PHYSICAL REVIEW VOLUME 163, NUMBER 2 10 NOVEMBER 1967

Structural Studies of Some Tellurium Compounds Using the Mössbauer Effect in Te^{125} and I^{129} Nuclei

M. Pasternak and S. Bukshpan
Nuclear Physics Department, Soreq Research Center, Yavne, Israel

(Received 23 May 1967)

Structural information on tellurium compounds was obtained from Mössbauer-effect data measured with Te^{129} sources. The compounds studied were tellurium metal, TeO_2, and $Te(NO_3)_4$. To check the reliability of the information obtained, experiments were also carried out using Te^{125} absorbers. It was found that for the tellurium compounds, but not for tellurium metal, the ratio of the quadrupole coupling of the Te^{129} sources to that of the Te^{125} absorbers was constant, despite the differences in the ligands and structural properties of these compounds as revealed by differences in their isomer shifts and asymmetry parameters It is concluded that the structure of TeO_2 (orthorhombic phase) resembles that of SeO_2, namely, a chain structure with three coordinated oxygens and an O—Te—O angle of 90°. From the significant magnitude of the asymmetry parameter, it is concluded that one of the Te—O bonds is longer than the other two. An appreciable anisotropy of the recoilless fraction was found in the case of TeO_2 and Te metal, confirming their chain character. For $Te(NO_3)_4$, the structure was found to be a tri- or tetrapyramid with the Te atom at the apex, equal Te—NO_3 bond distances, and a NO_3—Te—NO_3 angle close to 90°. The quadrupole moment of the Te^{125} first excited state was calculated and found to be -0.19 ± 0.02 b. The energy-level positions in the I^{129} quadrupole-split spectrum was calculated for intervals of 0.1 in η up to $\eta=1$. It is shown that from the greater sensitivity of some transitions to the value of η, it is possible to get quite accurate values of η.

I. INTRODUCTION

The Mössbauer effect (ME) in the Te^{125} nucleus is the only direct means for obtaining quadrupole-coupling values from which structural information on tellurium compounds can be obtained. The nuclear quadrupole resonance (NQR) technique,[1] with which more accurate values of e^2qQ are attainable, cannot be applied in this case, since all the ground-state spins of stable Te isotopes are 0 or $\frac{1}{2}$. The Te^{125} quadrupole coupling in various Te compounds has been measured (see Violet and Booth[2] and references therein). However, because of the intrinsically broad natural linewidth of the 37.6-keV line ($2\Gamma_{\text{nat}}=6.5\times10^{-7}$ eV$=5.5$ mm/sec) relative to the characteristic quadrupole splittings ($e^2qQ/4\approx3.7$ mm/sec) of Te compounds and the usual small experimental effects, accurate values of e^2qQ are difficult to measure.

In the present work, the ME associated with the 27.8-keV transition in I^{129} has been used with Te^{129} ($\beta^-\rightarrow I^{129}$) in various compounds as sources, and an unsplit CuI^{129} absorber (Fig. 1). Because of the more favorable spectroscopic properties of the I^{129} transition compared with Te^{125}, namely, narrower linewidth, high-spin transitions, and larger experimental effects, it is possible to deduce accurate values of the I^{129} quadrupole couplings as well as the asymmetry parameter η and the sign of the electric field gradient (efg), from which structural information on Te compounds might be inferred. In order to test the validity of the use of Te^{129} sources as another means for obtaining structural information on tellurium compounds, the quadrupole-coupling values were compared with those obtained with Te^{125} as absorbers (Fig. 2). The ratio of the quadrupole coupling of the source to that of the absorber should be conserved for the compounds in which the efg is not significantly altered by the β decay. The tellurium compounds used in this experiment were Te metal, TeO_2, and $Te(NO_3)_4$.

II. EXPERIMENTAL PROCEDURE

A. Sources and Absorbers

The TeO_2 and $Te(NO_3)_4$ absorbers and sources were prepared from spectroscopic pure materials of natural Te abundance. For the tellurium metal source, samples of enriched Te^{128} were used. The Te^{129} ($T_{1/2}=70$ min) sources were produced by irradiating the samples in the form of polystyrene pellets for 1 h in a thermal neutron flux of 10^{13} n/sec cm^2. The I^{129} ($T_{1/2}=1.6\times10^7$ yr) absorber was CuI (12 mg/cm^2 of I^{129}) obtained by reducing $CuSO_4$ with Na_2SO_3 in the presence of NaI^{129} solution.[3] The Te^{125} absorbers (3 mg/cm^2 of Te^{125}) were prepared by mixing the materials with glass powder. The 10 mCi source[4] of I^{125} ($T_{1/2}=78$ day), which populates the Te^{125} Mössbauer level by electron-capture decay, was electroplated on a Cu matrix.

From x-ray diffraction it was found that the TeO_2 was in the orthorhombic phase and the tellurium metal was crystalline.

B. Cryostats and Radiation Detection

The experiments were performed in a cryostat of Styrofoam where both source and absorber were kept at 80°K. Te^{129} sources were used for a 3–4 h period, and the 25.8-keV γ radiation was detected with a 1-mm-thick NaI(Tl) scintillator attached to a 6810 RCA

---

[1] T. P. Das and E. L. Hahn, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Suppl. 1.

[2] C. E. Violet and R. Booth, Phys. Rev. **144**, 225 (1966).

[3] Purchased from Oak Ridge, Isotopes Development Center.

[4] Purchased from New England Nuclear Corporation.

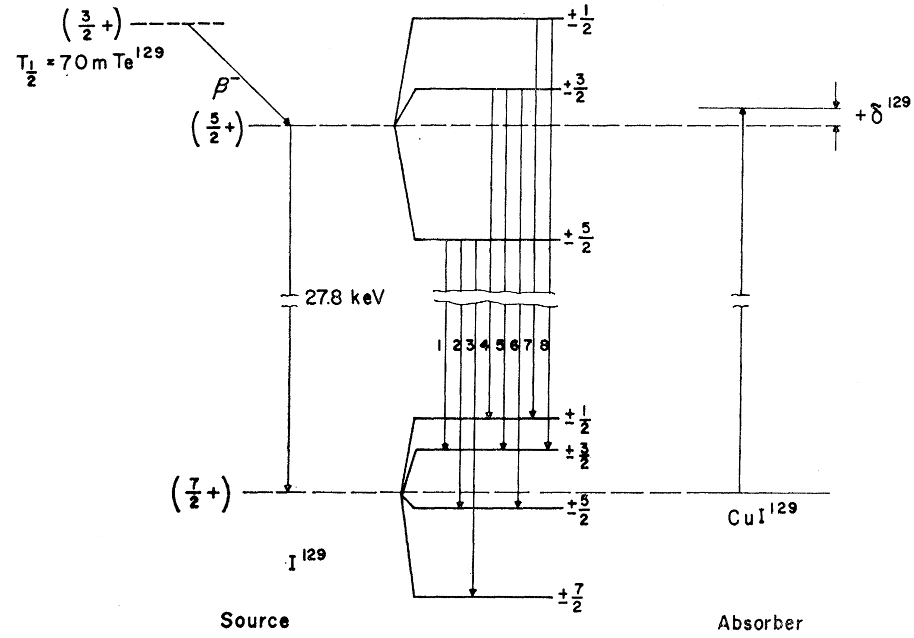

FIG. 1. Energy levels for a Te^{129} source and an I^{129} absorber. The splitting of the source levels corresponds to a negative quadrupole coupling.

photomultiplier. The 37.6-keV γ ray of the I^{125} source was analyzed with a 0.1-mm-thick NaI(Tl) scintillator by detecting its 7-keV escape peak.

The velocity system was of the constant accelerator type and the counts were stored in a 1024 CN TMC multichannel analyzer operated in the multiscaler mode.

III. EXPERIMENTAL RESULTS AND ANALYSIS OF DATA

The spectra of Te^{129}, $Te^{129}O_2$, $Te^{129}(NO_3)_4$, and $ZnTe^{129}$ sources against the CuI^{129} absorber are shown in Figs. 3–6. From the positions of the lines, the quadrupole coupling (magnitude and sign), the asymmetry parameter η, and the isomer shift δ were derived using the following relation:

$$E_{ij}=A[Rf(I^*,\, m_i^*,\, \eta)-f(I,\, m_j,\, \eta)]+\delta, \qquad (1)$$

where $A=e^2qQ_{\text{gnd}}/4$; $f(I,\, m,\, \eta)$ is related to the spin Hamiltonian eigenvalues for the case of non-axial-symmetric electric field, and R is the quadrupole moment ratio of I^{129} $(=Q_{\text{ex}}/Q_{\text{gnd}}=1.23)$.[5] The values of $f(I,\, m,\, \eta)$ have been numerically calculated by Cohen[6] for intervals of 0.1 in η. Using these values we computed the line positions E_{ij} presented in Table I. The dependence of E_{ij} on η is shown graphically in Fig. 7. We note that transitions 4 and 8 are quite sensitive to η.

From the experimental line positions, e^2qQ_{gnd} and δ were calculated using all the transitions except 4 and 8. Then by iteration, the η values were calculated from 4 and 8. Table II gives the values found for e^2qQ_{gnd}, the isomer shifts with respect to the standard ZnTe source, and η. The ground-state quadrupole coupling is expressed in terms of the quadrupole moment of the I^{127} ground state $[Q(129)/Q(125)=0.701]$, since most of the quadrupole coupling constants in iodine came from NQR measurements in I^{127}.

The spectra of $Te^{125}O_2$ and $Te^{125}(NO_3)_4$ absorbers are shown in Figs. 8 and 9 and the computed values of $e^2qQ(1+\frac{1}{3}\eta^2)^{1/2}$ are given in Table II. No measurements were made with tellurium metal absorber since this had been extensively studied.[2]

IV. DISCUSSION AND CONCLUSIONS

The electric field gradient eq_{mol} and the asymmetry parameter η are directly related to the electronic distribution in the molecule. According to Townes and

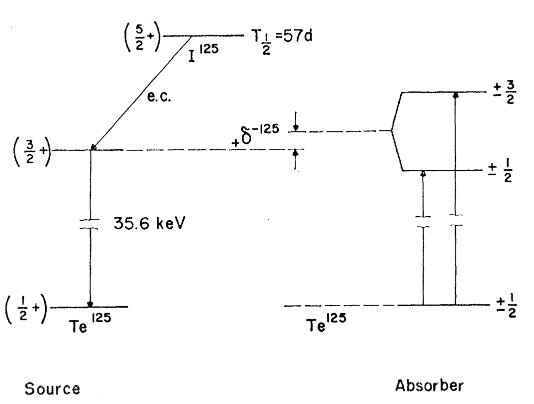

FIG. 2. Energy levels for a I^{125} source and a Te^{125} absorber. The splitting of the absorber levels corresponds to a positive quadrupole coupling.

---

[5] D. W. Hafemeister, G. De Pasquali, and H. De Waard, Phys. Rev. **135**, B1089 (1964).

[6] M. H. Cohen, Phys. Rev. **96**, 1278 (1954).

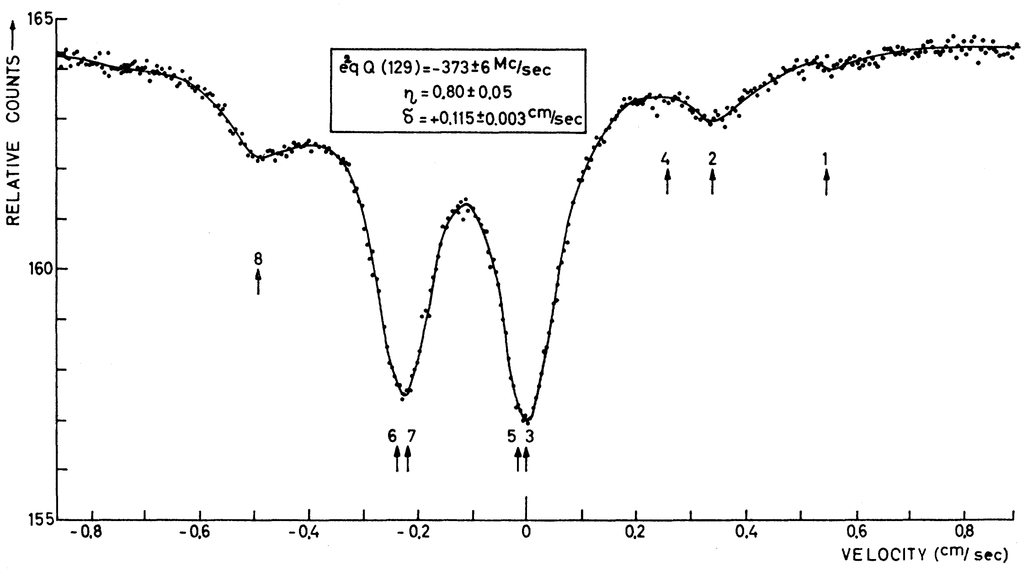

FIG. 3. Spectrum of Te^{129} (tellurium metal) source and CuI^{129} absorber at 80°K.

Dailey's theory,[7] one may express the measured eq_{mol} in the following way:

$$eq_{\text{mol}} = -U_p eq_{at} = U_p e\tfrac{4}{5}\langle 1/r^3\rangle, \tag{2}$$

where eq_{at} is defined as the efg due to the lowest p hole state in the closed shell, $\langle 1/r^3\rangle$ represents the averaging over the radial wave function, and U_p is a quantity depending on the electronic structure of the atomic environment. The quantity U_p is related to the p electron distribution in the x, y, and z direction (p_x, p_y, and p_z population) by the following expression[1]:

$$U_p = -U_z + \tfrac{1}{2}(U_x + U_y), \tag{3}$$

and η is given by

$$\eta = \frac{3}{2}\,\frac{U_x - U_y}{U_p}. \tag{4}$$

We shall use U_p and η as a probe for the structural environment of the iodine produced by the β decay of Te. To apply the information to the original Te compound we take into account that the value of $\langle 1/r^3\rangle$ will be changed as a result of the change in Z, since the averaging is now on the iodine radial wave function. Barnes and Smith[8] calculated the $\langle 1/r^3\rangle$ values of I and Te for the lowest p state, which is the main contributor to the efg, from the fine-structure data of atomic spectra. According to their calculations, the value for iodine will be larger than that of Te by approximately 20%.

A check whether the efg is changed as a result of the β decay can be made by comparing the quadrupole-coupling ratios R of the tellurium sources and absorbers. In the last column of Table II we see that for the two high ionic state compounds of Te [TeO_2 and $Te(NO_3)_4$], R is the same despite the differences in the ligands and structural properties of these compounds as revealed by the isomer shifts and asymmetry parameters. However for tellurium metal, R has a different value, showing that the efg in iodine situated in tellurium metal is considerably lower than that of the tellurium metal in the same environment.

A. Calculation of Q of the First Excited State of Te^{125}

Applying the assumption, which is supported by our experimental results, that U_p of TeO_2 and $Te(NO_3)_4$ is not changed by the nuclear transformation, one can calculate the quadrupole moment Q^{125} of the first excited state of Te^{125}. We may write the following expression for TeO_2:

$$R = 0.28 = \frac{q_{at}(\text{Te})}{q_{at}(\text{I})}\,\frac{Q^{125}}{Q^{127}}\,(1+\tfrac{1}{3}\eta^2)^{1/2}, \tag{5}$$

where Q^{127} is the quadrupole moment of the $\tfrac{5}{2}$ ground

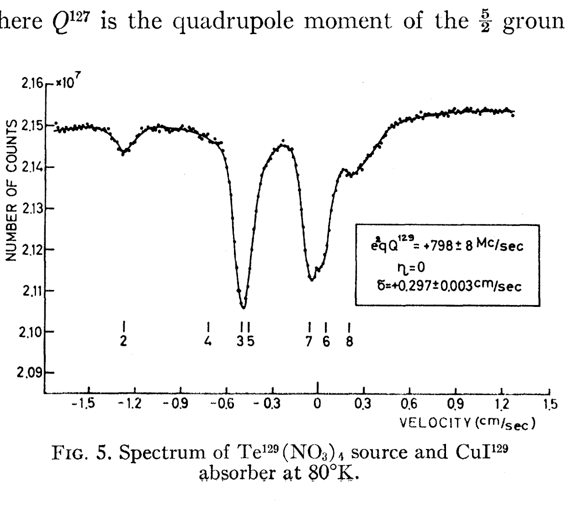

FIG. 5. Spectrum of $Te^{129}(NO_3)_4$ source and CuI^{129} absorber at 80°K.

---

[7] C. H. Townes and B. P. Dailey, J. Chem. Phys. **17**, 782 (1949).

[8] R. G. Barnes and W. V. Smith, Phys. Rev. **93**, 95 (1954).

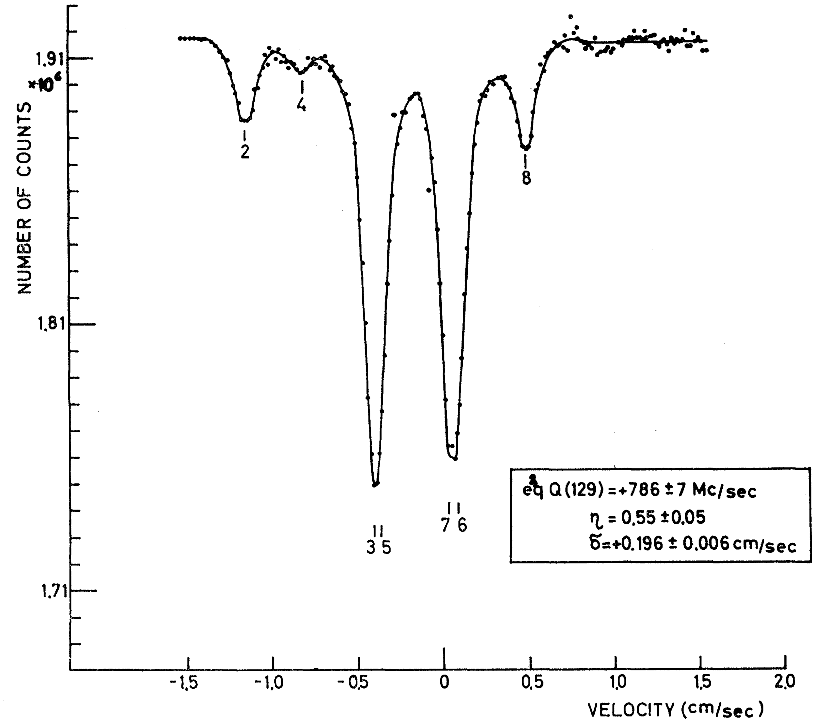

FIG. 4. Spectrum of $Te^{129}O_2$ (orthorhombic) source and CuI^{129} absorber at 80°K.

TABLE I. Energy positions of the eight transitions E_{ij} (in units of $e^2qQ/4$) in the quadrupole split spectrum of I^{129}, for values of η from 0 to 1, at intervals of 0.1. The square of the Clebsh-Gordan coefficients are given in the last line.

	Transition							
	$\frac{5}{2}\rightarrow\frac{3}{2}$	$\frac{5}{2}\rightarrow\frac{5}{2}$	$\frac{5}{2}\rightarrow\frac{7}{2}$	$\frac{3}{2}\rightarrow\frac{1}{2}$	$\frac{3}{2}\rightarrow\frac{3}{2}$	$\frac{3}{2}\rightarrow\frac{5}{2}$	$\frac{1}{2}\rightarrow\frac{1}{2}$	$\frac{1}{2}\rightarrow\frac{3}{2}$
η	1	2	3	4	5	6	7	8
0	1.654	1.087	0.230	0.469	0.178	−0.389	−0.269	−0.555
0.1	1.655	1.087	0.231	0.478	0.182	−0.386	−0.268	−0.564
0.2	1.645	1.085	0.232	0.505	0.180	−0.380	−0.264	−0.589
0.3	1.631	1.082	0.233	0.546	0.180	−0.369	−0.261	−0.627
0.4	1.616	1.079	0.236	0.600	0.183	−0.354	−0.256	−0.673
0.5	1.602	1.074	0.239	0.662	0.190	−0.338	−0.255	−0.727
0.6	1.589	1.068	0.243	0.729	0.192	−0.323	−0.254	−0.785
0.7	1.579	1.060	0.247	0.803	0.212	−0.307	−0.255	−0.846
0.8	1.573	1.052	0.253	0.877	0.228	−0.293	−0.258	−0.907
0.9	1.571	1.043	0.260	0.955	0.248	−0.280	−0.263	−0.970
1.0	1.572	1.032	0.267	0.035	0.270	−0.270	−0.267	−1.032
$\vert C.G\vert^2$	1	6	21	3	10	15	18	10

TABLE II. Experimental values of e^2qQ, η, and the isomer shift for Te^{129} sources, and $e^2qQ(1+\eta^2/3)$ for Te^{125} absorbers. The e^2qQ values of the sources are in terms of the I^{127} quadrupole moment, and the isomer shifts are with respect to the standard $ZnTe^{129}$ source. The quadrupole-coupling value for Te_2^{125} absorber was taken from Violet and Booth.[a] The last column gives the ratio R of the quadrupole couplings of the Te sources and absorbers.

	I^{129}			Te^{125}	
Compounds	$e^2qQ(127)$	η	Isomer shift (cm/sec)	$\vert e^2qQ(1+\eta^2/3)^{1/2}\vert$	R
Te_2	−532±10	0.80±0.05	+0.071±0.002	438±15	0.82
TeO_2	+1121±10	0.55±0.05	+0.152±0.001	309±10	0.28
$Te(NO_3)$	+1139±10	0	+0.252±0.001	316±10	0.28
CuI^{129}	0	0	−0.0446±0.0005		

[a] Reference 2.

state of I^{127}, which is -0.59 b,[9] the ratio $q_{at}(\mathrm{Te})/q_{at}(\mathrm{I}) = 0.85$,[8] and $\eta = 0.77$. From this we find

$$|Q^{125}| = 0.19 \pm 0.02\ b.$$

The same value, within the experimental error, is obtained from the $Te(NO_3)_4$ data.

In order to find the sign of Q^{125}, we must know the signs of e^2qQ^{125} and of the efg acting in Te^{125} (say in the case of TeO_2). To find the sign of e^2qQ^{125}, it is necessary to identify the $\frac{1}{2}\rightarrow\frac{1}{2}$ and the $\frac{3}{2}\rightarrow\frac{1}{2}$ transitions in Fig. 8. For that purpose we make use of the experimental data of Stepanov *et al.*[10] on $Te^{125}O_2$, where the experimental effect observed was larger than in our case. There it is seen that the less energetic absorption peak is stronger than the more energetic one. It has been shown[11] that in polycrystalline samples, the necessary and sufficient condition for deviation of the intensity from that predicted by the Clebsh-Gordan coefficients is anisotropy of the recoilless fraction; the intensity is not affected by such factors as the η parameter, for instance. In the case of the $Te^{129}O_2$ source (Fig. 4), where owing to the high-spin transitions it is possible to identify the various Δm transitions, we note that the peak corresponding to transition No. 2 ($\Delta m = 0$) significantly deviates from the intensity expected from the Clebsch-Gordan coefficients (see Table II). According to the latter, the ratio of peak 2 ($\Delta m = 0$) to peak 8 ($\Delta m = 1$) should be 6:10, whereas the experiment shows 7.5:10. We thus conclude that the $\Delta m = 0$ transition peaks in the $Te^{129}O_2$ source are amplified. Since we may expect that the lattice dynamics properties would not be affected after the β decay, we then identify the more intense absorption peak in Stepanov's spectrum as the $\frac{1}{2}\rightarrow\frac{1}{2}$ transition. Since this was the less energetic peak, e^2qQ^{125} is positive. The value of e^2qQ of the $Te^{129}O_2$ source is also positive, and since Q^{129} (and Q^{127}) is negative, the efg is negative, too. We finally conclude that

$$Q^{125} = -0.19 \pm 0.02\ \mathrm{b}.$$

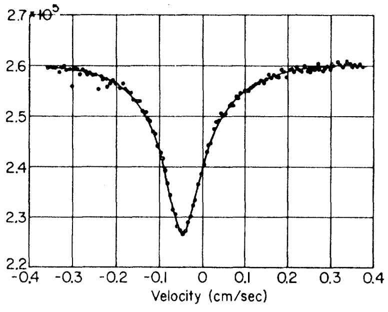

FIG. 6. Spectrum of $Zn^{66}Te^{129}$ source and CuI^{129} absorber at 80°K.

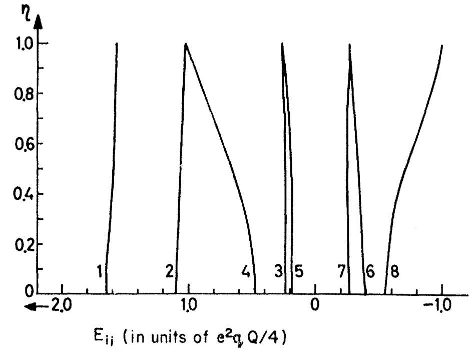

FIG. 7. Dependence of the energy positions on η.

The sign of the quadrupole moment is the same as for the odd-A nuclei in this region, extending from Sn up to Xe.[9] The value of Q^{125} is in agreement with that calculated by Violet *et al.*[12] ($|Q| = 0.20 \pm 0.03$) from the quadrupole coupling of Te^{125} metal, where they assumed *sp* hybridization of the covalent bond and calculated U_p from the bonding angle.

B. Chemical Structures

1. TeO_2

The quadrupole coupling of iodine in the Te position is larger than the values obtained for the iodate salts,[13] where e^2qQ ranges from 960 to 1000 Mc/sec. In the IO_3^- salts, the η parameter is very close to zero, which is consistent with their molecular structure—a regular tripyramid where the iodine is bound to three oxygens making OIO angles close to 90°. However, the values of e^2qQ and η obtained for the $Te^{129}O_2$ source are very similar to those for HIO_3 as measured by Livingston and Zeldes[14] by the NQR method. Their values for e^2qQ and η are 1126.6 Mc/sec and 0.47, respectively. HIO_3 lacks the threefold symmetry of the iodate salts, because one of the IO bonds is longer than the other two, and its structure may fit with that of SeO_2. The SeO_2 crystal is composed of chains, with the O-Se-O angle very close to 90° (see Fig. 10 [15]). The coordination number of Se is three, the third oxygen completing a tripyramid but with the third bond longer than those of the two bridging oxygens. We suggest the same structure for TeO_2. The isomer shift for TeO_2 is the

---

[9] G. H. Fuller and V. W. Cohen, *Nuclear Data Sheets*, compiled by K. Way *et al.* (Printing and Publishing Office, National Academy of Sciences-National Research Council Washington 25, D.C., 1965) Appendix I, p. 10.

[10] E. P. Stepanov, K. P. Aleshin, R. A. Manapov, B. N Samoilov, V. V. Sklyarevsky, and V. G. Stankevich, Phys. Letters **6**, 155 (1963).

[11] (a) V. I. Goldanskii, G. M. Gorodinski, S. V. Karyagin, L. A. Koryfko, L. M. Kryzhanski, and E. F. Suzdalov, Dokl. Akad. Nauk. SSSR **147**, 127 (1962). (b) P. Zory, Phys. Rev. **140**, A1401 (1965). (c) S. V. Karyagin, Dokl. Akad. Nauk SSSR **148**, 1102 (1963).

[12] C. E. Violet, R. Booth, and F. Wooten, Phys. Letters **5**, 230 (1963).

[13] E. C. Segel and R. G. Barnes, U.S. Atomic Energy Commission Report No. 520, 1962 (unpublished).

[14] R. Livingston and H. Zeldes, J. Chem. Phys. **26**, 351 (1957).

[15] W. Hückel, *Structural Chemistry of Inorganic Compounds* (Elsevier Publishing Co., New York, 1951), Vol. II, p. 483.

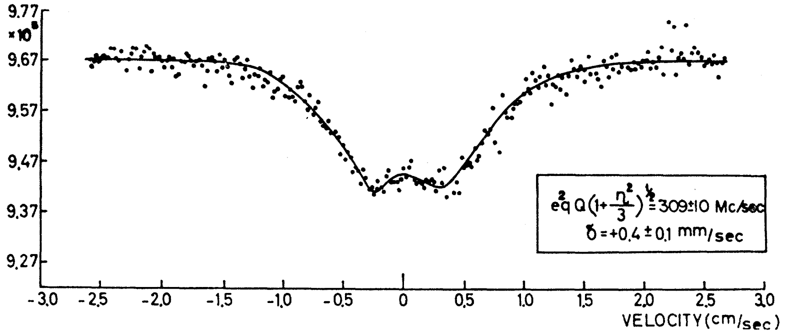

FIG. 8. Spectrum of $Te^{125}O_2$ (orthorhombic) absorber and I^{125} source electroplated on a Cu matrix, at 80°K.

same as that obtained for the KIO_3 [5] absorber, supporting the 90° angle of the O–Te–O bond.

The "Karyagin-Goldanskii" effect[11] observed in TeO_2, where the $\Delta m=0$ transitions are enhanced, shows that the recoilless fraction is anisotropic and in such a direction that the mean-square displacement perpendicular to the electric field axis[16,17] (which is in turn perpendicular to the plane formed by the three oxygens) is smaller than in the parallel direction. The "stiffening" of the mean-square displacement is thus in the direction of the Te–O bonds, suggesting again that TeO_2 has a chain structure similar to that of SeO_2.

The quadrupole-coupling value obtained for the $Te^{125}O_2$ orthorhombic phase absorber ($e^2qQ=309$ Mc/sec) is less than that found by Violet and Booth[2] for the tetragonal phase ($e^2qQ=415$ Mc/sec).

2. $Te(NO_3)_4$

No information is available in the literature on the structure of $Te(NO_3)_4$, but we may extract some data concerning the Te environment from the results obtained with the $Te^{129}(NO_3)_4$ source. We note the following:

(i) The efg is negative, which shows that the bonding is chiefly by p_x and p_y electrons.

(ii) The η parameter is zero, which points to a three- or fourfold symmetry.

(iii) The isomer shift with respect to ZnTe is positive and large, larger than that obtained for $Te^{129}O_2$.

(iv) From the line intensities no anisotropy is apparent in the recoilless fraction.

The positive and large value of the isomer shift shows that the bonding is chiefly by p electrons, thus the angle between the Te and the ligands will be close to 90°. From the relation between the isomer shift and the number of p holes (h_p) in the $5s^25p^6$ configuration,[18] namely,

$$\delta=0.136h_p-0.054\ (\text{cm/sec}), \qquad (3)$$

we find that h_p is 2.25. Therefore the iodine configuration will be $5s^25p^{3.75}$. If the coordination number of $Te(NO_3)_4$ is three, it means that of the $1.25e^-$ charge removed from the iodine, $0.41e^-$ may be attributed to each nitrate ligand. This is close to the values found in an earlier experiment[17] on ICl and I_2Cl_6 where it was deduced that $0.49e^-$ is removed from the I to each Cl.

The molecular structure is probably a pyramid with equal bond lengths ($\eta=0$), where the Te is situated at the top. If the structure were planar, the "lone pair" of electrons would produce a quadrupole coupling larger than that of the atomic iodine (2296 Mc/sec). The isotropic recoilless fraction does not sup-

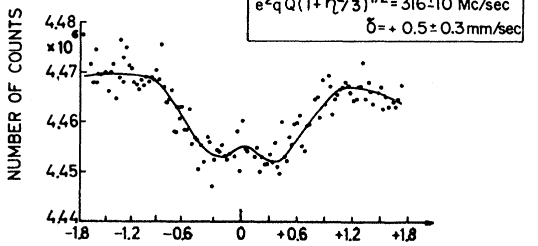

FIG. 9. Spectrum of $Te^{125}(NO_3)_4$ absorber and I^{125} source at 80°K.

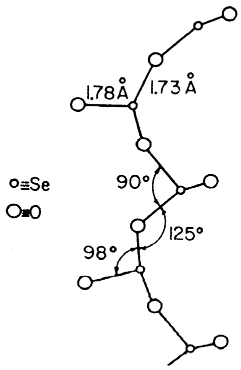

FIG. 10. Structure of SeO_2 chains.

---

[16] M. Pasternak, Israel Atomic Energy Commission Report No. IA-1106, 1966 (unpublished).

[17] M. Pasternak, thesis, 1966 (unpublished).

[18] M. Pasternak, A. Simopoulos, and Y. Hazoni Phys. Rev. 140, A1892 (1965).

port a chain structure as in the case of TeO_2 and tellurium metal.

3. Tellurium Metal

The efg in the iodine nucleus in Te metal is markedly less than that in the Te nucleus in the same environment (see Table II). This can be seen quantitatively from the values of $U_p(\mathrm{Te})$ and $U_p(\mathrm{I})$ which characterize the respective electronic distributions. The values of U_p were calculated from expression (1)

$$U_p = e^2q_{\mathrm{mol}}Q/e^2q_{\mathrm{at}}Q, \tag{4}$$

where the atomic quadrupole coupling of Te^{125} (537±40 Mc/sec) was calculated from the $\langle 1/r^3 \rangle$ data of Ref. 8 and from Q of the first excited state. From the e^2qQ values of Te^{125} and I^{127} given in Table II, we find that $|U_p(\mathrm{Te})| = 0.81$ and $U_p(\mathrm{I}) = +0.23$.

This reduction of U_p in iodine might be due to one of the following reasons: (a) highly ionic character of the I–Te bond, (b) a large *sp* hybridization fraction, and (c) considerable participation of p_x and p_y electrons in the bond (π bonding). The latter seems the most likely, the first two possibilities being readily excluded, as follows. (a) The observed isomer shift of 0.071 cm/sec is near to that obtained for molecular I_2 (see Ref. 18) (0.083 cm/sec). From relation (3) we find that $h_p = 0.92$, so that the iodine configuration will be $5s^2 5p^{5.08}$. This small ionicity ($I = 0.08$) is consistent with the small electronegativity difference between Te and I (see Ref. 19). (b) If *sp* hybridization occurred, the isomer shift would be markedly decreased, since the effect of *s* density on the I^{129} isomer shift is appreciably higher than and of opposite direction to that of the *p* density.[5] Also, the absence of *sp* hybridization is consistent with the positive value of $U_p(\mathrm{I})$, which suggests σ bonding along the I–Te1 axis (see Fig. 11). This implies that the iodine is bound chiefly to one Te atom. If the iodine were equally bound to both Te atoms (for instance by "bond switching") U_p would be negative and, because of the 103° angle, *sp* hybridization would be required.[20]

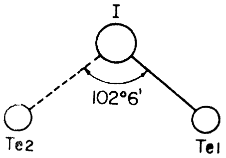

FIG. 11. The nearest Te neighbors of iodine. The main bonding is with Te1 (see text).

The large value of the asymmetry parameter, resulting from the interference of the neighboring Te atom, which breaks the cylindrical symmetry of the σ bond, suggests that a considerable I–Te2 bond is present. From the h_p η and U_p values we may calculate the *p* electron density at the iodine in the *z* (i.e., I–Te1), *y* (i.e., I–Te2), and *x* directions according to the following relations:

$$\eta = \tfrac{3}{2}(U_x - U_y)/U_p = 0.80,$$

$$U_p = -U_z + \tfrac{1}{2}(U_x + U_y) = 0.23,$$

$$h_p = 6 - (U_z + U_x + U_y) = 0.92. \tag{5}$$

From this set of equations we find the following values: $U_z = 1.54$, $U_y = 1.71$, and $U_x = 1.83$. From these results we conclude that the iodine atom (in the I^- state) is not bound to the two Te atoms in equal proportions but mainly to one of them (Te1). We note the importance of the isomer-shift data (h_p) without which the above information on the electron population distribution would not be deduced. We therefore conclude that the low value of $U_p(\mathrm{I})$ as compared with $U_p(\mathrm{Te})$ is due to the large fraction of π bonding involved in the I–Te1 bond.

As in the case of TeO_2, the tellurium metal spectrum (Fig. 3) suggests that the recoilless fraction is anisotropic. Here, too, absorption peak 2 ($\Delta m = 0$) is enhanced compared with peak 8, which points to a smaller mean-square displacement perpendicular to the I–Te1 direction. This property may be in the Te1-I-Te2 plane or perpendicular to it. The spectrum of Te^{125} metal, as measured by Stepanov *et al.*,[10] shows that the higher-energy absorption peak is enhanced. Since the quadrupole coupling of Te^{125} metal is positive, it means that the enhanced peak is the $\frac{3}{2} \rightarrow \frac{1}{2}$ ($\Delta m = 1$) transition, or the mean-square displacement perpendicular to the Te1–I–Te2 plane is smaller than that in the plane.

ACKNOWLEDGMENTS

We wish to thank S. Philippakis for carrying out the x-ray diffraction measurements and A. Simopoulos for valuable discussions.

---

[19] L. Pauling, *The Nature of the Chemical Bond*, (Cornell University Press, Ithaca, New York, 1963), 3rd ed.

[20] See Ref. 1, p. 141.