

isotopic frequency data to be satisfactory when the "trace" equations are intrinsically ill-conditioned. Ill-conditioning of these equations can be detected *a priori* by the occurrence of near linear dependences among the rows of the square matrix of which the i th row, corresponding to the i th isotope, consists of the $\frac{1}{2}n(n+1)$ elements $G_{11}^{(i)}$, $2G_{12}^{(i)}$, \dots , $2G_{1n}^{(i)}$, $G_{22}^{(i)}$, $2G_{23}^{(i)}$, \dots , $2G_{2n}^{(i)}$, \dots , $G_{nn}^{(i)}$.

(6) The above conclusions reveal that the "trace" method proposed by O'Reilly for the determination of vibrational force constants is of seriously limited applicability and that O'Reilly's application to HCN produces an unsatisfactory force field.

¹ E. J. O'Reilly, *J. Chem. Phys.* **48**, 1086 (1968).

² G. Strey, *J. Mol. Spectry.* **24**, 87 (1967).

³ D. E. Freeman, *J. Mol. Spectry.* **22**, 305 (1967).

Multiplicity of Force Constants in the Vibrational Analysis of Molecules

E. J. O'REILLY

*Department of Chemistry, University of North Dakota,
Grand Forks, North Dakota*

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There is a persistent error in the calculation of the numerical values of the force constants for the "double-root" solution of the HCN example in Ref. 1. The correct values are essentially as given by Freeman.² The numerical values of the $(L^\pm)^{-1}$ and B^\pm are then in error. The nonorthogonality of the B matrices was recognized and erroneously ascribed to "data inconsistency".¹

The significant part of Ref. 1 remains unaltered. The two different sets of force constants yield a difference in composition and "phase" of the normal coordinate associated with a given normal frequency as Freeman's results still indicate.

The extreme sensitivity of the trace method to error in the experimental data is recognized. An error of 200% on the interaction constant is hardly small.¹ The significant point remains, however, that the "trace method" is at present the only technique with a theoretical basis for deciding which of the two sets of force constants is correct. The phrase "in principle" was used throughout Ref. 1 in recognition of the practical limitations of the method.

¹ E. J. O'Reilly, *J. Chem. Phys.* **48**, 1086 (1968).

² D. E. Freeman, *J. Chem. Phys.* **49**, 4250 (1968), preceding Comment.

Errata

Erratum: Angular Distribution of Photoelectrons

[*J. Chem. Phys.* **48**, 942 (1968)]

J. COOPER AND R. N. ZARE

Joint Institute for Laboratory Astrophysics, Boulder, Colorado 80302

In the denominator of Eq. (2) a factor of 3 inadvertently appears. We thank Dr. U. Fano, Dr. R. S. Berry, and Dr. J. Tully for individually pointing out this error to us. The rest of the paper stands unchanged.

Erratum: Reactions of Negative Ions in the Gas Phase. III. The Formation of OCN^-

[*J. Chem. Phys.* **48**, 3828 (1968)]

JOHN G. DILLARD,* J. L. FRANKLIN, AND WILLIAM A. SEITZ
Department of Chemistry, Rice University, Houston, Texas

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The sentence following Eq. (5) should read: "The maximum intensity of Cl^- from CNCl occurred at an electron energy of 6.5 eV, so that the intensity of Cl^- was quite small in the electron energy range of O^- (about 2 and 4.2 eV maximum with N_2O and SO_2 , respectively)."

* Present address: Department of Chemistry, Virginia Polytechnic Institute, Blacksburg, Va.

Erratum: Exchange Effects in the Degenerate Perturbation Theory of Intermolecular Potentials

[*J. Chem. Phys.* **48**, 3639 (1968)]

DAVID A. MICHA

*Department of Physics and Institute of Pure and Applied Physical Sciences, University of California, San Diego,
La Jolla, California 92037*

The sentence including Eqs. (17) and (18) should be changed to read: "It is seen from Eq. (12) that we can always choose $\langle \Psi_{q'} | \Psi_q \rangle = N_q \delta_{q'q}$."

Delete the sentence starting on page 3641, Line 6.