**Sample jobs from ezDyson**

CH2, SF to IP [CH2 (1A1) → CH2+(2A1) ], Basis set; 6-31G\*

A graph of a graph

AI-generated content may be incorrect.

Formaldehyde, GS(HOMO)-IP, basis set: 6-31G\*

A graph of a graph

AI-generated content may be incorrect.

OH-, EE to IP [OH-\* → OH·], Basis set: 6-31G\*

A graph of a graph

AI-generated content may be incorrect.

NO, EA(B2) – GS [NO → NO+], Basis set aug-cc-pVTZ

A graph of a graph

AI-generated content may be incorrect.

H2O, GS(O1s) – IP, Basis set: cc-pVTZ

A graph of a graph

AI-generated content may be incorrect.

CO, GS(B1 or A1) to IP, Basis set: cc-pVDZ

A graph with different colored lines

AI-generated content may be incorrect.A graph of a graph

AI-generated content may be incorrect.

**DIPOLE bound anions photodetachment Xsc (0-2 eV)**

**A graph of a graph

AI-generated content may be incorrect.**

CCSD DBA cryosections for the set of molecules: they all have the overall shape

**Acetone**

**A graph with blue lines and dots

AI-generated content may be incorrect.A graph of a graph

AI-generated content may be incorrect.**

HF completely overestimates, good agreement CCSD-CC2

**Formamide**

**A graph of a graph

AI-generated content may be incorrect.**A graph with a purple line

AI-generated content may be incorrect.

Good agreement CCSD-CC2, HF completely different.

**Nitrobenzene (dba)**

**A graph of a graph

AI-generated content may be incorrect.A graph with a purple line

AI-generated content may be incorrect.**

Good agreement CCSD-CC2, HF completely different.

**Nitromethane**

**A graph of a graph

AI-generated content may be incorrect.**

Best HF result. Still, big disagreement w CCSD and CC2

**Pyridazine**

**VALENCE bound anions photodetachment Xsc (0-10eV)**

CCSD VBA crossections for the set of molecules.

A graph of different colored lines

AI-generated content may be incorrect.

**Azulene**

A graph of a graph

AI-generated content may be incorrect.

**Benzoquinone**

**A graph of a graph

AI-generated content may be incorrect.**

**1,3-Dicyanobenzene**

A graph of a graph

AI-generated content may be incorrect.A graph of a graph

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**Maleic anhydride**

**A graph of a graph

AI-generated content may be incorrect.**

**Nitrobenzene**

**A graph of a graph

AI-generated content may be incorrect.**

HF really bad, largest MO coeff in CCSD’s dyson is 0.63, in other molecules is >0.9

**Phenazine**

A graph of a graph

AI-generated content may be incorrect.

**Benzoquinone vba**

A graph of a graph

AI-generated content may be incorrect.

We get a better agreement between ccsd and cc2 if we set the ionitzation energies to the corresponding ones for each method and then shifting.

**Nitrobenzene**

A graph of a graph

AI-generated content may be incorrect.