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ADDITION/CORRECTION

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Correction to "Calculation of the O−H Stretching Vibrational Overtone Spectrum of the Water Dimer"

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There is a typographical error in the first column on the page 6307:

"The PES's were determined between −200 and +200 pm for the stretching coordinates ..." should be "The PES's were determined between −20 and +20 pm for the stretching coordinates ...".

Some rows in Table 3 on page 6308 had accidentally been mixed, leading to an error in the dipole moment surface. The correct values for the parameters are given below in Table 3.

Table 3. Corrections for Table 3

donor unit	y	z	donor unit	y	z
$\mu_{r_f\theta}$/D Å^{-1}	1.2484	0.1685	$\mu_{r_br_b\theta}$/D Å^{-2}	−2.7809	−1.7170
$\mu_{r_f\theta\theta}$/D Å^{-1}	0.7615	0.1356	$\mu_{r_br_b\theta\theta}$/D Å^{-2}	6.2824	3.2954
$\mu_{r_fr_f\theta}$/D Å^{-2}	−0.2607	−0.1883	$\mu_{r_fr_b}$/D Å^{-2}	−0.3718	0.7390
$\mu_{r_fr_f\theta\theta}$/D Å^{-2}	1.5804	0.3825	$\mu_{r_fr_br_b}$/D Å^{-3}	0.2454	0.2908
$\mu_{r_b\theta}$/D Å^{-1}	−1.9392	−0.3255	$\mu_{r_fr_fr_b}$/D Å^{-3}	−1.6691	0.2650
$\mu_{r_b\theta\theta}$/D Å^{-1}	1.0462	0.6180			

This error leads to an error in the transition intensity calculation in Table 4.

Some of the calculated energies are incorrect due to a programming error. The corrected energies for Table 4 on page 6310 are given here. This error changes the energies of the donor unit with methods AVTZ, AVQZ, and CP. Interpretations for the $|4\rangle_f|0\rangle_b|0\rangle$ and $|1\rangle_f|3\rangle_b|0\rangle$ states at the "CBS+CV+rel" level have been corrected. The corrected intensities are also included in Table 4.

Table 4. Corrections for Table 4

local mode assignment	AVTZ	AVQZ	CP	CBS+CV+rel	intensity
$\|00\rangle^+\|1\rangle$					27.5
$\|0\rangle_f\|0\rangle_b\|1\rangle$			1617.8		16.3
$\|00\rangle^+\|2\rangle$					0.2
$\|0\rangle_f\|0\rangle_b\|2\rangle$					1.6
$\|0\rangle_f\|1\rangle_b\|0\rangle$(85%) + $\|1\rangle_f\|0\rangle_b\|0\rangle$(13%)	3540.8	3553.5	3558.9		100
$\|10\rangle^+\|0\rangle$					3.1
$\|1\rangle_f\|0\rangle_b\|0\rangle$(85%) + $\|0\rangle_f\|1\rangle_b\|0\rangle$(13%)	3709.6	3727.1	3727.6		37.3
$\|10\rangle^-\|0\rangle$					22.2
$\|0\rangle_f\|1\rangle_b\|1\rangle$(82%) + $\|1\rangle_f\|0\rangle_b\|1\rangle$(12%)	5139.3	5153.0	5158.7		1.5
$\|10\rangle^+\|1\rangle$					0.047
$\|10\rangle^-\|1\rangle$					2.6
$\|1\rangle_f\|0\rangle_b\|1\rangle$(82%) + $\|0\rangle_f\|1\rangle_b\|1\rangle$(13%)	5306.7	5325.8	5326.6		3
$\|0\rangle_f\|1\rangle_b\|2\rangle$	6700.6	6713.8	6720.0		6.2×10^{-3}

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Table 4. Continued

local mode assignment	AVTZ	AVQZ	CP	CBS+CV+rel	intensity
$\|10\rangle^{+}\|2\rangle$					4.8×10^{-3}
$\|10\rangle^{-}\|2\rangle$					0.049
$\|1\rangle_f\|0\rangle_b\|2\rangle$	6870.6	6889.8	6890.9		0.031
$\|0\rangle_f\|2\rangle_b\|0\rangle$	6916.6	6937.3	6949.7		0.05
$\|20\rangle^{+}\|0\rangle$(75%) + $\|11\rangle^{+}\|0\rangle$(17%)					0.25
$\|2\rangle_f\|0\rangle_b\|0\rangle$(68%) + $\|1\rangle_f\|1\rangle_b\|0\rangle$(23%)	7178.5	7209.6	7212.2		0.66
$\|20\rangle^{-}\|0\rangle$					1.1
$\|1\rangle_f\|1\rangle_b\|0\rangle$(69%) + $\|2\rangle_f\|0\rangle_b\|0\rangle$(25%)	7304.4	7336.2	7339.9		0.073
$\|11\rangle^{+}\|0\rangle$(78%) + $\|20\rangle^{+}\|0\rangle$(18%)					5.8×10^{-3}
$\|0\rangle_f\|2\rangle_b\|1\rangle$	8498.8	8520.3	8533.0		0.033
$\|20\rangle^{+}\|1\rangle$(70%) + $\|11\rangle^{+}\|1\rangle$(16%)					1.2×10^{-3}
$\|20\rangle^{-}\|1\rangle$					0.11
$\|2\rangle_f\|0\rangle_b\|1\rangle$(63%) + $\|1\rangle_f\|1\rangle_b\|1\rangle$(22%)	8758.7	8791.1	8793.9		0.057
$\|1\rangle_f\|1\rangle_b\|1\rangle$(66%) + $\|2\rangle_f\|0\rangle_b\|1\rangle$(25%)	8881.7	8915.5	8919.5		0.018
$\|20\rangle^{+}\|1\rangle$(18%) + $\|11\rangle^{+}\|1\rangle$(74%)					9.5×10^{-6}
$\|0\rangle_f\|2\rangle_b\|2\rangle$(75%) + $\|0\rangle_f\|3\rangle_b\|0\rangle$(15%)	10024.5	10045.9	10060.8		1.4×10^{-3}
$\|0\rangle_f\|3\rangle_b\|0\rangle$(84%) + $\|0\rangle_f\|2\rangle_b\|2\rangle$(13%)	10121.0	10144.6	10163.8		3.1×10^{-3}
$\|30\rangle^{+}\|0\rangle$(77%) + $\|21\rangle^{+}\|0\rangle$(9%)					3.7×10^{-3}
$\|3\rangle_f\|0\rangle_b\|0\rangle$(67%) + $\|2\rangle_f\|1\rangle_b\|0\rangle$(12%)	10549.8	10592.1	10597.7		0.02
$\|30\rangle^{-}\|0\rangle$					0.036
$\|1\rangle_f\|2\rangle_b\|0\rangle$(68%) + $\|3\rangle_f\|0\rangle_b\|0\rangle$(15%)	10612.0	10654.0	10661.2		2.7×10^{-3}
$\|30\rangle^{+}\|0\rangle$(10%) + $\|21\rangle^{+}\|0\rangle$(80%)					1.6×10^{-3}
$\|2\rangle_f\|1\rangle_b\|0\rangle$(74%) + $\|1\rangle_f\|2\rangle_b\|0\rangle$(15%)	10823.6	10869.0	10875.5		3.8×10^{-3}
$\|21\rangle^{-}\|0\rangle$					4.4×10^{-3}
$\|0\rangle_f\|4\rangle_b\|0\rangle$	13086.5	13108.6	13136.6		1.1×10^{-3}
$\|40\rangle^{+}\|0\rangle$(72%) + $\|50\rangle^{+}\|0\rangle$(10%)					1.2×10^{-5}
$\|40\rangle^{-}\|0\rangle$(73%) + $\|50\rangle^{-}\|0\rangle$(10%)					1.7×10^{-3}
$\|4\rangle_f\|0\rangle_b\|0\rangle$	13799.4	13854.8	13857.9	13882.5	1.0×10^{-3}
$\|1\rangle_f\|3\rangle_b\|0\rangle$	13773.2	13817.1	13833.8	13841.8	9.0×10^{-5}
$\|3\rangle_f\|1\rangle_b\|0\rangle$(43%) + $\|2\rangle_f\|2\rangle_b\|0\rangle$(32%)	14064.4	14119.3	14129.0		2.4×10^{-4}
$\|31\rangle^{+}\|0\rangle$(55%) + $\|22\rangle^{+}\|0\rangle$(22%)					1.8×10^{-4}
$\|2\rangle_f\|2\rangle_b\|0\rangle$(50%) + $\|3\rangle_f\|1\rangle_b\|0\rangle$(38%)	14240.4	14297.5	14307.2		2.9×10^{-5}
$\|31\rangle^{-}\|0\rangle$					3.0×10^{-4}
$\|22\rangle^{+}\|0\rangle$(64%) + $\|31\rangle^{+}\|0\rangle$(27%)					2.6×10^{-6}
$\|0\rangle_f\|5\rangle_b\|0\rangle$	15893.5	15910.1	15948.6		3.4×10^{-4}
$\|50\rangle^{+}\|0\rangle$(54%) + $\|60\rangle^{+}\|0\rangle$(14%)					1.1×10^{-5}
$\|50\rangle^{-}\|0\rangle$(54%) + $\|60\rangle^{-}\|0\rangle$(14%)					7.3×10^{-5}

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