

## Universality behaviour for polarity formation in channel-type inclusion compounds

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Published online: 25 September 2008  
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### Erratum to: J Math Chem DOI 10.1007/s10910-008-9433-0

Table 1 in the original article is missing some text and characters. The table should read as follows:

| Table 1 Guest–guest and host–guest interaction energies | $E_{ij}$ | Range (kJ mol <sup>-1</sup> ) |
|---|----------|-------------------------------|
|   | $E_{AD}$ | –25.0 to 0.01                 |
|   | $E_{AA}$ | 0.01 to 10.0                  |
|   | $E_{DD}$ | –5.0 to 5.0                   |
|   | $E_{Cj}$ | –5.0 to 5.0                   |

In Eq. 6, a subscript character is missing; the equation should appear as follows:

$$P_{ij} = \frac{X e^{-\beta(E_{ij}+E_{Cj})}}{Z_i} \quad (6)$$

Figures 3 and 8 appear in color in the online version of the article. Where dashes appear in the captions of the original, there should be written out the corresponding color terminology.

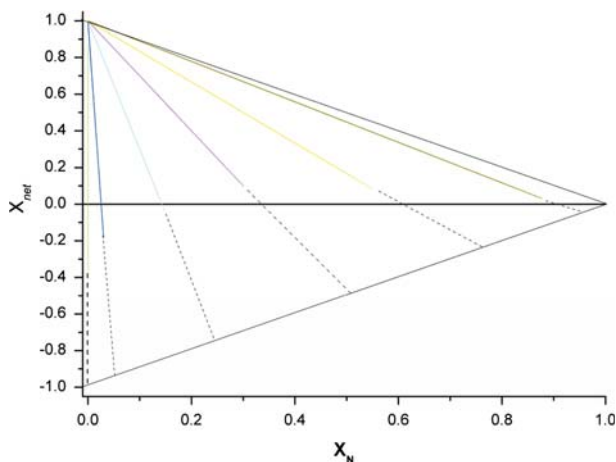
Therefore the caption to Fig. 3 should read:

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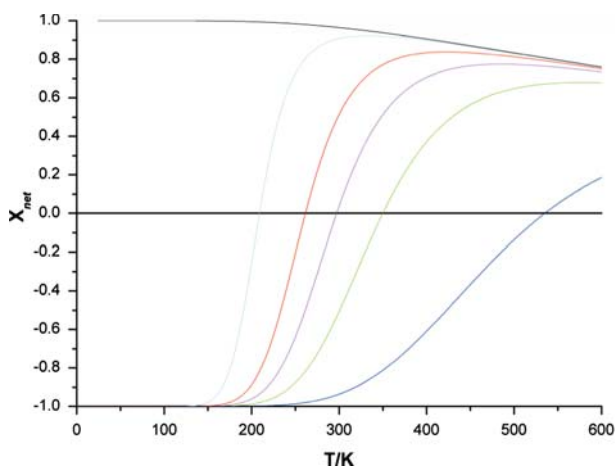
The online version of the original article can be found under doi:[10.1007/s10910-008-9433-0](https://doi.org/10.1007/s10910-008-9433-0).

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**Fig. 3** Net polarity  $X_{\text{net}}$ , as a function of  $X_N$ , the fraction of non-polar guests included in the crystal.  $X_{\text{net}}$  is plotted for various values of  $X_g$  (dark blue line:  $X_g = 0.05$ , light blue line:  $X_g = 0.25$ , purple line:  $X_g = 0.5$ , yellow line:  $X_g = 0.75$ , green line:  $X_g = 0.95$ ). Interactions energies were randomly chosen within the energy range given in Appendix 1. Dashed curves were obtained from calculations using an extended hypothetical energy range ( $-100 < E_{ij} < 100 \text{ kJ mol}^{-1}$ ). The solid black lines show the upper limits of  $X_{\text{net}}$  as a function of  $X_N$



**Fig. 8** The effect of temperature on polarity for various concentrations  $X_g$  (black line:  $X_g = 0$ , light blue line:  $X_g = 0.00001$ , red line:  $X_g = 0.0001$ , purple line:  $X_g = 0.0003$ , green line:  $X_g = 0.001$ , dark blue line:  $X_g = 0.01$ ). The interaction energies used for the calculations were  $E_{\text{AD}} = -25 \text{ kJ mol}^{-1}$ ,  $E_{\text{AA}} = 5 \text{ kJ mol}^{-1}$  and  $E_{\text{DD}} = -5 \text{ kJ mol}^{-1}$ . Surprisingly, a very small amount of neutral D- $\pi$ -D molecules in the gas phase can have a strong effect on polarity as temperature is varied

and the caption to Fig. 8 should read:

In Appendix 1, “Substituting Eqs. 3 and 3” should read “Substituting Eqs. 3 and 4”, and “Substituting Eq. 3 for the probabilities” should read “Substituting Eq. 6 for the probabilities”.