four parameters, more information is needed. Redington, Olson & Cross (1962) chose an OH distance of 0·95 Å and obtained an O–O distance of 1·475 (4) Å from their infrared spectra. Busing & Levy (1965) feel that a more reasonable choice would be 0·96 Å, giving r(O–O) = 1·467 (4) Å. The microwave data of Oelfke & Gordy (1969) lead to r(O–O) = 1·470 Å for r(OH) = 0·96 Å.

The value of r(O–O) in $(NH_4)_2C_2O_4.H_2O_2$ uncorrected for librational motion [1·452 (1) Å] is significantly shorter than the gas-phase value. Based on our estimate of the librational correction, about 0·004 Å, the difference between solid- and gas-phase O–O distances will barely be significant, [1·467 (4) − 1·456 (1)] Å = 0·011 (4) Å. We therefore feel that more reliable gas-phase data and a rigorous correction for thermal motion in the solid are needed to settle this question.

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On the Structures of $Y_2Zn_{\sim 9}$, $Gd_2Zn_{\sim 9}$, and Related Compounds*

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A number of $M_2X_{\sim 9}$ compounds exist where M is a rare-earth or Pu atom and X is Zn or Cd. They all have a hexagonal cell, or subcell, with a about 14 to 15·5 Å and c/a about 0·98. Many of the compounds have a superlattice which increases the a axis and may or may not lower the symmetry. $Gd_2Zn_{\sim 9}$ is an ordered example of the parent structure. $Y_2Zn_{\sim 9}$ has an occupational disorder but does not have a superlattice. $Pu_2Zn_{\sim 9}$, $Y_2Cd_{\sim 9}$ and $Ce_2Cd_{\sim 9}$ each have different superlattices, but so far none of these superstructures has been solved.

Introduction

Several $M_2X_{\sim 9}$ compounds are known where M is a large rare-earth or plutonium atom and X is a smaller zinc or cadmium atom. The structure of the compound $Pu_2Zn_{\sim 9}$ has been reported by Larson & Cromer (1966, 1967). Cramer & Wood (1967) in their study of the Pu–Zn system have designated this phase as η, and we use their nomenclature for $Pu_2Zn_{\sim 9}$ and similar phases. The η phase has a hexagonal subcell, probable space group $P6_3/mmc$. The previous work on ηPu–Zn gave what is best described as the average structure for the subcell, for it was recognized that the true cell has a doubled a axis.

By coincidence, at about the time the work on ηPu–Zn was started, Elliott & Lemons (1964) were making vapor pressure measurements on the Ce–Cd system at approximately the η composition. To interpret their data they proposed the existence of a large

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number of ordered phases having very small composition differences and coined the term 'microphase'. It was found that these Ce–Cd compounds were isostructural with the Pu–Zn η phase.

Roof & Elliott (1965) studied ηCe–Cd and observed several different crystal lattices in each of several alloy specimens. They found superlattices that multiplied the *a* axis by 3, 6, or 8 times but none that doubled *a* as in ηPu–Zn. Further, the symmetry of many of these superlattices was orthorhombic or monoclinic instead of hexagonal. The study provided independent evidence for the microphase concept.

The structure proposed for ηPu–Zn has two formula units of $Pu_{13}Zn_{58}$ in the cell, leading to the formula $Pu_2Zn_{8.92}$. Wang (1967) has published a paper on $Gd_{13}Zn_{58}$, another compound of this type. The structure given by Wang for ηGd–Zn is essentially the same as that of ηPu–Zn, but he described it in $P6_3mc$ rather than $P6_3/mmc$. If the origin is shifted by about $\frac{1}{4}$ along the *z* axis, if other small shifts are made, and if certain position sets are combined, Wang's structure of ηGd–Zn then corresponds quite closely to our structure of ηPu–Zn. In the reported structure of ηGd–Zn there are several errors and omissions in the distance table, the most notable being the Zn(10)–Zn(13) distance which should be 2·01 Å rather than 2·32 Å. Also, using Wang's parameters we do not calculate the same structure factors for ηGd–Zn. We suspect that the patch which he refers to for $x\bar{x}z$ positions was incorrectly made.

We decided to make a further study of η phases, in particular the compounds that have shown no evidence of a superlattice and one having a pronounced superlattice, in the hope of determining the changes which produce the long-range order.

Lott & Chiotti (1966) have reported Y–Zn and Ce–Zn compounds of this type. Mason & Chiotti (1970) have also reported the existence of ηPr–Zn. We have prepared and studied ηY–Zn and ηGd–Zn, neither of which has a detectable superlattice. We have also prepared ηY–Cd which has a fairly pronounced superlattice. In ηY–Cd the hexagonal *a* axis (but not the *b* axis) is doubled. This doubling leads to an orthorhombic cell of the same size as the hexagonal *C*-centered orthorhombic cell, but with a large number of added reflections which violate the *C*-centering conditions. A number of space groups could result, depending on which of the symmetry planes of the original hexagonal cell are preserved. In this case the space group is *Pbnn* (or *Pnna* in standard setting). Note that this space group is centric and unambiguously recognized by the systematic extinctions. Extensive twinning of this crystal could result in apparent hexagonal symmetry with a doubled *a* axis leading to the superlattice observed in ηPu–Zn. Cramer (1968) has stated that photomicrographs of ηPu–Zn show extensive twinning. Therefore, it is possible that our work on ηPu–Zn was done with a multiply twinned crystal having an orthorhombic superlattice of the type shown by ηY–Cd.

Experimental

Alloys of ηGd–Zn and ηY–Zn were made by arc melting and slowly cooling M_2X_9 stoichiometric mixtures of the elements. Rapid cooling was required to quench the ηY–Cd phase, which is probably not stable at room temperature. Further evidence of the instability of this phase is that whiskers of cadmium metal grow out from the surface after a few weeks. Such whiskers were also observed to form on ηCe–Cd. The alloys were crushed and single-crystal fragments were readily found.

Lattice constants were obtained from a least-squares analysis of the settings of 12 reflections measured with Mo $K\alpha_1$ radiation ($\lambda = 0{\cdot}70926$ Å) on an automated Picker diffractometer (Busing & Levy, 1967). The lattice constants for several η phase compounds are given in Table 1. The orientation, least-squares, and data

Table 1. *Lattice constants for η phase $M_2X_{\sim 9}$ compounds*

	a	*c*	*c/a*	Reference
Pu–Zn	14·43 Å	14·14 Å	0·980	Larson & Cromer (1967)
Ce–Zn	14·60	14·11	0·966	Lott & Chiotti (1966)
Y–Zn	14·24	14·00	0·959	This work
Gd–Zn	14·31	14·05	0·982	This work
Gd–Zn	14·35	14·21	0·990	Wang (1967)
Ce–Cd	15·75	15·55	0·987	Roof & Elliott (1965)
Y–Cd (hexagonal subcell)	15·34	15·22	0·992	This work
Y–Cd (orthorhombic)	$a=15{\cdot}34$,	$b=26{\cdot}59$,	$c=15{\cdot}22$ Å	

Table 2. *Refinements of* ηGd–Zn

Model	*R*	R_w	Number of parameters	Number of observations
$P6_3mc$, isotropic*	0·125	0·078	68	780
$P6_3mc$, anisotropic*	0·132	0·076	135	780
$P6_3/mmc$, isotropic	0·153	0·095	37	780
$P6_3/mmc$, anisotropic*	0·135	0·083	76	780

* Thermal parameters not all real

collection programs used by the automated diffractometer were local versions of the Oak Ridge system (Busing, Ellison, Levy, King & Roseberry, 1968). Step scans were made with 2-sec counts at each step and increments of 0·05° 2θ over a range of 2° plus the α_1–α_2 dispersion. Zr-filtered Mo $K\alpha$ radiation was used. For ηGd–Zn the crystal shape was approximated by several plane faces, and absorption corrections were made by using the method of Busing & Levy (1957) and a modification of Burnham's (1962) program. The volume of the crystal was $1{\cdot}6\times10^{-3}$ mm^3, and transmission factors varied from 0·011 to 0·072. For ηY–Zn, the intensity at 10° intervals around the diffraction vector was measured for several reflections having χ near 90°. These measurements which produced factors varying from 0·54 to 1·70, combined with a spherical absorption correction obtained from an average value of μR of 1·4 for the fragment, were used to make an empirical absorption correction. The absorption correction for both crystals was crude, but hopefully better than none.

For ηGd–Zn, 8350 reflections were measured within a maximum 2θ of 70°. Most reflections were measured

Table 3. *Final parameters for* ηGd–Zn

	x	y	z	B
Gd(1)	0	0	0	3·7 (5) Å^2
Gd(2)	0·2065 (2)	$-x$	0·0515 (4)	0·3 (1)
Gd(3)	0·5414 (3)	$-x$	$\frac{1}{4}$	0·3 (1)
Gd(4)	0·8715 (5)	$-x$	$\frac{1}{4}$	2·2 (2)
Zn(1)	0	0	$\frac{1}{4}$	3·1 (9)
Zn(2)	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	1·9 (8)
Zn(3)	$\frac{1}{3}$	$\frac{2}{3}$	0·0949 (18)	0·1 (3)
Zn(4)	0·3633 (7)	0·0362 (7)	0·1012 (7)	1·5 (1)
Zn(5)	0·0973 (6)	$-x$	0·1599 (10)	1·7 (2)
Zn(6)	0·0833 (10)	0·3666 (10)	0	1·1 (2)
Zn(7)	0·4372 (5)	$-x$	0·1395 (8)	0·5 (2)
Zn(8)	0·6011 (6)	$-x$	0·0527 (10)	0·8 (2)
Zn(9)	0·7626 (5)	$-x$	0·1606 (9)	0·9 (2)
Zn(10)	0·2692 (9)	$-x$	$\frac{1}{4}$	1·5 (4)
Zn(11)	0·8098 (12)	x	0	3·0 (3)
Zn(12)	$\frac{1}{2}$	$\frac{1}{2}$	0	3·0 (5)

$g=4{\cdot}2\ (4)\times10^{-6}$.

Table 4. *Interatomic distances in* ηGd–Zn

Standard deviations are about 0·01 Å for Gd–Zn and 0·02 Å for Zn–Zn distances.

Gd(1)–2Zn(1)	3·51 Å
–6Zn(5)	3·30
–6Zn(11)	2·72
Gd(2)– Zn(3)	3·20
–2Zn(4)	3·05
–2Zn(4)	3·13
– Zn(5)	3·10
–2Zn(6)	3·19
–2Zn(7)	3·15
–2Zn(8)	3·09
– Zn(9)	3·08
– Zn(10)	3·19
–2Zn(11)	3·16
–2Zn(12)	3·81
Gd(3)– Zn(2)	3·10
–4Zn(4)	3·10
–2Zn(6)	3·24
–2Zn(7)	3·01
–2Zn(8)	3·14
–4Zn(9)	3·08
–2Zn(12)	3·66
Gd(4)– Zn(1)	3·18
–4Zn(4)	3·23
–4Zn(5)	3·14
–2Zn(6)	3·24
–2Zn(9)	2·98
–4Zn(11)	3·86
Zn(1)–2Gd(1)	3·51
–3Gd(4)	3·18
–6Zn(5)	2·72
Zn(2)–3Gd(3)	3·10
–6Zn(8)	3·21
–6Zn(9)	2·69
Zn(3)–3Gd(2)	3·20
–3Zn(7)	2·65
–3Zn(8)	2·63
–3Zn(10)	2·70
Zn(4)– Gd(2)	3·13 Å
– Gd(2)	3·05
– Gd(3)	3·10
– Gd(4)	3·23
– Zn(4)	2·98
– Zn(5)	3·40
– Zn(6)	2·58
– Zn(7)	3·04
– Zn(8)	3·10
– Zn(9)	2·63
– Zn(11)	2·67
– Zn(12)	2·67
Zn(5)– Gd(1)	3·30
– Gd(2)	3·10
–2Gd(4)	3·14
– Zn(1)	2·72
–2Zn(4)	3·40
– Zn(5)	2·53
–2Zn(6)	2·86
–2Zn(11)	2·63
Zn(6)–2Gd(2)	3·19
– Gd(3)	3·24
– Gd(4)	3·24
–2Zn(4)	2·58
–2Zn(5)	2·86
– Zn(6)	2·86
–2Zn(7)	2·99
– Zn(10)	2·57
Zn(7)–2Gd(2)	3·15
– Gd(3)	3·01
– Zn(3)	2·65
–2Zn(4)	3·04
–2Zn(6)	2·99
– Zn(7)	3·10
– Zn(8)	2·86
–2Zn(10)	2·73
– Zn(12)	2·50
Zn(8)—2Gd(2)	3·09 Å
– Gd(3)	3·14
– Zn(2)	3·21
– Zn(3)	2·63
–2Zn(4)	3·10
– Zn(7)	2·86
– Zn(8)	2·81
–2Zn(9)	2·59
– Zn(12)	2·61
Zn(9)— Gd(2)	3·08
–2Gd(3)	3·08
– Gd(4)	2·98
– Zn(2)	2·69
–2Zn(4)	2·63
–2Zn(8)	2·59
– Zn(9)	2·51
Zn(10)–2Gd(2)	3·19
–2Zn(3)	2·70
–2Zn(6)	2·57
–4Zn(7)	2·73
–2Zn(10)	2·75
Zn(11)– Gd(1)	2·72
–2Gd(2)	3·16
–2Gd(4)	3·86
–2Zn(4)	2·67
–2Zn(5)	2·63
–2Zn(11)	2·73
Zn(12)–4Gd(2)	3·81
–2Gd(3)	3·66
–4Zn(4)	2·67
–2Zn(7)	2·50
–2Zn(8)	2·61

at four equivalent positions. Out of 2091 unique reflections, 780 were considered to be observed according to the criterion $(I-B)>3(I+B)^{1/2}$. The fact that very few reflections over 50° were observed is responsible for the large ratio of unobserved-to-observed reflections. A comparison of equivalent reflections gave:

$$R_F=\sum_n \sum_i |F_{i,n}-\bar{F}_i| \sum_n \sum_i F_{i,n}=0\cdot070\ ,$$

where the summations are over the n equivalent measurements of the ith unique reflection. For ηY–Zn, 7949 reflections were measured within a maximum 2θ of 50°. Most reflections were measured at 12 equivalent positions, and, out of 863 unique reflections, 507 were considered observed, as given above. For these compared and averaged data, $R_F=0\cdot121$. Weights were derived from counting statistics (Evans, 1961).

Least-squares calculations minimized $\sum w(F_o-F_c^*)^2$, where $F_c^*=KF_c\,.\,G(\theta,g,F_c,\bar{T})$, K is a scale factor, F_c is the ordinary calculated structure factor, and G is an extinction function (Zachariasen, 1963; Larson, 1970, equation 22) involving an extinction parameter g and the mean path length $\bar{T}$. An extinction parameter was not used for ηY–Zn, so $F_c^*=KF_c$ in this case. Discrepancy indices cited are $R=\sum|\Delta F|/\sum|F_o|$ and $R_w=(\sum w\Delta F^2/\sum wF_o^2)^{1/2}$ with unobserved reflections omitted. Scattering factors were from Cromer & Waber (1965) and dispersion corrections $\Delta f'$ and $\Delta f''$ were from Cromer (1965). Anisotropic thermal parameters were of the form:

$$\exp\left[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})\right]\ .$$

Results

ηGd–Zn

Isotropic and anisotropic least-squares refinements of ηGd–Zn were made starting with both the acentric structure proposed by Wang (1967) and the centric structure given for ηPu–Zn. The results are summarized in Table 2. Hamilton's (1965) R ratio test strongly favors the acentric structure. However, for several reasons we believe the centric structure to be correct. First, because of uncertainties in defining the shape of the crystal that we used, there are probably large systematic errors in the absorption corrections. In the acentric refinement, two of the Zn atoms had negative isotropic thermal parameters, and in the corresponding anisotropic refinement, 18 of the 23 atoms had unreal thermal parameters. In the centric anisotropic refinement, six of the 16 atoms had unreal thermal parameters, but all atoms had positive thermal parameters for the isotropic refinement. The unreal thermal parameters probably reflect the systematic errors in the absorption corrections. The second reason for favoring the centric structure is that, as shown later, ηY–Zn is probably centric. The strongest evidence that this phase

Table 5. *Refinements of* ηY–Zn

Model	R	R_w	Number of parameters	Number of observations
$P6_3mc$, isotropic*	0·119	0·086	68	507
$P6_3mc$, anisotropic*	0·100	0·064	135	507
$P6_3/mmc$, isotropic	0·136	0·096	37	507
$P6_3/mmc$, anisotropic*	0·108	0·073	76	507
$P6_3/mmc$, anisotropic (disordered)	0·090	0·066	81	507

*Thermal parameters not all real.

Table 6. *Final parameters for* ηY–Zn

	x	y	z	$\beta_{11}\times 10^5$	$\beta_{22}\times 10^5$	$\beta_{33}\times 10^5$	$\beta_{12}\times 10^5$	$\beta_{13}\times 10^5$	$\beta_{33}\times 10^5$
Y(1)	0	0	0	56 (147)	β_{11}	223 (273)	β_{11}	0	0
Y(2)	0·2062 (3)	$-x$	0·0517 (4)	243 (41)	β_{11}	172 (35)	273 (102)	30 (39)	$-\beta_{13}$
Y(3)	0·5425 (4)	$-x$	$\frac{1}{4}$	308 (60)	β_{11}	213 (55)	338 (151)	0	0
Y(4)	0·8723 (6)	$-x$	$\frac{1}{4}$	314 (71)	β_{11}	1323 (128)	309 (180)	0	0
Zn(1)	0	0	$\frac{1}{4}$	239 (113)	β_{11}	981 (203)	β_{11}	0	0
Zn(2)	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	378 (119)	β_{11}	410 (149)	β_{11}	0	0
Zn(3)	$\frac{1}{3}$	$\frac{2}{3}$	0·0952 (12)	295 (70)	β_{11}	221 (79)	β_{11}	0	0
Zn(4)	0·3661 (5)	0·0341 (5)	0·1005 (4)	499 (56)	322 (50)	286 (28)	146 (80)	−230 (78)	29 (70)
Zn(5)	0·0984 (4)	$-x$	0·1581 (7)	584 (64)	β_{11}	369 (55)	815 (153)	79 (55)	$-\beta_{13}$
Zn(6)	0·0860 (6)	0·3673 (6)	$\frac{1}{4}$	236 (63)	196 (60)	250 (43)	139 (107)	0	0
Zn(7)	0·4371 (3)	$-x$	0·1426 (6)	419 (56)	β_{11}	227 (47)	628 (130)	−31 (42)	$-\beta_{13}$
Zn(8)	0·6009 (4)	$-x$	0·0521 (6)	291 (51)	β_{11}	236 (52)	77 (122)	−10 (50)	$-\beta_{13}$
Zn(9)	0·7631 (4)	$-x$	0·1585 (6)	211 (44)	β_{11}	250 (51)	128 (113)	5 (43)	$-\beta_{13}$
Zn(10)	0·2701 (5)	$-x$	$\frac{1}{4}$	296 (71)	β_{11}	177 (69)	277 (169)	0	0
Zn(11)	0·8042	x	0	650 (68)	β_{11}	1072 (86)	450 (180)	628 (79)	$-\beta_{13}$
Zn(12)	$\frac{1}{2}$	$\frac{1}{2}$	0	841 (115)	β_{11}	551 (93)	1469 (182)	182 (79)	$-\beta_{13}$
Zn(13)	0	0	0·0938 (35)	229 (256)	β_{11}	320 (422)	β_{11}	0	0

Occupancy parameters:

Y(1)	0·62 (7)
Zn(13)	0·34 (6)

is centric, however, is that ηY–Cd, as mentioned earlier, has an unambiguously centric orthorhombic cell. It seems quite unlikely that long-range ordering to form a superlattice would cause a noncentric structure to become centric.

Table 3 gives the final parameters from the isotropic refinement of ηGd–Zn in the centric space group. The interatomic distances are shown in Table 4. Note that our shortest Zn–Zn distance is 2·50 Å. The shortest distance we found in the acentric model is 2·28 Å as opposed to 2·01 Å in Wang's (1967) model.

ηY–Zn

Isotropic and anisotropic refinements were again made in both space groups and the results are given in Table 5. The acentric model has 10 atoms with unreal anisotropic thermal parameters and two atoms with negative isotropic thermal parameters. In the centric anisotropic model, Y(1), at the origin, had a slightly negative $\beta_{11}[\sim -0{\cdot}2\sigma(\beta_{11})]$ and a very large β_{33} ($B=57$ Å^2). Y(4) also had a large $\beta_{33}(B=12$ Å$^2)$.

A difference Fourier map was calculated after the anisotropic centric refinement, and a large peak was found at 0,0,0·1. This peak was also quite evident in an observed electron density map. A final model was calculated with a fractional Y(1) atom at the origin and a fractional Zn(13) atom at 0,0,0·1. The value of *R* for this model is also given in Table 5. Final parameters are listed in Table 6 and interatomic distances are given in Table 7. A final difference Fourier map showed residual features varying from −5 to +5 e.Å^{-3} at positions near atomic sites. Observed and calculated

Table 7. *Interatomic distances in* ηY–Zn

Standard deviations are about 0·01 Å except as noted for Zn(13)

Y(1)—2Zn(1)	3·50 Å
-6Zn(5)	3·28
-6Zn(11)	2·79
Y(2)— Zn(3)	3·19
-2Zn(4)	3·06
-2Zn(4)	3·09
- Zn(5)	3·05
-2Zn(6)	3·15
-2Zn(7)	3·16
-2Zn(8)	3·08
- Zn(9)	3·04
- Zn(10)	3·19
-2Zn(11)	3·10
-2Zn(12)	3·79
Y(3)— Zn(2)	3·06
-4Zn(4)	3·06
-2Zn(6)	3·27
-2Zn(7)	3·00
-2Zn(8)	3·12
-4Zn(9)	3·07
-2Zn(12)	3·65
Y(4)— Zn(1)	3·15
-4Zn(4)	3·28
-4Zn(5)	3·13
-2Zn(6)	3·24
-2Zn(9)	2·98
-4Zn(11)	3·84
Zn(1)-2Y(1)	3·50
-3Y(4)	3·15
-6Zn(5)	2·75
Zn(2)-3Y(3)	3·06
-6Zn(8)	3·21
-6Zn(9)	2·70
Zn(3)-3Y(2)	3·19
-3Zn(7)	2·64
-3Zn(8)	2·62
-3Zn(10)	2·67
Zn(4)- Y(2)	3·09
- Y(2)	3·06
- Y(3)	3·06
Zn(4)- Y(4)	3·28 Å
- Zn(4)	2·94
- Zn(5)	3·40
- Zn(6)	2·59
- Zn(7)	2·98
- Zn(8)	3·06
- Zn(9)	2·63
- Zn(11)	2·63
- Zn(12)	2·60
Zn(5)- Y(1)	3·28
- Y(2)	3·05
-2Y(4)	3·13
- Zn(1)	2·75
-2Zn(4)	3·40
- Zn(5)	2·57
-2Zn(6)	2·83
-2Zn(11)	2·62
Zn(6)-2Y(2)	3·15
- Y(3)	3·27
- Y(4)	3·24
-2Zn(4)	2·59
-2Zn(5)	2·83
- Zn(6)	2·78
-2Zn(7)	2·96
- Zn(10)	2·55
Zn(7)-2Y(2)	3·16
- Y(3)	3·00
- Zn(3)	2·64
-2Zn(4)	2·98
-2Zn(6)	2·96
- Zn(7)	3·01
- Zn(8)	2·88
-2Zn(10)	2·69
- Zn(12)	2·53
Zn(8)-2 Y(2)	3·08
- Y(3)	3·12
- Zn(2)	3·21
- Zn(3)	2·62
-2Zn(4)	3·06
- Zn(7)	2·88
- Zn(8)	2·81
-2Zn(9)	2·58
Zn(8)— Zn(12)	2·59 Å
Zn(9)— Y(2)	3·04
-2Y(3)	3·07
- Y(4)	2·98
- Zn(2)	2·70
-2Zn(4)	2·63
-2Zn(8)	2·58
- Zn(9)	2·56
Zn(10)-2Y(2)	3·19
-2Zn(3)	2·67
-2Zn(6)	2·55
-4Zn(7)	2·69
-2Zn(10)	2·70
Zn(11)- Y(1)	2·79
-2Y(2)	3·10
-2Y(4)	3·84
-2Zn(4)	2·63
-2Zn(5)	2·62
-2Zn(11)	2·79
Zn(12)-4Y(2)	3·79
-2 Y(3)	3·65
-4 Zn(4)	2·60
-2 Zn(7)	2·53
-2 Zn(8)	2·59
Additional distances when Zn(13) is present.	
Zn(13)- Y(1)*	1·31 (5)
-3Y(4)	3·83 (3)
- Zn(1)	2·19 (5)
-3Zn(5)	2·59 (2)
-6Zn(11)	3·08 (2)
- Zn(13)	2·63 (10)
Y(4)—2Zn(13)	3·83 (3)
Zn(1)—2Zn(13)	2·19 (5)
Zn(5)— Zn(13)	2·59 (2)
Zn(11)-2Zn(13)	3·08 (2)

* Zn(13) and Y(1) not simultaneously present.

structure factors with the standard deviations in the observed values appear in Table 8 and 9.

Discussion

Both $M(1)$ and $M(4)$ are in rather roomy surroundings. The ηPu–Zn paper (Larson & Cromer, 1967) includes stereo drawings of the polyhedra about these atoms, and Table 10 contains the anisotropic B's for these atoms when refined as ordered structures in $P6_3/mmc$. It is probable that ηGd–Zn is a reasonably well-ordered example of the parent structure of this class. There are no anomalously large thermal parameters in this compound or other evidence for a disordered Gd(1) atom. In ηY–Zn there is a random substitution of pairs of

Table 8. *Observed and calculated structure factors for* ηGd–Zn

Unobserved structure factors are omitted; column headings are l, F_o/K, $F_c{}^*/K$ and $\sigma(F_o)$.

l	F_o/K	$F_c{}^*/K$	$\sigma(F_o)$
H= 0 K= 0			
0	0	5177	0
4	651	734	4
6	779	761	4
8	732	871	4
10	996	1185	4
12	550	745	6
14	355	553	8
16	177	408	15
18	175	148	15
20	736	924	6
H= 1 K= 0			
0	98	68	2
1	112	5	5
3	141	165	6
4	157	257	6
5	95	102	11
6	310	382	4
8	108	174	12
10	251	239	6
12	130	192	14
13	137	184	15
14	132	81	18
H= 1 K= 1			
6	203	265	7
8	126	124	14
10	165	147	15
14	129	142	21
H= 1 K= 2			
0	99	130	8
2	230	249	4
8	353	368	5
9	133	142	14
10	207	214	9
12	179	213	11
13	214	231	9
18	157	216	14
20	164	86	23
22	146	66	20
H= 1 K= 3			
2	112	90	8
3	148	164	6
4	105	117	8
6	124	88	15
8	192	227	8
16	160	154	18
18	168	189	23
H= 1 K= 4			
0	120	148	8
1	429	414	3
4	260	265	4
5	98	66	15
6	134	141	11
8	153	150	13
9	243	237	8
10	209	174	10
11	243	252	9
12	146	92	21
H= 1 K= 5			
0	329	374	3
1	200	175	6
2	344	283	4
4	301	295	5
7	311	308	6
8	650	618	4
12	381	295	7
13	199	203	13
16	188	146	16
18	211	230	15
H= 1 K= 6			
2	130	152	10
3	163	150	8
7	153	91	13
8	162	149	12
16	176	130	18
H= 1 K= 7			
0	300	305	4
1	244	252	6
2	141	77	13
3	156	154	12
4	493	447	4
5	203	190	10
6	676	564	4
7	213	170	10
9	179	94	20
10	196	255	14
11	181	150	16
14	234	237	13
16	175	207	26
20	186	203	25
H= 1 K= 8			
3	472	474	4
6	176	130	12
9	214	148	12
10	191	87	17
11	168	121	19
17	228	191	15
H= 1 K= 9			
6	175	112	15
H= 1 K= 10			
0	224	239	7
4	341	336	6
6	410	387	6
7	149	18	22
8	206	171	11
10	145	175	14
12	254	214	12
14	199	125	19
16	256	226	13
H= 1 K= 11			
0	132	174	16
2	262	266	7
3	233	250	8
8	144	142	22
9	193	151	13
18	196	146	19
H= 1 K= 12			
2	152	181	13
3	171	159	10
12	203	221	14
14	293	111	22
H= 1 K= 13			
1	309	310	6
6	143	131	16
9	223	233	11
10	271	240	9
11	275	253	10
H= 1 K= 14			
0	128	56	15
H= 1 K= 15			
0	124	182	16
3	136	166	15
8	171	116	18
9	179	134	18
10	211	191	12
H= 1 K= 16			
0	339	341	6
4	224	204	9
5	178	191	12
6	305	292	8
H= 1 K= 18			
7	157	149	15
H= 1 K= 19			
0	157	155	13
H= 2 K= 0			
0	92	25	5
1	301	314	3
5	472	447	3
6	138	201	8
7	555	597	3
8	471	302	4
9	202	139	8
10	267	231	7
11	248	220	7
12	191	165	10
H= 2 K= 0			
13	295	383	7
14	139	95	13
15	284	296	7
H= 2 K= 2			
0	315	238	7
4	649	659	3
6	291	264	6
10	152	247	18
16	199	221	15
H= 2 K= 3			
0	109	159	7
2	385	388	3
3	1102	1082	2
5	126	110	8
7	529	469	4
8	176	200	11
9	286	262	7
10	250	350	9
11	223	172	10
12	186	212	12
13	433	438	6
15	146	80	22
17	360	399	7
H= 2 K= 4			
0	347	361	3
3	367	371	3
4	393	363	3
7	133	50	13
8	165	147	13
9	154	50	22
11	188	108	20
15	178	195	16
H= 2 K= 5			
0	115	124	10
1	529	547	3
2	217	205	5
3	123	99	11
4	229	171	5
5	546	524	3
6	320	325	5
7	133	78	13
8	179	92	11
9	352	327	7
11	402	366	7
12	233	159	12
13	192	69	17
14	164	132	20
15	298	330	10
21	173	178	18
H= 2 K= 6			
0	190	209	5
1	145	170	7
2	564	568	3
3	191	172	7
5	157	148	10
7	236	208	9
8	344	310	7
12	268	302	11
13	281	218	11
18	241	265	13
20	196	96	22
H= 2 K= 7			
0	145	119	8
10	167	122	17
13	168	96	25
H= 2 K= 8			
0	145	208	9
1	668	679	3
5	562	515	4
7	146	81	20
8	173	133	14
9	534	457	6
10	348	275	8
11	559	502	6
12	162	66	25
15	333	376	11
19	210	167	17
H= 2 K= 9			
0	120	136	12
1	186	163	8
7	387	391	6
8	150	67	21
11	161	72	21
13	280	267	12
H= 2 K= 10			
3	287	298	6
5	238	240	9
7	182	177	12
8	216	153	11
9	166	119	15
10	216	167	12
12	227	151	18
15	180	120	25
17	210	193	20
H= 2 K= 11			
0	475	460	4
1	146	169	11
4	398	380	5
5	160	143	17
6	491	459	5
10	307	347	9
14	250	252	13
16	207	214	19
H= 2 K= 12			
3	190	235	10
H= 2 K= 13			
1	146	96	15
3	219	200	9
5	182	231	12
7	366	338	7
13	260	238	11
15	185	180	26
H= 2 K= 14			
0	179	142	10
1	268	277	7
5	375	392	6
6	150	141	22
8	153	39	20
9	229	179	11
11	229	189	14
H= 2 K= 15			
3	160	77	14
7	191	223	12
H= 2 K= 16			
0	181	230	13
2	251	259	8
8	193	185	14
H= 2 K= 17			
1	153	132	15
5	153	102	21
H= 2 K= 18			
3	199	235	11
H= 3 K= 0			
0	182	206	4
1	227	199	5
2	129	125	9
3	237	261	5
4	380	347	3
5	1609	1591	2
6	640	579	3
7	261	306	5
8	254	238	6
9	170	219	10
10	868	855	4
11	149	233	17
12	165	98	12
14	247	207	8
15	636	762	4
H= 3 K= 3			
0	1674	1696	3
2	316	279	4
4	426	343	4
6	419	372	6
8	222	212	12
10	716	689	7
12	249	232	15
H= 3 K= 3			
16	301	287	26
20	392	457	11
H= 3 K= 4			
0	178	253	5
1	184	168	5
2	149	128	6
6	154	194	10
7	147	90	13
9	408	381	5
10	181	150	19
12	189	170	15
13	229	267	14
17	218	167	15
18	172	175	21
H= 3 K= 5			
0	178	195	5
1	113	73	12
2	281	305	4
3	404	337	3
4	147	86	8
5	389	320	4
7	818	710	4
8	287	256	7
9	177	81	13
11	284	213	10
12	262	156	11
13	427	432	8
15	283	259	12
17	201	218	20
18	211	216	17
H= 3 K= 6			
0	127	145	10
2	217	190	6
3	288	243	5
4	128	110	17
5	838	763	3
6	196	156	9
7	303	179	7
10	425	357	7
15	428	362	9
H= 3 K= 7			
0	276	321	4
1	163	176	7
2	253	270	5
3	607	612	3
4	146	175	19
5	284	254	7
6	175	188	11
12	241	190	13
13	245	299	14
15	295	219	13
17	202	122	28
19	219	75	23
H= 3 K= 8			
1	131	151	13
2	368	390	4
4	622	174	9
6	373	335	6
10	246	223	11
12	375	396	9
13	254	208	14
18	222	190	22
H= 3 K= 9			
4	161	149	11
5	309	293	6
6	278	238	7
14	178	100	25
15	186	161	28
H= 3 K= 10			
2	294	279	5
3	355	365	5
4	166	70	10
5	186	173	10
7	606	543	5
8	289	270	8
13	458	418	8
14	209	141	22
17	245	228	16
18	216	230	23
H= 3 K= 11			
2	179	156	5
3	329	364	6
4	172	95	16
7	321	355	7
9	149	135	13
12	170	104	26
13	249	203	13
17	257	260	16
H= 3 K= 12			
1	216	207	7
5	220	216	5
9	173	171	17
11	221	228	13
15	195	168	22
H= 3 K= 13			
2	271	297	7
8	378	374	7
9	167	185	15
10	211	195	14
12	231	242	13
H= 3 K= 15			
1	297	309	7
4	332	315	7
6	178	182	14
9	221	203	12
11	208	191	14
H= 3 K= 16			
3	184	234	12
7	205	159	14
H= 3 K= 18			
0	278	278	8
4	231	217	10
H= 4 K= 0			
0	123	150	6
1	124	148	7
2	198	165	5
3	404	425	3
4	417	453	3
5	184	206	6
6	440	468	3
8	187	136	9
9	169	103	13
11	299	315	7
12	244	212	9
13	155	222	14
17	151	51	24
H= 4 K= 4			
0	443	457	5
4	310	278	6
6	474	424	6
12	335	231	13
14	198	139	25
16	222	168	21
H= 4 K= 5			
0	214	231	5
3	120	76	10
4	137	131	10
5	133	60	17
7	176	129	11
8	137	75	17
13	239	157	14
H= 4 K= 6			
1	144	153	9
2	120	115	15
4	182	155	8
6	363	306	6
7	253	210	8
8	338	317	7
10	269	155	10
13	226	119	22
14	338	252	11
H= 4 K= 7			
0	182	154	7
1	495	503	3
2	149	180	9
4	183	123	9
6	384	307	5
9	355	300	7
H= 4 K= 7			
10	198	140	13
11	493	350	7
19	196	82	27
H= 4 K= 8			
0	258	325	5
3	120	87	18
5	177	167	10
7	165	144	12
13	195	163	24
H= 4 K= 9			
2	127	142	14
12	186	94	22
H= 4 K= 10			
0	253	214	6
1	208	231	7
2	126	149	13
3	142	157	17
4	219	148	8
5	241	228	8
6	275	283	8
7	156	156	14
8	182	109	13
9	166	89	22
10	239	166	11
11	196	139	15
H= 4 K= 11			
3	150	166	18
5	151	120	14
8	249	212	9
10	234	169	12
H= 4 K= 12			
0	145	114	11
2	159	128	10
7	163	167	16
H= 4 K= 13			
0	446	465	4
1	132	112	14
4	181	215	12
5	186	160	11
10	164	109	19
12	193	113	21
H= 4 K= 14			
10	183	80	23
H= 4 K= 16			
5	144	110	20
H= 4 K= 17			
2	153	124	16
H= 5 K= 0			
0	564	623	2
1	186	177	5
2	1348	1327	2
3	532	509	3
4	106	119	16
5	262	236	5
6	228	269	6
8	742	706	4
9	306	357	7
10	182	154	16
11	210	189	12
12	545	583	5
13	186	110	17
18	438	525	6
20	208	213	13
22	268	313	10
H= 5 K= 5			
0	1139	1161	4
2	155	135	17
4	1119	1023	4
6	926	706	5
10	782	723	7
14	411	328	14
16	556	496	12
18	194	71	27
20	408	466	14
H= 5 K= 6			
0	129	222	11
1	186	200	8
3	291	323	5
5	137	82	16
6	289	300	6
8	165	159	13
10	479	323	6
12	215	147	16
14	225	103	20
15	203	60	28
16	199	104	25
17	213	220	24
H= 5 K= 7			
0	143	91	10
2	128	105	17
5	197	204	9
7	319	297	7
8	191	199	13
10	255	197	10
12	187	125	18
13	249	170	17
15	268	154	16
H= 5 K= 8			
0	181	268	8
1	532	516	4
4	287	260	6
5	676	635	4
6	273	259	7
9	440	367	6
10	247	196	10
11	406	380	8
14	220	152	20
15	478	432	9
16	241	185	25
H= 5 K= 9			
1	148	210	10
2	195	194	8
5	175	225	10
7	203	216	10
9	151	42	21
13	183	172	25
15	204	117	29
H= 5 K= 10			
0	421	473	4
2	514	513	4
3	151	65	12
6	151	92	15
8	306	314	8
10	408	200	13
12	303	288	11
H= 5 K= 11			
0	292	357	6
1	225	211	7
4	161	116	11
5	193	214	10
6	246	226	9
9	196	201	13
10	433	366	7
11	188	187	22
14	200	158	20
H= 5 K= 12			
2	213	218	8
4	154	112	15
8	253	202	10
12	237	175	13
H= 5 K= 13			
2	177	115	10
3	323	364	6
5	250	237	9
7	237	227	10
8	183	96	13
10	180	166	19
13	212	225	24
H= 5 K= 14			
0	310	286	6
4	213	175	10
5	145	84	20
6	163	167	20
10	216	232	22
H= 5 K= 15			
0	207	187	9
2	234	216	9
3	150	100	15
4	150	85	21
8	156	179	16
H= 5 K= 16			
2	173	229	11
H= 6 K= 0			
0	127	105	7
1	246	279	4
2	534	573	3
3	123	61	15
5	690	663	3
8	271	285	8
9	211	131	13
10	979	923	4
11	211	103	11
12	163	137	21
15	274	314	13
H= 6 K= 6			
0	795	849	5
2	117	21	25
4	227	172	11
8	285	209	11
10	398	333	10
12	295	136	15
16	210	128	42
H= 6 K= 7			
1	157	58	16
2	210	179	8
8	323	319	7
10	170	215	19
13	180	96	27
17	277	173	22
18	241	190	28
H= 6 K= 8			
3	159	118	13
4	162	129	11
7	295	304	7
8	167	164	13
11	164	110	21
12	200	154	15
13	207	150	18
H= 6 K= 9			
4	173	113	10
12	192	144	19
H= 6 K= 10			
2	218	266	8
3	227	223	8
4	312	329	6
8	371	307	6
12	414	310	8
13	223	197	21
H= 6 K= 11			
2	267	282	7
8	205	168	16
12	259	240	13
14	185	109	21
H= 6 K= 12			
0	208	185	8
4	282	249	7
6	171	167	13
H= 6 K= 13			
2	134	58	21
3	231	266	8
7	175	219	14
H= 6 K= 14			
6	169	125	18
7	171	169	17
H= 6 K= 15			
0	182	202	15
1	171	156	11
6	178	108	15
H= 6 K= 16			
2	211	257	10
H= 7 K= 0			
0	228	316	4
1	177	210	6
2	310	282	4
3	203	215	7
4	212	213	8
5	136	169	21
7	607	592	4
8	340	378	7
11	166	118	21
13	433	394	7
14	200	184	13
17	184	165	20
18	213	275	16
20	173	164	22
H= 7 K= 7			
0	459	490	7
4	468	472	6
6	174	161	14
12	164	132	26
16	332	231	19
H= 7 K= 8			
2	154	103	13
3	390	394	5
5	248	239	8
7	204	185	13
8	160	78	17
9	172	138	15
10	172	115	21
15	204	127	21
17	258	194	19
H= 7 K= 9			
0	133	28	14
3	218	292	8
7	244	191	9
13	226	164	15
H= 7 K= 10			
2	142	117	19
5	353	357	6
6	157	138	18
10	417	363	7
15	218	168	18
H= 7 K= 11			
0	167	209	11
2	175	187	10
8	178	190	13
H= 7 K= 12			
12	186	69	23
H= 7 K= 13			
5	403	416	6
6	180	165	13
10	225	205	13
H= 7 K= 14			
3	159	114	15
5	146	154	21
H= 8 K= 0			
0	106	63	14
2	290	298	5
3	877	897	3
4	213	191	9
5	171	132	12
6	145	166	19
7	563	522	5
8	269	255	9
9	187	217	15
10	223	128	11
12	317	273	9
13	386	387	8
15	164	136	25
17	452	442	7
H= 8 K= 8			
0	515	512	7
4	411	387	7
6	331	290	9
10	373	422	11
14	221	195	13
16	269	218	34
H= 8 K= 9			
3	261	254	7
7	176	166	14
H= 8 K= 10			
3	261	235	7
5	208	239	10
7	319	288	7
8	208	225	11
13	258	248	12
H= 8 K= 11			
1	240	225	8
5	367	392	6
6	149	99	19
9	201	192	15
11	185	172	18
H= 8 K= 12			
3	151	130	14
7	204	200	11
H= 8 K= 13			
0	188	246	10
2	213	236	9
8	222	236	12
H= 8 K= 14			
1	162	123	15
5	232	254	10
H= 9 K= 0			
0	647	685	3
1	178	180	8
3	153	243	10
4	149	187	17
6	158	66	19
7	150	86	18
8	217	144	11
9	160	170	21
10	172	224	16
12	175	95	17
H= 9 K= 9			
10	147	32	34
H= 9 K= 10			
2	167	97	12
H= 9 K= 12			
1	137	105	17
5	162	146	13
H= 10 K= 0			
0	376	399	4
1	269	263	6
2	693	750	3
4	369	366	5
6	298	286	7
7	228	164	10
8	475	513	6
10	302	304	9
12	270	289	10
13	296	268	10
14	190	142	22
16	236	161	14
17	204	184	22
18	410	414	9
H= 10 K= 10			
0	729	763	6
2	159	108	22
10	292	282	13
H= 10 K= 11			
4	139	16	19
8	179	110	13
H= 11 K= 0			
0	190	162	10
2	387	473	5
3	165	153	10
4	414	414	5
7	329	336	7
8	571	529	5
12	503	413	7
16	231	176	14
17	211	189	17
18	301	278	12
H= 11 K= 11			
0	420	439	8
2	131	31	31
4	260	232	12
6	214	179	14
H= 11 K= 12			
2	153	137	13
H= 12 K= 0			
0	172	176	9
1	245	319	7
6	250	258	8
9	200	165	12
10	289	261	9
11	231	138	11
14	208	102	19
H= 13 K= 0			
0	192	201	10
2	220	328	8
3	516	563	4
4	172	190	12
5	176	193	11
7	268	193	8
8	184	163	12
12	285	246	10
13	295	352	10
15	225	205	14
17	188	167	23
H= 14 K= 0			
2	181	182	10
4	169	154	13
13	174	116	22
H= 15 K= 0			
0	440	416	5
1	133	159	16
2	154	165	12
4	441	394	5
6	250	320	8
10	293	315	9
H= 16 K= 0			
3	165	188	13
6	236	242	9
7	159	243	14
8	228	220	10
10	183	176	16
H= 17 K= 0			
0	148	194	15
6	174	167	13
H= 18 K= 0			
0	161	179	15
1	264	258	7
5	266	250	8
7	177	164	18
9	195	208	14
13	208	187	16
H= 19 K= 0			
2	213	220	10

Table 9. *Observed and calculated structure factors for* ηY–Zn

Column headings are l, F_o/K, F_c, 10 $\sigma(F_o)$. A minus sign preceding F_o means 'less than' and the value given is that derived from $3\sigma(I)$.

l	F_o/K	F_c	10 $\sigma(F_o)$
H= 0 K= 0			
0	0	4476	0
2	-37	27	0
4	170	226	31
6	655	465	24
8	645	662	25
10	635	724	24
12	484	513	50
14	227	281	99
16	105	35	178
H= 1 K= 0			
0	148	104	11
1	61	35	18
2	-37	4	0
3	60	56	28
4	95	123	20
5	-39	37	0
6	234	272	14
7	182	191	16
8	57	53	39
9	94	75	24
10	184	185	14
11	-65	5	0
12	78	57	61
13	-64	16	0
14	88	53	57
15	-72	16	0
16	-74	51	0
H= 1 K= 1			
0	77	77	34
2	-40	34	0
4	63	66	37
6	114	113	24
8	137	128	25
10	209	216	16
12	-65	5	0
14	92	75	46
16	-72	11	0
H= 1 K= 2			
0	-44	12	0
1	49	42	35
2	-41	38	0
3	55	73	30
4	66	76	25
5	-41	10	0
6	99	122	19
7	59	67	35
8	151	158	13
9	98	110	19
10	120	115	24
11	-65	30	0
12	-66	37	0
13	157	158	21
14	-70	36	0
15	-71	22	0
16	-72	12	0
H= 1 K= 3			
0	-43	36	0
1	-41	13	0
2	-44	37	0
3	95	107	19
4	62	51	28
5	-40	9	0
6	87	76	22
7	-45	20	0
8	67	61	47
9	-59	30	0
10	100	106	29
11	-65	34	0
12	134	121	24
13	-69	14	0
14	-72	71	0
15	-72	48	0
16	91	75	46
H= 1 K= 4			
0	88	125	46
1	261	267	12
2	-41	31	0
3	46	52	44
4	144	189	16
5	241	239	13
6	64	66	31
7	-56	35	0
8	75	79	26
9	116	113	25
10	125	123	24
11	136	101	28
12	-68	47	0
13	-70	36	0
14	-70	53	0
15	92	77	43
H= 1 K= 5			
0	375	347	18
1	182	156	14
2	279	267	13
3	257	235	13
4	217	201	14
5	51	34	54
6	107	119	18
7	120	123	17
8	428	425	10
9	91	71	33
10	-65	31	0
11	-68	64	0
12	197	195	19
13	-73	61	0
14	-72	69	0
15	-73	40	0
H= 1 K= 6			
0	66	55	60
1	86	73	25
2	91	85	23
3	78	68	27
4	59	47	37
5	-60	15	0
6	83	76	31
7	119	107	27
8	145	153	22
9	70	81	50
10	97	93	32
11	-68	29	0
12	-70	29	0
13	-73	48	0
14	-73	16	0
H= 1 K= 7			
0	74	32	45
1	170	174	16
2	106	107	22
3	133	133	18
4	227	219	13
5	194	193	14
6	406	402	14
7	162	167	21
8	-64	7	0
9	92	85	35
10	-68	18	0
11	107	81	30
12	-71	7	0
13	-71	26	0
14	105	89	36
H= 1 K= 8			
0	85	56	46
1	76	77	35
2	-63	47	0
3	314	333	12
4	-68	31	0
5	78	75	48
6	136	138	25
7	-69	15	0
8	-68	9	0
9	129	128	28
10	-71	54	0
11	90	68	44
12	-71	16	0
13	-73	17	0
H= 1 K= 9			
0	120	52	59
1	-67	4	0
2	-66	7	0
3	93	46	39
4	76	64	45
5	-68	37	0
6	-69	63	0
H= 1 K= 9			
7	-68	4	0
8	-69	23	0
9	-71	12	0
10	90	54	49
11	-73	2	0
12	-73	39	0
H= 1 K= 10			
0	268	292	23
1	-67	13	0
2	-69	67	0
3	-69	17	0
4	246	242	18
5	82	83	43
6	239	208	18
7	-70	22	0
8	131	112	29
9	-72	20	0
10	-74	40	0
11	-74	18	0
H= 1 K= 11			
0	96	100	61
1	67	77	41
2	146	139	25
3	189	189	21
4	-72	53	0
5	-71	20	0
6	-72	26	0
7	-73	34	0
8	96	77	40
9	155	140	26
10	-73	11	0
H= 1 K= 12			
0	-73	11	0
1	-71	11	0
2	-70	14	0
3	121	103	32
4	116	93	33
5	-74	19	0
6	-74	6	0
7	-73	33	0
8	-74	19	0
H= 1 K= 13			
0	-73	25	0
1	226	191	19
2	-74	16	0
3	-73	40	0
4	-74	4	0
5	-75	63	0
6	189	161	23
H= 1 K= 14			
0	145	76	38
1	-74	21	0
2	-73	5	0
H= 2 K= 0			
0	-41	12	0
1	-40	53	0
2	-51	53	0
3	-41	48	0
4	62	31	49
5	327	340	13
6	131	115	18
7	310	308	15
8	269	269	16
9	182	169	15
10	177	178	30
11	201	211	24
12	81	70	70
13	151	159	31
14	95	88	52
15	180	184	30
16	-73	21	0
H= 2 K= 2			
0	146	22	58
2	-39	9	0
4	439	448	16
6	151	149	22
8	-54	22	0
10	-63	30	0
12	-67	10	0
14	-69	17	0
16	102	99	61
H= 2 K= 3			
0	75	61	37
1	-41	4	0
2	240	247	12
3	816	804	11
4	-46	55	0
5	-46	16	0
6	62	42	31
7	229	228	11
8	-56	30	0
9	186	191	20
10	125	139	26
11	132	128	26
12	84	93	47
13	198	198	21
14	-70	12	0
15	-71	21	0
H= 2 K= 4			
0	390	338	17
1	-46	23	0
2	85	78	23
3	261	261	13
4	295	302	13
5	47	43	50
6	-48	14	0
7	-55	15	0
8	70	68	33
9	79	81	43
10	-67	7	0
11	91	63	50
12	60	69	52
13	95	44	45
14	-71	27	0
15	-71	31	0
H= 2 K= 5			
0	84	76	38
1	365	340	12
2	250	243	14
3	86	69	23
4	107	103	21
5	204	199	13
6	130	119	17
7	89	93	25
8	94	92	35
9	157	153	23
10	87	70	47
11	178	178	23
12	140	140	28
13	83	73	62
14	-72	51	0
15	103	103	39
H= 2 K= 6			
0	110	120	31
1	132	144	19
2	296	289	14
3	139	151	17
4	-59	35	0
5	122	133	20
6	-59	5	0
7	164	166	23
8	107	48	31
9	-67	49	0
10	-67	52	0
11	-69	10	0
12	87	71	42
13	175	166	25
14	-73	36	0
H= 2 K= 7			
0	88	71	41
1	106	51	28
2	86	78	30
3	80	77	30
4	70	59	33
5	-66	28	0
6	46	65	35
7	-66	47	0
8	90	71	53
H= 2 K= 7			
9	-70	30	0
10	95	78	44
11	-69	7	0
12	-72	45	0
13	-71	56	0
H= 2 K= 8			
0	-66	20	0
1	362	440	16
2	-66	7	0
3	-66	48	0
4	-66	61	0
5	183	174	23
6	-66	11	0
7	79	81	55
8	109	124	34
9	243	225	19
10	115	118	33
11	264	237	19
12	102	89	44
13	-72	27	0
H= 2 K= 9			
0	108	136	49
1	125	142	31
2	77	71	56
3	-68	53	0
4	75	53	52
5	-66	17	0
6	-71	31	0
7	214	206	22
8	-72	13	0
9	-73	6	0
10	-73	4	0
11	-72	48	0
12	-74	9	0
H= 2 K= 10			
0	-71	48	0
1	-68	17	0
2	-69	19	0
3	157	146	26
4	-69	57	0
5	148	139	26
6	-72	45	0
7	-75	43	0
8	104	79	60
9	106	87	38
10	46	93	53
H= 2 K= 11			
0	184	172	30
1	116	123	31
2	-70	19	0
3	-70	18	0
4	176	165	24
5	116	104	34
6	264	228	19
7	-72	9	0
8	-74	15	0
9	85	70	59
H= 2 K= 12			
0	-72	19	0
1	-75	51	0
2	-70	29	0
3	122	105	36
4	-72	54	0
5	-72	15	0
6	-74	23	0
7	-73	11	0
H= 2 K= 13			
0	86	46	67
1	88	71	50
2	-72	7	0
3	86	59	55
4	-74	13	0
H= 3 K= 0			
0	-48	54	0
1	98	104	21
2	46	63	42
3	177	191	18
4	211	221	15
5	1263	1308	12
6	758	774	13
7	209	202	17
8	215	217	14
9	66	28	40
10	568	592	17
11	85	62	54
12	110	115	39
13	-67	14	0
14	267	250	23
15	376	376	20
16	-74	67	0
H= 3 K= 3			
0	1481	1471	20
2	277	262	17
4	627	629	16
6	143	125	27
8	121	111	26
10	302	301	23
12	159	151	35
14	-70	53	0
H= 3 K= 4			
0	296	283	19
1	169	166	15
2	-44	34	0
3	58	62	31
4	-45	1	0
5	75	78	29
6	98	110	22
7	90	91	25
8	207	201	20
9	127	132	27
10	63	77	44
11	-68	4	0
12	88	77	55
13	152	140	27
14	-73	35	0
15	-72	6	0
H= 3 K= 5			
0	166	130	24
1	72	42	31
2	129	118	18
3	118	133	20
4	157	168	15
5	224	220	13
6	-59	14	0
7	425	424	15
8	-66	76	0
9	125	120	29
10	-69	75	0
11	168	153	24
12	-73	52	0
13	171	161	25
14	-72	18	0
H= 3 K= 6			
0	-59	20	0
1	71	64	33
2	142	146	18
3	205	212	14
4	-59	24	0
5	496	517	15
6	230	231	19
7	207	209	20
8	63	35	62
9	62	53	55
10	192	191	22
11	-70	17	0
12	-71	14	0
13	-72	39	0
14	96	70	53
H= 3 K= 7			
0	214	227	21
1	124	139	19
2	152	175	30
3	311	350	17
4	-68	69	0
5	141	152	27
6	115	128	31
7	95	104	37
8	-69	31	0
H= 3 K= 7			
9	-69	24	0
10	82	62	55
11	-71	25	0
12	87	80	51
13	96	72	42
H= 3 K= 8			
0	-66	42	0
1	85	106	47
2	103	121	37
3	-66	14	0
4	-65	32	0
5	-68	17	0
6	97	119	40
7	137	116	30
8	127	116	30
9	-69	12	0
10	113	95	37
11	-72	54	0
12	131	100	31
H= 3 K= 9			
0	96	83	58
1	-67	68	0
2	-69	56	0
3	-69	29	0
4	90	87	45
5	170	164	24
6	181	166	24
7	-72	6	0
8	-71	10	0
9	-72	37	0
10	-73	32	0
11	-72	43	0
H= 3 K= 10			
0	-72	58	0
1	87	77	45
2	180	180	23
3	156	140	27
4	86	86	52
5	-73	85	0
6	-71	9	0
7	312	294	18
8	141	125	36
9	-72	26	0
H= 3 K= 11			
0	-67	76	0
1	-69	49	0
2	109	114	37
3	173	150	25
4	103	64	41
5	-71	36	0
6	-73	17	0
7	153	128	26
8	-74	9	0
H= 3 K= 12			
0	-69	5	0
1	103	81	36
2	88	62	53
3	-71	46	0
4	-74	11	0
5	81	51	61
H= 4 K= 0			
0	99	114	51
1	113	107	19
2	106	111	21
3	307	297	14
4	363	366	14
5	196	202	16
6	366	373	15
7	147	137	22
8	152	152	23
9	102	85	27
10	-64	28	0
11	227	221	23
12	171	166	28
13	-72	55	0
14	-72	49	0
15	85	71	65
16	-74	42	0
H= 4 K= 4			
0	592	560	27
2	-45	7	0
4	162	170	21
6	243	253	18
8	85	68	64
10	132	112	39
12	174	174	34
14	94	81	66
H= 4 K= 5			
0	159	178	30
[illegible]	-60	11	0
1	-49	11	0
2	-58	40	0
3	-57	49	0
4	102	100	23
5	-60	36	0
6	-65	29	0
7	161	161	23
8	115	125	32
9	109	118	33
10	-68	44	0
11	-64	54	0
12	91	69	49
13	163	154	27
14	-73	27	0
H= 4 K= 6			
0	-62	48	0
1	111	118	23
2	118	129	22
3	87	94	45
4	87	125	44
5	98	88	39
6	201	220	21
7	102	102	33
8	180	175	23
9	-68	4	0
10	141	121	28
11	-70	35	0
12	-72	41	0
13	-72	33	0
H= 4 K= 7			
0	128	162	42
1	304	306	17
2	106	115	35
3	-60	13	0
4	114	110	33
5	119	125	32
6	283	284	18
7	-69	41	0
8	-69	16	0
9	164	169	23
10	101	91	40
11	245	227	20
12	-73	13	0
H= 4 K= 8			
0	146	210	39
1	-66	40	0
2	-66	12	0
3	127	147	32
4	-72	47	0
5	115	123	35
6	-68	33	0
7	90	92	47
8	81	80	54
9	109	93	44
10	-73	22	0
11	-71	39	0
H= 4 K= 9			
0	-68	15	0
1	81	74	49
2	-71	22	0
3	-69	7	0
4	-71	46	0
5	-69	46	0
6	-71	25	0
7	107	101	37
8	-72	35	0
9	101	74	46
10	-72	5	0
H= 4 K= 10			
0	118	135	43
1	179	173	25
2	95	116	44
3	101	106	40
4	98	101	46
5	151	153	29
6	162	171	24
7	119	112	35
8	104	87	46
H= 4 K= 11			
0	-70	22	0
1	-70	30	0
2	-72	8	0
3	160	161	27
4	95	74	60
5	-74	76	0
6	-73	30	0
H= 4 K= 12			
0	90	111	62
1	-72	1	0
2	112	97	38
3	-73	44	0
H= 5 K= 0			
0	559	524	19
1	217	181	15
2	1048	1017	13
3	513	494	14
4	86	66	27
5	249	242	18
6	144	114	21
7	78	80	29
8	430	423	17
9	276	276	21
10	-71	47	0
11	186	168	27
12	273	275	22
13	-74	59	0
14	97	81	50
15	-74	59	0
H= 5 K= 5			
0	631	705	23
2	95	104	37
4	594	656	20
6	627	456	21
8	-70	27	0
10	305	292	24
12	-71	10	0
H= 5 K= 6			
0	93	96	53
1	161	198	26
2	-66	35	0
3	87	64	43
4	-65	38	0
5	-67	52	0
6	171	161	23
7	134	133	28
8	-67	38	0
9	-66	22	0
10	246	225	19
11	-70	29	0
12	90	53	58
H= 5 K= 7			
0	100	132	52
1	84	101	48
2	-66	63	0
3	-66	11	0
4	-68	6	0
5	103	102	38
6	-71	64	0
7	167	161	26
8	86	52	63
9	-69	19	0
10	117	104	35
11	84	52	60
H= 5 K= 8			
0	-67	31	0
1	250	291	19
2	-69	56	0
3	-67	32	0
4	141	151	29
5	267	275	19
6	100	104	42
7	-71	42	0
8	-71	27	0
9	196	180	23
10	-71	42	0
H= 5 K= 9			
0	-67	8	0
1	110	121	34
2	86	66	51
3	-70	15	0
4	-71	19	0
5	146	131	30
6	-71	9	0
7	115	110	36
8	-73	9	0
9	-73	22	0
H= 5 K= 10			
0	269	277	25
1	-70	33	0
2	282	252	18
3	106	86	38
4	-72	31	0
5	-76	34	0
6	94	60	51
7	-72	63	0
H= 5 K= 11			
0	158	155	37
1	67	63	60
2	80	45	58
3	-72	56	0
4	-74	67	0
H= 6 K= 0			
0	-64	25	0
1	520	499	14
2	498	477	14
3	69	48	34
4	-46	8	0
5	342	305	15
6	-74	57	0
7	-62	56	0
8	194	188	26
9	294	287	21
10	601	656	17
11	266	257	23
12	-71	60	0
13	-75	61	0
14	-72	24	0
15	80	82	82
H= 6 K= 6			
0	496	641	34
2	75	75	83
4	103	124	56
6	-67	34	0
8	159	163	38
10	241	229	29
H= 6 K= 7			
0	-67	32	0
1	91	104	42
2	-68	21	0
3	-68	53	0
4	-68	70	0
5	-66	54	0
6	-70	14	0
7	-64	12	0
8	118	106	34
9	-71	34	0
10	65	86	48
H= 6 K= 8			
0	-69	47	0
1	-68	3	0
2	-69	24	0
3	-69	40	0
4	-73	71	0
H= 6 K= 8			
5	-73	31	0
6	-72	36	0
7	137	115	31
8	-74	43	0
9	-73	4	0
H= 6 K= 9			
0	-70	45	0
1	-70	26	0
2	-72	68	0
3	-71	2	0
4	138	140	31
5	139	125	30
6	-72	12	0
7	-73	7	0
H= 6 K= 10			
0	-71	45	0
1	-72	12	0
2	128	115	31
3	92	83	44
4	199	169	23
5	-76	29	0
H= 7 K= 0			
0	267	249	28
1	185	175	18
2	212	201	17
3	78	42	56
4	133	140	20
5	70	43	42
6	-63	33	0
7	377	383	20
8	184	166	27
9	-67	12	0
10	-69	42	0
11	119	124	41
12	66	63	79
13	244	243	26
14	139	126	37
H= 7 K= 7			
0	333	383	42
2	-72	61	0
4	342	346	21
6	101	82	61
8	-72	1	0
H= 7 K= 8			
0	-69	26	0
1	-70	37	0
2	84	56	63
3	202	193	22
4	-71	5	0
5	139	139	31
6	-72	24	0
7	-69	27	0
H= 7 K= 9			
0	100	68	56
1	88	56	56
2	-71	2	0
3	110	84	37
4	-72	25	0
5	-73	5	0
H= 8 K= 0			
0	294	142	27
1	78	55	37
2	173	172	20
3	575	577	13
4	136	113	23
5	77	85	72
6	-67	56	0
7	264	262	22
8	117	126	50
9	106	78	43
10	103	86	45
11	93	85	56
12	166	162	33
13	142	141	38
H= 8 K= 8			
0	174	194	68
2	-71	63	0
4	144	160	41
H= 9 K= 0			
0	489	489	21
1	137	134	36
2	-68	41	0
3	123	141	38
4	146	205	27
5	-66	41	0
6	156	163	30
7	101	81	46
8	126	114	37
9	115	84	49
10	83	59	75
11	-68	50	0
12	101	85	51
13	114	97	45
H= 10 K= 0			
0	217	270	51
1	237	260	23
2	422	441	19
3	-68	6	0
4	298	314	22
5	102	94	47
6	199	177	26
7	178	157	29
8	229	205	25
9	-75	35	0
10	151	151	39
11	-62	25	0
12	109	102	48
H= 11 K= 0			
0	158	172	62
1	-71	2	0
2	289	286	22
3	-72	24	0
4	321	310	21
5	-71	50	0
6	-69	102	0
7	123	112	42
8	357	336	21
9	-74	1	0
10	102	59	82
11	105	89	59
H= 12 K= 0			
0	87	74	131
1	186	186	28
2	-70	51	0
3	-71	35	0
4	-72	14	0
5	-72	5	0
6	109	112	48
7	-74	14	0
8	-74	16	0
9	132	108	41
H= 13 K= 0			
0	156	99	71
1	65	61	83
2	129	111	40
3	310	313	22
4	118	96	45
5	97	82	53
6	-73	63	0
7	116	95	55
H= 14 K= 0			
0	-78	31	0
1	-72	45	0
2	-71	47	0
3	89	69	65
4	152	139	36
5	-76	26	0

Zn(13) atoms for approximately one-third of the Y(1) atoms at the origin. There is no evidence for substitution at Y(4), so the large thermal parameter is either real or a reflection of a positional disorder of the Y atom in the large cage. When Zn(13) atoms are present they are only 2·19 Å from Zn(1) at $0,0,\frac{1}{4}$. Zn(1) is then probably pushed away to about $z=0{\cdot}28$ and the large β_{33} for Zn(1) is more a result of positional disorder than of thermal motion. Zn(13) atoms cannot simultaneously be at $0,0,z$ and $0,0,\frac{1}{2}-z$ positions. Attempts to refine fractional Zn(1) atoms at $z=\frac{1}{4}$ and $z=\frac{1}{4}+\Delta$ were unsuccessful.

Table 10. *Anisotropic B_i for M(1) and M(4) thermal ellipsoids for several compounds refined in $P6_3/mmc$*

The large B is parallel to the c axis in all cases.

	M(1)	*M*(4)
ηPu–Zn	2·4 Å²	1·2 Å²
	2·4	1·9
	4·2	13·8
ηGd–Zn	4·1	1·5
	4·1	0·7
	6·7	4·4
ηY-Cd	0·8	0·9
	0·8	2·3
	2·9	20·7
ηY–Zn	0·0	2·0
	0·0	1·7
	57·5	11·9
ηY–Zn (disordered)	0·3	1·9
	0·3	1·9
	1·8	10·4
	Zn(13)	
	1·4	
	1·4	
	2·5	

An example of random occupational disorder in the parent structure is thus given by ηY–Zn. The compounds ηPu–Zn, Y–Cd and Ce–Cd are examples of small, ordered changes in the parent structure. Unfortunately, we have so far been unable to solve the complete structure of ηY–Cd. We have carried out refinements starting with the parent ηGd–Zn structure and ignoring the reflections which cannot be indexed with the hexagonal lattice. The resulting B_i for Y(1) and Y(4) are also given in Table 10. There is no suggestion of substitution at the Y(1) site, but there is strong evidence for an anomaly at the Y(4) site. Additional anomalies are at the Cd(11) and Cd(12) sites, for Cd(11) is extremely anisotropic and Cd(12) has such large apparent thermal motion that it is probably absent entirely. The ordered changes that produce the superlattice in this compound are thus most likely associated with the Y(4), Cd(11) and Cd(12) sites.

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