Mercury

- First released September 2001
- Visualisation, particularly of organic crystal structures. Replacement for Pluto...
Mercury

- First released September 2001
- Visualisation, particularly of organic crystal structures. Replacement for Pluto...
- Grown significantly during that time:
  - A hub for components of the CSD System
  - Can search the CSD in a number of ways within Mercury
    - from visualisation to interrogation and exploration...
Mercury 1.0, 2001
Mercury 4.0, 2019
Some overlooked features? Some favourites...
It’s the simple things

- Do you load .cif files into Mercury a lot?
It’s the simple things

- Do you look at chiral molecules a lot?
It’s the simple things

- Do you select parts of molecules often (to change display styles for example?)
- Alt-Left Mouse button invokes lasso selection
It’s the simple things

- Do you look at hydrogen bonds a lot?
- Colour by distance
It’s the simple things

• Disordered structures?

“Suppression” is our term for disordered atoms
It’s the simple things

- Select by SMARTS
It’s the simple things

• Make pictures for publications or slides?
It’s the simple things

• Make pictures for publications or slides?
It’s the simple things

• Work with coordination metals?

Recent update!
And a little more involved

- Molecule Overlay

- 2 molecules in the asymmetric unit and want to compare their conformations?
And a little more involved

- Overlaying more than 2 structures?

Multiple structures dialog allows you to “freeze” and hide the overlaid molecules

Last molecule selected is the one that moves
And a little more involved

- Want to overlay molecules from different structures? (and you don’t want to use structure overlay)

Select substructure
And a little more involved

- Do you want to find all crystal structures containing a particular molecule?
  - Solid form landscape of paracetamol, ethanol solvates, anything with a common substructure, not just packing features...
And a little more involved

- Do you build subsets of structures based on a particular property? Cut and paste from Excel....

|    | Refcode | spacegr | zprime | mol_co | molecule | active1 | laxis | maxis | saxis | Im_rati | Is_ratic | ms_rati | shape | Atoms | Aroma | Ring | A |
|----|---------|---------|--------|--------|----------|---------|-------|-------|-------|---------|----------|---------|-------|-------|-------|-----|
| 54 | ABAGUG  | P21/c   | 0.5    | 1269.882 | 1269.882 | 1269.882 | 20.021 | 16.593 | 15.394 | 1.207   | 1.301   | 1.078   | 0.054 | 180   | 6    | 36  |
| 134| ABAZUA  | P21/c   | 0.5    | 556.5447 | 556.5447 | 556.5447 | 19.086 | 12.307 | 11.725 | 1.551   | 1.628   | 1.05    | 0.055 | 80    | 6    | 36  |
| 148| ABECAL  | P21/n   | 0.5    | 354.4418 | 354.4418 | 354.4418 | 20.035 | 9.386  | 3.592  | 2.135   | 5.577   | 2.613   | 0.13  | 46    | 6    | 35  |
| 166| ABEFOE  | P2/n    | 0.5    | 618.7596 | 618.7596 | 618.7596 | 13.965 | 12.457 | 9.76   | 1.121   | 1.431   | 1.276   | 0.091 | 82    | 6    | 36  |
| 167| ABEFOE01| P2/n    | 0.5    | 618.7596 | 618.7596 | 618.7596 | 13.965 | 12.457 | 9.76   | 1.121   | 1.431   | 1.276   | 0.091 | 82    | 6    | 36  |
| 175| ABEGEV  | P-1     | 0.5    | 620.7754 | 620.7754 | 620.7754 | 14.918 | 13.838 | 13.373 | 1.078   | 1.116   | 1.035   | 0.069 | 84    | 6    | 36  |
| 186| ABEHEW  | Pbca    | 0.5    | 744.746  | 744.746  | 744.746  | 16.922 | 15.583 | 10.971 | 1.09    | 1.549   | 1.42    | 0.084 | 95    | 6    | 36  |
| 191| ABEHOG  | P21/n   | 0.5    | 700.6936 | 700.6936 | 700.6936 | 15.065 | 14.07  | 10.708 | 1.071   | 1.407   | 1.314   | 0.087 | 88    | 6    | 36  |
| 283| ABERJI  | P21/n   | 0.5    | 694.7266 | 694.7266 | 694.7266 | 15.2   | 15.144 | 10.921 | 1.004   | 1.392   | 1.387   | 0.091 | 86    | 6    | 36  |
| 308| ABIBES  | P21/c   | 0.5    | 452.756  | 492.756  | 492.756  | 14.536 | 12.656 | 9.833  | 1.148   | 1.509   | 1.314   | 0.09  | 54    | 6    | 36  |

Property in this column is the number of aromatic rings in molecule. Chosen structures with 6 aromatic rings.
And a little more involved

- Do you build subsets of structures based on a particular property? Cut and paste from Excel... into Mercury
And a little more involved

- Editing a structure
  - Invert a structure/Invert a molecule
  - Removing symmetry by choosing a subgroup
  - Changing the space group setting: $P2_1/n$ to $P2_1/c$
And a little more involved

- Do you explore structural changes due to phase transitions?
- FIZPEL/ FIZPEL01

Mirror symmetry relationship formalised in \( \text{P2}_1/c \)

Transformed to subgroup P-1

\( \text{P-1} \)

\( \text{Low temp} \)
And a little more involved

- Sketch a molecule and generate a conformation
And a little more involved

• Sketch a molecule and generate a conformation....
Too many to mention:

- Custom view
- Powder pattern simulation
- Links to Isostar, GOLD, Mogul etc
- Motif searching and hydrogen bond propensity calculations
- More info dialog
  - Nearest Miller Plane
  - Selecting atoms from Atoms list
- MOPAC – point group symmetry
Acknowledgements – too many to mention

• Many thanks to all the developers, testers and documentation-writers at CCDC
• Many thanks to you for suggesting enhancements and new features .......and reporting bugs

Thank you!