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The Structure and Bijvoet Ratios of Cadmium Selenide

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The structure of cadmium selenide has been determined from X-ray intensity data obtained with extended-face crystals. The wurtzite parameter u was found to be 0·37679 ± 0·00012. Comparison of the intensities of equivalent reflexions provided a test for the internal consistency of the measurements. Equivalent reflexions in two specimens differed on average by 1·4 and 0·6% from the mean measured intensity, attesting to the high internal consistency of measurements from extended-face crystals. Comparison of 36 structure factors derived from data obtained from both specimens showed their average deviation from the mean to be 0·9%. An attempted least-squares refinement of the dispersion corrections of both atoms from observed Bijvoet ratios failed, presumably on account of correlation. When the dispersion corrections of one atom were held constant, it did prove possible to refine the dispersion corrections of the other atom.

Introduction

The use of an extended crystal face in accurate intensity measurements has recently been discussed in a number of papers (Mair, Prager & Barnea, 1971*a*,*b*; Barnea, 1975). Integrated intensities measured by this method are used here to determine the structure and Bijvoet ratios of cadmium selenide.

Cadmium selenide crystallizes in the polar space group $P6_3mc$ and has the wurtzite structure (Zachariasen, 1926). The two atoms in the unit cell are assigned the special positions 2(*b*); the cadmium atoms occupy the sites $(\frac{1}{3},\frac{2}{3},0)$ and $(\frac{2}{3},\frac{1}{3},\frac{1}{2})$, while the selenium atoms are at $(\frac{1}{3},\frac{2}{3},u)$ and $(\frac{2}{3},\frac{1}{3},\frac{1}{2}+u)$. A refinement of the structure including anisotropic harmonic thermal vibrations requires six variables: the scale factor, the wurtzite parameter u, and the temperature parameters β_{11}(Cd), β_{33}(Cd), β_{11}(Se), and β_{33}(Se). Symmetry requires that $\beta_{11}=\beta_{22}=2\beta_{12}$ and that $\beta_{13}=\beta_{23}=0$ for both atoms.

Experimental

Sample preparation

A single crystal of cadmium selenide, oriented from its cleavage habit, was embedded in a brass ring filled with Araldite. In order to extract the air bubbles, the Araldite was allowed to set under vacuum. A flat face parallel to the (100) planes was then polished with the aid of emery paper of decreasing coarseness placed on a flat glass surface. Kerosene was used as a lubricant during this stage of the polishing. The surface was then successively polished with 10, 1 and 0·05 μm Buehler micropolish. The micropolish was embedded in a Buehler polishing cloth (40-7008) and Diabort-Micro Dialute was used as a lubricant. During the final stages, polishing was alternated with etching in a mixture of orthophosphoric acid, hydrochloric acid and chromic oxide until the surface remained flat to within one fringe of sodium light when viewed against an optical flat. The polished 0·7 × 0·4 cm face had a mirror finish and was parallel to the (100) planes to within about 0·5°. Back-reflexion Laue photographs of the oriented crystal exhibited a pattern of sharp spots. However, after data collection was completed, it was found that Laue photographs with the crystal slightly misoriented showed one set of symmetry-related reflexions to be split. Another specimen was, therefore, prepared and an additional set of data collected. In this specimen a 1·3 × 0·9 cm face was parallel to the (110) planes. Back-reflexion photographs revealed a pattern of sharp, unsplit reflexions. Both specimens were more than 3 mm thick. We shall refer to the two specimens as Nos. 1 and 2. Both crystals were mounted with the polished face perpendicular to the axis of the goniometer head (Fig. 1). Photographic work and counter scans showed no evidence of polytypism. Chemical analysis of the crystals showed that they contained less than 0·5 wt% sulphur.

Measurement procedure

Integrated intensities were measured on a General Electric XRD-6 four-circle diffractometer with a

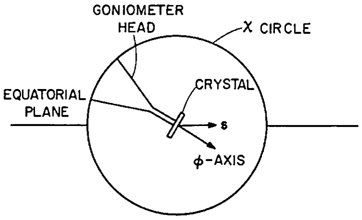

Fig. 1. Crystal mounted with face perpendicular to φ axis. Note that the cross-section of the crystal platelet shown in the diagram is not in general parallel to any of the faces forming the platelet edges.

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quarter-circle Eulerian cradle. The GE molybdenum X-ray tube was powered by a stabilized Philips PW 1320 generator. All measurements were carried out with the direct beam completely intercepted by the crystal. A monochromator of our design was mounted on the counter arm between the specimen and the scintillation counter. The 004 reflexion of a pyrolytic graphite crystal (supplied by the Union Carbide Corporation) was used to monochromate the diffracted beams. The monochromator crystal was mounted in the nondispersive configuration. The measurements were carried out at 21 ± 3°C. The unit-cell dimensions used were $a=4{\cdot}299$, $c=7{\cdot}010$ Å (National Bureau of Standards, 1957).

Integrated intensities were measured by the following procedure. Reflexions were located with the aid of computed values of the 2θ, φ, χ angles (ω was set to zero to correspond to symmetric reflexion). The reflexions were maximized and the diffracted beam was centred with the aid of half-slits in the diffracted-beam collimator. (The diffracted-beam collimator aperture was found to be too small to accept the entire diffracted beam; the collimator was therefore removed during the actual measurement.) A θ–2θ scan was used to measure the integrated intensity. A scanning range of $3\frac{1}{3}^\circ$ 2θ starting $1\frac{1}{2}^\circ$ 2θ below the peak maximum was found to be satisfactory for all but the highest-angle reflexions. All integrated intensity measurements were repeated at least once. Background counts were taken 3° 2θ below and above the peak maximum and averaged. In order to eliminate absorption effects due to miscut, the same reflexion was remeasured with $\varphi'=\varphi+180^\circ$ and $\chi'=-\chi$ (we refer to the position in which the normal to the crystal face is in the plane of incidence as the $\chi=0$ position). All measured reflexions were within the octant $-45^\circ<\chi<45^\circ$. The two integrated intensity measurements were averaged after background subtraction and the Lorentz–polarization correction was applied to these averages. No attempt was made to subtract the contribution due to thermal diffuse scattering.

Internal consistency of the measurements

Two equivalent reflexions were measured for each set of $\{hkl\}$ and $\{hk\bar{l}\}$ values [in the polar space group $P6_3mc$, when dispersion effects cannot be neglected, the intensities of the hkl reflexions differ from those of the $hk\bar{l}$ reflexions (Harrison, Jeffrey & Townsend, 1958)]. The extent to which the intensities of equivalent reflexions agreed was taken to be a measure of the internal consistency of the measurements for each specimen. 66 reflexions and their equivalents were

Table 1. *Observed and calculated structure factors and structural parameters from the least-squares refinement of* CdSe *data obtained from specimen No.* 1

hkl	F_o	F_c	ΔF	*hkl*	F_o	F_c	ΔF
321	14·13	14·11	0·02	612	7·18	6·89	0·29
$32\bar{1}$	16·99	17·20	−0·21	$61\bar{2}$	6·29	5·99	0·30
322	16·66	16·65	0·01	$\bar{5}17$	7·20	7·35	−0·15
$32\bar{2}$	15·25	15·28	−0·03	$\bar{5}1\bar{7}$	5·53	5·35	0·28
412	30·46	30·66	−0·20	$\bar{6}13$	13·20	13·12	0·08
$41\bar{2}$	27·99	28·01	−0·02	$\bar{6}1\bar{3}$	14·20	13·99	0·21
414	4·27	4·38	−0·11	$\bar{4}42$	11·60	11·67	−0·07
$41\bar{4}$	3·73	3·72	0·01	$\bar{4}4\bar{2}$	9·98	10·06	−0·08
332	24·10	24·26	−0·16	526	9·64	9·46	0·18
$33\bar{2}$	21·77	21·86	−0·09	$52\bar{6}$	11·21	11·17	0·04
$\bar{4}21$	9·54	9·56	−0·02	$\bar{6}15$	12·21	12·16	0·05
$\bar{4}2\bar{1}$	12·15	12·20	−0·05	$\bar{6}1\bar{5}$	11·63	11·44	0·19
$\bar{4}23$	22·62	22·67	−0·05	$\bar{5}33$	10·50	10·68	−0·18
$42\bar{3}$	23·80	23·81	−0·01	$\bar{5}3\bar{3}$	11·31	11·45	−0·14
416	18·26	18·34	−0·08	$\bar{6}23$	9·60	9·65	−0·05
$41\bar{6}$	20·99	20·73	0·26	$\bar{6}2\bar{3}$	10·46	10·38	0·08
$\bar{5}11$	8·63	8·46	0·17	$\bar{5}28$	11·28	11·47	−0·19
$\bar{5}1\bar{1}$	11·13	10·98	0·15	$\bar{5}2\bar{8}$	11·39	11·55	−0·16
$\bar{5}12$	10·74	10·47	0·30	712	8·78	8·73	0·05
$\bar{5}1\bar{2}$	9·65	9·34	0·31	$71\bar{2}$	7·38	7·38	0·01
$\bar{4}25$	20·40	20·41	−0·01	$\bar{6}25$	9·02	9·06	−0·04
$\bar{4}2\bar{5}$	19·56	19·45	0·11	$\bar{6}2\bar{5}$	8·50	8·47	0·03
$\bar{4}32$	8·43	8·46	−0·03	627	3·71	3·80	−0·09
$\bar{4}3\bar{2}$	7·49	7·45	0·04	$62\bar{7}$	2·54	2·52	0·02
515	18·43	18·33	0·10	716	4·97	5·16	−0·19
$51\bar{5}$	17·84	17·42	0·42	$71\bar{6}$	6·19	6·31	−0·12
$\bar{4}33$	16·15	16·23	−0·08	718	6·34	6·50	−0·16
$\bar{4}3\bar{3}$	17·18	17·20	−0·02	$71\bar{8}$	6·49	6·56	−0·07
$\bar{5}22$	15·67	15·79	−0·12	813	4·87	4·92	−0·05
$\bar{5}2\bar{2}$	13·87	13·84	0·03	$81\bar{3}$	5·32	5·36	−0·04
$\bar{5}16$	6·23	6·29	−0·06	815	4·78	4·73	0·05
$\bar{5}1\bar{6}$	7·29	7·30	−0·01	$81\bar{5}$	4·33	4·37	−0·04
$\bar{4}35$	14·80	14·88	−0·08				
$\bar{4}3\bar{5}$	14·00	14·07	−0·07				

Structural parameters

$u=0{\cdot}37667\pm0{\cdot}00015$

$B_{11}(\text{Cd})=1{\cdot}46\pm0{\cdot}02$ Å^2

$B_{33}(\text{Cd})=1{\cdot}67\pm0{\cdot}08$

$B_{11}(\text{Se})=1{\cdot}19\pm0{\cdot}02$

$B_{33}(\text{Se})=0{\cdot}99\pm0{\cdot}12$

Scale factor = 1·000 ± 0·004

$R=0{\cdot}0088$

measured for specimen No. 1 and 77 for specimen No. 2. The average deviation of the intensity of a reflexion from the mean value of the two equivalent reflexions was 1·4% for specimen No. 1 and 0·6% for specimen No. 2.

Analysis of data

The observed integrated intensities were analysed by the crystallographic least-squares program (Busing, Martin & Levy, 1963), modified to include dispersion corrections [the values used were those of Cromer & Liberman (1970)] and to calculate (rather than interpolate) the values of the atomic scattering factors at the appropriate value of $\sin\theta/\lambda$ using the polynomial expansion of Doyle & Turner (1968). The latter modification has been found to result in somewhat lower estimated standard deviations. For a structure consisting of light atoms and including low-angle data the effect of replacing the usual interpolation procedure by the polynomial expansion could well be more significant.

Table 1 lists the observed and calculated structure factors for specimen No. 1 (equivalent reflexions have been averaged), as well as the final values of the parameters of the structure obtained from the least-squares refinement. Equal weight was given to all observations. The discrepancy index $R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ was 0·009. Similarly, Table 2 summarizes the results for specimen No. 2. The discrepancy index for specimen No. 2 was 1·6%. We found it at first rather surprising that the data from specimen No. 2 which showed considerably better agreement between equivalent reflexions should lead to a higher discrepancy index (as well as to a larger standard deviation of an observation of unit weight). We concluded, however, that this would be entirely reasonable if equivalent reflexions were similarly affected by some source of systematic error (such as inhomogeneity of the crystal surface or some geometrical factor). Indeed, inspection of Table 2 shows that the values of $\Delta F=F_o-F_c$ for pairs of hkl and $hk\bar{l}$ reflexions are in most instances similar in both magnitude and sign. This trend is certainly less prevalent in Table 1.

Comparison of the two tables shows the structural parameters derived from the two sets of data to be in very good agreement. The estimated standard deviations for specimen No. 2 are generally larger than those for No. 1. The particularly large estimated standard deviations of the B_{33} values are due to correlation between these parameters. This correlation is larger for the set of reflexions observed with specimen No. 2 (0·97, compared with 0·92 for specimen No. 1). Table 3 is the result of a combined refinement of the entire data. Here the correlation between the B_{33} decreased to 0·80.

Table 2. *Observed and calculated structure factors and structural parameters from the least-squares refinement of cadmium selenide data from specimen No.* 2

hkl	F_o	F_c	ΔF
$42\bar{1}$	12·53	12·16	0·37
421	9·92	9·57	0·35
422	12·23	11·60	0·63
$42\bar{2}$	10·95	10·43	0·52
$42\bar{3}$	23·75	23·56	0·19
423	22·70	22·42	0·28
510	13·85	14·25	−0·40
$51\bar{1}$	10·82	10·94	−0·12
511	8·39	8·48	−0·49
512	10·15	10·38	−0·23
$51\bar{2}$	9·20	9·27	−0·07
$51\bar{3}$	20·98	21·07	−0·09
513	19·89	19·99	−0·10
425	20·28	20·16	0·12
$42\bar{5}$	19·08	19·22	−0·14
600	23·46	23·65	−0·19
$60\bar{2}$	15·04	15·33	−0·29
602	17·07	17·36	−0·29
$43\bar{1}$	8·81	8·92	−0·11
431	6·59	6·72	−0·13
515	18·01	18·09	−0·08
$51\bar{5}$	16·99	17·20	−0·21
432	8·46	8·38	0·08
$43\bar{2}$	7·48	7·39	0·09
$43\bar{3}$	17·11	16·97	0·14
433	16·29	16·01	0·28
522	15·48	15·64	−0·16
$52\bar{2}$	13·58	13·72	−0·14
$51\bar{6}$	7·10	7·15	−0·05
516	6·26	6·14	0·10
427	8·10	7·99	0·11
$42\bar{7}$	5·96	5·86	0·10
$61\bar{1}$	7·16	7·32	−0·16
611	5·25	5·36	−0·11
435	14·75	14·66	0·09
$43\bar{5}$	13·73	13·86	−0·13
$51\bar{7}$	5·11	5·23	−0·12
517	7·07	7·24	−0·17
$61\bar{3}$	13·70	13·78	−0·08
613	12·83	12·92	−0·09
700	7·21	7·48	−0·27
526	9·27	9·21	0·06
$52\bar{6}$	10·68	10·92	−0·24
442	11·68	11·53	0·15
$44\bar{2}$	9·89	9·93	−0·04
615	11·76	11·95	−0·19
$61\bar{5}$	11·00	11·25	−0·25
532	5·98	5·58	0·40
$53\bar{2}$	5·28	4·79	0·49
$53\bar{3}$	11·20	11·26	−0·06
533	10·52	10·50	0·02
$62\bar{3}$	10·40	10·20	0·20
623	9·70	9·48	0·22
535	9·92	9·80	0·12
$53\bar{5}$	9·22	9·18	0·04
$52\bar{8}$	11·62	11·40	0·22
528	11·53	11·31	0·22
625	9·10	8·89	0·21
$62\bar{5}$	8·65	8·31	0·34
$54\bar{3}$	7·66	7·62	0·04
543	7·12	7·04	0·08
632	6·90	7·10	−0·20
$63\bar{2}$	5·86	5·95	0·09
545	6·80	6·68	0·12
$54\bar{5}$	6·29	6·21	0·08
$72\bar{3}$	6·17	6·30	−0·13
723	5·68	5·80	−0·12
718	6·17	6·40	−0·23
$71\bar{8}$	6·22	6·46	−0·24
416	18·16	17·98	0·18
$41\bar{6}$	19·99	20·38	−0·39
803	6·28	6·39	−0·11
$80\bar{3}$	6·88	6·93	−0·05
712	8·71	8·60	0·11
$71\bar{2}$	7·38	7·28	0·10
815	4·75	4·61	0·14
$81\bar{5}$	4·42	4·26	0·16

Structural parameters

$u=0{\cdot}37686\pm0{\cdot}00023$

$B_{11}(\mathrm{Cd})=1{\cdot}45\pm0{\cdot}02$ Å^2

$B_{33}(\mathrm{Cd})=2{\cdot}04\pm0{\cdot}38$

$B_{11}(\mathrm{Se})=1{\cdot}24\pm0{\cdot}02$

$B_{33}(\mathrm{Se})=0{\cdot}63\pm0{\cdot}35$

Scale factor $=1{\cdot}000\pm0{\cdot}009$

$R=0{\cdot}016$

Table 3. *Structure parameters from the combined least-squares refinement of* CdSe *data obtained from both specimens*

$u = 0\cdot37679 \pm 0\cdot00012$
$B_{11}(\mathrm{Cd}) = 1\cdot46 \pm 0\cdot02$ Å^2
$B_{33}(\mathrm{Cd}) = 1\cdot77 \pm 0\cdot05$
$B_{11}(\mathrm{Se}) = 1\cdot21 \pm 0\cdot02$
$B_{33}(\mathrm{Se}) = 0\cdot96 \pm 0\cdot08$
$R = 0\cdot0136$

Another comparison of the two sets of measurements is afforded by considering the measure of agreement between the structure factors of the 36 reflexions observed with both crystals; the average deviation of the two structure factors from their mean is 0·9%.

An attempt to determine the possible effect of the unknown monochromator polarization was made. The data was re-processed with the assumption that the monochromator is perfect. The resulting changes in all the structural parameters were within one standard deviation; only the change in the scale factor was somewhat larger. We ascribe this insensitivity to the polarization to the short wavelength of the radiation used and to the fact that the measurements were relative rather than absolute.

Inspection of our tables shows that no extinction correction was required for either specimen. The widths of the Bragg peaks indicated that we were dealing with crystals which were by no means perfect. Nevertheless, we found the agreement with kinematic theory better than we might have expected [similar observations were made in studies of CsCl (Barnea & Post, 1966) and $BaTiO_3$ (Harada, Pedersen & Barnea, 1970)]. A more detailed investigation of the most intense low-angle reflexions of specimen No. 2 indicated that they exhibited moderate extinction which could, moreover, be accounted for by Zachariasen's theory (1967) (see also Mair & Barnea, 1975*a*). Inclusion of this data in the refinement resulted in no significant change of the structural parameters. Since this data was not obtained under exactly the same conditions, we have not included it in our tables. A more detailed study of extinction in an extended-face crystal has been carried out by one of the authors (Barnea, 1974) and will be published in due course. The effect of extinction on the Bijvoet ratios in our study here is certainly negligible.

The effects of anomalous dispersion

The very satisfactory agreement between the observed and calculated structure factors led us to a more detailed consideration of anomalous dispersion effects in cadmium selenide. Previous investigations of these effects in substances with the wurtzite structure are restricted to zinc oxide, in which they are relatively small and hence difficult to measure. This may have been the cause of some of the difficulties encountered by Harrison, Jeffrey & Townsend (1958) in attempting to account for the results of their experiment. More recent measurements of the intensities of zinc oxide (Abrahams & Bernstein, 1969) are in better accord with predictions based on the refined structural parameters and theoretically calculated dispersion corrections. However, even in this investigation (the primary purpose of which was a redetermination of the structure of ZnO) the magnitudes of the observed intensities of 12 out of a total of 40 reported Friedel pairs are reversed, *i.e.* the reflexion which is predicted to be more intense is in fact observed to be the less intense.

In our approach to this problem, we attempted to extract experimental dispersion corrections from the observed Bijvoet ratios (Peerdeman, van Bommel & Bijvoet, 1951) formed by the difference between the observed intensities of hkl and $hk\bar{l}$ reflexions divided by their average intensity. These Bijvoet ratios were compared with calculated ratios and the differences between the observed and calculated values were minimized by an iterative least-squares procedure in which the dispersion corrections were allowed to vary. In calculating the Bijvoet ratios and their derivatives with respect to the dispersion corrections, we used the

Table 4. *Observed Bijvoet ratios B_o compared with B_c values calculated by the least-squares analysis of the data of specimen No.* 2

hkl	$10^2 B_o$	Deviation from mean	$10^2 B_c$
421	−46·05	0·54	−46·93
422	21·99	0·40	20·68
423	− 9·04	0·77	− 9·63
416	−19·47	0·70	−23·98
511	−49·80	3·21	−49·83
512	19·75	1·52	22·05
425	12·20	0·14	9·29
431	−56·47	0·64	−55·53
515	11·72	1·06	9·83
432	24·25	0·30	24·73
433	− 9·73	0·13	−11·47
522	26·15	1·16	25·60
516	−25·29	0·25	−28·92
427	59·51	0·21	57·07
611	−59·94	2·67	−61·13
435	14·19	0·61	10·86
517	62·84	0·79	59·72
613	−13·27	0·78	−12·63
442	32·90		29·33
526	−28·21	0·10	−32·56
615	13·34	0·23	11·82
533	−12·36	1·63	−13·70
623	−13·80	1·03	−14·20
535	14·54	0·42	12·70
625	11·88	1·78	13·11
543	−14·62	0·33	−15·55
632	32·53	0·48	34·61
545	15·47	0·62	14·18
712	32·96	1·36	32·65
718	− 1·89	0·09	− 1·82
803	−17·97	0·26	−15·95
723	−16·75	0·51	−16·32
815	14·89	0·37	15·28

Refined dispersion corrections for selenium

$$f'_{\mathrm{Se}} = 0\cdot177 \pm 0\cdot007$$
$$f''_{\mathrm{Se}} = 2\cdot19 \pm 0\cdot03$$

usual kinematic expression for the intensities, theoretically calculated atomic scattering factors (Doyle & Turner, 1968) determined from their polynomial expansion and the structural and thermal parameters obtained in our structure analysis. All observations were given equal weight.

Table 4 lists the experimental Bijvoet ratios for specimen No. 2 and values calculated with the dispersion corrections derived from the data by the least-squares analysis. The experimental values are in all but one case an average of two ratios obtained from different sets of equivalent reflexions, *i.e.* from the pair hkl and $hk\bar{l}$ and from the pair khl and $kh\bar{l}$. The deviation from this average, also listed in the table, provides an indication of the reliability of our measurements.

All our attempts to refine simultaneously the four dispersion corrections failed. This was apparently because of strong correlation between the real and imaginary dispersion corrections of the two atoms respectively. It did, however, prove possible to refine the dispersion corrections of any one of the atoms, convergence being achieved after a few cycles. The K absorption edges of cadmium (0·46 Å) and selenium (0·98 Å) being approximately equidistant from the incident Mo $K\alpha$ radiation, we chose arbitrarily to refine the dispersion corrections of selenium and retained the theoretical values (Cromer & Liberman, 1970) for cadmium. The data from specimen No. 2 refined easily, converging within a few cycles. The values obtained were: $f'_{\rm Se} = -0{\cdot}177 \pm 0{\cdot}006$ and $f''_{\rm Se} = 2{\cdot}19 \pm 0{\cdot}03$. The errors cited are estimated standard deviations. To these one must add the effect of the uncertainty in the u parameter. This was determined by inserting in the least-squares program the limiting values of u. With allowance for these the values become: $-0{\cdot}18 \pm 0{\cdot}13$ and $2{\cdot}19 \pm 0{\cdot}04$. The data from specimen No. 1 yielded the values: $-0{\cdot}47 \pm 0{\cdot}14$ and $2{\cdot}11 \pm 0{\cdot}04$. The data from specimen No. 2 had the lower discrepancy index. The values calculated theoretically by Cromer & Liberman (1970) are $f'_{\rm Se} = -0{\cdot}178$ and $f''_{\rm Se} = 2{\cdot}223$.

Conclusions

The structure of CdSe has recently been discussed, together with other wurtzite structures, by Lawaetz (1972) and, in a different context, by Mair & Barnea (1975*b*). The u parameter determined in our study is consistent with its expected magnitude and with the position of cadmium selenide within the series of wurtzite compounds.

The advantages of using extended-face crystals, particularly in measurements involving highly absorbing crystals, are quite apparent, as is the need for careful monitoring of the preparation of the face used. The use of more than one sample, though not essential to the method, can be instructive providing an external test of the reliability of the results. In our instance it has also given us the opportunity to obtain a reduction in the correlation of the B_{33} temperature parameters.

The attempted refinement of dispersion corrections from the Bijvoet ratios has highlighted the difficulties of such a program: nonconvergence of the refinement, due apparently to correlation; a not unexpected sensitivity of the real part of the dispersion correction to the quality of the data; the effect of the uncertainty of the position parameter on the real dispersion correction (which can perhaps be avoided by working with zinc blende rather than wurtzite crystals). All these complications cause us to view our dispersion correction results with caution – we can, at most, state that we have observed no great or systematic differences between observed and calculated Bijvoet ratios in CdSe with Mo $K\alpha$ radiation.

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