STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

**Volume 76 (2020)**

**Supporting information for article:**

# Interplay between packing, dimer interaction energy and morphology in a series of tricyclic imide crystals

**Maura Malinska, Aleksandra Kieliszek, Anna E. Kozioł, Barbara Mirosław and Krzysztof Woźniak**

# Interplay between packing, dimer interaction energy, and morphology in series of tricyclic imide crystals

Maura Malinska,[*,†] Aleksandra Kieliszek,[†,‡] Anna E. Kozioł,[¶] Barbara Mirosław,[¶] and Krzysztof Woźniak[†]

†*Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Poland*

‡*Faculty of Physics, University of Warsaw, Warsaw, Poland*

¶*Faculty of Chemistry, Maria Curie-Sklodowska University, Lublin, Poland*

E-mail: mmalinska@chem.uw.edu.pl

Phone: +48 22 55 26356

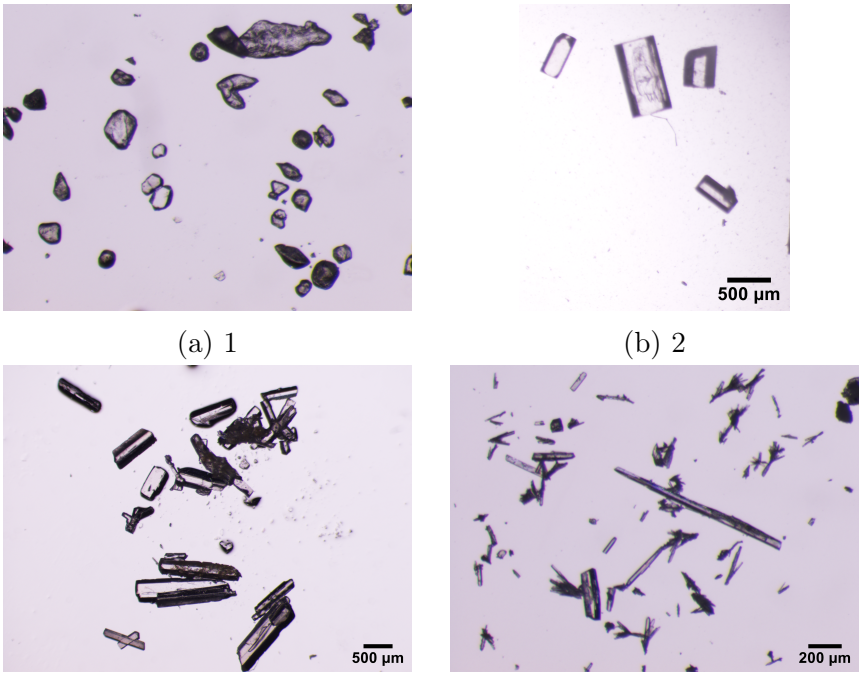
## List of Figures

# List of Tables



Table S1: Summary of slice energies, attachment energies [kJ mol$^{-1}$] and morphological importance (M.I. [%]) for surfaces of 1

| Facets | {100} | {11-1} | {010} |
|---|---|---|---|
| d | 8.5 | 5.4 | 7.8 |
| $E_{sl}$ | -117.1 | -76.0 | -83.6 |
| $E_{att}$ | -41.5 | -82.7 | -75.0 |
| M.I | 34 | 5 | 5 |




(a) 1 (b) 2

(c) 4 (d) 5

Figure S1: Morphology of 1, 2, 4 and 5

Table S2: Summary of slice energies, attachment energies [kJ mol$^{-1}$] and morphological importance (M.I. [%]) for surfaces of 2

| Facets | {100} | {011} | {11-1} | {110} |
|---|---|---|---|---|
| d | 11.4 | 13.7 | 17.8 | 14.6 |
| $E_{sl}$ | -122.7 | -81.8 | -100.3 | -100.1 |
| $E_{att}$ | -58.2 | -99.1 | -80.6 | -80.8 |
| M.I | 14 | 6 | 6 | 5 |

Table S3: Summary of slice energies, attachment energies [kJ mol$^{-1}$] and morphological importance (M.I. [%]) for surfaces of 3

| Facets | {10-1} | {011} | {11-1} | {002} |
|---|---|---|---|---|
| d | 12.4 | 13.3 | 16.0 | 17.6 |
| $E_{sl}$ | -140.3 | -123.5 | -121.4 | -130.3 |
| $E_{att}$ | -69.1 | -85.9 | -89.5 | -79.0 |
| M.I | 14 | 8 | 4 | 10 |

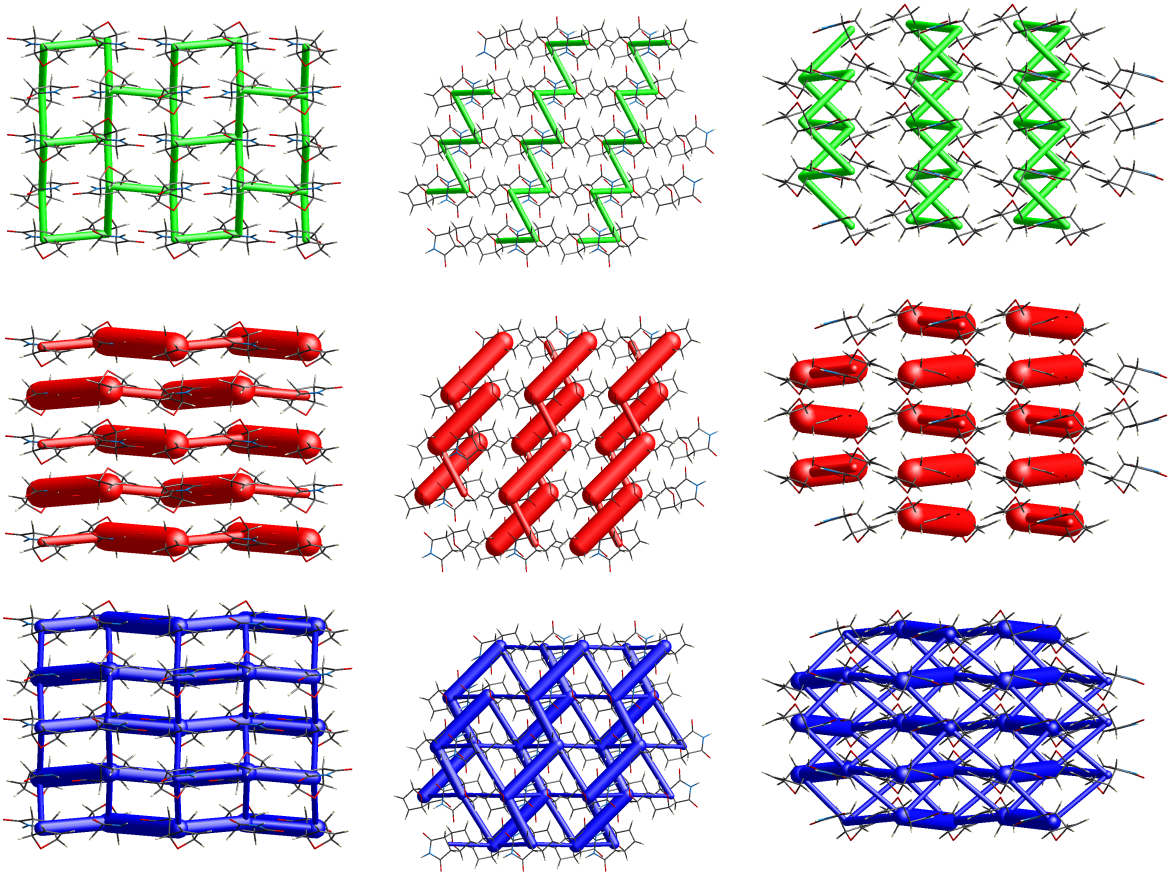


Figure S2: Energy frameworks generated for the 1 crystal. Line thickness indicates the interaction energy value (the thicker the line the greater the energy). In rows dispersion energy (green), electrostatic energy (red) and total energy (blue). Views are presented along the X axis (1st column), Y axis (2nd column) and Z axis (3rd column).

Table S4: Summary of slice energies, attachment energies [kJ mol$^{-1}$] and morphological importance (M.I. [%]) for surfaces of 4

| Facets | {001} | {10-1} | {010} | {100} | {111} | {011} | {110} |
|---|---|---|---|---|---|---|---|
| d | 7.0 | 15.0 | 12.2 | 13.2 | 16.6 | 13.9 | 15.2 |
| $E_{sl}$ | -136.3 | -198.3 | -162.8 | -187.0 | -194.0 | -189.0 | 184.2 |
| $E_{att}$ | -252.8 | -190.8 | -226.3 | -202.0 | -195.1 | -200.1 | 204.9 |
| M.I | 9 | 8 | 7 | 7 | 7 | 7 | 5 |

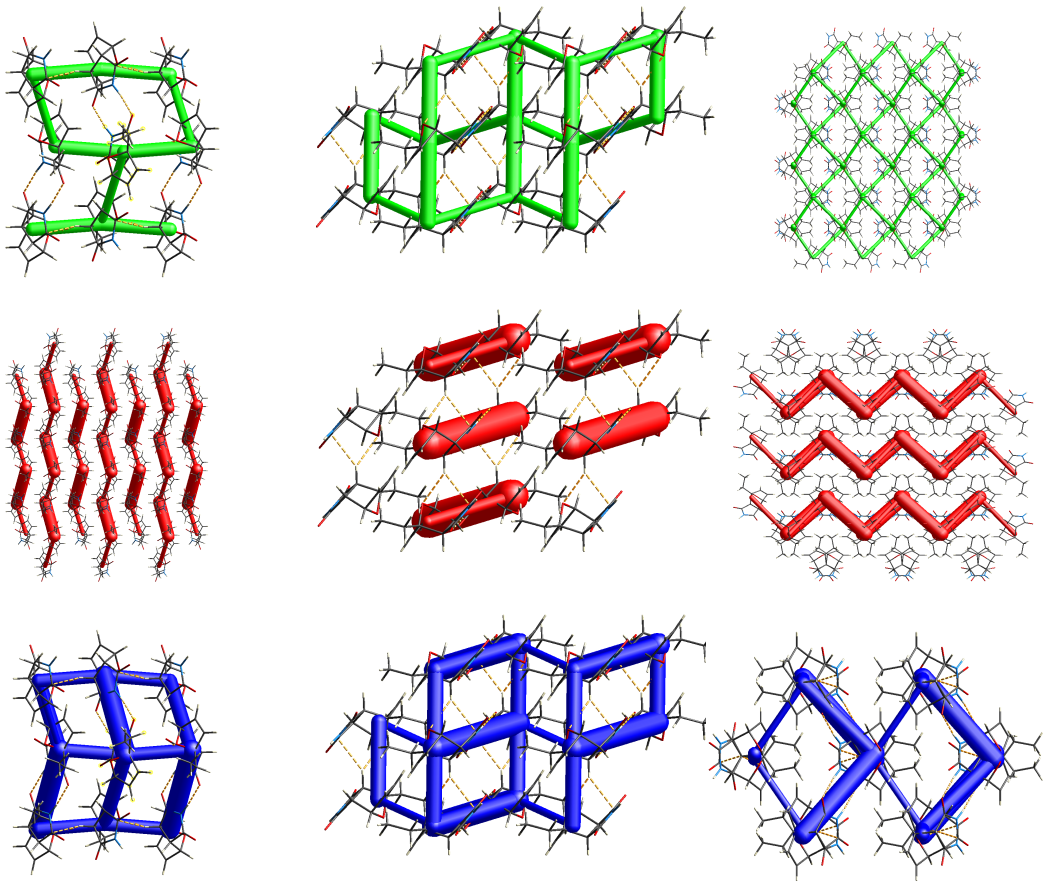


Figure S3: Energy frameworks generated for the 2 crystal. Line thickness indicates the interaction energy value (the thicker the line the greater the energy). In rows dispersion energy (green), electrostatic energy (red) and total energy (blue). Views are presented along the X axis (1st column), Y axis (2nd column) and Z axis (3rd column).

Table S5: Summary of slice energies, attachment energies [kJ mol$^{-1}$] and morphological importance (M.I. [%]) for surfaces of 5

| Facets | {10-1} | {002} | {011} |
|---|---|---|---|
| d | 8.5 | 5.4 | 7.8 |
| $E_{sl}$ | -313.7 | -301.3 | -268.1 |
| $E_{att}$ | -105.6 | -117.9 | -151.1 |
| M.I | 20 | 15 | 8 |

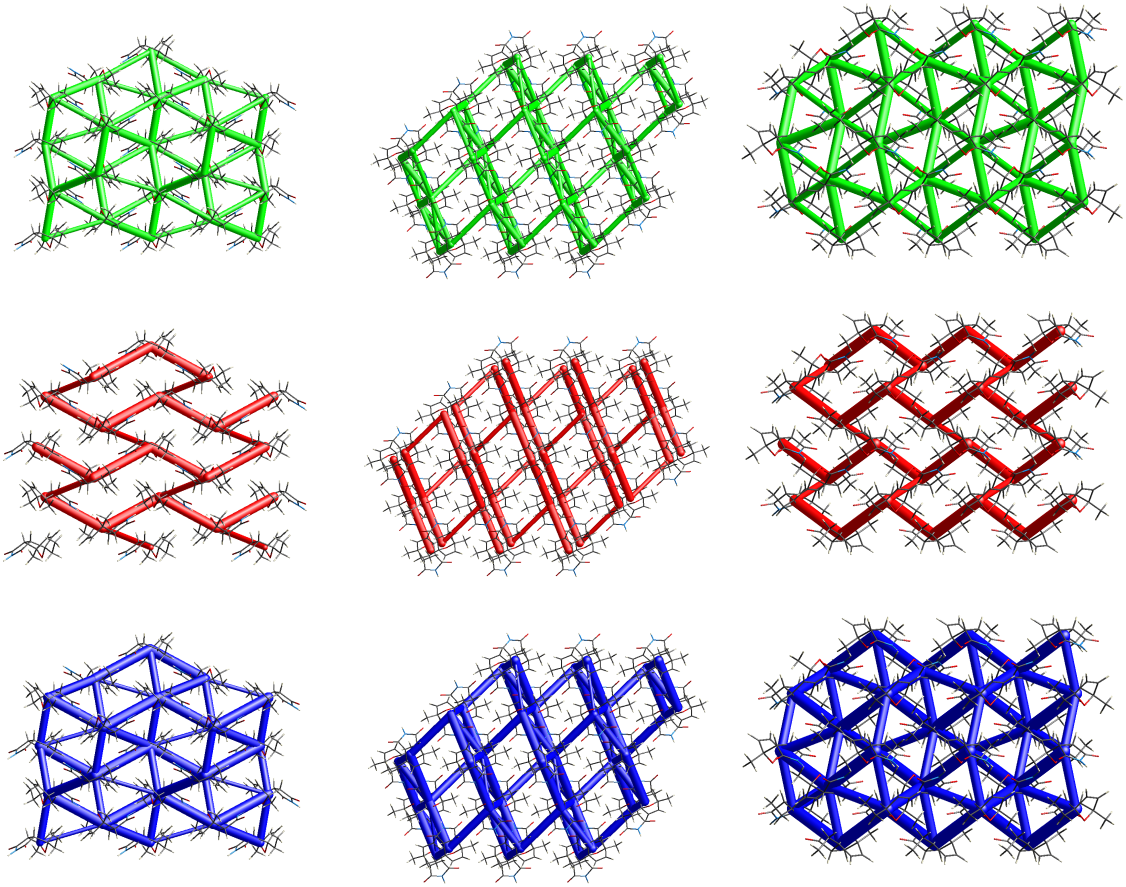


Figure S4: Energy frameworks generated for the 3 crystal. Line thickness indicates the interaction energy value (the thicker the line the greater the energy). In rows dispersion energy (green), electrostatic energy (red) and total energy (blue). Views are presented along the X axis (1st column), Y axis (2nd column) and Z axis (3rd column).

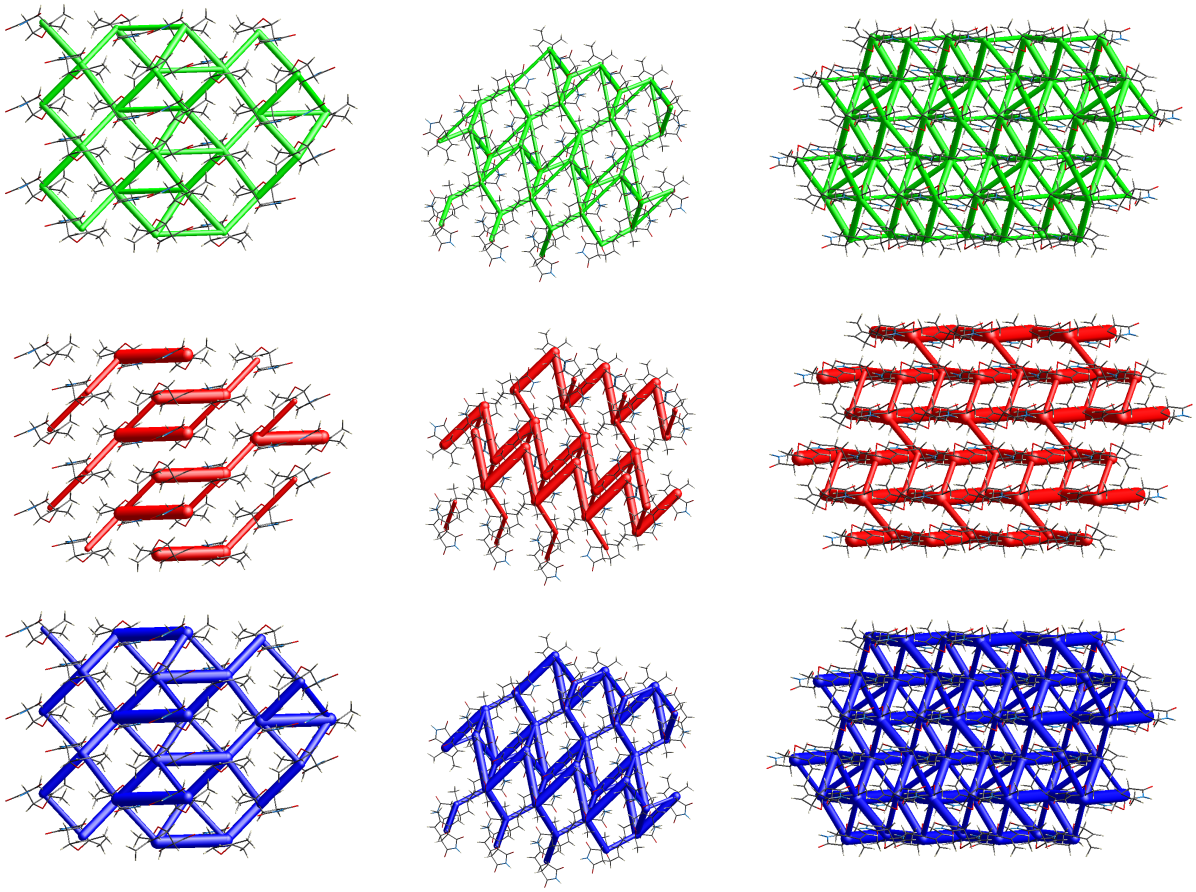


Figure S5: Energy frameworks generated for the 4 crystal. Line thickness indicates the interaction energy value (the thicker the line the greater the energy). In rows dispersion energy (green), electrostatic energy (red) and total energy (blue). Views are presented along the X axis (1st column), Y axis (2nd column) and Z axis (3rd column).

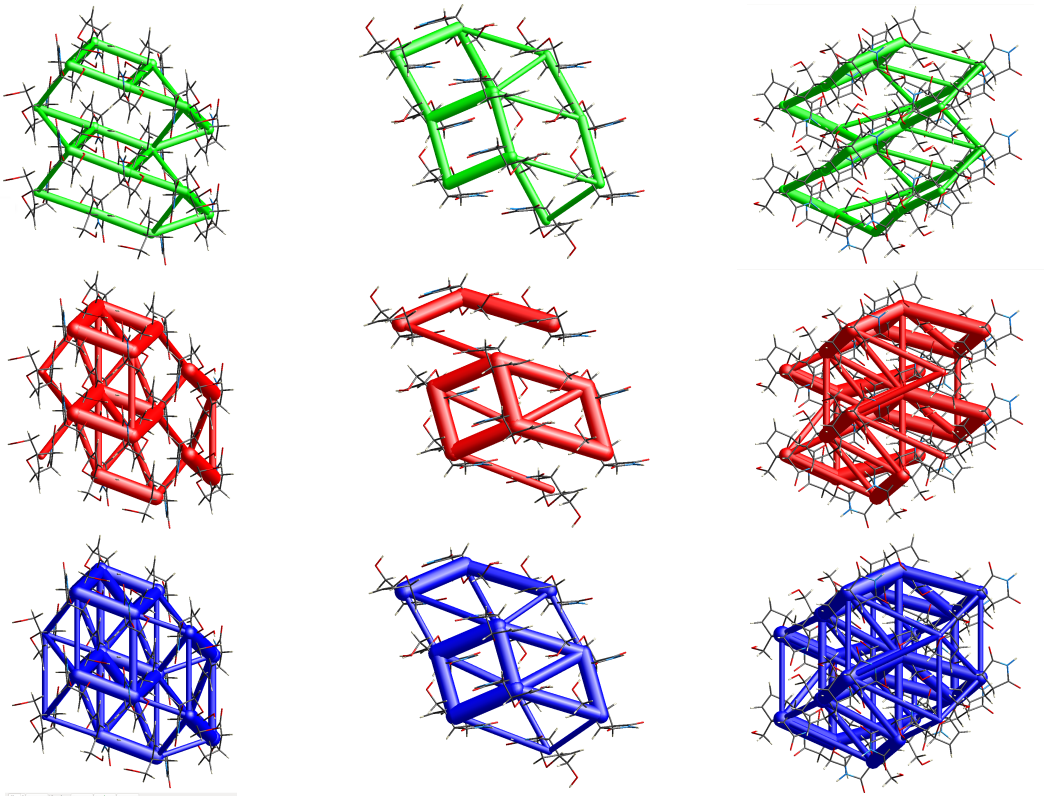
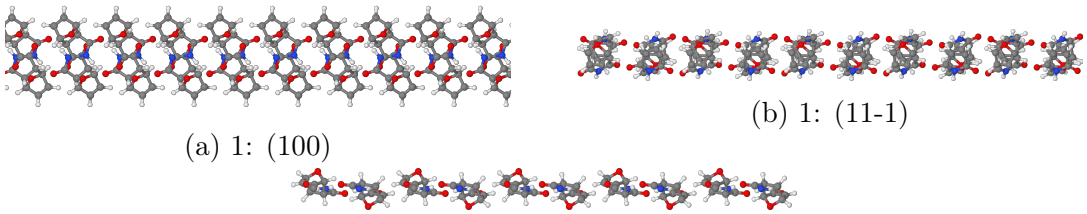


Figure S6: Energy frameworks generated for the 5 crystal. Line thickness indicates the interaction energy value (the thicker the line the greater the energy). In rows dispersion energy (green), electrostatic energy (red) and total energy (blue). Views are presented along the X axis (1st column), Y axis (2nd column) and Z axis (3rd column).

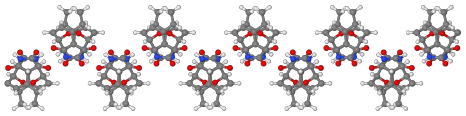


(a) 1: (100)

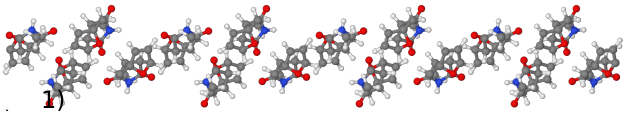
(b) 1: (11-1)

(c) 1: (010)

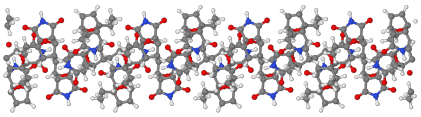
Figure S7: The most morphologically important facets of the 1 crystal visualised with the aid of Jmol.



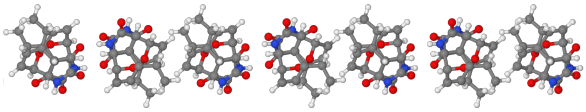
(a) 2: (100)



(b) 2: (011)

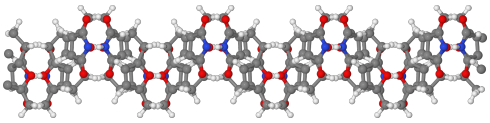


(c) 2: (11-1)

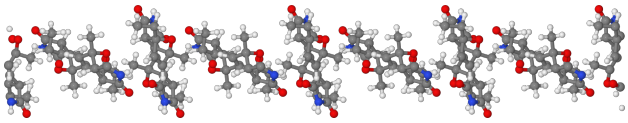


(d) 2: (110)

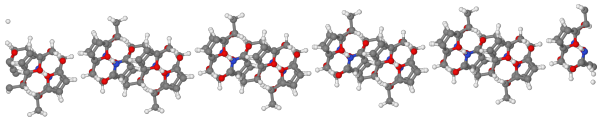
Figure S8: The most morphologically important facets of 2 crystals visualised with the aid of Jmol.



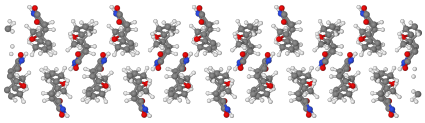
(a) 3: (10-1)



(b) 3: (011)

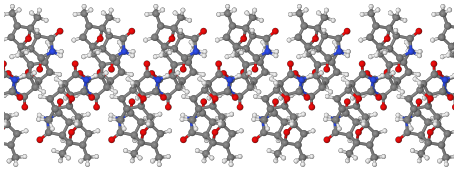


(c) 3: (11-1)

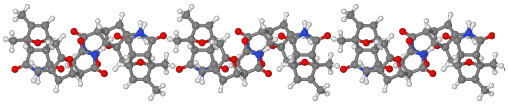


(d) 3: (002)

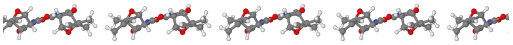
Figure S9: The most morphologically important facets of 3 crystals visualised with the aid of Jmol.



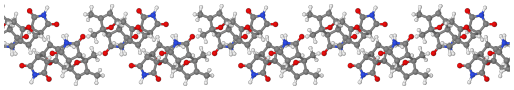
(a) 4: (001)



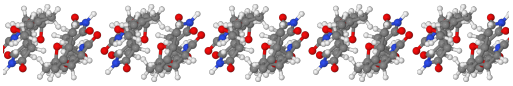
(b) 4: (10-1)



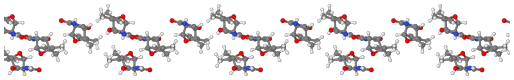
(c) 4: (010)



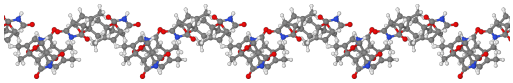
(d) 4: (100)



(e) 4: (111)

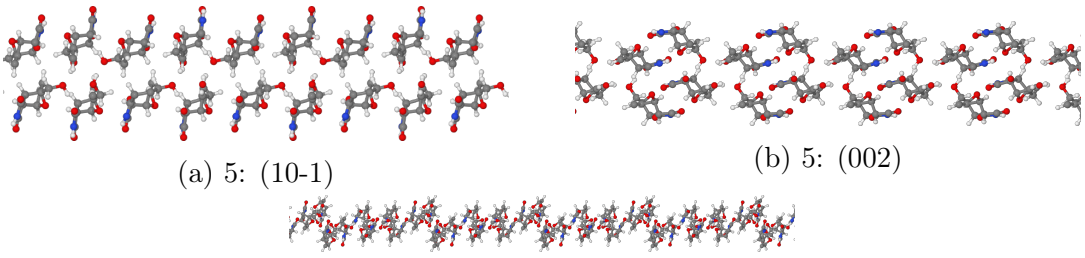


(f) 4: (011)



(g) 4: (110)

Figure S10: The most morphologically important facets of 4 crystals visualised with the aid of Jmol.



(a) 5: (10-1)

(b) 5: (002)

(c) 5: (011)

Figure S11: The most morphologically important facets of 5 crystals visualised with the aid of Jmol.