

TABLE I. Molecular parameters for the isotopic species of CH₂CFCI.*

	(a+c)/2	(a-c)/2	κ
CH ₂ CFCI ¹⁶	7065.00	3616.62	-0.542724
CH ₂ CFCI ¹⁷	7030.91	3650.42	-0.568678

* The number of significant figures quoted appears to be justified by the very close agreement of the five transitions of $J < 6$ for the Cl³⁵ species. This would indicate that the deviations of about a megacycle in the $J \geq 6$ transitions, which are consistent in sign, may be accounted for in terms of centrifugal distortion.

TABLE II. CH₂CFCI¹⁶ transitions.

Transition	Frequency calculated (Mc)	Frequency observed
1 ₀₁ →2 ₁₂	21,026.7	21,026.70
2 ₁₂ →3 ₀₃	20,214.2	20,214.29
6 ₄₃ →7 ₃₄	22,420.4	22,419.13
2 ₁₂ →2 ₂₁	21,699.7	21,699.70
3 ₁₃ →3 ₂₂	24,362.3	24,362.48
5 ₀₅ →5 ₁₄	24,601.4	24,601.24
6 ₁₆ →6 ₂₄	20,392.4	20,391.51
6 ₂₄ →6 ₃₃	24,896.3	24,895.46
7 ₁₆ →7 ₂₅	25,657.3	25,656.30
7 ₂₅ →7 ₃₄	23,897.8	23,896.29
CH ₂ CFCI ¹⁷ transitions		
1 ₀₁ →2 ₁₂	20,822.8	20,822.8
8 ₄₄ →9 ₃₅	22,848.8	22,852.40
2 ₁₂ →2 ₂₁	21,902.5	21,902.50
3 ₁₃ →3 ₂₂	24,427.4	24,427.38

ties χ are products of eQ and $(\partial^2 V / \partial a^2)$ and $(\partial^2 V / \partial b^2)$, the appropriate components of the molecular field gradient at the Cl nucleus. a and b are the principal axes of least and intermediate moments of inertia, respectively.

The assignments were initially made solely on the basis of the observed multiplet structure. Particularly helpful in this regard were certain of the Q -branch transitions of $J > 2$, which appear as quadruplets of lines with a ratio of certain component separations which is determined only by the J value involved. Figure 1 shows the 6₂₄→6₃₃ multiplet; the ratio of the differences A and B agreeing with that calculated from the first-order formulas for a 6→6 transition. Although a P or R branch transition gives rise to a similar quadruplet, the ratio of spacings depends on the quadrupole coupling factors of the two levels involved and will not usually be confused with that expected for any Q -branch transition. The amount of the separation depends, however, on the magnitude of the individual coupling factors, so that, due to limitations of resolution, some of the transitions may appear as singlet or doublet lines.

Because the a axis is very nearly parallel to the C-Cl bond, one may calculate with reasonable assurance -74.4 ± 2 mc/sec. as the value of the quadrupole coupling along the bond.

The corresponding deuterated compound is now being prepared, with whose results we hope to determine the structure of the molecule.

We wish to express our gratitude to Dr. M. Prober of this laboratory for the preparation of the compounds used in this investigation. We also wish to thank Miss V. G. Thomas for her assistance with the numerical computations involved in this work.

¹ J. K. Bragg, Phys. Rev. **74**, 533 (1948); J. K. Bragg and S. Golden, Phys. Rev. **75**, 735 (1949).

Erratum: A Theory of Pressure Absorption

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SOME numerical values must be corrected as follows: The experimental intensity of the Q -branch of O₂ band near 1556 cm⁻¹ is 4.4×10^6 cm⁻¹ instead of 4.0×10^8 cm⁻¹, at 1 atm. Thus

$\beta^2 + (11/30)\gamma^2$ in (6) must be assumed to be 1.9×10^{-52} in order to explain the above experimental results.

The estimation of the intensity ratio of the quadrupole absorption to the pressure absorption must be revised as follows,

$$1: \left(\frac{c}{\nu}\right)^2 \frac{n}{R_0^3} \left(\beta^2 + \frac{11}{30}\gamma^2\right) \approx 1:10^4.$$

Coherent Scattering of X-Rays by Atoms with More Than One Electron According to the One-Electron Theory and the Positron Theory

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THERE is no doubt that the "one-electron theory" and the "positron theory" cannot give identical expressions for the coherent scattering of x-rays by atoms. Recently Halpern and Hall¹ announced the results of this calculation, which exhibited this fact, but from the very beginning it is clear that the one-electron theory cannot give rise, for example, to the terms due to vacuum polarization. The real problem consists therefore in determining the order of magnitude of the differences in the results of the two theories.

On the other hand, it is evident that these differences may be separated into two classes from the beginning: Those which are encountered for the atom with many electrons as well as for the hydrogen atom and those which are specific to the atom with many electrons, and which are due, if they exist, to the interactions between electrons. The terms of the first class are to be looked for in the "one-particle parts" (in the sense defined by Schwinger²), the other in the two- and many-particle parts. It is these latter terms we tried to find.

Let N be the number of electrons, $\varphi_1 \varphi_2 \dots$ the wave functions of a single electron in the field of the nucleus. Let

$$\psi(x) = \sum a_n \varphi_n \exp(iE_n)$$

be the matter field, H the coupling between the matter field and the transverse electromagnetic field, and H^c the Coulomb interaction of the electrons. We introduce S and T by

$$\partial S / \partial t = H, \quad \partial T / \partial t = \frac{1}{2} i [S, H] - H_{\text{self}}^c \text{ and } \epsilon(t) = \pm 1 \text{ if } t \geq 0.$$

H^c shall be treated as a perturbation. To the one-particle parts of $\frac{1}{2} i [S, H]$ which give to the well-known terms (Waller):

$$\sum_{z=1}^N \sum_{i=1}^N \varphi_i^* (\alpha \cdot A_0) \varphi_z \varphi_z^* (\alpha \cdot A_1) \varphi_i / (E_z - E_i \pm |k|), \quad (1)$$

we must add the two-particle terms of

$$\frac{1}{2} i^2 [S, (S, H^c - H_{\text{self}}^c)] + i(T, H^c - H_{\text{self}}^c) \\ = -\frac{1}{2} \int \{ [H^c(t) - H_{\text{self}}^c(t), H(t')] \} \epsilon(t-t') \epsilon(t'-t'') dt' dt''.$$

As the calculation shows, this is equivalent to replacing in (1) the function φ by $\varphi + \varphi'$, where φ' , for instance, is given by

$$\varphi'_i = \sum_{\lambda \neq i} \sum_{j \neq i} \varphi_\lambda \frac{\langle \lambda j | H^c - H_{\text{self}}^c | i j \rangle}{E_i - E_\lambda}.$$

In other words, the scattering due to the i th electron is to be calculated for an electron moving in the field of the nucleus and the mean field of the other electrons. But this is exactly the result of the one-electron theory, if the interaction between electrons is treated as a perturbation.

Thus, we are led to the following conclusion: If there is a non-negligible difference between the results of the one-electron theory and the positron theory, this difference cannot be attributed to the interaction of the electrons within the atom.

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¹ O. Halpern and H. Hall, Phys. Rev. **75**, 1322 (1949).

² J. Schwinger, Phys. Rev. **75**, 651 (1949).