
THE PREDICTION OF VALENCE FORCE CONSTANTS AND VIBRATION FREQUENCIES FOR $XY_6(O_h)$ MOLECULES, USING THE EFFECTIVE NUCLEAR CHARGE MODEL

Manuel FERNÁNDEZ-GÓMEZ, Juan J. LÓPEZ-GONZÁLES
and Manuel MARTÍNEZ-SÁNCHEZ

*Department of Physical-Chemistry, University of Granada,
University College Santo Reino, 23071 Jaen, Spain*

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Ohwada's effective nuclear charge model has been extended to the calculation of valence force constants for $XY_6(O_h)$ molecules. To achieve this the potential energy function has had to be expressed in terms of independent force constants for which it has been necessary to eliminate the *gem*- and *tree*-redundancies that exist between the displacement coordinates. The vibration frequencies predicted by the use of these constants agree well in general with experimental observations.

The calculation of valence force constants by empirical means falls short due to the difficulty in obtaining sufficient experimental data (vibration frequencies, isotopic shifts, Coriolis zeta constants, *etc.*) and in like manner a mathematical approach to the problem, which calls for the expression of complicated wavefunctions, makes it equally difficult to obtain *a priori* constants values. For these reasons it is commonly accepted that a simple and general model, capable of predicting reliable force constants in polyatomic molecules, is highly desirable.

To this end Ken Ohwada, in a recent publication¹, has put forward a semi-empirical model for the calculation of valence force constants in polyatomic molecules, which he calls the effective nuclear charge model (ENCM). The model has been applied to various molecular structures: bent and linear XY_2 (refs^{1,2}), pyramidal XY_3 (ref.³), tetrahedral XY_4 (ref.⁴), pseudo-tetrahedral XY_3Z (ref.⁵), planar XY_2Z (ref.⁶), and to some complex ions of tetrahedral symmetry⁷ and of D_{4h} and D_{5h} symmetry⁸. The aim of this present work is to extend the application of the model to neutral octahedral XY_6 molecules.

THEORETICAL

Expression of the Potential Energy Function for XY_6 Molecules

Ohwada has constructed his model¹ by making use of the Hellmann and Feynman's theorem^{9,10} and also by separating the electronic density function into two terms,

one for the electrons which adhere closely to the movements of the nucleus and one for those that move more freely¹¹. The resulting intramolecular potential function can be expressed as

$$V = \sum_{i \neq j} \frac{Z_i^* Z_j^*}{R_{ij}} + \sum_{j \neq k} \frac{Z_j^* Z_k^*}{q_{jk}} - N(r, R), \quad (1)$$

where Z_i^* and Z_j^* represent the effective nuclear charges defined from the expressions for the force constants of homonuclear, diatomic molecules derived from the second-order perturbation theory¹², R_{ij} and q_{jk} are the distances between bonded atoms and adjacent but not directly bonded atoms, respectively, and $N(r, R)$ is the energy of the electrons that do not follow the movement of the nucleus closely.

In order to obtain the expressions for the force constants as a function of the effective nuclear charges, Eq. (1) is expanded in a power series so that, if the second order contribution of the term $N(r, R)$ is disregarded, we obtain the expression for the potential

$$V = V_0 - \sum_{i \neq j} \left[\frac{Z_i^* Z_j^*}{R_{ij}^3} + \frac{1}{R_{ij}} \left(\frac{\partial N}{\partial R_{ij}} \right)_0 \right] (R_{ij} \Delta R_{ij}) + \frac{1}{2} \sum_{i \neq j} \left(\frac{2Z_i^* Z_j^*}{R_{ij}^3} \right) (\Delta R_{ij})^2 - \\ - \sum_{j \neq k} \left(\frac{Z_j^* Z_k^*}{q_{jk}^3} \right) (q_{jk} \Delta q_{jk}) + \frac{1}{2} \sum_{j \neq k} \left(\frac{2Z_j^* Z_k^*}{q_{jk}^3} \right) (\Delta q_{jk})^2 + \dots \quad (2)$$

Some of the linear terms in Eq. (2) can be got rid of if we take into account the *gem*-redundancy relationship¹³ that exists between Δq_{jk} and ΔR_{ij} and ΔR_{jk} , given by the general expression

$$\Delta q_{jk} = s_{jik} \Delta R_{ij} + s_{kij} \Delta R_{ik} + (t_{jik} t_{kij} R_{ij} R_{ik})^{1/2} \Delta \Phi_{jk} + \\ + [t_{jik} (\Delta R_{ij})^2 + t_{kij} (\Delta R_{ik})^2 - s_{jik} s_{kij} R_{ij} R_{ik} (\Delta \Phi_{jk})^2 - \\ - 2t_{jik} t_{kij} (\Delta R_{ij}) (\Delta R_{ik}) + 2t_{jik} s_{kij} (\Delta R_{ij}) (R_{ik} \Delta \Phi_{jk}) + \\ + 2t_{kij} s_{jik} (\Delta R_{ik}) (R_{ij} \Delta \Phi_{jk})] / 2q_{jk}, \quad (3)$$

where

$$s_{jik} = (R_{ij} - R_{ik} \cos \Phi_{jk}) / q_{jk} \quad (4a)$$

$$s_{kij} = (R_{ik} - R_{ij} \cos \Phi_{jk}) / q_{jk} \quad (4b)$$

$$t_{jik} = R_{ij} \sin \Phi_{jk} / q_{jk} \quad (4c)$$

$$t_{kij} = R_{ik} \sin \Phi_{jk} / q_{jk}. \quad (4d)$$

For an octahedral molecule, such as that shown in Fig. 1, the equilibrium distances, q_{jk} , are $2R$ or $(2)^{1/2} R$, depending upon whether the atoms in question are collinear

or not. In the former case the value of the parameters s_{jik} and t_{kij} are 1 and 0, respectively and in the latter case both parameters have the same value, $(2)^{-1/2}$. Thus the *gem*-redundancy can be expressed in the following two equations

$$\Delta q_{jk} = (\Delta R_{ij} + \Delta R_{ik}) - (R \Delta \Phi_{jk}^2)/4 \quad (5a)$$

$$\Delta q_{jk} = (2)^{-1/2} (\Delta R_{ij} + \Delta R_{ik} + R \Delta \Phi_{jk}) + (2)^{-1/2} (\Delta R_{ij}^2 + \Delta R_{ik}^2 - R^2 (\Delta \Phi_{jk})^2 - 2 \Delta R_{ij} \Delta R_{ik} + 2R \Delta R_{ij} \Delta \Phi_{jk} + 2R \Delta R_{ik} \Delta \Phi_{jk})/4R \quad (5b)$$

for collinear and non-collinear atoms, respectively.

If Eqs (5a) and (5b) are introduced into Eq. (2), without using any terms of higher order than the quadratic, because we are treating the vibration as being harmonic, then the potential function can be expressed as

$$\begin{aligned} V = V_0 - \sum_i \left[\frac{Z^* Z_i^*}{R^2} - \frac{(2)^{1/2} Z^{*2}}{R^2} + \left(\frac{\partial N}{\partial R_i} \right)_0 \right] (\Delta R_i) - \sum_{i,j \neq \pi} \frac{Z^{*2}}{2(2)^{1/2} R} (\Delta \Phi_{ij}) + \\ + \frac{1}{2} \sum_i \left(\frac{2Z^* Z_i^*}{R^3} + \frac{Z^{*2}}{(2)^{1/2} R^3} + \frac{Z^{*2}}{4R^3} \right) (\Delta R_i)^2 + \frac{1}{2} \sum_{i,j \neq \pi} \frac{3Z^{*2}}{4(2)^{1/2} R} (\Delta \Phi_{ij})^2 + \\ + \sum_{\substack{i < j \\ \text{non-} \\ \text{collinear}}} \frac{3Z^{*2}}{4(2)^{1/2} R^3} (\Delta R_i) (\Delta R_j) + \sum_{\substack{i < j \\ \text{collinear}}} \frac{Z^{*2}}{4R^3} (\Delta R_i) (\Delta R_j) + \\ + \sum_{i,j \neq \pi} \frac{Z^{*2}}{4(2)^{1/2} R^2} (\Delta R_i) (\Delta \Phi_{ij}), \end{aligned} \quad (6)$$

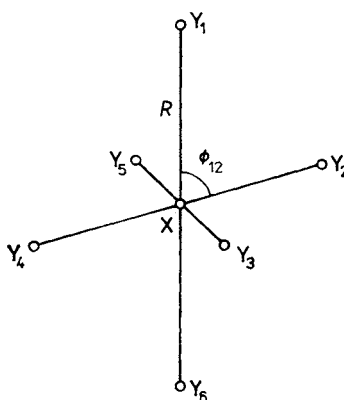


FIG. 1

Spatial arrangement of the atoms and internal coordinates for an octahedral $XY_6(O_h)$ molecule

where Z^* and Z_1^* represent the effective nuclear charges of the peripheral and central atoms, respectively, and the subindices refer to the peripheral atoms involved in the corresponding displacement coordinates.

The introduction of Eqs (5a) and (5b) into Eq. (6) provides a series of linear terms representing angular deformations, between which *tree*-redundancies must exist¹³, as is always the case when the atom is bonded at four or more sites. We have obtained the explicit form of these *tree*-redundancy relationships¹⁶ by generalising the method proposed by Cihla and Plíva¹⁴ and Califano¹⁵ in such a way as to respect the equivalence which, for reasons of symmetry, must exist between the various different interbond angles. The resulting expression for the octahedral XY_6 molecules is

$$\begin{aligned}
 & 2(\Delta\Phi_{12} + \Delta\Phi_{13} + \Delta\Phi_{14} + \Delta\Phi_{15} + \Delta\Phi_{23} + \Delta\Phi_{25} + \Delta\Phi_{26} + \Delta\Phi_{34} + \\
 & \quad + \Delta\Phi_{36} + \Delta\Phi_{45} + \Delta\Phi_{46} + \Delta\Phi_{56}) + (\Delta\Phi_{12} \Delta\Phi_{13} + \Delta\Phi_{12} \Delta\Phi_{15} + \\
 & \quad + \Delta\Phi_{12} \Delta\Phi_{23} + \Delta\Phi_{12} \Delta\Phi_{25} + \Delta\Phi_{13} \Delta\Phi_{14} + \Delta\Phi_{13} \Delta\Phi_{23} + \Delta\Phi_{13} \Delta\Phi_{34} + \\
 & \quad + \Delta\Phi_{14} \Delta\Phi_{15} + \Delta\Phi_{14} \Delta\Phi_{34} + \Delta\Phi_{14} \Delta\Phi_{45} + \Delta\Phi_{15} \Delta\Phi_{25} + \Delta\Phi_{15} \Delta\Phi_{45} + \\
 & \quad + \Delta\Phi_{23} \Delta\Phi_{26} + \Delta\Phi_{23} \Delta\Phi_{36} + \Delta\Phi_{25} \Delta\Phi_{26} + \Delta\Phi_{25} \Delta\Phi_{56} + \Delta\Phi_{26} \Delta\Phi_{36} + \\
 & \quad + \Delta\Phi_{26} \Delta\Phi_{56} + \Delta\Phi_{34} \Delta\Phi_{36} + \Delta\Phi_{34} \Delta\Phi_{46} + \Delta\Phi_{36} \Delta\Phi_{46} + \Delta\Phi_{45} \Delta\Phi_{46} + \\
 & \quad + \Delta\Phi_{45} \Delta\Phi_{56} + \Delta\Phi_{46} \Delta\Phi_{56}) = 0. \quad (7)
 \end{aligned}$$

Using an undetermined Lagrange multiplier, Eq. (7) can be introduced into Eq. (6), a process which eliminates all the dependence relationships that exist among the displacement coordinates and thus gets rid of the linear terms in Eq. (6). In this particular case the undetermined Lagrange multiplier, or intramolecular tension parameter¹⁷, is given as

$$k = Z^{*2}/4(2)^{1/2} R. \quad (8)$$

So, the potential function of Eq. (6) can be written as

$$\begin{aligned}
 V = V_0 + \frac{1}{2} \sum_i \left(\frac{2Z^*Z_1^*}{R^3} + \frac{Z^{*2}}{(2)^{1/2} R^3} + \frac{Z^{*2}}{4R^3} \right) (\Delta R_i)^2 + \frac{1}{2} \sum_{i,j \neq \pi} \frac{3Z^{*2}}{4(2)^{1/2} R} (\Delta\Phi_{ij})^2 + \\
 + \sum_{\substack{i < j \\ \text{non-} \\ \text{-collinear}}} \frac{3Z^{*2}}{4(2)^{1/2} R^3} (\Delta R_i) (\Delta R_j) + \sum_{\substack{i < j \\ \text{collinear}}} \frac{Z^{*2}}{4R^3} (\Delta R_i) (\Delta R_j) + \\
 + \sum_{i,j \neq \pi} \frac{Z^{*2}}{4(2)^{1/2} R^2} (\Delta R_i) (\Delta\Phi_{ij}) + \sum \frac{Z^{*2}}{4(2)^{1/2} R} (\Delta\Phi_{ij}) (\Delta\Phi_{ki}), \quad (9)
 \end{aligned}$$

where the last sum is the second term of Eq. (7).

It is worth emphasising that, as a result of the introduction of the *gem*- and *tree*-redundancies, the potential function of Eq. (2), becomes, in Eq. (9), an almost general valence function.

Expression and Evaluation of Valence Force Constants

From the potential function as expressed in Eq. (9) it is a simple step to arrive at the explicit expressions for the valence force constants as described below.

Bond Stretching,

$$f_r = \frac{2Z^*Z_1^*}{R^3} + \frac{Z^{*2}}{(2)^{1/2}R^3} + \frac{Z^{*2}}{4R^3} \quad (10a)$$

Angle Deformation,

$$f_\phi = \frac{3Z^{*2}}{4(2)^{1/2}R} \quad (10b)$$

Stretch–Stretch interaction,
(non-collinear bonds)

$$f_{rr} = \frac{3Z^{*2}}{4(2)^{1/2}R^3} \quad (10c)$$

Stretch–Stretch interaction,
(collinear bonds)

$$f'_{rr} = \frac{Z^{*2}}{4R^3} \quad (10d)$$

Stretch–Deformation interaction,
(angles other than π)

$$f_{r\phi} = \frac{Z^{*2}}{4(2)^{1/2}R^2} \quad (10e)$$

Deformation–Deformation interaction,
(as shown by Eq. (9))

$$f_{\phi\phi} = \frac{Z^{*2}}{4(2)^{1/2}R} \quad (10f)$$

To calculate the valence force constants by means of these expressions it is necessary to introduce the values for the equilibrium lengths of the bonds, R , of the polyatomic molecules in question, and the effective nuclear charges, Z^* , calculated beforehand by using the force constants of homonuclear diatomic molecules.

If the effective nuclear charges are originally expressed in elementary units (eu) and the equilibrium bond lengths in angstroms (Å), then Eqs (10a–10f) have to be multiplied by the conversion factor $2.3097 \text{ mdyn } \text{Å}^2 (\text{eu})^{-2}$ and as a result the force constants f_r , f_{rr} , and f'_{rr} will be expressed in $\text{mdyn } \text{Å}^{-1}$, the constants f_ϕ and $f_{\phi\phi}$ in $\text{mdyn } \text{Å}$ and $f_{r\phi}$ in mdyn , or, if preferred all the constants can be expressed in terms of $\text{mdyn } \text{Å}^{-1}$ if they are put into scale by using the equilibrium distance, R ($1 \text{ Å} = 10^{-10} \text{ m}$; $1 \text{ Nm}^{-1} = 10^{-2} \text{ mdyn } \text{Å}^{-1}$).

In this study we have applied the ENCM to several specific octahedral molecules, *i.e.* the hexafluorides of sulphur, selenium, tellurium, molybdenum, and wolfram. In order to arrive at an approximation of the effective nuclear charges of these elements we used the data pertaining to the corresponding homonuclear diatomic molecules¹⁸, except in the cases of wolfram and molybdenum, which were calculated from the crystal compressibility¹⁹. The resulting effective nuclear charges are shown in Table I, together with the corrected values used to achieve a better adjustment between the predicted and the experimental results, which appear alongside in brackets. With these effective nuclear charges calculated it is now possible to reach a value for the valence force constants, according to Eqs (10a–10f) and these appear in Table II.

The equilibrium distances for SF_6 have been taken from Brunet and Perez²⁰, for SeF_6 from Bartell and Jin²¹, for TeF_6 from Abramowitz and Levin²², and for MoF_6 and WF_6 from Seip and Seip²³.

Calculation of Frequencies

In order to obtain the vibration frequencies from the calculated force constants we followed Wilson's **GF** method²⁴, taking the symmetrized elements of the **G** and **F**

TABLE I
Effective nuclear charges

Element	Z^* , eu ^a
F	1.69 (1.38)
S	2.69 (2.62)
Se	2.76 (3.10)
Te	2.89 (4.32)
Mo	3.00 (5.57)
W	3.20 (6.06)

^a $1 \text{ eu} = 3.33564 \cdot 10^{-10} \text{ C}$.

matrices from Nakamoto²⁵, the numerical values of which are shown in Tables III and IV, respectively.

Once the numerical values for the \mathbf{F} and \mathbf{G} matrices have been obtained, the frequencies can then be calculated by means of the roots of the secular determinant $|\mathbf{GF} - E\lambda| = 0$.

The vibration frequencies thus arrived at, together with the experimental frequencies, are shown in Table V.

The experimental values for SeF_6 , for the A_{1g} and E_g modes of SF_6 and TeF_6 , and for the T_{2g} and T_{2u} modes of TeF_6 have been taken from Bosworth, Clark, and Rippon²⁶, while the values for the T_{1u} and T_{2u} modes of SF_6 and TeF_6 and the T_{2g} and T_{2u} modes of SF_6 are provided by Claassen, Goodman, Holloway, and Selig²⁷, and the data concerning MoF_6 and WF_6 come from McDowell, Shermann, Asprey, and Kennedy²⁸ and McDowell and Asprey²⁹, respectively.

As can be seen, the agreement between the calculated and the experimental values is generally quite acceptable qualitatively and even on occasions quantitatively.

CONCLUSION

As our results show the ENCM provides a useful means of calculating an initial reliable series of valence force constants relying, in principle, only upon strictly geometrical data concerning the polyatomic molecule. These force constants can then be used as input in an iterative refinement process, such as those described in the literature, refs^{30,31} for example, designed to lead to an acceptable fitting with the experimentally observed frequencies.

As Ohwada has commented¹, the reasons for the imperfect fitting of our calculated values to the experimental ones may be due to the disregard for the contribution of the $N(r, R)$ term to the force constants values, to the poor transferability of

TABLE II
Valence force constants (in $\text{mdyn } \text{\AA}^{-1}$)^a for XY_6 molecules

Molecule	$R, \text{\AA}$	f_r	f_{rr}	f'_{rr}	f_ϕ	$f_{\phi\phi}$	$f_{r\phi}$
SF_6	1.58	5.30	0.59	0.28	0.59	0.20	0.20
SeF_6	1.68	5.01	0.49	0.23	0.49	0.16	0.16
TeF_6	1.84	5.10	0.37	0.17	0.37	0.12	0.12
MoF_6	1.82	4.94	0.23	0.11	0.23	0.08	0.08
WF_6	1.83	5.23	0.22	0.11	0.22	0.07	0.07

^a 1 $\text{mdyn} = 10^{-8}$ N, 1 $\text{\AA} = 10^{-10}$ m.

TABLE III

The symmetrized elements of the **G** matrix (in amu⁻¹)

Molecule	μ_x^a amu ⁻¹	$G(A_{1g})$	$G(E_g)$	$G_{11}(T_{1u})$	$G_{12}(T_{1u})$	$G_{22}(T_{1u})$	$G(T_{2g})$	$G(T_{2u})$
SF ₆	0.03118	0.05264	0.05264	0.11501	-0.12475	0.35477	0.21054	0.10527
SeF ₆	0.01266	0.05264	0.05264	0.07797	-0.05066	0.20659	0.21054	0.10527
TeF ₆	0.00784	0.05264	0.05264	0.06331	-0.03135	0.16797	0.21054	0.10527
MoF ₆	0.01042	0.05264	0.05264	0.07348	-0.04169	0.18865	0.21054	0.10527
WF ₆	0.00544	0.05264	0.05264	0.06351	-0.02175	0.14878	0.21054	0.10527

^a $\mu_y = 0.05264 \text{ amu}^{-1}$, $1 \text{ amu} = 1.66043 \cdot 10^{-27} \text{ kg}$. μ_x and μ_y represent the inverse of the atomic masses of the central and peripheral elements, respectively.

TABLE IV

The symmetrized elements of the **F** matrix (in m dyn Å⁻¹)

Molecule	$F(A_{1g})$	$F(E_g)$	$F_{11}(T_{1u})$	$F_{12}(T_{1u})$	$F_{22}(T_{1u})$	$F(T_{2g})$	$F(T_{2u})$
SF ₆	7.94	4.39	5.02	0.40	0.99	0.59	0.19
SeF ₆	7.19	4.27	4.78	0.32	0.81	0.49	0.17
TeF ₆	6.77	4.53	4.92	0.24	0.61	0.37	0.13
MoF ₆	5.96	4.59	4.83	0.16	0.39	0.23	0.07
WF ₆	6.23	4.39	5.13	0.14	0.36	0.22	0.08

TABLE V

Calculated and observed (in brackets) frequencies (in cm⁻¹)

Vibration	SF ₆	SeF ₆	TeF ₆	MoF ₆	WF ₆
$\nu_1(A_{1g})$	842 (774)	801 (708)	778 (697)	729 (741)	746 (772)
$\nu_2(E_g)$	626 (642)	617 (658)	636 (671)	640 (652)	641 (678)
$\nu_3(T_{1u})$	1 042 (939)	791 (778)	748 (752)	772 (741)	739 (712)
$\nu_4(T_{1u})$	566 (614)	485 (436)	403 (325)	326 (264)	299 (252)
$\nu_5(T_{2g})$	459 (525)	417 (402)	365 (312)	285 (318)	283 (320)
$\nu_6(T_{2u})^a$	188 (347)	171 (263)	150 (201)	116 (117)	115 (128)

^a Experimental values estimated from overtone transitions.

the effective nuclear charges from the diatomic to the polyatomic molecule, and to a slight uncertainty concerning the observed frequencies.

For these reasons we believe that the calculated results might be improved upon if the effective nuclear charges were obtained in a more reliable way, such as, for example, by using Mulliken's population analysis³². Nevertheless, despite these limitations, we believe that the effective nuclear charge model is a simple, general, and reasonable manner of calculating valence force constants.

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