

relationship for compounds containing only these elements. For C_nH_b compounds this expression estimates 75.0% of entries with $E \leq 5\%$, the highest value for all families. However, deviations are marked for aromatic compounds in which there are important π - π interactions between the delocalized π -systems (Hunter & Sanders, 1990). On the other hand, for compounds containing N and/or O atoms, the number of entries with $E \leq 5\%$ decreases, possibly due to the existence of C—H...O and N—H...O contacts in the crystal structures (Desiraju, 1991; Taylor & Kennard, 1984), which produces a more compact crystal packing and a decrease in the average volume per atom. This effect also occurs in compounds containing F atoms in which there are contacts of the types C—H...F and N—H...F (Taylor & Kennard, 1982; Emerson, Román, Luque, Gutiérrez-Zorrilla & Martínez-Ripoll, 1991). In this latter case the average volume per atom decreases and the more accurate formula is $F_{1/2}$ in which the average volume (12 \AA^3) is smaller than that in $F_{1/3}$ (14 \AA^3).

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