mechanism of hydrolysis (Bartlett & Ando, 1970) of derivatives of bicyclo[3.2.0]hept-2-en-6-one. Related crystal structures (Friedrichsen, Debaerdemaeker, Bottcher, Hahnemann & Schmidt, 1983; Murray-Rust, Murray-Rust & Brown, 1979; Gordon, Pluscek & Ondetti, 1981; Goldstein, Vannes, Houge, Frisque-Hesbain, Wiaux-Zamar, Ghosez, Germain, Declercq, Van Meerssche & Arrieta, 1981).

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SHORT COMMUNICATION

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Acta Cryst. (1988). C**44**, 395–396

On the structure of Ca_8In_3.

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Abstract

The crystal structure of Ca_8In_3, recently described in space group $P1$, has been more satisfactorily refined in $P\bar{1}$. Although the structure is little changed, adding the center of symmetry has eliminated near-singularities in the least-squares matrix, leading to e.s.d.'s that are approximately one-quarter as large as those previously reported.

Recently, the crystal structure of Ca_8In_3 was described (Fornasini, 1987) in the non-centrosymmetric space group $P1$ [$a = 9{\cdot}606$ (2), $b = 9{\cdot}717$ (2), $c = 9{\cdot}782$ (2) Å, $\alpha = 69{\cdot}65$ (2), $\beta = 78{\cdot}85$ (2), $\gamma = 60{\cdot}34$ (1)°, $Z = 2$]. The author considered the centrosymmetric space group $P\bar{1}$, but was unable to obtain refinement below an R value of 0·33. Hence, refinement was carried out in space group $P1$ leading to an R of 0·027 for 2789 reflections.

We have experienced no difficulty in carrying out the refinement in space group $P\bar{1}$. The center of symmetry was created by fixing atoms In(3) and In(5) at (0,0,0) and $(0,\frac{1}{2},\frac{1}{2})$ respectively. The other atoms were shifted accordingly ($x-0{\cdot}6668$, $y-0{\cdot}1626$, $z-0{\cdot}4985$). Full-matrix least-squares refinement quickly led to an R of 0·038. With the addition of a secondary-extinction parameter, further refinement resulted in a final R of 0·0276 for the 2789 reflections (recovered

Table 1. *Coordinates and* U_{eq} *values (all* $\times 10^4$*), space group* $P\bar{1}$

$U_{eq} = \frac{1}{3}\sum_i\sum_j |U_{ij}(a_i^* a_j^*)(\mathbf{a}_i.\mathbf{a}_j)|$.

	x	y	z	U_{eq}(Å^2)
In(3)	0	0	0	154 (1)
In(5)	0	5000	5000	171 (1)
In(1,4)	3352 (0·5)	−1621 (0·5)	4999 (0·4)	160 (1)
In(2,6)	3359 (0·5)	3402 (0·5)	−272 (0·4)	155 (1)
Ca(1,8)	3496 (1)	−2709 (2)	−1078 (1)	179 (2)
Ca(2,6)	2989 (2)	−2 (2)	1098 (1)	182 (2)
Ca(3,4)	3297 (2)	2013 (2)	3493 (1)	181 (2)
Ca(5,10)	220 (2)	981 (2)	−3521 (1)	186 (3)
Ca(7,9)	444 (2)	−3783 (2)	1094 (1)	181 (2)
Ca(11,15)	3332 (2)	2101 (2)	−2980 (1)	252 (3)
Ca(12,16)	1213 (2)	−3469 (2)	−2998 (1)	248 (3)
Ca(13,14)	3965 (2)	−4390 (2)	3301 (1)	216 (2)

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from SUP 43571) and 104 parameters. The $P1$ model of Fornasini involves 197 parameters.

Despite the change in space group, the $P\bar{1}$ structure reported here (Table 1)* differs little from the $P1$ structure of Fornasini (1987); indeed, all coordinates agree (after translation of the origin) within 0·04 Å. Thus, the coordination polyhedra described by Fornasini are little changed and the structure remains complex. However, 'the low symmetry, very unusual for an intermetallic phase' is not quite so low. In addition, the $P\bar{1}$ structure shows coordinate e.s.d.'s that are smaller by factors of about $\frac{1}{4}$ – due, of course, to the removal of the near-singularities inherent in refining an approximately centrosymmetric model in a non-centrosymmetric space group.

The $P\bar{1}$ model considered by Fornasini (1987), which was derived by 'direct methods', apparently differs from our model in that the two atoms In(1) and In(6), rather than In(3) and In(5), were located on centers of symmetry (0,0,0 and $0,\frac{1}{2},\frac{1}{2}$). In that model, the In atoms map fairly closely – within 0·3 Å – onto the In atoms in our model; however, many of the Ca atoms do not. It seems likely that further pursuit of the $P\bar{1}$ model of Fornasini, perhaps using difference maps, might have led to the correct structure.

* A list of anisotropic U_{ij} values has been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44474 (1 p.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Notes and News

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