Summary DFT Calculations NONCOV

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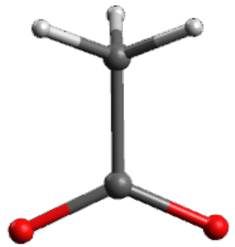
Molecules

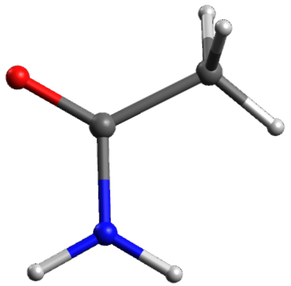
Anion, cation and polar H donor used with different aromatics

Anion Pi



Cation Pi

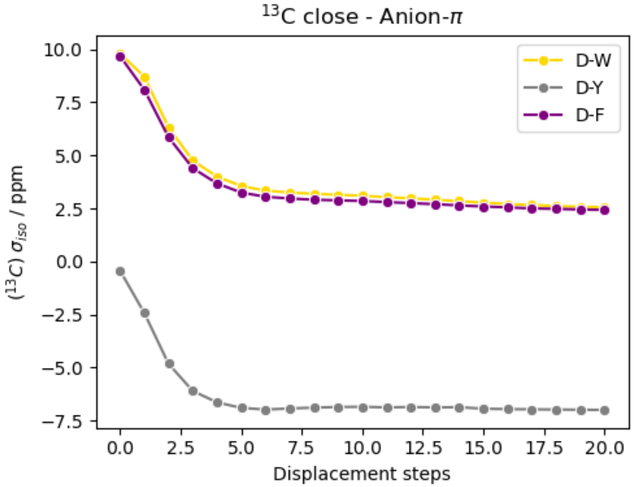
Hp Pi

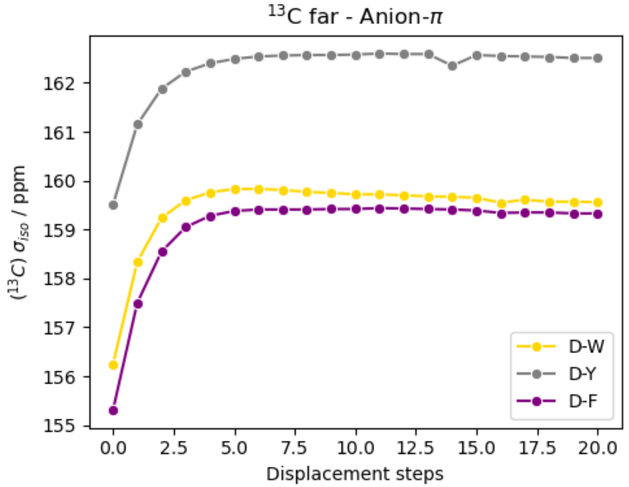


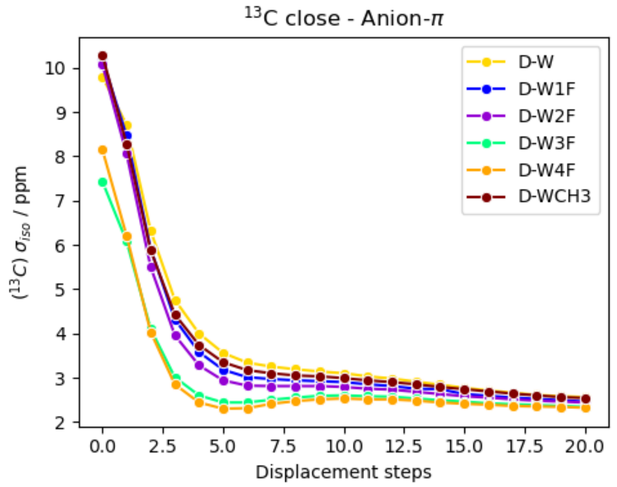
These molecules have been placed on top of three aromatic moieties representing aromatic amino acids and then they have been moved up to 5 Angstroems away from the original position in the direction normal to the aromatic plane.

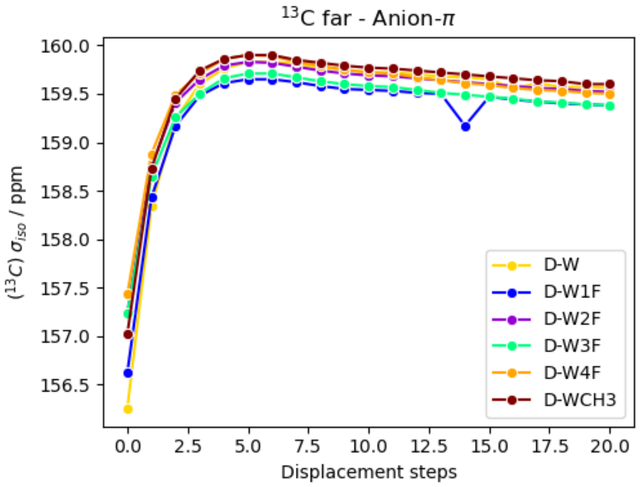
Anion-pi interaction

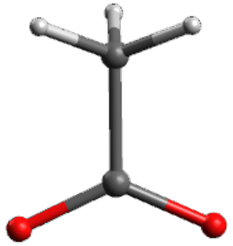
Aspartic acid vs. different aromatics and progressive fluorination





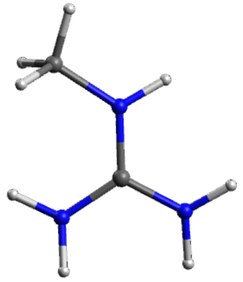


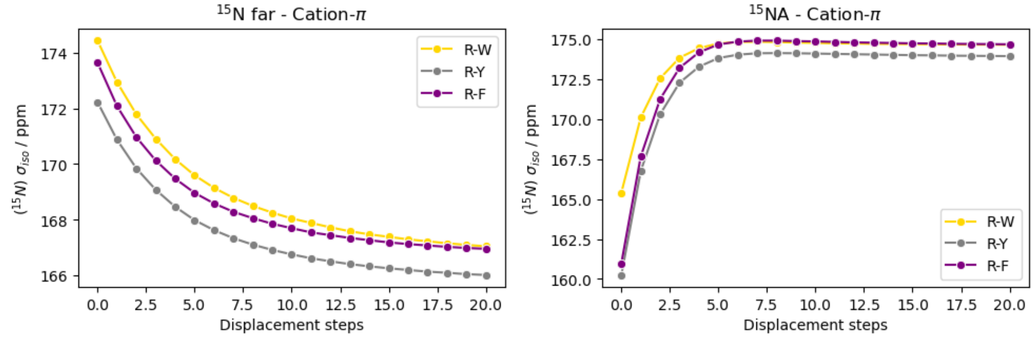


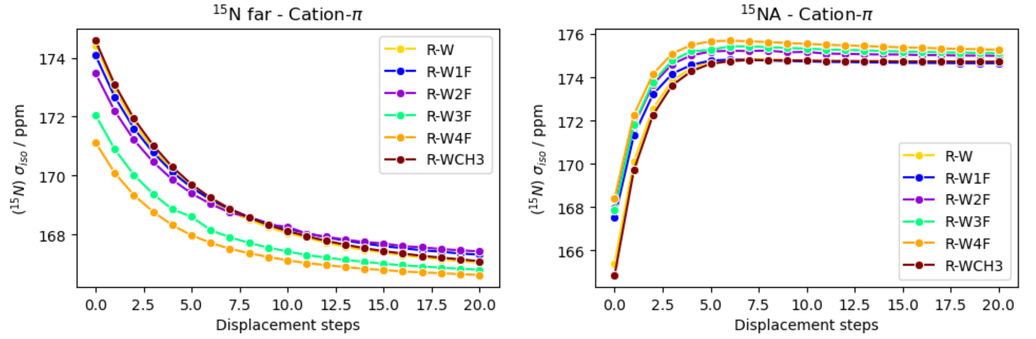


Cation-pi interaction

Arginine vs. different aromatics and progressive fluorination







Hp-pi interaction

Asparagine vs. different aromatics and progressive fluorination