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**Exploration and Optimization in Crystal Structure Prediction: Combining Basin Hopping with Quasi-Random Sampling**

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Computational data related to landscapes of predicted crystal structures (Table D1) have been deposited in a series of files that can be accessed via DOI XXXXX.

Table D1. Predicted crystal structures of the single component crystal structures of molecules benzamide, glycine and tetracyanoethylene with relative lattice energies (Erel) within 10 kJ mol-1 of the corresponding global minimum. Each file is named by the molecule (bzamid = benzamide; glycin = glycine; tcyety = tetracyanoethylene) and space group number. Predicted crystal structures in CIF format are provided within the zip files, with calculated energies given in the corresponding txt files.

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| --- | --- |
| File name | File content description |
| bzamid\_2 | benzamide predicted crystal structures in space group 2 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| bzamid\_4 | benzamide predicted crystal structures in space group 4 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| bzamid\_14 | benzamide predicted crystal structures in space group 14 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| bzamid\_15 | benzamide predicted crystal structures in space group 15 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| bzamid\_19 | benzamide predicted crystal structures in space group 19 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| bzamid\_43 | benzamide predicted crystal structures in space group 43 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| bzamid\_88 | benzamide predicted crystal structures in space group 88 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| tcyety\_2 | tetracyanoethylene predicted crystal structures in space group 2 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| tcyety\_4 | tetracyanoethylene predicted crystal structures in space group 4 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| tcyety\_14 | tetracyanoethylene predicted crystal structures in space group 14 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| tcyety\_15 | tetracyanoethylene predicted crystal structures in space group 15 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| tcyety\_19 | tetracyanoethylene predicted crystal structures in space group 19 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| tcyety\_43 | tetracyanoethylene predicted crystal structures in space group 43 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| tcyety\_88 | tetracyanoethylene predicted crystal structures in space group 88 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| glycin\_2 | glycine predicted crystal structures in space group 2 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| glycin\_4 | glycine predicted crystal structures in space group 4 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| glycin\_14 | glycine predicted crystal structures in space group 14 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| glycin\_15 | glycine predicted crystal structures in space group 15 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| glycin\_19 | glycine predicted crystal structures in space group 19 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| glycin\_43 | glycine predicted crystal structures in space group 43 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| glycin\_88 | glycine predicted crystal structures in space group 88 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |

Table D2. Predicted crystal structures of the TTBI with relative lattice energies (Erel) within 10 kJ mol-1 of the corresponding global minimum. Each file is named by the molecule (ttbi) and space group number. Predicted crystal structures in CIF format are provided within the zip files, with calculated energies given in the corresponding txt files.

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| File name | File content description |
| ttbi\_2 | TTBI predicted crystal structures in space group 2 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_4 | TTBI predicted crystal structures in space group 4 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_14 | TTBI predicted crystal structures in space group 14 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_15 | TTBI predicted crystal structures in space group 15 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_19 | TTBI predicted crystal structures in space group 19 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_43 | TTBI predicted crystal structures in space group 43 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_77 | TTBI predicted crystal structures in space group 77 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_86 | TTBI predicted crystal structures in space group 86 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |
| ttbi\_88 | TTBI predicted crystal structures in space group 88 with lattice energies within 110 kJ mol-1 of the global energy minimum in this space group. |

Table D3. Predicted crystal structures of the co-crystal systems PYRPMA and XAFQAZ with relative lattice energies (Erel) within 10 kJ mol-1 of the corresponding global minimum. Each file is named by the co-crystal, using the Cambridge Structural Database reference code (pyrpma; xafqaz) and space group number. Predicted crystal structures in CIF format are provided within the zip files, with calculated energies given in the corresponding txt files.

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| File name | File content description |
| pyrpma\_2 | PYRPMA predicted crystal structures in space group 2 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| pyrpma\_4 | PYRPMA predicted crystal structures in space group 4 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| pyrpma\_14 | PYRPMA predicted crystal structures in space group 14 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| xafqaz\_14 | XAFQAZ predicted crystal structures in space group 14 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| xafqaz\_43 | XAFQAZ predicted crystal structures in space group 43 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |
| xafqaz\_88 | XAFQAZ predicted crystal structures in space group 88 with lattice energies within 10 kJ mol-1 of the global energy minimum in this space group. |