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Synthesis and crystal structure of a new polymorph of diisopropylammonium trichloroacetate, $C_8H_{16}Cl_3NO_2$

Abstract

$C_8H_{16}Cl_3NO_2$, monoclinic, $P2_1$ (no. 4), $a = 9.1804(5)$ Å, $b = 19.4133(10)$ Å, $c = 13.9191(7)$ Å, $\beta = 90.593(3)^\circ$, $V = 2480.6(2)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0605$, $wR_{ref}(F^2) = 0.1387$, $T = 296(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Needle, colorless
Size:	$0.51 \times 0.12 \times 0.05$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.72 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
$\theta_{\max}$, completeness:	29° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	56285, 13160, 0.064
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 11276
$N(\text{param})_{\text{refined}}$:	521
Programs:	DIAMOND [1], Bruker programs [2], SHELX [3, 4]

The asymmetric unit of the title crystal structure is shown in the figure. Ellipsoids are drawn at the 50% probability level [1]. Tables 1 and 2 contain details on the crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of the material

In a typical experiment 0.50 g (3.06 mmol) trichloroacetic acid and 0.30 g (3.00 mmol) diisopropylamine (*dip*) were mixed in a petri dish. The mixture emits a white smoke. After a few days two types of colourless crystals (cubes and needles) form in the solution. Recrystallization from ethanol yields cube crystals only, whereas the needle crystals were obtained from an 2-propanol solution. Preliminary X-ray experiments showed that the cubes represent an orthorhombic phase, whereas the needle crystals show monoclinic symmetry. The IR and Raman spectra show the typical bands and signals for the diisopropylammonium (*dipH*) cation [5] and the trichloroacetate (TCA) anion [6].

The **Raman spectrum** was measured using a Bruker MULTIRAM spectrometer; Nd:YAG-Laser at 1064 nm;

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
Cl1	−0.0416(2)	0.74558(11)	0.38100(18)	0.0533(6)
Cl2	−0.1031(2)	0.72644(10)	0.17835(17)	0.0464(5)
Cl3	0.19028(18)	0.74415(9)	0.24514(14)	0.0346(4)
Cl4	0.48392(19)	0.31158(9)	0.36335(13)	0.0337(4)
Cl5	0.70476(16)	0.31718(8)	0.51192(12)	0.0260(3)
Cl6	0.40384(19)	0.32273(9)	0.56281(14)	0.0356(4)
Cl7	0.38638(19)	0.34106(10)	0.10267(13)	0.0359(4)
Cl8	0.67175(17)	0.30574(9)	0.03859(13)	0.0312(4)
Cl9	0.4305(2)	0.30275(9)	−0.09573(13)	0.0374(4)
Cl10	−0.0458(2)	0.74599(9)	−0.14238(13)	0.0372(4)
Cl11	0.17593(16)	0.73766(8)	−0.28623(12)	0.0264(3)
Cl12	−0.1222(2)	0.71626(11)	−0.34082(14)	0.0424(5)
O1	−0.0930(5)	0.5990(2)	0.2968(4)	0.0262(10)
O2	0.1496(5)	0.6018(3)	0.2954(4)	0.0291(11)
O3	0.4064(5)	0.4546(2)	0.4569(3)	0.0227(9)
O4	0.6490(5)	0.4564(2)	0.4524(4)	0.0258(10)
O5	0.4136(5)	0.4573(2)	−0.0326(4)	0.0266(10)
O6	0.6542(5)	0.4419(2)	−0.0445(3)	0.0250(10)
O7	0.1464(5)	0.6025(2)	−0.2026(3)	0.0270(10)
O8	−0.0960(5)	0.5935(3)	−0.2161(4)	0.0295(11)
N1	−0.0632(5)	0.4731(3)	0.3915(4)	0.0192(10)
H11	−0.150574	0.465323	0.416383	0.023*
H12	−0.068586	0.512666	0.359394	0.023*
N2	0.4350(5)	0.5822(3)	0.3634(3)	0.0165(10)
H21	0.431481	0.542184	0.394495	0.020*
H22	0.347104	0.589479	0.337804	0.020*
N3	0.1257(5)	0.4979(3)	−0.0673(4)	0.0185(10)
H31	0.126573	0.530349	−0.112468	0.022*
H32	0.215037	0.480215	−0.063898	0.022*
N4	−0.3762(5)	0.5492(3)	−0.1778(4)	0.0181(10)
H41	−0.286179	0.565930	−0.181151	0.022*
H42	−0.375421	0.516328	−0.133219	0.022*
C1	0.0437(7)	0.4824(3)	0.4734(4)	0.0198(12)
H1A	0.138835	0.494873	0.447191	0.024*
C2	−0.0121(7)	0.5423(3)	0.5341(5)	0.0251(14)
H2A	−0.106087	0.530858	0.559225	0.038*
H2B	−0.020012	0.582840	0.494959	0.038*
H2C	0.054655	0.550749	0.586335	0.038*
C3A	0.0596(7)	0.4173(4)	0.5305(5)	0.0254(14)
H3A	−0.032501	0.405386	0.557934	0.038*
H3B	0.130252	0.424129	0.580955	0.038*
H3C	0.091292	0.380811	0.489177	0.038*
C4	−0.0328(7)	0.4166(3)	0.3201(4)	0.0199(12)
H4A	−0.041102	0.372094	0.352856	0.024*
C5	−0.1517(7)	0.4211(4)	0.2429(4)	0.0248(13)
H5A	−0.147518	0.465336	0.212213	0.037*
H5B	−0.245263	0.415234	0.271930	0.037*
H5C	−0.136994	0.385586	0.196012	0.037*
C6	0.1192(7)	0.4232(3)	0.2811(5)	0.0247(13)
H6A	0.132037	0.468534	0.254857	0.037*
H6B	0.133466	0.389511	0.231698	0.037*
H6C	0.188832	0.415928	0.332047	0.037*
C7	0.0289(7)	0.6272(3)	0.2902(4)	0.0173(11)
C8	0.0201(7)	0.7070(3)	0.2743(5)	0.0276(14)
C9	0.5408(7)	0.5750(3)	0.2831(4)	0.0201(12)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H9A	0.637591	0.564877	0.309888	0.024*
C10	0.4906(8)	0.5144(4)	0.2212(5)	0.0277(14)
H10A	0.490368	0.473194	0.259332	0.042*
H10B	0.555907	0.508779	0.168382	0.042*
H10C	0.394070	0.523177	0.197099	0.042*
C11	0.5476(8)	0.6413(4)	0.2259(5)	0.0287(15)
H11A	0.451188	0.654091	0.205356	0.043*
H11B	0.607905	0.634700	0.170779	0.043*
H11C	0.587986	0.677200	0.265505	0.043*
C12	0.4637(7)	0.6381(3)	0.4364(4)	0.0208(12)
H12A	0.453061	0.682893	0.404715	0.025*
C13	0.6167(7)	0.6328(4)	0.4780(5)	0.0263(14)
H13A	0.629964	0.588359	0.506945	0.039*
H13B	0.630808	0.667989	0.525659	0.039*
H13C	0.686237	0.638802	0.427592	0.039*
C14	0.3457(7)	0.6314(3)	0.5127(5)	0.0243(13)
H14A	0.251382	0.633708	0.482487	0.037*
H14B	0.355499	0.668312	0.558301	0.037*
H14C	0.356203	0.588099	0.545324	0.037*
C15	0.5299(6)	0.4295(3)	0.4608(4)	0.0169(11)
C16	0.5327(6)	0.3481(3)	0.4766(5)	0.0210(12)
C17	0.0941(7)	0.5324(3)	0.0280(4)	0.0216(13)
H17A	0.110305	0.498831	0.079549	0.026*
C18	−0.0624(7)	0.5565(4)	0.0316(5)	0.0300(15)
H18A	−0.085286	0.570166	0.095948	0.045*
H18B	−0.125806	0.519603	0.012020	0.045*
H18C	−0.075593	0.594948	−0.010987	0.045*
C19	0.2026(7)	0.5911(4)	0.0408(5)	0.0288(15)
H19A	0.188324	0.624334	−0.009563	0.043*
H19B	0.299959	0.573285	0.038049	0.043*
H19C	0.187768	0.612782	0.101901	0.043*
C20	0.0248(7)	0.4423(3)	−0.1001(4)	0.0216(13)
H20A	−0.073546	0.461530	−0.106559	0.026*
C21	0.0759(7)	0.4188(3)	−0.1991(5)	0.0261(14)
H21A	0.084891	0.458133	−0.240509	0.039*
H21B	0.006228	0.387262	−0.226115	0.039*
H21C	0.168733	0.396421	−0.192829	0.039*
C22	0.0205(8)	0.3826(3)	−0.0306(5)	0.0271(14)
H22A	0.117748	0.366222	−0.018742	0.041*
H22B	−0.037362	0.346069	−0.057618	0.041*
H22C	−0.021560	0.397435	0.028769	0.041*
C23	0.5283(7)	0.4234(3)	−0.0264(4)	0.0185(12)
C24	0.5067(7)	0.3470(3)	0.0044(4)	0.0203(12)
C25	−0.4132(7)	0.5164(3)	−0.2728(4)	0.0191(12)
H25A	−0.399566	0.550728	−0.323549	0.023*
C26	−0.5681(7)	0.4915(4)	−0.2774(5)	0.0248(13)
H26A	−0.589773	0.466219	−0.219971	0.037*
H26B	−0.580948	0.462058	−0.332238	0.037*
H26C	−0.632592	0.530252	−0.282805	0.037*
C27	−0.3039(7)	0.4587(4)	−0.2873(5)	0.0267(14)
H27A	−0.206900	0.477091	−0.283993	0.040*
H27B	−0.320011	0.437862	−0.349002	0.040*
H27C	−0.315667	0.424672	−0.237895	0.040*
C28	−0.4748(7)	0.6060(3)	−0.1443(4)	0.0190(12)
H28A	−0.573531	0.587656	−0.137251	0.023*
C29	−0.4787(8)	0.6648(3)	−0.2161(5)	0.0250(14)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H29A	−0.381170	0.679821	−0.228696	0.038*
H29B	−0.533880	0.702328	−0.190291	0.038*
H29C	−0.523629	0.649277	−0.274865	0.038*
C30	−0.4182(7)	0.6296(4)	−0.0455(4)	0.0238(13)
H30A	−0.410404	0.590544	−0.003480	0.036*
H30B	−0.484580	0.662488	−0.018927	0.036*
H30C	−0.324062	0.650480	−0.052432	0.036*
C31	0.0208(7)	0.6246(3)	−0.2215(4)	0.0200(12)
C32	0.0096(7)	0.7026(3)	−0.2483(4)	0.0190(12)

RT-InGaAS-detector; $4000\text{--}70\text{ cm}^{-1}$: 3062(w), 2986(v(C—H), s), 2962(s), 2940(v(C—H), vs), 2745(w), 2492(w), 1678($\nu_{as}(\text{COO}^-)$, m), 1456($\delta(\text{C—H})$, m), 1428($\delta(\text{C—H})$, m), 1322($\nu_{sym. \text{COO}^-}$, m), 1181(w), 1099(w), 954 (w), 912(w), 832(m), 804(s), 733($\delta(\text{COO}^-)$, m), 670(m), 471(m), 443(s), 422(COO^- , vs) 318, 275 ($\delta_{as}(\text{CCl}_3)$, s), 194 ($\rho_s(\text{CCl}_3)$, s), 119(w). **IR data** collected on a Digilab FT3400 spectrometer using a MIRacle ATR unit (Pike Technologies); $4000\text{--}560\text{ cm}^{-1}$: 3062(v(CH_3), s), 2985 (v(C—H), s), 2946(m), 2890(m), 2694(m), 2585(w), 2498(m), 2446(w), 1657 ($\nu_{as}(\text{COO}^-)$, vs), 1615(sh), 1504(w), 1464(w), 1399(m), 1380(w), 1354(m), 1319($\nu_s(\text{COO}^-)$, vs), 1149(m), 1102(m), 823($\nu_{as}(\text{CCl}_3)$, s), 735($\delta_a(\text{COO}^-)$, s), 673(m) {w = weak, m = medium, s = strong, vs = very strong}.

Experimental details

The data collection followed the standard procedures of the APEX2 user interface. For data integration and reduction a strategy using the narrow frame algorithm for 3D profile modelling was applied [2]. Structure solution and completion of the structural model was performed using the SHELX software package [3, 4]. Hydrogen atoms were included in last stages of refinement using a riding model with constrained U_{iso} parameters [4]. It should be noted that the Flack parameter determined using 4522 Parsons' quotients [7] was 0.12(2) for this Cl-containing structure measured using Mo radiation. Despite significant deviation from zero, no inversion twin was refined.

Comment

Some simple diisopropylammonium (*dipH*) salts have attracted attention as ferroelectric materials [8–13]. The aforementioned studies almost exclusively focused on some of the corresponding halogenides. Newer developments point to *dipH* salts based on oxygen-containing counter anions like perchlorate [14, 15] or trifluoromethylsulfonate to provide interesting physical properties [16]. For the *dipH* perchlorate [17], as well as for the methanesulfonate [5], we have presented

some basic structural features many years ago. Generally, the structural chemistry of simple *dipH* salts dates back in the nineties of the last century [18]. The *dipH* halogenides and some other directly related salt structures, which were characterized, all feature hydrogen bonded chains [19–27]. Even though the physical properties associated with temperature depending phase transitions have only been recently reported, the fact that this class of compounds exhibits polymorphism for almost each compound has been shown earlier. {chloride: [18, 20]; bromide: [22, 23]; iodide [24, 25]}. Furthermore, *dipH* salts are able to incorporate various solvent molecules [26–28]. This contribution forms part of our long-standing interest in hydrogen-bonded *dipH* halogenides and pseudo halogenide [19, 22, 24, 26], *dipH* salts with oxygen-containing counter anions [5, 17, 29] and a limited number of *dipH* halogenidometallates [30, 31]. Furthermore, hydrogen-bonded trichloroacetate salts are also materials with interesting properties [32–34]. Many of the chain-type hydrogen bonded polymers like *dipHI*, *dipHCl*, *dipHBr*, *dipH[HF₂]* etc. crystallize in the space group $P2_12_12_1$. In these structures hydrogen-bonded chains run along two crystallographically axes and thus are perpendicular to each other. From a structural point of view the already reported structure of diisopropylammonium trichloroacetate (*dipH* TCA) exactly features such hydrogen-bonded, perpendicularly crossed chains [35].

We here report a second polymorph of *dipH* TCA. The asymmetric unit contains four crystallographically independent *dipH* cations and four TCA counter anions (*cf.* the figure). Similarly to other *dipH* salts, hydrogen-bonded chains of cations and anions are formed. The $\text{N}\cdots\text{O}$ distances within these hydrogen bonds fall in the narrow range of $2.777(7)\text{--}2.811(7)\text{ \AA}$. The graph set descriptor for the hydrogen bonding motif in the title structure is $\text{C}^2_2(6)$ [36]. Anions and cations are both ordered and their geometric parameters are all in the expected ranges. The isopropyl groups are individually rotated around the C—N bonds to fill the needs of packing, which is typical for the *dipH* salts.

To verify that the $Z' = 4$ situation is true we furthermore analyzed some key features of the title structure. In detail, the two crystallographically independent chains (chain 1: N1, N2, O1–O4; chain 2: N3, N4, O5–O8) feature significantly different geometries (*cf.* figure [1]). For example the $\text{N}\cdots\text{N}$ distances in chain 1 are $5.059(7)$ and $5.082(7)\text{ \AA}$, whereas the corresponding distances are $4.944(7)$ and $4.941(7)\text{ \AA}$ in chain 2. The same is true for the $\text{N}\cdots\text{N}\cdots\text{N}$ angles [chain 1: $129.7(1)^\circ$; chain 2: $136.5(1)^\circ$]. We had proposed that the general rules of hydrocarbon chain packing [37] can be retrieved sometime in the packing of a *dipH* salt [17]. Obviously, in the case of the title structure, optimization procedures during the crystallization process lead to a packing with $Z' = 4$.

The comparison of the asymmetric unit of the title structure with the orthorhombic polymorph **1** shows that the content is doubled. Another obvious difference of the title structure compared to the orthorhombic polymorph **1** of *dipH* TCA [34] is that in the polymorph **1** one crystallographically independent TCA anion shows disorder of the CCl₃ group, whereas the other one appears ordered. The most interesting observation is, that the hydrogen bonded chains run both along the crystallographic *a* direction in the title structure which is in glaring contrast to polymorph **1** in which the chains run along two directions, which are perpendicular to each other.

A solid-state phase transition between the orthorhombic polymorph **1** and the new monoclinic polymorph **2** seems unlikely given the fact that it would require a complete structural rearrangement, as the arrangement of crossed chains in **1** will not be reorganized to the parallel arrangement found in the title structure. However, it may be of interest to set up an advanced study to investigate the potential temperature and pressure dependence of structural changes for both polymorphs. Finally, it was surprising to us that in the case of *dipH* TCA two chain type structures are observed, whereas in the case of *dipH* trifluoroacetate and the corresponding pentafluoropropionate [29] as well as acetates with bulkier substituents [38, 39], hydrogen-bonded cyclic moieties, composed of two cations and two anions, are observed.

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