

states. This structure becomes apparent when comparing H^+ energy distributions resulting from ionization of H_2 , HD, and D_2 (HD background). In particular the H^+ energy distribution produced from HD at $\sim 1.9 \text{ v/\AA}$ exhibits three peaks which do not exist in the spectrum from H_2 . These peaks have field-dependent energy separations from the main peak of $\sim 1.7, 6.0, \text{ and } 12.6 \text{ eV}$. They occur because for HD the center of mass and center of charge are not coincident, producing a torque on those HD^+ ions with axis skewed from the field. Viewed from the C of M, the molecule ion moves as though it were a variable length pendulum with the equilibrium orientation, H atom down-field. For molecules ionized with H atom up-field, the dissociative probability is enhanced as the HD^+ swings through the equilibrium orientation, producing secondary peaks corresponding to $1/2, 3/2, \text{ and } 5/2$ pendulum swings. H^+ from HD appears before H^+ from H_2 .

¹A. J. Jason, Phys. Rev. 156, 266 (1967).

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BE 5 Ab-Initio LCAO-MO-SCF Calculations on Energetic Compounds: Five-Member Heterocyclics and Nitrobenzene.*
HARRY J. T. PRESTON and JOYCE J. KAUFMAN, The Johns Hopkins University.--Ab-initio LCAO-MO-SCF calculations were performed for pyrrole, pyrazole and imidazole with a Gaussian basis C, N $9^5P \rightarrow 4^5P$, H $4^5P \rightarrow 3^5P$. The total energies (pyrrole, $-208.7764415 \text{ a.u.}$; pyrazole, $-224.7400665 \text{ a.u.}$; imidazole, $-224.7580246 \text{ a.u.}$) indicated pyrazole to be less stable than imidazole in agreement with experiment. Comparison of the ab-initio results with those of less rigorous methods showed that ZDO methods, such as CNDO and INDO, did not reproduce correctly either the MO energy levels or population analyses. An ab-initio LCAO-MO-SCF calculation was carried out for nitrobenzene with a somewhat smaller basis set, C, N, O $7^5P \rightarrow 3^5P$, H $3^5P \rightarrow 2^5P$. The less rigorous ZDO methods again did not give agreement with the ab-initio results.

*Submitted by JOYCE J. KAUFMAN.

BE 6 The Pair Potential for Water. J. G. LANE and H. W. LEIDECKER, American U.--We have investigated the determination of the intermolecular pair potential for water using the thermodynamic properties of the dilute vapor and structural features predicted by Hartree-Fock calculations of the potential. In order to correctly represent the angle dependence of the pair interaction, we have generated for the first time the explicit angle dependent multipole functions necessary to describe the water charge distribution through dipole-octupole and quadrupole-quadrupole terms. A comparison of several point charge models for the pair potential with truncated multipole series descriptions of the same models indicates the failure of the truncated multipole series to correctly represent the point charge interaction in the range of intermolecular separation near the equilibrium position. Nevertheless a "multipole" potential model consisting of a Lennard-Jones spherically symmetric part plus the angle dependence of dipole-dipole, dipole-quadrupole, dipole-octupole, and quadrupole-quadrupole interactions using moments correct for water and adjusted to fit the second virial coefficient gives good agreement with the energy minimum and force constants obtained from HF calculations.

BE 7 Second Order Perturbation Treatment of Some One-electron Diatomic Molecules. FRANK C. SANDERS and AHMAD A. MAHOOTCHI, Southern Illinois University.--Wave functions for the ground states of the H_2^+ and HeH^+ molecular ions are obtained through second order in perturbation theory. The calculations are carried out for some alternative zero-order Hamiltonians. Estimates of the ground state energies complete through fifth order are computed and the convergence of the alternative perturbation series are examined. Applications to more complex molecular systems are discussed.

BE 8 Optical Constants of Water in the Infrared.*
DUDLEY WILLIAMS and HARRY D. DOWNING, Kansas State U.--Several years ago Irvine and Pollack¹ pointed out the

lack of reliable values of the optical constants n and k of water in the infrared and pointed out the desirability of further quantitative studies. Since then there have been numerous measurements of these quantities by various experimental techniques in our laboratory and elsewhere; we give a critical survey of the results and attempt to formulate curves presenting the present "best values". Throughout most of the spectrum between the visible and the radio-frequency region both n and k have been determined to within one or two percent; the resulting spectra can be interpreted in general terms and provide information concerning the intermolecular lattice structure of water in the liquid state.

*Supported by the Office of Naval Research.

¹W. H. Irvine and J. B. Pollack, Icarus 8, 324 (1968).

BE 9 Electronic Transitions Involving Triplet Systems of ZrO Molecule. L. SCHOONVELD and S. SUNDARAM, Univ. of Illinois, Chicago, Ill.--In view of the importance of the spectra of ZrO molecule for astrophysical applications, a systematic review of all available experimental data on the electronic transitions of the molecule has been made. The triplet systems $C^3\Delta-X^3\Delta$, $B^3\Pi-X^3\Delta$, and $A^3\Phi-X^3\Delta$ have been analysed and a consistent set of vibrational constants $\omega_e, \omega_e x_e$ have been derived. They are given below:

| State | ω_e | $\omega_e x_e$ |
|-------------|------------|----------------|
| $C^3\Delta$ | 819.83 | 3.150 |
| $B^3\Pi$ | 845.58 | 3.602 |
| $A^3\Phi$ | 856.12 | 3.430 |
| $X^3\Delta$ | 937.36 | 3.487 |

Using Morse type eigenfunctions, Franck-Condon factors and r-centroids have been calculated. Also, RKR and Morse potential curves have been generated for all the four triplet states of the molecule ZrO.

BE 10 Accuracy Limitation of Saturated Absorption Optical Frequency Standards by Transverse Doppler Effect. J. L. HALL, CH. BORDÉ,* and C. V. KUNASZ, Joint Institute for Laboratory Astrophysics, National Bureau of Standards and Univ. of Colorado.--Despite the remarkable frequency stability¹ and spectral resolution² achieved with suitable laser techniques, the accuracy capability of potential optical frequency standards will be importantly limited by the second order Doppler shift. Using the density matrix, numerical lineshape calculation of Bordé et al.³ (which explicitly treats the molecular free flight through the probing laser field), we calculate the effective second order Doppler shifts vs detuning and can then average over the modulation waveform. For example, for the case of equal collision, transit and radiative interaction times we find a preliminary average squared velocity of $.84 \text{ u}^2$ at line center and $.99 \text{ u}^2$ at the half-power points. Here $u^2 = 2kT/M$. At 10 times lower pressure and power, these averages are 0.30 u^2 and 0.49 u^2 . An average velocity of $y \cdot u^2 \rightarrow$ a relative frequency shift of $-1/2(u^2/c^2)y = -y \cdot 1.7 \cdot 10^{-12}$ for methane at room temperature.

*Laboratoire de Physique des Lasers, Paris.

¹S.N. Bagaev and V.P. Chebotayev, JETP Lett. 16, 433 (1972).

²J.L. Hall and Ch. Bordé, Phys. Rev. Lett. 30, 1101 (1973).

³Ch. Bordé, D.G. Hummer, C.V. Kunasz and J.L. Hall, to be published.

BE 11 Speed of Light from Molecular Spectroscopic Data Recent Microwave and Infrared Measurements for HCl & CO
PETER K.L. YIN and K. NARAHARI RAO, Department of Physics, The Ohio State University, Columbus, Ohio 43210-- The most recent studies in the submillimeter wave region¹ corrected the previous measurements² for $H^{35}Cl$ by 4 Mc/sec . This indicated a possibility for a similar error¹ in the infrared measurements³ because both the previous measurements in the microwave and infrared regions led