Supplementary information

Corrugated Layered Heptazine-based Carbon Nitride: The Lowest Energy Modifications of C$_3$N$_4$ Ground State

J. Gracia*, P. Kroll

Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX 76019-0065, USA.

* Institut fur Anorganische Chemie, Rheinisch-Westfalische Technische Hochschule (RWTH), Aachen, Professor-Pirlet-Strasse 1,

52056, Aachen, Germany.

*corresponding author: Eindhoven University of Technology, Schuit Institute of Catalysis. Department of Inorganic Chemistry and Catalysis. P.O. Box 513 5600 MB Eindhoven, The Netherlands; (email) j.m.graciabudria@tue.nl; (phone) +31 40 247 4924; (fax) +31 40 247 3481
Crystallographic information as extracted from computation

\textit{g-h-Heptazine.aiMD}

\textbf{Crystal data}

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**h-ThSi$_2$.Heptazine**

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**h-ThSi2.Heptazine.Coplanar**

Crystal data

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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**h-ThSi₂.Triazine.Coplanar**

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**g-h-Heptazine**

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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\textit{g-h-Heptazine.Coplanar}

\textit{Crystal data}

\begin{align*}
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\alpha &= 90^\circ \\
\beta &= 90^\circ \\
\gamma &= 90^\circ \\
\end{align*}

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\textit{g-m-Heptazine}
Supplementary material (ESI) for Journal of Materials Chemistry
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Crystal data

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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g-h-Triazine

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g-h-Triazine.Coplanar

Crystal data
g-o-Triazine

Crystal data

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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Supplementary material (ESI) for Journal of Materials Chemistry
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*g-o-Triazine.Coplanar*

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\text{c} = 8.04096 \text{ Å} & \quad \gamma = 90^\circ \\
\end{align*}
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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)
**Crystal data**

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\[
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**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)**

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c = 12.00537 \text{ Å}
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**Alpha**

**Crystal data**

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)

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**Beta**

**Crystal data**

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)
## Will-II

**Crystal data**

$I-43d$

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c & = 5.44378 \text{ Å} \\
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\beta & = 90^\circ \\
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\end{align*}
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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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## Dsph

**Crystal data**

$P-43m$

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\end{align*}
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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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*Spinel*

**Crystal data**

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Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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