A visualization of the anomeric effect from crystal structures.

Henry Rzepa

Affiliation not available

April 17, 2023
A visualization of the anomeric effect from crystal structures.

HENRY RZEP A
I also include a further constraint, that the diffraction data must be collected below 140K. The hotspot moves to ~55/60° indicating values free of some vibrational noise.

Interestingly, replacing oxygen with nitrogen reveals relatively few examples of the effect (C(NR)4 is an exception). Replacing O by divalent S produces only 13 hits, with the surprising result (below) that in all of them only one S sets up an anomeric interaction. Arguably, the number of examples is too low...
Most diffractometers measure low angle scattering of X-rays by high density electrons. These are the core electrons associated with a nucleus rather than the valence electrons associated with lone pairs. Hence very few positions of valence lone pairs have ever been crystallographically measured.