STRYCHNIDINE SUCCINIDATE SHOWS SIMILAR SELF-ASSEMBLY TO STRYCHNINE SALTS

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Close structurally related, naturally occurring alkaloids - strychnine and brucine - are known as powerful resolving agents. Surprisingly, there are no data available on separating procedures involving strychnine and brucine derivatives. Strychnidine is a readily available, less toxic, equally stable and enantiomerically pure derivative of strychnine. Here we report the structural study carried out for a crystal of the salt of strichnidine with succinic acid. This salt forms orthorhombic crystals resembling, for many reasons, some strychnine salts crystals. It is built from alternate strychnidinium and succinidate bilayers. Strychnidine molecules are separated by hydrogen bonded sheets comprising succinic acid molecules, or more precisely succinic acid anions, where one hydrogen atom of the carboxyl groups is disociated. The succinic acid anions form infinite hydrogen bonded chains in a-direction. The strychnidine molecules pack back to back with their hydrophobic surfaces allowing the protonated amine nitrogen atoms to hydrogen bond with the carboxylate oxygen atoms (Fig. 1).

Such situation was observed previously for strychnine-carboxylic acid salts [1-3], and also for inorganic salts of strychnine [4].

The structure has interesting hydrogen bonding scheme, especially when it comes to the carboxylic acid fragment. Examining the CSD (Ver. 5.26) one may find as many as 2050 entries for carboxylic acids structures in which H-bonds are formed between a carboxyl group and a carbonyl oxygen atom from another carboxyl group. In the case of coexistence in a structure both carboxyl and carboxylate groups it is very likely that these groups will form a connection (853 entries in CSD). Very often the double and the single bonds in a carboxylate group could be easily distinguished and hence the negative charge could be ascribed to the particular oxygen [5]. In Table 1, the hydrogen bond geometry and the geometry of both carboxyl and carboxylate groups are shown. One may conclude that the C–O bond lengths in the carboxyl group (C4A–O3A and C4A–O4A) are of the usual values for C–OH and C=O, respectively. In the case of carboxylate group, however, the situation is more complicated. Searching for similar structures in CSD - it means having the same conformation of the carboxyl group and bonded it to a carboxylate anion - one may observe that only few of them have lengths longer then 1.285 Å and hardly ever around 1.300 Å. In our case the lengths of 1.298(2) and 1.230(2) Å, respectively, are close to a single and a double C–O bond lengths in a carboxyl group, respectively. As it might be expected, the hydrogen bonds are formed only between the best donors (O–H and N–H) and the oxygen atoms of higher localized electron density - O$^-$.

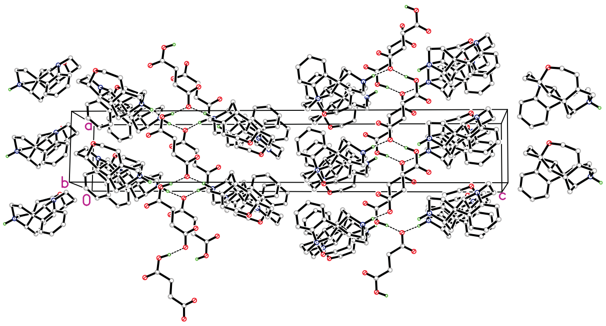

Fig. 1. Packing diagram of the title compound showing hydrogen bonds as the dashed lines. Only the hydrogen atoms involved in hydrogen bonding are shown.

Table 1. Selected geometric parameters (Å).

O1A—C1A	*1.298 (2)*	*O3A—C4A*	*1.324 (2)*
O2A—C1A	*1.230 (2)*	*O4A—C4A*	*1.213 (2)*

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N19—H19···O1A	1.02(2)	1.69(2)	2.700(2)	170.0(19)
N19—H19···O2A	1.02(2)	2.54(2)	3.225(2)	123.5(16)
O3A—H3A···O1A^{i}	0.98(3)	1.63(3)	2.598(2)	173(2)

Symmetry codes: (i) *x*+1, *y*, *z*.

References

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