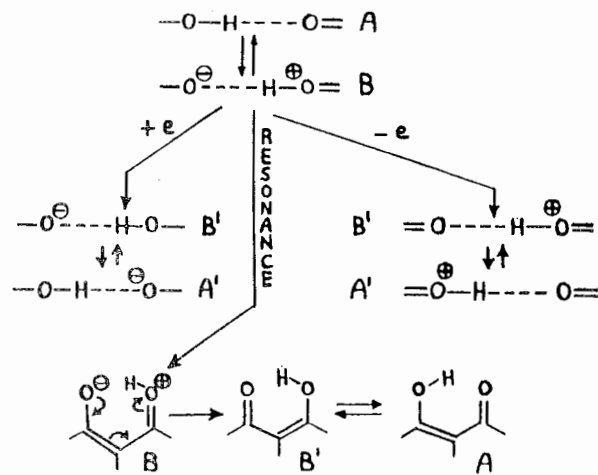


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connecting the two O atoms by a resonant system able to transmit the charges; (ii) by adding an electron to B; (iii) by removing an electron from B (see scheme). Experimental proves of such statement will be given at the meeting for all strong O-H...O bonds retrievable from the Cambridge Structural Database.

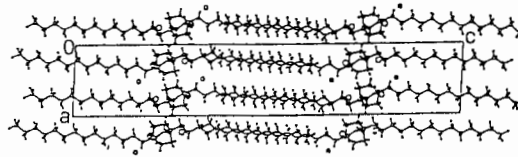


PS-06.04.08 QUATERNARY ALKYL HALIDE SALTS OF 1,4-DIAZABICYCLO[2.2.2]OCTANES WITH HALIDE ANION CONDUCTIVITY. By M. Yasui¹, R. Yamazaki¹, F. Iwasaki¹, T. Nogami¹, N. Kamiya² and H. Iwasaki², ¹Dept. of Applied Physics and Chemistry, The Univ. of Electro-Communications, Chofu, Tokyo 182, Japan, ²The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama 351-01, Japan.

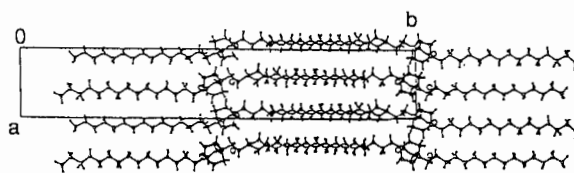
A series of quaternary alkyl halide salts of 1,4-diazabicyclo[2.2.2]octanes (DABCO) exhibited first-order phase transition in the temperature range of 62-100°C and showed halide anion conductivity in the high temperature phase (Shimizu, J. *et al.*, 1986, Bull. Chem. Soc. Jpn, **59**, 1443-1448). The phase transition temperature (Tc) and heats of transition showed a so-called even-odd number effect of carbon number which was also observed for a series of long chain alkanes and alcohols. In this study, we have investigated the crystal structures of *N,N'*-ditetradecyl-1,4-diazabicyclo[2.2.2]octane dibromide (I) and a dipentadecyl derivative (II). In each crystal, one dimension of the unit cell was very long and crystals showed instabilities against the X-ray irradiation, so that the intensity data from single crystals were collected on the IPD-WAS (Weissenberg type diffractometer with Imaging Plate, N. Kamiya *et al.*, 1990, Acta Cryst. **A46** Suppl., C10). The molecular structures of (I) and (II) have similar features. Two alkyl chains have *trans*-zigzag conformation, and dihedral angles between the planes of alkyl carbons are 128 and 157° for (I) and (II), respectively. Two bromide anions reside near the DABCO ring. Alkyl chains form sheet-like structures in crystals. In spite of the difference of chain length, the number of van der Waals contacts between alkyl chains in (I) is slightly larger than that in (II). This fact may explain the even-odd number effect that the heat of transition of (I) was greater than that of (II). In the powder X-ray diffraction patterns for (I) and (II) which were measured at the temperature near Tc, sharp diffraction peaks for the high temperature phase appeared at lower 2θ angles. At the temperature beyond the Tc, diffraction peaks assigned for short axes directions disappeared, although the sharp peaks for long axis direction still remained. Thus disorder along short axes just as the liquid-crystal arose from the phase transition.

Crystal Data

	(I)	(II)
Formula	2Br ⁺ C ₃₄ H ₇₀ N ₂ ²⁻ · 0.5H ₂ O	2Br ⁺ C ₃₆ H ₇₄ N ₂ ²⁻
Fw	666.75	694.80
Color	Colorless	Colorless
Crystal system	monoclinic	orthorhombic
Space group	P2 ₁ /c	P2 ₁ 2 ₁ 2 ₁
a/Å	8.720(1)	8.792(5)
b	8.789(2)	52.046(7)
c	49.298(8)	8.727(2)
β/°	93.83(2)	90.00
V/Å ³	3770(1)	3993(1)
Z	4	4
Reflections measured	9499	10125
observed	3675	2385
R	0.0650	0.0650



(I)



(II)

PS-06.04.09 POLYMORPHIC STRUCTURES AND PHASE TRANSITIONS OF N-PICRYLANILINE DERIVATIVES By K. Taguchi, M. Hirota, K. Maeda, M. Yasui and F. Iwasaki*, Dept. of Applied Physics and Chemistry, The Univ. of Electro-Communications, Chofu-shi, Tokyo 182, Japan

N-picryl-p-toluidine (I) and N-(2,4-dinitrophenyl)-o-anisidine (II) crystallize in two modifications, orange and red forms. The condition to crystallize each form is very subtle, so that it is by chance which form can be obtained and the coexistence of these forms is often observed. The orange crystals of both I and II turns red just below the melting points. After the orange crystals melt completely, the red crystals are obtained by cooling. Crystal structures of these polymorphic forms have been determined in order to study on the relationships between molecular interactions and polymorphic transition.

	I _o	I _r	II _o	II _r
Color	Orange	Red	Orange	Red
Cr. system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Sp. group	P2 ₁ /a	P2 ₁ /c	P2 ₁ /a	P2 ₁
a / Å	16.475(3)	13.107(4)	15.546(8)	15.693(2)
b	6.007(1)	17.739(4)	4.220(1)	10.981(3)
c	15.203(3)	6.090(2)	16.747(4)	3.842(1)
β / °	114.12(1)	102.16(3)	122.31(1)	98.39(2)
V / Å ³	1373.2(4)	1384.2(8)	1287.0(7)	655.0(2)
Z	4	4	4	2
Dx / gcm ⁻³	1.539	1.527	1.493	1.467
Radiation	MoKα	MoKα	CuKα	MoKα
No. ref.	2188	1434	1234	866
R	0.052	0.106	0.120	0.079
Solvent	acetone	acetone+CCl ₄	benzene+EtOH	acetone

The molecular structures of I_o and I_r are very similar. Intramolecular NH...O hydrogen bond is formed between anilino and nitro groups. On the other hand the molecules of II_o and II_r are rotational isomers. In II_r NH group is hydrogen-bonded to nitro and methoxy groups bifurcatedly, while in II_o the hydrogen