Crystal Structure Studies on Arylsulphonamides and *N*-Chloro-Arylsulphonamides

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The effect of ring substitution and *N*-chlorination on the molecular geometry of arylsulphonamides and *N*-chloro-arylsulphonamides have been studied by determining the crystal structures of 2-methyl-4-chloro-benzenesulphonamide (**2M4CBSA**) and the sodium salt of *N*-chloro-2-methyl-4-chloro-benzenesulphonamide (**NaNC2M4CBSA**). The results are analyzed along with the crystal structures of benzenesulphonamide, 4-methyl-benzenesulphonamide and 4-chloro-benzenesulphonamide. The crystal structure of **NaNC2M4CBSA** has also been compared and correlated with the crystal structures of the above compounds and those of the sodium salts of *N*-chloro-benzenesulphonamide, *N*-chloro-4-methyl-benzenesulphonamide, *N*-chloro-4-chloro-benzenesulphonamide and *N*-chloro-2,4-dichloro-benzenesulphonamide. The crystal system, space group, formula units and lattice constants in Å of the new structures are: **2M4CBSA**: triclinic, $P1$, $Z = 4$, $a = 7.9030(10)$, $b = 8.6890(10)$, $c = 13.272(2)$, $\alpha = 100.680(10)^\circ$, $\beta = 98.500(10)^\circ$, $\gamma = 90.050(10)^\circ$; **NaNC2M4CBSA**: monoclinic, $C2/c$, $Z = 4$, $a = 10.9690(10)$, $b = 6.7384(6)$, $c = 30.438(2)$, $\beta = 98.442(7)^\circ$. The structure of 2M4CBSA is quite complex with four molecules in its asymmetric unit. The S-N bond length slightly decreases with substitution of electron-withdrawing groups, while the effect is more pronounced with disubstitution. The structure of **NaNC2M4CBSA** confirms that there is no interaction between nitrogen and sodium, and Na^+ is attached to one of the sulphonyl oxygen atoms. The Na^+ coordination sphere involves oxygen atoms from water moleculess of crystallization and neighbouring molecules. The S-N distance of 1.586 Å for the compound is consistent with a S-N double bond. The molecules are held together by hydrogen bonds with distances varying from 2.12 to 2.85 Å.

Key words: Crystal Structure; 2-Methyl-4-chloro-/*N*-Chloro-2-methyl-4-chloro-benzenesulphonamide.