P—W—P^{iii}	176,03 (16)	P—C1—C2	117,3 (9)
P—W—P^{iv}	89,7 (15)	C1—C2—C3	117,3 (12)
P—W—P^{v}	84,0 (15)	C4—C3—C2	121,8 (16)
W—P—F1	116,1 (3)	C5—C4—C3	117,3 (14)
W—P—F2	115,7 (2)	C4—C5—C6	123,1 (14)
W—P—C1	126,8 (3)	C1—C6—C5	118,6 (15)
F1—P—F2	95,6 (3)	C6—C1—C2	121,8 (12)
F1—P—C1	97,6 (5)		

Symmetriebezeichnungen: (i) $1 - y, 1 + x - y, z$; (ii) $-x + y, 1 - x, z$; (iii) $1 - y, 1 - x, \frac{1}{2} - z$; (iv) $-x + y, y, \frac{1}{2} - z$; (v) $x, 1 + x - y, \frac{1}{2} - z$.

Zur Sammlung der Reflexintensitäten wurde ein plättchenförmiger Kristall mit Silikonfett in einer Glaskapillare angeheftet. Einer möglichen Zersetzung des Kristalls wurde durch Nachstopfen weiterer kristalliner Substanz entgegengewirkt. Die Lösung des Phasenproblems erfolgte durch Direkte Methoden in der aufgrund der Auslöschungsbedingung hhl mit $l = 2n + 1$ wahrscheinlichen Raumgruppe $P\bar{3}1c$. Es konnten ein Wolfram- und ein Phosphoratom aus der E Map und die Fluor- und Kohlenstoffatome eines PF_2Ph Liganden der anschließenden Differenzfouriersynthese entnommen werden. Die Verfeinerung des Strukturmodells erfolgte mit anisotropen Temperaturkoeffizienten für alle Nichtwasserstoffatome. Die H-Lagen wurden mit idealisierter Geometrie fixiert und mit einem gemeinsam verfeinerten isotropen Temperaturfaktor versehen.

In den kanalartigen Hohlräumen um die c-Achse bleibt auf einer Lage der Punktsymmetrie 2 eine maximale Restelektronendichte von 1,3 e Å^{-3} übrig. Einige unabhängige experimentelle Befunde deuten hier auf den Einbau von Solvensmolekülen hin. Neben der erwähnten Trübung der Kristalloberfläche während der Lagerung wurden unterschiedliche Debye-Scherrer-Aufnahmen des pulverförmigen Ausgangsprodukts und der umkristallisierten Substanz beobachtet. Einen noch deutlicheren Hinweis lieferte eine rasterelektronenmikroskopische Untersuchung, bei der die Einkristalle unter dem Einfluß von Vakuum und Elektronenstrahl förmlich zersprangen. In der anschließend durchgeführten Röntgenfluoreszenzanalyse konnte im Gegensatz zum Pulver Sauerstoff nachgewiesen werden. Hinweise auf den Einbau von Methylenchlorid wurden weder massenspektrometrisch noch mittels Röntgenfluoreszenzanalyse erhalten. Aufgrund dieser Ergebnisse wurde die Restelektronendichte in den weiteren Verfeinerungen als Sauerstofflage eines fehlgeordneten H_2O-Moleküls behandelt. Die geometrische Anordnung und die niedrige Elektronendichte führen zu einem Fehlordnungsmodell, bei dem ein Sauerstoffatom auf die drei alternativen Lagen $x, -x, \frac{1}{4}$; $x, 2x, \frac{1}{4}$; $-2x, -x, \frac{1}{4}$ verteilt ist. Berücksichtigt man die Zähligkeit der Punktlage des Sauerstoffs, so resultiert für den untersuchten Kristall insgesamt die Zusammensetzung $W(PF_2Ph)_6.H_2O$.

Datensammlung: *CAD*-4 *Software* (Enraf-Nonius, 1989). Gitterverfeinerung: *CAD*-4 *Software* (Enraf-Nonius, 1989). Datenreduktion: *MolEN* (Fair, 1990). Lösung der Struktur mit Programm: *SHELXS*86 (Sheldrick, 1985). Verfeinerung der Struktur mit Programm: *SHELX*76 (Sheldrick, 1976). Zeichenprogramme: *SCHAKAL*88 (Keller, 1988); *ORTEP* (Davenport, Hall & Dreissig, 1990). Programme zur Berechnung der geometrischen Daten und zur Erstellung der Tabellen: *ORFFE*4 (Busing, Martin, Levy, Brown, Johnson & Thiessen, 1977); *KRISTALL-ST* (Tebbe, 1992).

Wir danken dem Fonds der Chemischen Industrie und dem Bundesminister für Forschung und Technologie für die Förderung dieser Arbeit.

Die Liste der Strukturfaktoren, anisotropen Verschiebungsfaktoren, H-Atom Koordinaten und vollständigen geometrischen Daten sind bei der IUCr (Aktenzeichen: SE1039) hinterlegt. Kopien sind erhältich durch: The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Literatur

Busing, W. R., Martin, K. O., Levy, H. A., Brown, G. M., Johnson, C. K. & Thiessen, W. E. (1976). *ORFFE4*. Oak Ridge National Laboratory, Tennessee, VStA.

Cloke, F. G. N., Fyne, P. J., Gibson, V. C., Green, M. L. H., Ledoux, M. J., Perutz, R. N., Dix, A., Gourdon, A. & Prout, K. (1984). *J. Organomet. Chem.* **277**, 61-73.

Crump, W & Gilles, T. (1992). *SDF-CIF. Ein Programm zur Erstellung des CIF aus internen Archiv-Files.* Univ. Köln, Deutschland.

Davenport, G., Hall, S. R. & Dreissig, W. (1990). *ORTEP: Oak Ridge Thermal Elipsoid Plot. Xtal* 3,0 *Reference Manual*, herausgegeben von S. R. Hall & J. M. Stewart. Univ. Western Australia, Australien, und Maryland, VStA.

Enraf-Nonius (1989). *CAD-4 Software. Version* 5.0. Enraf-Nonius, Delft, Niederlande.

Fair, C. K. (1990). *MolEN. An Interactive Intelligent System for Crystal Structure Analysis.* Enraf-Nonius, Delft, Niederlande.

Keller, E. (1988). *SCHAKAL88. Fortran Program for the Graphical Representation of Molecular and Crystallographic Models.* Univ. Freiburg, Deutschland.

Krampe, W., Kruck, Th. & Tebbe, K.-F. (1989). *Chem. Ber.* **122**, 1477-1480.

Rabinovich, D. & Parkin, G. (1990). *J. Am. Chem. Soc.* **112**, 5381-5383.

Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination.* Univ. Cambridge, England.

Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures.* Univ. Göttingen, Deutschland.

Siegers, B. (1993). Dissertation, Universität zu Köln, Deutschland.

Tebbe, K.-F. (1992). *KRISTALL-ST. Ein Programmsystem zur Erstellung von Eingabefiles, Tabellen und Pulverdiagrammen.* Univ. Köln, Deutschland.

Acta Cryst. (1994). **C50**, 1076–1079

Sodium Galactarate and Potassium Galactarate

Tooru Taga, Tatsuo Shimada and Norio Mimura

Faculty of Pharmaceutical Sciences, Kyoto University, Sakyo-ku, Kyoto 606-01, Japan

(*Received* 25 *October* 1993; *accepted* 26 *January* 1994)

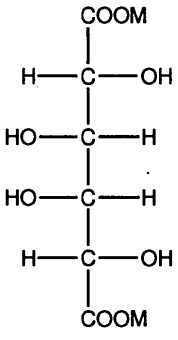
Abstract

In both title crystals, $2Na^+.C_6H_8O_8^{2-}$ and $2K^+.C_6H_8O_8^{2-}$, the galactarate ion is centrosymmetrical and has a fully extended molecular conformation. The Na ion is coordinated to six O atoms to form a distorted bipyramidal octahedron, with Na$\cdots$O distances in the range 2.260 (2)–

2.451 (2) Å, while the K ion is surrounded by six O atoms in a largely distorted triangular antiprismatic arrangement, with K···O distances in the range 2.688 (4)–2.871 (5) Å. A number of three-center hydrogen bonds have been found for both the Na and the K salt crystals.

Comment

Binding of carbohydrates to cations in the solid state and in aqueous solution is important because of its biological implications. The coordination of the divalent Ca, Ba and Mg cations with the galactarate ion in the solid state has been established (Sheldrick, Mackie & Akrigg, 1989; Sheldrick & Mackie, 1989), along with the coordination of the Ca and K cations with the glucarate ion (Taga & Osaki, 1976; Burden, Mackie & Sheldrick, 1985; Taga, Kuroda & Osaki, 1977). The present study concerns the structures of monovalent cation salts of the galactarate ion, (I).



(I) M = Na, K

In both the Na and the K salt crystals, the asymmetric unit consists of a cation and one half of a galactarate ion. As shown in Fig. 1, the galactarate ion has an extended *trans*-zigzag conformation and the carboxyl group has a periplanar conformation for the α-hydroxyl atom O(2) about the C(1)—C(2) bond [the torsion angle O(11)—C(1)—C(2)—O(2) is 5.1 (7)° for the Na salt and 9.3 (8)° for the K salt]. The molecular conformation is similar to that in both the acid form (Jeffrey & Wood, 1982) and the divalent cation salts (Sheldrick, Mackie & Akrigg, 1989; Sheldrick & Mackie, 1989), although the glucarate ion in the K salt has a different molecular conformation than that in the Ca salt (Taga, Kuroda & Osaki, 1977).

Bond distances and angles have normal values for carbohydrates (Table 2). The Na ion is coordinated to six O atoms to form a distorted bipyramidal octahedron, with Na···O distances in the range 2.260 (2)–2.451 (2) Å (Fig. 2*a*). The O(11) and O(2) atoms in the coordination shell belong to the same molecule. On the other hand, the K ion is coordinated to six O atoms in a largely distorted triangular antiprismatic arrangement, with K···O distances in the range 2.688 (8)–2.871 (9) Å; the six O atoms belong to different molecules (Fig. 2*b*). In the crystal of the Na salt, the atom O(3) is hydrogen-bonded to the atom O(12^{ix}) and the O(2) hydroxyl group forms a three-center hydrogen bond (Jeffrey & Saenger, 1991) with the atoms O(12^{viii}) and O(3) [O(12^{viii})···H(O2)···O(3) is 121 (4)° and the sum of the three angles about H(O2) is 360°]. In the crystal of the K salt, the O(2) hydroxyl group makes a three-center hydrogen bond to O(12^{i}), with a minor intramolecular hydrogen bond to O(11) [O(12^{i})···H(O2)···O(11) is 92 (2)° and the sum of the three angles about H(O2) is 355°]. Also, the O(3) hydroxyl group makes a three-center hydrogen bond to O(11^{ii}), with a weak hydrogen bond to O(12^{ii}) in the same carboxyl group [O(11^{ii})···H(O3)···O(12^{ii}) is 65 (2)° and the sum of the three angles about H(O3) is 358°].

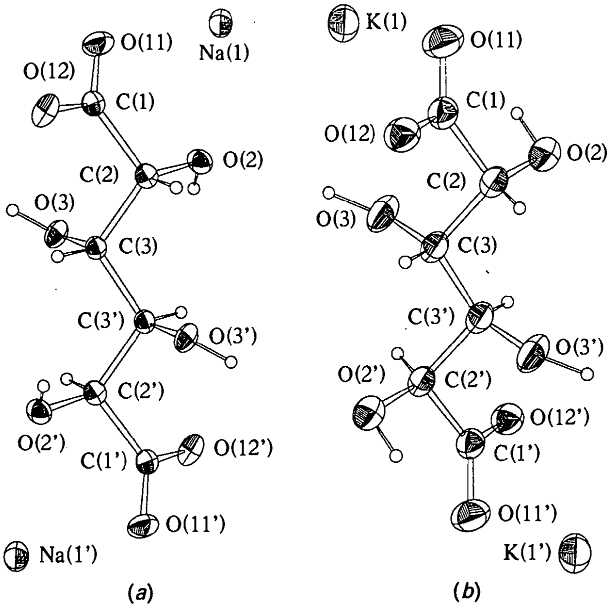


Fig. 1. Perspective views of the title compounds showing the numbering of the atoms. The asymmetric unit contains one half of the galactarate ion. The displacement ellipsoids are drawn at the 50% probability level.

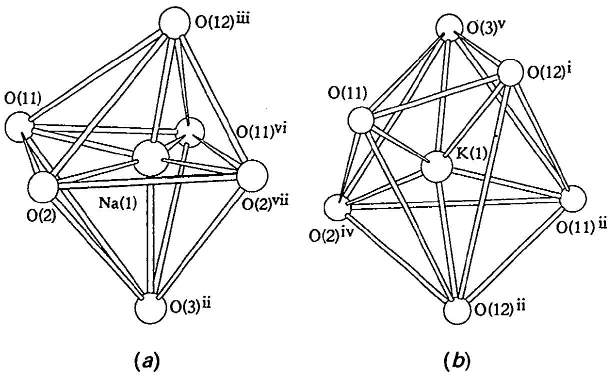


Fig. 2. Coordination of (*a*) the Na ion with six O atoms involving Na···O distances in the range 2.260–2.451 Å, and of (*b*) the K ion involving six O atoms with K···O distances in the range 2.688–2.871 Å.

Experimental

Sodium Galactarate

Crystal data

$2Na^+.C_6H_8O_8^{2-}$
$M_r = 254.10$
Monoclinic
$P2_1/c$
$a = 7.827$ (1) Å
$b = 8.351$ (1) Å
$c = 8.951$ (1) Å
$\beta = 132.90$ (1)°
$V = 428.6$ Å^3
$Z = 2$
$D_x = 1.969$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 24 reflections
$\theta = 35$–$40°$
$\mu = 2.412$ mm^{-1}
$T = 297.0$ K
Prism
0.26 × 0.23 × 0.15 mm
Colourless

Data collection

Rigaku AFC-5*RU* diffractometer
$\theta/2\theta$ scans
Absorption correction: none
842 measured reflections
743 independent reflections
637 observed reflections $[F > 3\sigma(F)]$

$R_{\rm int} = 0.019$
$\theta_{\rm max} = 65°$
$h = -8 \rightarrow 7$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 10$
3 standard reflections monitored every 150 reflections intensity variation: none

Refinement

Refinement on F
$R = 0.045$
$wR = 0.053$
$S = 0.63$
637 reflections
90 parameters
Only coordinates of H atoms refined, all from $\Delta\rho$ map
Calculated weights $w = 1/[\sigma^2(F) + 0.023F^2]$

$(\Delta/\sigma)_{\rm max} = 0.02$
$\Delta\rho_{\rm max} = 0.37$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.30$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Potassium Galactarate

Crystal data

$2K^+.C_6H_8O_8^{2-}$
$M_r = 286.32$
Monoclinic
$P2_1/c$
$a = 5.004$ (1) Å
$b = 7.173$ (1) Å
$c = 13.140$ (2) Å
$\beta = 93.96$ (1)°
$V = 470.5$ Å^3
$Z = 2$
$D_x = 2.021$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 25$–$38°$
$\mu = 9.41$ mm^{-1}
$T = 297.0$ K
Prism
0.40 × 0.35 × 0.25 mm
Colorless

Data collection

Rigaku AFC-5*RU* diffractometer
$\theta/2\theta$ scans
Absorption correction: spherical, $\mu r = 3.2$
968 measured reflections
846 independent reflections
730 observed reflections $[F > 3\sigma(F)]$

$R_{\rm int} = 0.033$
$\theta_{\rm max} = 65°$
$h = 0 \rightarrow 5$
$k = 0 \rightarrow 8$
$l = -14 \rightarrow 14$
3 standard reflections monitored every 150 reflections intensity variation: none

Refinement

Refinement on F
$R = 0.063$
$wR = 0.078$
$S = 0.91$
730 reflections
90 parameters
Only coordinates of H atoms refined, all from $\Delta\rho$ map
Calculated weights $w = 1/[\sigma^2(F) + 0.023F^2]$

$(\Delta/\sigma)_{\rm max} = 0.24$
$\Delta\rho_{\rm max} = 0.73$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.55$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{\rm eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	$B_{\rm eq}$
Na salt				
Na(1)	0.2553 (2)	0.5507 (2)	0.2414 (2)	1.78 (7)
C(1)	0.0467 (6)	0.2031 (4)	0.1605 (5)	1.3 (2)
C(2)	0.2832 (6)	0.1798 (4)	0.3761 (5)	1.3 (2)
C(3)	0.3873 (5)	0.0189 (4)	0.3917 (5)	1.2 (2)
O(11)	0.0179 (4)	0.3185 (3)	0.0562 (4)	2.1 (1)
O(12)	−0.1059 (4)	0.1003 (3)	0.1036 (3)	1.9 (1)
O(2)	0.4410 (4)	0.3069 (2)	0.4382 (3)	1.5 (1)
O(3)	0.4412 (4)	0.0233 (3)	0.2675 (3)	1.6 (1)
K salt				
K(1)	0.0282 (3)	0.3070 (2)	0.1800 (1)	2.97 (4)
C(1)	0.553 (1)	0.1476 (9)	0.3594 (5)	2.3 (2)
C(2)	0.476 (1)	0.2389 (9)	0.4586 (5)	2.2 (2)
C(3)	0.525 (1)	0.4494 (9)	0.4505 (4)	2.3 (2)
O(11)	0.3758 (9)	0.0675 (7)	0.3040 (3)	3.2 (1)
O(12)	0.7905 (9)	0.1633 (6)	0.3397 (3)	2.6 (1)
O(2)	0.2138 (9)	0.1984 (7)	0.4858 (3)	2.7 (1)
O(3)	0.355 (1)	0.5253 (7)	0.3706 (3)	3.0 (1)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and hydrogen-bonding geometry* (Å, °)

Na salt			
Na(1)—O(11)	2.402 (3)	Na(1)—O(11$^{\rm vi}$)	2.260 (2)
Na(1)—O(12$^{\rm iii}$)	2.382 (4)	Na(1)—O(2)	2.424 (2)
Na(1)—O(2$^{\rm vii}$)	2.451 (2)	Na(1)—O(3$^{\rm ii}$)	2.441 (4)
C(1)—C(2)	1.525 (4)	C(2)—O(2)	1.424 (5)
C(1)—O(11)	1.251 (5)	C(3)—O(3)	1.433 (7)
C(1)—O(12)	1.263 (5)	C(3)—C(3′)	1.521 (4)
C(2)—C(3)	1.528 (5)		
C(2)—C(1)—O(11)	119.3 (3)	C(3)—C(2)—O(2)	110.7 (4)
C(2)—C(1)—O(12)	115.1 (3)	C(2)—C(3)—O(3)	109.1 (3)
O(11)—C(1)—O(12)	125.6 (2)	C(2)—C(3)—C(3′)	112.5 (3)
C(1)—C(2)—C(3)	109.9 (3)	O(3)—C(3)—C(3′)	107.2 (3)
C(1)—C(2)—O(2)	112.5 (3)		

D—H···A	H···A	D···A	D—H···A
O(2)—H(O2)···O(12$^{\rm viii}$)	2.21 (7)	2.867 (4)	136 (6)
O(2)—H(O2)···O(3)	2.51 (7)	2.819 (4)	103 (4)
O(3)—H(O3)···O(12$^{\rm ix}$)	1.81 (6)	2.660 (3)	166 (4)

K salt

K(1)—O(11)	2.871 (5)	K(1)—O(11^{iii})	2.772 (5)
K(1)—O(12^{i})	2.688 (4)	K(1)—O(12^{ii})	2.730 (4)
K(1)—O(2^{iv})	2.775 (5)	K(1)—O(3^{v})	2.833 (4)
C(1)—C(2)	1.532 (9)	C(2)—C(3)	1.535 (9)
C(1)—O(11)	1.248 (7)	C(3)—C(3′)	1.525 (8)
C(1)—O(12)	1.239 (7)		
C(2)—C(1)—O(11)	118.9 (5)	C(3)—C(2)—O(2)	112.0 (5)
C(2)—C(1)—O(12)	116.1 (5)	C(2)—C(3)—O(3)	109.9 (5)
O(11)—C(1)—O(12)	125.0 (6)	C(2)—C(3)—C(3′)	111.9 (5)
C(1)—C(2)—C(3)	108.1 (5)	O(3)—C(3)—C(3′)	108.9 (5)
C(1)—C(2)—O(2)	114.8 (5)		

D—H···*A*	H···*A*	*D*···*A*	*D*—H···*A*
O(2)—H(O2)···O(12^{i})	1.87 (5)	2.770 (6)	160 (5)
O(2)—H(O2)···O(11)	2.38 (5)	2.741 (6)	103 (4)
O(3)—H(O3)···O(11^{ii})	1.78 (6)	2.756 (6)	164 (5)
O(3)—H(O3)···O(12^{ii})	2.25 (5)	2.978 (6)	129 (4)

Symmetry codes: (i) $x - 1, y, z$; (ii) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$ (iii) $-x, \frac{1}{2} + y, \frac{1}{2} - z$; (iv) $x, \frac{1}{2} - y, z - \frac{1}{2}$; (v) $-x, \frac{1}{2} + y, \frac{1}{2} - z$; (vi) $-x, 1 - y, -z$; (vii) $1 - x, 1 - y, 1 - z$; (viii) $1 + x, \frac{1}{2} - y, \frac{1}{2} + z$; (ix) $-x, -y, -z$.

Data were collected using *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). The structures were solved using *MULTAN*88 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1988). Structure refinement, geometric calculations and preparation of the figures were performed using *KPPXRAY* (Taga, Masuda, Higashi & Iizuka, 1991) on a FACOM M1900 computer at the Data Processing Center, Kyoto University, Japan. *EDCIF-J* (Osaki & Taga, 1993) was used to prepare the material for publication.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: AS1094). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Burden, C., Mackie, W. & Sheldrick, B. (1985). *Acta Cryst.* C**41**, 693-695.

Jeffrey, G. A. & Saenger, W. (1991). *Hydrogen Bonding in Biological Structures*, pp. 20-24. New York: Springer-Verlag.

Jeffrey, G. A. & Wood, R. A. (1982). *Carbohydr. Res.* **108**, 205-211.

Main, P., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1988). *MULTAN88. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Molecular Structure Corporation (1988). *MSC/AFC Diffractometer Control Software.* MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Osaki, K. & Taga, T. (1993). *J. Crystallogr. Soc. Jpn*, **35**, 223-224.

Sheldrick, B. & Mackie, W. (1989). *Acta Cryst.* C**45**, 1072-1073.

Sheldrick, B., Mackie, W. & Akrigg, D. (1989). *Acta Cryst.* C**45**, 191-194.

Taga, T., Kuroda, Y. & Osaki, K. (1977). *Bull. Chem. Soc. Jpn*, **50**, 3079-3083.

Taga, T., Masuda, K., Higashi, T. & Iizuka, H. (1991). *KPPXRAY. Kyoto Program Package for X-ray Crystal Structure Analysis.* Kyoto Univ., Kyoto, Japan.

Taga, T. & Osaki, K. (1976). *Bull. Chem. Soc. Jpn*, **49**, 1517-1520.

Acta Cryst. (1994). C**50**, 1079–1084

Two 4-Nitropyridine *N*-Oxide Adducts: $(C_5H_4N_2O_3)_2.AgNO_3$ and $(C_5H_4N_2O_3)_2.Co(NO_3)_2.4H_2O$

MURIEL BAGIEU-BEUCHER, YVETTE LE FUR,
JEAN-PIERRE LEVY AND JACQUES PÉCAUT

Laboratoire de Cristallographie, associé à l'Université Joseph Fourier, CNRS, BP 166, 38042 Grenoble, CEDEX, France

(*Received* 8 *July* 1993; *accepted* 1 *November* 1993)

Abstract

Two new addition compounds of the optically non-linear molecule 4-nitropyridine *N*-oxide (NPO) have been synthesized and characterized: bis(4-nitropyridine *N*-oxide)silver nitrate and bis(4-nitropyridine *N*-oxide)cobalt nitrate tetrahydrate. Their structural features are described and compared, in particular the arrangement of the NPO molecules, the type of linkage in the inorganic entities (the cationic polyhedra and the nitrate anions) which make up the host matrice for the organic molecules and the hydrogen-bonding scheme contributing to the packing cohesion. Certain characteristics of both these centrosymmetric structures are also discussed with respect to some non-linear optical NPO derivatives.

Comment

It has been shown in previous studies (Nicoud & Twieg, 1987) that aromatic molecules, characterized by a strong charge transfer occurring between a donor and an acceptor substituent and by a small ground-state dipole moment, can lead to non-linear optical materials if, of course, the non-centrosymmetry of the crystal structure is assured. Effectively, these molecular features give a high molecular first-order hyperpolarizability. Besides, a small dipole almost cancels the electrostatic interactions between molecules and consequently may prevent centrosymmetric arrangement of the molecules while facilitating the growth of good quality crystals (chemical feasibility).

4-Nitropyridine *N*-oxide (NPO) displays both the required properties: an important electronic charge transfer from the *N*-oxide group to the nitro group and a quasi-cancelled total dipole moment. Nevertheless, its crystal structure is centrosymmetric. So, the aim of the molecular engineering of efficient non-linear optically related compounds is to find either supplementary substituents for the aromatic ring, or other entities which do not disturb the charge-transfer mechanism and remove the centrosymmetry from the NPO structure. The former possibility

Acta Crystallographica Section C
ISSN 0108-2701 ©1994