

A DTA STUDY OF PHENOLS

Part 1 Halophenols

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A comprehensive DTA study is reported of 17 halophenols and of the corresponding p-nitrobenzoylchloride 3,5-dinitrobenzoylchloride and p-phenylazobenzoylchloride derivatives, prepared "in-situ" by heating intimate mixtures of phenol and acid chloride in the DTA system. The thermal analysis data, in particular, the derivative formation temperatures, are interpreted in terms of the inductive, mesomeric and steric effects associated with the ring substituents of the phenol and acid chloride and the extent of inter- and intramolecular hydrogen-bonding existing in these systems. The DTA data collectively provide a reference base for the identification and characterization of halophenols via thermal analysis.

Phenols are of primary concern as environmental pollutants. These compounds are components of numerous commercial products such as pesticides [1] wood preservatives [2, 3] fungicides [4, 5] disinfectants [6] and dyes [7, 8]. Further, phenols are often by-products of industrial processes, such as coke ovens and tar distilleries [9, 10] petrochemical industries [11, 12] kraft pulp mill bleaching effluents [13, 14] and coal liquefaction plants [15].

Analytical methods available for the characterization and determination of phenols in the solid state are few in number. Infrared [16-19] and photoelectron spectroscopy [20] have been applied to structure evaluation of numerous phenols; however, classical spectroscopic techniques have limited applicability to the characterization of the components of a phenol mixture, due to overlap of the characteristic spectral bands.

The old, familiar characterization procedure of derivative formation and determination of the melting point thereof, has been applied to phenols.

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Various derivatives such as urethans, acetates, phenylethers and, in particular, acid chlorides [21, 22] have been used as a basis for the classical characterization of phenols. For example, the p-nitrobenzoylchloride (p-NBC) and 3,5-dinitrobenzoylchloride (3,5-dNBC) and p-phenylazobenzoylchloride (p-PABC) derivatives of phenols are synthesised via the Schotten-Baumann benzoylation reaction [23]:



However, the toxicity of the required solvent, pyridine, together with the low product yield after recrystallisation makes this characterization procedure unattractive.

Crandall and Pennington [24] have reported a brief DSC study of phenol, resorcinol and eugenol and the corresponding p-nitrophenylbenzoate derivatives. This study is suggestive of a general characterization procedure for phenols in the solid state. It is proposed here that characterization of a phenol or of the components in a phenol mixture be based upon a DTA study of individual phenols together with the in-situ formation of the corresponding p-NBC, 3,5-dNBC and p-PABC derivatives.

This Paper is the first of a series reporting an intensive DTA study of a wide variety of phenols and phenol derivatives. The "in-situ" derivative formation principle is proposed as a unique and simple thermal analysis characterization procedure for phenols generally.

Experimental

Chemicals

Phenols were obtained from Aldrich Chemical Co. UK. The sources of pNBC, 3,5-dNBC and p-PABC were Hopkin and Williams, Riedel and Haën AG and BDH, UK, respectively. Indium metal was obtained from Rigaku-Denki, Japan-mp. 156.6° [25] and benzoic acid was BDH (AR grade)-mp. 122.4° [26].

Instrumentation and associated procedures

The DTA system used throughout was the Rigaku-Denki modular Thermal Analysis System (Type-Thermoflex 8085). The DTA head was of the Boesma design and employed Pt/Pt, 13% Rh thermocouples as temperature sensors. Temperatures were determined from DTA profiles using the ASTM, EMF Tables. Sample and the alumina reference-in the mass range (8.0 ± 5.0 mg) were contained in crimped, disposable aluminium crucibles (2.5×2.5 mm), pierced with a 0.1 mm diameter escape hole and were heated at a rate at 10 deg min^{-1} in a dry, static air atmosphere.

Encapsulation of the sample and reference improves the detail of DTA profiles; essentially eliminates thermal lag [27], prevents vaporization and/or oxidation at low temperatures and during melting, assists the formation of a uniform liquid film [27]. Inhomogeneity of sample, packing density, and the extent of filling crucibles are known factors which influence DTA reproducibility [27] and are critical factors in analytical DTA applications. Tapping [27] of sample and reference in crucibles prior to encapsulation are known to eliminate these effects.

In the case of phenol/acid chloride mixtures, the mass of acid chloride used was sufficient for complete 1:1 reaction and is calculated from the following simple formulae: p-PABC : ($x + 1.6x$): p-NBC ($x + 1.3x$) and 3,5-dNBC ($x + 1.5x$) when $x =$ mass of phenol. Phenol and acid chloride were intimately ground in a mortar prior to encapsulation.

The DTA sensitivity range was $10 \mu\text{V FSD}$ and the chart speed was 2.5 mm min^{-1} . Temperature calibration of the system was effected using indium metal and benzoic acid. An overall reproducibility of 1-2% is estimated.

The thermomicroscopy system used was a Mettler Hot-Stage FP-2 Microscope. The heating rate used was 10 deg min^{-1} to parallel that of the DTA studies. Precision in temperature measurement was $\pm 0.1^\circ$. Calibration of the system was effected using benzoic acid as standard.

Data analysis: A typical DTA profile for a phenol/acid chloride derivative is shown schematically in Fig. 1. The peaks are assigned in sequence as:

1. Acid chloride mp.
2. Phenol mp. (Peaks 1 and 2 may interchange or be superimposed depending on the system involved).
3. Derivative formation temperature, (T_D).
4. Derivative mp.
5. Derivative decomposition (exo- or endothermic). ΔT_f corresponds to the derivative formation range. DTA peaks are defined in terms of onset (T_1), peak (T_2) and offset (T_3) temperatures, as shown in Fig. 2. The onset and offset temperatures are defined at

the respective points on the DTA profile which correspond to discernible deviations from the recognized base line.

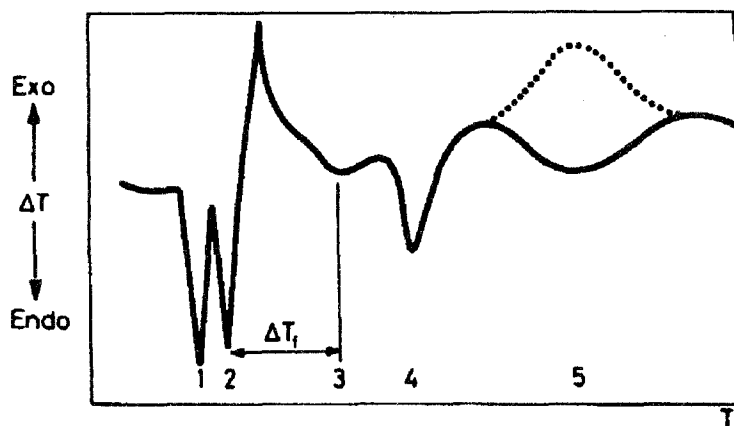


Fig. 1 Generalised DTA profile for a phenol/acid chloride derivative

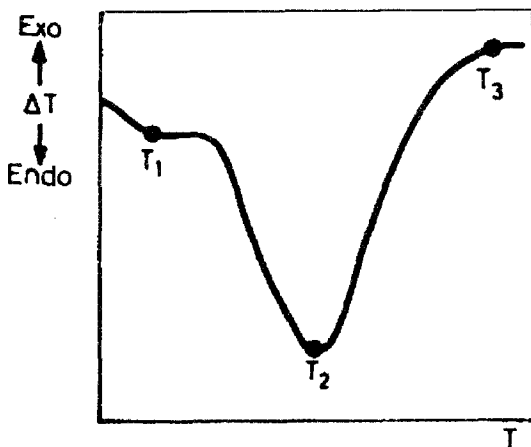


Fig. 2 Peak definition temperatures

Results and discussion

The DTA profile analysis data for the temperature calibration standards - indium metal and benzoic acid, are given in Table 1. On the basis of these data, no temperature corrections are necessary since the melting points of these standards, as determined by DTA, are within 0,4% of the accepted corresponding values.

Table 1 Peak definition temperatures for DTA standard reference materials

DTA standard	Peak definition temperatures, °C		
	onset	peak	offset
In (metal)	152	156 ^a	160
benzoic acid	117	122 ^a	127
	190	246	283

^a normal mp

The DTA profile analysis data for the acid chlorides, used in the synthesis of phenol derivatives, are given in Table 2. The first set of data in each case correspond to the melting point of the compound studied and act as reference data in the subsequent analysis of the DTA profiles of phenol derivatives.

Table 2 Peak definition temperatures for p-PABC, p-NBC and 3,5-dNBC

Acid chloride	Peak definition temperatures, °C		
	onset	peak	offset
p-PABC	88	94 ^a	108
	221	256	283
p-NBC	66	72 ^a	84
	99	159	200
3,5-dNBC	65	70 ^a	84
	182	204	243

^a normal mp

The DTA profile analysis data for 17 halophenols and the corresponding p-PABC, p-NBC and 3,5-dNBC derivatives are recorded in Table 3. All transitions are endothermic, except when marked (EXO) exothermic. Even without characterization of the individual peaks, these data collectively constitute a comprehensive source reference for the subsequent characterization of halophenols by DTA. It is simply necessary to derive a

Table 3 Peak definition temperatures for halophenols and the corresponding p-PABC, p-NBC and 3,5-dNBC derivatives

Phenol		Peak definition temperatures, °C		
		onset	peak	offset
2,6-dichloro-	parent	60	67	72
		94	152	165
	p-PABC	46	54sh	
			57	95
		95	108	117
		117	*138	155
		204	219	237
	p-NBC	237	247	271
		30	54	70
		72	98sh	
			*128	177
		177	209EXO	246
	3,5-dNBC	30	57	58
		58	61	73
		81	116	126
126		*145	155	
155		190	203	
3,4-dichloro-	parent	56	67	82
		154	189	206
	p-PABC	41	63	86
		86	94EXO	103
		103	116	137
		137	*148	167
		178	217	255
	p-NBC	40	62	76
		100	119sh	
			*139	166
		186	209	263
		43	64	78
	3,5-dNBC	103	131sh	
			*166	185
		189	226	282
3,5-dichloro-	parent	65	68	80
		96	175	191
	p-PABC	40	50	55
		55	60	73

Table 3 cont.

Phenol		Peak definition temperatures, °C			
		onset	peak	offset	
3,5-dichloro	p-NBC	73	107EXO	108	
		108	112	128	
		141	*151	162	
		181	206	242	
		26	34	39	
		39	47	70	
	3,5-dNBC	p-NBC	96	115sh	
				*171	193
			193	219	246
		3,5-dNBC	26	34sh	
				60	73
			73	80EXO	96
			96	131sh	
				*160	175
			183	218	263
2,3,6-trichloro-	parent	46	58	72	
		114	185	210	
		p-PABC	41	57	70
			70	84	96
			100	*106	114
	121		138sh		
			165	170	
	p-NBC	170	176EXO	195	
		26	42sh		
			54	70	
		72	83sh		
			*123	134	
	3,5-dNBC	138	170	187	
		27	43sh		
			56	70	
73		84	99		
127		*142	163		
169	188	201			
2,3,5-trichloro-	parent	50	62	75	
		114	171	188	
	p-PABC	41	61	77	

Table 3 cont.

Phenol		Peak definition temperatures, °C		
		onset	peak	offset
	EXO drift to	96	102	111
		111	*126	130
		130	145	162
	p-NBC	28	44sh	
			55	71
73		85sh		
		*128	146	
	149	163	181	
2,3,5-trichloro-	3,5-dNBC	29	46sh	
			57	76
		81	96	118
		139	*163	179
		179	196	231
2,4,5-trichloro	parent	53	68	80
		110	194	205
	p-PABC	54	67	
			89sh	99
		109	116sh	
			*126	160
		171	193	209
	p-NBC	36	57	69
		72	101sh	
			*128	145
		145	189	203
	3,5-dNBC	42	54sh	
			66	74
		90	112	121
129		*157	169	
173		200	236	
2,4,6-trichloro-	parent	64	68	81
		114	180	197
	p-PABC	52	63	
			75sh	87
		87	102	117
		140	*153	172
		172	206EXO	220
	p-NBC	38	58	66

Table 3 cont.

Phenol		Peak definition temperatures, °C		
		onset	peak	offset
2,4,6-trichloro-	p-NBC	68	86sh *108sh	
			136	148
	3,5-dNBC	154	155	166
		43	66	74
		84	99	107
		128	*138	146
	146	159	178	
2,3,4-trichloro-	parent	63	84	95
		107	175	191
	p-PABC	57	73	76
		76	110sh *160	172
		206	261	289
	p-NBC	46	67	
			73sh	84
		85	106	129
		149	*166	182
		194	277	291
		3,5-dNBC	47	69
		92	74sh 117sh *169	84 186
		198	264	284
	3,5,4,5-trichloro-	parent	89	101
127			207	225
p-PABC		45	60	67
		67	72	89
EXO drift to		97	110sh *121	135
		135	151	172
		p-NBC	48	64
		86	89	93
		93	113	131
		160	*176	198
		211	259	283
3,5-dNBC		52	67	76
		92	94	99
	114	128	137	

Table 3 cont.

Phenol		Peak definition temperatures, °C		
		onset	peak	offset
3,4,5-trichloro-	3,5-dNBC	176	*190	200
		213	242	267
2,3,4,6-tetrachloro-	parent	49	70	87
		104	213	226
	p-PABC	38	50sh	
			65	80
	EXO drift to	86	91	102
		102	*108	122
		139	161	177
	p-NBC	30	46	55
		59	79	99
		130	*144	166
		181	206	231
	3,5-dNBC	36	53	60
		63	81	102
		137	*160	174
174		198	223	
2,3,4,5-tetrachloro-	parent	86	98	112
		148	207	220
	p-PABC	68	76	82
		82	86	99
	EXO drift to	101	105	110
		110	*131	153
		189	201	234
	p-NBC	28	38	47
		47	60	69
		69	76	89
		159	*170	179
	3,5-dNBC	184	196	209
		30	40	49
		53	64	70
		97	107	117
		154	*177	187
187	206	218		
2,3,5,6-tetrachloro-	parent	110	115	130
		145	223	233
	p-PABC	70	82	86
		86	91	108

Table 3 cont.

Phenol		Peak definition temperatures, °C		
		onset	peak	offset
2,3,5,6-tetrachloro-	p-PABC	108	115sh	
			*137	152
		167	204	228
	p-NBC	44	52	67
		68	81sh	
			89	115
		153	*181	189
	3,5-dNBC	189	194EXO	222
		42	54	66
		83	86sh	
		90	107	
	157	*185	209	
	218	221	264	
2,3,4,5,6-pentachloro-	parent	182	188	206
		213	238	252
	p-PABC	70	95	107
		128	136	140
		140	144	150
		182	*197	212
	p-NBC	212	237EXO	259
		43	52	67
		75	130	
			145sh	165
		165	*186	204
	3,5-dNBC	204	259EXO	286
		61	68	79
		83	147	151
		EXO drift to	153	156
	175		*194	200
206	289		304	
4-bromo	parent	62	63	71
		100	160	170
	p-PABC	41	52	59
		59	61	76
		113	141	152
		152	*171	181
	p-NBC	181	196	215
		28	39	64
		88	128sh	137

Table 3 cont.

Phenol		Peak definition temperatures, °C		
		onset	peak	offset
4-bromo-	p-NBC	156	*182	200
		200	246EXO	248
	3,5-dNBC	30	43sh	
			61	76
		135	150	170
		170	*193	199
	226	259	268	
2,4,6-tribromo-	parent	82	95	110
		120	180	198
	p-PABC	58	64	72
		74	87	97
		97	*116	131
	p-NBC	131	194	212
		40	59sh	
			67	73
		73	86	111
		143	*157	166
		174	204	230
	3,5-dNBC	50	67	73
		77	80	91
		91	121	140
		154	*178	191
228		264sh		
		304	340	
2,3,4,5,6-pentabromo-	parent	219	224	230
		286	318	332
	p-PABC	84	96	102
		140	145	151
		151	154	166
	p-NBC	166	*181	203
		64	73	81
		141	143	151
		151	168	182
		182	*200	214
		244	291	323
	3,5-dNBC	57	67	73
		139	143	147
		147	160	168

Table 3 cont.

Phenol		Peak definition temperatures, °C		
		onset	peak	offset
		174	*191	214
		238	298	321
2,4,6-triiodo-	parent	152	159	170
		208	283	312
	p-PABC	81	93	103
		124	134	
			143sh	148
		162	*171	175
		175	199	207
		219	238EXO	284
	p-NBC	61	72	80
		102	128	
			138sh	140
		147	*163	191
		191	203	219
		227	235	241
3,5-dNBC	61	69	74	
	121	151	159	
		166sh		
		*186	199	
	215	228	234	

sh shoulder, * derivative melting point (confirmed by hot stage microscopy)

cross-matrix of DTA data related to heating the parent phenol, the phenol/p-PABC mixture, the phenol/p-NBC mixture and the phenol/3,5-dNBC mixture and compare with similar data, in terms of peak definition temperatures, as reported herein. Thus from the bank of DTA data given in Table 3, halophenols in the solid state can be rapidly identified and characterized and this aspect is the principal value of such data.

For the quick identification and characterization of phenols, the melting points of the halophenols and of the corresponding p-PABC, p-NBC and 3,5-dNBC derivatives are summarized in Table 4. Corresponding literature melting points of these compounds, are included when available. Interpretation of the various peaks in the DTA profiles of the halophenols and the corresponding derivatives is generally in accordance with the sequence of events shown schematically in Fig. 1. This procedure is illustrated with reference to the DTA profiles of the p-NBC derivatives of 4-bromophenol,

Table 4 Melting points of halophenols and the corresponding derivatives

Phenol	Melting point (°C)			
	Parent	p-PABC	p-NBC	3,5-dNBC
2,6-dichloro-	67	138	128	145
3,4-dichloro-	67	148	139	166
3,5-dichloro-	68	151	171	161
2,3,6-trichloro-	58	106	123	142
2,3,5-trichloro-	62	126	128	163
2,4,5-trichloro-	68	126	128	157
2,4,6-trichloro-	68	153	108	139
			105 ^a	136 ^b
2,3,4-trichloro-	84	160	166	169
3,4,5-trichloro-	101	121	176	190
2,3,4,6-tetrachloro-	70	108	144	160
2,3,4,5-tetrachloro-	98	131	170	177
2,3,5,6-tetrachloro-	115	137	181	185
2,3,4,5,6-pentachloro-	188	197	186	194
4-bromo-	64	171	182	193
		167 ^d	180 ^c	191 ^c
2,4,6-tribromo-	95	118	157	178
		116 ^d	153 ^c	174 ^c
2,3,4,5,6-pentabromo-	224	181	200	191
2,4,6-triiodo-	159	171	163	186
				181 ^c

^a From Ref. 21 ^b From Ref. 22 ^c From Ref. 21, 22 ^d From Ref. 35

2,4,6-tribromophenol and 2,3,4,5,6-pentabromophenol shown in Fig. 3. A common feature exhibited is that an intimate mixture of a phenol and a derivative-forming agent results in a depression of the melting point of both components. For the 4-bromophenol/p-NBC mixture, the individual melting points of the phenol and p-NBC cannot be differentiated and a single melting point occurs at 39° followed by derivative formation (T_D) at 128°, derivative melting at 182°C and exothermic derivative decomposition at 246°.

For the 2,4,6-tribromophenol/p-NBC system, the melting points of p-NBC and the phenol occur at 59 and 67° respectively, followed by derivative formation (T_D) at 86° and derivative melting and endothermic decomposition at 157 and 204° respectively. For the 2,3,4,5,6-pentabromophenol/p-NBC system, the melting points of p-NBC and the phenol occur at 73 and

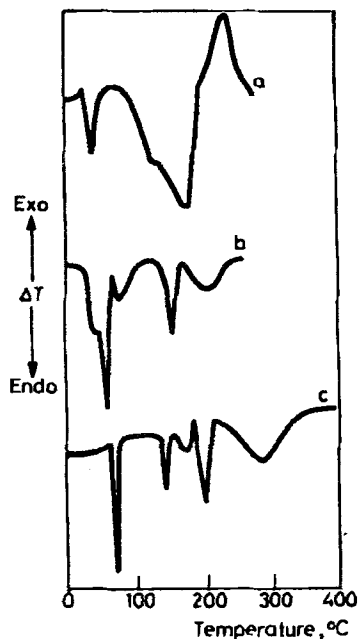


Fig. 3 DTA profiles of the p-NBC derivatives
 a) 4-bromophenol
 b) 2,4,6-tribromophenol
 c) 2,3,4,5,6-pentabromophenol

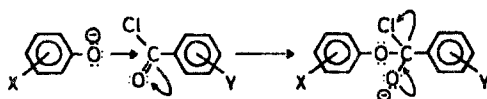
143° respectively, followed by derivative formation at 168° and derivative melting and endothermic decomposition at 200 and 291° respectively.

Various anomalies occur in this general sequence of thermal events relating to the heating of a phenol/derivative-forming agent. In some cases, mutual reaction between the phenol and the derivative-forming agent occurs prior to the melting of the derivative, as is the case for the 3,4-dichlorophenol/p-PABC mixture - the 94° exothermic peak signifies commencement of derivative formation. In other cases an exothermic commencement of derivative formation occurs after both phenol and derivative-forming agent have melted - for the 3,5-dichlorophenol/p-PABC and 3,5-dNBC mixtures, such exotherms appear at 107 and 80° respectively. In some cases (T_D) is not well defined - for example, with the 3,4-dichlorophenol/p-NBC and 2,3,4-trichlorophenol/p-PABC and 2,3,4-trichlorophenol/3,5-dNBC derivatives. Stepwise decomposition of derivatives may occur, as with the 2,6-dichlorophenol/p-PABC, 2,3,6-

trichlorophenol/p-PABC, 2,4,6-trichlorophenol/p-NBC and 2,4,6-tribromophenol/3,5-dNBC derivatives.

Similar interpretations can be given to the other composite data given in Table 3. It should be noted that in all cases of derivative formation, a parallel sequence of events was noted by heating intimate mixtures of the parent phenol and the derivative-forming agent in a hot-stage microscope. However, elucidation of the derivative formation temperature (T_D), in the majority of cases was not as readily achieved as the derivative melting point.

In order to interpret the trends in these extensive DTA as related to derivative formation, it is necessary to review the mechanism of the Schotten-Baumann derivative formation reaction [23]. In these classical reactions, phenoxide ion acts as a nucleophile and attacks the carbonyl centre of the acid chloride with subsequent formation of a derivative and release of chloride anion:



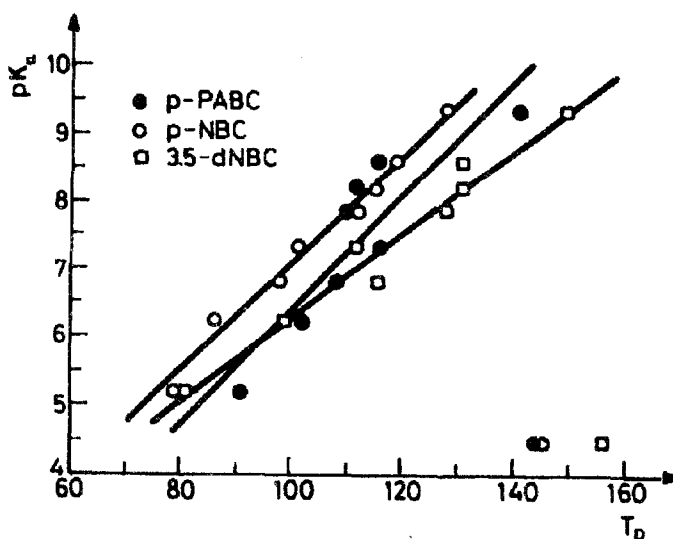
A tetrahedral intermediate is involved- the formation of which is favoured by the presence of electron withdrawing substituents Y on the acid chloride, but is hindered by bulky ortho X and Y substituents on the phenol and acid chloride respectively. Thus, the ease of derivative formation depends on the respective acidic and basic strengths of the acid chloride and phenoxide ion. These primary influencing factors are augmented by second order hydrogen bonding effects. Phenols are known to be strongly H-bonded in the solid state - for example, 2,3-, 2,5- and 2,6-dimethylphenols form intermolecular H-bonding chains within a 3-fold spiral matrix [28]. Intramolecular H-bonds are possible in phenols containing a highly electronegative ortho-substituent [16]. Such hydrogen-bonding reduces the acidic strength of the phenol and hence reduces the tendency to derivative formation.

Intermolecular hydrogen bonding is also possible between phenol and acid chloride of the type $-O-H\cdots Cl-$, $-O-H\cdots ONO$ and $O-H\cdots N=N$. Bulky ortho substituents X on the phenol inhibit these H-bonding processes [16].

A preliminary indication that the ease of derivative formation is dependent on the phenol acidity is revealed by pK_a [29-31]/ T_D relationships (Table

Table 5 pK_a data for halophenols and T_D data for the corresponding derivatives

Phenol	pK_a^a	T_D		
		P-PABC	p-NBC	3,5-dNBC
2,3,4,5,6-pentachloro-	4.50	144	145	156
2,3,4,6-tetrachloro-	5.22	91	79	81
2,4,6-trichloro-	6.23	102	86	99
2,6-dichloro-	6.80	108	98	116
2,4,5-trichloro-	7.33	116	101	112
3,4,5-trichloro-	7.84	110	113	128
3,5-dichloro-	8.18	112	115	131
3,4-dichloro	8.60	116	119	131
4-bromo-	9.34	141	128	150

^a From Refs. 29-31**Fig. 4** pK_a/T_D relationships for halophenol systems

5, Fig. 4) for halophenols and the corresponding p-PABC, p-NBC derivatives. From these data, it is apparent that the derivative formation temperature (T_D) decreases as phenol acidity increases - due consideration is given to the approximation of comparison of phenol acidity in water with derivative formation in the solid state. The trend appears to be a general one - for

example, for the tri-halophenols studied, the derivative formation temperatures increase in the order:

2,4,6-trichlorophenol < 2,4,6-tribromophenol < 2,4,6-triiodophenol

as noted for the corresponding 3,5-dNBC derivatives with corresponding T_D of 99, 121 and 166° respectively. This trend reflects the decreasing acidic strength of these phenols due to a progressive decrease in halo substituent electronegativity, and an increase in intramolecular H-bonding between phenolic and ortho halo groups [32].

For a particular phenol, the general order of derivative formation temperatures is: p-NBC < p-PABC < 3,5-dNBC, which reflects the reverse order of the Lewis acid strengths of the acid chlorides. For example, 2,6-dichlorophenol, the p-PABC, p-NBC and 3,5-dNBC derivative formation temperatures are 108, 98 and 116° respectively.

In the case where second-order H-bonding effects predominate, anomalous trends in derivative formation temperatures result. For example, from the DTA profiles for bromophenol/p-NBC mixtures shown in Fig. 3, the order in T_D is: 2,4,6-tribromophenol < 4-bromophenol < 2,3,4,5,6-pentabromophenol:

($T_D = 86, 128$ and 168° respectively). On the basis of the number of bromo substituents, the lowest T_D should correspond with the 2,3,4,5,6-pentachlorophenol/p-NBC derivative. The observed trend in T_D for these phenols is explained in terms of the relative intermolecular H-bonding effects operating. -O-H---X- intermolecular H-bonding in tri-halophenols is known to be weak [33]; whereas that in 4-bromophenol is known to be strong [34]. It is inferred that the acid strength of 2,3,4,5,6-pentabromophenol is reduced by strong inter- and intramolecular H-bonding.

The dominant effect of intramolecular H-bonding is apparent in the relatively high T_D for the derivatives of ortho substituted halophenols, for example, the relatively high T_D for the 2,6-dichlorophenol/3,5-dNBC derivative (116°). Also, considerable steric hindrance to the formation of the transition intermediate occurs in these systems.

Hence, trends in the DTA data for halophenol/p-NBC, 3,5-dNBC and p-PABC derivatives can be adequately explained in terms of inductive, mesomeric and steric effects associated with the ring substituents of the phenol and acid chloride and the extent of inter- and intramolecular H-bonding present in these systems.

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Zusammenfassung - An 17 Halophenolen und den entsprechenden p-Nitrobenzoylchlorid-, 3,5-Dinitrobenzoylchlorid- und p-Phenylazobenzoylchlorid-Derivativen wurde eine vergleichende DTA-Studie durchgeführt. Diese Substanzen wurden durch Erhitzen in niger Gemische aus Phenol und Sauerchloriden im DTA-System "in situ" hergestellt. Die DTA-Ergebnisse, insbesondere die Bildungstemperatur der Derivate wurden als Funktion des induktiven, mesomeren und sterischen Effektes in Verbindung mit den Substituenten an

Phenol und Säurechlorid sowie der Stärke der in diesem System gegenwärtigen intra- und intermolekularen Wasserstoffbrückenbindungen interpretiert. Die DTA-Daten im ganzen stellen Referenzdaten für die Identifizierung und Charakterisierung von Halophenolen mittels Thermoanalyse dar.