

Analyzing diffuse scattering with supercomputers (Correction)

T. M. MICHELS-CLARK,^{a,b*} V. E. LYNCH,^b C. M. HOFFMANN,^b J. HAUSER,^c
T. WEBER,^d R. HARRISON^e AND H. B. BÜRGI^{c,f}

^aLawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, ^bOak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, USA, ^cDepartment of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012, Bern, Switzerland, ^dETH Zürich, Laboratorium f. Kristallographie, Wolfgang-Pauli-Str. 10, 8093 Zürich, Switzerland, ^eStony Brook University, Department of Applied Mathematics & Statistics, Stony Brook, NY 11794-3600, USA, and ^fUniversity of Zürich Department of Chemistry, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland. E-mail: tmichels-clark@ion.chem.utk.edu

The paper by Michels-Clark, T. M. *et al.* [*J. Appl. Crystallogr.* (2013), **46**, 1616-1625], contains misleading errors which are corrected here. The numerical results reported in that paper and the conclusions given there are not affected and remain unchanged. The transition probabilities in Table 1 (rows 4, 5, 7, 8) and Figure 2 (rows 1 and 2) of the original paper were different from those used in the numerical calculations. Corrected transition probabilities as used in the computations are given in Table 1.(revised) and Figure 2.(revised). The Δ parameter in the stacking model expresses the preference for the fifth layer in a five layer stack to be eclipsed with respect to the first layer. This statement corrects the original text on p. 1622, lines

4-7. In the original Fig. 2 the helicity of the layer stacks b_L and b_R in rows 3 and 4 had been given as opposite to those in rows 1, 2 and 5. Fig. 2.(revised) shows rows 3 and 4 corrected to correspond with rows 1, 2 and 5.

Table 1. (Revised) The transition matrix $\mathbf{T}$ of probabilities for extending the left-hand column of four-layer motifs into the top row of new four-layer motifs. Once a new motif is formed by adding a new fifth layer, the first layer and thus the first motif are dropped. The meaning of the symbols is described in the original paper, T. M. et al. [*J. Appl. Crystallogr.* (2013), **46**, 1616-1625].

from \ to	... eb_L	... eb_R	... ee	... b_Lb_R	... b_Lb_L	... b_Le	... b_Rb_L	... b_Rb_R	... b_Re
eb_L	0	0	0	$t - \frac{\Delta}{2}$	$c - \frac{\Delta}{2}$	$e_1 + \Delta$	0	0	0
eb_R	0	0	0	0	0	0	$t - \frac{\Delta}{2}$	$c - \frac{\Delta}{2}$	$e_1 + \Delta$
ee	$\frac{1-e_2}{2}$	$\frac{1-e_2}{2}$	e_2	0	0	0	0	0	0
b_Lb_R	0	0	0	0	0	0	t	c	e_1
b_Lb_L	0	0	0	t	c	e_1	0	0	0
b_Le	$\frac{1-e_2}{2} - \Delta$	$\frac{1-e_2}{2} + \Delta$	e_2	0	0	0	0	0	0
b_Rb_L	0	0	0	t	c	e_1	0	0	0
b_Rb_R	0	0	0	0	0	0	t	c	e_1
b_Re	$\frac{1-e_2}{2} + \Delta$	$\frac{1-e_2}{2} - \Delta$	e_2	0	0	0	0	0	0

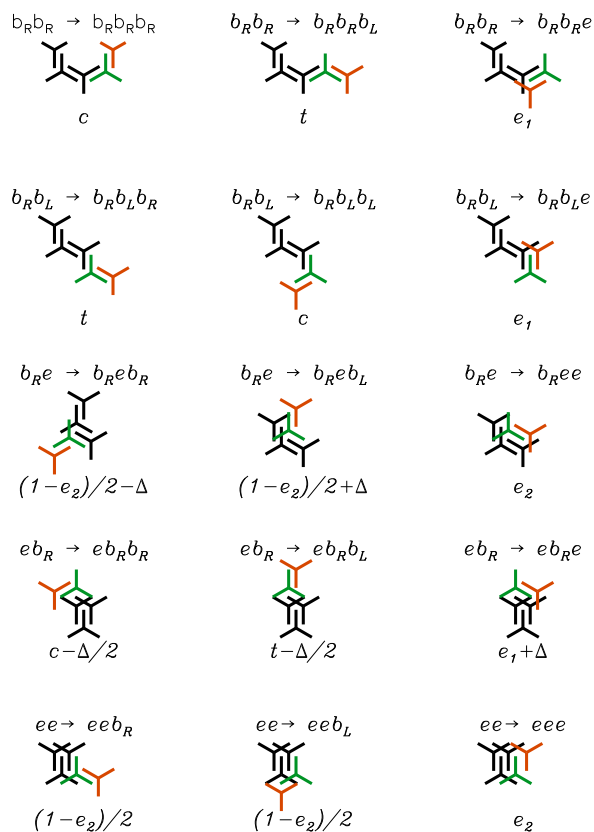


Fig. 2. (Revised; color online) Examples of unique five-layer stacking motifs: layers 1, 2, 3 in solid black from left to right, layer 4 in green, and layer 5 in red. In the actual crystal structure overlapping arms of molecules in neighboring layers sit on top of each other, but are slightly displaced here for clarity. The symbols above each motif describe the four- and five-layer stacks. The abbreviations b_L , b_R , e (bent left, bent right, eclipsed) characterize the three possible three-layer stacks. A four-layer stack is defined by two symbols, and a five layer-stack by three symbols. Respective transition probabilities from four- to five-layer stackings are given at the bottom of each motif.