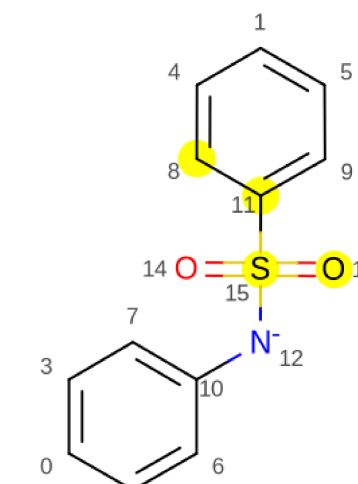
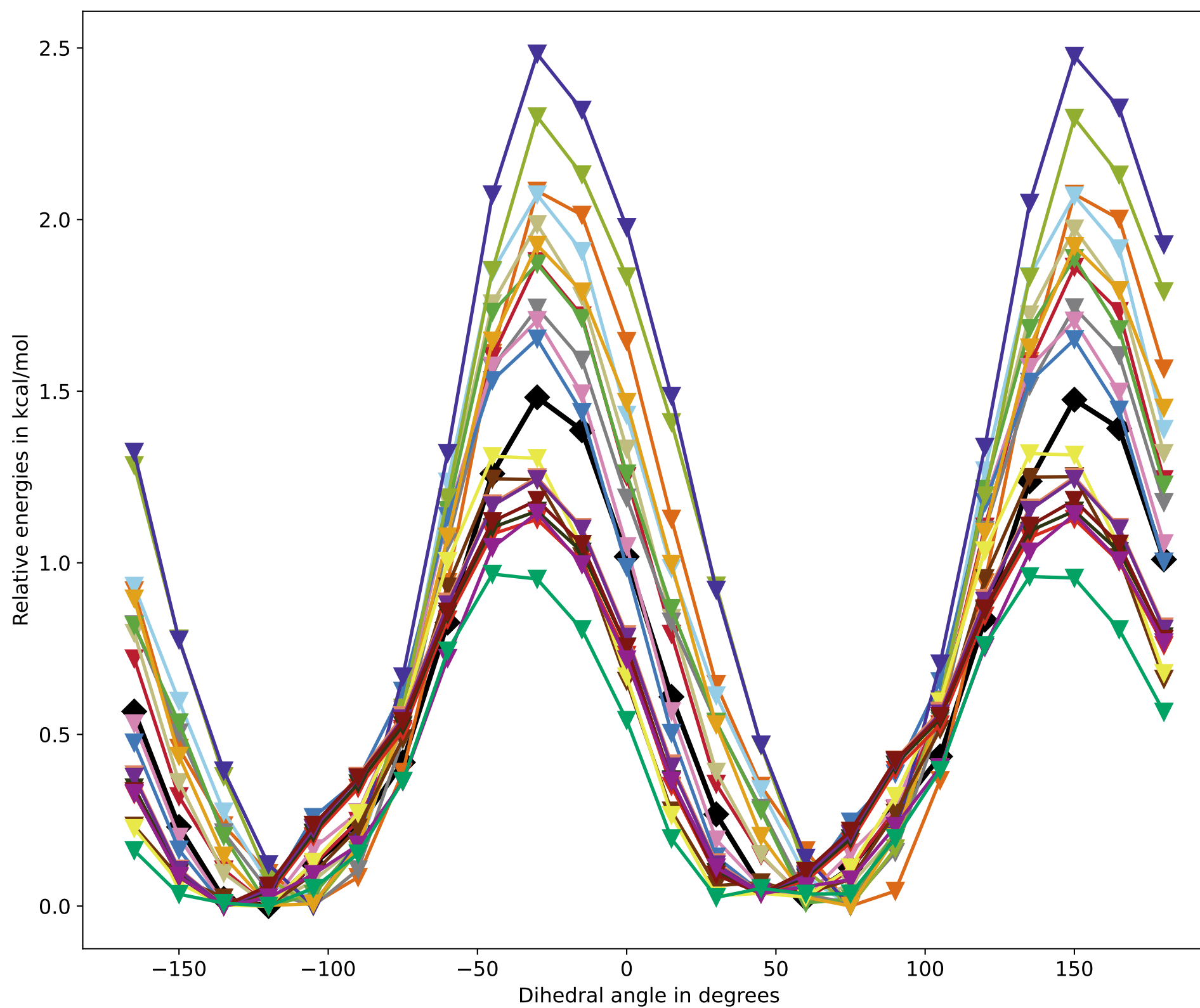
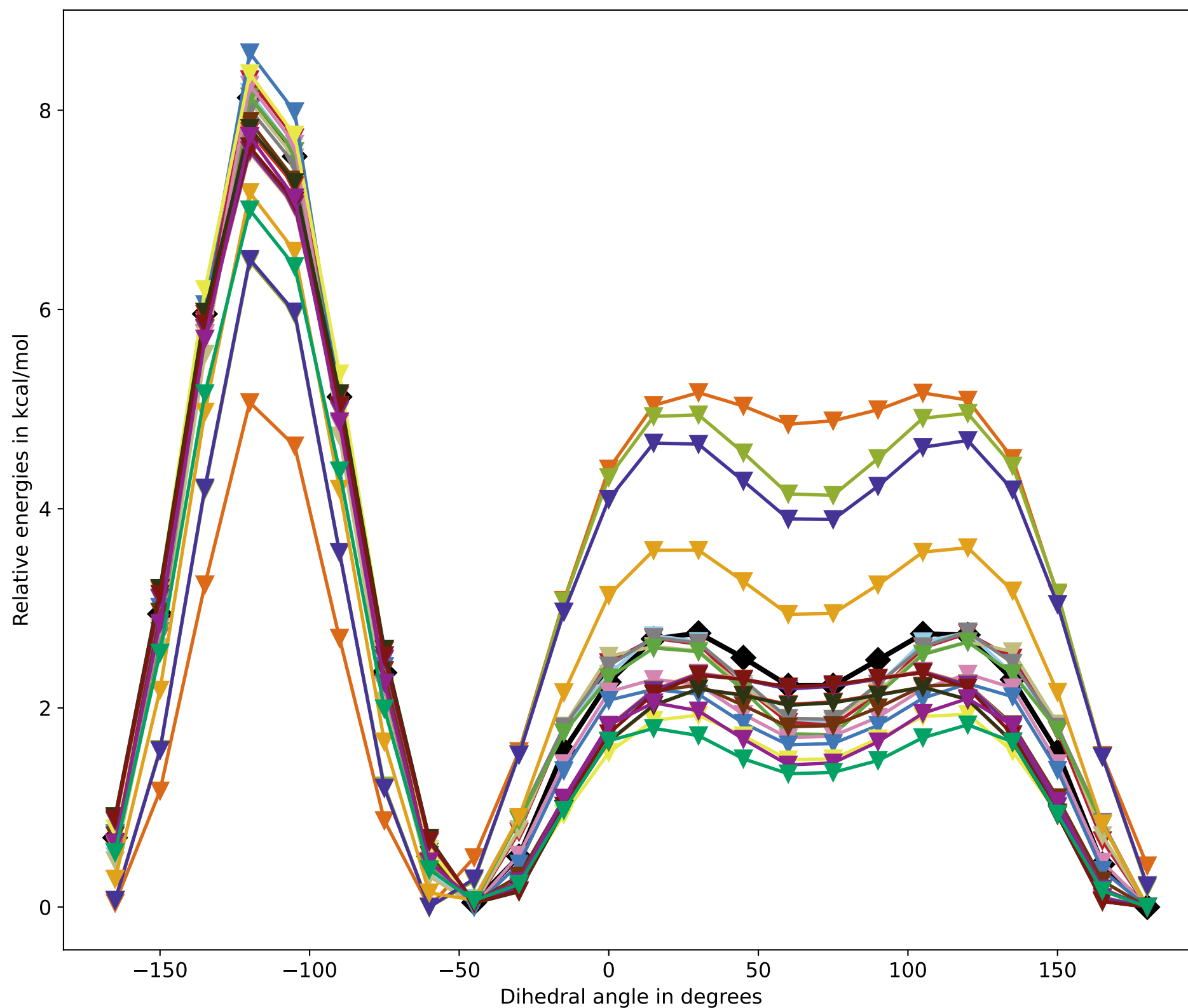
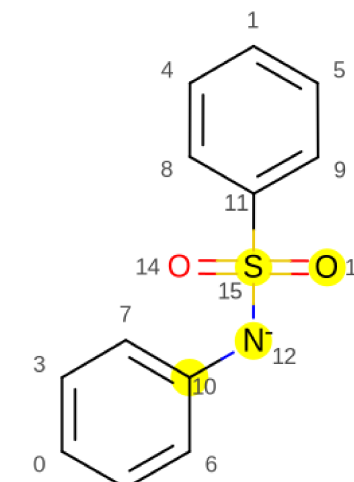


Charged molecule



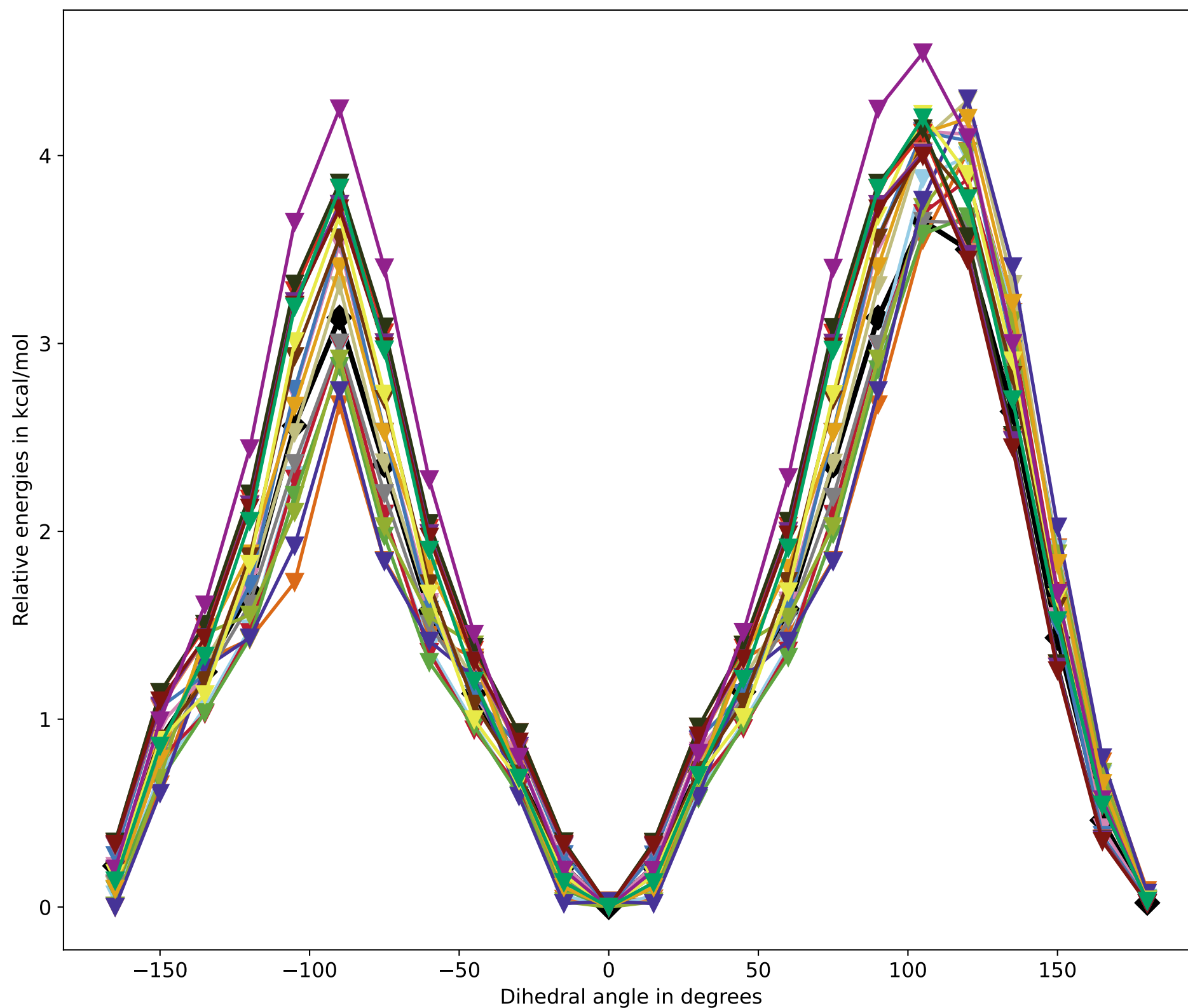
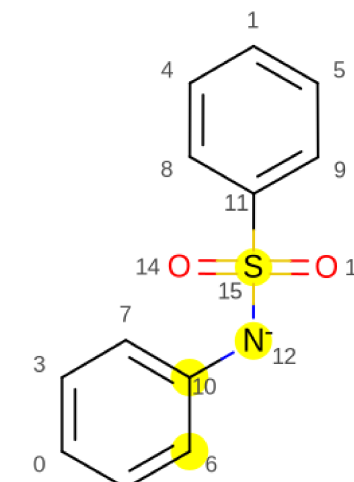
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- ▾ m05-2x-d3/dzvp
- ▾ m06-2x-d3/dzvp
- ▾ m08-hx-d3/dzvp
- ▾ wb97m-d3bj/dzvp
- ▾ wb97m-v/dzvp
- ▾ pw6b95-d3bj/dzvp
- ▾ pw6b95-d3/dzvp
- ▾ mp2/aug-cc-pvtz
- ▾ mp2/heavy-aug-cc-pvtz
- ▾ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ▾ b3lyp-d3bj/dzvp
- ▾ b3lyp-nl/dzvp
- ▾ b3lyp-d3bj/def2-tzvp
- ▾ b3lyp-d3bj/def2-tzvppd
- ▾ b3lyp-d3bj/def2-tzvpp
- ▾ b3lyp-d3bj/def2-qzvp
- ▾ b3lyp-d3bj/6-31+g**
- ▾ b3lyp-d3bj/6-311+g**

Charged molecule



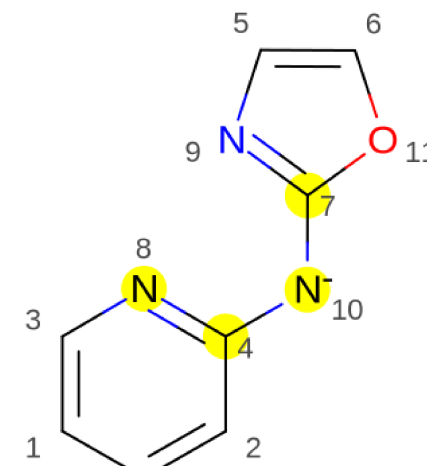
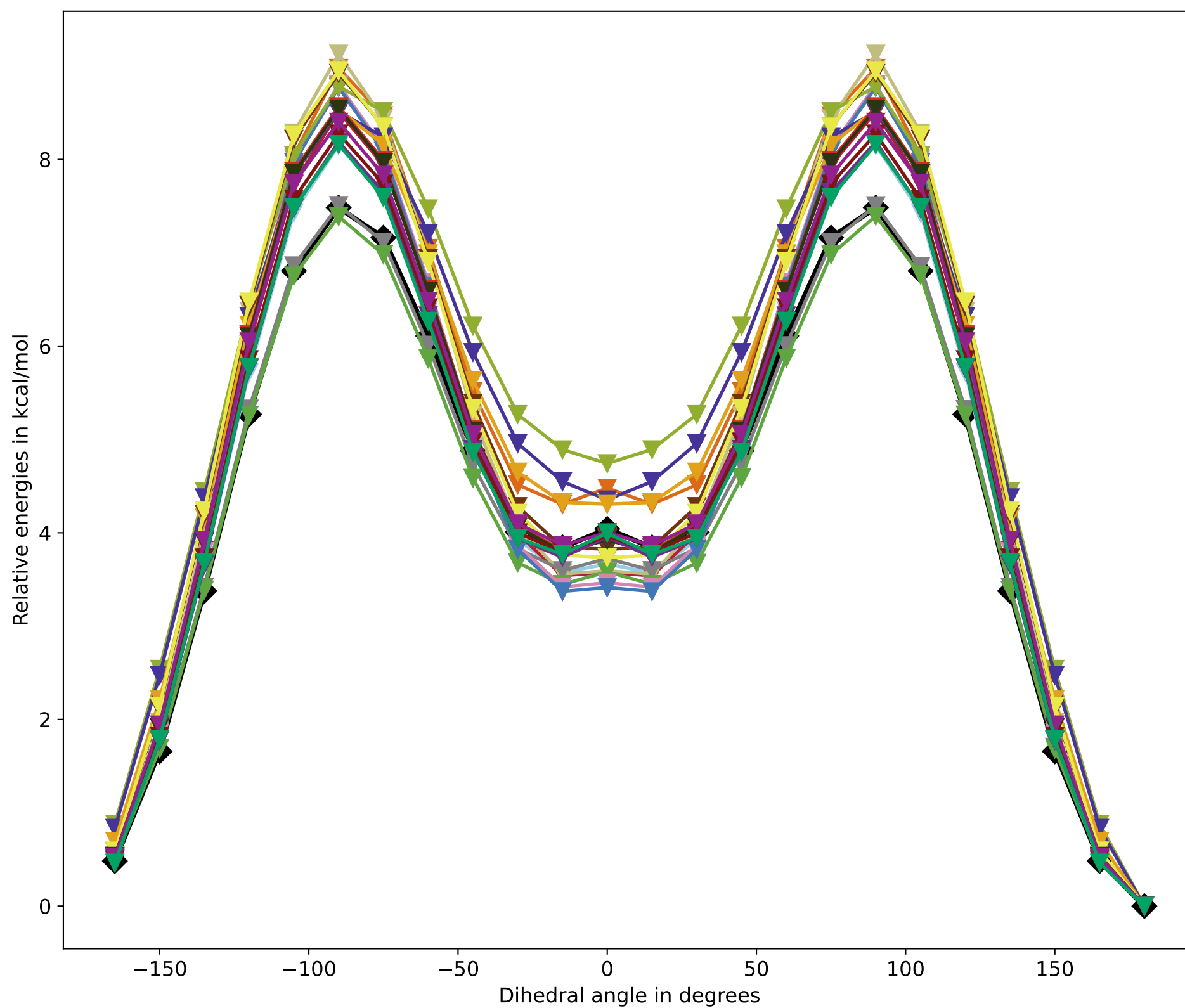
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- ▾ wb97m-v/dzvp
- ▾ pw6b95-d3bj/dzvp
- ▾ pw6b95-d3/dzvp
- ▾ mp2/aug-cc-pvtz
- ▾ mp2/heavy-aug-cc-pvtz
- ▾ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ▾ b3lyp-d3bj/dzvp
- ▾ b3lyp-d3bj/def2-tzvp
- ▾ b3lyp-d3bj/def2-tzvppd
- ▾ b3lyp-d3bj/def2-qzvp
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Charged molecule



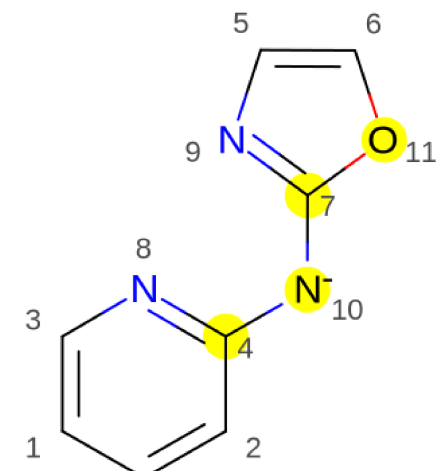
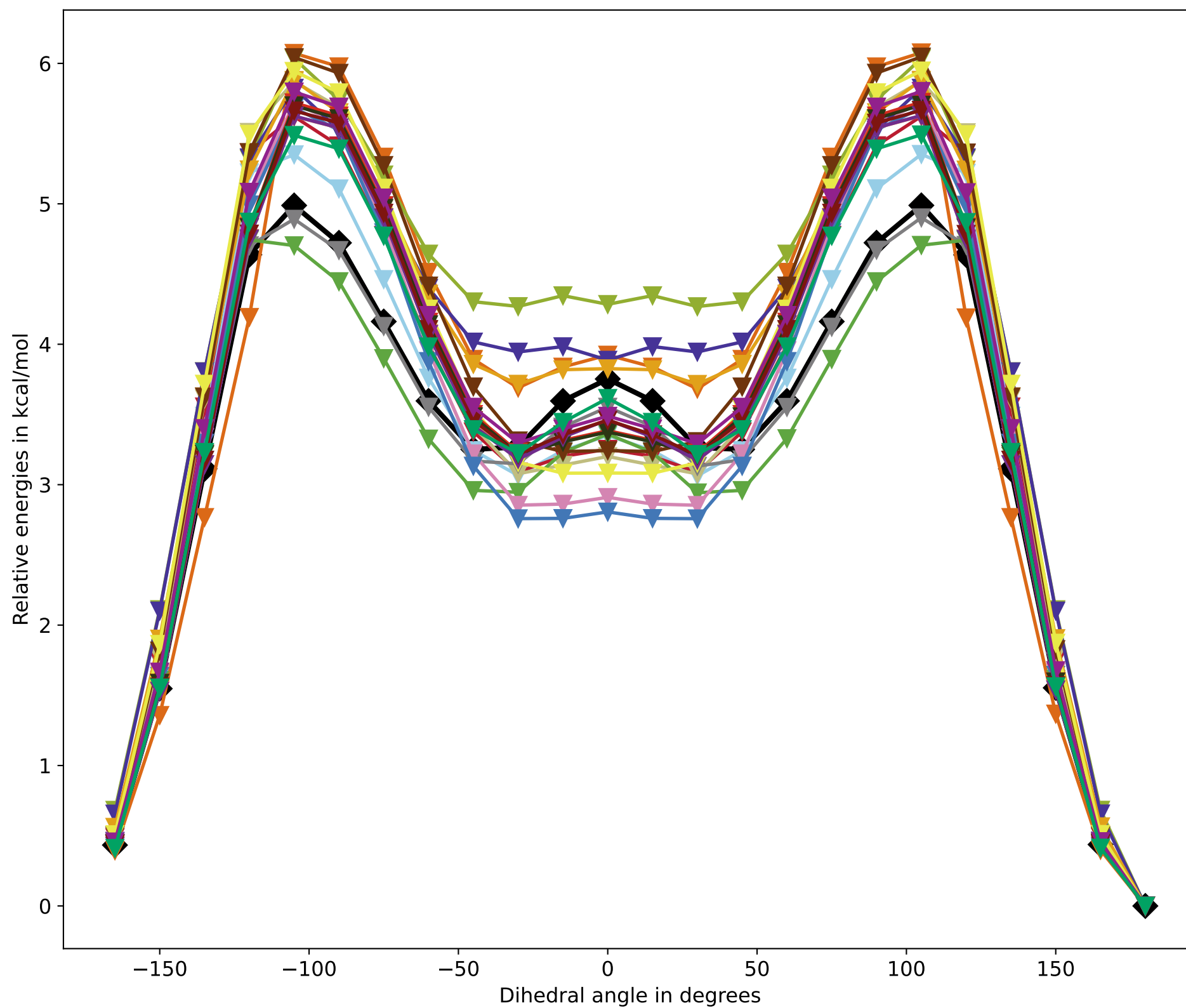
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
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- b3lyp-d3bj/6-311+g**

Charged molecule



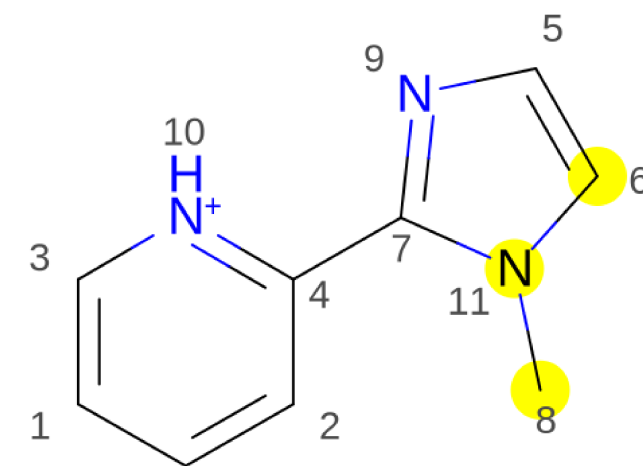
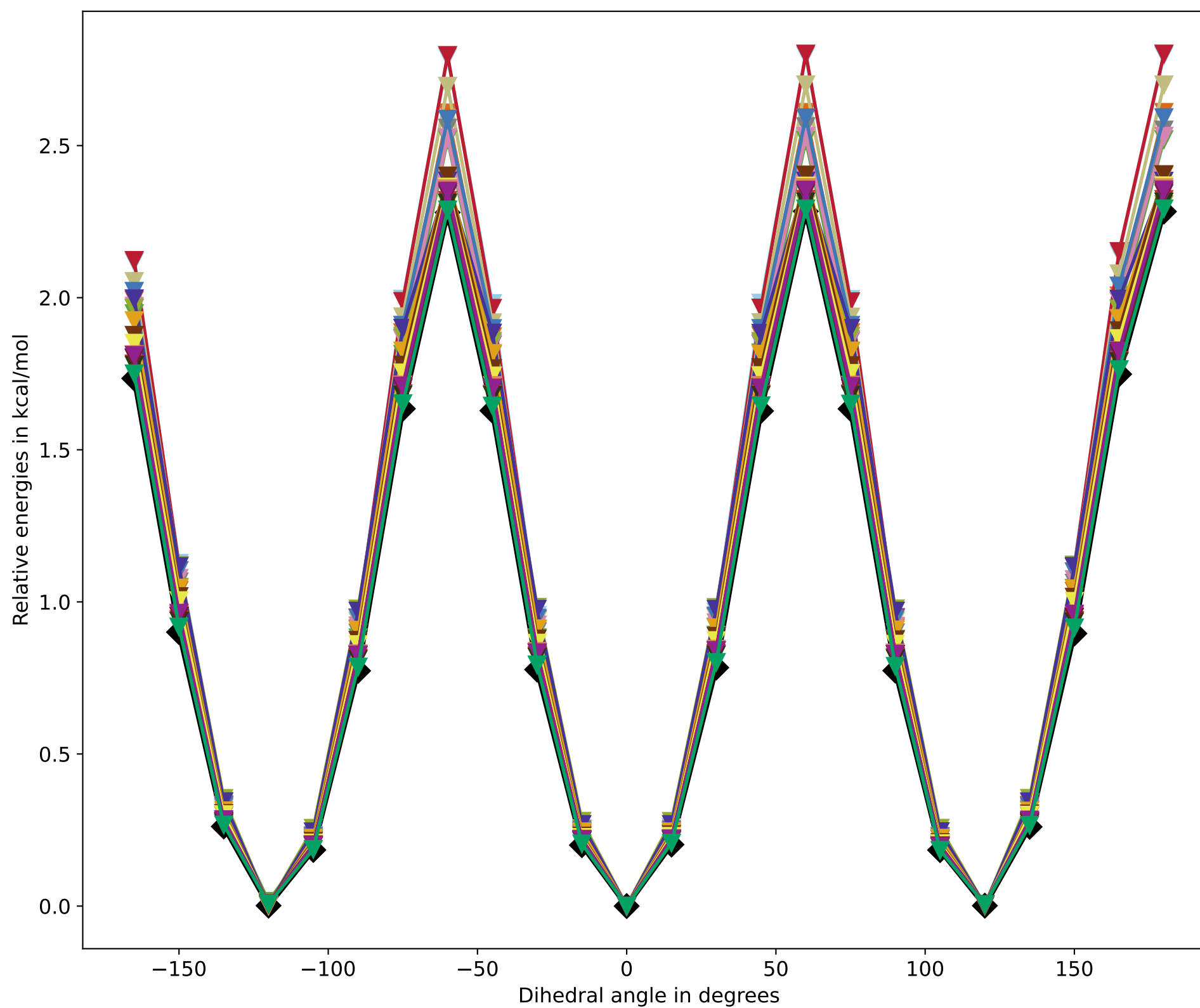
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
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- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
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Charged molecule



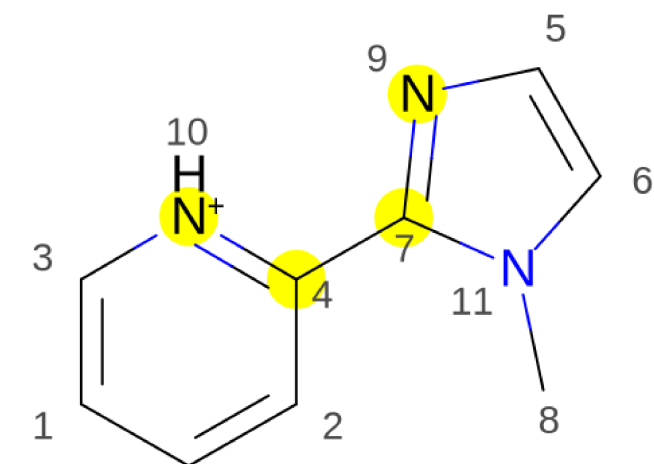
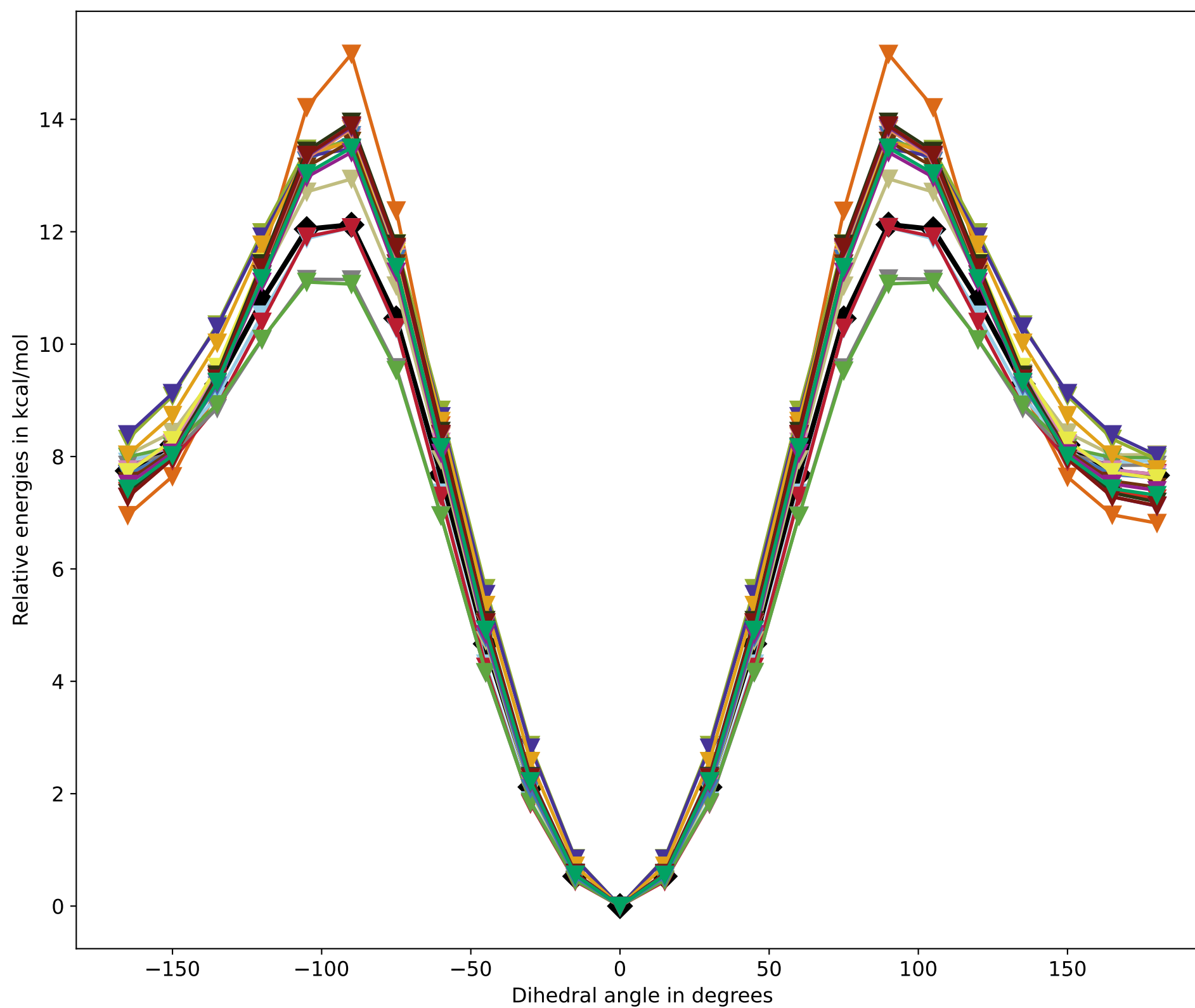
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- m06-2x-d3/dzvp
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
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Charged molecule



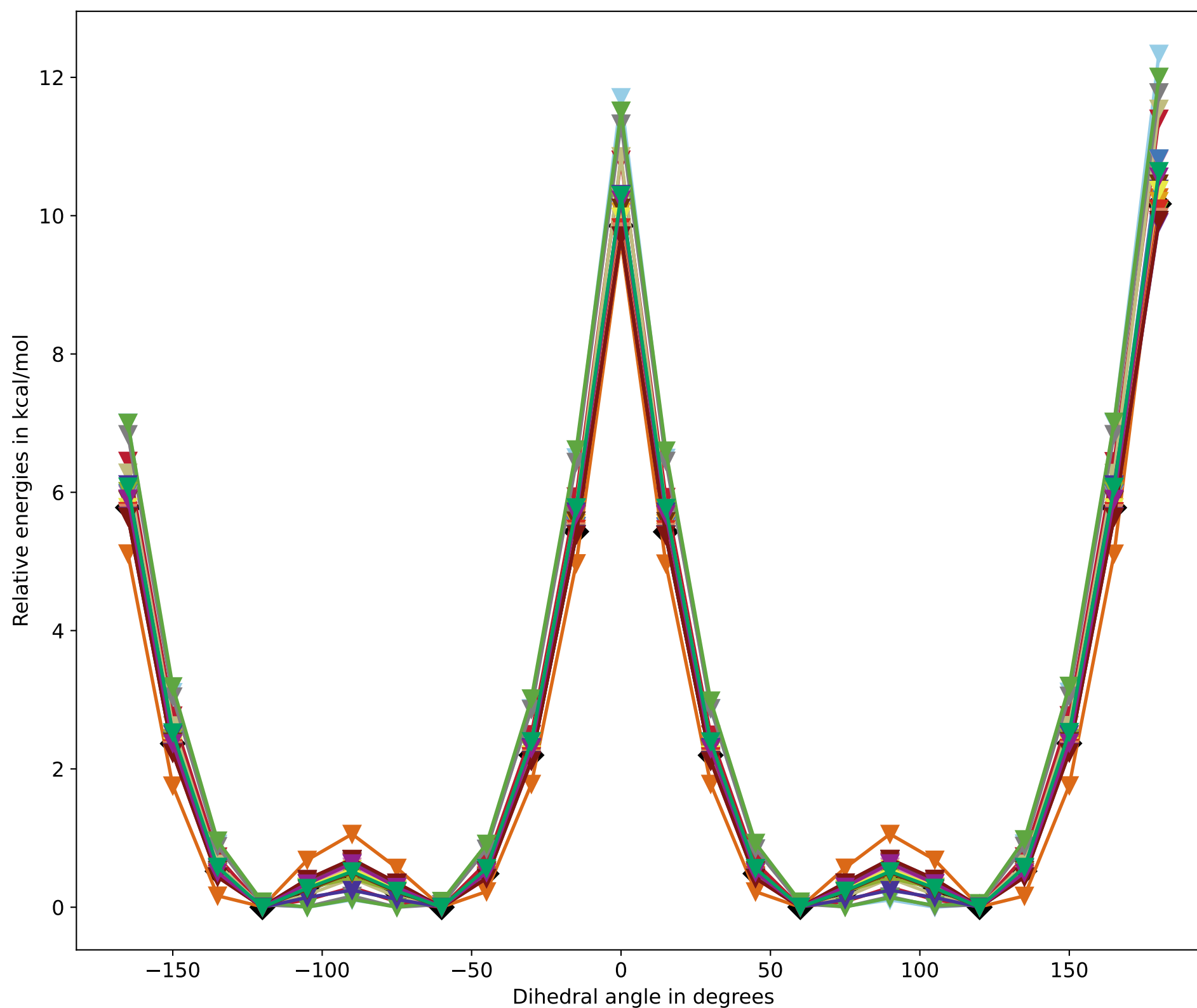
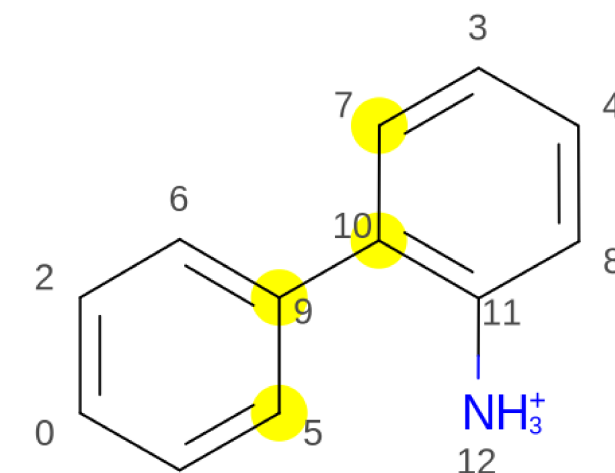
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- m08-hx-d3/dzvp
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Charged molecule



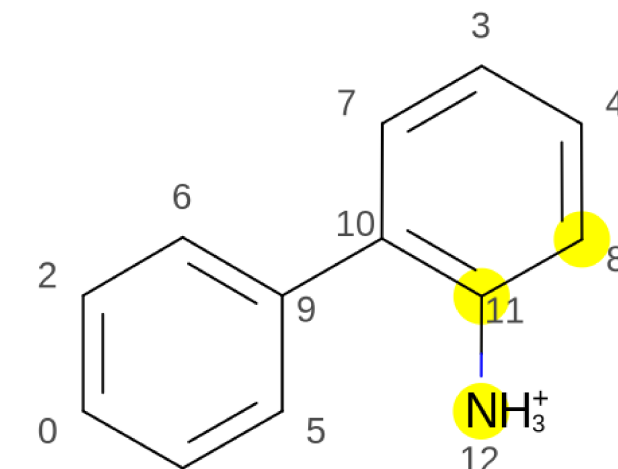
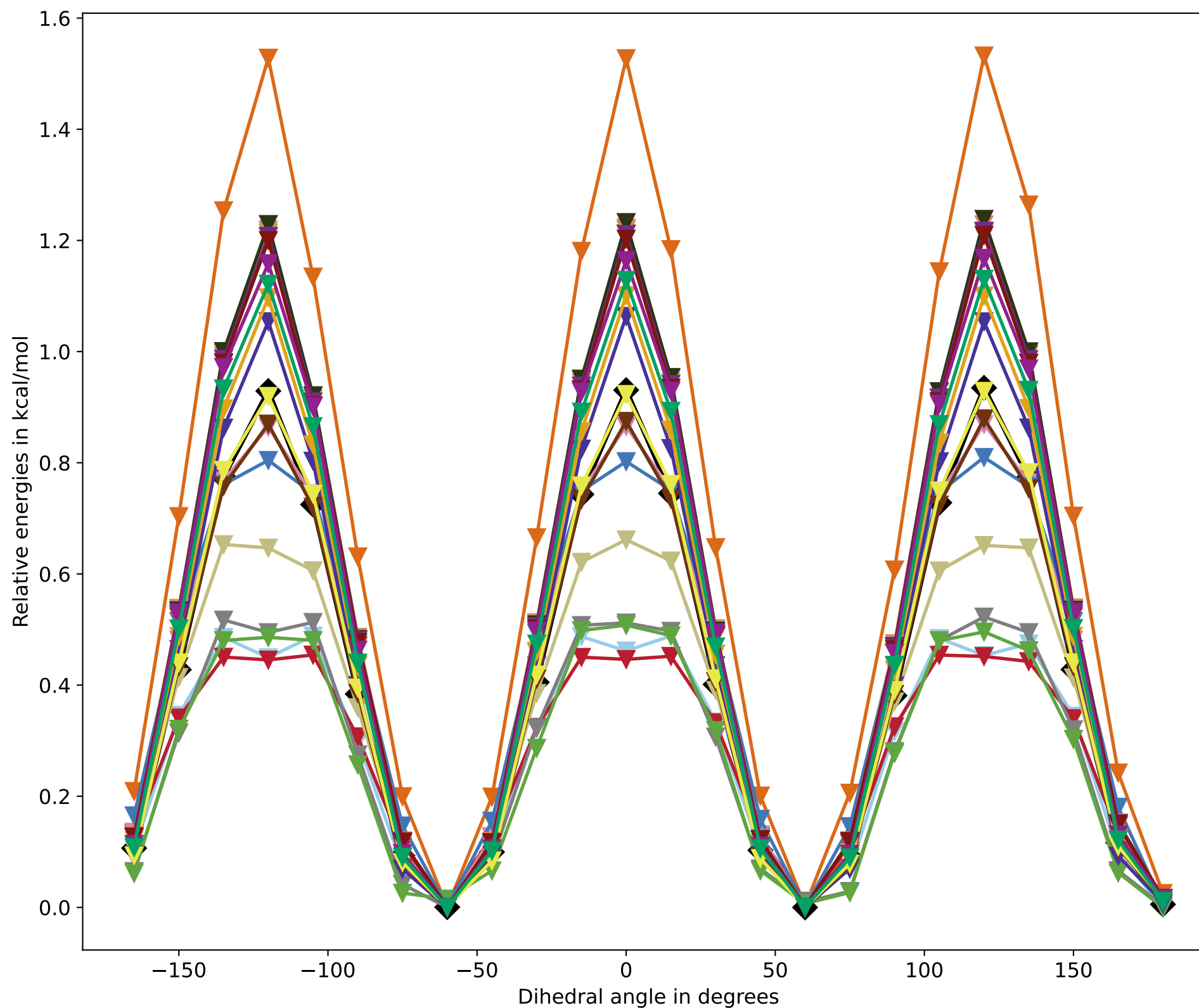
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- m06-2x-d3/dzvp
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- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Charged molecule



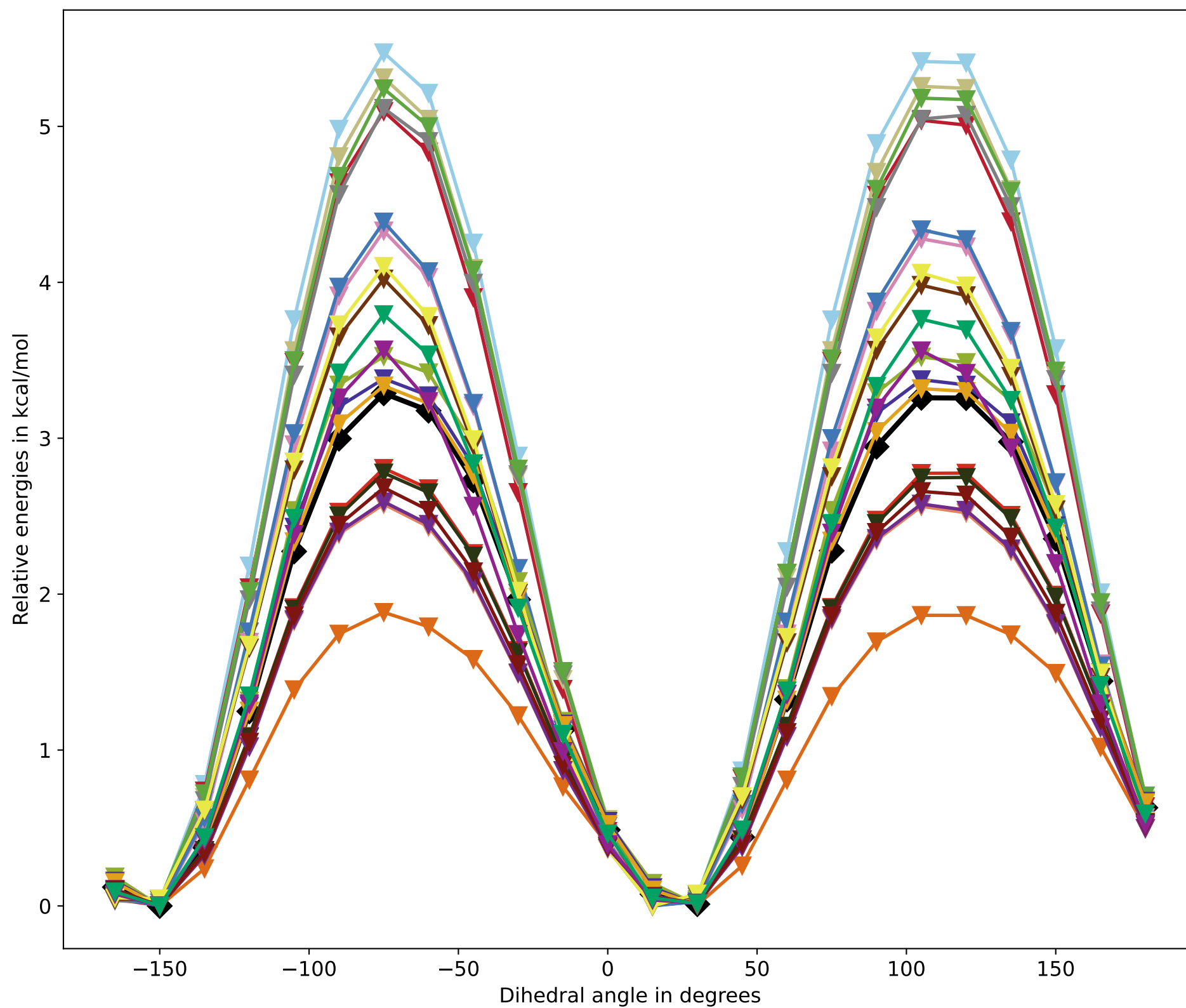
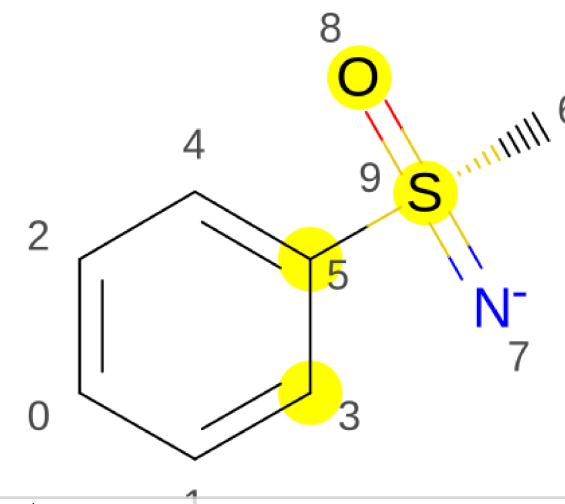
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- ▴ wb97m-v/dzvp
- ▴ pw6b95-d3bj/dzvp
- ▴ pw6b95-d3/dzvp
- ▴ mp2/aug-cc-pvtz
- ▴ mp2/heavy-aug-cc-pvtz
- ▴ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ▴ b3lyp-d3bj/dzvp
- ▴ b3lyp-nl/dzvp
- ▴ b3lyp-d3bj/def2-tzvp
- ▴ b3lyp-d3bj/def2-tzvppd
- ▴ b3lyp-d3bj/def2-tzvppp
- ▴ b3lyp-d3bj/def2-qzvp
- ▴ b3lyp-d3bj/6-31+g**
- ▴ b3lyp-d3bj/6-311+g**

Charged molecule



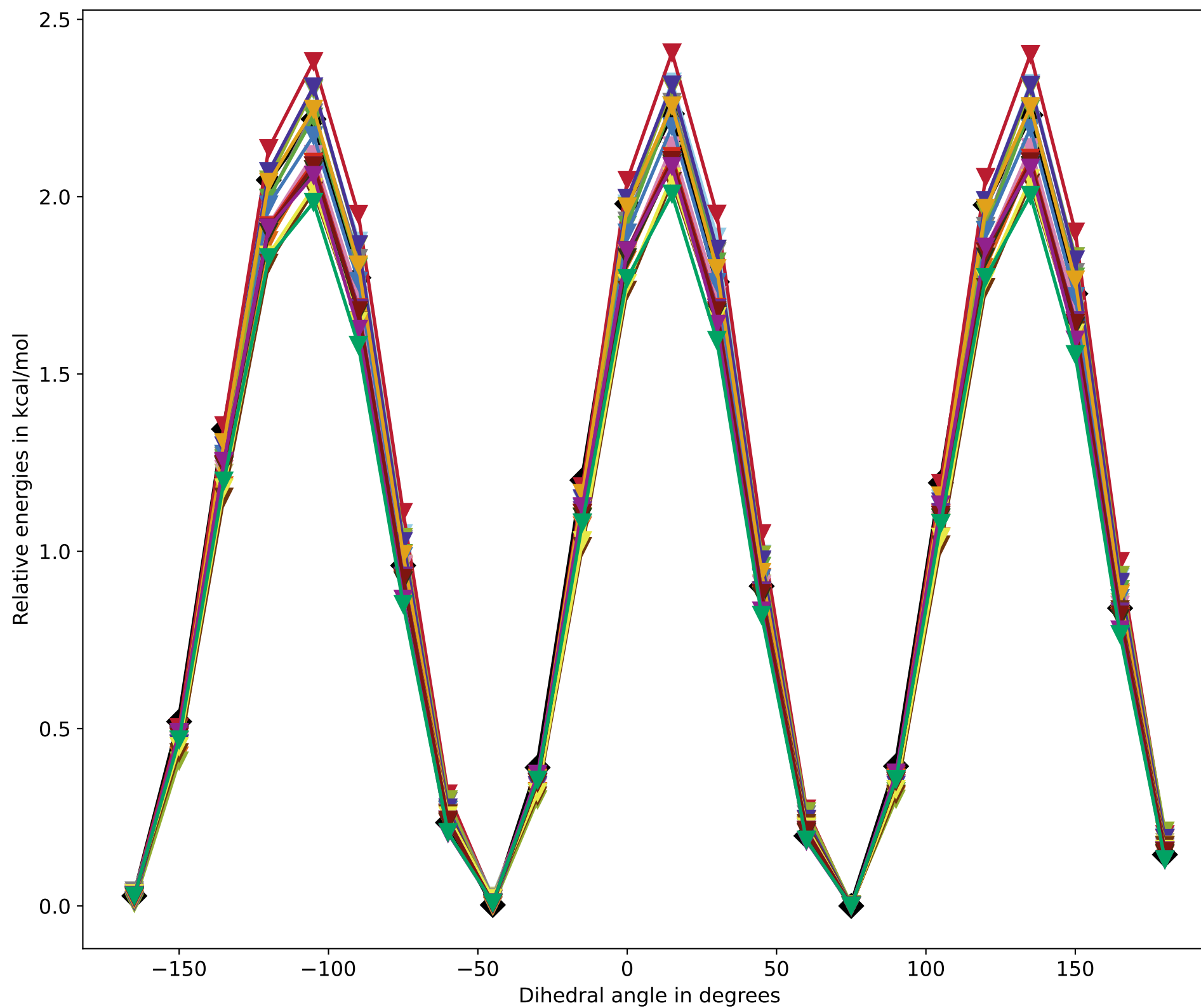
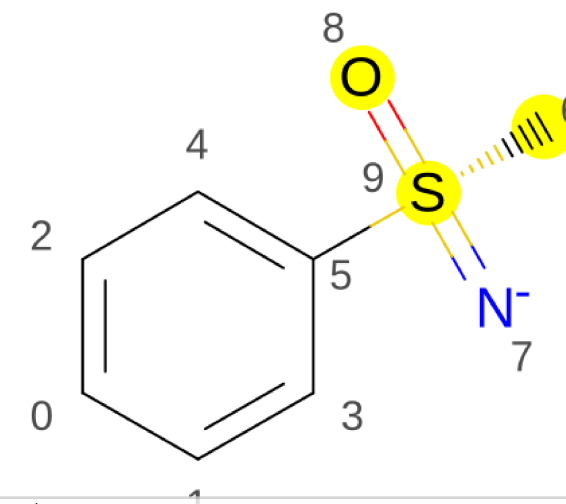
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- m08-hx-d3/dzvp
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Charged molecule



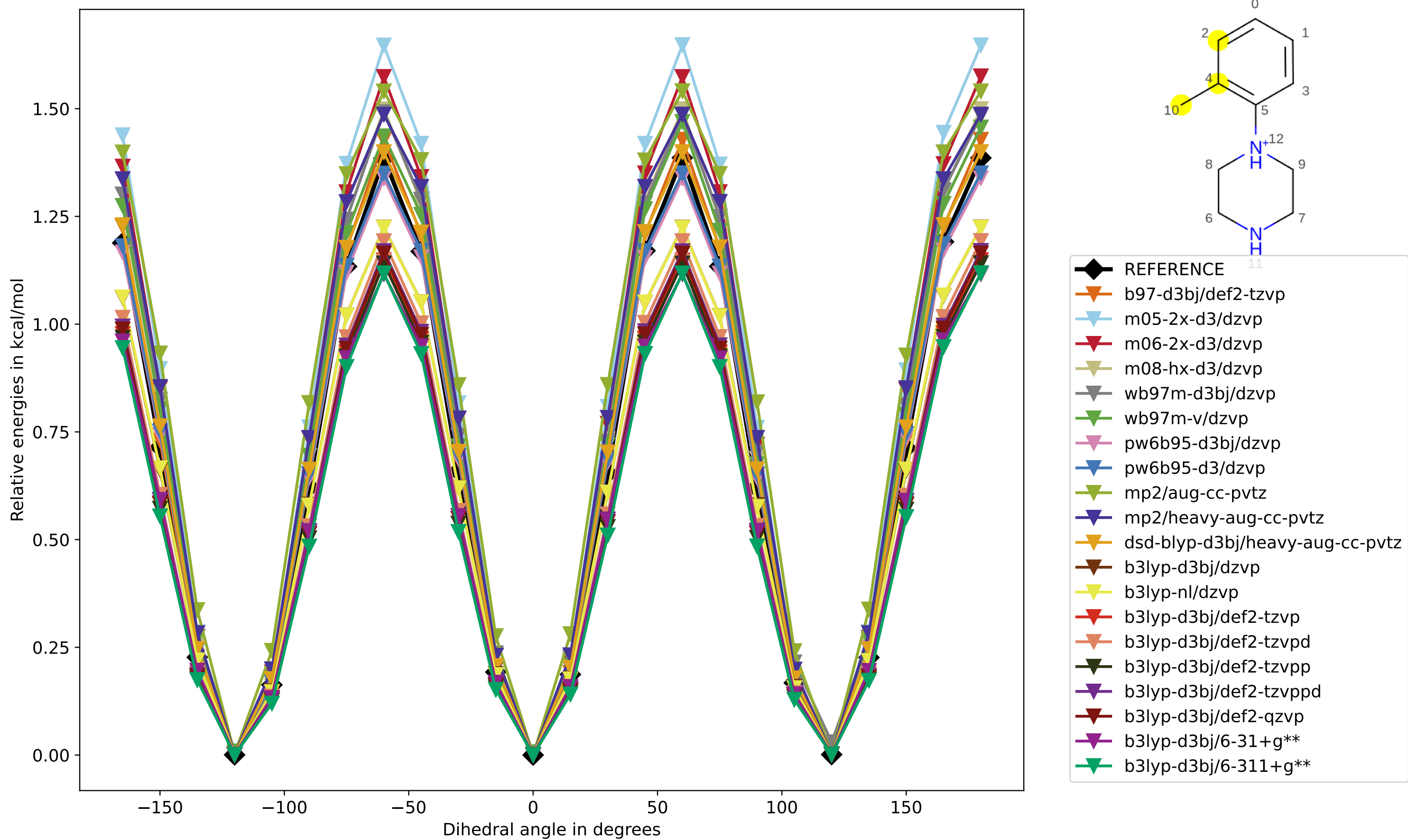
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Charged molecule

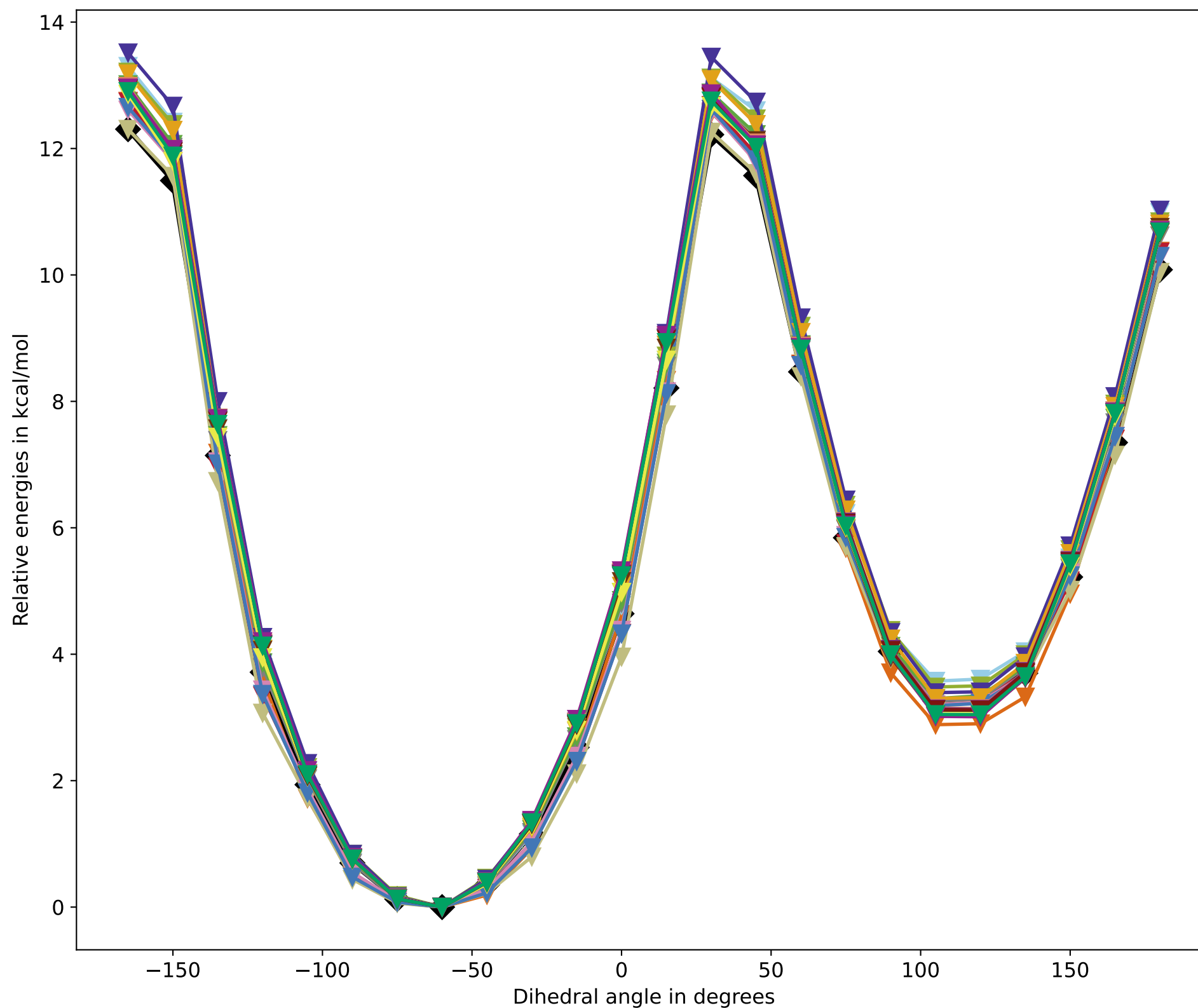
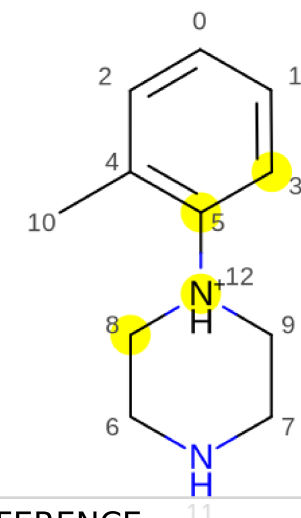


- REFERENCE
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- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
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- b3lyp-d3bj/def2-tzvppd
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- b3lyp-d3bj/6-311+g**

Charged molecule

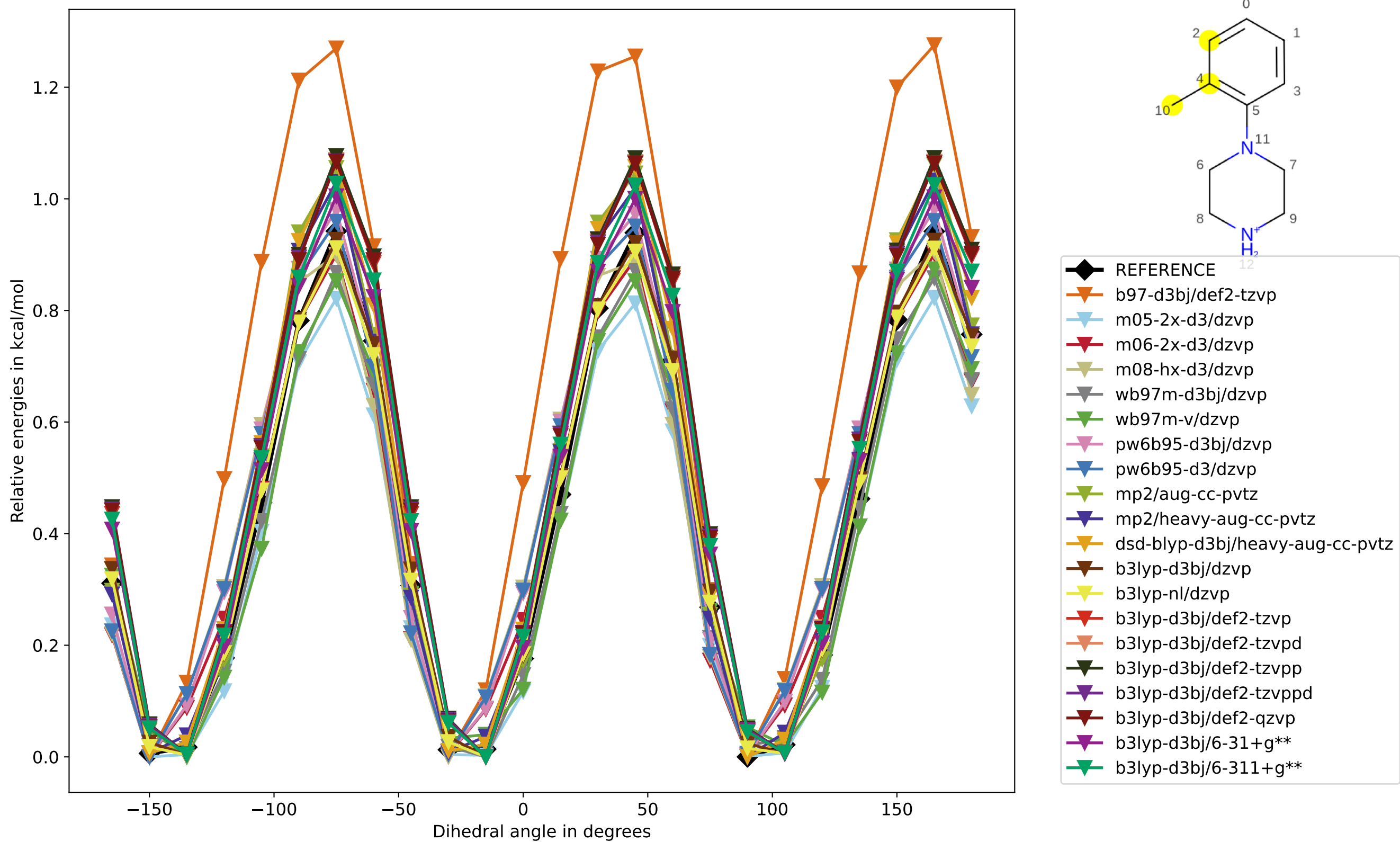


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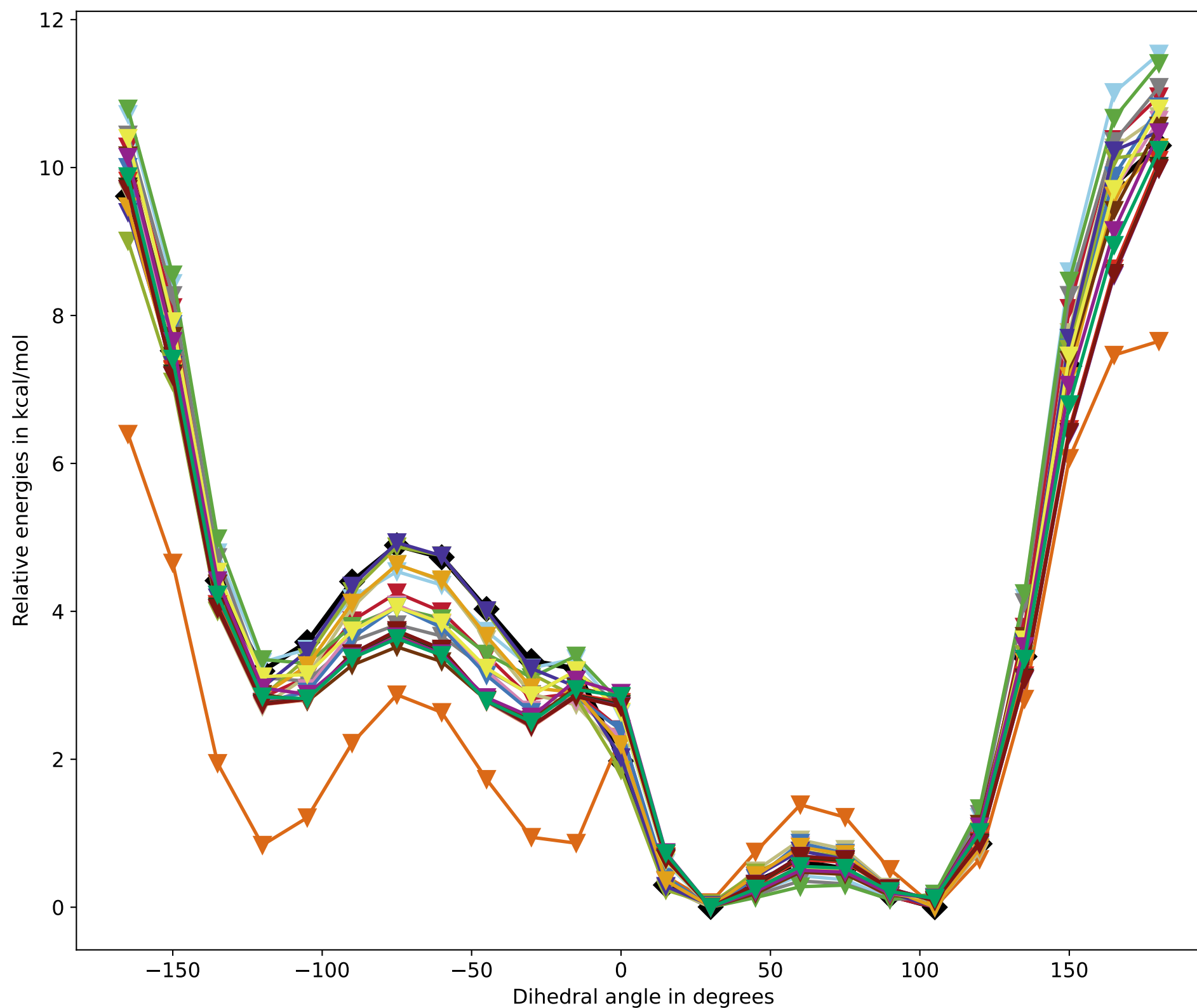
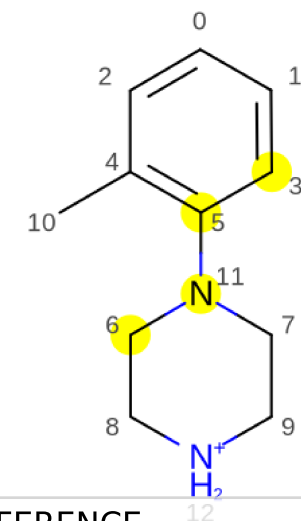


- REFERENCE
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- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
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- b3lyp-d3bj/6-311+g**

Charged molecule

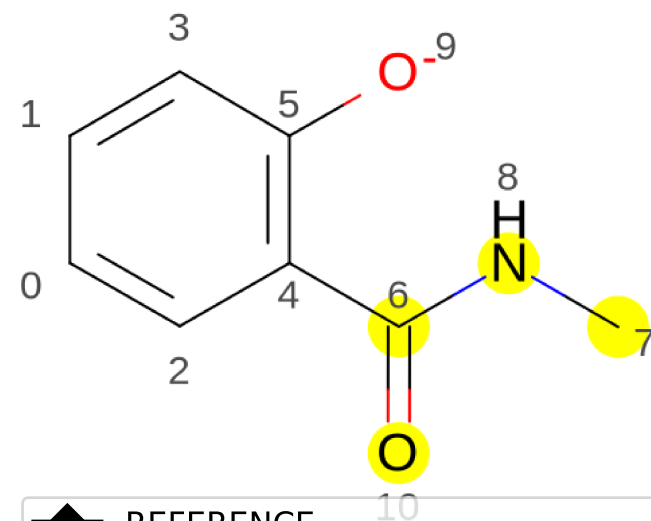
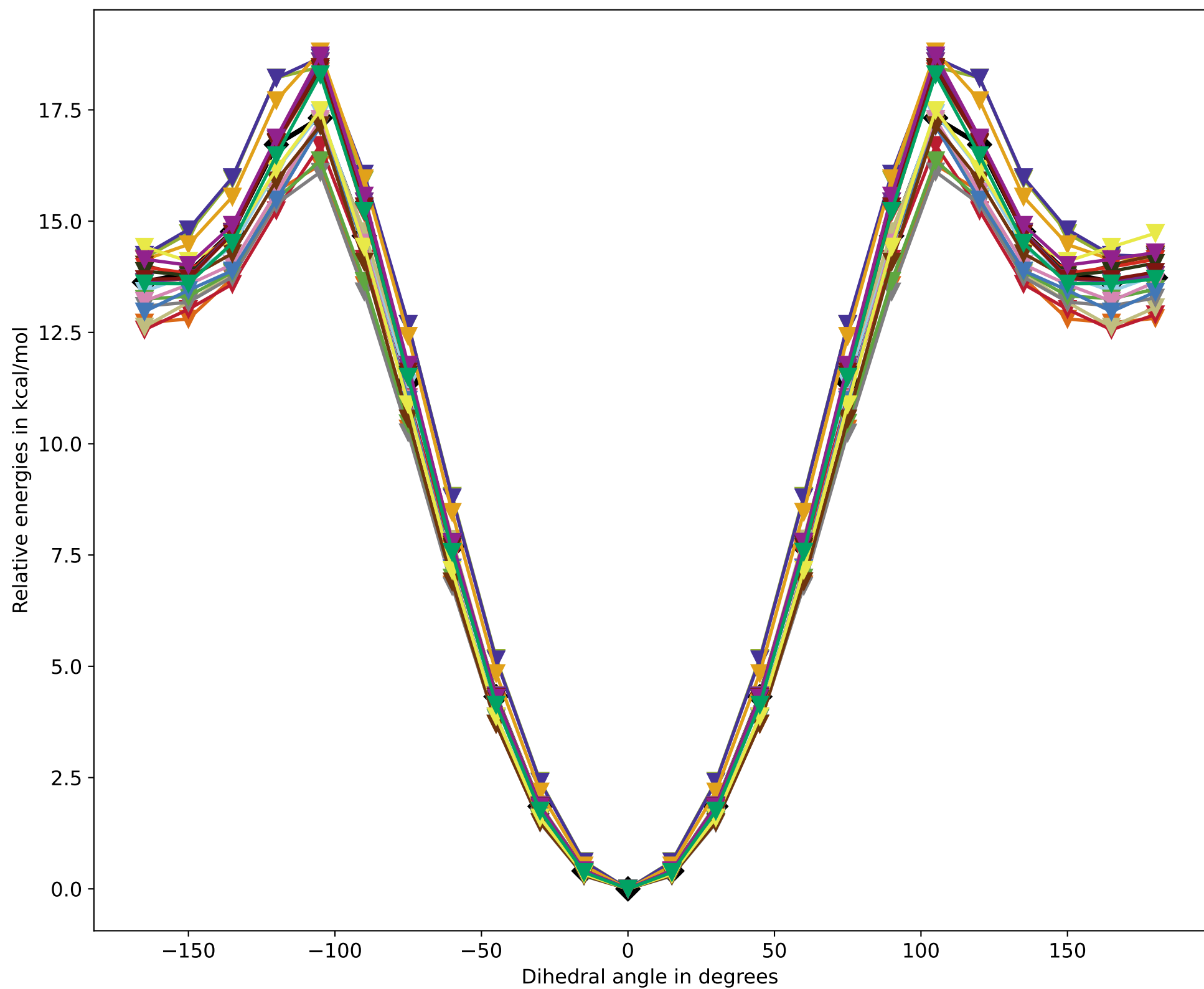


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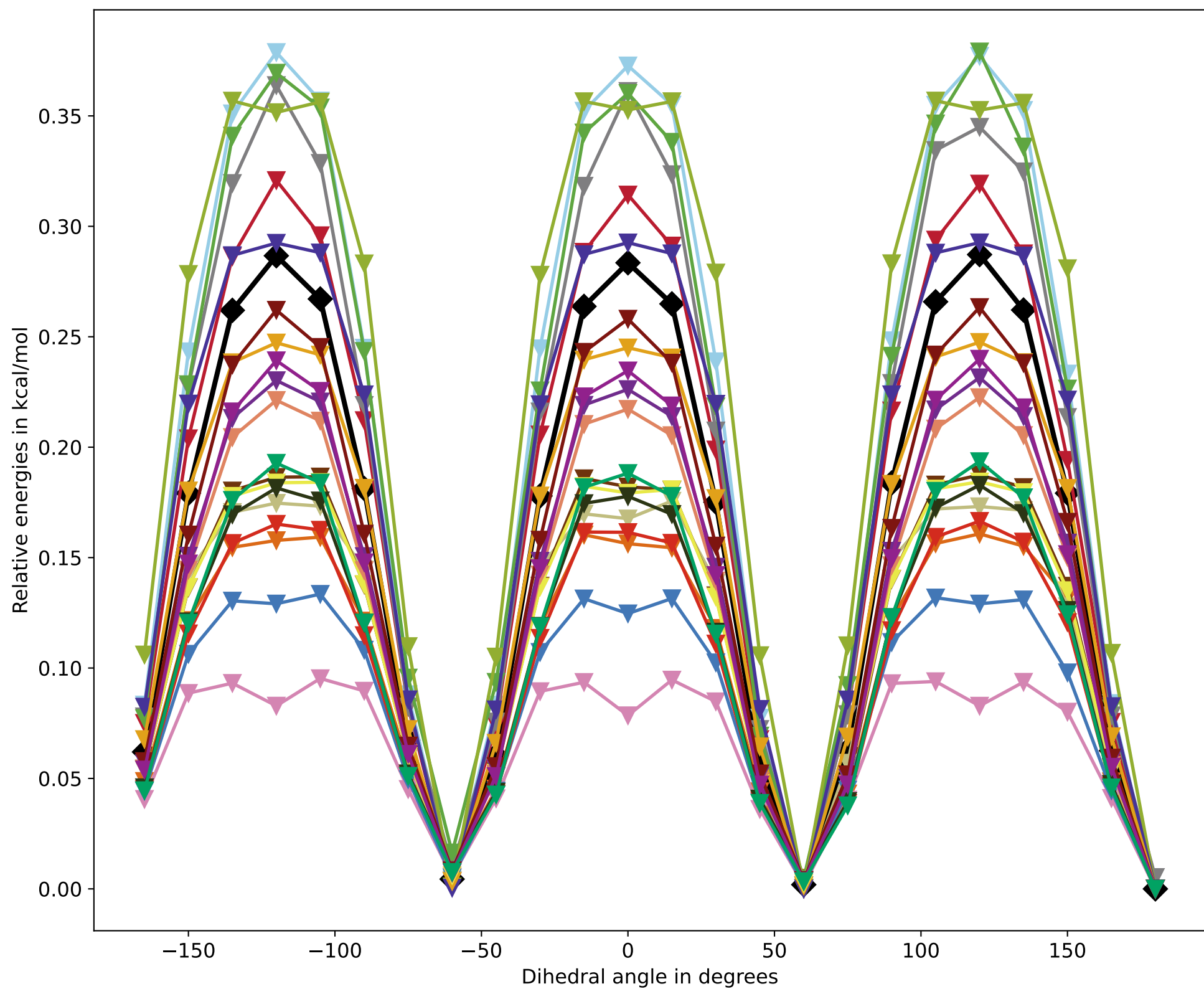
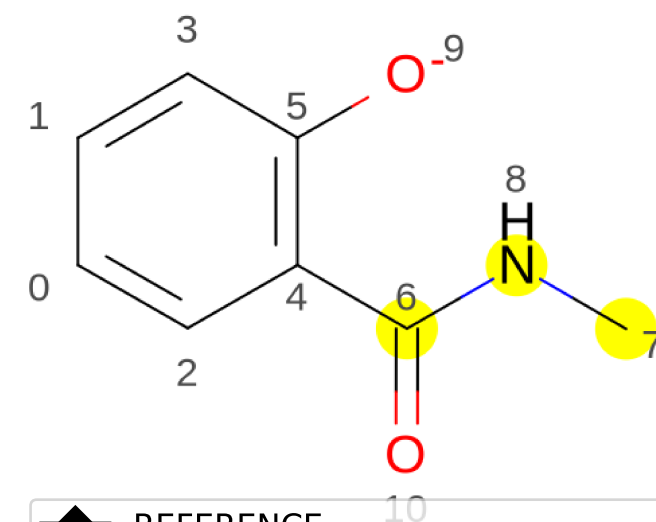
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
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- b3lyp-d3bj/def2-tzvppd
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- b3lyp-d3bj/6-311+g**

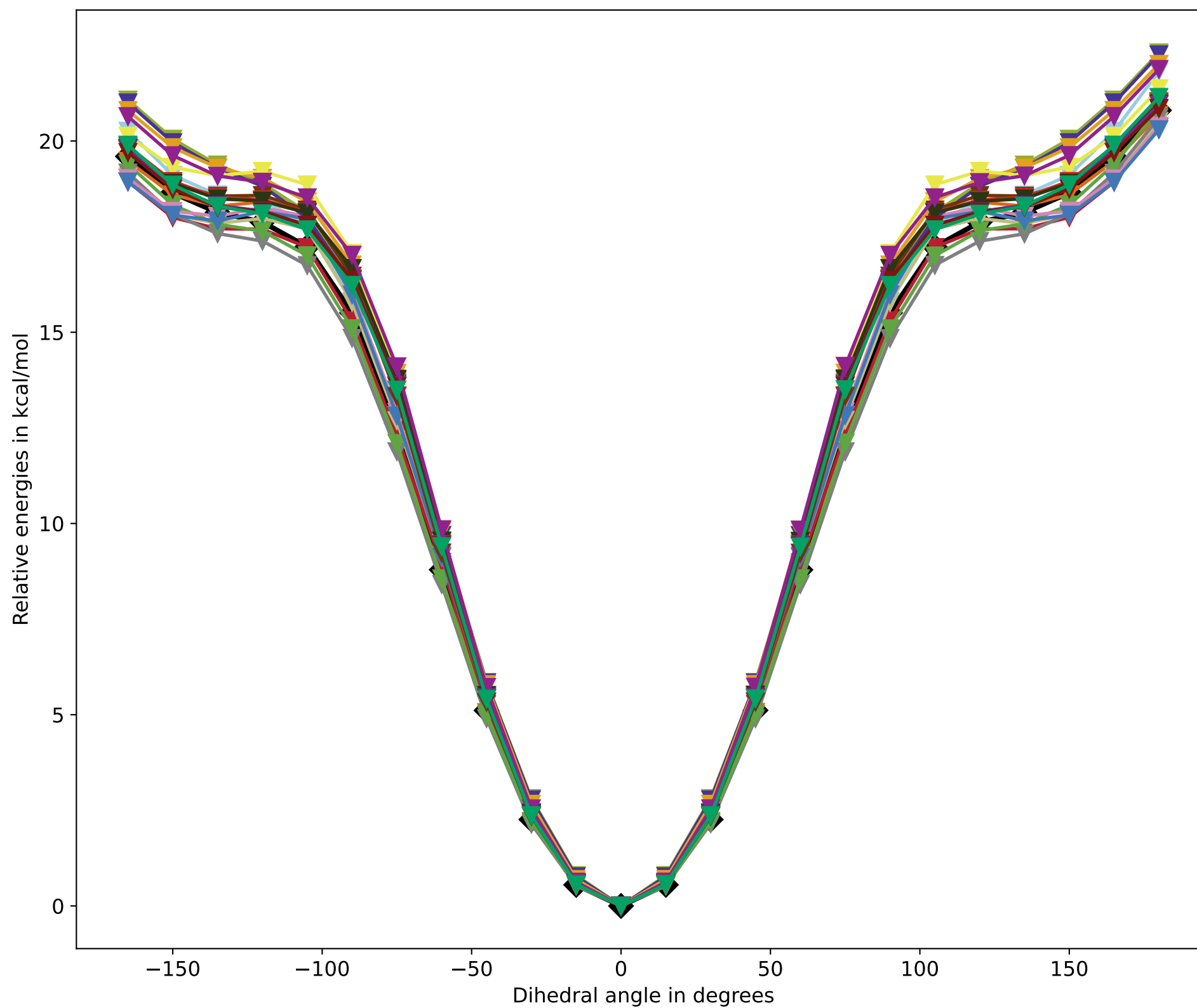
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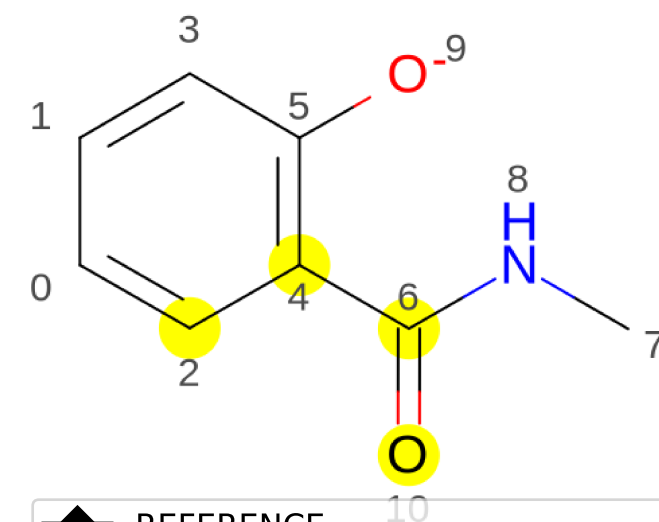
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- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
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- b3lyp-d3bj/def2-tzvp
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- b3lyp-d3bj/def2-tzvppd
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- b3lyp-d3bj/6-311+g**

Charged molecule



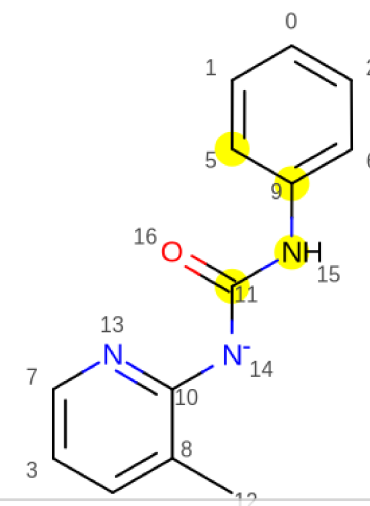
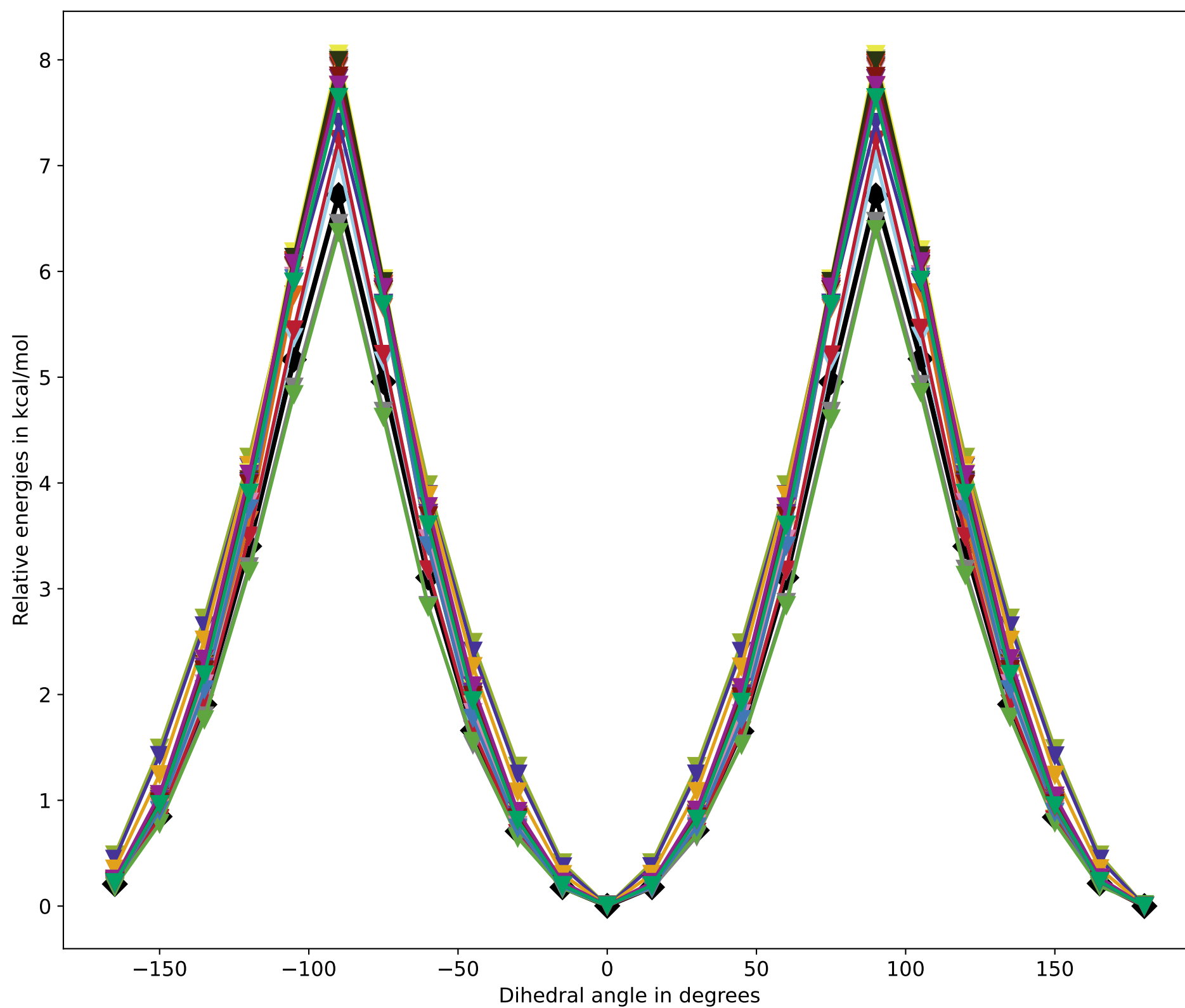


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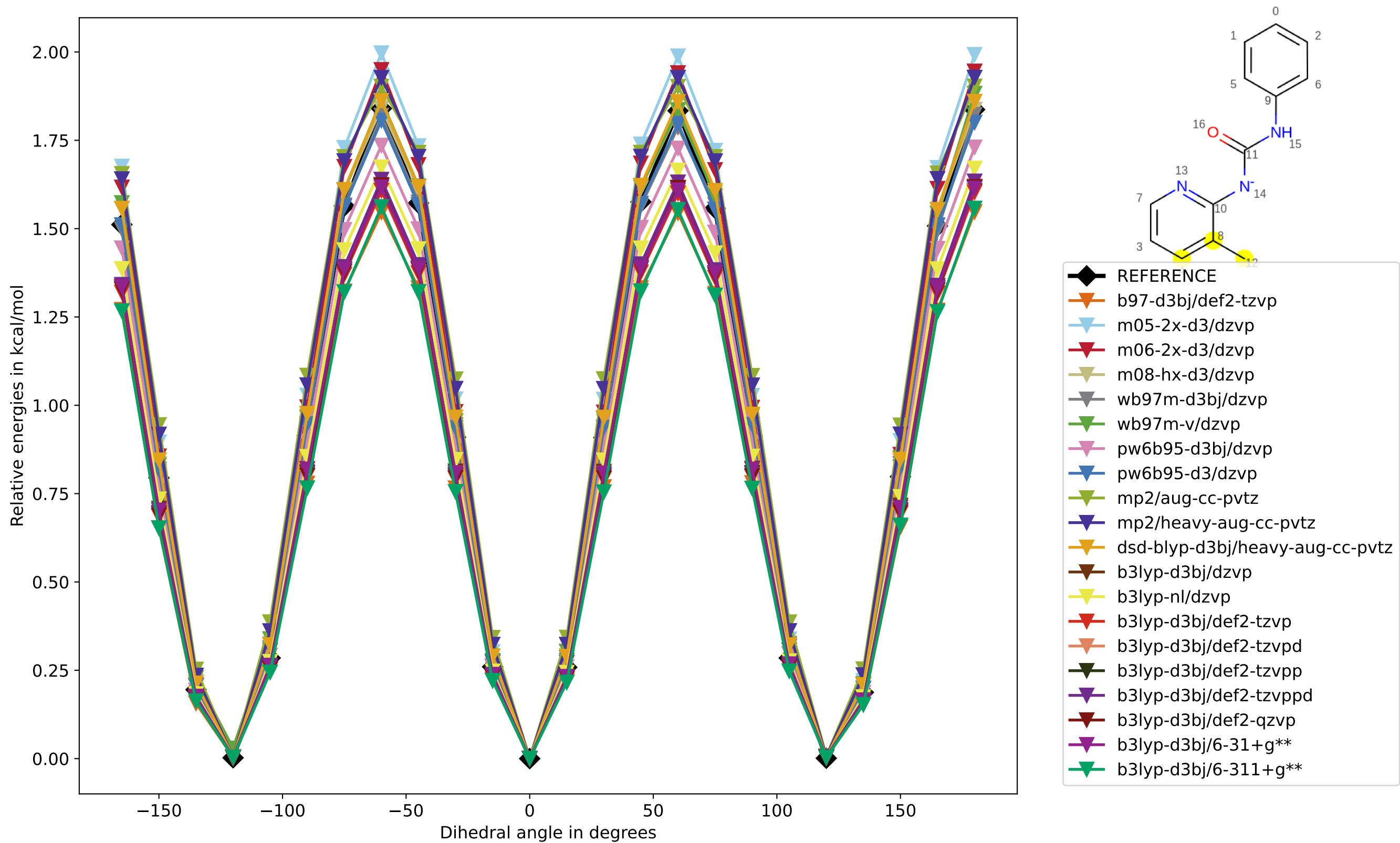
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- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
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- b3lyp-d3bj/def2-tzvp
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- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Charged molecule

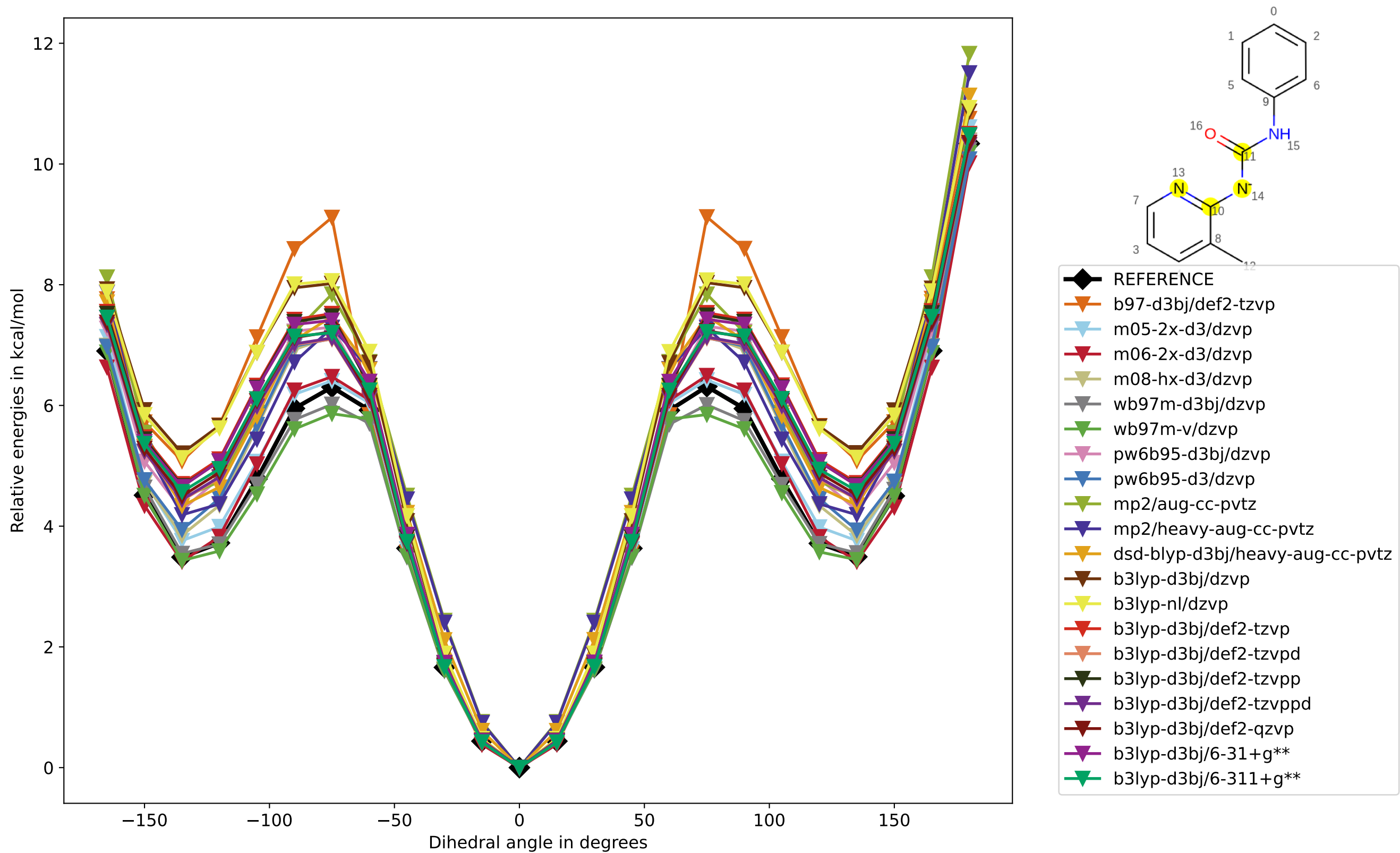


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- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

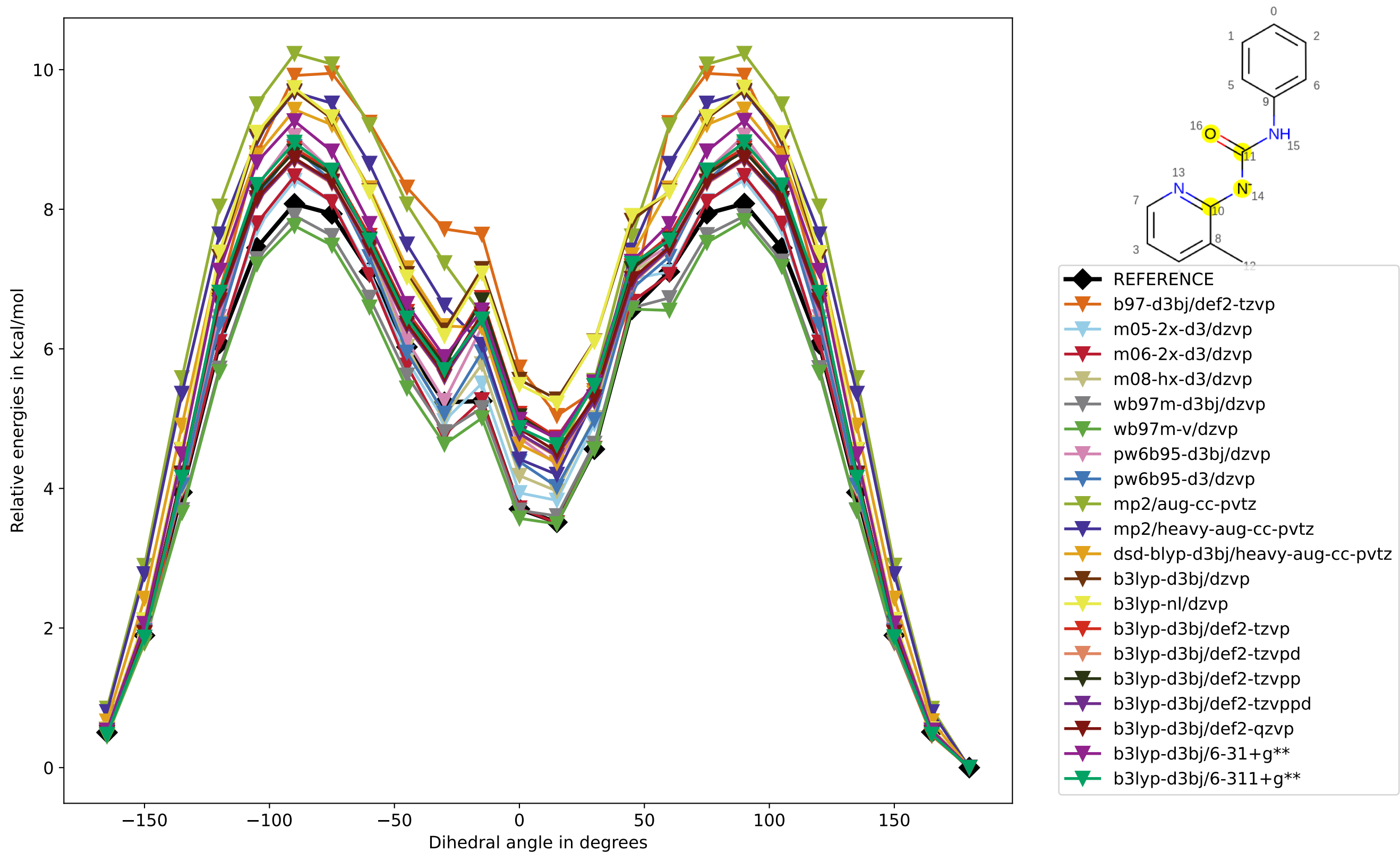
Charged molecule



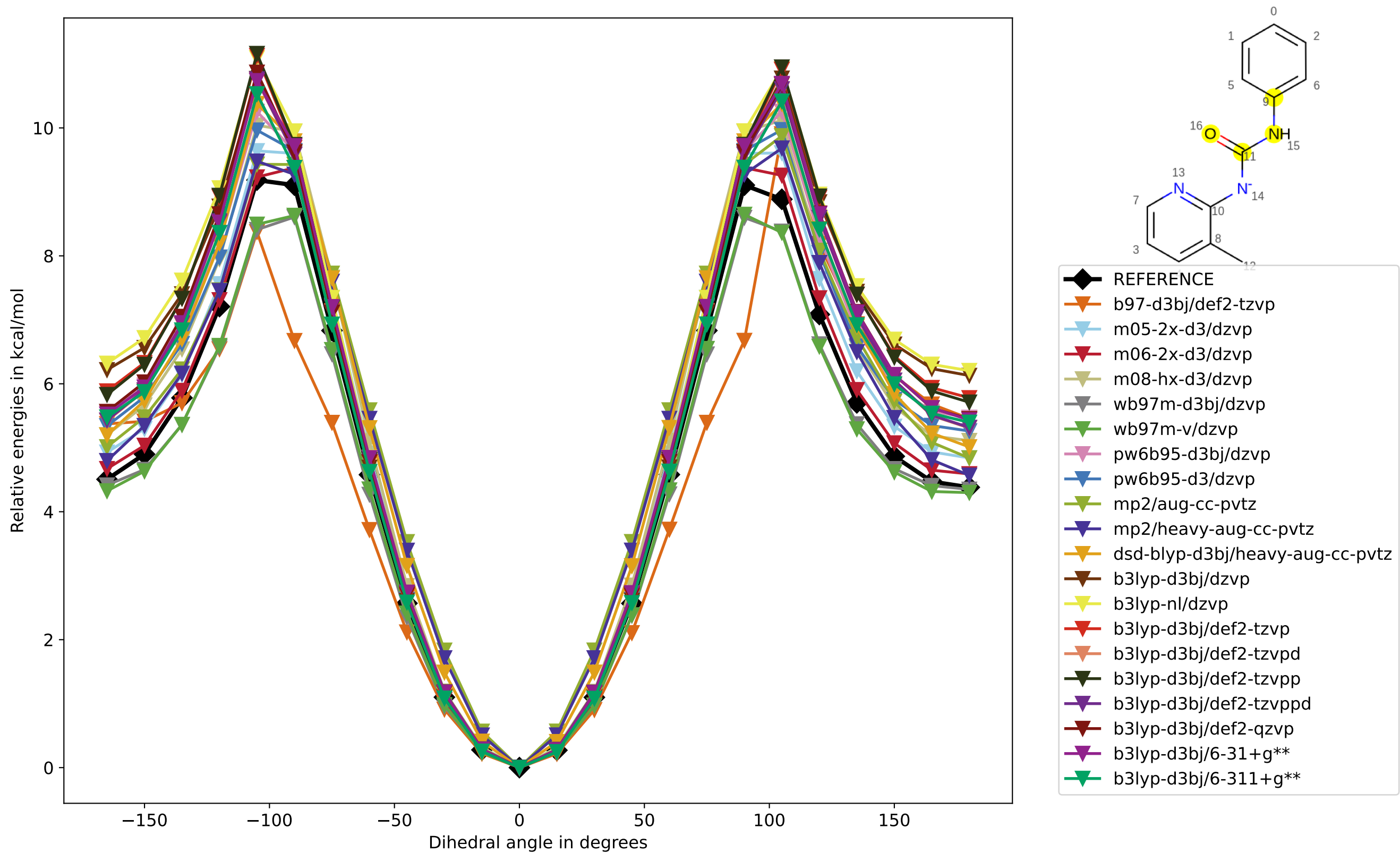
Charged molecule



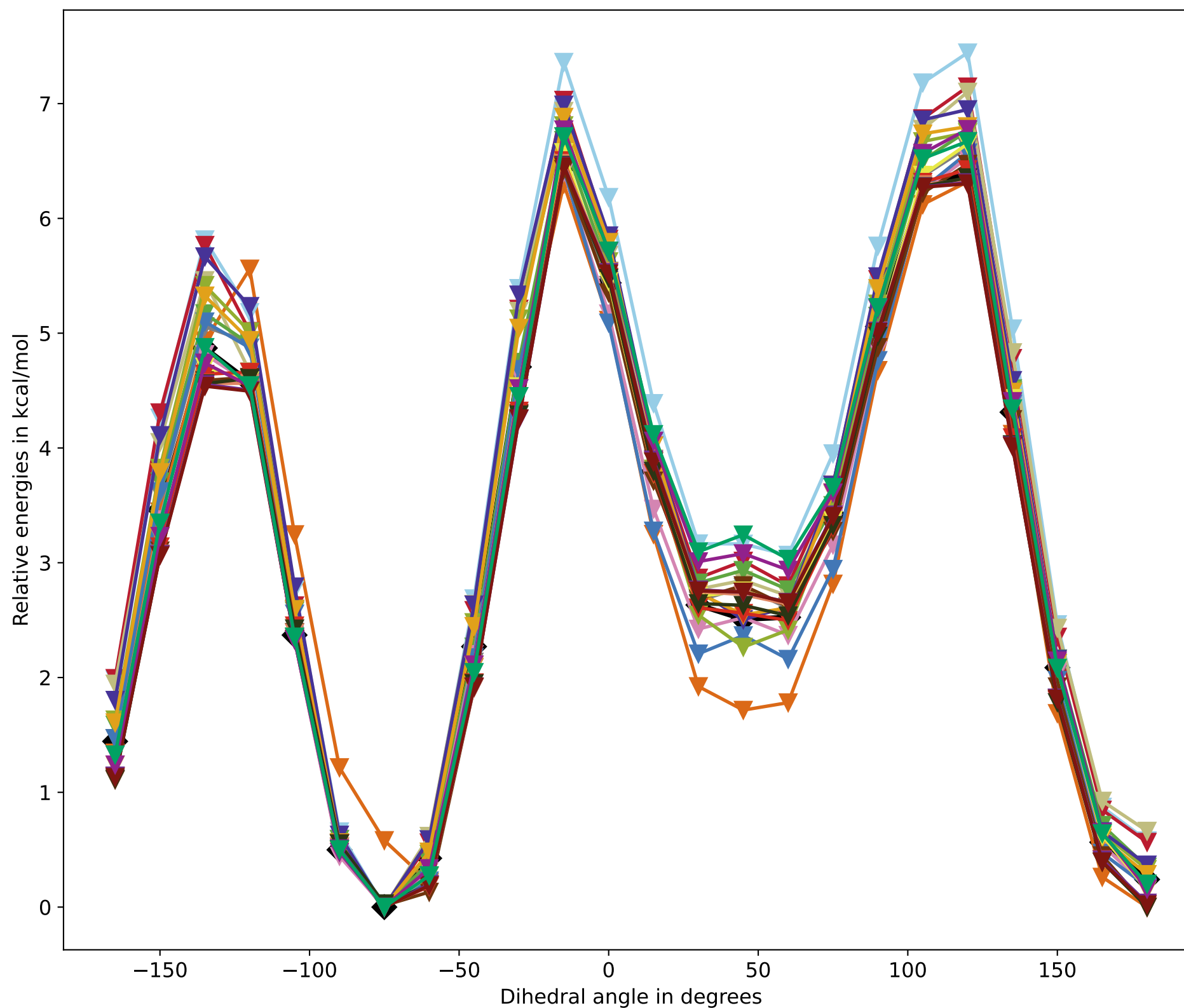
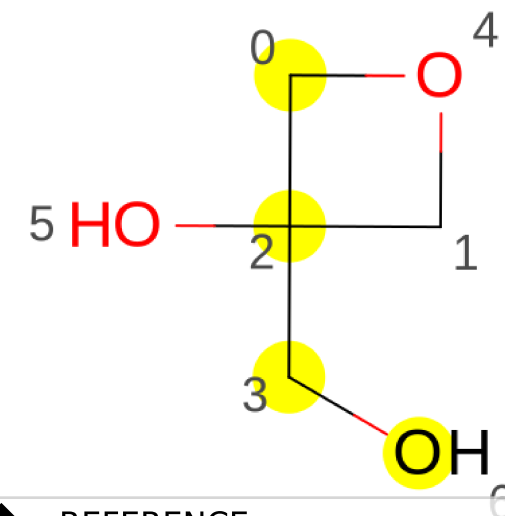
Charged molecule



Charged molecule

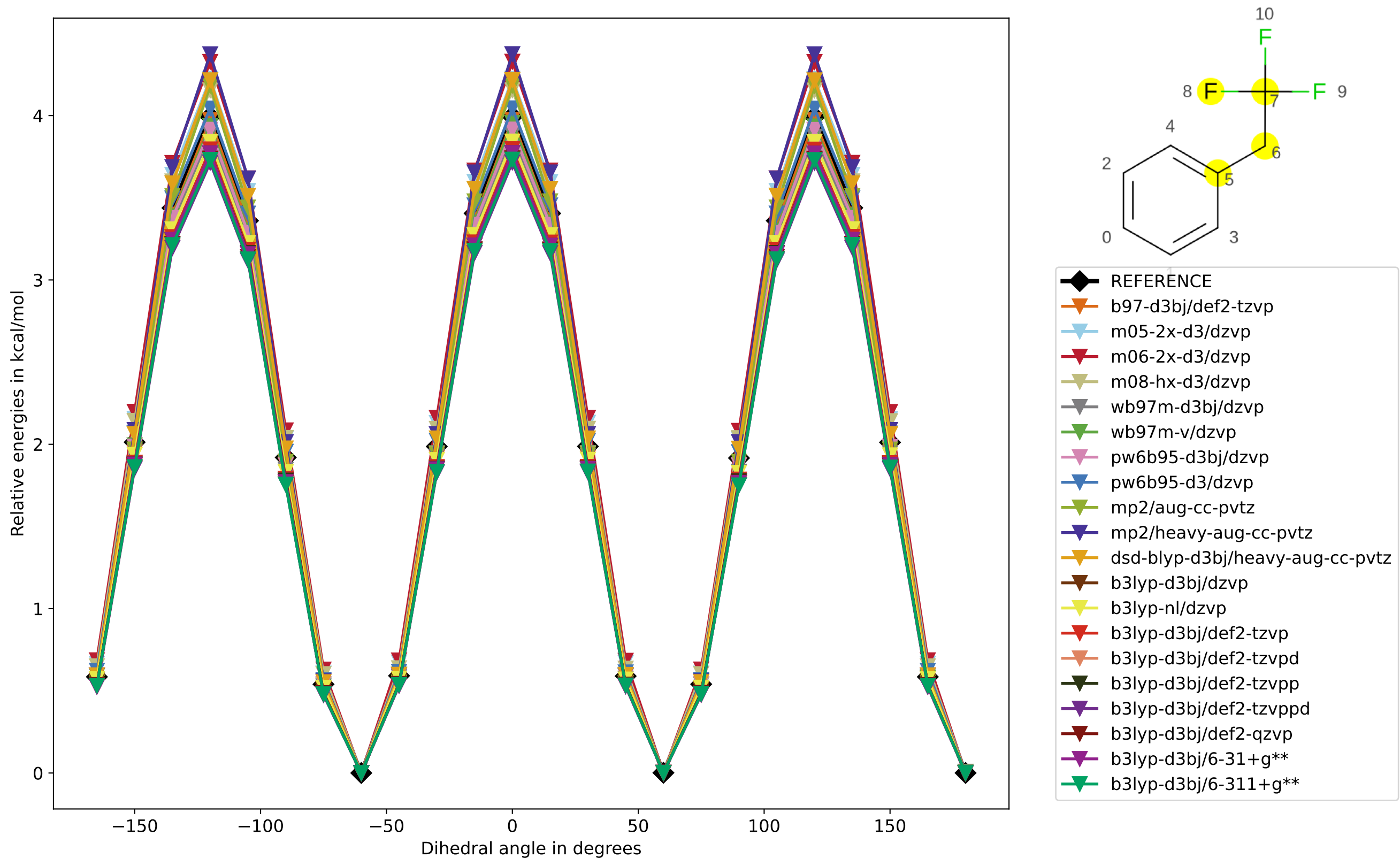


Neutral molecule

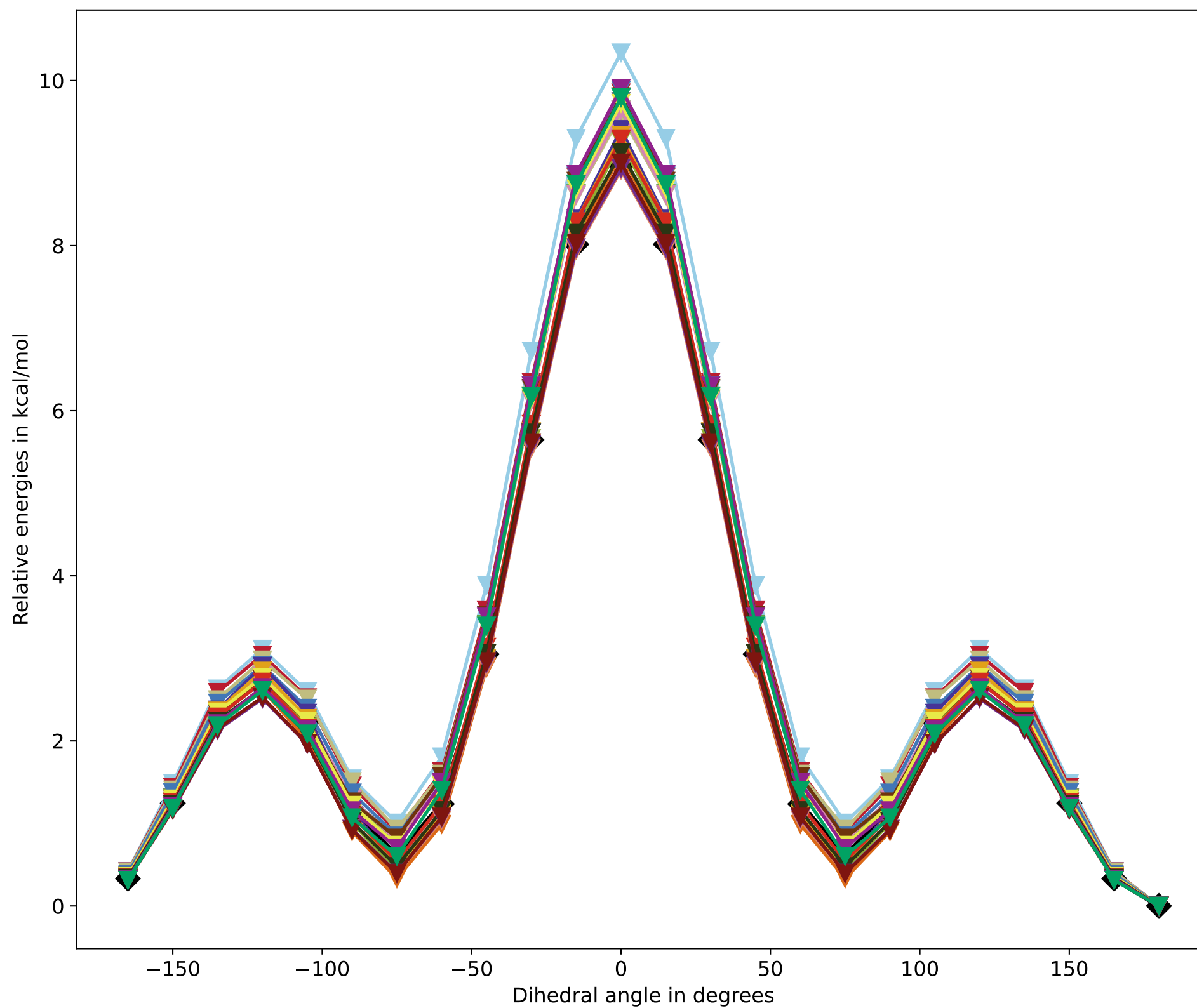


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

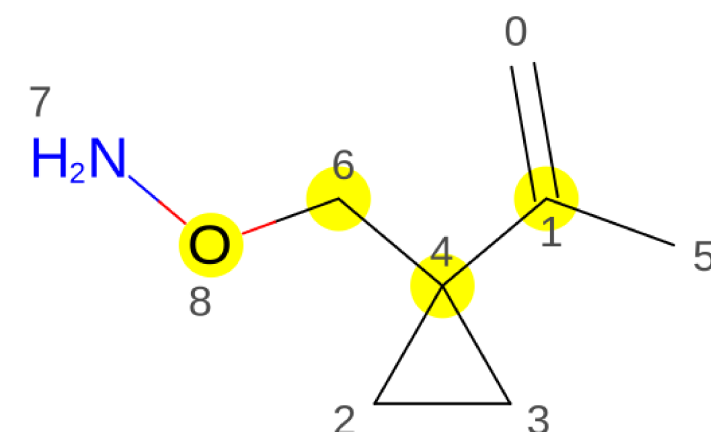
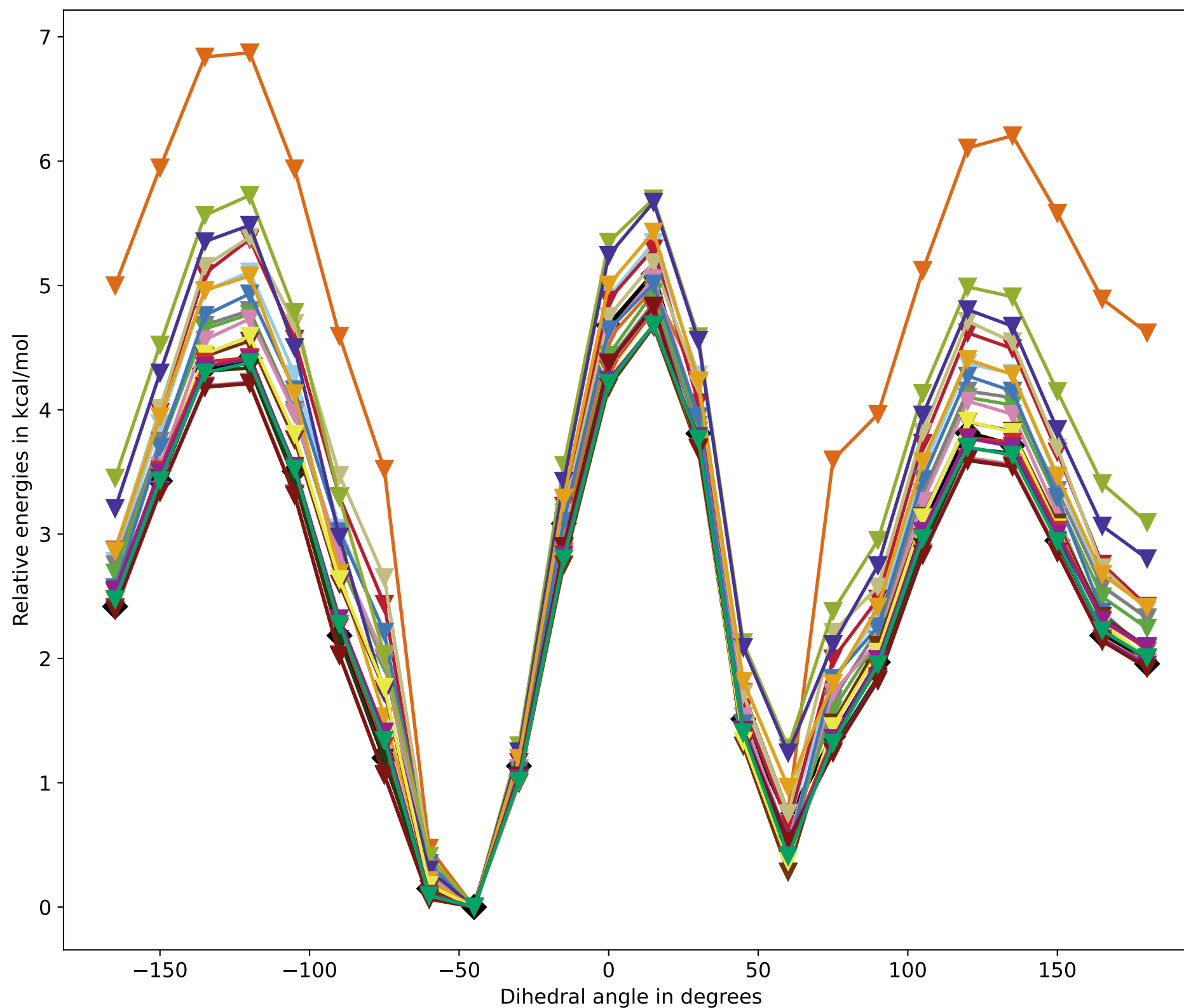
Neutral molecule



Neutral molecule

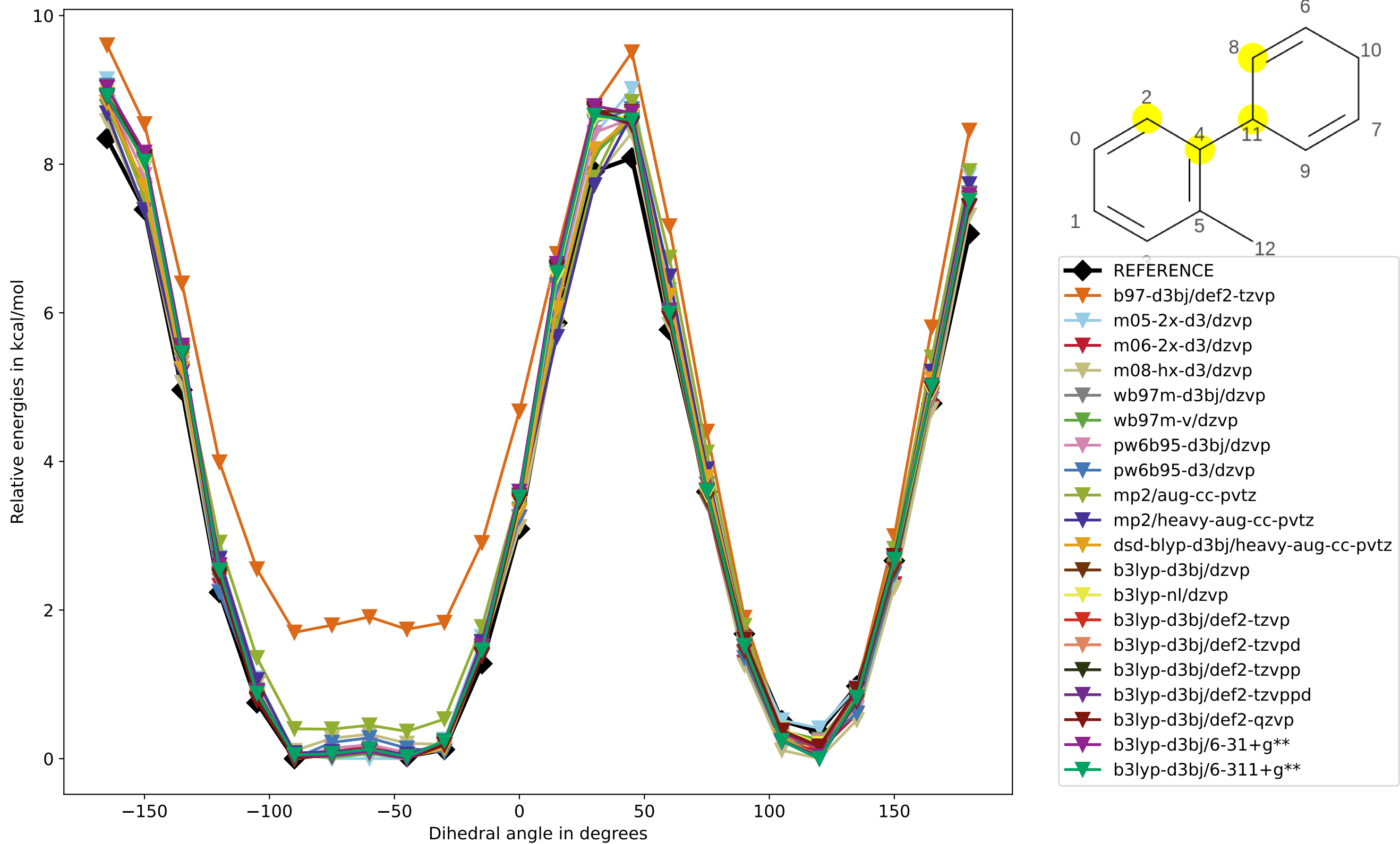


Neutral molecule

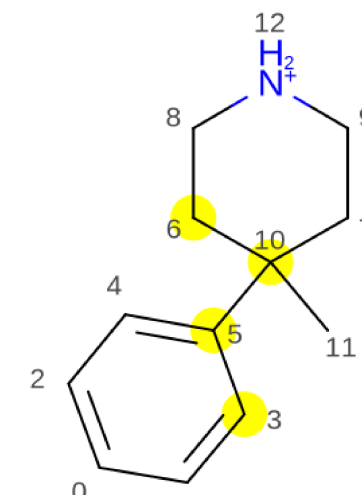
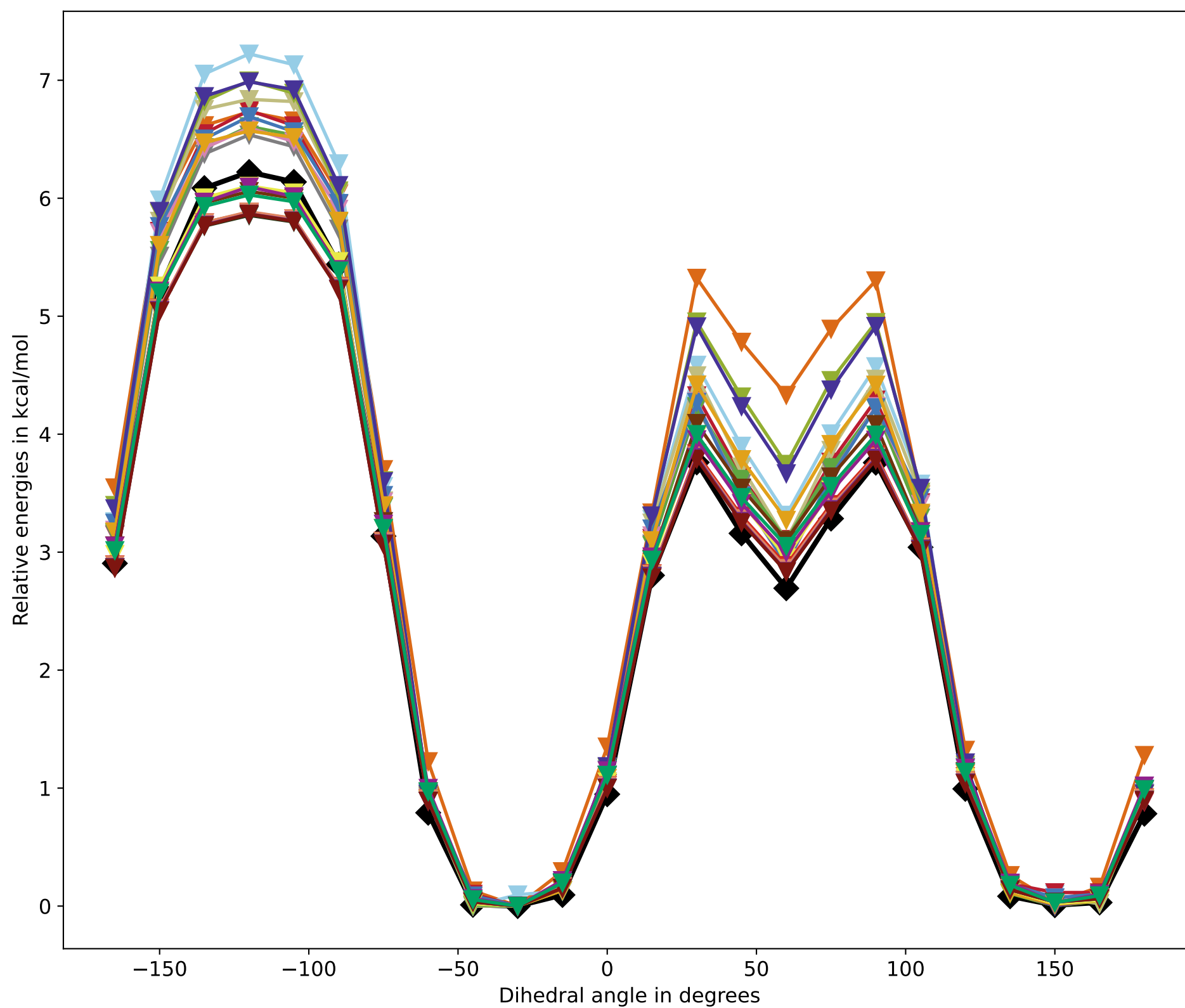


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvdpd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule

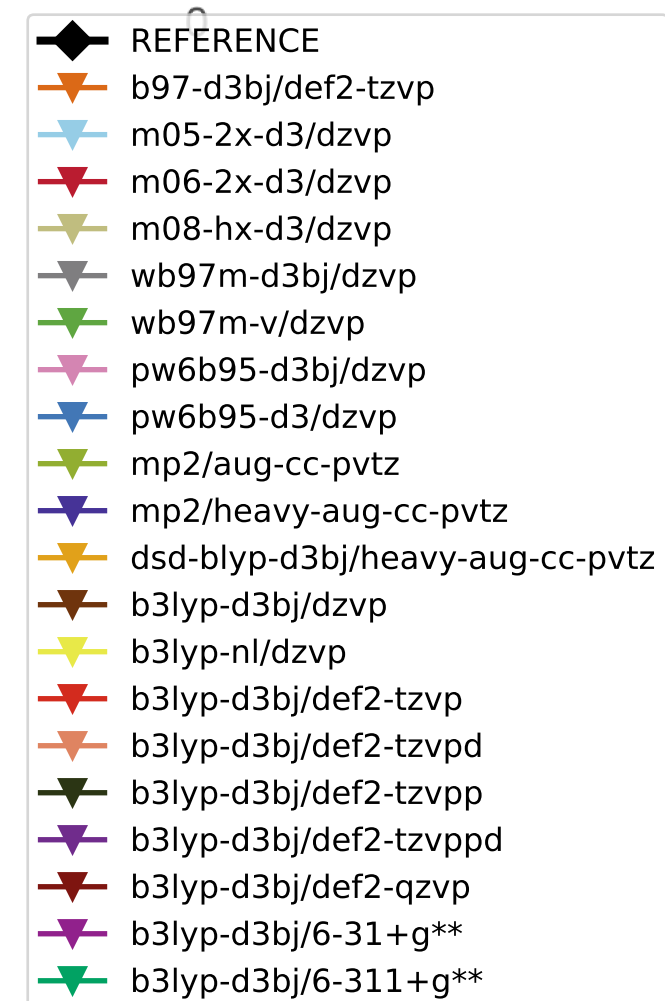
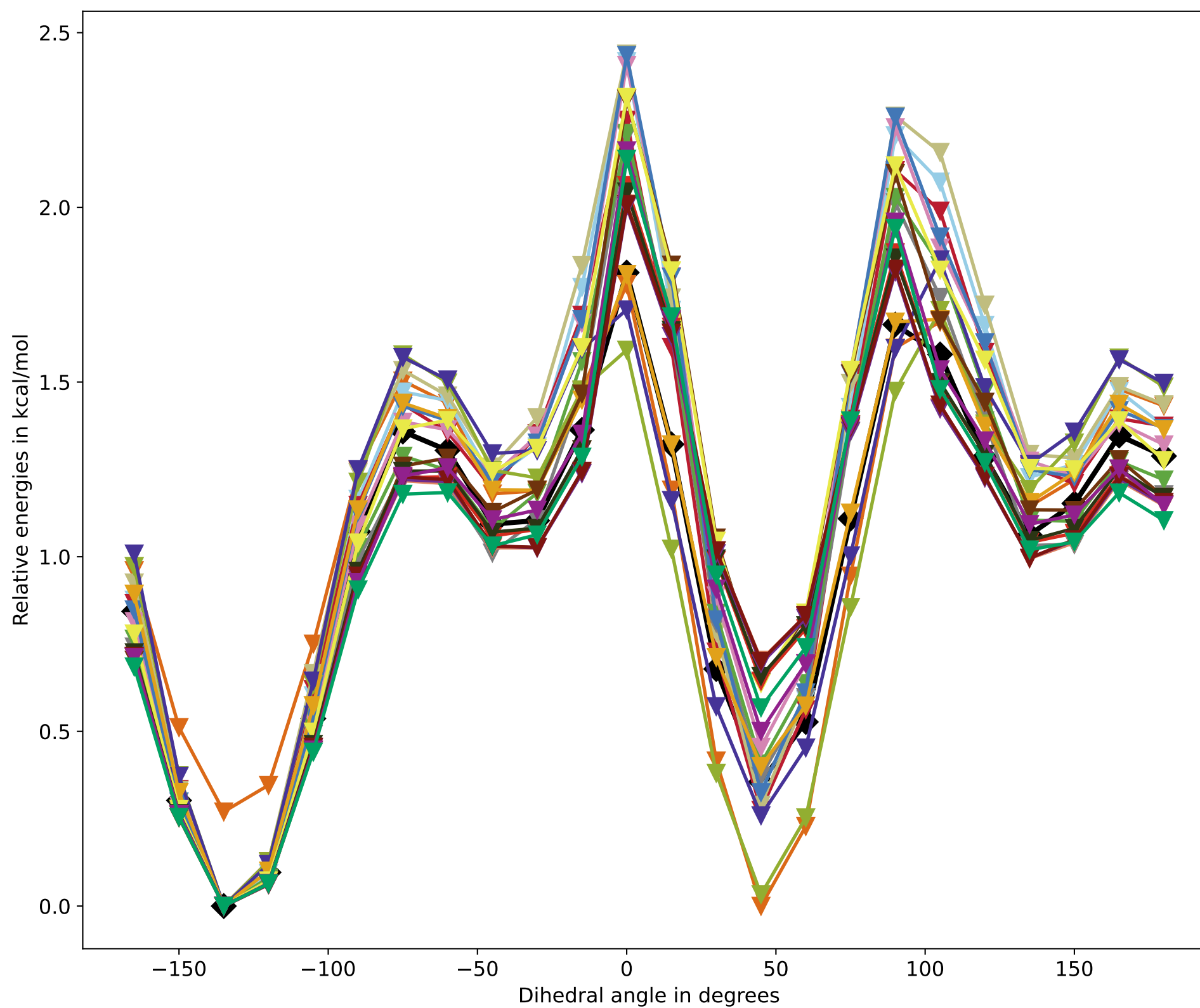
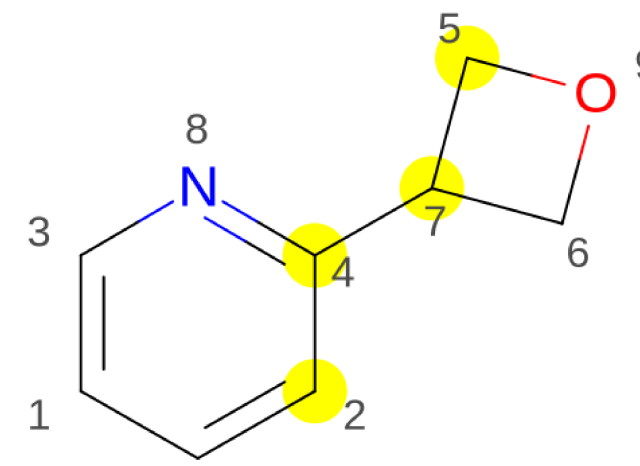


Charged molecule

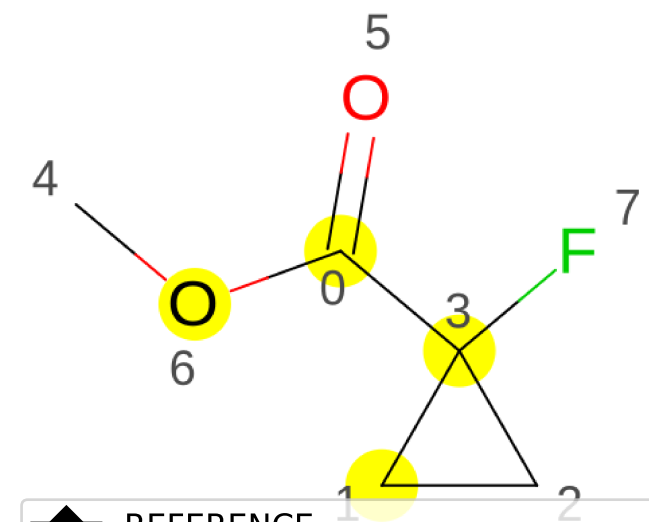
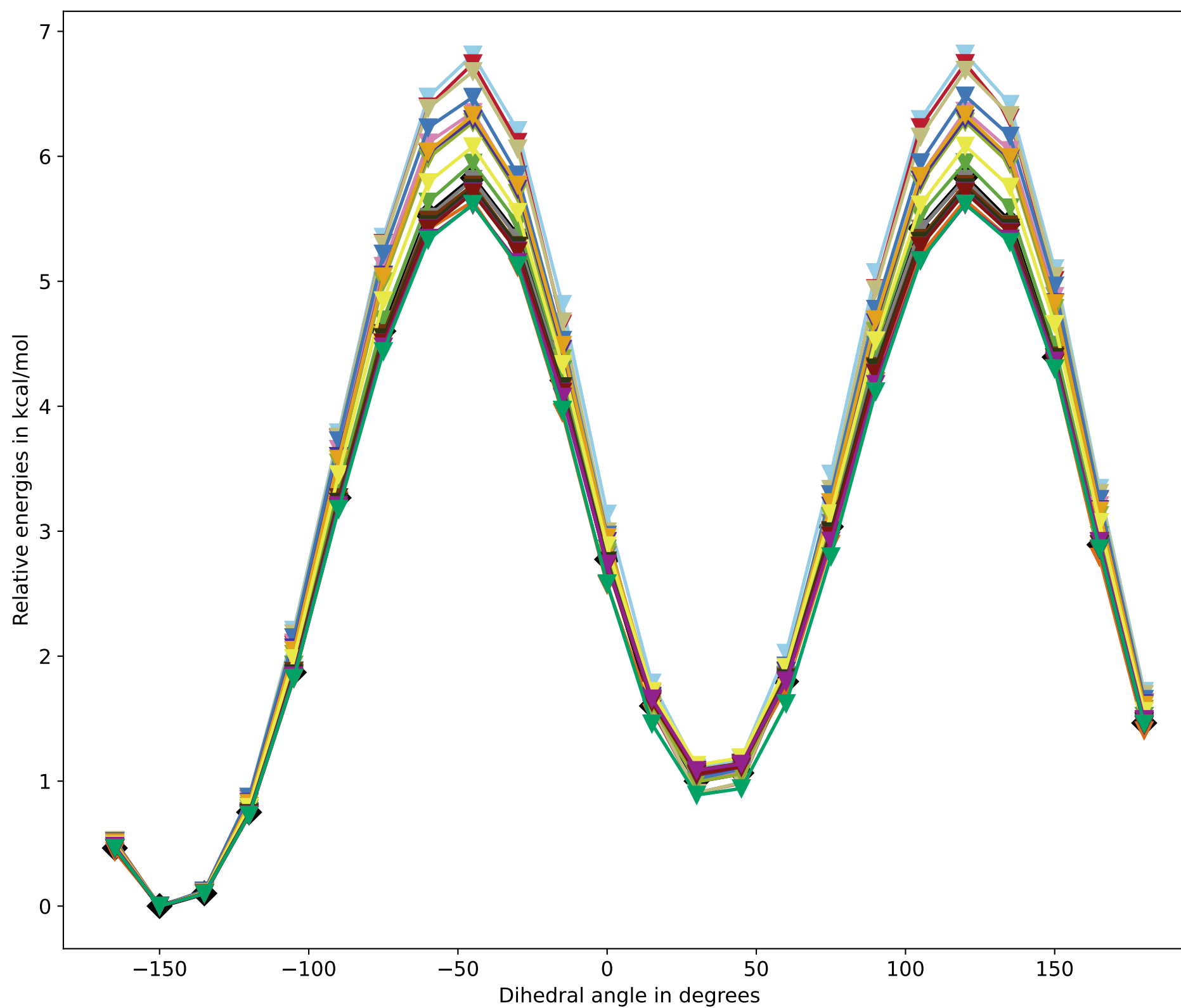


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

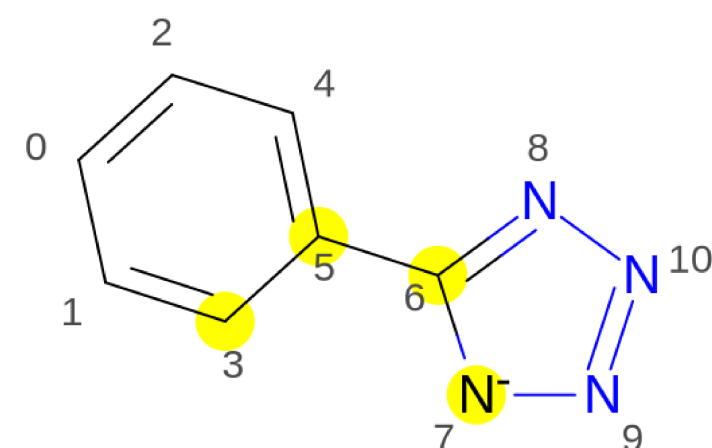
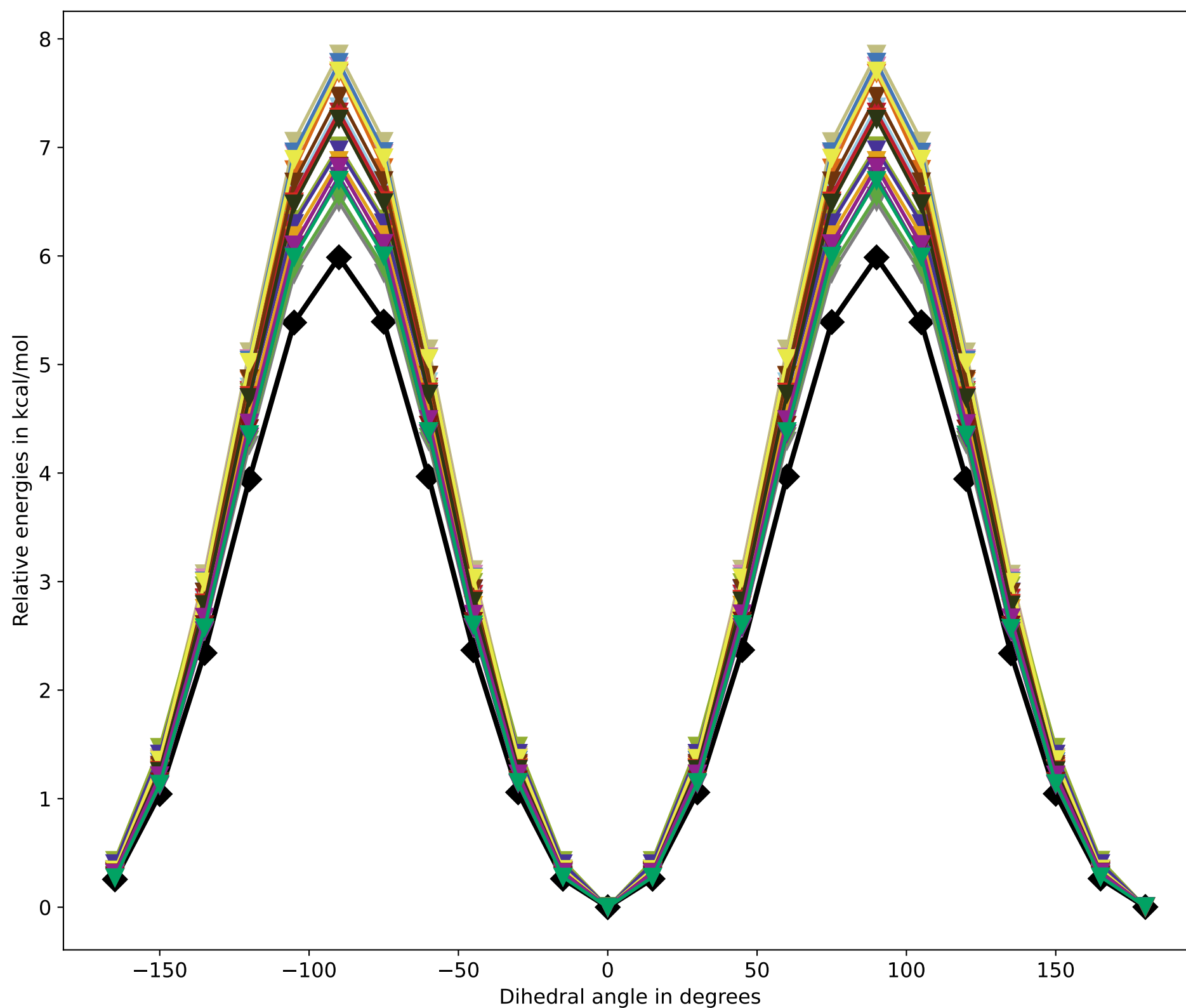
Neutral molecule



Neutral molecule

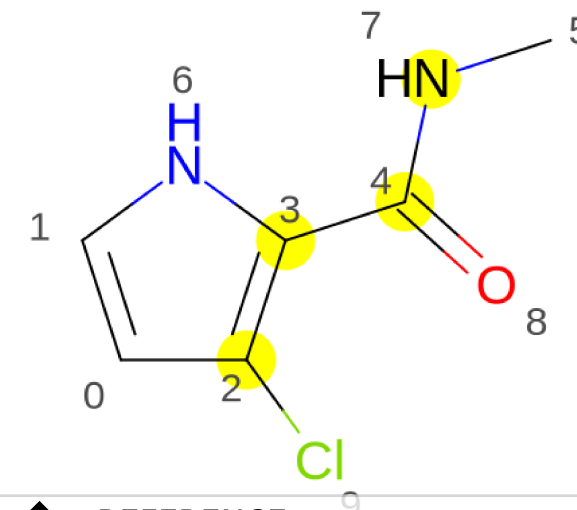
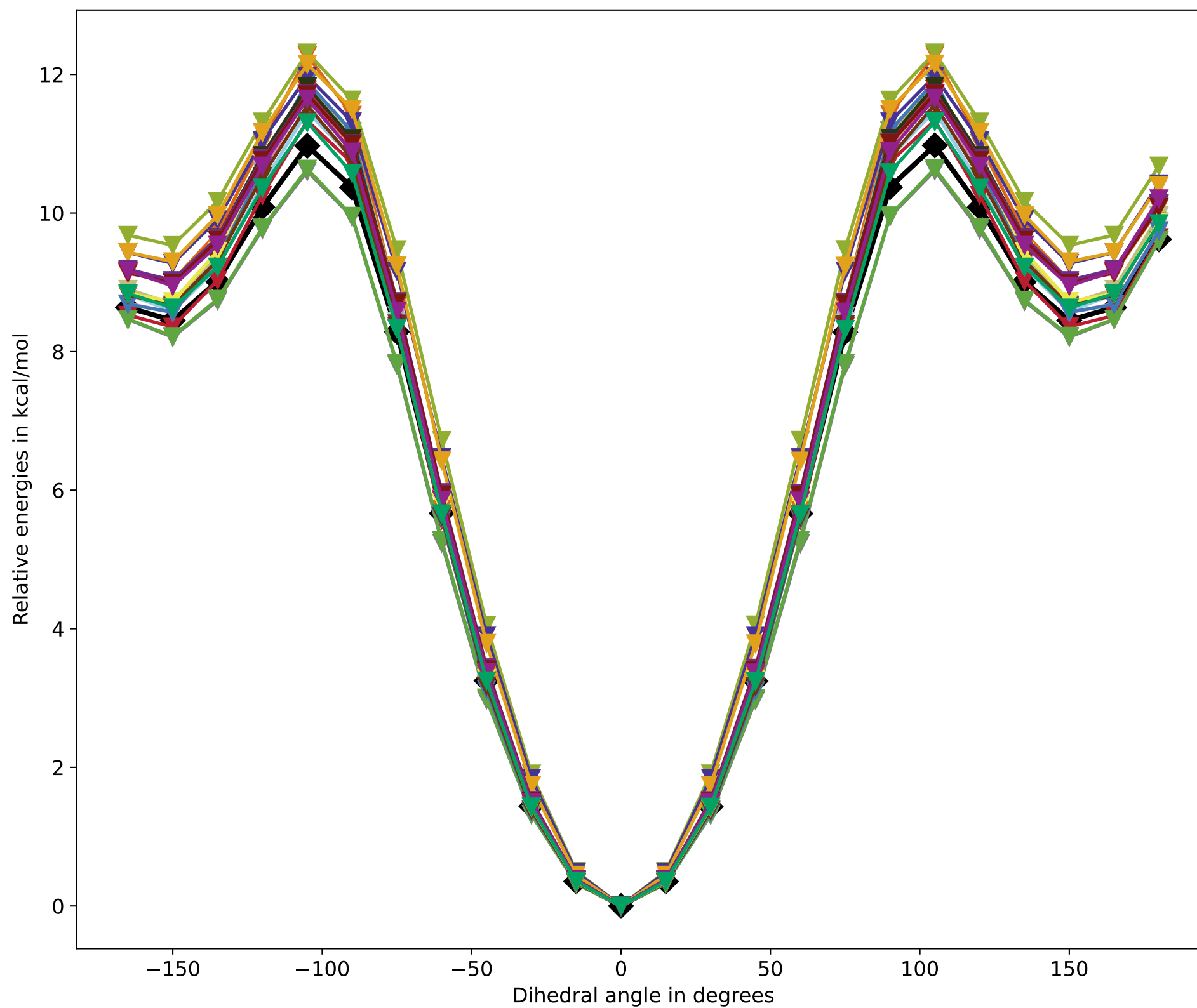


Charged molecule



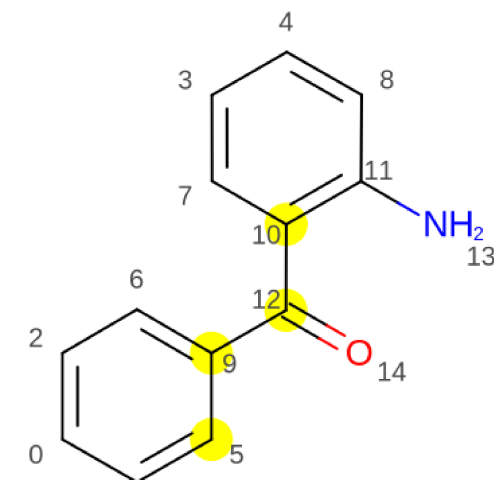
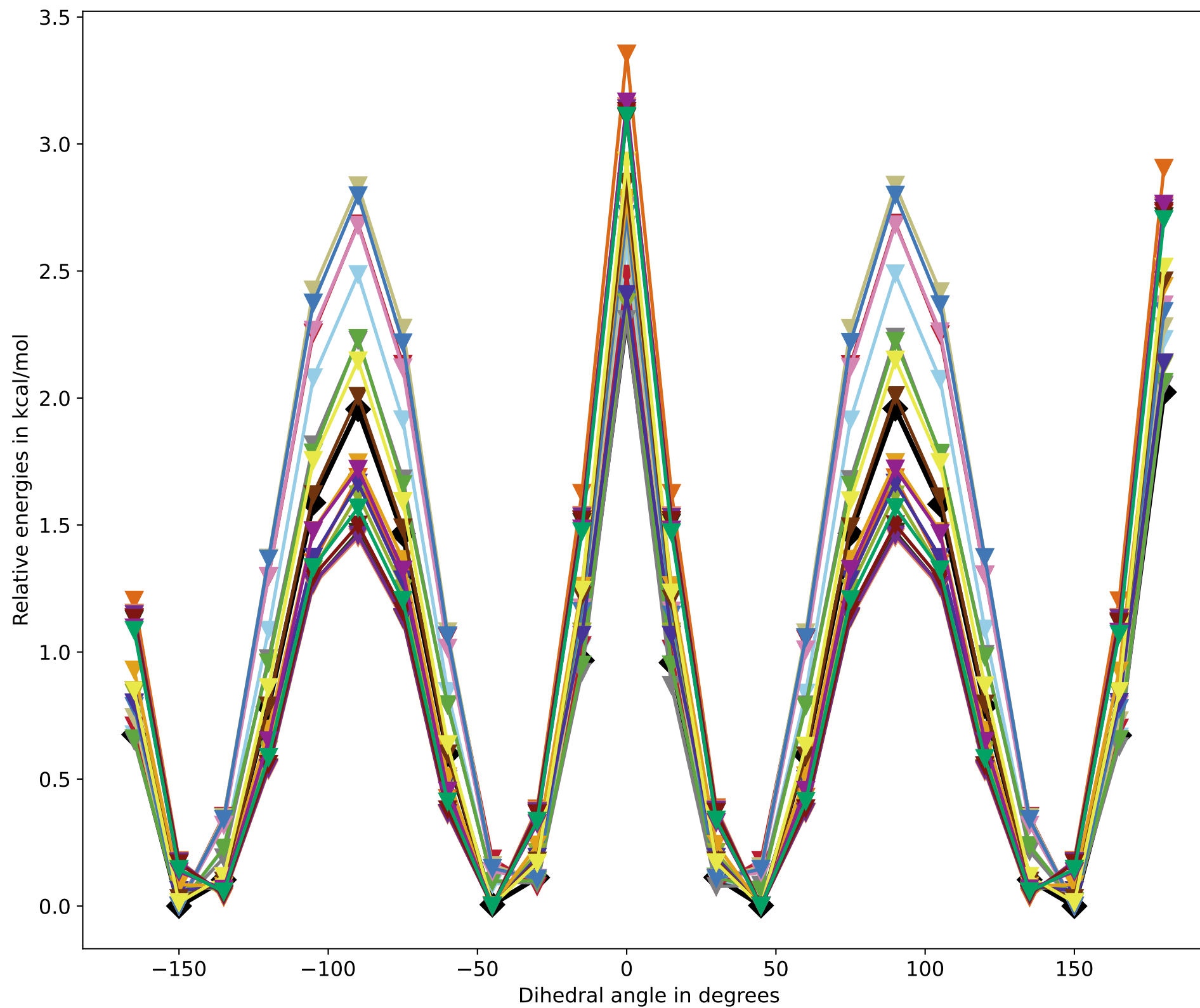
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvpp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule



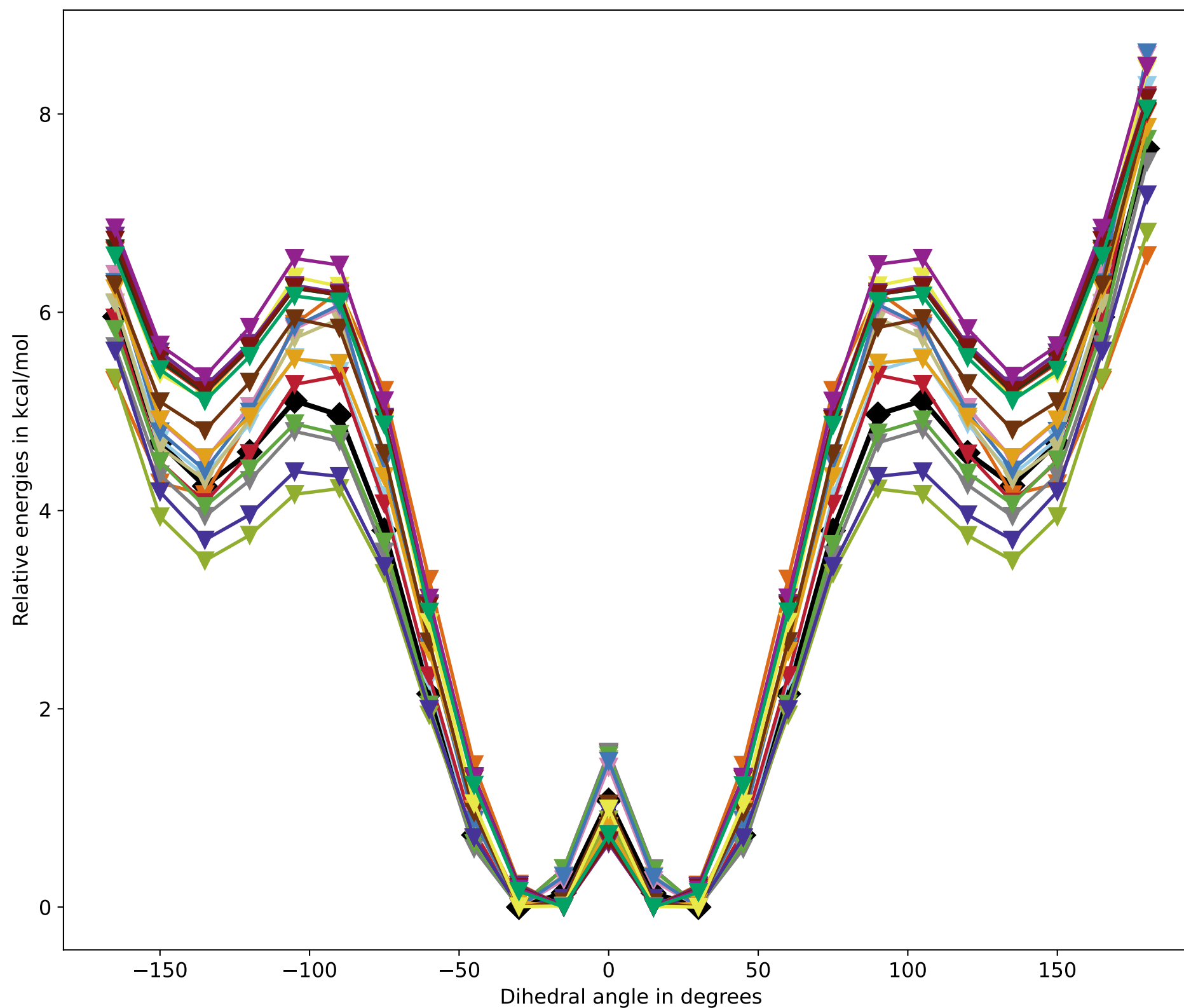
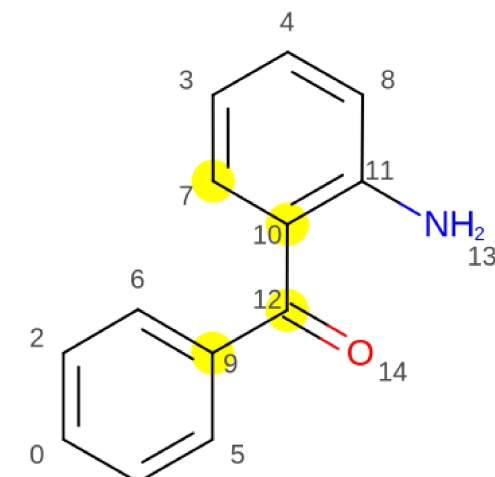
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule



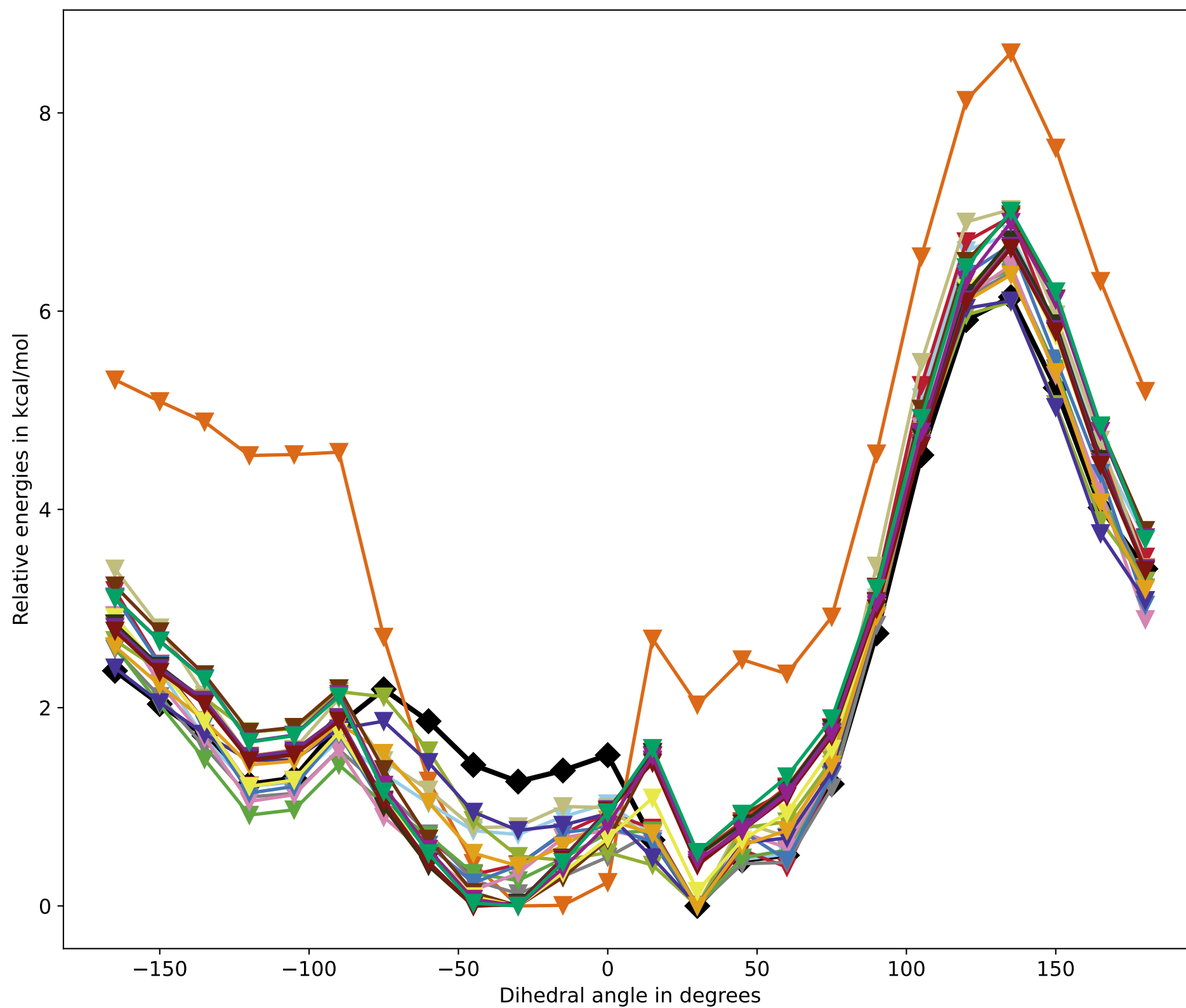
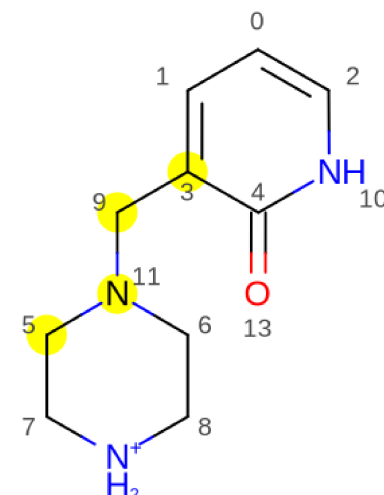
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule



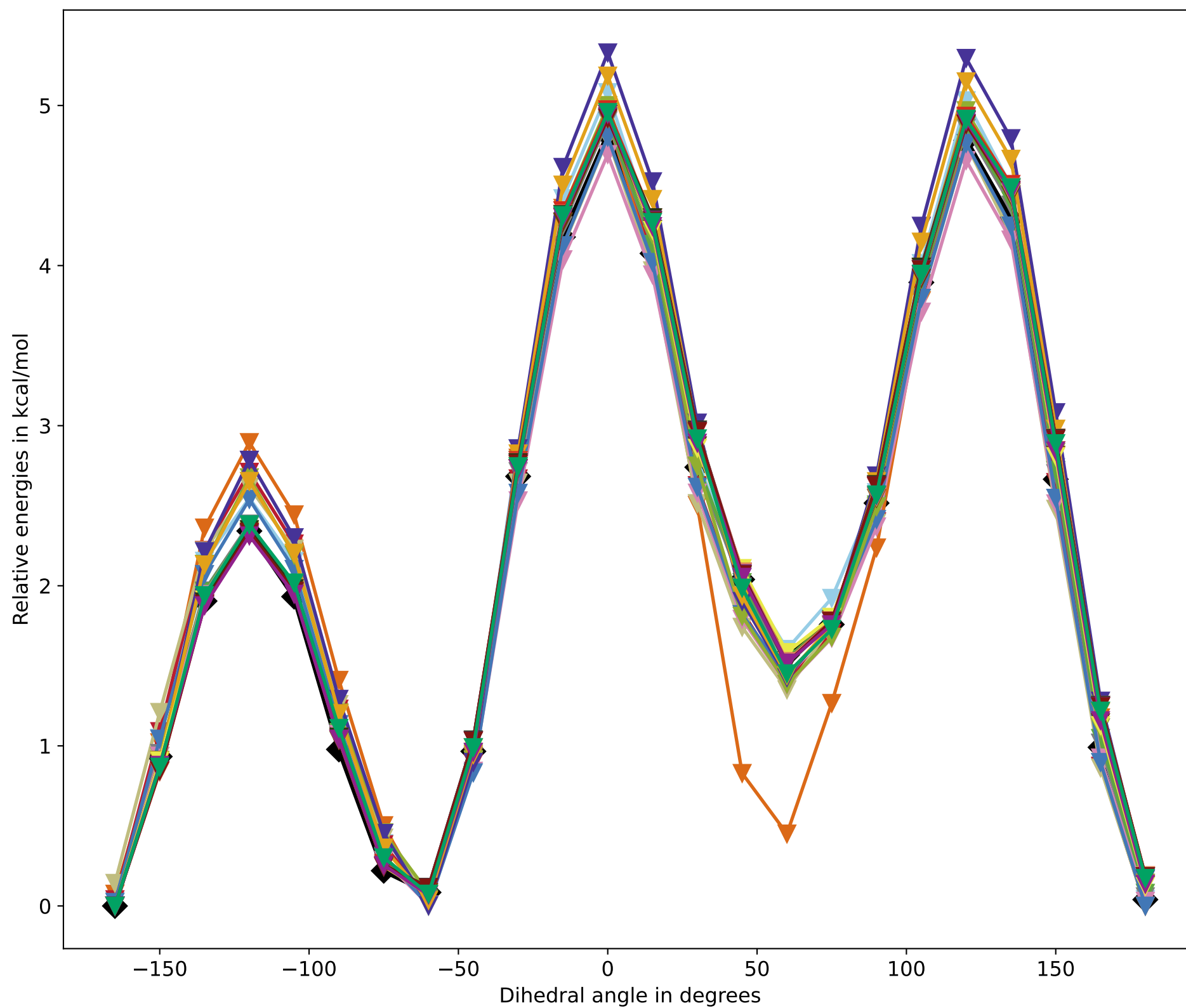
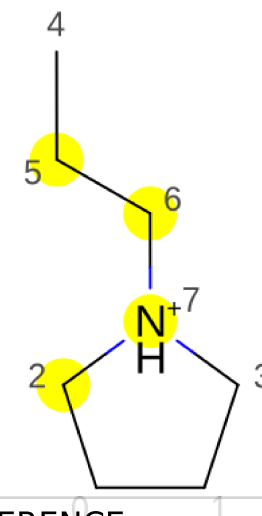
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvpp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Charged molecule



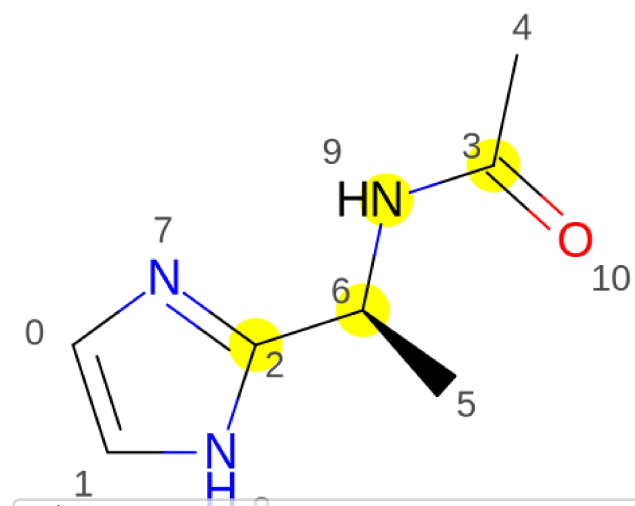
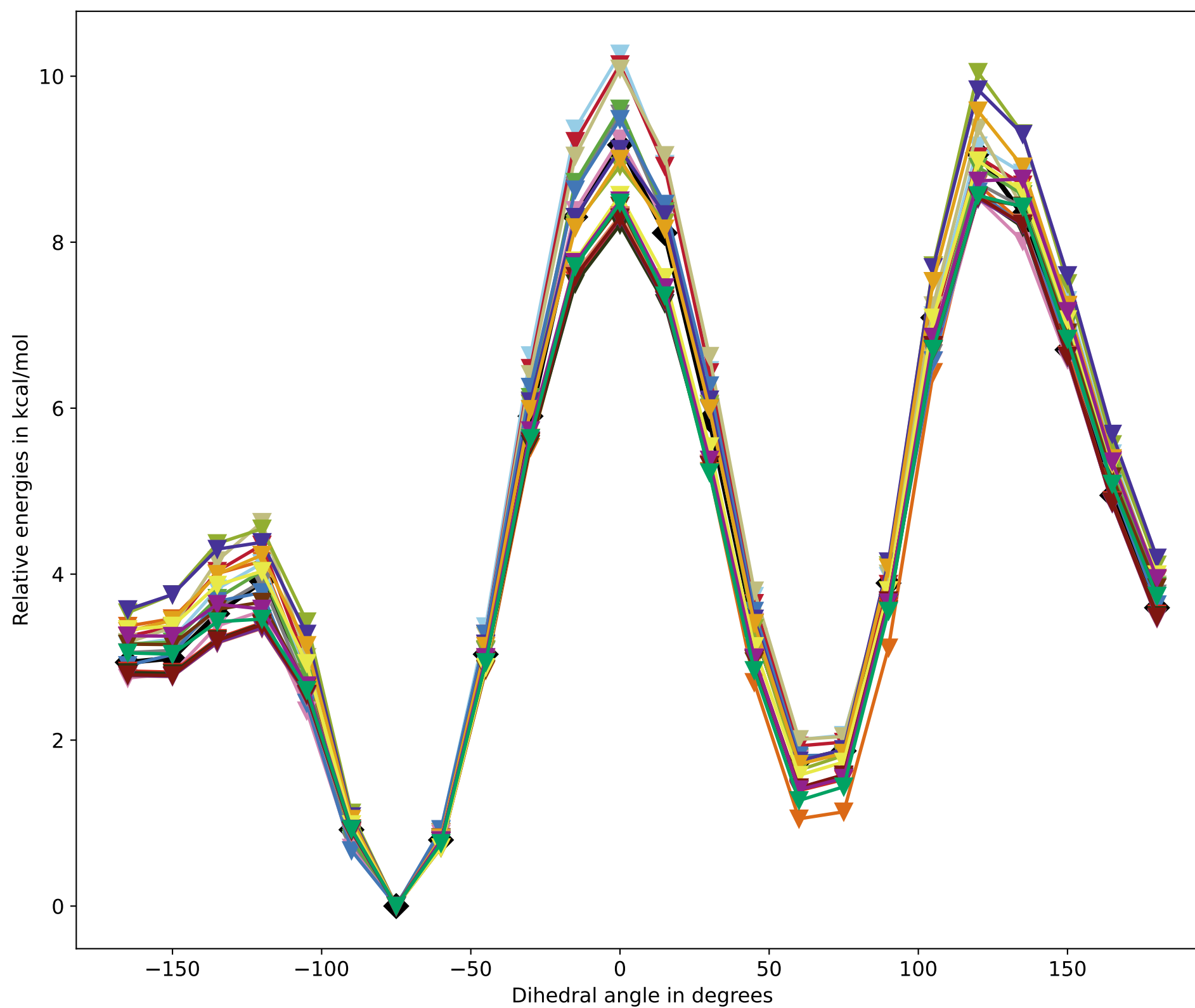
- ◆ REFERENCE
- ▲ b97-d3bj/def2-tzvp
- ▼ m05-2x-d3/dzvp
- ▼ m06-2x-d3/dzvp
- ▼ m08-hx-d3/dzvp
- ▼ wb97m-d3bj/dzvp
- ▼ wb97m-v/dzvp
- ▼ pw6b95-d3bj/dzvp
- ▼ pw6b95-d3/dzvp
- ▼ mp2/aug-cc-pvtz
- ▼ mp2/heavy-aug-cc-pvtz
- ▼ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ▼ b3lyp-d3bj/dzvp
- ▼ b3lyp-nl/dzvp
- ▼ b3lyp-d3bj/def2-tzvp
- ▼ b3lyp-d3bj/def2-tzvppd
- ▼ b3lyp-d3bj/def2-tzvppd
- ▼ b3lyp-d3bj/def2-qzvp
- ▼ b3lyp-d3bj/6-31+g**
- ▼ b3lyp-d3bj/6-311+g**

Charged molecule



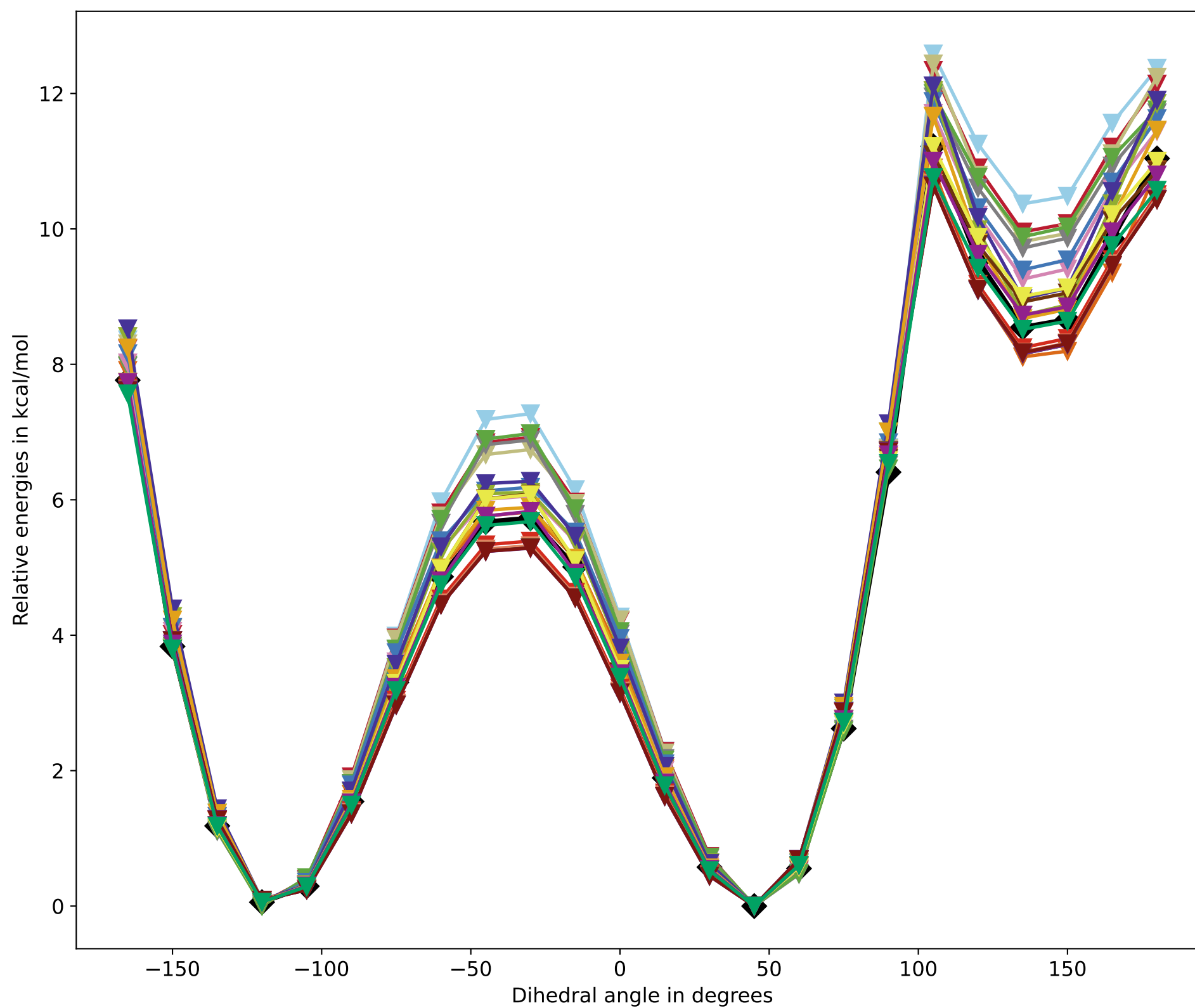
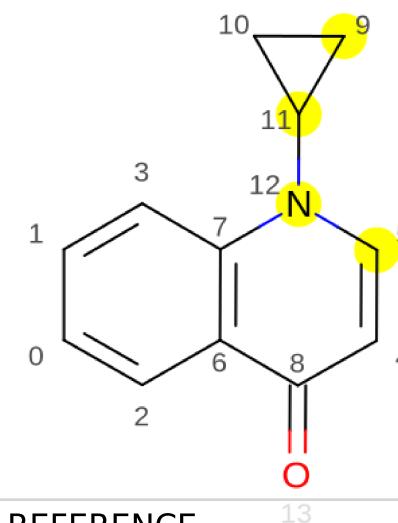
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule



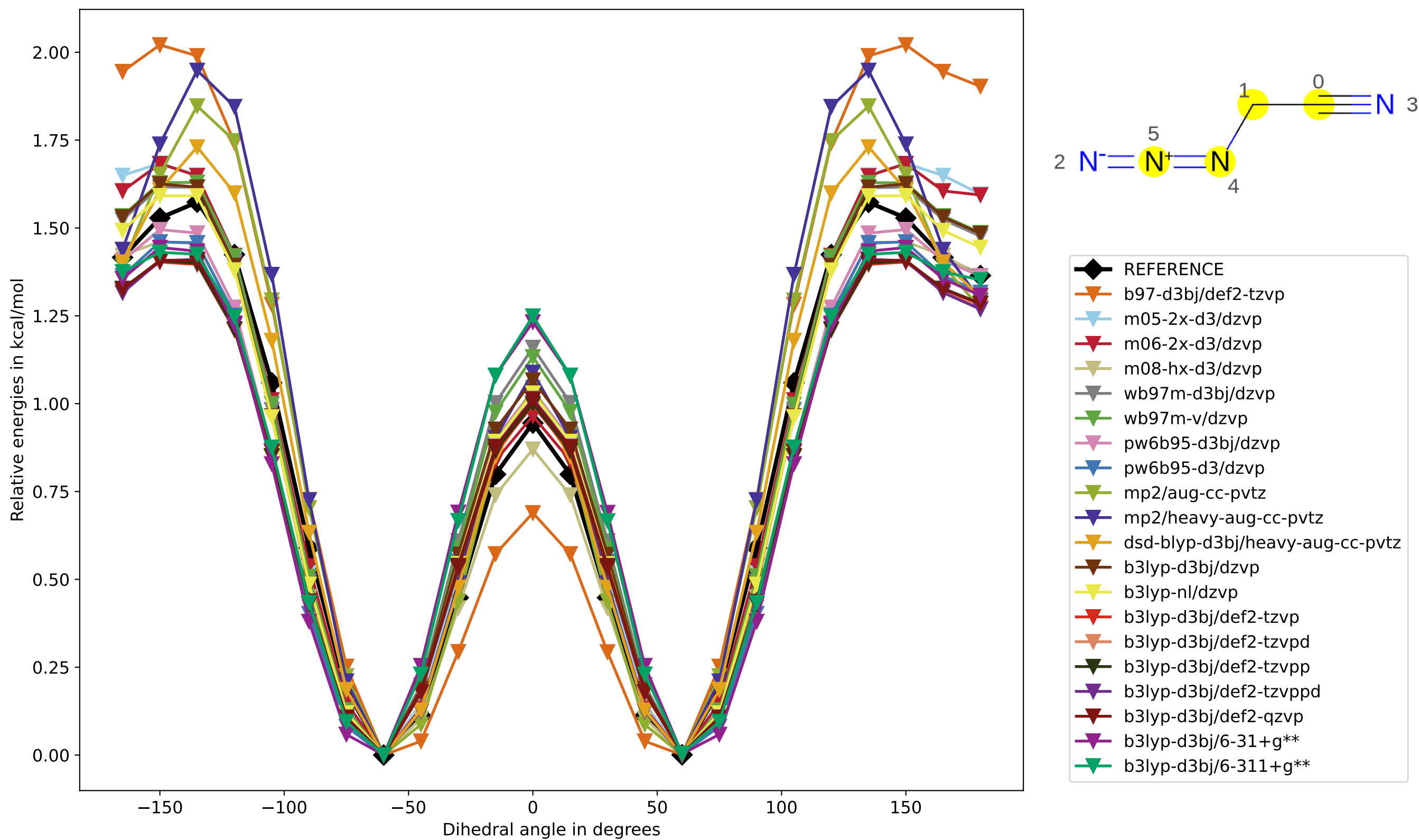
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppp
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule

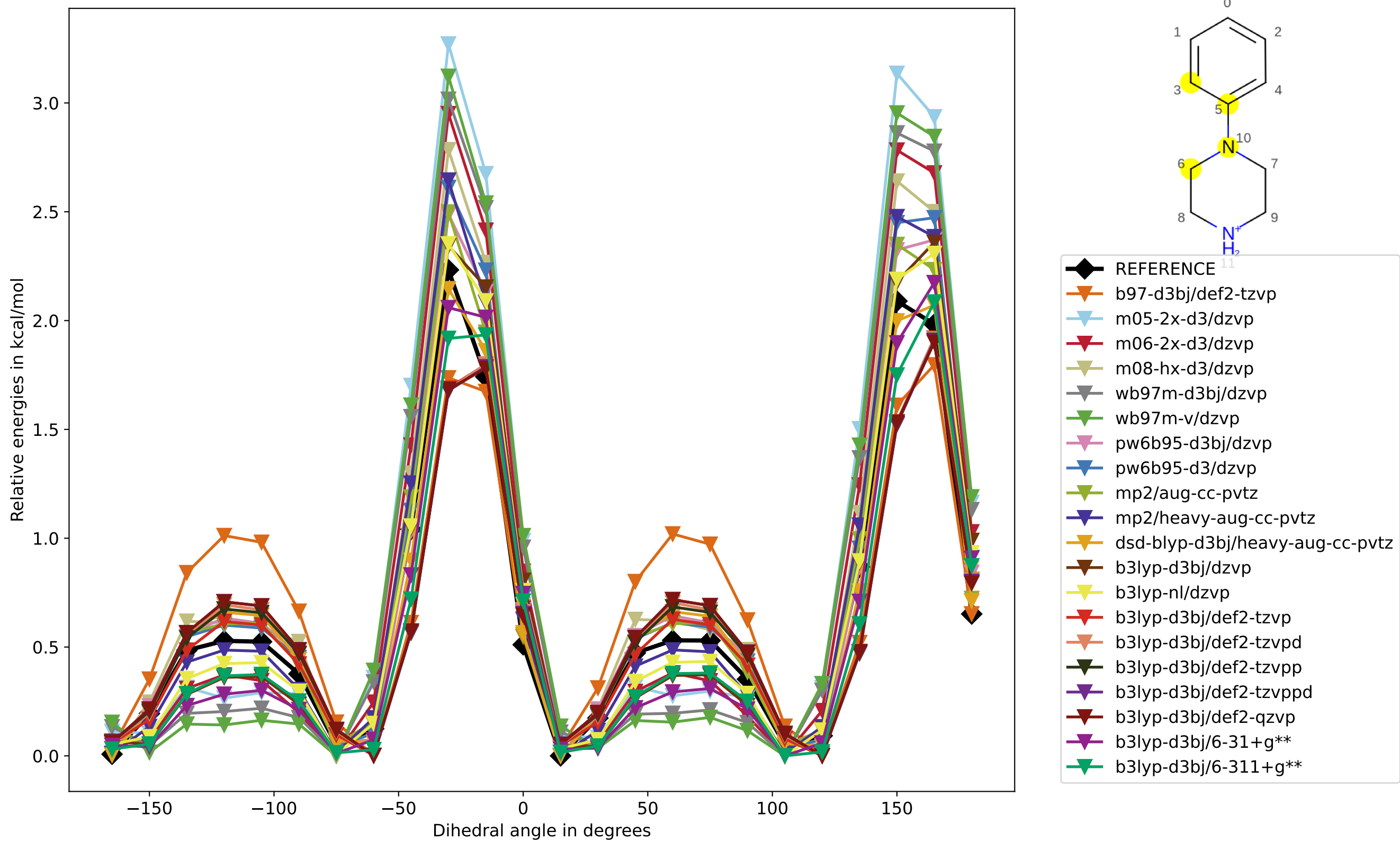
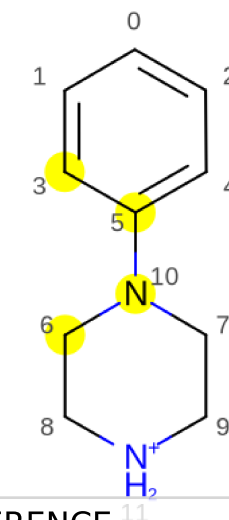


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

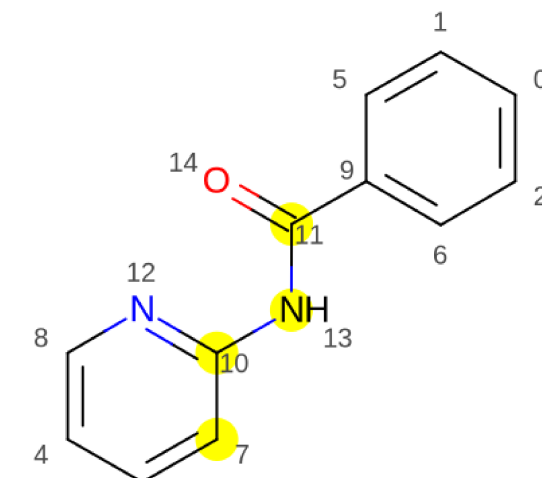
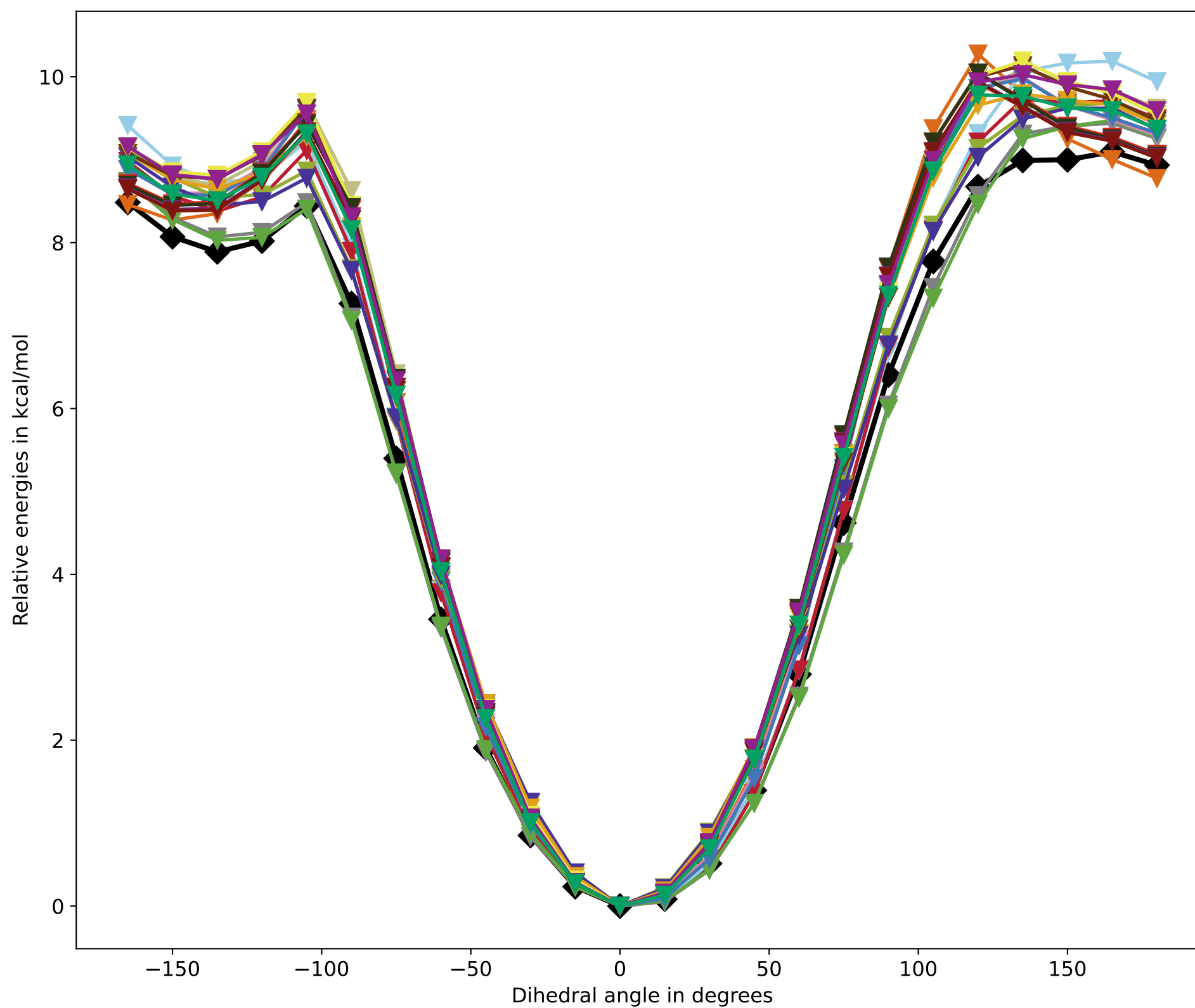
Charged molecule



Charged molecule

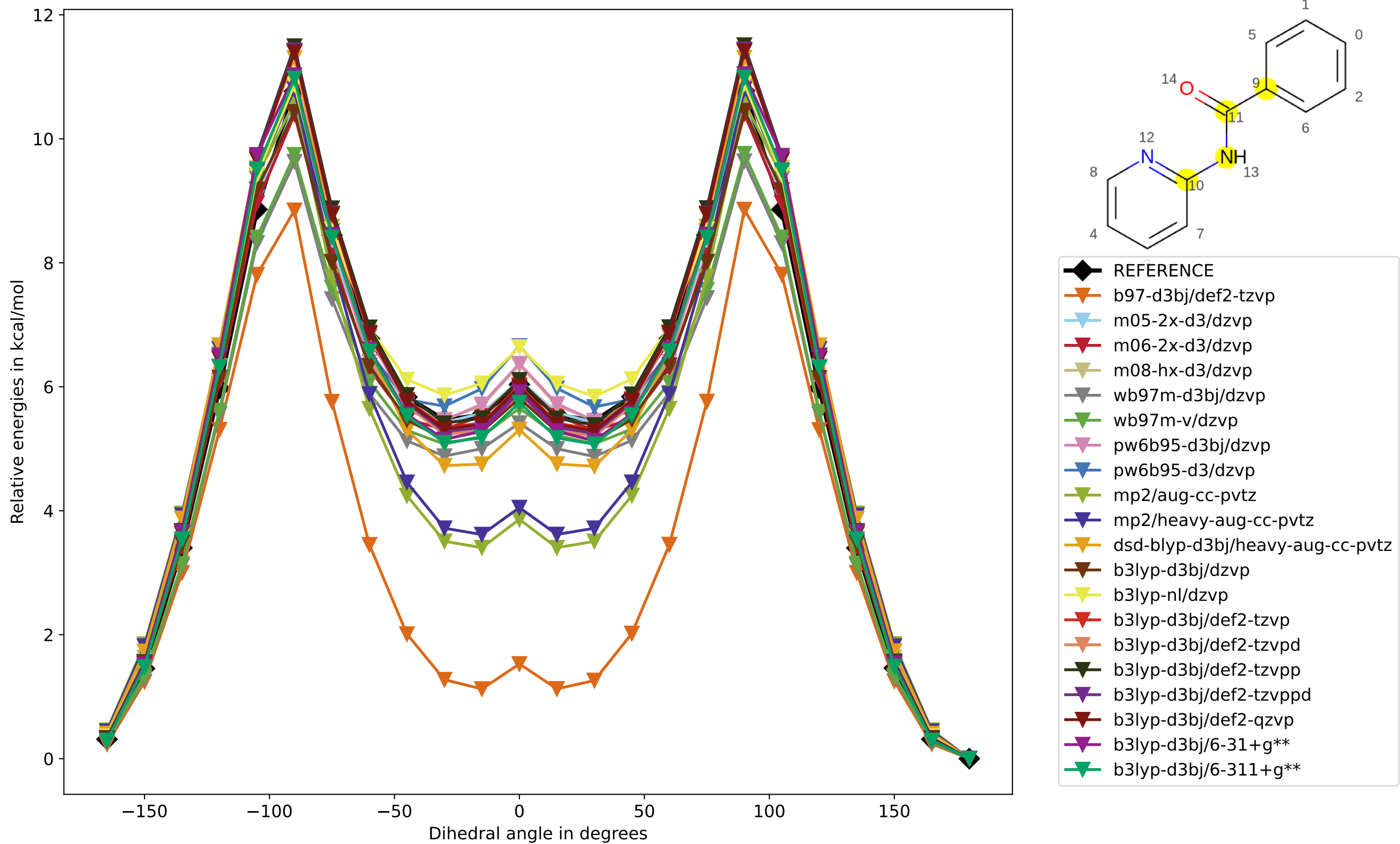
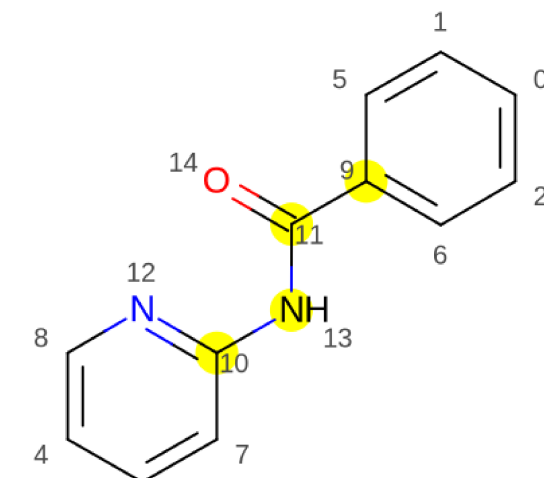


Neutral molecule

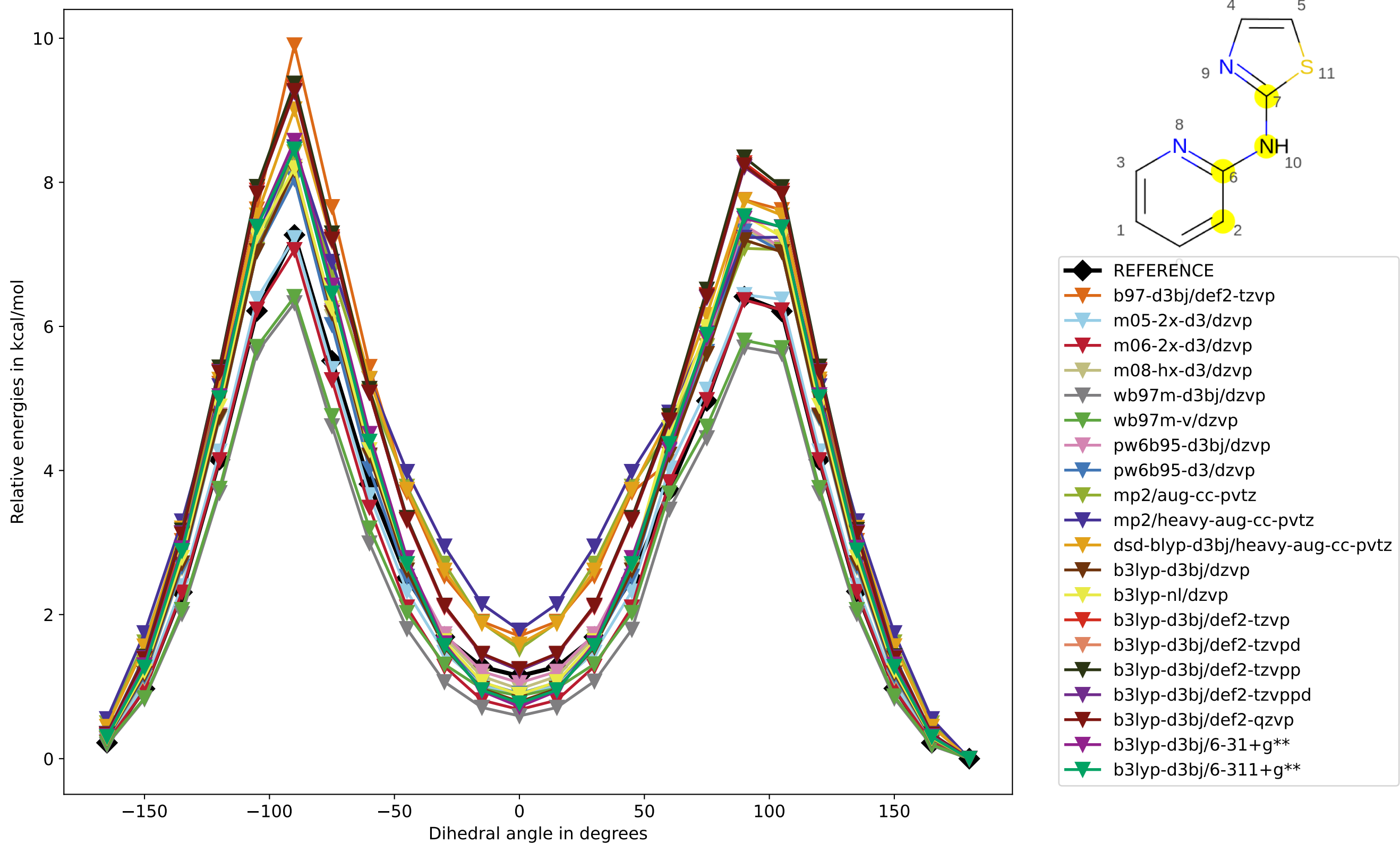
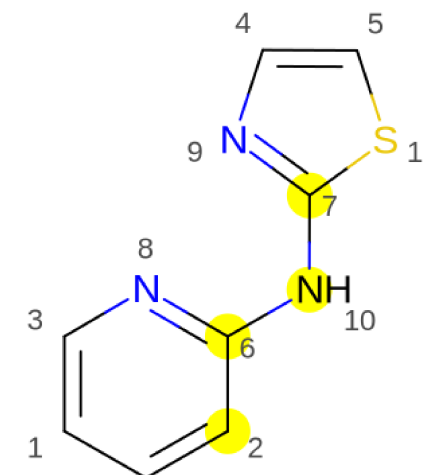


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

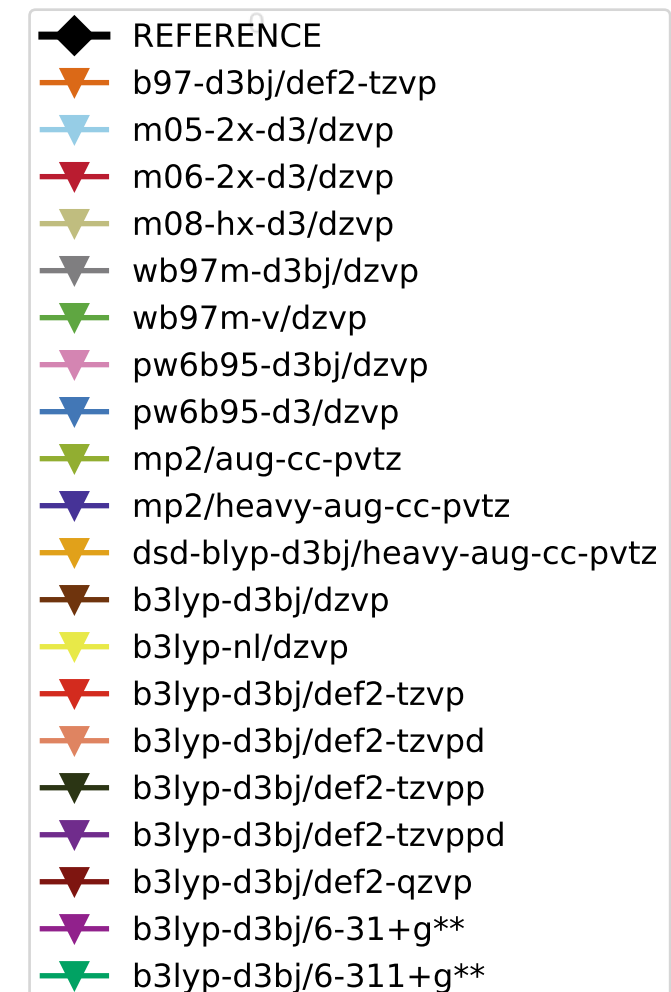
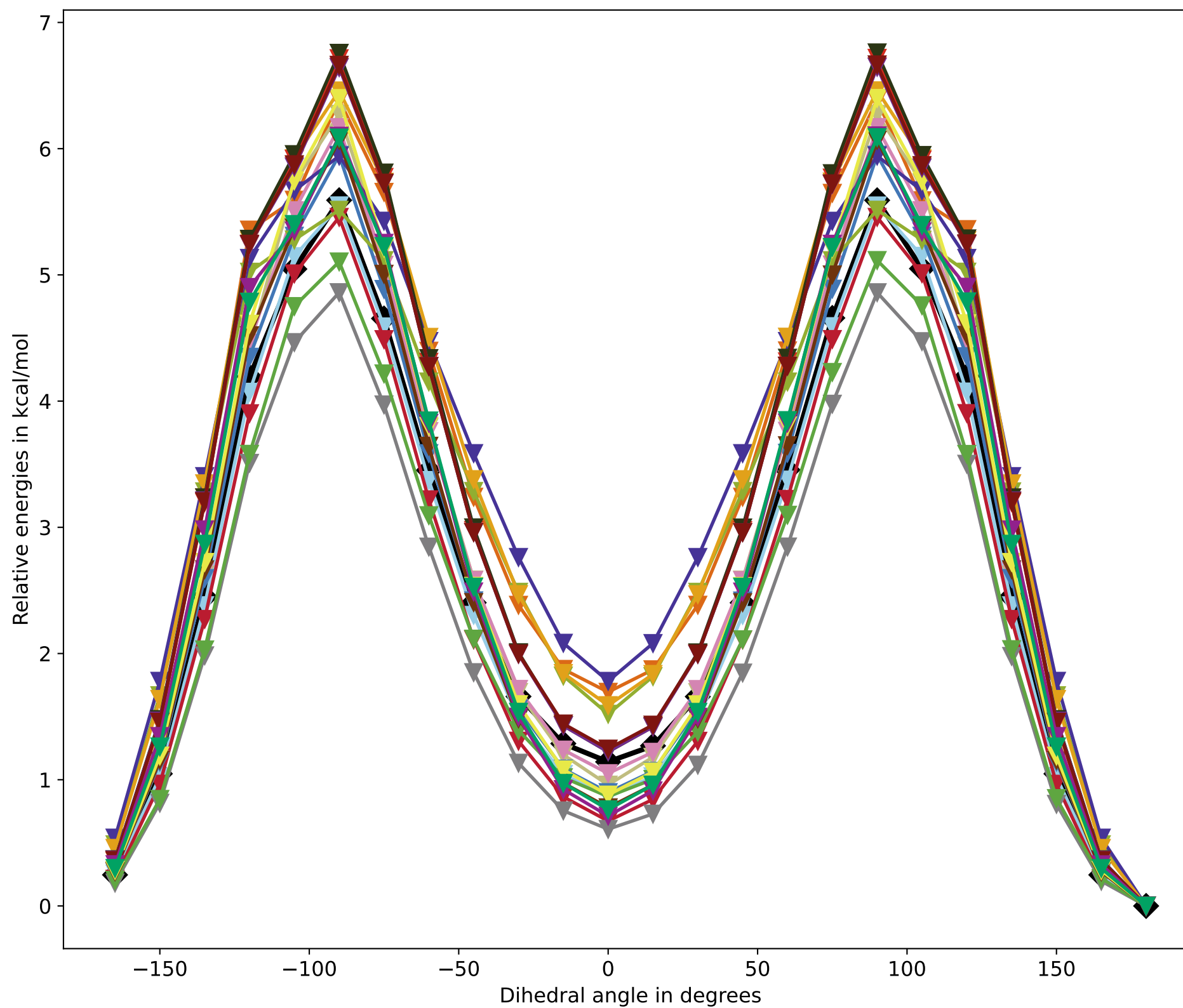
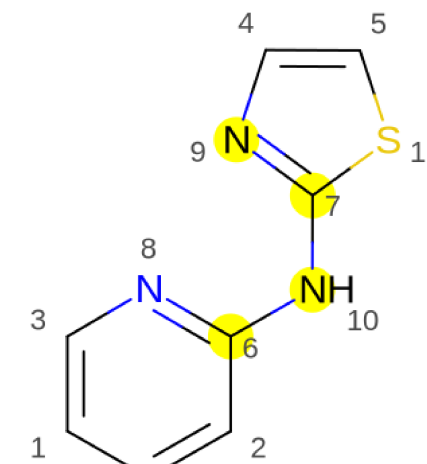
Neutral molecule



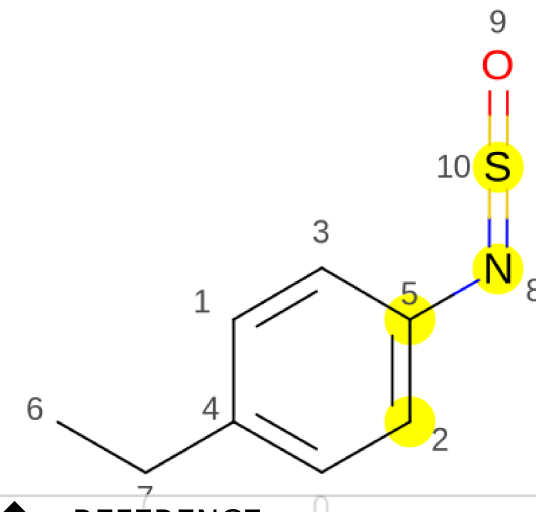
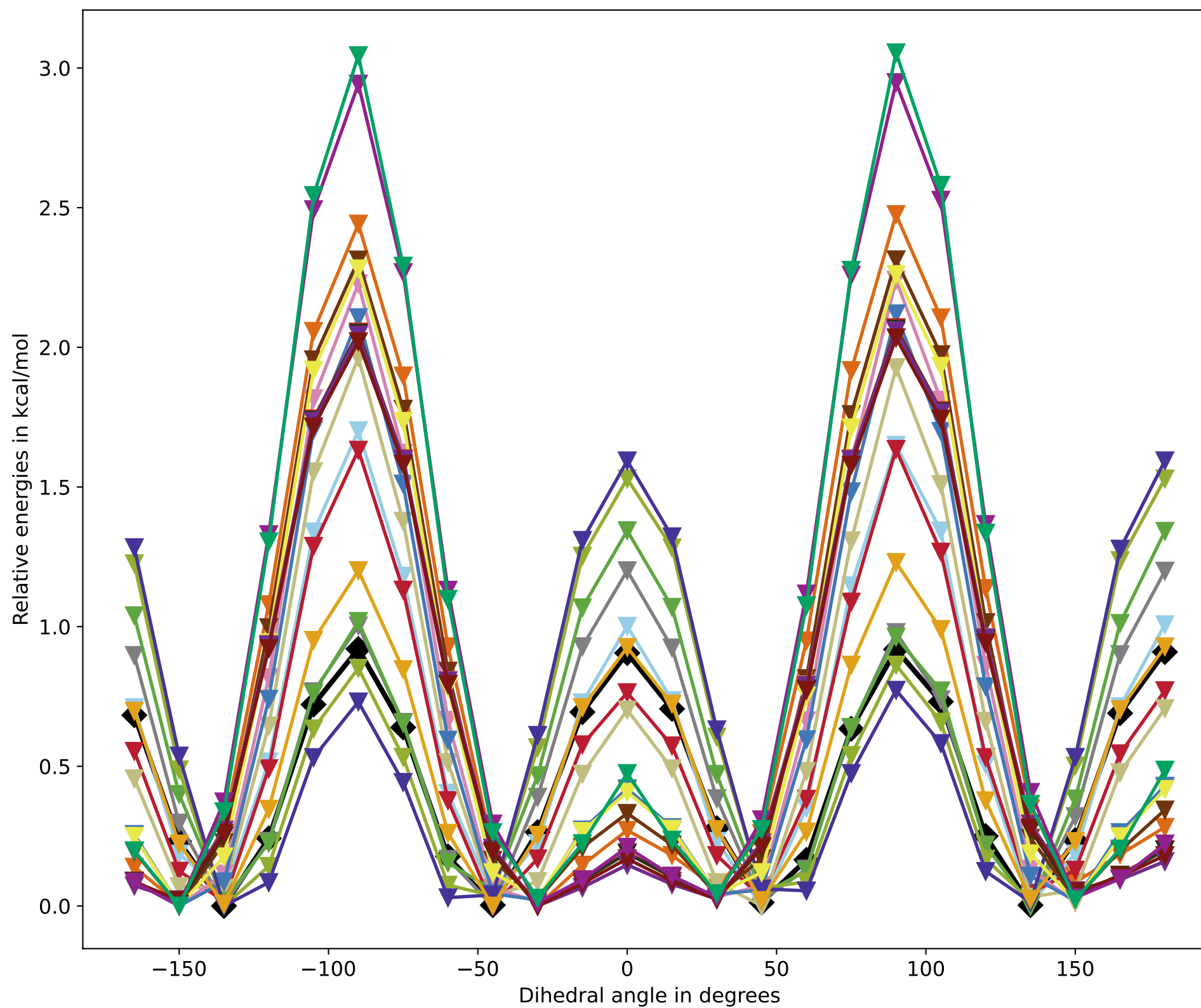
Neutral molecule



Neutral molecule

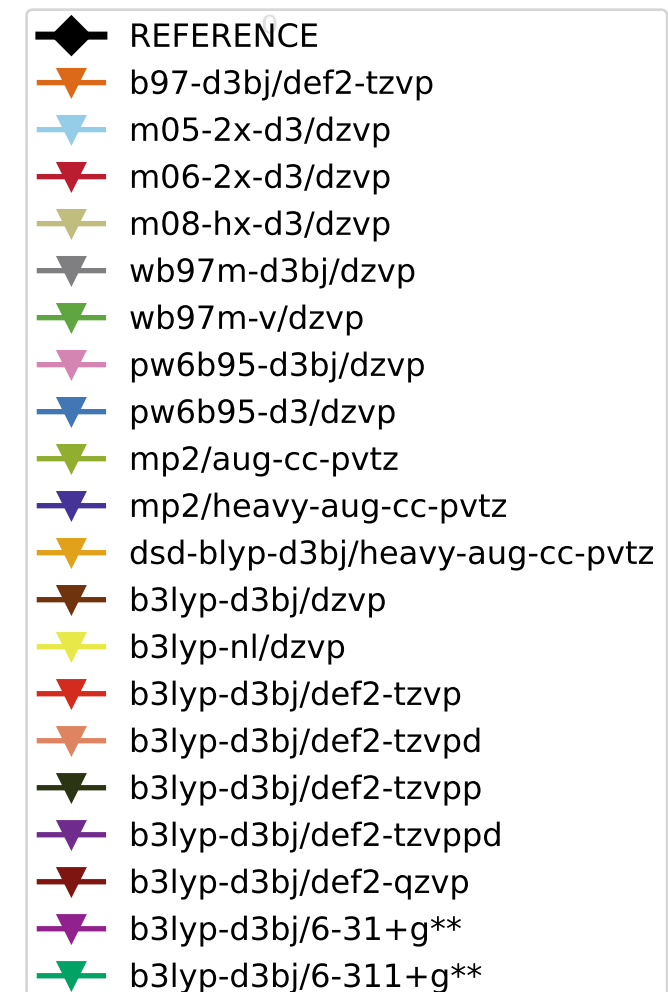
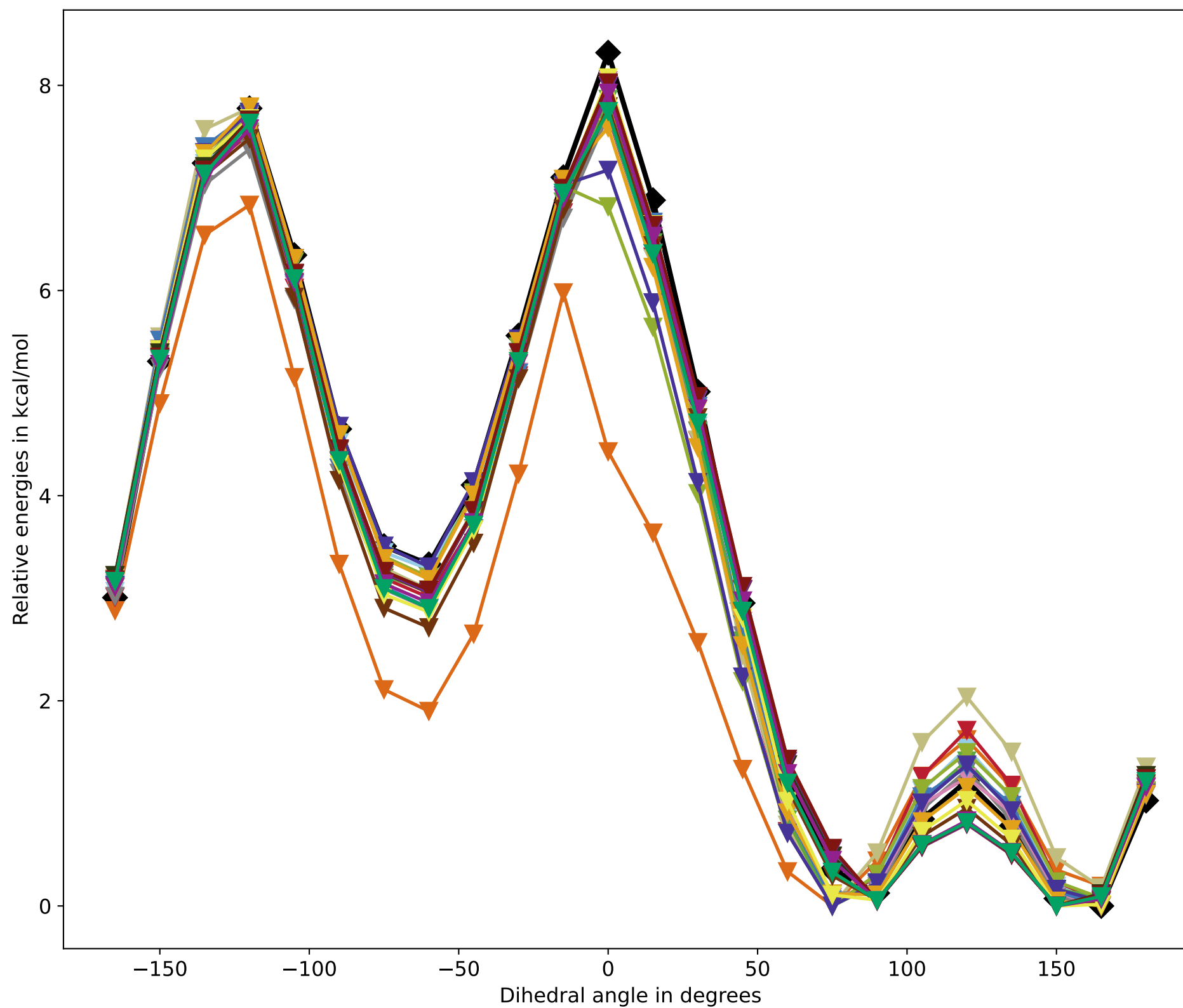
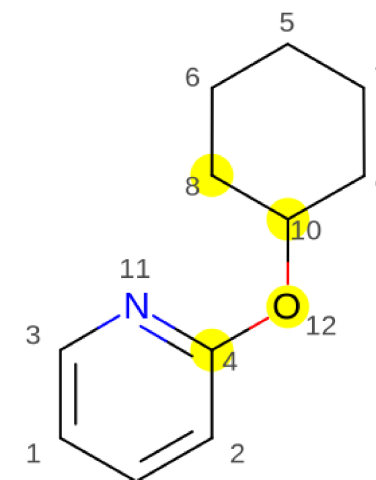


Neutral molecule

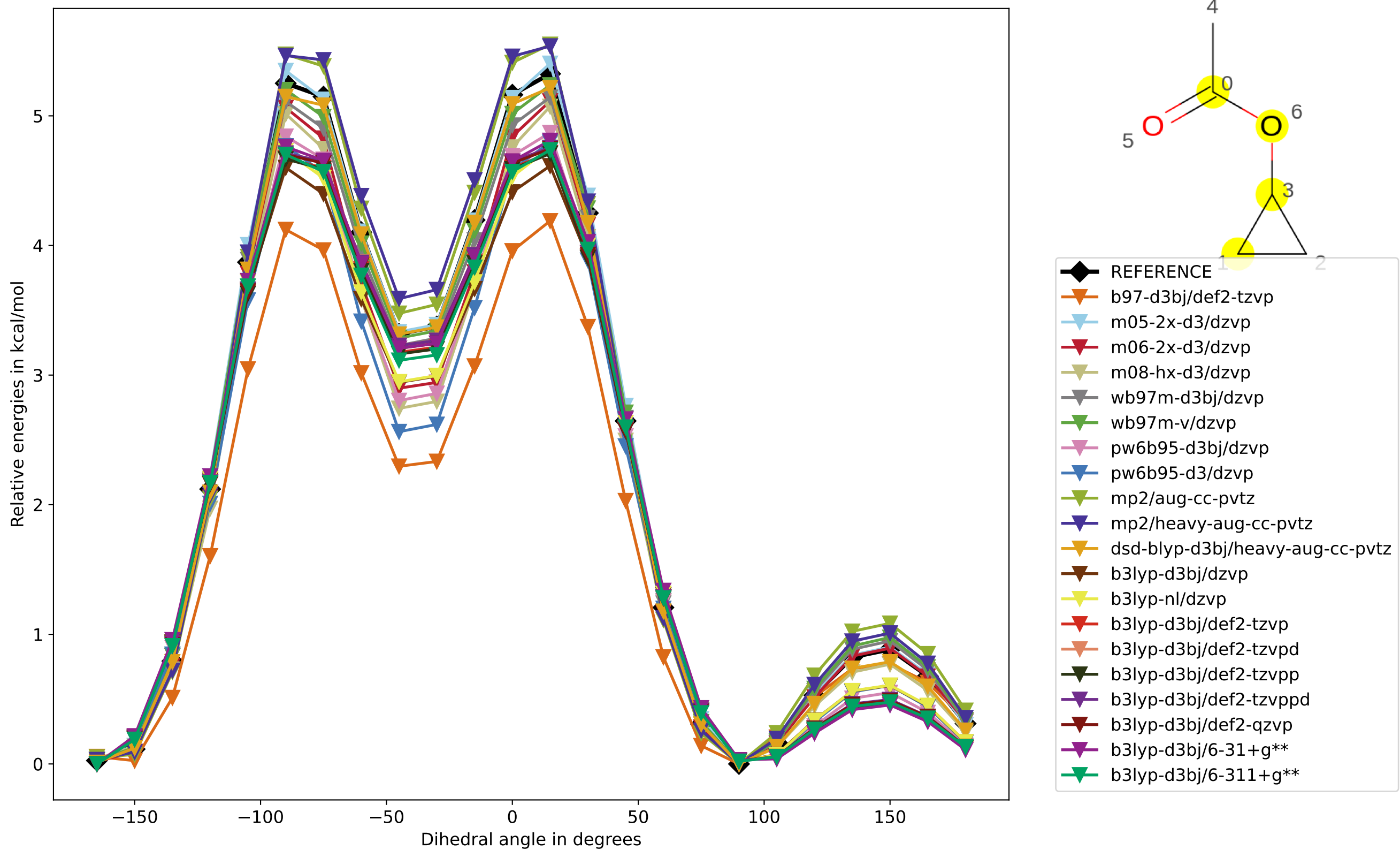


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

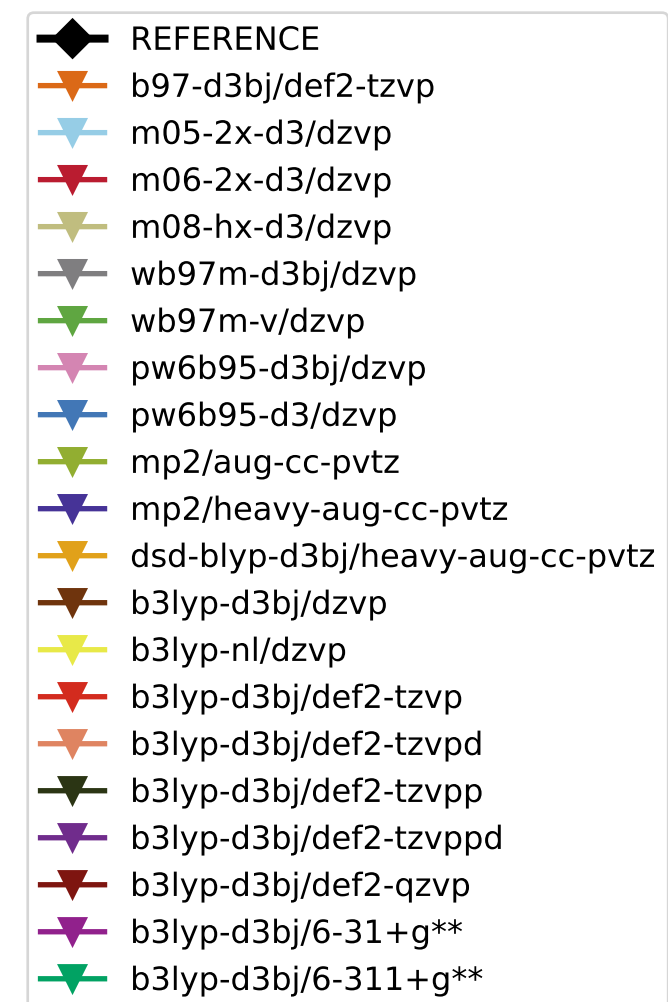
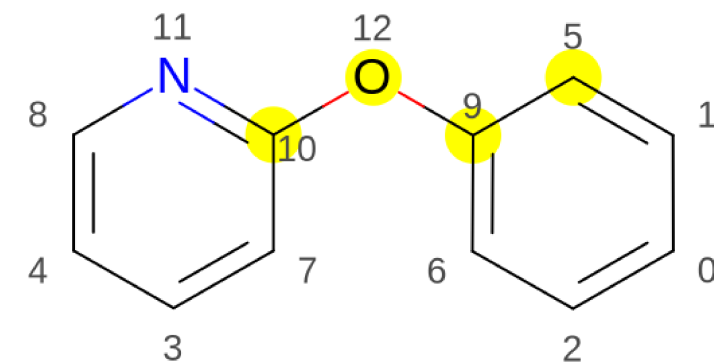
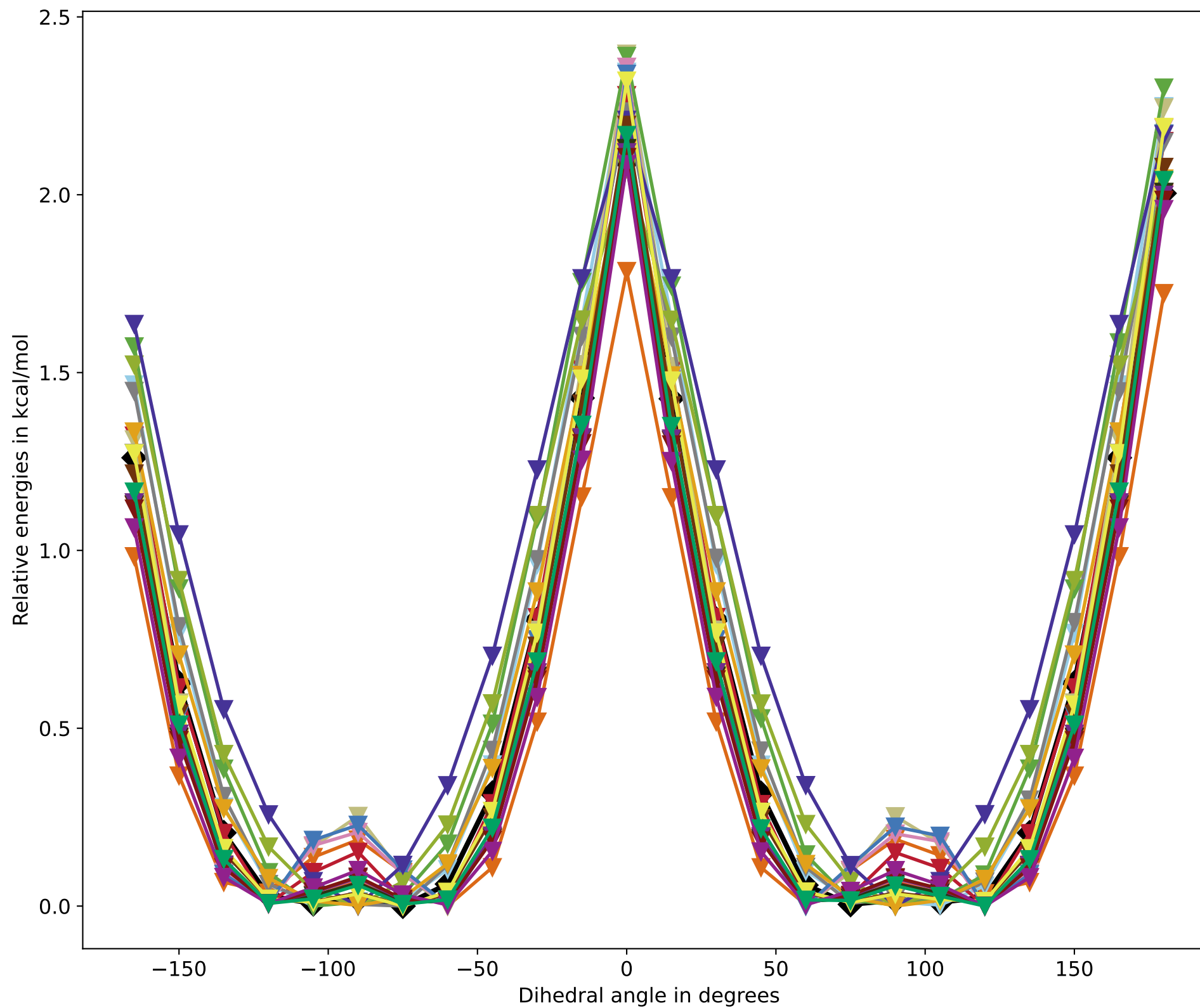
Neutral molecule



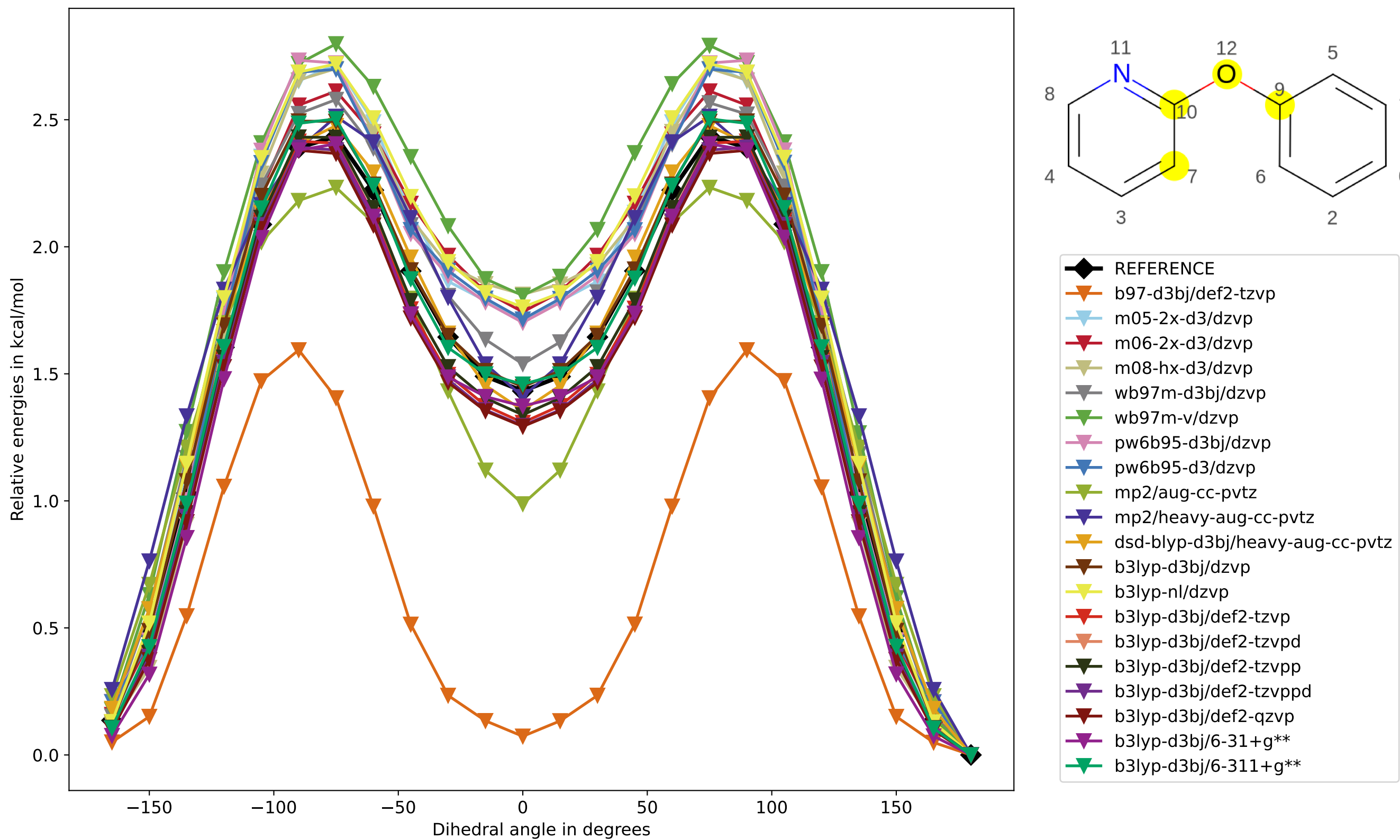
Neutral molecule



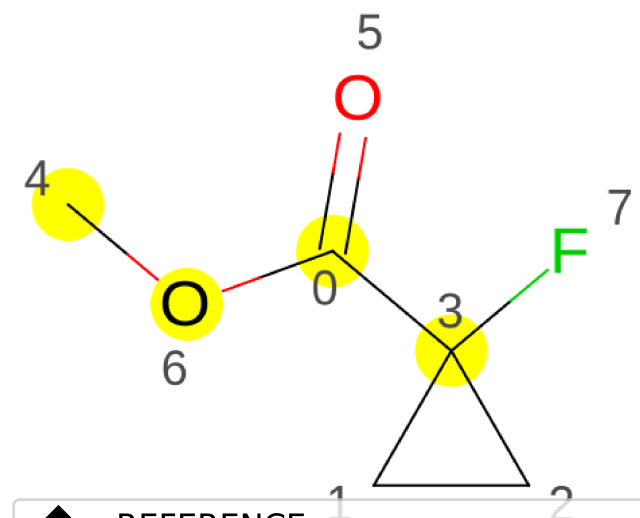
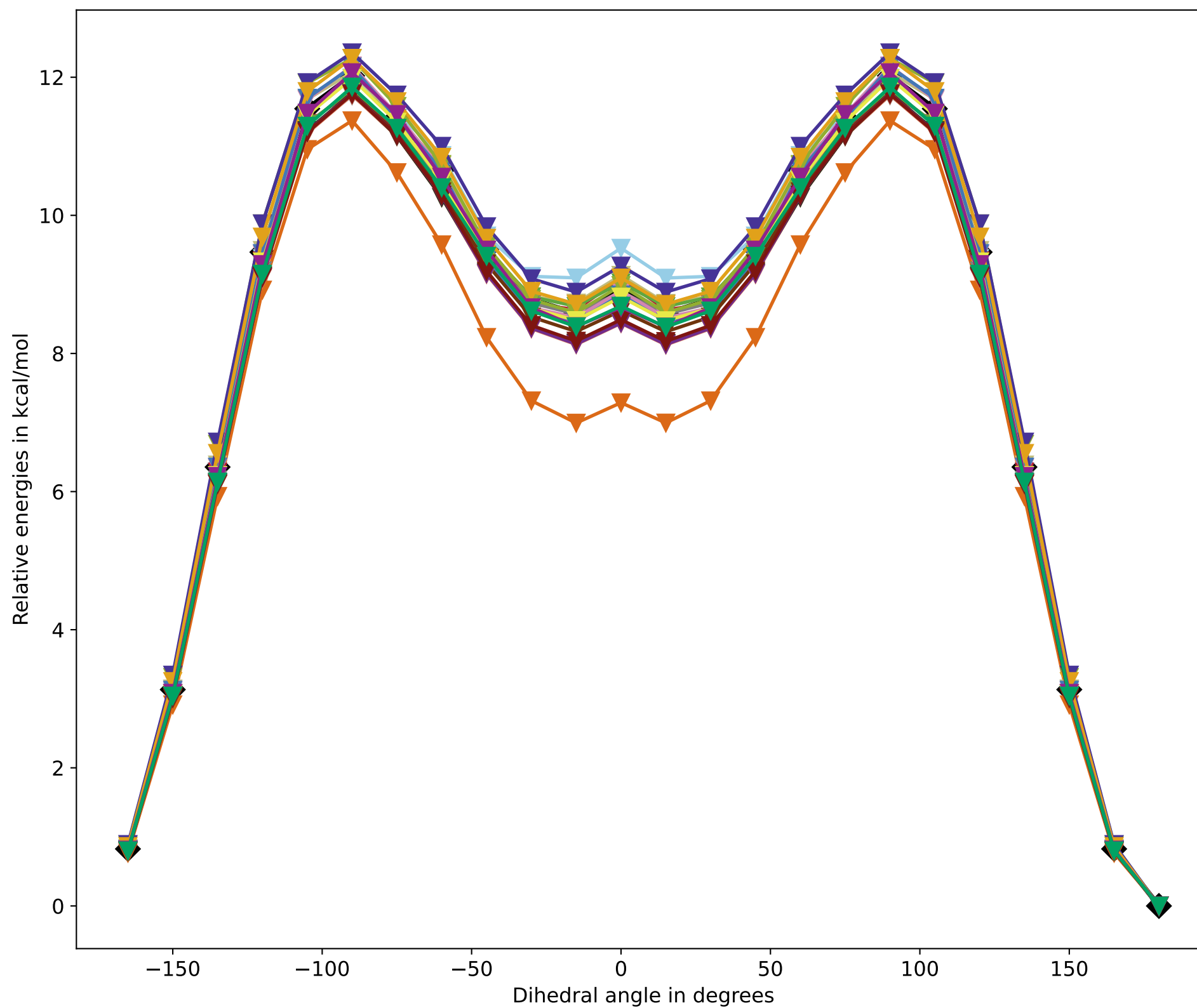
Neutral molecule



Neutral molecule

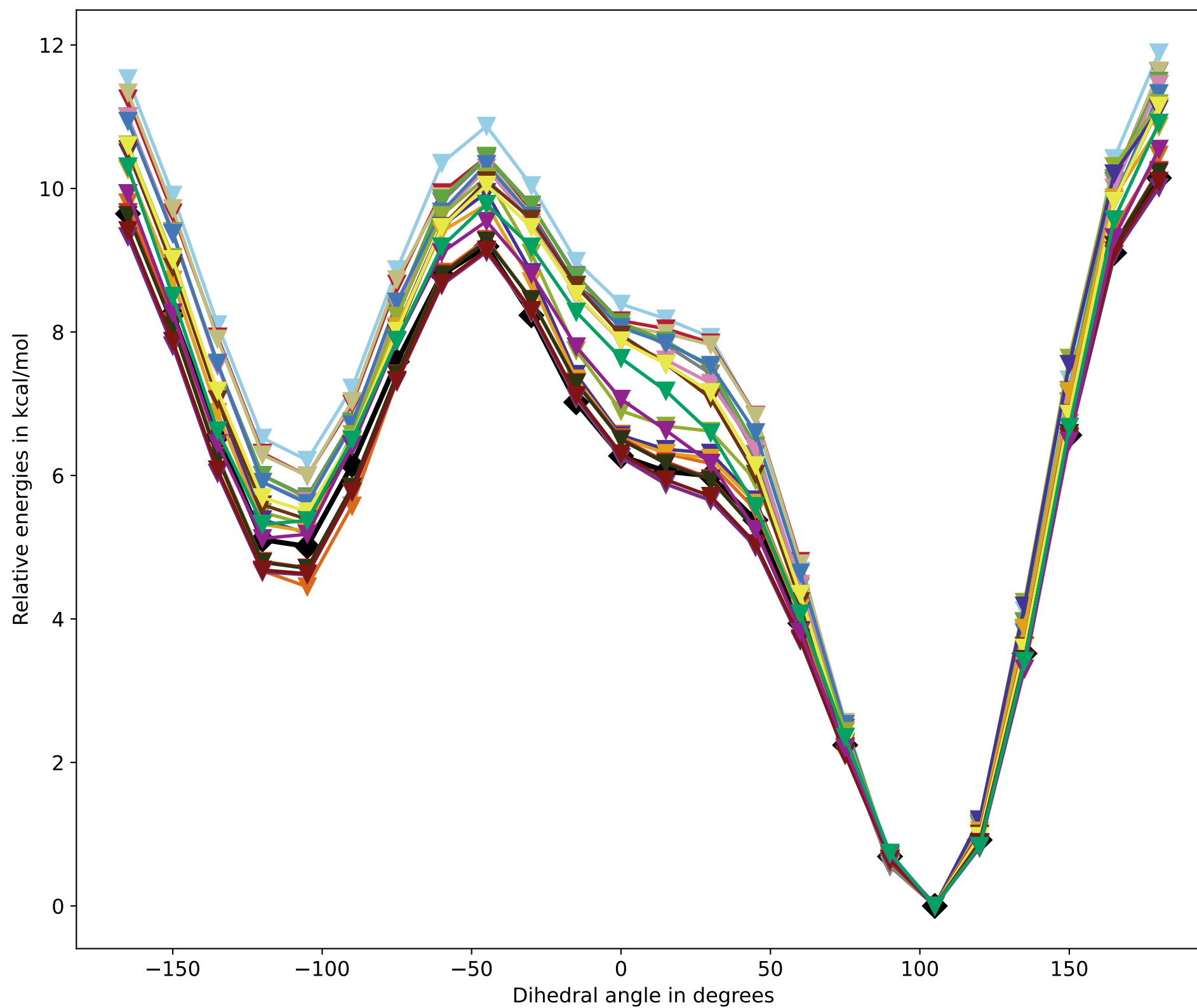
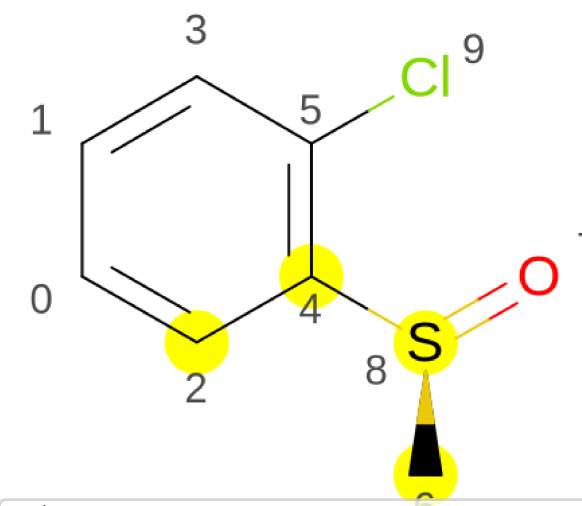


Neutral molecule

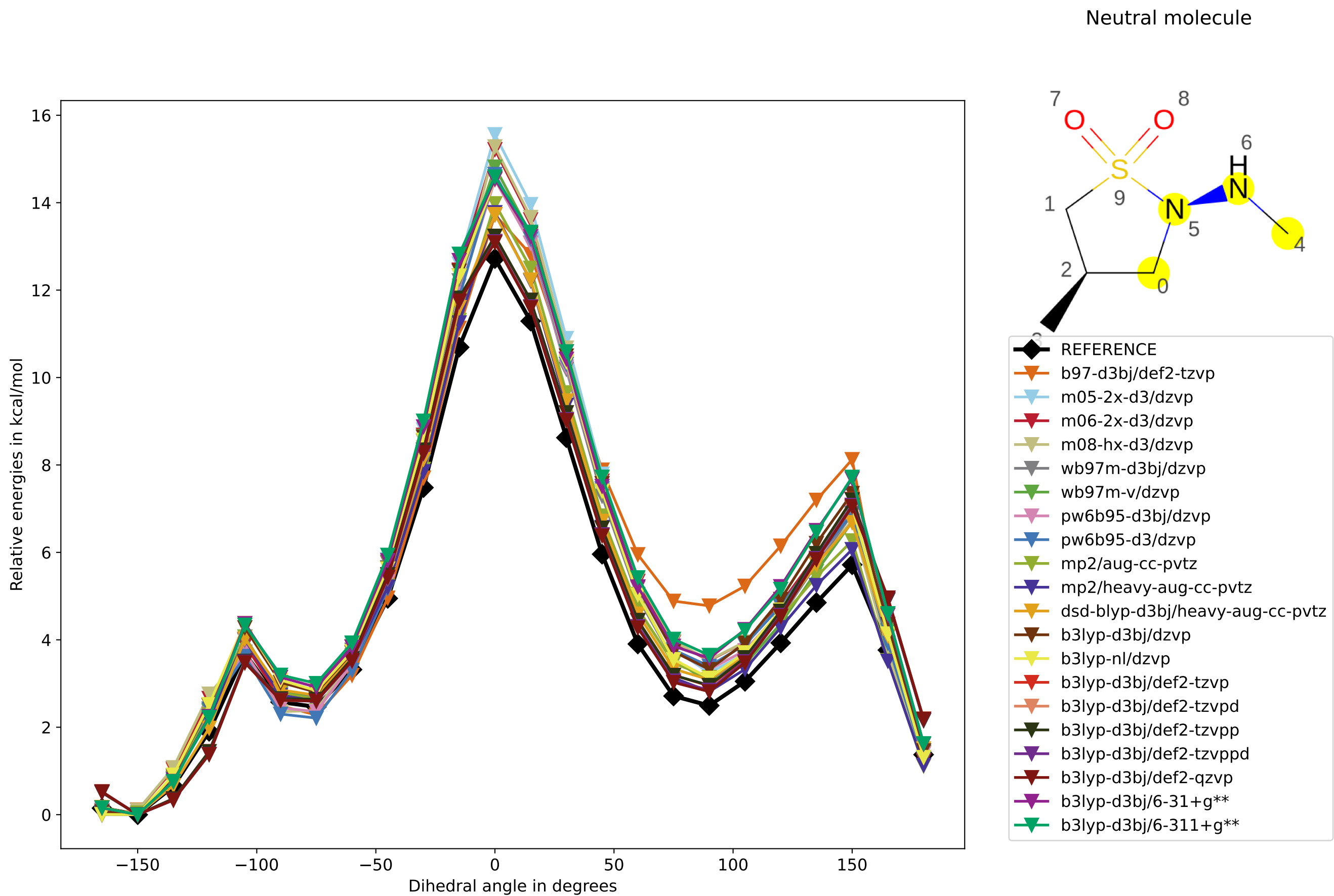


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

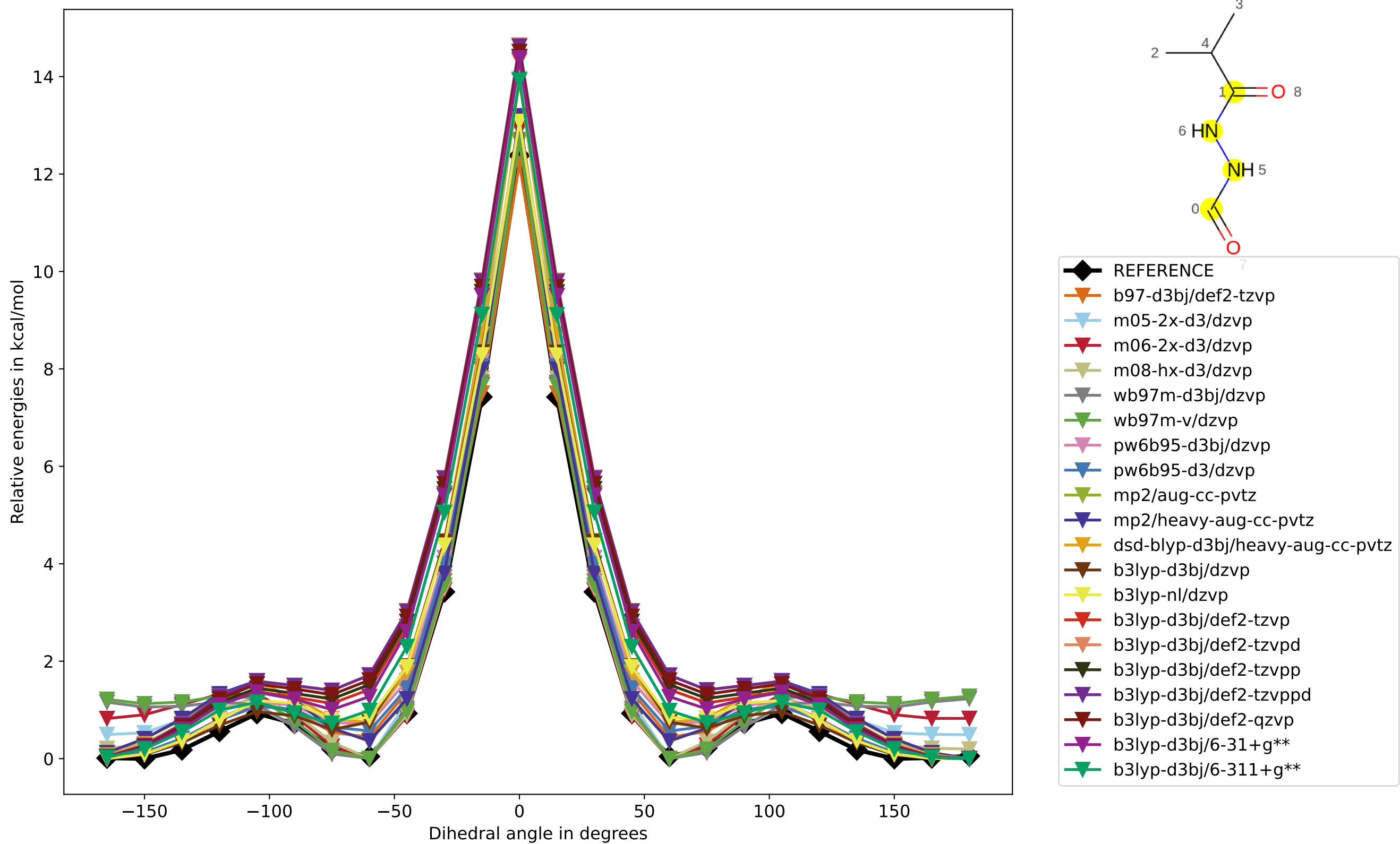
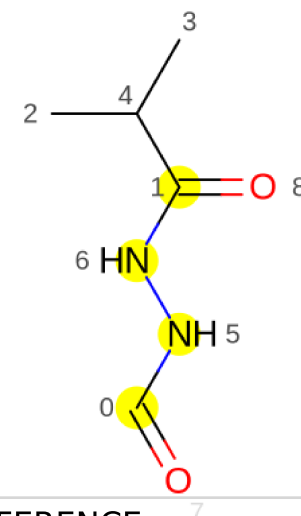
Neutral molecule



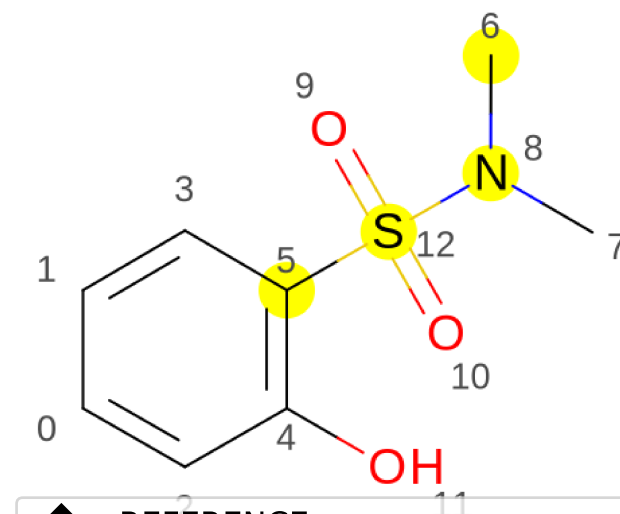
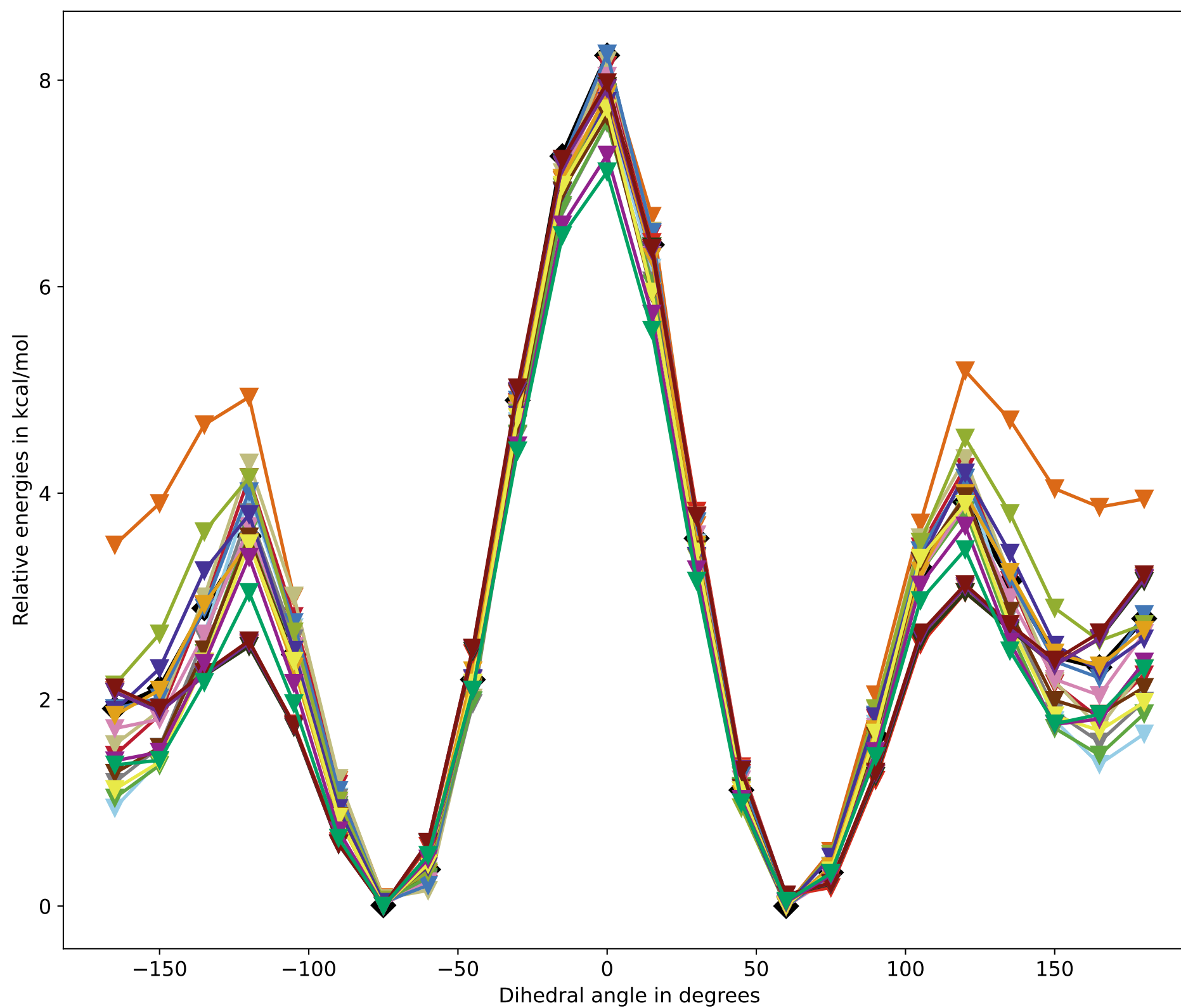
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**



Neutral molecule

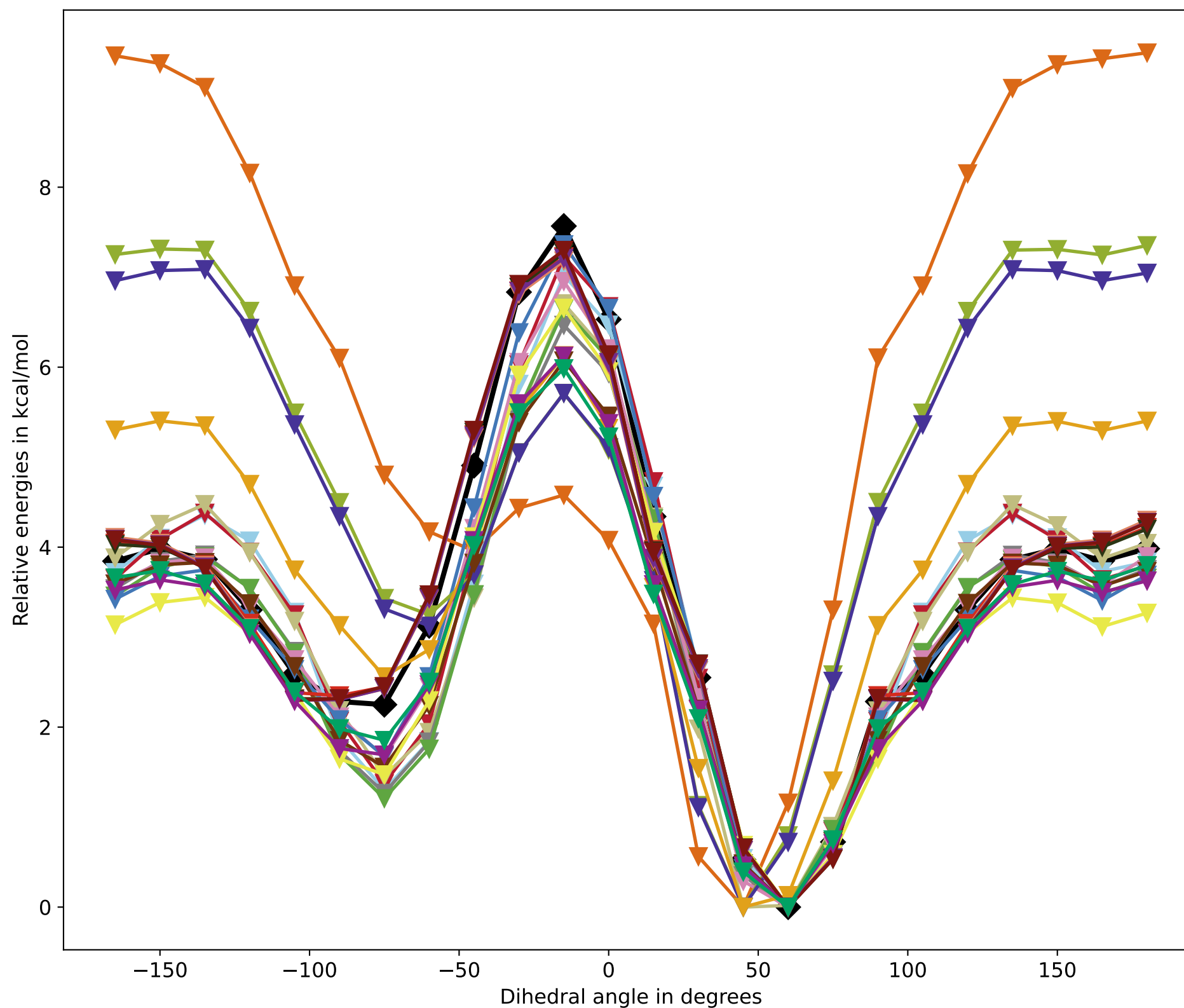
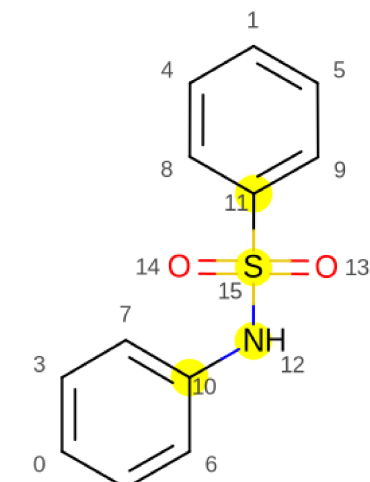


Neutral molecule



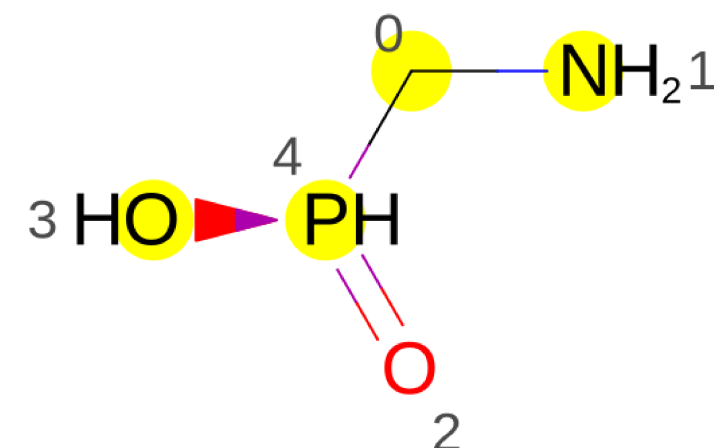
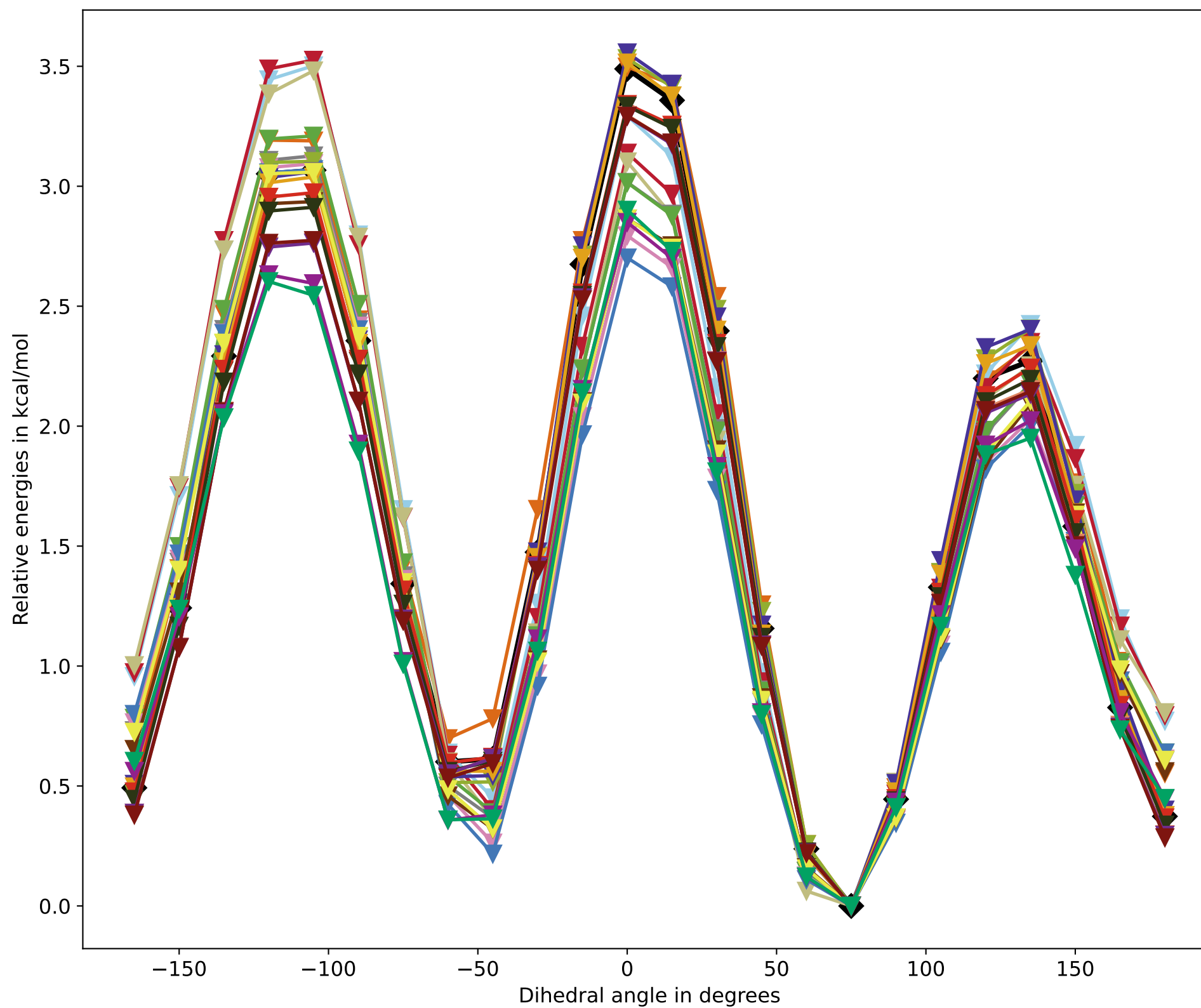
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule



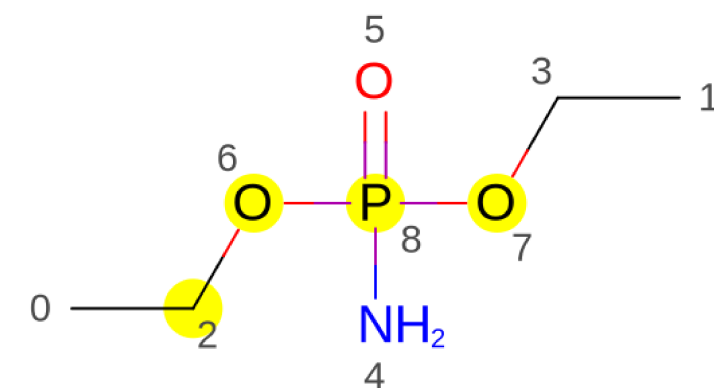
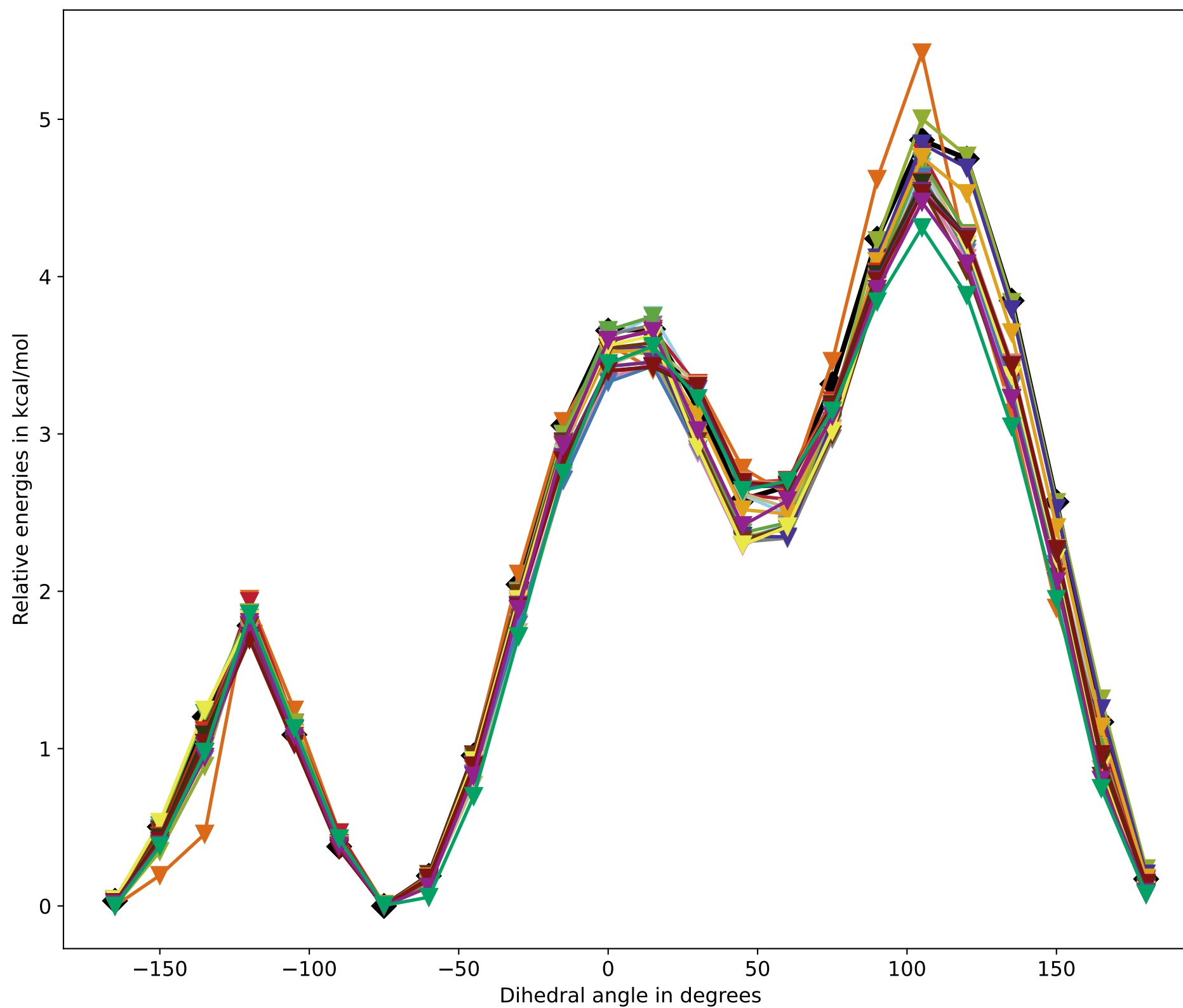
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule



- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule



- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**

Neutral molecule

