

Erratum: The intramolecular vibrations of the ammonia water complex. A matrix isolation study [J. Chem. Phys. 9 1, 6604 (1989)]

Anders Engdahl and Bengt Nelander

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(b) The second deviation is noticed at the high energy region (where it is less expected), where the classical curve performs one additional wiggle before continuing to increase with the energy, as does the QM curve.

(c) As for the main energy range, it is seen that the classical curve rounds off the sharp corners created by the QM treatment, but other than that, the two curves overlap very nicely. The round-off is a smearing type process, which can be related to the quantization of the vibrational state and/or to the fact that partial cross sections were calculated within an angular range rather than strict differential cross sections.

The conclusion from this comparison is that even the most detailed observable magnitude, namely, the state-to-state back differential cross section, in the second lightest

reactive system seems to exhibit mainly quasiclassical features.

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ERRATA

Erratum: The intramolecular vibrations of the ammonia water complex. A matrix isolation study [*J. Chem. Phys.* **91**, 6604 (1989)]

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The title of this paper should be:
"The intermolecular vibrations of the ammonia water complex. A matrix isolation study."

The abstract should read:

The infrared spectrum of the ammonia water complex has been recorded from 10 to 4000 cm⁻¹ for complexes trapped in neon and krypton matrices. Spectra have been observed for NH₃ or ND₃ complexed with H₂O, HDO, and D₂O. The observed intermolecular fundamentals are compared with frequencies calculated from a rigid-molecule harmonic oscillator model.

In addition, *intramolecular* in the first sentence of the

introduction and in the head of Table III should be changed to *intermolecular*. The Eckart conditions on page 6608 should read:

$$M_R \rho \times \frac{d\rho}{dt} + I_A \cdot \omega_A + I_B \cdot \omega_B = 0.$$

The last formula on page 6608 should read:

$$2T = \dot{Q}^+ (S^+)^{-1} T S^{-1} \dot{Q} = \dot{Q}^+ T_Q \dot{Q}$$

The question mark after 2753.7 in Table I should be removed. In Ref. 6: Vol. 16 is missing.

Erratum: The multiconfigurational spin tensor electron propagator method: Electron affinities of Li, Na, and K [*J. Chem. Phys.* **91**, 5451 (1989)]

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The second sentence of the second paragraph on page 5452 should read: "Therefore, a unitary transformation¹ (within each set of orbital types-inactive, active, and excited) is carried out on the converged MCSCF orbitals by dia-

gonalizing the corresponding (*a_i, a_j*) subblock of block 1 of the *M* matrix."

In the first paragraph of column II, page 5452, the EA of K was reported incorrectly as 0.486 eV. It should read 0.496

eV as reported in Table II.

In Table I, a d exponent of K^{-1} was reported as 0.037. It should read 0.37. Footnote c should read: "Reference 13. The second s and p functions are uncontracted." Also, footnote e in this table should read: "Reference 15 [$6s5p$] contraction. The second p function is uncontracted."

In the third paragraph on page 5453, we incorrectly reported the square of the MCSCF wave function amplitudes for the $3s^2$ and $3p^2$ configurations in Na^- and for the $4s^2$ and $4p^2$ configurations in K^{-1} . The corrected sentences should read: "The MCSCF expansion amplitude squared for the $2s^2$

and $2p^2$ configurations of Li^- are 0.870 and 0.105, respectively; for Na^- the MCSCF expansion amplitude squared for the $3s^2$ and $3p^2$ configurations are 0.887 and 0.087, respectively; and for $K^{-1}4s^2$ and $4p^2$ amplitude squared are 0.868 and 0.107, respectively. As the results by Ortiz compared to MCSTEP show, perturbational approaches to the electron propagator are not nearly as reliable as multiconfigurational-based approaches even at this level of configuration mixing. When the mixing of two or more configurations is even greater, perturbational approaches are invalid."

Erratum: Picosecond fluorescence depletion spectroscopy. III. Intramolecular vibrational relaxation in the excited electronic state of *p*-cyclohexylaniline [J. Chem. Phys. 92, 1004 (1990)]

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Equation (1) was incorrectly printed; this equation should read:

$$I(t) = 1 - \exp\left(\frac{-t}{t_1}\right)\left(1 - \frac{y}{2}\right) - \frac{y}{2} \exp\left(\frac{-t}{t_2}\right) \cos\left(\frac{2\pi t}{p}\right). \quad (1)$$

Erratum: Swelling equilibria for ionized temperature-sensitive gels in water and in aqueous salt solutions [J. Chem. Phys. 92, 2061 (1990)]

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