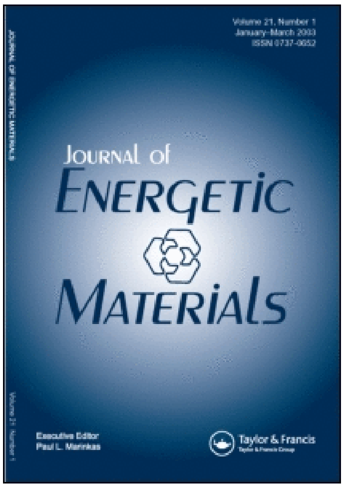

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Crystal chemistry study on nitrobenzenes Part 2. hydrogen bonding, stability and density

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CRYSTAL CHEMISTRY STUDY ON NITROBENZENES §

Part 2. HYDREGEN BONDING, STABILITY AND DENSITY

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ABSTRACT

In crystal structures of nitrobenzenes, intramolecular hydrogen bonding increases the molecule's stability, planarity and packing coefficient. The head-to-tail pattern of intermolecular hydrogen bonding favours the antiparallel packing of the molecular assemblies and close packing. The geometry of the C-H linkage alpha to the NO_2 group is discussed in connecting to the molecular stability. The relation between the crystal density and hydrogen bonding is discussed.

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INTRODUCTION

In part 1 of this series[1], the molecular conformation and packing energy were discussed. Among various interactions between non-bonded atoms, Van Der Waals interactions are universal. In polar compounds like nitrobenzenes, electrostatic interactions usually need consideration. For halogen- or sulphur-containing compounds, the special halogen-halogen or sulphur-sulphur interactions[2,3] are also important in some cases. However, the hydrogen bonding(HB) is the strongest interaction in most of cases if it exists in the structure of a molecular crystal. In our database containing 79 crystal structures of nitrobenzenes[1], there are 23 nitroanilines and 12 nitrophenols, in which hydrogen bonding plays important role. To study the relation between hydrogen bonding and properties, intramolecular geometry was calculated and related to the molecular planarity, stability and density. The packing type resulted from intermolecular hydrogen bonding was analysed and related to the close packing. The interaction between NO_2 group and its alpha C-H linkage was geometrically discussed.

INTRAMOLECULAR HYDROGEN BONDING

The main results concerning hydrogen bonding were listed in table 1. The same numbering was used as in the previous

Table 1a. Hydrogen Bonding in Nitroanilines*

No.	Groups	μ	P_N	P_A	d_{ON}	d_{CC}	d_{NC}	d_{CD}	d_{OD}	d_{OH}	D_{HB}	D_M	R_{OD}	δ_H	δ_O	Form	SO
		(D)			(	in	0.001	Å)	(	in	0.01	Å	)	(in	e)		
17	N A N A N V		1	2	1233	1435	1436	1331	257	186	15	42					
			3	2	1234	1429	1421	1331	255	182	17						
			3	4	1241	1437	1421	1321	254	182	23		321			$R_1^2(4)$	S
			5	4	1238	1429	1455	1321	262	188	22		302			$R_1^2(4)$	G
18	N A N A N F		1	2	1230	1441	1464	1315	259	190	14	18	308	.267	-.230	$R_2^2(6)$	T
			3	2	1233	1440	1433	1315	252	177	11			.276	-.220		
			3	4	1237	1424	1433	1319	251	177	7			.274	-.220		
			5	4	1230	1425	1456	1319	261	189	17		299	.261	-.233	$R_1^2(4)$	G
21	N A N	1.93	1	2	1222	1429	1459	1339	261	189	3	5	300	.253	-.230	$R_2^1(4)$	G
			3	2	1227	1426	1452	1339	262	193	7						
22	N A N A N	1.44	1	2	1235	1386	1514	1323	259	186	4	7		.263	-.240		
			3	2	1262	1467	1415	1323	252	174	5		297	.273	-.223	$R_2^2(6)$	T
			3	4	1242	1472	1415	1317	252	175	5			.274	-.215		
			5	4	1259	1392	1433	1317	260	189	6		325	.264	-.236	$R_1^2(4)$	G
24	N X		1	2	1229	1400	1459	1395	266	196	16	27					
28	N K N U		1	6	1245	1432	1434	1322	261	183	13	55					
			1′	6′	1237	1409	1425	1339	262	192	6						
32	N N N R		1	6	1233	1422	1452	1331	264	198	12	44	301			$R_2^2(7)$	G
			1′	6′	1236	1428	1449	1335	260	190	7		289			$R_2^1(4)$	G
33	N U N M B		1	2	1197	1416	1428	1320	261	183	5	37	313			$R_2^2(12)$	I
40	N A	4.17	1	2	1216	1355	1490	1371	267	204	3	9	300	.235	-.229	D	I
			1′	2′	1223	1421	1428	1350	263	201	4		302			D	I
41	N N A	5.85	3	4	1250	1404	1442	1352	262	192	3	5	305	.215	-.185	C(6)	S
													300	.254	-.207	$R_2^1(4)$	T
43	N A N A N A	0.00	1	2	1236	1436	1417	1309	249	175	6	7	293			$R_2^2(6)$	T
			3	2	1243	1448	1417	1309	249	173	5						
			3	4	1246	1437	1417	1319	248	175	5		295			$R_2^2(6)$	T
			5	4	1239	1446	1422	1319	251	175	6						
			5	6	1243	1435	1422	1331	248	171	5		293			$R_2^2(6)$	T
			1	6	1260	1440	1417	1331	250	174	8						
44	N N N A	2.87	1	6	1219	1429	1475	1340	263	192	15	15	309	.259	-.221	C(6)	S
			5	6	1230	1428	1463	1340	262	191	5		309	.266	-.229	$R_1^2(4)$	G
45	N A N N N		1	2	1214	1428	1461	1312	262	191	5	14					
			3	2	1217	1434	1467	1312	272	204	24		303			$R_1^2(4)$	G
47	N A N A N O		1	2	1276	1442	1409	1320	249	166	12	36	300			$R_2^2(6)$	S
			3	2	1240	1435	1423	1320	259	190	18		294			$R_2^2(6)$	T
			3	4	1247	1437	1423	1313	250	182	14						
			5	4	1248	1420	1462	1313	254	184	30		324			$R_1^2(4)$	S
19	N U B											29	306			$R_2^1(4)$	G
20	N C A											3	305			C(8)	G
23	N S	9.62										39					
31	N U											11	306	.202	-.211	$R_1^2(4)$	G
34	N X M											58	286			C(4)	G
35	N A	4.89										4	327	.201	-.208	$R_1^2(4)$	T
36	N U M											17	308			C(7)	T

Table 1 (continued)

No.	Groups	μ (D)	P_N	P_A	d_{ON}	d_{CC}	d_{NC}	d_{CD}	d_{OD}	d_{OH}	D_{HB}	D_M	R_{OD}	δ_H	δ_O	Form	SO
					(in 0.001 Å)				(in 0.01 Å)					(in e)			
39	N A	6.37										3	307	.206	-.214	$R^2_2(6)$	G
46	N O A											2	295	.186	-.210	$R^2_2(6)$	T

Statistics from table 1a		d_{ON}	d_{CC}	d_{NC}	d_{CD}	d_{OD}	d_{OH}	D_{HB}	D_M
	ave.	1236	1427	1441	1328	258	185	10	23
	r.m.s.	15	21	24	18	6	9	7	17
	max.	1276	1448	1514	1395	272	204	30	55
	min.	1197	1355	1409	1309	248	166	3	5

Table 1b. Hydrogen Bonding in Nitrophenols*

No.	Groups	μ (D)	P_N	P_O	d_{ON}	d_{CC}	d_{NC}	d_{CD}	d_{OD}	d_{OH}	D_{HB}	D_M	R_{OD}	δ_H	δ_O	Form	SO
					(in 0.001 Å)				(in 0.01 Å)					(in e)			
47	N A N A N O		5	6	1276	1414	1409	1332	249	166	19	36	312			C(6)	S
48	N N O B											7	293			C(8)	G
50	N N O C		3	4	1235	1406	1464	1333	255	174	4	7		.279	-.231		
51	N N O	3.31	3	4	1237	1407	1449	1343	261	180	2	4		.266	-.228	C(6)	S
52	N O N	3.89	1	2	1242	1399	1457	1337	256	169	6	11					
													319	.278	-.214	C(6)	G
55	N O P		1	2	1256	1398	1454	1354	256	169	3	10		.264	-.241		
58	N O C		1	2	1240	1401	1442	1342	259	174	1	1	303	.267	-.239	C(6)	S
59	N O	3.22	1	2	1234	1395	1457	1339	259	173	1	1		.264	-.240		
60	N N N O	1.51	1	6	1227	1412	1456	1312	255	176	6	13	296	.285	-.206	C(6)	S
			1′	6′	1232	1385	1449	1358	256	170	2	12					
46	N O A											2	295	.186	-.210	$R^2_2(6)$	T
56	N O	3.93										1	295	.215	-.210	$R^2_1(4)$	T
57	N O	5.09										5	284			C(8)	G
Statistics from table 1b		ave.			1242	1402	1449	1339	256	172	5	11					
		r.m.s.			15	9	16	13	3	4	6	11					
		max.			1276	1414	1464	1358	261	180	19	36					
		min.			1227	1385	1409	1312	249	166	1	1					

* No. : Same numbering as in part 1.
μ : Dipole moment in Debye. P_N, P_A & P_O stand for the positions where the corresponding groups are located, respectively. A prime is used to distinquish conformationally different molecules in the asymmetric unit. For d_{ON}, d_{CC}, d_{NC}, d_{CD}, d_{OH} see Fig. 1. d_{OD} and R_{OD}: Distance between donor and oxygen atoms involved in intra- and intermolecular HB, respectively. Form: Pattern type of intermolecular HB[5]. SO: Symmetry operator relating molecules linked by intermolecular HB. (T: Translation, S: Screw rotation, G: Glide reflection, I: Inversion). For Groups, D_{HB}, D_M, δ_H and δ_O see text.

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paper[1] for comparision reason. The short notation for substituents used in column Groups were: A NH_2, B Br, C Cl, F F, K CF_3, M CH_3, N NO_2, O OH, P OCH_3, R NH-NH_2, S $N(CH_3)_2$, T $C(CH_3)_3$, U $NHCH_3$, V $CONH_2$, W NF_2, X $NHCOCH_3$, Z N_3 and blank for H atom. The substituents were ordered from positions 1 to 6. For each intramolecular HB, listed were the involved distances whose meaning could be seen from Fig. 1.

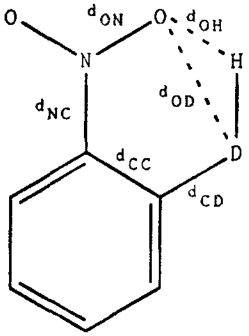


Fig. 1

Intramolecular HB

(D for donor N or O)

The D_{HB} and D_M respectively are the r.m.s. deviations from the best mean plane of the benzene ring for the atoms in the 6-member intramolecular HB ring and the whole molecule, calculated as:

$$D = (\sum_i d_i^2 /n)^{1/2}$$

where d_i is the distance to the mean benzene plane for the atom i and n is the number of atoms involved.

It is well known that intramolecular hydrogen bonding stablizes the molecule, as also shown by the impact experimental data[4].

The HB rings are essentially planar with a few exceptions having the r.m.s. deviation up to 0.3 Å. However, a significant improvement in the molecular planarity can be seen for this subclass of nitrobenzens when comparing the D_M data of related structures (see table 2), for example, m-dinitrobenzene(No. 3, in which there is no hydrogen bonding) with its ortho substituted derivatives Nos. 21, 41, 51, 52 (in which intramolecular HB

Table 2 Density and packing Coefficient in Nitrobenzenes

No.	Groups	D_X (g/cm^3)	C_K	D_M (Å)	NO.	Groups	D_X (g/cm^3)	C_K	D_M (Å)
10	N	1.378	.715	.02	41	N N A	1.626	.751	.05
15	N N	1.571	.728	.46	52	N O N	1.704	.753	.01
59	N O	1.492	.734	.01	21	N A N	1.627	.753	.05
40	N A	1.447	.742	.09	64	N N C	1.799	.768	.30
24	N X	1.436	.737	.27	13	N N N	1.675	.720	1.29
80	N G	1.471	.734	.24	60	N N N O	1.771	.745	.13
3	N N	1.574	.728	.14	44	N N N A	1.772	.768	.15
56	N O	1.476	.728	.12	32	N N N R	1.773	.775	.46
35	N A	1.435	.734	.04	68	N N N C	1.772	.717	.43
67	N C	1.576	.721	.02	16	N N N M	1.653	.741	1.18
37	N S	1.286	.714	.17	22	N A N A N	1.837	.801	.07
4	N N	1.617	.748	.09	14	N M N M N	1.632	.757	.51
57	N O	1.425	.729	.03	69	N C N C N	1.932	.741	.46
39	N A	1.425	.729	.03	45	N A N N N	1.859	.767	.14
31	N U	1.367	.726	.94	43	N A N A N A	1.936	.848	.07
23	N S	1.354	.747	.15	47	N A N A N O	1.889	.809	.36
9	N M	1.284	.691	.11	18	N A N A N F	1.944	.810	.18
75	N G	1.491	.745	.02	17	N A N A N V	1.887	.799	.65
51	N N O	1.667	.750	.04	8	N N N N N N	1.987	.768	.65

is involved). Similiar effect could be observed when comparing structure No.13 with structures Nos. 60,44,22,45,43,47.

More planar molecules are packed more efficiently. It could best be seen by comparing the C_K and D_M data in table 2 for structural isomers. The packing coefficient C_K is the ratio of the volume actually occupied by molecules in crystal to the total crystal volume^5. The larger the C_K, the more efficiently the molecules are packed. Structures Nos. 15,3 and 4, and also Nos. 23 and 37 are good examples because in the structures there is neither intra- nor intermolecular HB and thus the difference in their C_K are originated from the difference in their planarity.

INTERMOLECULAR HYDROGEN BONDING

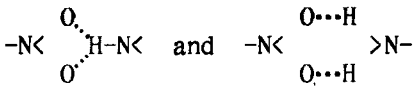
The H atoms in amine or phenolic OH group can take part in either intra- or intermolecular hydrogen bonding and sometimes in both of them. The relevant terms were listed in the remaining part of table 1.

The δ_H and δ_O respectively are the atomic partial charges for H and O atoms involved in intermolecular HB. They were calculated at STO-3G level by using the crystal structure data and the Gaussian-82 program.Since the corresponding values for the H atoms other than those involed in HB are in the range of 0.05-0.10 electrons(not listed in table 1), the δ_H values are very high and the H atoms are right sites to form intermolecular HB.

Since the position for the H atom measured by X-ray diffraction is generally less accurate than the "heavy" atom, listed were R_{OD}, the distance between the O atom in NO_2 group and the donor atom instead of H atom.

When comparing with the intramolecular HB, the intermolecular HB is relatively weak, as shown by the d_{OD} and R_{OD} data. The latter is very close to or even greater than the sum of Van Der Waals radii of the atoms involved, particularly for the cases in which the H atom has been involved in intramolecular HB. However, the intermolecular HB plays a crucial role in the molecular packing, pending on its pattern taken in individual crystal structure.

The term Form in table 1 respesents the intermolecular HB pattern. The notation was taken from Etter[8], that is, R for ring, C for chain, D for finite molecular aggregate. The numbers in subscript, superscript and parenthesis are the numbers of H atoms, acceptor atoms and the total atoms involved. For example, $R_1^2(4)$ and $R_2^2(6)$ are the short notations respectively for the HB patterns:



$$-N<\begin{matrix}O\cdots\\ \\ O\cdots\end{matrix}H-N< \quad \text{and} \quad -N<\begin{matrix}O\cdots H\\ \\ O\cdots H\end{matrix}>N-$$

The last column SO is the symmetry operator,which relates the two hydrogen bonded molecules, that is, T for translation, S for screw rotation, G for glide reflection and I for inversion. If the SO for the individual intermolecular HB is T or S or G, by symmetry the result must be an infinite molecular chain extended throughout the whole crystal structure. If the SO is inversion or pure rotation or reflection or rotoinversion, generally only finite molecular aggregate is the result. The combination of the individual HB patterns in given structure shall determine the structure type for the crystal, and various crystal properties.

Since most of the intermolecular HB in structures studied take the head-to-tail form (see above scheme), a strong polar chain results in as shown by the column μ in table 1, the experimental values of dipole moment[7].Strong polar chains favour antiparallel packing mode and therefore centersymmetric space groups[3]. It increases the packing closeness to lower the potential energy. The above could best be seen by comparing the data of packing energy (PE,see previous paper[1]) for structural isomers. For nitrophenols, the PE values are -17.50,-21.89 and -23.61 kcal/mol respectively for the ortho-, meta- and para-isomers. In the crystal of the o-nitrophenol (No.59), there is no intermolecular HB. For the m-nitrophenol (No.56) the intermolecular HB is weak, but for the p-nitrophenol (No.57), it is strong and the dipole moment is large. The corresponding data for nitroanilines (Nos. 40, 35, and 39) are -21.50, -23.11 and -24.09 kcal/mol, respectively. The unity of high crystal density and good stability as explosives in nitroanilines can be explained in term of HB in their crystals.

THE ALPHA C-H LINKAGE

In a comprehensive study on impact sensitivity of explosives with structure, Kamlet and Adolph[4] have concluded the importance of alpha C-H linkage in the impact experiment. In our database[1], there are 20 structures in each of which the alpha C-H linkage appears.

The twist angles τ of the NO_2 group with the benzene ring plane in the above 20 structures are in the range of 13° to 90° , with an average being 56.0° (29.66°), the parenthetical value being the associated r.m. s. scatter (For τ value see previous paper[1]). For the NO_2 groups having an alpha C-H linkage and another non-hydrogen ortho group, the average τ is 78.3° (9.8°), some of which are close to 90° . The NO_2 group perpendicular to the benzene ring is found in the structure No. 12 (2,4,5,6-tetramethyl-1,3-dinitrobenzene). In the structure, one of the H atoms in the alpha C-H linkage is positioned in the benzene plane, and therefore, is equally exposed to the two O atom in the NO_2 group. Although the positions for H atom have less reliability, it is assumed that the H atom could be positioned so that a local minimum potential energy is achieved like the above case. Under the condition in impact experiment, the H atom becomes the preferred site of intra- or intermolecular oxidative attack for NO_2 group and the activation energy for the reaction involving HONO formation could be lowered due to the local atomic circumstances and the ease of rotation around the C-C single bond. Similiar situation could be observed in sturctures Nos. 11,6,14,22 and 5. Very accurate measurement on the H atom position is needed to construct a precise pictu-

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