the interpretation of $(|F_Q|^2/|F_P|^2)F_P$ (Ramachandran & Srinivasan, 1970) and from n successive convolutions of $|F_Q|^2/|F_P|^2$ terms one can evaluate the contribution to peak heights as $(\Sigma_Q/\Sigma_P)^n f_X$. A lot of lesser peaks from this synthesis in more general positions will contribute to the general background.

The results of numerical summation for R_P and R_Q, Table 2, showed that in the range of convergence the peak heights of P and Q atoms are not very sensitive to the value of Σ_Q/Σ_P. The P enhancement obtained from the first approximation and the Σ_Q/Σ_P dependence of the Q peak heights from the second approximation are overestimated. But all of this is derived for the rather limited range of Σ_Q/Σ_P.

Table 2. *The numerical values of R_P and R_Q obtained by summation of the first* 51 *terms* ($k_{\max} = 50$) *of the expansion*

$|F_Q|/|F_P|$	R_P	R_Q
0·00	1·000	0·500
0·10	1·002	0·499
0·20	1·010	0·498
0·30	1·023	0·494
0·40	1·040	0·490

The fact that the peak heights are almost insensitive to Σ_Q/Σ_P shows that the γ' synthesis is a very good tool for location of unknown atoms and for refinement of atom positions and electron density (especially as $2F_o - F_c$ synthesis) in the final stages of structure determination and no special synthesis seems to be necessary.

References

MAIN, P. (1979). *Acta Cryst.* A**35**, 779–785.

RAMACHANDRAN, G. N. & SRINIVASAN, R. (1970). *Fourier Methods in Crystallography.* London: Wiley–Interscience.

Acta Cryst. (1984). A**40**, 162

The consequences of the neglect of TDS correction for temperature parameters: erratum.

By ANDREW W. STEVENSON, *School of Physics, University of Melbourne, Parkville, Victoria* 3052, *Australia* and JIMPEI HARADA, *Department of Applied Physics, Nagoya University, Chikusa-ku, Nagoya* 464, *Japan*

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Abstract

In the paper by Stevenson & Harada [*Acta Cryst.* (1983), A**39**, 202–207] the calculated values of Δ' (and consequently $\delta\bar{B}$) in Table 1 are in error. For KCl and BaF_2 the conventional (rather than primitive) unit-cell volumes were mistakenly used when calculating q_{ZB}. For CdS and CdSe the factor used to get q'_{ZB} from q_{ZB} was incorrect. The new (corrected) Table 1 is given below. The agreement between $\delta\bar{B}$ and $\delta\bar{B}_{\text{obs}}$ is, with the new $\delta\bar{B}$ values, generally better; with $\delta\bar{B}$ for KCl closer to the $\delta\bar{B}_{\text{obs}}$ value given by Cooper & Rouse [*Acta Cryst.* (1968), A**24**, 405–410], namely 0·16 Å^2. The calculated value of the '*overall*' temperature parameter for CdS becomes 1·29 Å^2. It should also be noted that there is a factor of 2 missing from the denominator of equation (15).

Table 1. *Details for comparison of experimental and theoretical Δ' values for each of four studies*

The size of the detector aperture is given with the width first in each case.

	Experimental conditions										
				Lattice parameters				Results			
	Scan mode	Scan width (°θ)	Detector aperture (°)	a (Å)	c (Å)	q_s (Å^{-1})	q_{ZB} (Å^{-1})	Δ'	Δ'_{obs}	$\delta\bar{B}$ (Å^2)	$\delta\bar{B}_{\text{obs}}$ (Å^2)
KCl	ω	2·5	1·5 × 1·5	6·290	–	0·1702	0·9837	0·073	0·087 (0·105)	0·14	0·16 (0·20)
CdS	ω–2θ	3·0	2·0 × 1·5	4·136	6·713	0·1991	0·8413	0·080	0·057	0·11	0·08
CdSe	ω–2θ	3·0	2·0 × 1·5	4·299	7·010	0·1991	0·8081	0·083	0·072	0·12	0·11
BaF_2	ω–2θ	2·4	2·2 × 3·2	6·196	–	0·1682	0·9986	0·062	0·066	0·05	0·05

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