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$_6$H$_4$SO$_2$NH$_2$) and 4-bromo-benzenesulphonamide (4-BrC$_6$H$_4$SO$_2$NH$_2$) and analyzing the results along with the structures of 4-methylbenzenesulphonamide (4-CH$_3$C$_6$H$_4$SO$_2$NH$_2$), 4-fluorobenzene-sulphonamide (4-FC$_6$H$_4$SO$_2$NH$_2$) and 4-aminobenzenesulphonamide (4-NH$_2$C$_6$H$_4$SO$_2$NH$_2$). The crystal type, space group, formula units and lattice constants in Å of new structures are: (4-ClC$_6$H$_4$SO$_2$NH$_2$): 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$_6$H$_4$SO$_2$NH$_2$): monoclinic, $P2_1/n$, $Z =$ 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$^\circ$ and C(6)-C(1)-S-N: $-$108.5$^\circ$. 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.