electrons within molecules. Then letting $|\phi_i\rangle$ be a normalized Slater determinant for the Z electrons of molecule i and letting $|\phi_1\cdots\phi_N\rangle$ be the product of one such for each molecule, the trace becomes

$$\mathrm{Tr}O=[(Z!)^N/(NZ)!]\sum_{\text{states}}\sum_{\alpha}{}'\sum_{\beta}{}'\delta_\alpha\delta_\beta \times\langle\phi_1\cdots\phi_N|P_\alpha OP_\beta|\phi_1\cdots\phi_N\rangle.$$

Next we let the sums over reassignments revert to being sums over all permutations and divide by $(Z!)^{2N}$ to compensate, obtaining

$$\mathrm{Tr}O=[(Z!)^N(NZ)!]^{-1}\sum_{\text{states}}\sum_{\alpha}\sum_{\beta}\delta_\alpha\delta_\beta \times\langle\phi_1\cdots\phi_N|P_\alpha OP_\beta|\phi_1\cdots\phi_N\rangle.$$

This formula is an example of a form in which summation over states of molecule 1 is not done independently of summation over states of the other molecules.

We want now to stop summing over "states" of the whole gas and instead to use uncorrelated summations over the states of the individual molecules of the gas. When we do this we will include each state of the whole gas $(NZ)!/(Z!)^N$ times and therefore put in a factor to compensate, obtaining

$$\mathrm{Tr}O=[(NZ)!]^{-2}\sum_{\phi_1}\cdots\sum_{\phi_N}\sum_{\alpha}\sum_{\beta}\delta_\alpha\delta_\beta \times\langle\phi_1\cdots\phi_N|P_\alpha OP_\beta|\phi_1\cdots\phi_N\rangle.$$

Note that all the one-molecule determinants are still being formed of one-electron orbitals taken from a single complete orthonormal set. In the above expression, terms vanish due to antisymmetrization if they contain a given orbital more than once.

We want next to convert the sum over states of molecule i $(i=1, 2, \cdots, N)$ from its present form involving arbitrary one-electron orbitals to a form incorporating orbitals which are appropriate to the molecule, e.g., a form incorporating the Hartree–Fock ground and bound excited-state orbitals together, perhaps, with some "low"-energy scattering states. To this end let u_i be a unitary transformation which converts each determinant $|\phi_i\rangle$ based on the earlier arbitrary orbitals into a determinant $|\lambda_i\rangle$, appropriate to molecule i. Then the product

$$u\equiv\prod_{i=1}^{N}u_i$$

is again unitary. We observe further that the functions $|\phi_1\cdots\phi_N\rangle$ constitute an orthonormal basis for a certain function space and that the summation over them in the preceding equations constitutes a trace in that space. Then using the fact that $uu^+=1$ and that the trace is unchanged by a cyclic permutation of the operators and writing $u_i|\phi_i\rangle=|\lambda_i\rangle$, we have

$$\mathrm{Tr}O=[(NZ)!]^{-2}\sum_{\lambda_1}\cdots\sum_{\lambda_N}\sum_{\alpha}\sum_{\beta} \times\langle\lambda_1\cdots\lambda_N|P_\alpha OP_\beta|\lambda_1\cdots\lambda_N\rangle.$$

Then assuming that $[O, P_\beta]=0$ and using the fact that the operator $(NZ)!^{-1}\sum_\alpha\delta_\alpha P_\alpha$ is idempotent and that the one-molecule states $|\zeta_i\rangle$ are antisymmetric, we have

$$\mathrm{Tr}O=[(Z!)^N/(NZ)!]\sum_{\lambda_1}\cdots\sum_{\lambda_N}\sum_{\alpha}{}'\delta_\alpha \times\langle\lambda_1\cdots\lambda_N|P_\alpha O|\lambda_1\cdots\lambda_N\rangle,$$

where the primed sum is again just over reassignments of electron variables among the molecules.

[1] L. T. Klauder, Jr., J. Chem. Phys. **46**, 3369 (1967).

Errata

Erratum: Electron Paramagnetic Resonance of Beef Heart Ferricytochrome c

[J. Chem. Phys. **48**, 2049 (1968)]

IRVING SALMEEN AND GRAHAM PALMER

Biophysics Research Division, Institute of Science and Technology, The University of Michigan, Ann Arbor, Michigan

The values for λ, μ and R, calculated to fit the experimental g values, are not unique as was implied, because the matrix to be diagonalized can be multiplied by an arbitrary constant without changing the eigenfunctions.

Although there are no unique values for λ, μ, and R, we can find limits. One limit corresponds to choosing the free-ion value for the spin–orbit coupling, viz., $\lambda=420$ cm^{-1}, $\mu=1110$ cm^{-1}, and $R=625$ cm^{-1}. The other limit is set using Zerner and Gouterman's[1] estimate of 80% covalency which corresponds to $\lambda=340$ cm^{-1}, $\mu=900$ cm^{-1}, and $R=500$ cm^{-1}.

[1] M. Zerner and M. Gouterman, Theoret. Chim. Acta **6**, 363 (1966).

Erratum: Ion Motion in Tetrafluoroborate Salts. I. NH_4BF_4 and ND_4BF_4

[J. Chem. Phys. **47**, 2577 (1967)]

A. P. CARON, D. J. HUETTNER, J. L. RAGLE, L. SHERK, AND T. R. STENGLE

Department of Chemistry, University of Massachusetts, Amherst, Massachusetts

The y axes of Figs. 1–3 are mislabeled, and observed relaxation times are a factor of (exactly) 10 longer

than shown. The results and conclusions of the paper are unaffected by this typographical error.

The text (page 2579) incorrectly refers to the ordinates of these figures as abscissa.

The equation below Eq. (5) (page 2579) should read

$$(\tau T_1)^{-1} = (1.2384\times 10^{10})_{FF} + (3.0339\times 10^{10})_{BF}.$$

The correct version of this equation was used in the analysis presented in Eq. (6).

Erratum: Vibrational Structuring in Optical Activity. II. "Forbidden" Character in Circular Dichroism

[J. Chem. Phys. **43**, 3609 (1965)]

OSCAR E. WEIGANG, JR.

Richardson Chemical Laboratories, Department of Chemistry, Tulane University, New Orleans, Louisiana

The left-hand side of Eq. (A18) should read $\hbar^2 R_K^{(2)} R_K$.

The final expression of Eq. (A26) should have the additional term

$$\sum_r \sum_s \mathrm{Im}\{\mathbf{C}_r\cdot\mathbf{B}_s\}(\hbar/i)(0\mid Q_r P_s\mid 0) = \sum_r \mathrm{Im}\{\mathbf{C}_r\cdot\mathbf{B}_r\}\xi_r\hbar\omega_r,$$

which arises from application of the commutation relation

$$H^K Q_s - Q_s H^K = (\hbar/i)P_s.$$

P is the momentum conjugate to Q_s.

Equation (A27) then follows from a neglect of terms containing $(l_K{}^{rs}-\delta_{rs}l_N{}^{rr})$, where the definition of the weighted mean frequency $\bar{\omega}$, Eq. (22), should be corrected to read

$$\hbar\bar{\omega} = \sum_r \mathrm{Im}\{\mathbf{C}_r\cdot\mathbf{B}_r\}\xi_r\hbar\omega_r / \sum_r \mathrm{Im}\{\mathbf{C}_r\cdot\mathbf{B}_r\}\xi_r.$$

Agreement with the analogous term in Eq. (99) of Ref. 2 is thus complete.

The author is grateful to Glen M. Robinson for critically reviewing the derivations.

Erratum: Infrared Spectrum and Internal-Rotation Barrier of Nitroethylene

[J. Chem. Phys. **46**, 1200 (1967)]

K. R. LOOS AND HS. H. GÜNTHARD

Laboratorium für Physikalische Chemie, Eidg. Techn. Hochschule, Zürich, Switzerland

In the calculation of the barrier to internal rotation an error occurred. Table XI should be replaced by

TABLE XI. Internal-rotation barrier heights.

Molecule	Harmonic approx. (cm^{-1} cal/mole)		Mathieu treatment (cm^{-1} cal/mole)	
H_2CCHNO_2	1250±50	3570±140	1300±50	3720±140
H_2CCDNO_2	1260±50	3600±140	1308±50	3740±140

On p. 1206 the following corrections should be made:

(i) ··· the reduced moment of inertia for the NO_2 group is calculated to be 7.94 amu·Å² for the d_0 and 9.45 amu·Å² for the d_1 isotope.

(ii) ··· a table of Mathieu eigenvalues has been calculated for functions having a period $\cos 2\phi$ and s values of 612 and 732 were obtained for the d_0 and d_1 isotope, respectively.

(iii) ··· in a barrier value of approximately 3720 cal/mole for nitroethylene-d_0.