JCTC Journal of Chemical Theory and Computation

Erratum

Rigorous Extraction of the Anisotropic Multispin Hamiltonian in Bimetallic Complexes from the Exact Electronic Hamiltonian. [*J. Chem. Theory Comput. 6,* 55–65 (2010)]. By Rémi Maurice,* Nathalie Guihéry, Roland Bastardis, and Coen de Graaf.

Table 4. Two typographical errors are worth noting:

• The matrix elements $\langle 2, -2|H_{mod}|0, 0\rangle$, $\langle 2, 2|H_{mod}|0, 0\rangle$, $\langle 0, 0|H_{mod}|2, -2\rangle$, and $\langle 0, 0|H_{mod}|2, 2\rangle$, that were reported as $[2/(\sqrt{3})](E_a - E_{ab})$ in the published version, are equal to $[1/(\sqrt{3})](2E_a - E_{ab})$.

• The matrix elements $\langle 1, -1|H_{mod}|1, 1\rangle$ and $\langle 1, 1|H_{mod}|1, -1\rangle$, that were reported as $-E_a - E_{ab}$ in the published version, are equal to $-E_a + E_{ab}$.

The entire corrected version of the matrix is presented. All results and exploitations reported in the article used the correct expressions.

Table 4. Matrix Elements of the Model Hamiltonian for Bimetallic Ni(II) Complexes with Magnetic Anisotropy in the Coupled $|S, M_S\rangle$ Basis

$\|S, M_S\rangle$	$\|2, -2\rangle$	$\|2, -1\rangle$	$\|2, 0\rangle$	$\|2, 1\rangle$	$\|2, 2\rangle$
$\langle 2, -2\|$	$J + (2/3)(D_a + D_{ab})$	0	$[\sqrt{(2/3)}](E_a + E_{ab})$	0	0
$\langle 2, -1\|$	0	$J - (1/3)(D_a + D_{ab})$	0	$E_a + E_{ab}$	0
$\langle 2, 0\|$	$[\sqrt{(2/3)}](E_a + E_{ab})$	0	$J - (2/3)(D_a + D_{ab})$	0	$[\sqrt{(2/3)}](E_a + E_{ab})$
$\langle 2, 1\|$	0	$E_a + E_{ab}$	0	$J - (1/3)(D_a + D_{ab})$	0
$\langle 2, 2\|$	0	0	$[\sqrt{(2/3)}](E_a + E_{ab})$	0	$J + (2/3)(D_a + D_{ab})$
$\langle 1, -1\|$	0	0	0	0	0
$\langle 1, 0\|$	0	0	0	0	0
$\langle 1, 1\|$	0	0	0	0	0
$\langle 0, 0\|$	$[1/(\sqrt{3})](2E_a - E_{ab})$	0	$[(\sqrt{2})/3](2D_a - D_{ab})$	0	$[1/(\sqrt{3})](2E_a - E_{ab})$
	$\|1, -1\rangle$	$\|1, 0\rangle$	$\|1, 1\rangle$	$\|0, 0\rangle$	
$\langle 2, -2\|$	0	0	0	$[1/(\sqrt{3})](2E_a - E_{ab})$	
$\langle 2, -1\|$	0	0	0	0	
$\langle 2, 0\|$	0	0	0	$[(\sqrt{2})/3](2D_a - D_{ab})$	
$\langle 2, 1\|$	0	0	0	0	
$\langle 2, 2\|$	0	0	0	$[1/(\sqrt{3})](2E_a - E_{ab})$	
$\langle 1, -1\|$	$-J - (1/3)(D_a - D_{ab})$	0	$-E_a + E_{ab}$	0	
$\langle 1, 0\|$	0	$-J + (2/3)(D_a - D_{ab})$	0	0	
$\langle 1, 1\|$	$-E_a + E_{ab}$	0	$-J - (1/3)(D_a - D_{ab})$	0	
$\langle 0, 0\|$	0	0	0	$-2J$	

CT100053G

10.1021/ct100053g
Published on Web 02/16/2010

Published on Web 02/16/2010