

Correction to “From Hexaphenylbenzene to 1,2,3,4,5,6-Hexacyclohexylcyclohexane”

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J. Am. Chem. Soc. **2020**, *142* (30), pp 12916–12920. DOI: [10.1021/jacs.0c04956](https://doi.org/10.1021/jacs.0c04956)



Cite This: *J. Am. Chem. Soc.* **2020**, *142*, 17810–17810



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Supporting Information

We recently reported the hydrogenation of hexaphenylbenzene toward partially hydrogenated hexacyclohexylbenzene (HCB) as well as fully hydrogenated 1,2,3,4,5,6-hexacyclohexylcyclohexane (HCC). The block-shaped crystal of HCC showed an orthorhombic space group *Pbcn* (four molecules per unit cell) with C_i or C_2 symmetry. During refinement, some atoms of the central ring appeared in split positions. Two disordered C_2 -symmetric six-membered rings of cyclohexane were assumed as a model for the two conformations. With the approbated restraints/constraints, the refinement of the HCC model converged well.

After publication, re-inspection of the bond angles and lengths suggested that the structure is rather due to an overlapping of different orientations of cyclohexene units. Final refinement of the new model, 1,2,3,4,5,6-hexacyclohexylcyclohexene (HCCE), was performed without restraints/constraints and also converged rapidly (revised Figure 3, below). Both models of HCC and HCCE have nearly the same *R*-values, but the latter shows a geometry indicating one double bond in the central six-membered ring.

As a consequence, HCC in the original paper should be replaced by HCCE, and the stereochemical conclusions about HCC are inappropriate. The title should be revised to “Hydrogenation of Hexaphenylbenzene”. The discussions of

the HCC crystal should be removed, and Figure 3 should be updated to show HCCE as presented herein.

The first sentence of Abstract should now read, “The hydrogenation of hexaphenylbenzene was studied, affording novel partially hydrogenated hexacyclohexylbenzene (HCB) as well as 1,2,3,4,5,6-hexacyclohexylcyclohexene (HCCE).”

The first sentence of the concluding paragraph should be revised to “In conclusion, the hydrogenation of hexaphenylbenzene was successfully achieved, furnishing the partially hydrogenated hexacyclohexylbenzene (HCB) and the 1,2,3,4,5,6-hexacyclohexylcyclohexene (HCCE).”

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/jacs.0c09797>.

Crystallographic data of HCB and HCCE (CIF)

■ ACKNOWLEDGMENTS

We thank Prof. Robert A. Pascal of Tulane University for careful examination of the crystal structure and contribution to this Correction.

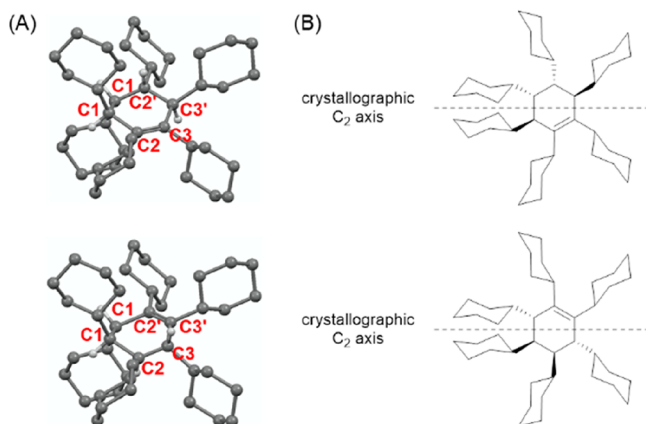


Figure 3. (A) Single-crystal structures of HCCE in the unit cell. (B) Corresponding molecular configurations of HCCE.

Published: September 29, 2020

