

data alone without introducing arbitrary and unwarranted assumptions. However, observed distributions of structural parameters found in different crystal environments do provide qualitative information about the shapes of low-energy regions of potential energy surfaces and can thus be related to ratios of corresponding restoring forces. We have outlined a general scheme indicating how this information might be obtainable.

Perhaps a parallel can be drawn with molecular mechanics models, widely used for estimating structural and energetic properties of molecules. These are just more or less elaborate schemes of representing inter- and intramolecular perturbations on a standard fragment characterized by a standard geometry and a standard force field. As far as the structures alone are

concerned, the force constants may be scaled upward or downward without change; it is only their ratios that matter.

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SHORT COMMUNICATION

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Gitterenergieberechnungen zur Ermittlung der wahrscheinlichsten Strukturtypen für Verbindungen MX_6 .
Druckfehlerberichtigung. Von WOLFGANG WILLING und ULRICH MÜLLER, *Fachbereich Chemie der Universität Marburg, Hans-Meerwein-Strasse, D-3550 Marburg, Bundesrepublik Deutschland*

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Abstract

Printer's errors in the article by Willing & Müller [*Acta Cryst.* (1988), **B44**, 1–6] are corrected. On page 2, the second sentence of the second paragraph should read: 'Wir betrachten nur intermolekulare Wechselwirkungen, die interatomaren Potentiale innerhalb eines Moleküls werden nicht

berücksichtigt'. In the bottom right of Fig. 1, the height of the layers, reading from top to bottom, should be: 3/4, 1/4 and –1/4.

Alle Daten sind in der Zusammenfassung gegeben.

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