

ADDITIONS AND CORRECTIONS

2006, Volume 110A

Kristine L. Carlson, Stephen L. Lowe, Mark R. Hoffmann, and Kathryn A. Thomasson*: Theoretical UV Circular Dichroism of Cyclo(L-Proline-L-Proline)

Page 1928. Figure 2 incorrectly identified the ϕ and ψ angles. The corrected figure appears below. The values for the angles are unchanged.

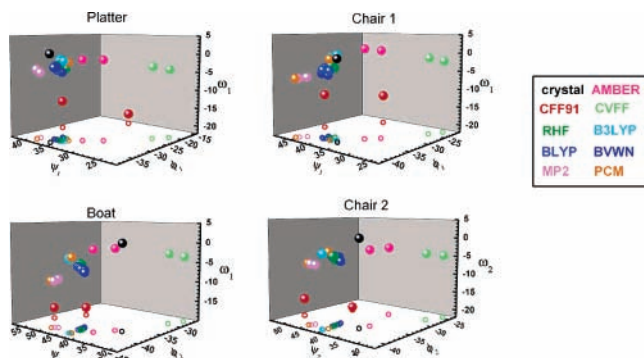


Figure 2. Dihedral angles of cyclo(L-Pro-L-Pro) in the three conformations. “Platter” and “Boat” denote the dihedral angles of the platter and boat conformations, respectively. The platter and boat conformations have C_2 symmetry, so both residues in each dipeptide have identical dihedral angles. “Chair 1” denotes the dihedral angles of one proline unit, and “Chair 2” denotes the dihedral angles of the other proline unit in the chair conformation. The spheres locate ϕ , ψ , and ω three-dimensionally, and the open circles represent the two-dimensional shadow on the ϕ/ψ wall.

Supporting Information Available:

(Page 1932) The tables of dihedral angles, Table 1a and Table 2a, mistakenly had the ϕ and ψ angles transposed. The corrected tables are included as Supporting Information to this Correction and are available free of charge via the Internet at <http://pubs.acs.org>.

10.1021/jp061761c
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2004, Volume 104A

M. Capitelli, G. Colonna, and F. Esposito*: On the Coupling of Vibrational Relaxation with the Dissociation–Recombination Kinetics: From Dynamics to Aerospace Applications

Page 8933. In the cited paper we report in eqs 10 and 11 the analytical expression of the $N_2(\nu) + N$ multi-quantum dissociation

rates as a function of the gas temperature and the vibrational quantum number ν . The coefficients are reported in Table 1. In this table two columns are missing. In this correction we report the complete table.

TABLE 1

j	$i = 0$	$i = 1$	$i = 2$	$i = 3$	$i = 4$
0	-29.8534	-175.5599	526.1455	1402.1769	67.6086
1	0.4177	5.1058	-15.7695	-40.0537	-1.9758
2	-3.7076×10^{-2}	-3.7157×10^{-2}	0.1186	0.2842	1.4665×10^{-2}
3	2.4664×10^{-3}				
4	-6.9381×10^{-5}				
5	8.6006×10^{-7}				
6	-3.9160×10^{-9}				

10.1021/jp061804p
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2005, Volume 109A

Vanessa Audette Lynch, Steven L. Mielke,* and Donald G. Truhlar*: High-Precision Quantum Thermochemistry on Nonquasiharmonic Potentials: Converged Path-Integral Free Energies and a Systematically Convergent Family of Generalized Pitzer–Gwinn Approximations

An exponent of 3/2 was omitted from the last factor on the right-hand side of eq 4 and the first factor on the right-hand side of eq 20. The corrected equations are

$$Q_{m'_a m'_b m'_c m'_d}^{P=1}(T) = Q_{m_a m_b m_c m_d}^{P=1}(T) \left(\frac{m'_a m'_b m'_c m'_d}{m_a m_b m_c m_d} \right)^{3/2} \left(\frac{m_a + m_b + m_c + m_d}{m'_a + m'_b + m'_c + m'_d} \right)^{3/2} \quad (4)$$

and

$$\prod_{j=1}^F \frac{\omega_j}{\omega'_j} = \left(\frac{\sum_i m_i}{\sum_i m'_i} \right)^{3/2} \left(\frac{I_{x' y' z'}}{I_{x y z}} \right)^{1/2} \prod_i^{\text{#atoms}} \left(\frac{m'_i}{m_i} \right)^{3/2} \quad (20)$$

The results and discussion were not affected by these errors.

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