 74.15°. The material has a density of 1.58 gram per cc. The axial lengths as measured were a = 10.25 A, b = 9.37 A, c = 6.68 A. These dimensions give a calculated 2.8 molecules per unit cell, an impossible situation. The first spot on the first layer line of the a axis rotation shows an interplanar spacing of 9.11, which is incompatible with a = 10.25 A. Careful inspection of one of the a-axis rotation runs indicated faint spots intermediate between the zero and first layer lines with repeat intervals of approximately 16.75 and 32 A. This implies a tripling of the a-axis to yield a = 30.75 A. On this basis the dimensions of the monoclinic unit cell are:

a 30.75 A
b 9.37 A
c 6.68 A
β 74.15°
Unit cell volume, 1.852×10^{-21} cm^3
Unit cells per cc, 5.400×10^{20}
Density, 1.58 g. per cc
Molecules per cc., 4.525×10^{21}
Molecules per unit cell, 8.38 or 8

Possible indexing of the powder pattern is indicated in Table I, where some of the fits are not close, indicating again the possibility of some confusion in choice of axes. A zone axis might have been chosen for a, but even this should have given consistent indexing.

Table II shows the respective unit cell dimensions of calcium succinate, hydroxyapatite, and collagen.

TABLE I

X-RAY DIFFRACTION POWDER PATTERN OF CALCIUM SUCCINATE TRIHYDRATE

d in A	Intensity	Index	d, calc.
8.7	M 1	110	8.93
6.95	M 3	101	6.67
6.5	M 4	310	6.42
		001	
5.35	M	011	5.29
4.85	F	020	4.69
4.45	M	220	4.47
3.87	F	420	3.95
3.68	F	3.33 a s β202	3.33
3.42	F		
3.32	M 2	202	3.33
2.84	F	410	2.90
2.73	F	222	2.72
2.61	F	022	2.64
2.53	F		
2.45	F	1200	2.48
2.37	F	040	2.34
2.21	F	440	2.24
2.15	F	003	2.14
2.10	F	013	2.09
2.03	F		
1.94	F	550	1.99
1.86	F	050	1.874
1.78	F		

TABLE II

COMPARISON OF UNIT CELL DIMENSIONS

	Class	a	b	c	β
Calcium Succinate Trihydrate	Monoclinic	30.75	9.37	6.68	74.15°
Hydroxyapatite (3)	Hexagonal	9.40	9.40	6.93	
Collagen, dry (4)	Spiral (pseudohexagonal)	10.6	10.6	28.6	
Collagen, wet (5)	("Orthorhombic" as calc. from data given)	49.85	37.3	28.6	

It is possible to visualize a two-dimensional isomorphism between calcium succinate and hydroxyapatite on the basis of the close correspondence of the *b* and *c* axes in the two compounds, which might possibly serve as a means of anchoring the calcium succinate in the bone. With respect to wet collagen, the *a* axis of calcium succinate is of the same order of magnitude as the *c* axis of collagen, but interpretation is difficult in view of doubt as to the structure of wet collagen.

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