THE 'CENTERPIECE' APPROACH: A HIGH-THROUGHPUT THERMODYNAMIC TOOL FOR LOHC AND BIOSYNTHETIC FUEL TECHNOLOGIES

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Conventional group-additivity (GA) methods often fail for complex cyclic and polycyclic molecules because ring strain and substitution effects are difficult to parametrize. To address this, we present the "centerpiece" approach — a refined GA variation that utilizes a well-characterized experimental "core" molecule to mimic the target structure, followed by the addition or removal of precisely calibrated fragments.

The reliability of this method is demonstrated across several key LOHC and biofuel families:

- Aromatic & Naphthenic Carriers: Dicyclohexylmethane and perhydro-dibenzyltoluene (errors ≤ 1–2 kJ·mol^{-1}).
- N-Heterocycles: 6,7-benzindole and its perhydrogenated (8H- and H_{12}-) forms, including methyl-substituted decahydroquinolines.
- Oxygenated Biomass Derivatives: Methoxy- and ethoxy-derivatives of bicyclohexane, decalin, indane, and benzofuran.

In all cases, the calculated enthalpies of formation (gas/liquid), vaporization, and sublimation align with both experimental data and high-level G4 quantum-chemical results within combined uncertainties. The approach effectively resolves literature contradictions and provides the precise hydrogenation/dehydrogenation enthalpies required for LOHC screening.

The "centerpiece" method is a "pen-and-paper" fast-prediction tool that requires only reliable data for the core molecule. Its integration with quantum chemistry creates a robust hybrid toolbox for the rapid, low-cost design of next-generation hydrogen storage and sustainable fuel technologies.

Keywords: chemical thermodynamics, group additivity, centerpiece approach, LOHC, enthalpy of formation, hydrogen storage, renewable fuels.

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