CROATICA CHEMICA ACTA CCACAA **63** (1) 79—86 (1990)

CCA-1922

YU ISSN 0011-1643
UDC 548.312
Original Scientific Paper

Description of Molecular Distortions III. Trigonally-Planar XY_3 Molecules

Kostadin Trenčevski

Institute of Mathematics, Faculty of Science, Cyril and Methodius University, Skopje, Yugoslavia

and

*Vladimir Petruševski**

Institute of Chemistry, Faculty of Science, Cyril and Methodius University, Skopje, Yugoslavia

Received May 18, 1988

Second-rank tensors were used to calculate the degree of distortion for the NO_3 ions in a number of crystalline compounds. All NO_3 ions appear to be strictly planar, as found in a previous study[1]. A significant correlation, between the main components of the tensor and the wavenumbers of the components of the antisymmetric stretching vibration (ν_3) of the NO_3 ion, was found.

INTRODUCTION

In previous studies[2,3] two independent methods for the description of distortions of tetrahedral molecules were introduced. The possible advantages of these two methods over the existing ones[4-8] were then discussed.

The method of Baur[4] can be easily extended to trigonally-planar XY_3 molecules. The same can be done with the method of Murray-Rust *et al.*[5-7]. We have calculated the distortions of about 40 NO_3 ions[1] using these two methods. Unfortunately, neither the distortion indices[4] nor the displacent vectors[5-7] could be correlated with the frequencies** of the components of the antisymmetric stretching vibrations of the nitrate ions. Therefore, in this work we made an attempt to correlate spectroscopic and crystallographic data, by the method introduced previously[2].

MATHEMATICAL METHOD

As the method was described in detail elsewhere[2], only a brief summary of the general ideas will be given here. Let us, first, consider an XY_3-type molecule. The following notation is used:

---

* to whom correspondence should be addressed

** Frequencies of NO_3 stretchings, even for non-distorted ions, depend on N—O distances; hence, a »compressed« NO_3 ion should show higher stretching frequencies, compared with the values obtained for a »free« ion.

$$\overrightarrow{XY}_1 = \mathbf{p} = \{p_1, p_2, p_3\}$$
$$\overrightarrow{XY}_2 = \mathbf{q} = \{q_1, q_2, q_3\}$$
$$\overrightarrow{XY}_3 = \mathbf{s} = \{s_1, s_2, s_3\}$$
$$T_{ij} = \sum_{i,j} p_i \cdot p_j / |p|^\delta + q_i \cdot q_j / |q|^\delta + s_i \cdot s_j / |s|^\delta \qquad i, j \in \{1, 2, 3\} \tag{1}$$

The right-hand side of equation (1) is a tensorial quantity. In other words, a tensor defined by equation (1) may be adjoined to a molecule. Quantity δ is a constant; its value was fixed at 12[2], assuming that the behaviour of the covalent and overlap forces (*i. e.* their dependence on the interatomic distance) is analogous. The strong repulsion of the atoms — typical of noble gases, due to overlap forces — may be understood as a result of »antibonding«. As the atoms move towards each other, electrons are forced to fill up antibonding orbitals of the forming »molecule«, a simple consequence of the Pauli exclusion rule. On the other hand, when a bonding between two atoms is chemically favourable, one can explain it, similarly, as a result of filling-up bonding orbitals. Hence, the covalent and the overlap forces may be viewed (to a first approximation) as forces of common origin, but different sign. Alternatively, δ may be treated as an empirical constant[2].

Several different situations may occur:

a) The XY_3 molecule has exactly D_{3h} symmetry. In this case, the tensor is diagonal, with $T_{11} = T_{22}$; $T_{33} = 0$. This tensor defines a circular cylinder.

b) Let the XY_3 molecule have C_{3v} symmetry. The tensor is diagonal with $T_{11} = T_{22} \neq T_{33}$. This tensor defines an ellipsoid of revolution.

c) Let the molecule be planar with C_s symmetry. By diagonalization, one obtains $T'_{11} \neq T'_{22}$; $T'_{33} = 0$. This tensor defines elliptical cylinder (the same holds for planar molecules with C_1 site-symmetry; primes are used to denote the principal values of the tensor, after diagonalization).

d) Let, finally, the symmetry of the molecule be C_1 (*i. e.* the molecule has no symmetry at all). Again, by diagonalization one obtains: $T'_{11} \neq T'_{22} \neq \neq T'_{33}$ and the tensor defines an ellipsoid with three different axes. The same result is obtained for bent XY_3 molecules with C_s symmetry.

Departure of the XY_3 molecule from complanarity is determined by the value of T'_{33}, *i. e.* the condition $T'_{33} > 0$ has to be fulfilled for non-planar molecules. On the other hand, the departure from threefold symmetry is determined by $|T'_{11} - T'_{22}| > 0$.

It seems reasonable* to define the distortion of the molecules (NO_3^- ions — in this study) in the following way:

$$D_t = (1 - b/a)^2 \tag{2}$$

Quantity D_t in the above equation is the distortion of the molecule, $a^2 = 1/T'_{11}$ and $b^2 = 1/T'_{22}$ (a and b are chosen so that $a > b$). In fact, a and b are the semi-major axes of the ellipsoid (the elliptical cylinder, in this case) defined by tensor T_{ij}. Distortion D_t defined as above, is scaled between 0 and 1.

---

* Almost all ions (the only exception is the NO_3 ion in the structure of $Cd(NO_3)_2 \cdot 4H_2O$) are very strictly planar, since $T'_{33} = 0$. This finding is in agreement with our earlier results[1] obtained by different methods.

Some special types of small distortions are discussed in Appendix 1. The corresponding equations for approximate calculations of D_t in these special cases are also derived.

RESULTS AND DISCUSSION

In this study, 35 nitrate ions in different crystalline compounds were investigated. The results are presented in Table I. This Table also contains the values for distortion indices[4] and displacement vectors[7] which are given for comparison. For most of the studied compounds, there is a correspondence between the distortions obtained by the three methods. A detailed analysis of such and similar correlations will be published in a separate paper. This paper deals only with the spectra-structural correlations.

TABLE I

Distortions of NO_3^- ions. Results obtained by various methods

Compound	DI(NO)	DI(ONO)	DI(OO)	D_3(E)/Å	D_4(E)/°	$Dt \cdot 10^5$	Ref.
NO_3^- free	0.0000	0.0000	0.0000	0.0000	0.000	0	9
$NaNO_3$	0.0000	0.0000	0.0000	0.0000	0.000	0	10
NH_4NO_3(III)	0.0011	0.0025	0.0010	0.0024	0.551	16	11
KNO_3	0.0018	0.0010	0.0003	0.0042	0.230	25	12
$Al(NO_3)_3 \cdot 9D_2O''$	0.0034	0.0016	0.0020	0.0082	0.360	73	13
$Al(NO_3)_3 \cdot 9D_2O'''$	0.0064	0.0050	0.0061	0.0149	1.251	160	13
$AgNO_3$(I)	0.0067	0.0053	0.0064	0.0152	1.326	176	14
$LiNO_3 \cdot 3H_2O$	0.0073	0.0115	0.0032	0.0167	2.535	520	15
$Al(NO_3)_3 \cdot 9D_2O'$	0.0093	0.0080	0.0012	0.0220	1.959	683	13
$Mg(NO_3)_2 \cdot 2H_2O$	0.0097	0.0101	0.0063	0.0253	2.388	736	16
$Hg(OH)NO_3$	0.0111	0.0060	0.0019	0.0269	1.411	931	17
$Ce(NO_3)_3 \cdot 6H_2O'$	0.0090	0.0186	0.0069	0.0229	4.287	1094	18
NH_4NO_3(IV)	0.0160	0.0003	0.0078	0.0364	0.063	1133	19
$UO_2(NO_3)_2 \cdot 6H_2O''$	0.0103	0.0242	0.0098	0.0237	5.340	1323	20
$Ca(NO_3)_2 \cdot 4H_2O'$	0.0128	0.0106	0.0006	0.0316	2.603	1396	21
$Ce(NO_3)_3 \cdot 6H_2O''$	0.0127	0.0145	0.0026	0.0310	3.213	1461	18
$Ni(NO_3)_2 \cdot 2H_2O$	0.0149	0.0113	0.0039	0.0350	2.634	1646	22
$La(NO_3)_3 \cdot 6H_2O'$	0.0133	0.0204	0.0059	0.0337	4.658	1914	23
$La(NO_3)_3 \cdot 6H_2O''$	0.0153	0.0152	0.0021	0.0356	3.512	1924	23
$Ca(NO_3)_2 \cdot 4H_2O''$	0.0128	0.0225	0.0079	0.0327	5.420	1937	21
$Co(NO_3)_2 \cdot 2H_2O$	0.0148	0.0206	0.0053	0.0343	4.537	1987	24
$La(NO_3)_3 \cdot 6H_2O'''$	0.0167	0.0157	0.0035	0.0427	3.555	2322	23
$Cd(NO_3)_2 \cdot 4H_2O$	0.0147	0.0566	0.0308	0.0342	12.689	2880	25
$Ni(NO_3)_2 \cdot 4H_2O'$	0.0235	0.0207	0.0038	0.0542	4.732	3382	26
$Ni(NO_3)_2 \cdot 4H_2O''$	0.0235	0.0203	0.0025	0.0547	4.486	3410	26
$Th(NO_3)_4 \cdot 5H_2O'$	0.0212	0.0270	0.0062	0.0505	6.036	3926	27
$Ce(NO_3)_3) \cdot 6H_2O'''$	0.0235	0.0214	0.0026	0.0542	4.862	4161	18
$UO_2(NO_3)_2 \cdot 6H_2O'$	0.0224	0.0303	0.0077	0.0515	6.673	4261	20
$Th(NO_3)_4 \cdot 5H_2O''$	0.0233	0.0313	0.0079	0.0540	6.910	4607	27
$Sn(NO_3)_4''$	0.0301	0.0381	0.0090	0.0696	8.404	7104	28
$Sn(NO_3)_4'$	0.0358	0.0418	0.0086	0.0825	9.266	9420	28
$LiNO_3$	0.0365	0.0409	0.0076	0.0856	9.009	9642	29
$Sn(NO_3)_4''''$	0.0419	0.0453	0.0078	0.0972	10.196	12296	28
$Sn(NO_3)_4'''$	0.0452	0.0481	0.0086	0.1056	10.603	13763	28
NO_2^+ in N_2O_5	1.3333	0.3333	0.6667	∞	73.485	100000	30

In the study of the sulfate-ion distortions[2], a highly significant correlation between the main components (eigenvalues) of the tensor and the components of the antisymmetric stretching vibration (ν_3) was found. It was assumed that a similar correlation should exist in the case of nitrate-ion too. In order to check this assumption, 67 pairs of data (cf. Table II) were included in the

TABLE II

Pairs of T'_{ii} — ν_3 *data, included in the regression*

Compound	T'_{ii}/Å^{-10}	ν/cm^{-1}	Ref.
NO_3^- »free«	0.1674	1390	31
	0.1674	1390	
$NaNO_3$	0.1715	1395	32
	0.1715	1395	
NH_4NO_3(III)	0.1743	1378^a	33
	0.1787	1412^a	
KNO_3	0.1653	1345	34
	0.1705	1361	
	0.1521	1327^b	
	0.1638	1334^b	
$Al(NO_3)_3 \cdot 9D_2O$	0.1693	1355^b	35
	0.1730	1385^b	
	0.1808	1392^b	
	0.1837	1425^b	
$AgNO_3$(I)	0.1645	1320^c	36
	0.1792	1382^c	
$LiNO_3 \cdot 3H_2O$	0.1540	1332	32
	0.1789	1416	
$Mg(NO_3)_2 \cdot 2H_2O$	0.1406	1334	37
	0.1682	1460	
Hg((OH)NO_3	0.1478	1305	38
	0.1810	1396	
	0.1346	1350^d	
	0.1477	1350^d	
$Ce(NO_3)_3 \cdot 6H_2O$	0.1528	1350^d	39
	0.1905	1465^d	
	0.1911	1465^d	
	0.2124	1465^d	
NH_4NO_3(IV)	0.1619	1310^a	40
	0.2027	1446^a	
	0.1289	1297	
$UO_2(NO_3)_2 \cdot 6H_2O$	0.1422	1333	28
	0.1816	1497	
	0.2048	1536	
	0.1338	1368^d	
$Ca(NO_3)_2 \cdot 4H_2O$	0.1356	1368^d	41
	0.1720	1440^d	
	0.1830	1440^d	
$Ni(NO_3)_2 \cdot 2H_2O$	0.1335	1310	32
	0.1757	????^{e}	
	0.1390	1330^d	
	0.1405	1330^d	
$La(NO_3)_3 \cdot 6H_2O$	0.1409	1330^d	30
	0.1893	1470^d	
	0.1899	1470^d	
	0.1935	1470^d	
$Co(NO_3)_2 \cdot 2H_2O$	0.1320	1320	32
	0.1789	????^{e}	

To be continued

Table II continued

Compound	$T'_{ii}/\mathrm{Å}^{-10}$	ν/cm^{-1}	Ref.
$Cd(NO_3)_2 \cdot 4H_2O$	0.1438	1335	42
	0.2086	1450	
	0.1298	1310[d]	
$Ni(NO_3)_2 \cdot 4H_2O$	0.1304	1310[d]	32
	0.1953	1460[d]	
	0.1957	1460[d]	
	0.1293	1292	
$Th(NO_3)_4 \cdot 5H_2O$	0.1402	1323	32
	0.2096	1506	
	0.2180	1520	
	0.1054	1170	
	0.1075	1190	
	0.1107	1240	
$Sn(NO_2)_4$	0.1151	1262	43
	0.2058	1556	
	0.2397	1610	
	0.2549	1622	
	0.2664	1653	
$LiNO_3$ — ab initio	0.0911	1264[f]	29
	0.1916	1524[f]	
NO_2^+	0.0000	—	28
	0.4775	2375	

[a] Frequencies refer to deuterated compound
[b] Frequencies refer to protiated compound
[c] The given frequencies are the mean of the IR-active components
[d] Frequency at the band centroid
[e] Uncertain assignment
[f] Experimental frequencies

regression analysis. Data for the NO_2^+ ion were also included, the last being an example of an NO_3^- ion with extremely large distortion*. Several two-parameter functions were tested. The best result (see Figure 1) was obtained for a linear function of the type:

$$(\nu/\mathrm{cm}^{-1}) = 2901 \cdot (T'_{ii}/\mathrm{A}^{-10}) + 907.4 \qquad (3)$$

with a correlation coefficient $r^2 = 0.94$. Although the correlation coefficient for the power-type function:

$$(\nu/\mathrm{cm}^{-1}) = 2641 \cdot (T'_{ii}/\mathrm{A}^{-10})^{0.3541} \qquad (3')$$

is lower ($r^2 = 0.86$), one should expect that this function to be more realistic, because it retains its physical significance throughout the whole range of possible T_{ii}' values.

It is noticeable that the points in Figure 1 are considerably scattered. There could be several reasons for this finding: (i) the accuracy of the crystal structures is, perhaps, the most important one (e. g. the accuracy of the NO_2NO_3 structure[30] should be considered as rather low); (ii) in certain cases there may be some doubt about the band assignment, since under the C_1 local symmetry of the NO_3^- ion all of the stretching vibrations are »mixed«

---

* NO_2^+ ion can be visualized as an NO_3^- ion in which one of the N—O bonds is infinitely elongated, *i. e.* one oxygen atom is removed.. The nitrogen and the remaining two oxygens, as a result of strong repulsion (or »rehybridization«), form linear nitronium cation.

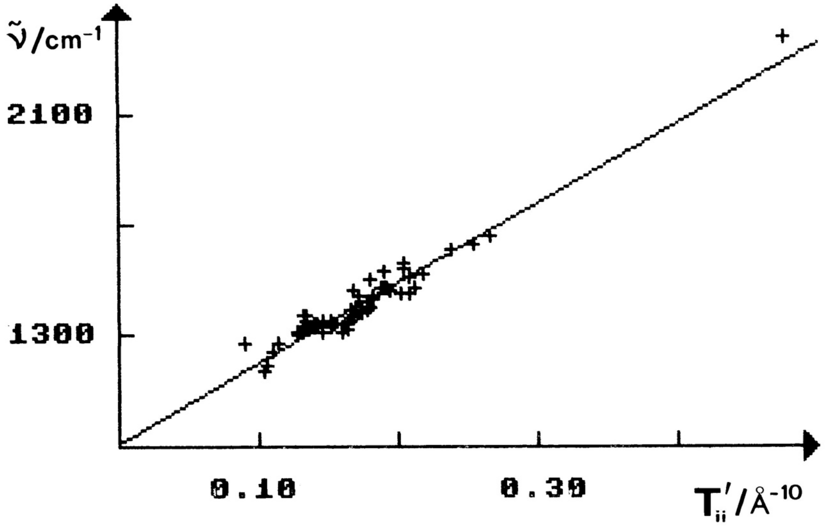

Figure 1. Linear regression of T'_{ii} vs ν_3.

to some extent; (iii) the large thermal vibrations of the atoms are also important, the N—O distances not being corrected for thermal motion. For instance, the shorter N—O distances in the structure of ND_4NO_3 [44], compared with the N—O distance in the free ion, are most probably a result of thermal vibrations; (iv) a very important point may be the existence of the correlation field splitting, in the spectra of crystals. Unfortunately, it is not possible to obtain frequencies of the NO_3 stretchings »free«, so to say, from various crystal effects (the mentioned correlation field splitting, LO-TO splittings, different frequencies for different **k**, as a result of the dispersion of phonon curves, etc.), in the same manner as sulfates[2] were »isomorphously« isolated in the corresponding selenates (there is no other XY_3 ion isomorphous with NO_3). A rough estimate of the »free« frequency could be the mean frequency of all factor-group components. These are known for very few compounds, the accuracy of the corresponding structure being, often, very low. The statistical size of the sample, therefore, would be too small, if such cases were the only ones to be analysed; (v) finally, the effect of the surroundings on the NO_3 stretching frequencies, was not considered at all. Thus, a more sophisticated approach seems neccesary for more reliable results and this is going to be the aim of our further study on the description of molecular distortions.

Acknowledgement. — The authors are indebted to Dr Biljana Minčeva-Šukarova and Prof. Bojan Šoptrajanov for their critical reading of the manuscript. The financial support of the Community for Scientific Activities of the Socialist Republic of Macedonia is also acknowledged.

APPENDIX

Let us consider a special type of distortion: the Y atoms are at the corners of an equilateral triangle, and the atom X is at a distance ϱ away from the centre. The coordinate system may be chosen in such a way that the atomic coordinates wil have the values:

$$Y_1\,(0, r);\quad Y_2\,(-r\sqrt{3/2}, -r/2);\quad Y_3\,(r\sqrt{3/2}, -r/2);\quad X\,(\varrho\cdot\cos\varphi, \varrho\cdot\sin\varphi)$$

with $\varrho \ll r$.

Let λ_1 and λ_2 be the main components of tensor T_{ij}. Their value may be obtained by solving the determinantal equation:

$$\begin{vmatrix} T_{11}-\lambda & T_{12} \\ T_{21} & T_{22}-\lambda \end{vmatrix} = 0 \tag{i}$$

$$\lambda_{1,2} = [T_{11} + T_{22} \pm \sqrt{(T_{11}-T_{22})^2 + 4T_{12}}]/2 \tag{ii}$$

As $T_{11} - T_{22} \approx 0$ and, also, $T_{12} \approx 0$, one obtains:

$$\frac{\lambda_1}{\lambda_2} \approx 1 + 2\cdot\frac{\sqrt{(T_{11}-T_{22})^2 + 4\cdot T_{12}^2}}{T_{11}+T_{22}} \tag{iii}$$

For the components of tensor T_{ij}, disregarding the higher order terms, one obtains:

$$T_{11} \approx (3r^2/2 - 3\delta r\varrho\cdot\sin\varphi/4)/r^\delta$$

$$T_{22} \approx (3r^2/2 + 3\delta r\varrho\cdot\sin\varphi/4)/r^\delta$$

$$T_{12} \approx (-3\delta r\varrho\cdot\cos\varphi/4)/r^\delta$$

Equation (iii) can now be solved, the result being:

$$\frac{\lambda_1}{\lambda_2} \approx 1 + \delta\cdot\frac{\varrho}{r} \tag{iv}$$

Thus, the ratio of the eigenvalues is independent of the polar angle. Substituting $\lambda_1 = 1/b^2$ and $\lambda_2 = 1/a^2$, the following simple equation for the total distortion of the molecule is obtained:

$$D_f = \left(\frac{\delta\varrho}{2r}\right)^2 \tag{v}$$

Since this type of distortion is independent of φ, it is called isotropic distortion. Among the 35 NO_3^- ions studied, the nitrate ion in KNO_3 and one of the nitrate ions in $Ca(NO_3)_2\cdot 4H_2O$ (cf. Table I), may be considered as isotropic. There is no evidence that these two ions show any unusual spectral properties, as compared to the others.

All calculations were performed on a COMMODORE 128 microcomputer with a program written in Basic. The listing of the program is available upon request, from the authors.

REFERENCES

1. G. Kostovski adn V. Petruševski, *XIVth Yugoslav Congress of Students of Pure and Applied Chemistry with International Participation. Abstracts*, Bor (1985) 110b.
2. V. Petruševski and K. Trenčevski, *Croat. Chem. Acta* **59** (1986) 867.
3. V. Petruševski and B. Soptrajanov, *J. Mol. Struct.* **175** (1988) 349.
4. W. H. Baur, *Acta Crystallogr.* **B30** (1974) 1195.
5. P. Murray-Rust, H. B. Bürgi and J. D. Dunitz, *Acta Crystallogr.* **B34** (1978) 1787.
6. P. Murray-Rust, H. B. Bürgi and J. D. Dunitz, *Acta Crystallogr.* **B34** (1978) 1793.
7. P. Murray-Rust, H. B. Bürgi and J. D. Dunitz, *Acta Crystallogr.* **A35** (1979) 703.
8. W. A. Dollase, *Acta Crystallogr.* **A30** (1974) 513.
9. J. C. Moore and J. P. Devlin, *J. Chem. Phys.* **68** (1978) 826.
10. G. L. Paul and A. W. Pryor, *Acta Crystallogr.* **B27** (1971) 2700.
11. C. S. Choi and H. J. Prask, *Acta Crystallogr.* **B38** (1982) 2324.

12. J. K. Nimmo and B. W. Lucas, *J. Phys. C.* **6** (1973) 201.
13. K. Hermansson, *Acta Crystallogr.* **C39** (1983) 925.
14. C. S. Gibbons and J. Trotter, *J. Chem. Soc. (A)* (1976) 2058.
15. K. Hermansson, J. O. Thomas, and I. Olovsson, *Acta Crystallogr.* **B36** (1980) 1932.
16. B. Ribár, F. Gabela, R. Herak, und B. Prelesnik, *Z. Kristallogr.* **137** (1973) 290.
17. B. Matković, B. Ribár, B. Prelesnik, and R. Herak, *Inorg. Chem.* **13** (1974) 3006.
18. N. Milinski, B. Ribár, and M. Satarić, *Cryst. Struct. Comm.* **9** (1980) 473.
19. C. H. Choi, J. E. Mapes, and E. Prince, *Acta Crystallogr.* **B28** (1972) 1357.
20. J. C. Taylor and M. H. Mueller, *Acta Crystallogr.* **19** (1965) 536.
21. A. Leclaire et J.-C. Monier, *Acta Crystallogr.* **B33** (1977) 1861.
22. B. Ribár and N. Milinski, *Z. Kristallogr.* **144** (1976) 126.
23. B. Eriksson, L.O. Larsson, L. Niinsto, and J. Valkonen, *Inorg. Chem.* **19** (1980) 1207.
24. B. Ribár, N. Milinski, R. Herak, N. Krstanović, and S. Djurić, *Z. Kristallogr.* **144** (1976) 133.
25. B. Matković, B. Ribár, and B. Zelenko, *Acta Crystallogr.* **21** (1966) 719.
26. B. Morosin and T. Haseda, *Acta Crystallogr.* **B35** (1979) 2856.
27. T. Ueki, A. Zalkin, and D. H. Templeton, *Acta Crystallogr.* **20** (1966) 836.
28. C. D. Garner, D. Sutton, and S. C. Wallowork, *J. Chem. Soc. (A)* (1967) 1949.
29. V. G. Solomoniak and S. P. Konovalov, *Z. Strukt. Khim.* **24** (1983) 11 (Russ.).
30. E. Grison, K. Eroks et J. L. de Vries, *Acta Crystallogr.* **3** (1950) 290.
31. G. Herzberg, *Molecular Spectra and Molecular Structure. II. Infrared and Raman Spectra of Polyatomic Molecules*, Van Nostrand, New York (1956).
32. S. D. Ross, *Inorganic Infrared and Raman Spectra,* McGraw-Hill, London (1972).
33. G. J. Kearley and S. F. A. Kettle, *J. Phys. Chem.* **86** (1982) 4007.
34. D. M. Adams and S. K. Sharma, *J. Chem. Soc. Faraday Trans. 2,* **76** (1981) 1263.
35. I. I. Kondilenko, P. A. Korotkov, and N. G. Golubeva, *Z. Prikl. Spektr.* **24** (1976) 532 (Russ.).
36. C. H. Huang and M. C. Brooker, *Spectrochim. Acta* **32A** (1976) 1715.
37. T.-C. G. Chang and D. E. Irish, *Can. J. Chem.* **51** (1973) 118.
38. R. P. J. Cooney and J. R. Hall, *Aust. J. Chem.* **25** (1972) 1159.
39. B. N. Ivanov-Emin, Z. K. Odinec, B. E. Zaicev, V. M. Akimov, M. Arias de Paskual, and A. I. Ezhov, *Z. Neorg. Khim.* **24** (1979) 2637 (Russ.).
40. G. J. Kearley and S. F. A. Kettle, *J. Chem. Phys.* **73** (1980) 2129.
41. I. I. Kondilenko, P. A. Korotkov, and N. G. Golubeva, *Z. Prikl. Spektr.* **20** (1974) 1028 (Russ.).
42. M. T. Carrick, D. W. James, and W. H. Leong, *Aust. J. Chem.* **36** (1983) 223.
43. D. W. Amos and G. W. Flewwet, *Spectrochim. Acta* **30A** (1974) 453.
44. B. W. Lucas, M. Ahtee, and A. W. Hewat, *Acta Crystallogr.* **B35** (1979) 1038.

SAŽETAK

Opis molekularnih distorzija III. Trigonsko-planarne XY_3 molekule

K. Trenčevski i V. Petruševski

Primijenjeni su tenzori drugoga reda u izračunavanju stupnja distorzije iona NO_3^- u nizu kristalnih spojeva. Utvrđena je pouzdana korelacija između glavnih komponenata tenzora i valnih brojeva antisimetričnih isteznih vibracija (ν_3) iona NO_3^-.