

## Erratum: "Solvent Effects on Geminal H–H Couplings: A New Method for Determining Signs of Coupling Constants"

Stanford L. Smith and Richard H. Cox

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# Erratum: "Thermal-Energy Ion-Neutral Reaction Rates. IV. Nitrogen-Ion Charge-Transfer Reactions with CO and CO<sub>2</sub>"

[J. Chem. Phys. **44**, 4537 (1966)]F. C. FEHSENFELD, A. L. SCHMELTEKOPF, AND  
E. E. FERGUSON*Institute for Telecommunication Sciences and Aeronomy  
Environmental Science Services Administration, Boulder, Colorado*

WE have discovered that our data for the charge-transfer reactions of nitrogen ions with NO and CO were inadvertently interchanged. Table I on p. 4538 should read as shown.

TABLE I. Measured rate constants.

Reaction	Rate constant (cm <sup>3</sup> /sec) at 300°K
N <sup>+</sup> +CO <sub>2</sub> →CO <sub>2</sub> <sup>+</sup> +N+0.75 eV	1.3×10 <sup>-9</sup>
N <sub>2</sub> <sup>+</sup> +CO <sub>2</sub> →CO <sub>2</sub> <sup>+</sup> +N <sub>2</sub> +1.79 eV	9×10 <sup>-10</sup>
N <sup>+</sup> +CO→CO <sup>+</sup> +N+0.53 eV	5×10 <sup>-10</sup>
N <sub>2</sub> <sup>+</sup> +CO→CO <sup>+</sup> +N <sub>2</sub> +1.57 eV	7×10 <sup>-11</sup>

The CO reactions listed in the original Table I actually referred to the NO reactions as follows:



and



These NO charge-transfer reaction-rate-constant measurements agree well with our earlier measurements<sup>1</sup> (which gave 11% and 24% lower rate constants for N<sup>+</sup> and N<sub>2</sub><sup>+</sup>, respectively). The value of the rate constant for the N<sub>2</sub><sup>+</sup>+CO<sub>2</sub> charge transfer agrees with a recent measurement of Warneck<sup>2</sup> to within 10%. The N<sub>2</sub><sup>+</sup>+CO reaction was measured using isotopic N<sub>2</sub>. Both the <sup>15</sup>N<sup>15</sup>N and <sup>15</sup>N<sup>14</sup>N ions were measured, leading to the same rate constant.

We are indebted to Dr. Warneck for a discussion which led to our discovery of the above error.

<sup>1</sup> P. D. Goldan, A. L. Schmeltkopf, F. C. Fehsenfeld, H. I. Schiff, and E. E. Ferguson, J. Chem. Phys. **44**, 4095 (1966).  
<sup>2</sup> P. Warneck, GCA Tech. Rept. No. 66-13-N, GCA Technology Division, Bedford, Mass., July 1966.

# Erratum: "Gaussian Wavefunctions for the 10-Electron Systems. III. OH<sup>-</sup>, H<sub>2</sub>O, H<sub>3</sub>O<sup>+</sup>"

[J. Chem. Phys. **43**, 3550 (1965)]

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ON account of an error in one of the integral evaluation routines the computations for H<sub>2</sub>O in the basis (95/31) and (53/31), for H<sub>3</sub>O<sup>+</sup> in the basis (95/31), and for OH<sup>-</sup> in the basis (95/31) are slightly in error. All other computations are correct as reported, in particular those containing *d* orbitals. A short table of corrected results is given below.

TABLE I. Total energy and dipole moment of H<sub>2</sub>O, H<sub>3</sub>O<sup>+</sup>, and OH<sup>-</sup> in a Gaussian basis. OH distance equals 1.8 a.u. Total energy and dipole moment in atomic units.

	Basis	HOH angle	Total energy	Dipole moment
H <sub>2</sub> O	(95/31)	105°	-76.03308	0.9556
H <sub>2</sub> O	(53/31)	105°	-75.59039	0.9035
H <sub>3</sub> O <sup>+</sup>	(95/31)	120°	-76.32028	...
H <sub>3</sub> O <sup>+</sup>	(95/31)	118°06'	-76.32014	...
OH <sup>-</sup>	(95/31)	...	-75.36669	0.5145

# Erratum: "Solvent Effects on Geminal H-H Couplings: A New Method for Determining Signs of Coupling Constants"

[J. Chem. Phys. **45**, 2848 (1966)]

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IN Table III, p. 2852, the column headed *J<sub>trans</sub>* should be headed *J<sub>cis</sub>*; that headed *J<sub>cis</sub>* should be headed *J<sub>trans</sub>*.