Lawrence Berkeley National Laboratory

Recent Work

Title

DETERMINATION OF STRUCTURE BY ISOTOPIC SUBSTITUTION IN MOLECULES WITH SYMMETRICALLY EQUIVALENT ATOMS

Permalink

<https://escholarship.org/uc/item/31t3r76v>

Author

Chutjian, Ara.

Publication Date

1964-04-01

University of California

Ernest O. Lawrence
Radiation Laboratory

DETERMINATION OF STRUCTURE BY ISOTOPIC SUBSTITUTION IN
MOLECULES WITH SYMMETRICALLY EQUIVALENT ATOMS

TWO-WEEK LOAN COPY

*This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 5545*

Berkeley, California

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Rept. sub. for pub. in the
Journal of Molecular Spectros-
copy.

UCRL-11230

UNIVERSITY OF CALIFORNIA
Lawrence Radiation Laboratory
Berkeley, California
AEC Contract No. W-7405-eng-48

DETERMINATION OF STRUCTURE BY ISOTOPIC SUBSTITUTION IN
MOLECULES WITH SYMMETRICALLY EQUIVALENT ATOMS

Ara Chutjian

April 1964

DETERMINATION OF STRUCTURE BY ISOTOPIC SUBSTITUTION IN
MOLECULES WITH SYMMETRICALLY EQUIVALENT ATOMS*

Ara Chutjian†

Department of Chemistry and Inorganic Materials
Research Division, Lawrence Radiation
Laboratory, University of California
Berkeley, California

April 1964

ABSTRACT

Kraitchman's well-known equations relate changes in moments of inertia upon single isotopic substitution to the location of the substituted atom. These relations are here extended to the case of multiple isotopic substitution on a set of symmetrically equivalent atoms.

*Support received from the U. S. Atomic Energy Commission is gratefully acknowledged.

†National Science Foundation Predoctoral Fellow, 1962-64.

DETERMINATION OF STRUCTURE BY ISOTOPIC SUBSTITUTIONS IN
MOLECULES WITH SYMMETRICALLY EQUIVALENT ATOMS

Ara Chutjian

List of Symbols Used

μ	Greek mu	(lower case)
ω	Greek omega	"
Δ	Greek delta	(upper case)
Σ	Greek sigma	"
χ	Script X	
ψ	Script Y	
σ	Greek sigma	(lower case)

The determination of molecular structure from isotopic substitutions of single atoms in a molecule may be conveniently carried out by means of relations formulated by Kraitchman (1). His approach may be extended to provide simple relations applicable to multiple isotopic substitutions of symmetrically equivalent nuclei for cases in which the whole molecule has, for example, S_{nv} or C_{nv} symmetry. This extended treatment will be useful since it is easier experimentally to prepare compounds in which all of the equivalent nuclei have been substituted, rather than a number less than the full set.

Many polatomic molecules have nuclei which are transformed into one another under the symmetry operations of the molecular point group (2). One may generate all these equivalent nuclei by first assigning coordinates to one of the set, and then performing the necessary reflections and rotations (proper and improper) linking this "chosen" atom to the others. Thus, the two hydrogen atoms in water are equivalent under the C_2 rotation and σ_v reflections; and the six hydrogens in staggered ethane are related by the S_6 rotation-reflection operation. Also, it can be shown from the character table of the point group exactly which moments and products of inertia will not be affected by the substitution.

COORDINATE SYSTEM

We may use Kraitchman's method of defining an arbitrary coordinate system for the substituted molecule, while still making calculations with respect to the center of mass of the parent molecule. If we let r_1 represent the distance of the i^{th} atom from the arbitrary origin, r_1^0 its distance from the center of mass of the parent molecule, and $\bar{r}$ the distance of the center of mass from the origin, then $r_1 = r_1^0 + \bar{r}$.

In the center-of-mass system, the inertia tensor is

$$\underline{I}^{\circ} = \sum m_i (r_i^{\circ 2} \underline{1} - \underline{r}_i \underline{r}_i) \quad (1)$$

where $\underline{1}$ is the unit dyad

$$\underline{1} = \begin{pmatrix} 11 & 0 & 0 \\ 0 & jj & 0 \\ 0 & 0 & kk \end{pmatrix}.$$

If we write $\underline{r}_i^{\circ} = \underline{r}_i - \underline{r}$, let M be the mass of the parent molecule, and use the center-of-mass relations $\sum m_i \underline{r}_i / M = \underline{r}$, and $\sum m_i \underline{r}_i^{\circ} = 0$, then $\underline{I}^{\circ}$ can be expressed in the arbitrary coordinate system as

$$\underline{I}^{\circ} = \sum m_i (r_i^2 \underline{1} - \underline{r}_i \underline{r}_i) - (1/M) [(\sum m_i \underline{r}_i) \cdot (\sum m_i \underline{r}_i) \underline{1} - (\sum m_i \underline{r}_i)(\sum m_i \underline{r}_i)]$$

which has elements

$$I_{xx}^{\circ} = \sum m_i (y_i^2 + z_i^2) - (\sum m_i y_i)^2 / M - (\sum m_i z_i)^2 / M \quad (2a)$$

$$I_{xy}^{\circ} = - \sum m_i x_i y_i + (\sum m_i x_i)(\sum m_i y_i) / M, \text{ etc.} \quad (2b)$$

In the trivial case in which the arbitrary origin is the center of mass, only the first terms in I_{xx} , I_{xy} , etc., remain, and we have the usual form given by Eq. (1).

If we have chosen the principal axes of the parent molecule, the inertia tensor will be diagonal, with the principal moments of inertia about the three axes along the diagonal. In the most general case, isotopic substitution will cause a net translation and rotation of the parent principal axes corresponding to different diagonal elements, and the introduction of off-diagonal products of inertia.

A simplification results however, in that we obtain non-zero changes only for those tensor elements which belong to the totally symmetric representations. That is, the inertial ellipsoids of both the parent and the substituted molecule must be unaffected by the group operations of the molecule, so no tensor elements can be introduced into the inertia tensor of the substituted molecule which change sign under any of the symmetry operations. Since, for the simple examples shown here, at most only one of the products xy , xz and yz transform as the symmetric representation (in the C_{2h} point group), only one plane described by the principal axes of the parent molecule may be rotated by substitutions, and we need diagonalize only a 2×2 tensor to get the new principal axes of the substituted molecule.

Also, since the inertial ellipsoid has the same symmetry as the nuclear framework, certain symmetry axes of the molecule will be principal axes of the ellipsoid, and certain planes of symmetry will contain two axes of the ellipsoid (3). This will enable us to equate certain coordinates of our "chosen" atom to zero since it will lie on one (or more) of the principal axes. These and further points will be illustrated in the examples that follow.

For notation, we will denote the coordinates (referred to the center of mass of the parent molecule) and mass of the isotopic atom as (x,y,z) and $m + \Delta m$ respectively, where m is the mass of the parent atom. Since the bond lengths will be constant in our treatment, the sums in Eqs. (2a) and (2b) will run over the coordinates and masses of the parent molecule whose moments of inertia are denoted by I_x , etc., and over the mass differences Δm and coordinates (x,y,z) of the isotopes in the substituted

molecules, whose moments of inertia are referred to as I'_x , etc.

NUCLEI RELATED BY C_N ROTATIONS

If N atoms are related by an N -fold proper rotation C_N , we may choose the z -axis, say, as the axis of rotation and assign the coordinates of the "chosen" atom as (x, y, z) . In this case, the coordinates of the k th atom of the equivalent set are, letting $k\omega = 2\pi k/N$,

$$\begin{pmatrix} x_k \\ y_k \\ z_k \end{pmatrix} = \begin{pmatrix} \cos k\omega & -\sin k\omega & 0 \\ \sin k\omega & \cos k\omega & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

and the differences $I'_x - I_x = \Delta I_{xx}$ in the moments of inertia become

$$\begin{aligned} \Delta I_{xx} = \Delta m x^2 \sum_{k=1}^N \sin^2 k\omega + 2\Delta m xy \sum \sin k\omega \cos k\omega \\ + \Delta m y^2 \sum \cos^2 k\omega + \mu_N z^2. \end{aligned} \quad (3a)$$

Here we have used the fact that $\sum y_k = 0$, $\sum z_k = Nz$ since only z transforms as A_1 , and the abbreviation $\mu_N = M(N\Delta m)/(M + N\Delta m)$.

Likewise,

$$\begin{aligned} \Delta I_{yy} = \Delta m x^2 \sum \cos^2 k\omega - 2\Delta m xy \sum \cos k\omega \sin k\omega \\ + \Delta m y^2 \sum \sin^2 k\omega + \mu_N z^2 \end{aligned} \quad (3b)$$

$$\Delta I_{zz} = N\Delta m (x^2 + y^2) \quad (3c)$$

For the products of inertia, we have the relation $\sum x_k = 0$, and thus

$$\Delta I_{xy} = -(\Delta m/2)(x^2 - y^2) \sum \sin 2k\omega - \Delta m xy \sum \cos 2k\omega \quad (3d)$$

$$\Delta I_{xz} = -\Delta m xz \sum \cos k\omega + \Delta m yz \sum \sin k\omega \quad (3e)$$

$$\Delta I_{yz} = -\Delta m xz \sum \sin k\omega - \Delta m yz \sum \cos k\omega \quad (3f)$$

If the molecule is planar, then one of the principal axes will be perpendicular to the plane, and one of the coordinates of the chosen atom will be zero. If the out-of-plane axis is the z-axis, then many of the terms in Eqs. (3a) to (3f) will be zero, and we get the familiar result that $\Delta I_{zz} = \Delta I_{xx} + \Delta I_{yy}$.

NUCLEI RELATED BY S_N ROTATIONS

If the nuclei are related by an improper rotation operation where the plane of reflection is perpendicular to the N-field rotation axis (again taken to be the z-axis), then the k th equivalent atom has coordinates

$$\begin{pmatrix} x_k \\ y_k \\ z_k \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & (-1)^k \end{pmatrix} \begin{pmatrix} \cos k\omega & -\sin k\omega & 0 \\ \sin k\omega & \cos k\omega & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$= \begin{pmatrix} x \cos k\omega - y \sin k\omega \\ x \sin k\omega + y \cos k\omega \\ (-1)^k z \end{pmatrix}$$

This differs from the C_n case in the inversion of the z coordinate for alternate atoms during the reflection operation.

We will not make the assumption here that $\sum x_k = \sum y_k = 0$, but will retain these terms in the expressions for ΔI_{xx} , etc., so that we have

$$\Delta I_{xx} = \Delta m \sum_k x_k^2 \sin^2 k\omega + 2\Delta mxy \sum_k \sin k\omega \cos k\omega + \Delta my^2 \sum_k \cos^2 k\omega$$

$$+ N\Delta mz^2 - ((\Delta m)^2/M + N\Delta m) \left[\left(\sum_k y_k \right)^2 + z^2 \left(\sum_k (-1)^k \right)^2 \right] \quad (4a)$$

$$\Delta I_{yy} = \Delta mx^2 \sum_k \cos^2 k\omega - 2\Delta mxy \sum_k \sin k\omega \cos k\omega + \Delta my^2 \sum_k \sin^2 k\omega$$

$$+ N\Delta mz^2 - ((\Delta m)^2/M + N\Delta m) \left[\left(\sum_k x_k \right)^2 + z^2 \left(\sum_k (-1)^k \right)^2 \right] \quad (4b)$$

$$\Delta I_{zz} = N\Delta m(x^2 + y^2) - ((\Delta m)^2/M + N\Delta m) \left[(\Sigma x_k)^2 + (\Sigma y_k)^2 \right] \quad (4c)$$

$$\Delta I_{xy} = -(\Delta m/2)(x^2 - y^2) \Sigma \sin 2k\omega - \Delta mxy \Sigma \cos 2k\omega + ((\Delta m)^2/M + N\Delta m) \left[(\Sigma x_k)(\Sigma y_k) \right] \quad (4d)$$

$$\Delta I_{xz} = \Delta mxz \Sigma (-1)^k \cos k\omega + \Delta myz \Sigma (-1)^k \sin k\omega + ((\Delta m)^2/M + N\Delta m) \left[(\Sigma x_k)(\Sigma z_k) \right] \quad (4e)$$

$$\Delta I_{yz} = -\Delta mxz \Sigma (-1)^k \sin k\omega - \Delta myz \Sigma (-1)^k \cos k\omega + ((\Delta m)^2/M + N\Delta m) \left[(\Sigma y_k)(\Sigma z_k) \right] \quad (4f)$$

EXAMPLES WITH C_N ROTATIONAL SYMMETRY

WX_2 Molecules, C_{2v} Group

Atoms 1 and 2 in Fig. 1 are related by the C_2 rotation about the z-axis and if we assign the coordinates of atom 1 as $(x, 0, z)$, then from Eqs. (3a), (3b) and (3c), we get

$$\Delta I_{xx} = \mu_2 z^2$$

$$\Delta I_{zz} = 2\Delta mx^2$$

$$\Delta I_{yy} = 2\Delta mx^2 + \mu_2 z^2 = \Delta I_{xx} + \Delta I_{zz}$$

All of the products of inertia are zero, as can be seen either by explicit substitution in Eqs. (3d), (3e) and (3f), or from the fact that none of the products xy , xz , or yz transforms as A_1 .

The coordinates of atom 1 are then

$$x^2 = \frac{1}{2\Delta m} \Delta I_{zz}$$

$$z^2 = \frac{1}{\mu_2} (\Delta I_{yy} - \Delta I_{zz}) = \frac{1}{\mu_2} (\Delta I_{xx})$$

Only the square of the coordinates can be obtained, and the sign to be given them must be determined through other structural information.

WXY₃ Molecules, C_{3v} Group

Here we can make use of the fact that the molecule has a σ_v plane through one of the three symmetrically equivalent nuclei and the W-X bond. This plane must then contain two of the principal axis, and the third must be perpendicular to it. If we take the z axis along the W-X bond, and have atom 1 lie in the xz plane, then its coordinates will be (x,0,z)(see Fig.2).

The tensor elements are then

$$\Delta I_{xx} = \frac{3}{2} \Delta m x^2 + \mu_3 z^2$$

$$\Delta I_{yy} = \frac{3}{2} \Delta m x^2 + \mu_3 z^2 = \Delta I_{xx}$$

$$\Delta I_{zz} = 3 \Delta m x^2$$

$$\Delta I_{xy} = \Delta I_{xz} = \Delta I_{yz} = 0$$

So that

$$x^2 = \frac{1}{3\Delta m} \Delta I_{zz}$$

$$z^2 = \mu_3^{-1} \left(\Delta I_{xx} - \frac{\Delta I_{zz}}{2} \right)$$

were the rotor actually planar, then z = 0, and we would get

$$\Delta I_{zz} = 3\Delta m x^2 = \Delta I_{xx} + \Delta I_{yy}.$$

X₆ Molecules, D_{6h} Group

The z axis is taken along the C₆ rotational axis, and the y and x axes lie in the σ_h plane and are directed along the C'₂ and C''₂ symmetry axes (or, alternatively, the yz and xz planes form the σ_d and σ_v reflection planes, respectively). The coordinates of the generating atom then become

(0,y,0) as shown in Fig. 3, and we get

$$\Delta I_{xx} = \Delta I_{yy} = 3\Delta m y^2$$

$$\Delta I_{zz} = \Delta I_{xx} + \Delta I_{yy} = 6\Delta m y^2$$

$$\Delta I_{xy} = \Delta I_{xz} = \Delta I_{yz} = 0$$

and so

$$y^2 = \frac{1}{3\Delta m} (\Delta I_{xx})$$

EXAMPLES WITH S_N ROTATIONAL SYMMETRY

Formaldehyde, C_s Group

Formaldehyde illustrates the case where two equivalent protons are related by a reflection operation. In this configuration, the COH group lies in the reflection plane, otherwise the molecule would have no symmetry at all. The coordinates of atom 1 in Fig. 4 are taken as (x,y,z), and those of atom 2 are just (x,y,-z).

In this point group, both x and y transform as A' , as well as xy (which introduces the ΔI_{xy} correction), and we find from Eqs. (4),

$$\Delta I_{xx} = \mu_2(y^2 + z^2) + (4(\Delta m)^2/M + 2\Delta m)z^2 = \mu_2 y^2 + 2\Delta m z^2$$

$$\Delta I_{yy} = \mu_2(x^2 + z^2) + (4(\Delta m)^2/M + 2\Delta m)z^2 = \mu_2 x^2 + 2\Delta m z^2$$

$$\Delta I_{zz} = \mu_2(x^2 + y^2)$$

$$\Delta I_{xy} = -\mu_2 xy$$

$$\Delta I_{yz} = \Delta I_{xz} = 0$$

The inertia tensor now has off-diagonal elements, and is given by

$$\begin{pmatrix} I'_x & 0 \\ & I'_y \\ 0 & I'_z \end{pmatrix} = \begin{pmatrix} I_x + \mu_2 y^2 + 2\Delta m z^2 & -\mu_2 xy & 0 \\ -\mu_2 xy & I_y + \mu_2 x^2 + 2\Delta m z^2 & 0 \\ 0 & 0 & I_z + \mu_2 (x^2 + y^2) \end{pmatrix}$$

The z element is diagonal, and we have immediately that

$$x^2 + y^2 = \mu_2^{-1} (\Delta I_{zz}) \quad (5)$$

We can diagonalize the 2 X 2 submatrix by noting that both the trace and determinant of the tensors must be invariant under the similarity transformation, so that, letting $\chi = I_x + 2\Delta m z^2$ and $y = I_y + 2\Delta m z^2$, we get

$$I'_x + I'_y = \chi + y + \mu_2 (x^2 + y^2) \quad (6)$$

$$I'_x I'_y = (\chi + 2\Delta m z^2)(y + 2\Delta m z^2) - \mu_2^2 x^2 y^2 \quad (7)$$

From Eqs. (5) and (6), we get

$$z^2 = \frac{1}{4\Delta m} (\Delta I_{xx} + \Delta I_{yy} - \Delta I_{zz}).$$

And using this result in Eq. (7), we have that

$$x^2 = \frac{I'_x I'_y - \chi y - y \Delta I_{zz}}{\mu_2 (I'_x - I'_y)};$$

$$y^2 = \frac{I'_x I'_y - \chi y - \chi \Delta I_{zz}}{\mu_2 (I'_y - I'_x)}$$

$W_{22}X_2Y_2$ Molecules, C_{2h} Group

This class of molecules includes the planar trans-disubstituted ethylenes, as shown in Fig. 5. Atoms 1-2, 3-4, and 5-6 are all equivalent pairs. None of the coordinates transform as A_g , and xy is the only

off-diagonal product that belongs to this representation. The z-axis is taken out of the plane of the molecule, and the reflection σ_h is the xy plane.

Since atoms 1 and 2 are related by the S_2 (inversion) operation, we can assign the coordinates to 1 as (x,y,0) and get

$$\Delta I_{xx} = 2\Delta m y^2$$

$$\Delta I_{yy} = 2\Delta m x^2$$

$$\Delta I_{zz} = 2\Delta m(x^2 + y^2) = \Delta I_{xx} + \Delta I_{yy}$$

$$\Delta I_{xy} = -2\Delta m xy$$

$$\Delta I_{xz} = \Delta I_{yz} = 0$$

so we have

$$I = \begin{pmatrix} I_x + 2\Delta m y^2 & -2\Delta m xy & 0 \\ -2\Delta m xy & I_y + 2\Delta m x^2 & 0 \\ 0 & 0 & I_z + 2\Delta m(x^2 + y^2) \end{pmatrix}$$

Diagonalizing the 2 X 2 submatrix as before, we find that

$$y^2 = \left(\frac{1}{2\Delta m}\right) \frac{(I'_x - I_y)(I'_y - I_y)}{I_x - I_y}$$

$$y^2 = \left(\frac{1}{2\Delta m}\right) \frac{(I'_x - I_x)(I'_y - I_x)}{I_y - I_x}$$

X_2Y_6 Molecules, D_{3d} Group

This symmetry class is that for staggered ethane, and if we orient the z-axis along the S_6 rotational axis, and the y axis so that the chosen atom 1 lies in the xz plane, we get

$$\Delta I_{xx} = 3\Delta m(x^2 + 2z^2) = \Delta I_{yy}$$

$$\Delta I_{zz} = 6 \Delta m x^2$$

$$\Delta I_{xy} = \Delta I_{xz} = \Delta I_{yz} = 0$$

Thus

$$z^2 = \frac{1}{6\Delta m} (\Delta I_{yy} - \Delta I_{zz}/2),$$

$$x^2 = \frac{1}{6\Delta m} (\Delta I_{zz}).$$

The results of these six examples are conveniently summarized in Table I according to the number of equivalent atoms and the symmetry point group.

Table I - SUMMARY OF RESULTS FOR MULTIPLE SUBSTITUTIONS^a

N	Symmetry	Type	ΔI_{xx}	ΔI_{yy}	ΔI_{zz}	ΔI_{xy}
2	C_{2v}	WX_z	$\mu_2 z^2$	$\Delta I_{xx} + \Delta I_{zz}$	$2\Delta m x^2$	0
3	C_{3v}	WXY_3	$\frac{3}{2} \Delta m x^2 + \mu_3 z^2$	ΔI_{xx}	$3\Delta m x^2$	0
6	D_{6h}	X_6	$3\Delta m y^2$	ΔI_{xx}	$2\Delta I_{xx}$	0
2	C_s	CH_3CHO	$\mu_2 y^2 + 2\Delta m z^2$	$\mu_2 x^2 + 2\Delta m z^2$	$\mu_2 (x^2 + y^2)$	$-\mu_2 xy$
2	C_{2h}	$W_2X_2Y_2$	$2\Delta m y^2$	$2\Delta m x^2$	$\Delta I_{xx} + \Delta I_{yy}$	$-2\Delta m xy$
6	D_{3d}	X_2Y_6	$3\Delta m (x^2 + 2z^2)$	ΔI_{xx}	$6\Delta m x^2$	0

^a Δm is the mass difference in the isotopes, and $\mu_N = \frac{M(N\Delta m)}{M + N\Delta m}$.

The axes are as defined in the text and M is the total mass of the molecule in each case.

ACKNOWLEDGMENT

The author is very grateful to Dr.D.R. Herschbach for suggesting the problem and for making many helpful comments. This work was performed under the auspices of the U. S. Atomic Energy Commission.

REFERENCES

1. K. Kraitichman, Am. J. Phys., 21, 17 (1953).
2. G. Herzberg, Infrared and Raman Spectra, p. 131., Van Nostrand, Princeton, New Jersey, 1945.
3. Ibid., p. 13.

FIGURE CAPTIONS

- Fig. 1 WX_2 Configuration of C_2 Symmetry
- Fig. 2 WXY_3 Configuration of C_{3v} Symmetry. The z-axis is the C_3 Rotation Axis.
- Fig. 3 Benzene-like X_6 Configuration of D_{6h} Symmetry
- Fig. 4 Configuration of Formaldehyde. The COH Group lies in the σ_h symmetry plane passing through atom 3.
- Fig. 5 C_{2h} Configuration. Atoms 1, 2 and 3, 4 are related by the S_2 operation.
- Fig. 6 Staggered Ethane Configuration of D_{3d} Symmetry.

MU - 33746

Fig. 1.

MU-33747

Fig. 2.

MU - 33748

Fig. 3.

MU-33749

Fig. 4.

MU-33750

Fig. 5.

MU-33751

Fig. 6.

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

- A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or
- B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.