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# Accurate Calculation of Heats of Formation for Conjugated and Cage Systems

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**Abstract**: The calculation method of the accurate heats of formation for conjugated and cage systems has been reviewed, by choosing suitable reference compound and designing isodesmic reaction and taking examples of tetrazole derivatives and polysubstitut cubanes (i. e. the tetrazole and the cubane cage skeleton is not broken). It is pointed that the application of the group addition method to calculate the heats of formation is restricted in some case, for example, to calculate the heats of formation for polynitrocubanes.
**Key words**: heat of formation; isodesmic reaction; conjugated system; tetrazole derivative; cage compound; polysubstitute cubane; density functional theory method

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