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**Supporting information for article:**

# Invariom-model refinement and Hirshfeld surface analysis of well-ordered solvent-free dibenzo-21-crown-7

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**Table S1** Invarioms employed.

| Atoms | Invariom |
|---|---|
| C2, C3, C12, C13, C15, C16, C18, C19, C28, C29 | C1o1c1h1h |
| C5, C10, C21, C26 | 6-C#6c[#6c1o]#6c[#6c1h]1o |
| C6, C7, C8, C9, C22, C23, C24, C25 | 6-C#6c[#6c1o]#6c[#6c1h]1h |
| H2a, H2b, H3a, H3b, H12a, H12b, H13a, H13b, H15a, H15b, H16a, H16b, H18a, H18b, H19a, H19b, H28a, H28b, H29a, H29b | H1c[1o1c1h] |
| H6, H7, H8, H9, H22, H23, H24, H25 | H@6c |
| O1, O14, O17 | O1c1c |
| O4, O11, O20, O27 | O@6c1c |

**Table S2** Interaction energies for neighbouring molecules as computed using DFT [B3LYP/6-31G(d,p)].

| | *N* | Symmetry operator | *R* | $E'_{ele}$ | $E'_{pol}$ | $E'_{dis}$ | $E'_{rep}$ | $E_{tot}$ |
|---|---|---|---|---|---|---|---|---|
| | 2 | *x*, *y*, *z* | 4.98 | –29.7 | –6.6 | –109.1 | 68.8 | –88.8 |
| | 1 | –*x*, –*y*, –*z* | 8.23 | –2.4 | –0.9 | –33.3 | 15.4 | –22.6 |
| | 2 | *x*, –*y*+½, *z*+½ | 11.69 | –7.9 | –1.6 | –31.8 | 23.4 | –22.9 |
| | 2 | *x*, –*y*+½, *z*+½ | 12.37 | –7.5 | –1.5 | –28.9 | 21.4 | –21.0 |
| | 2 | –*x*, *y*+½, –*z*+½ | 11.56 | –6.1 | –1.3 | –17.1 | 12.8 | –14.4 |
| | 2 | –*x*, *y*+½, –*z*+½ | 11.75 | –1.1 | –0.3 | –14.5 | 9.4 | –8.2 |
| | 1 | –*x*, –*y*, –*z* | 8.96 | –11.0 | –1.9 | –38.0 | 27.7 | –29.1 |
| | 1 | –*x*, –*y*, –*z* | 11.41 | –0.1 | –0.2 | –11.6 | 2.2 | –9.0 |
| | 1 | –*x*, –*y*, –*z* | 12.93 | –3.6 | –0.5 | –6.8 | 4.6 | –7.2 |

Colour codes referring to Figure S2; *N:* number of neighbours of given type; symmetry operator for the wave function in relation to central molecule; *R*: distance between molecular centroids in Å, *E*′: unscaled electrostatic (ele), polarisation (pol), dispersion (dis), and exchange-repulsion (rep) energies in kJ mol$^{-1}$; $E_{tot}$: scaled total interaction energy in kJ mol$^{-1}$.

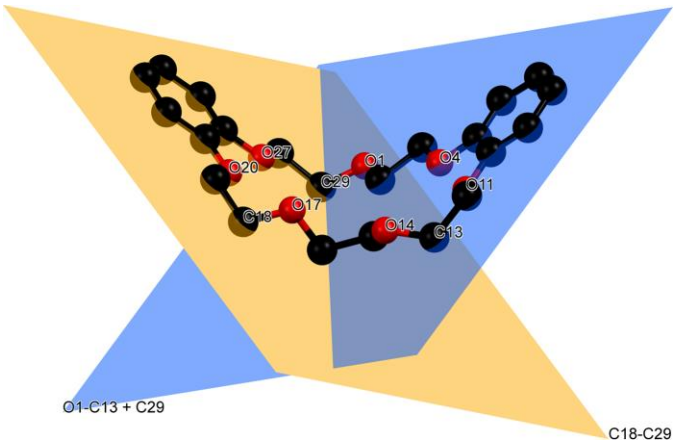


**Figure S1** Boat-like conformation of (I) in the crystal with governing least-squares planes, one including C18–C29 (orange) and one including O1–C13 as well as C29 (blue). Ball-and-stick representation with arbitrary radii (black: carbon, red: oxygen, hydrogen atoms omitted for clarity).

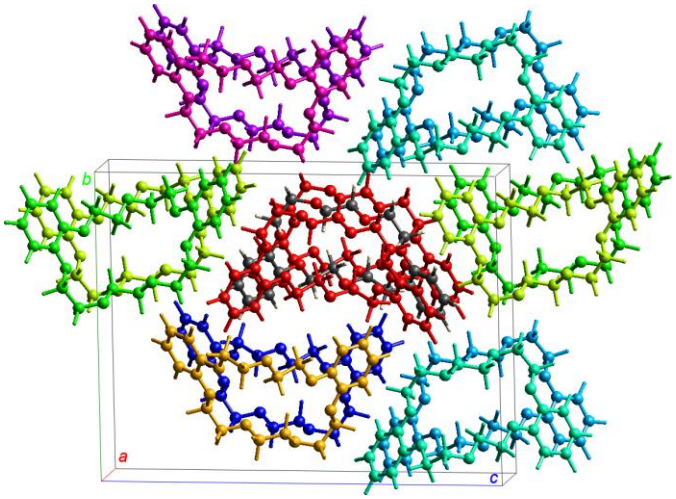


**Figure S2** Molecular cluster for computation of interaction energies with colour-coded molecules (*cf.* Table S2). Ball-and-stick representation with arbitrary radii (central molecule with colour differentiation for elements).