Crystal Structure Studies on *p*-Substitutedbenzenesulphonamides 4-X-$C_6H_4SO_2NH_2$ (X = CH_3, NH_2 F, Cl or Br)

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Effect of ring substitution on the crystal structures of *p*-substitutedbenzenesulphonamides, *p*-$XC_6H_4SO_2NH_2$ (X = F, Cl, Br, CH_3 or NH_2) has been studied by determining the crystal structures of 4-chlorobenzenesulphonamide (4-$ClC_6H_4SO_2NH_2$) and 4-bromobenzenesulphonamide (4-$BrC_6H_4SO_2NH_2$) and analyzing the results along with the structures of 4-methylbenzenesulphonamide (4-$CH_3C_6H_4SO_2NH_2$), 4-fluorobenzene-sulphonamide (4-$FC_6H_4SO_2NH_2$) and 4-aminobenzenesulphonamide (4-$NH_2C_6H_4SO_2NH_2$). The crystal type, space group, formula units and lattice constants in Å of new structures are: (4-$ClC_6H_4SO_2NH_2$); monoclinic, $P2_1/n$, $Z = 4$, $a = 6.6276(10)$, $b = 16.219(3)$, $c = 7.5716(10)$, $\beta = 93.387(14)^\circ$; (4-$BrC_6H_4SO_2NH_2$): monoclinic, $P\,2_1/n$, $Z = 4$, $a = 6.5660(10)$, $b = 16.4630(10)$, $c = 7.6900(10)$, $\beta = 92.760(10)^\circ$. Orientation of the amine group with respect to the phenyl ring is given by the torsion angles C(2)-C(1)-S-N: 70.9° and C(6)-C(1)-S-N: −108.5°. Similarly, the orientation of S, O(1) and O(2) with respect to the ring are given by torsion angles. The comparison of bond lengths and bond angles of 4-fluoro-, 4-chloro-, 4-bromo-, 4-methyl- and 4-amino-benzenesulphonamides reveal that the S-N and C-S bond lengths decrease with the introduction of electron-withdrawing substituents such as F, Cl or Br, while these groups do not have significant effects on the S-O distances. The effect on ring C-C distances was not uniform. Substitution of F, Cl or Br decreases the O-S-N bond angle, but increases the O-S-N, N-S-C(1) and C(3)-C(4)-C(5) bond angles.

Key words: Crystal Structures; 4-Chloro- and 4-Bromo-benzenesulphonamide.