

## Diels-Alder reaction volumes in the solid state and solution

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### Abstract

The densities of anthracene, tetracyanoethylene, maleic anhydride, N-phenylmaleineimide, trans, trans-1,4-diphenylbuta-1,3-diene, and their Diels-Alder adducts were measured in the solid state and in solution at 25°C. The reaction volumes in the solid state were calculated from the difference in molar volumes. They turned out to be low, close to each other (-4 to -11 cm<sup>3</sup> mol<sup>-1</sup>), and slightly different from the reaction volumes (-8±1 cm<sup>3</sup> mol<sup>-1</sup>) calculated from the van der Waals radii. The reaction volumes in solutions (-15 to -32 cm<sup>3</sup> mol<sup>-1</sup>) were found from the difference in partial molar volumes of the reactants in dioxane, acetonitrile, and 1,2-dichloroethane. The experimental Diels-Alder reaction volumes in solution are determined not only by the formation of new bonds in an adduct: a considerably higher contribution (to 75%) is made by a change in the volume of intermolecular empty spaces in solution on going from reactants to adducts. © 2004 Springer Science+Business Media, Inc.

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### Keywords

Diels-Alder reaction, Intrinsic reaction volume, Packing coefficient, Pressure effect, Reaction volume in solid state, Reaction volume in solution