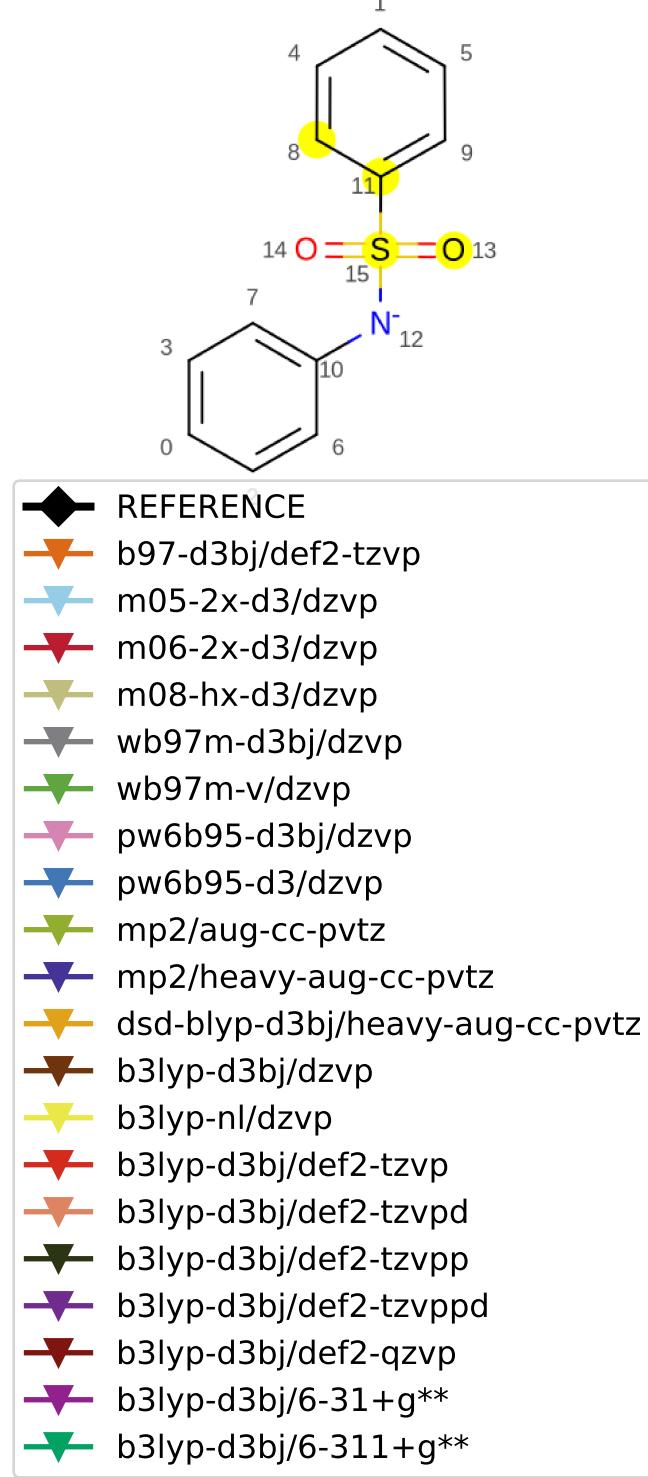
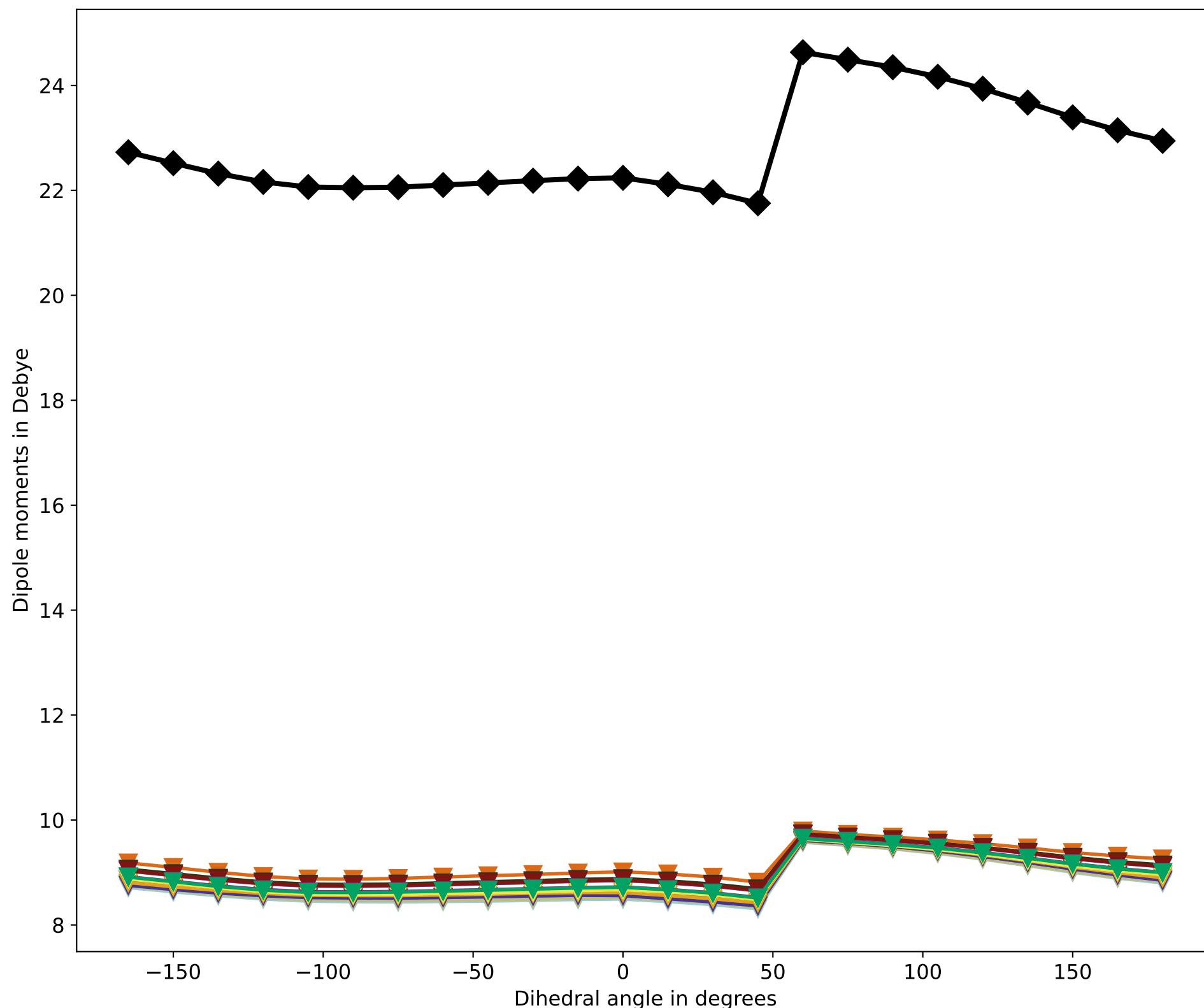
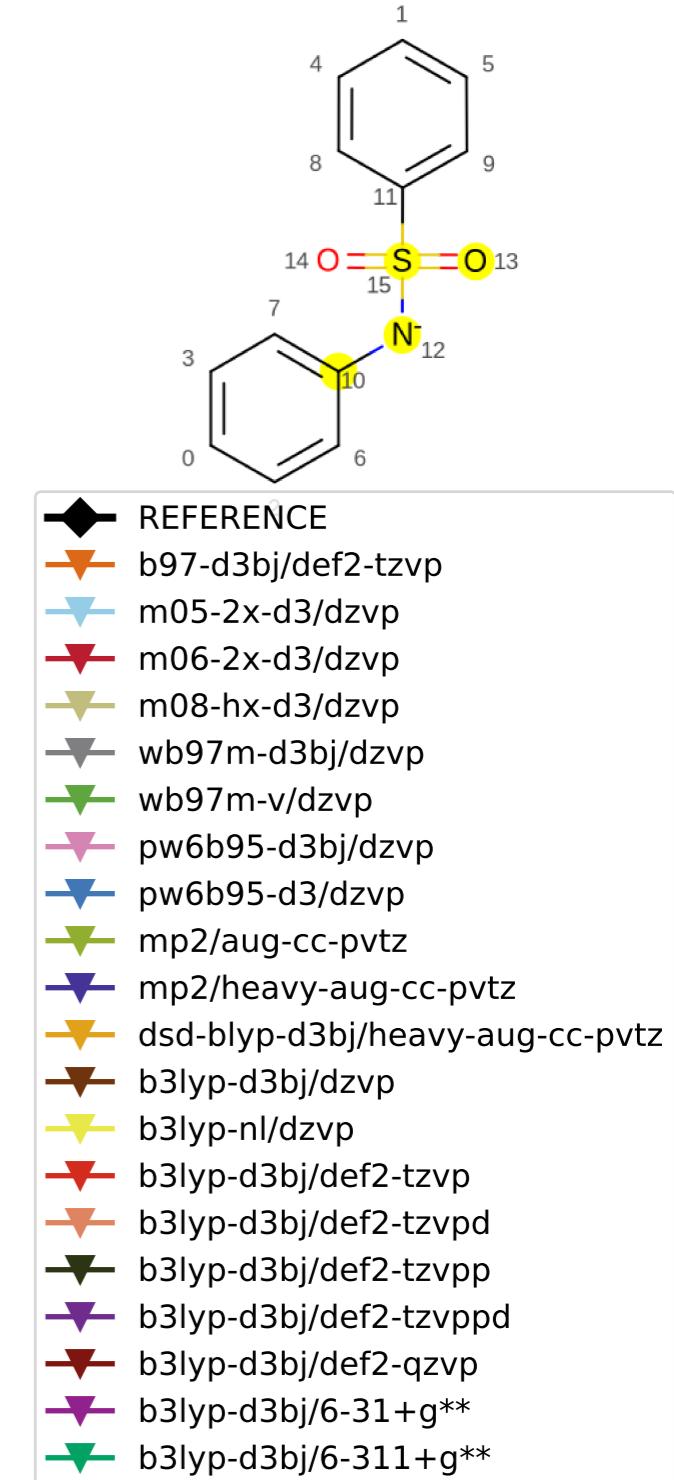
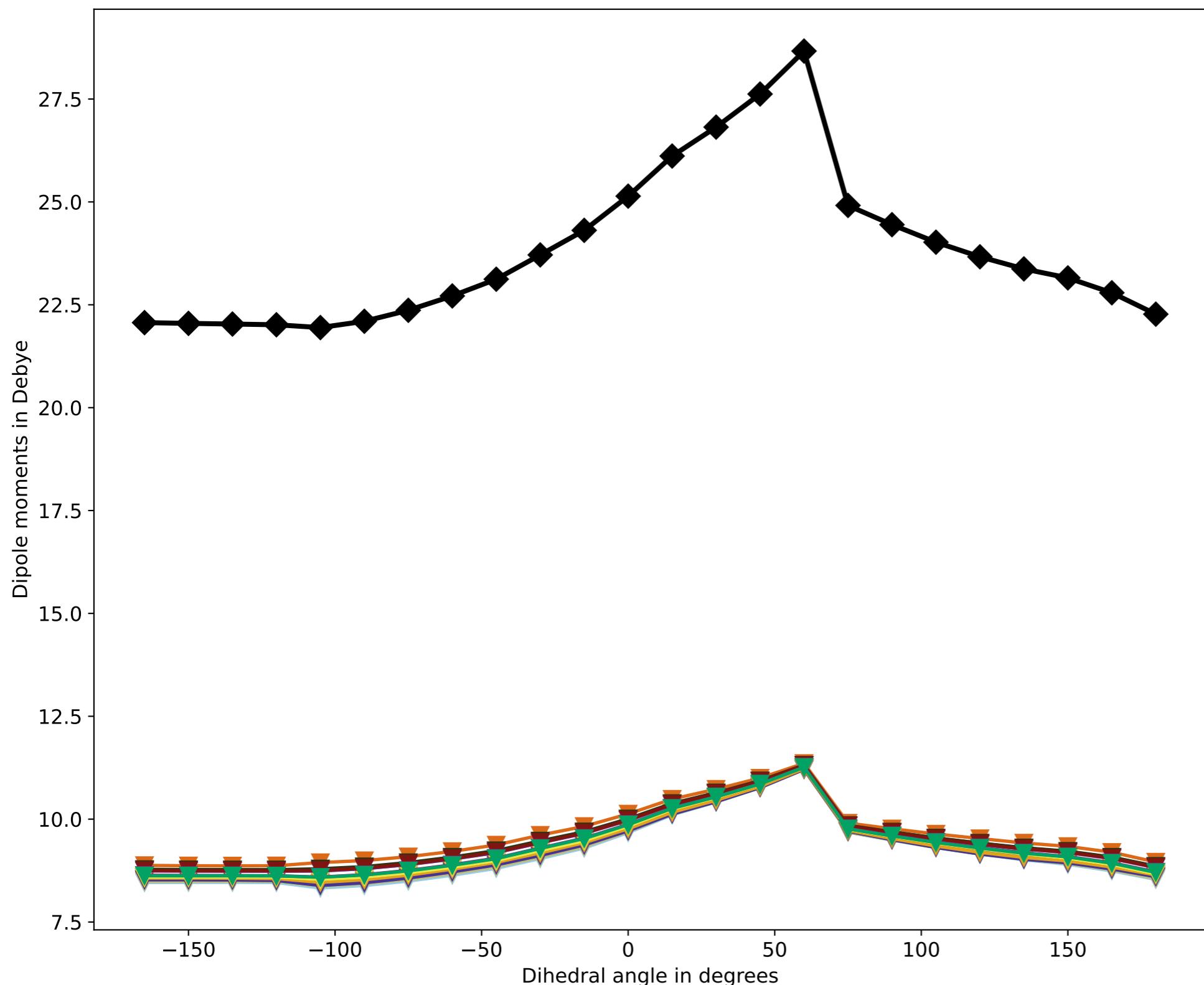


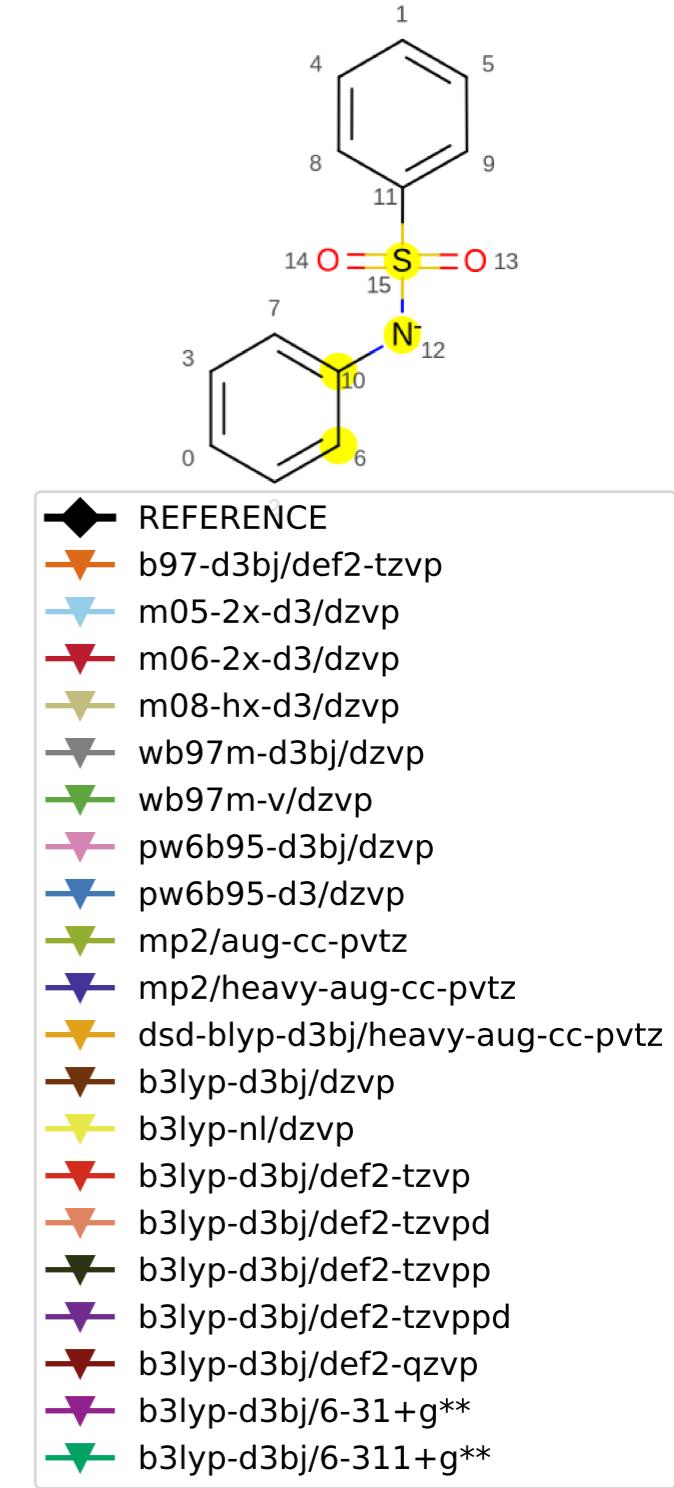
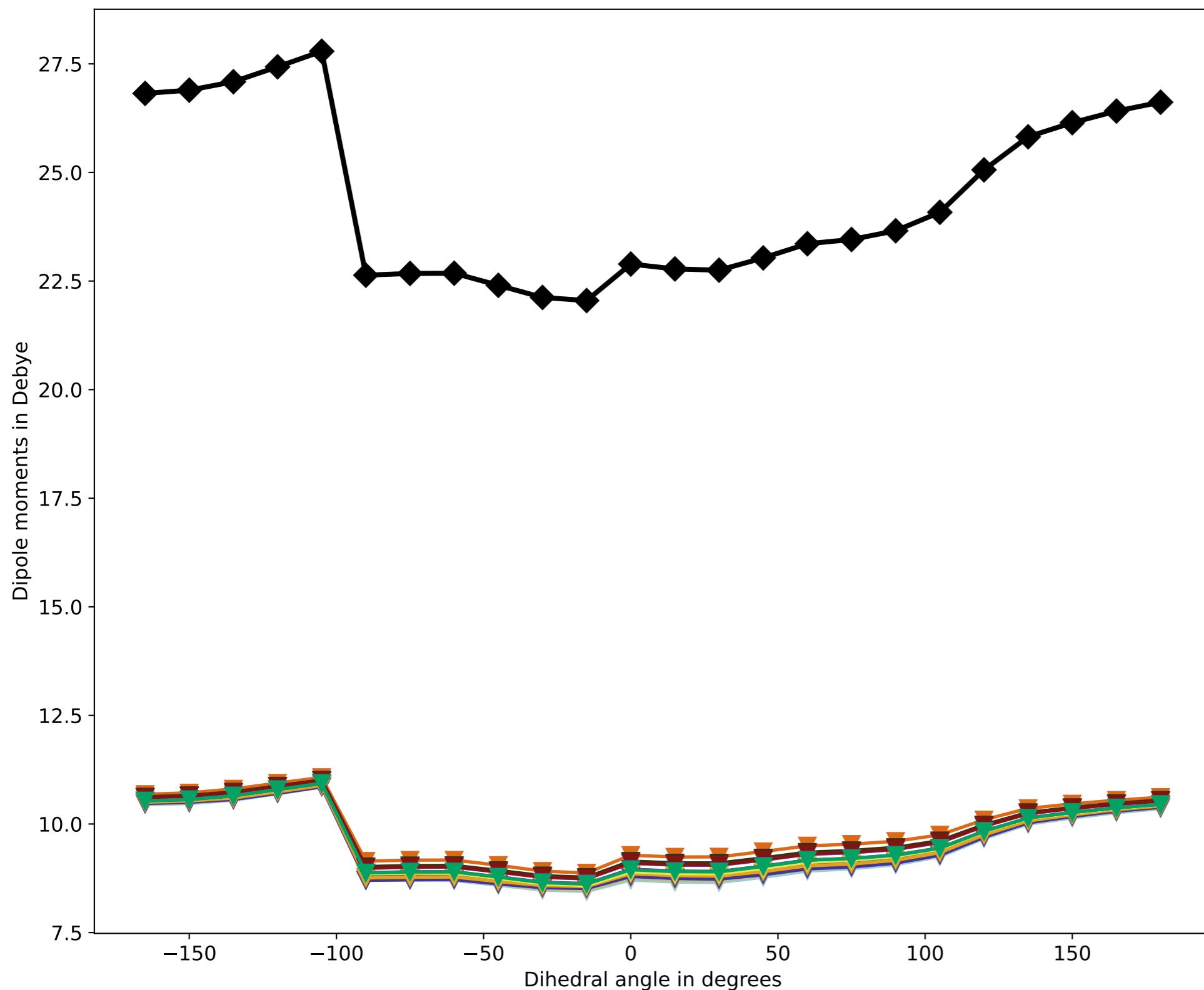
Charged molecule



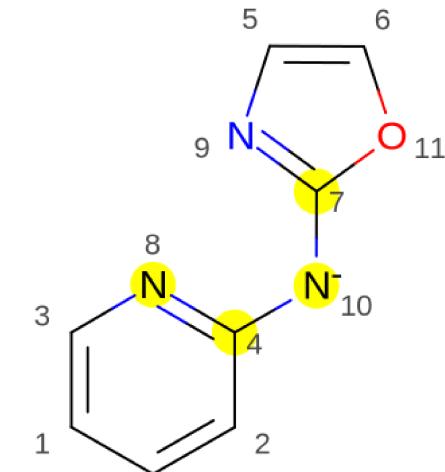
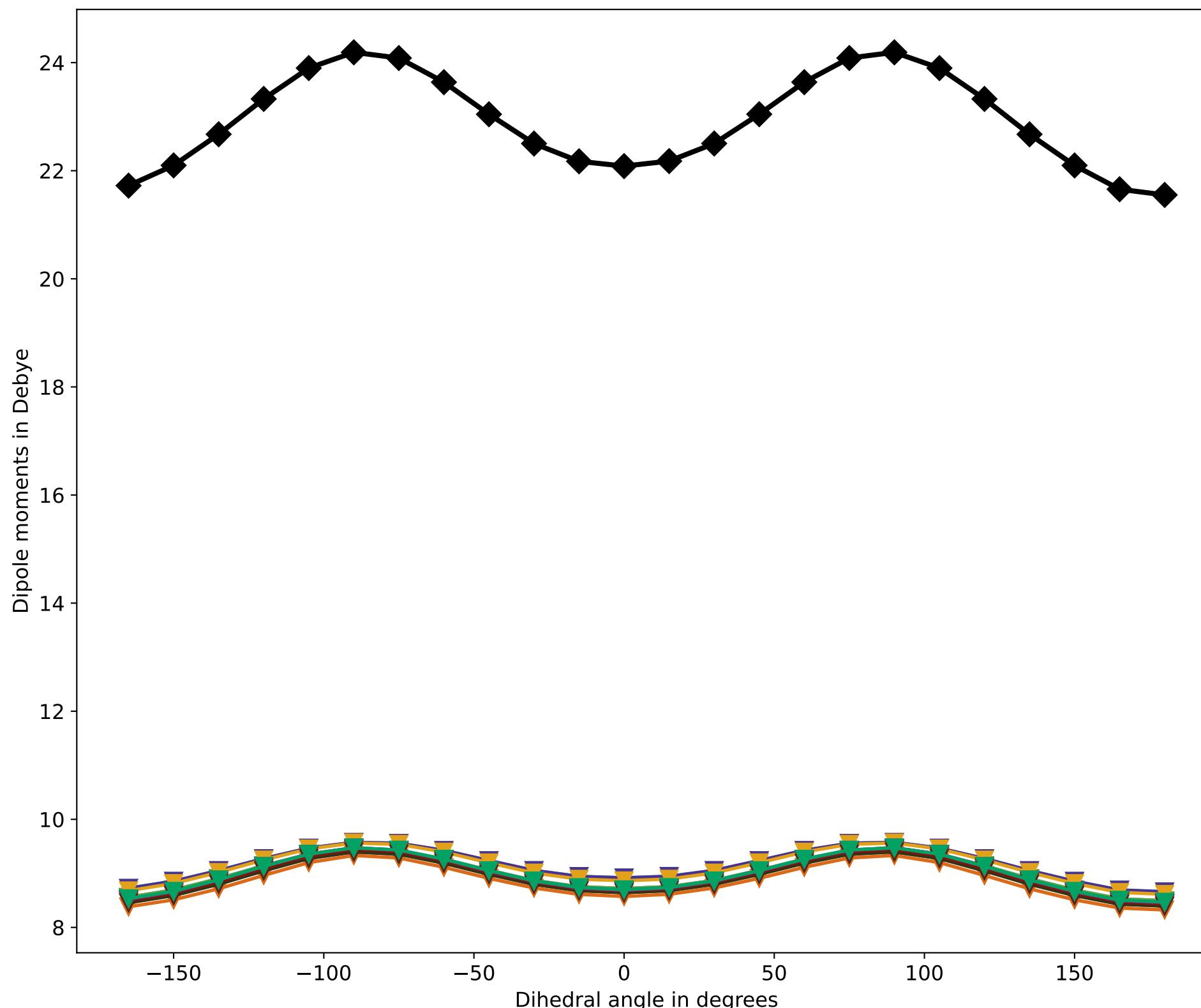
Charged molecule



Charged molecule

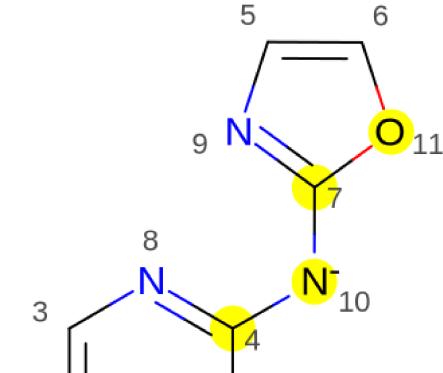
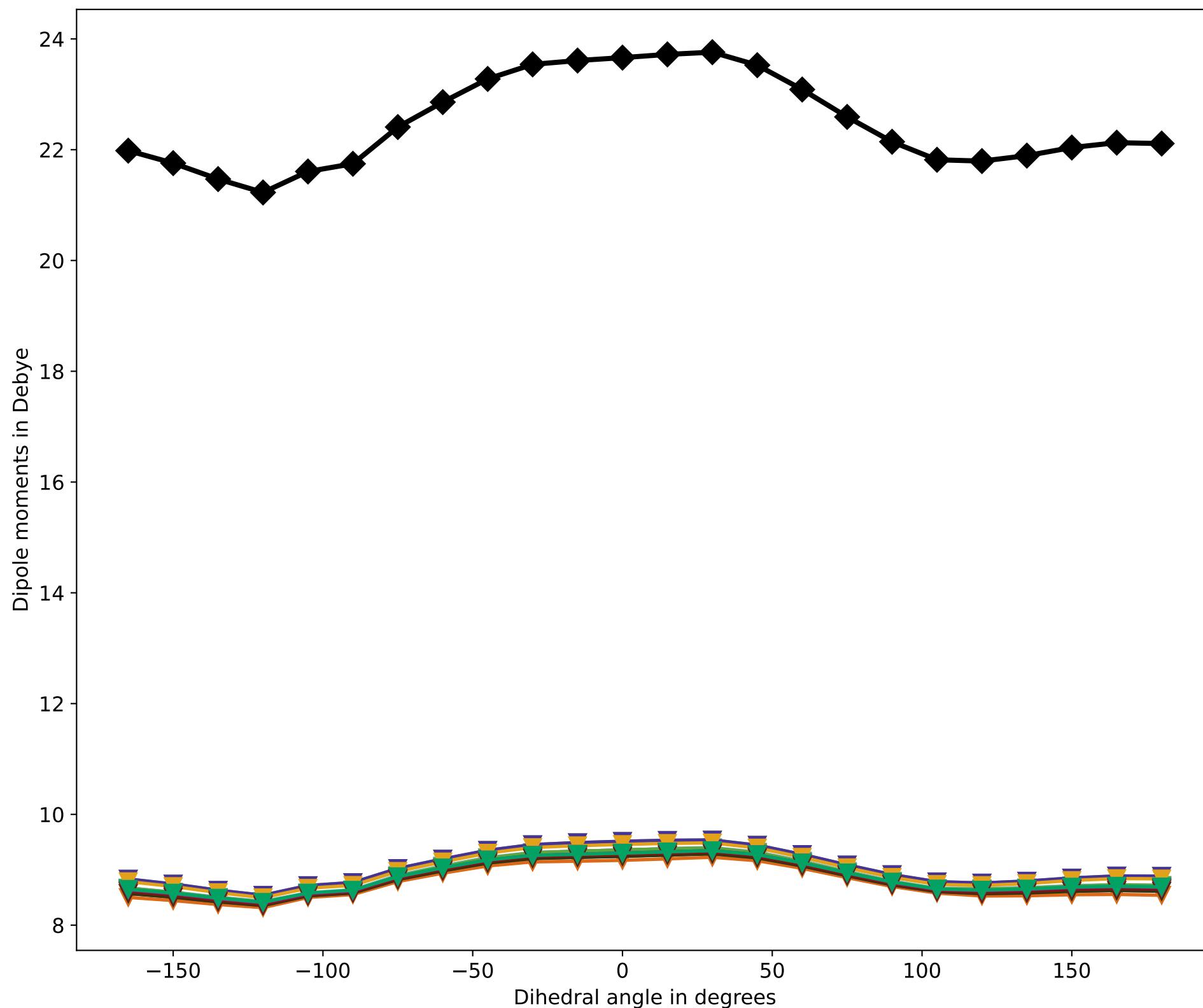


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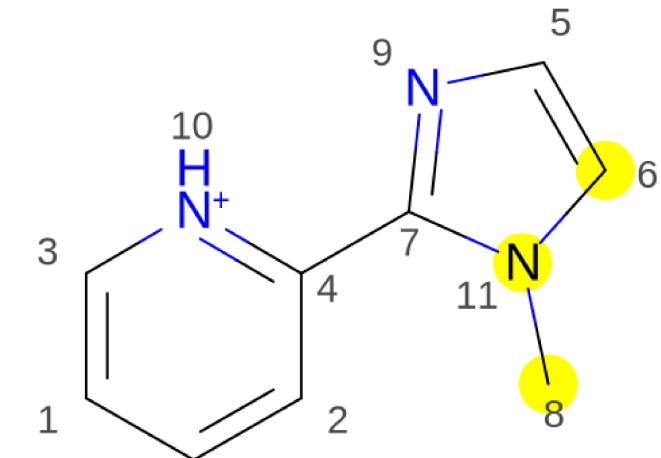
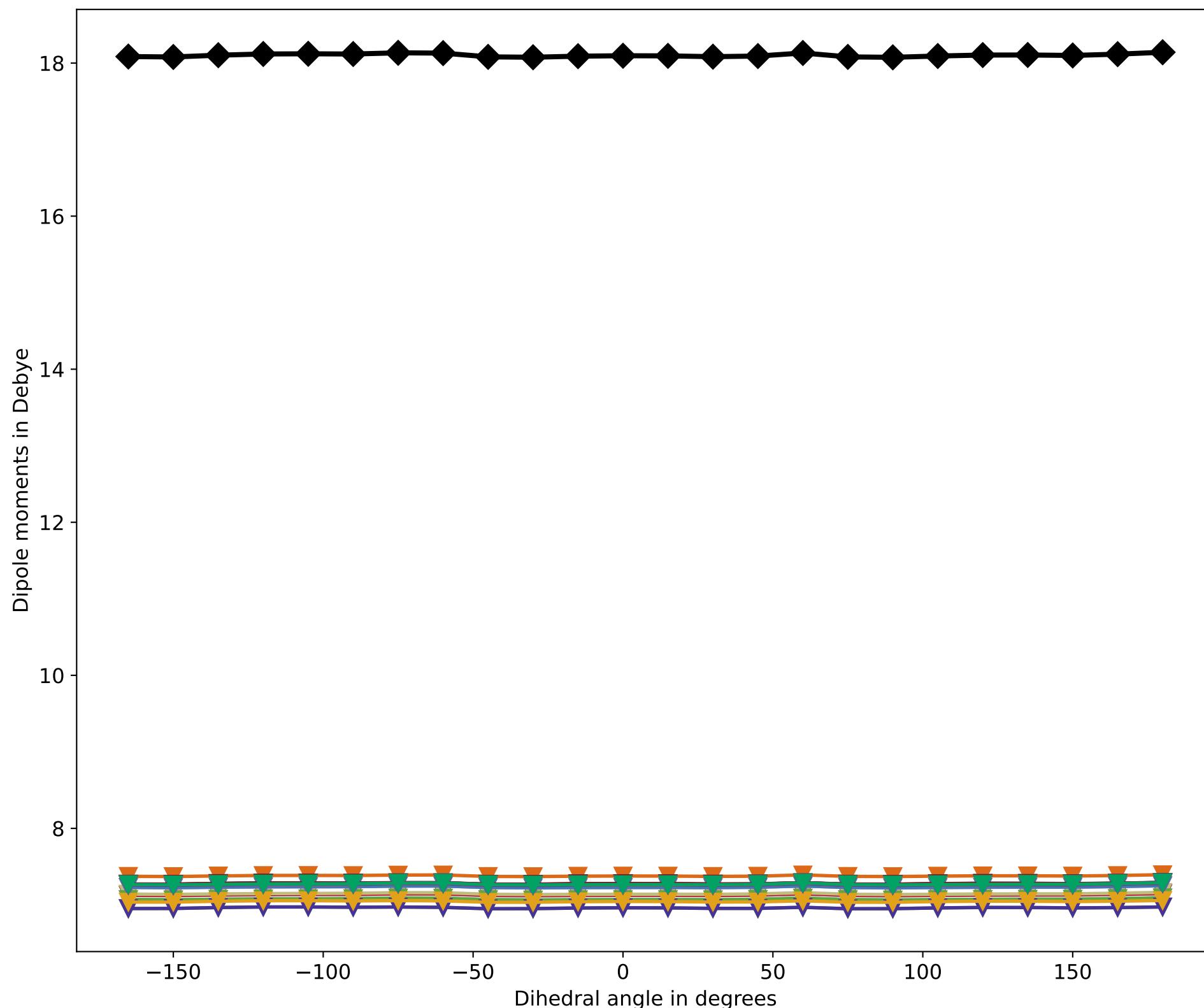
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp (red triangle)
- ◆ b3lyp-d3bj/def2-tzvpd (orange triangle)
- ◆ b3lyp-d3bj/def2-tzvpp (black triangle)
- ◆ b3lyp-d3bj/def2-tzvppd (purple triangle)
- ◆ b3lyp-d3bj/def2-qzvp (dark red triangle)
- ◆ b3lyp-d3bj/6-31+g** (pink triangle)
- ◆ b3lyp-d3bj/6-311+g** (green triangle)

Charged molecule



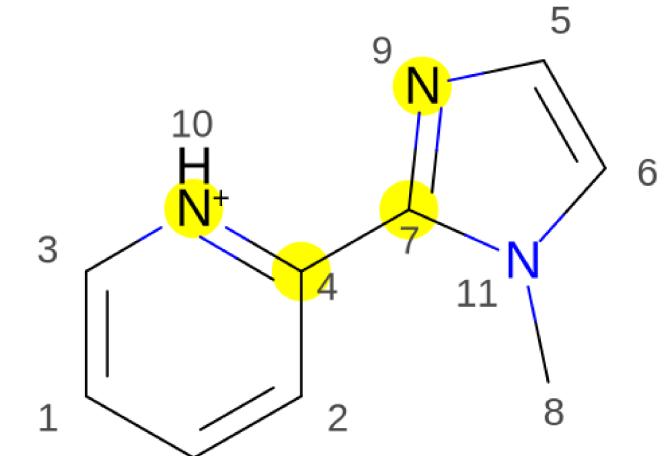
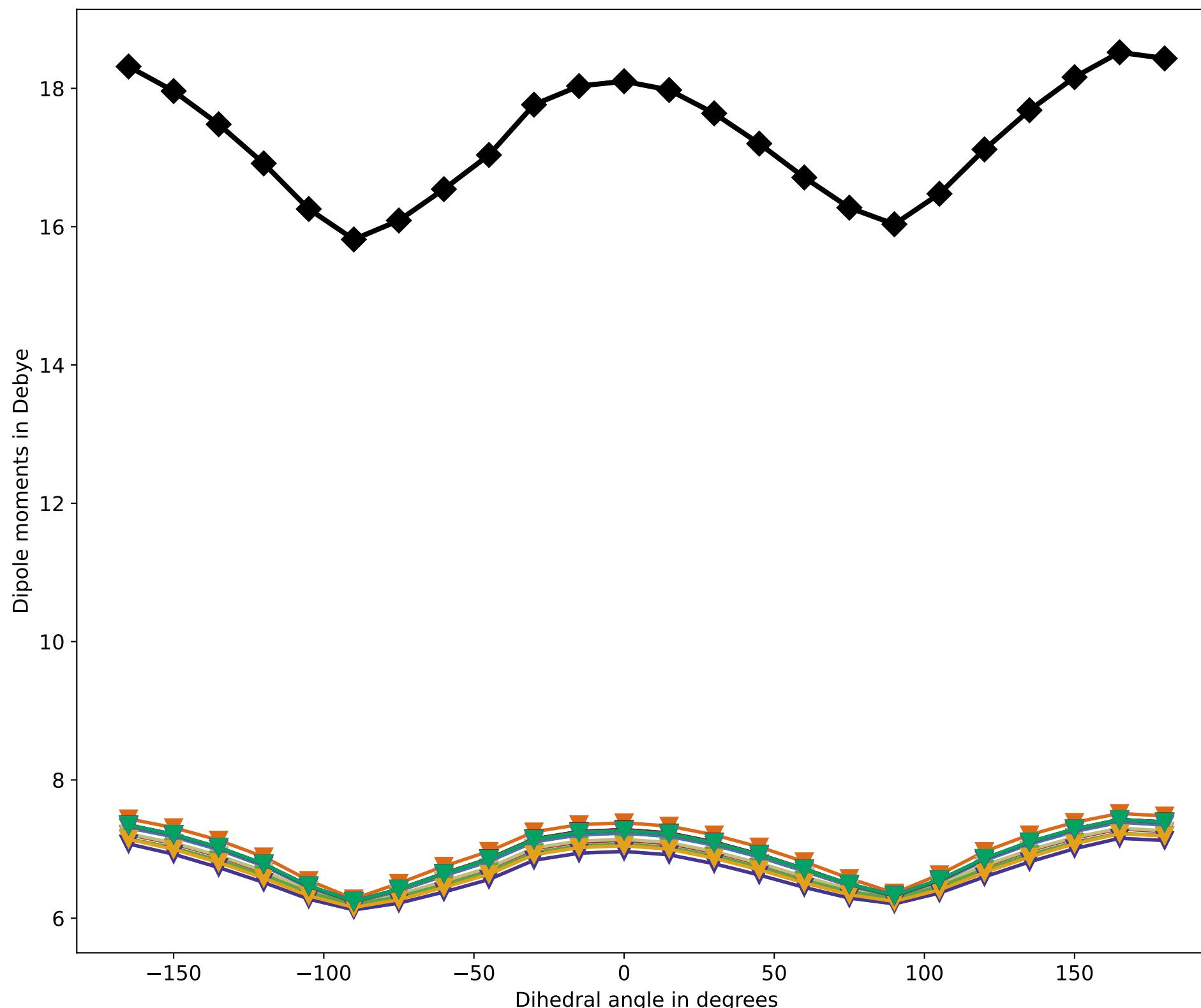
- ◆ REFERENCE
- ▲ b97-d3bj/def2-tzvp
- △ m05-2x-d3/dzvp
- ▼ m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- ▲ wb97m-d3bj/dzvp
- ▼ wb97m-v/dzvp
- ▼ pw6b95-d3bj/dzvp
- ▲ pw6b95-d3/dzvp
- ▲ mp2/aug-cc-pvtz
- ▲ mp2/heavy-aug-cc-pvtz
- ▲ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ▲ b3lyp-d3bj/dzvp
- ▲ b3lyp-nl/dzvp
- ▲ b3lyp-d3bj/def2-tzvp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

Charged molecule



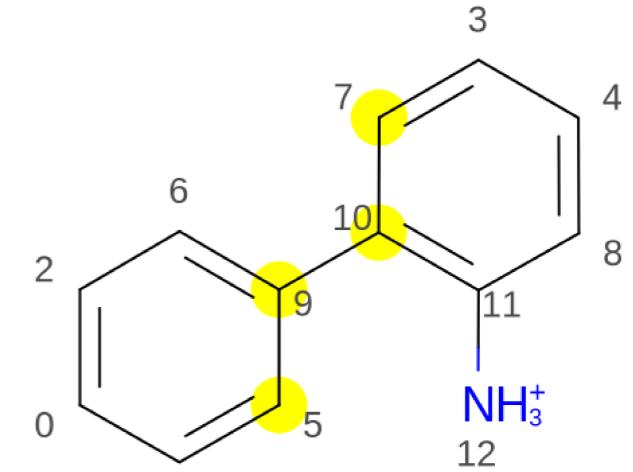
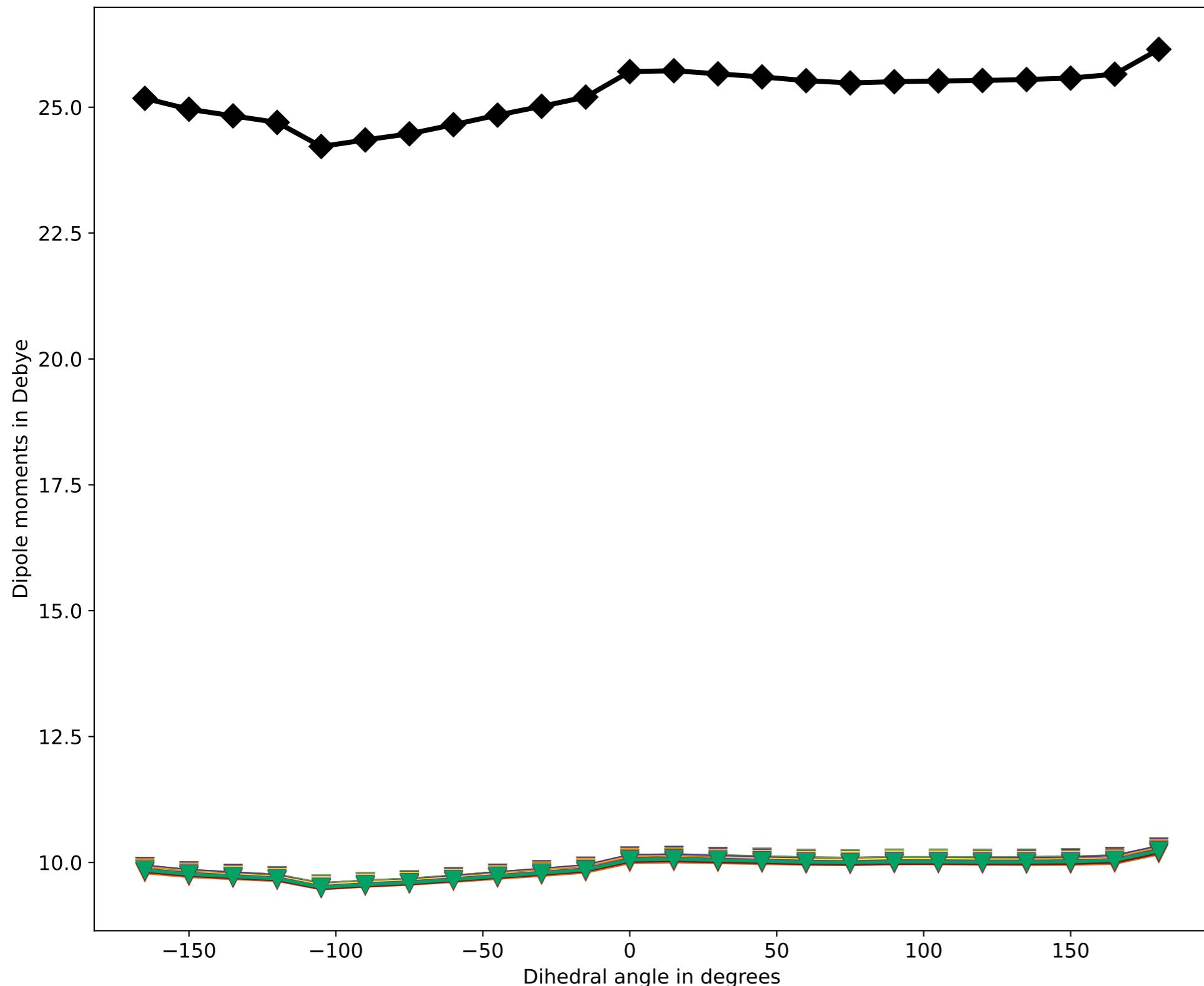
- ◆ REFERENCE
- b97-d3bj/def2-tzvp
- ▲ m05-2x-d3/dzvp
- ▼ m06-2x-d3/dzvp
- ◀ m08-hx-d3/dzvp
- ▬ wb97m-d3bj/dzvp
- ▬ wb97m-v/dzvp
- ▬ pw6b95-d3bj/dzvp
- ▬ pw6b95-d3/dzvp
- ▬ mp2/aug-cc-pvtz
- ▬ mp2/heavy-aug-cc-pvtz
- ▬ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ▬ b3lyp-d3bj/dzvp
- ▬ b3lyp-nl/dzvp
- ▬ b3lyp-d3bj/def2-tzvp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

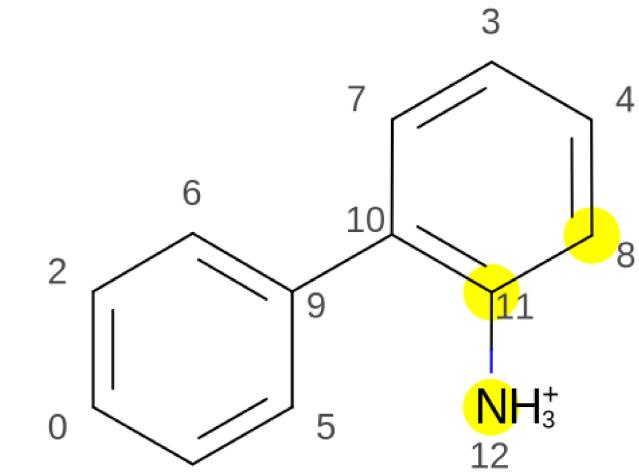
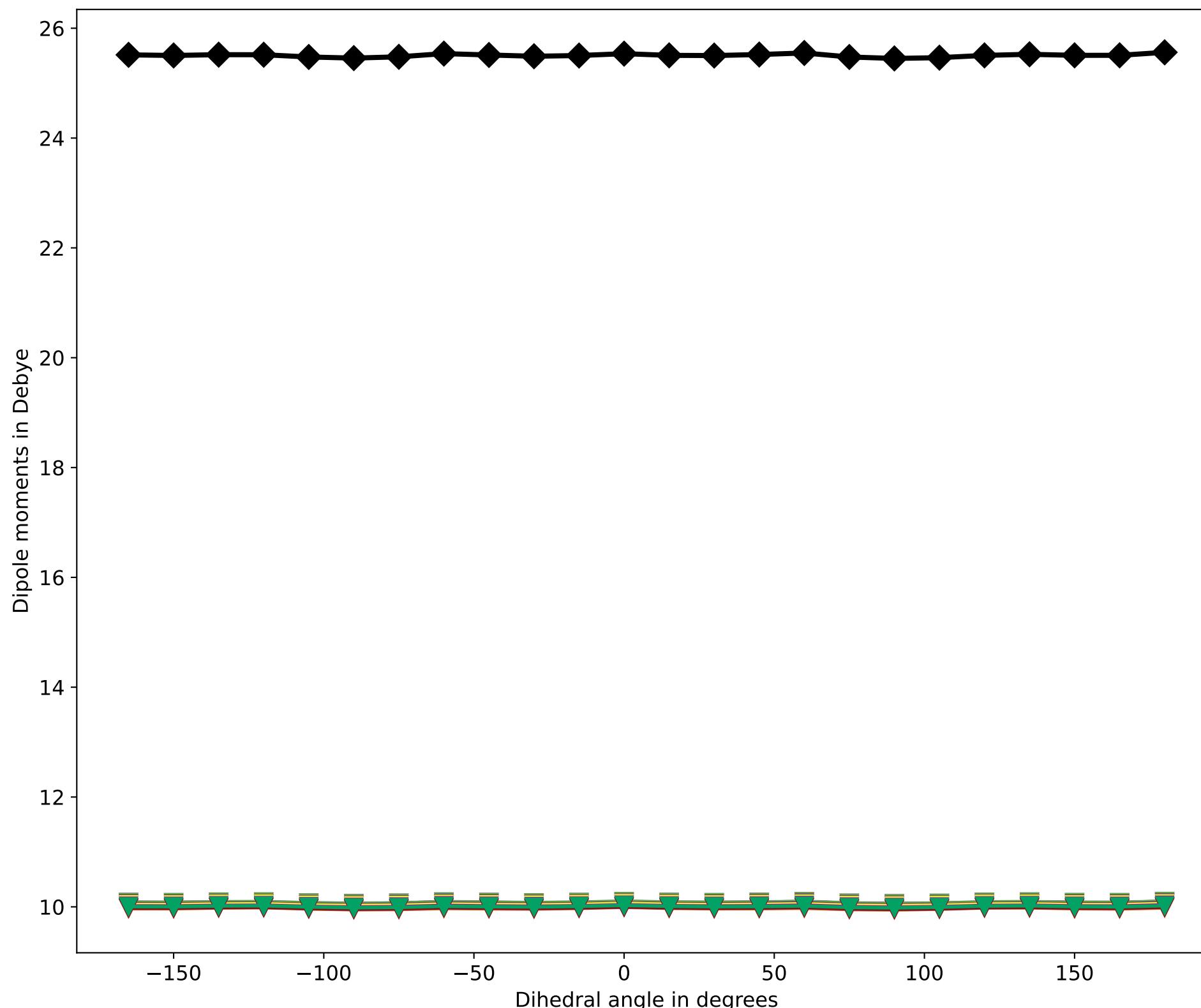
Charged molecule



- ◆ REFERENCE

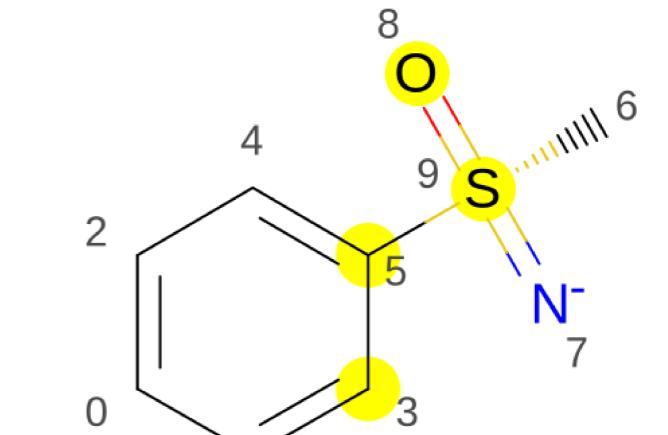
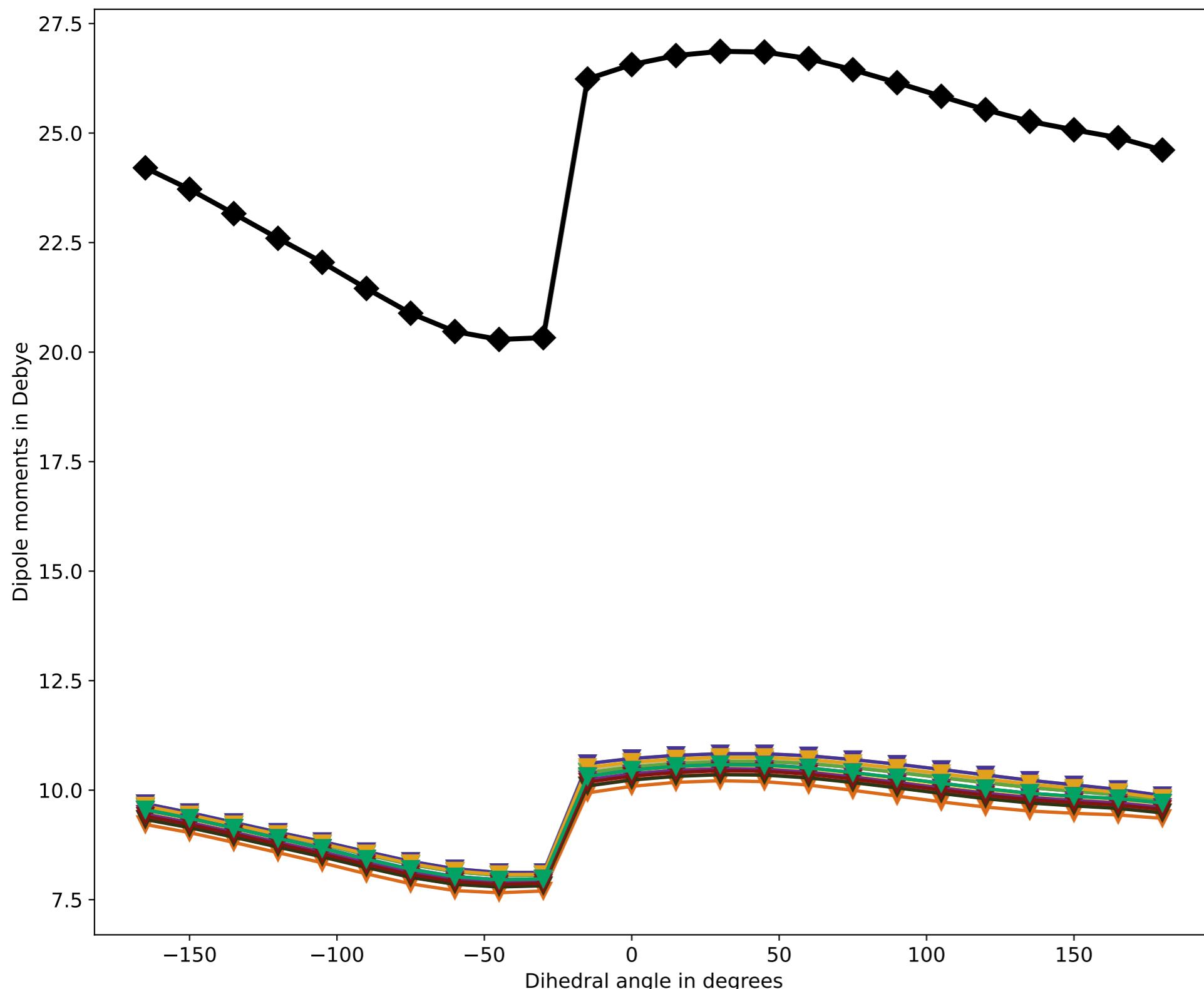
 - ◆ b97-d3bj/def2-tzvp
 - ◆ m05-2x-d3/dzvp
 - ◆ m06-2x-d3/dzvp
 - ◆ m08-hx-d3/dzvp
 - ◆ wb97m-d3bj/dzvp
 - ◆ wb97m-v/dzvp
 - ◆ pw6b95-d3bj/dzvp
 - ◆ pw6b95-d3/dzvp
 - ◆ mp2/aug-cc-pvtz
 - ◆ mp2/heavy-aug-cc-pvtz
 - ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
 - ◆ b3lyp-d3bj/dzvp
 - ◆ b3lyp-nl/dzvp
 - ◆ b3lyp-d3bj/def2-tzvp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

Charged molecule



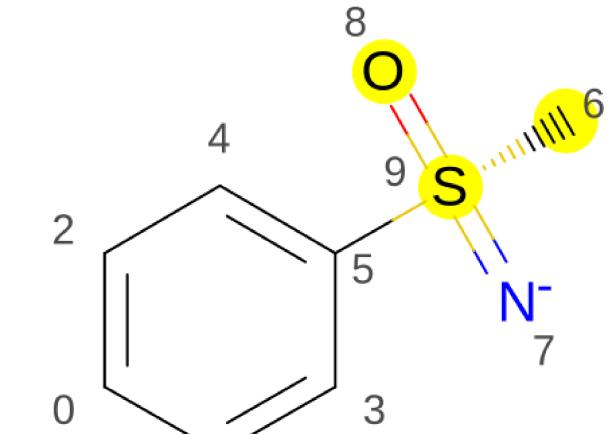
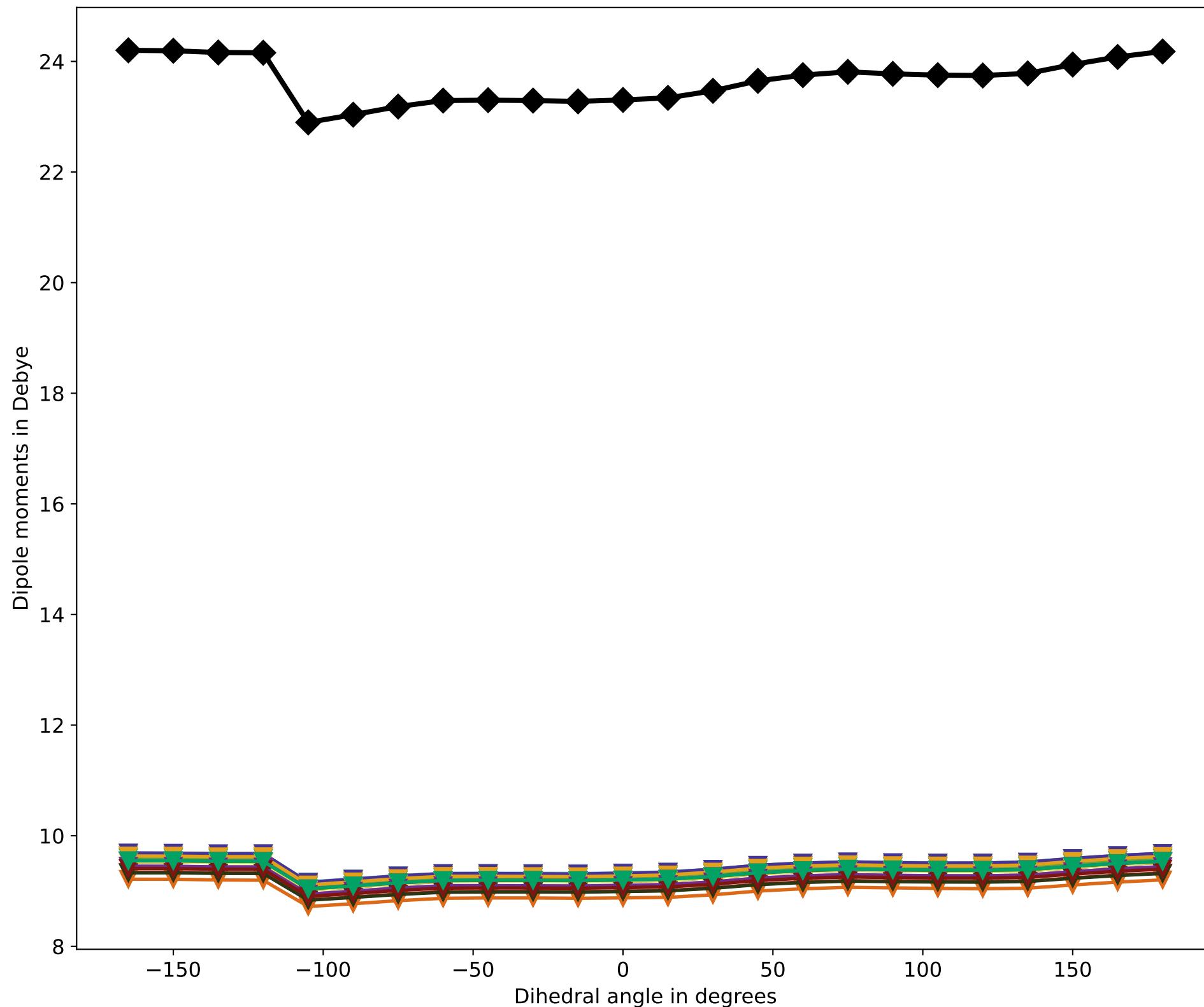
- ◆ REFERENCE
- ▼ b97-d3bj/def2-tzvp
- △ m05-2x-d3/dzvp
- ▲ m06-2x-d3/dzvp
- ▽ m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- ▲ wb97m-v/dzvp
- ▼ pw6b95-d3bj/dzvp
- ▲ pw6b95-d3/dzvp
- ▲ mp2/aug-cc-pvtz
- ▲ mp2/heavy-aug-cc-pvtz
- ▲ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ▲ b3lyp-d3bj/dzvp
- ▲ b3lyp-nl/dzvp
- ▲ b3lyp-d3bj/def2-tzvp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

Charged molecule



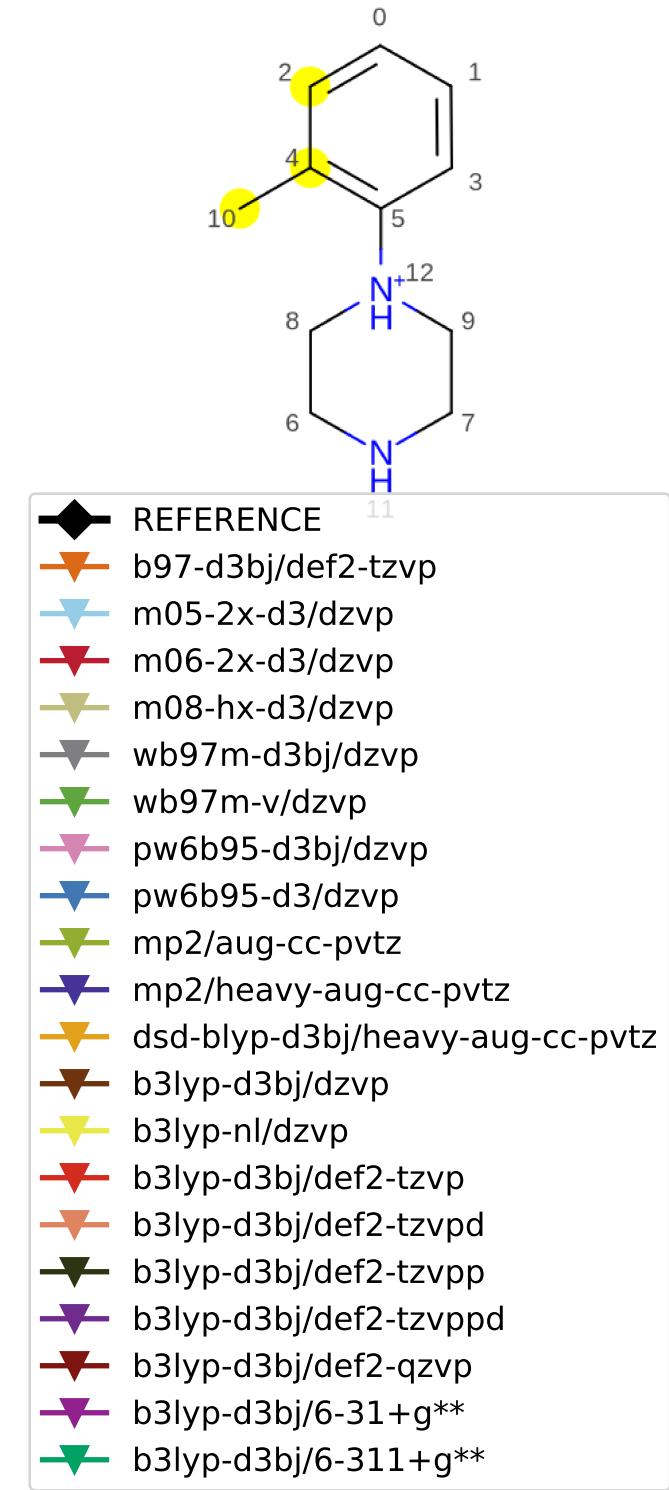
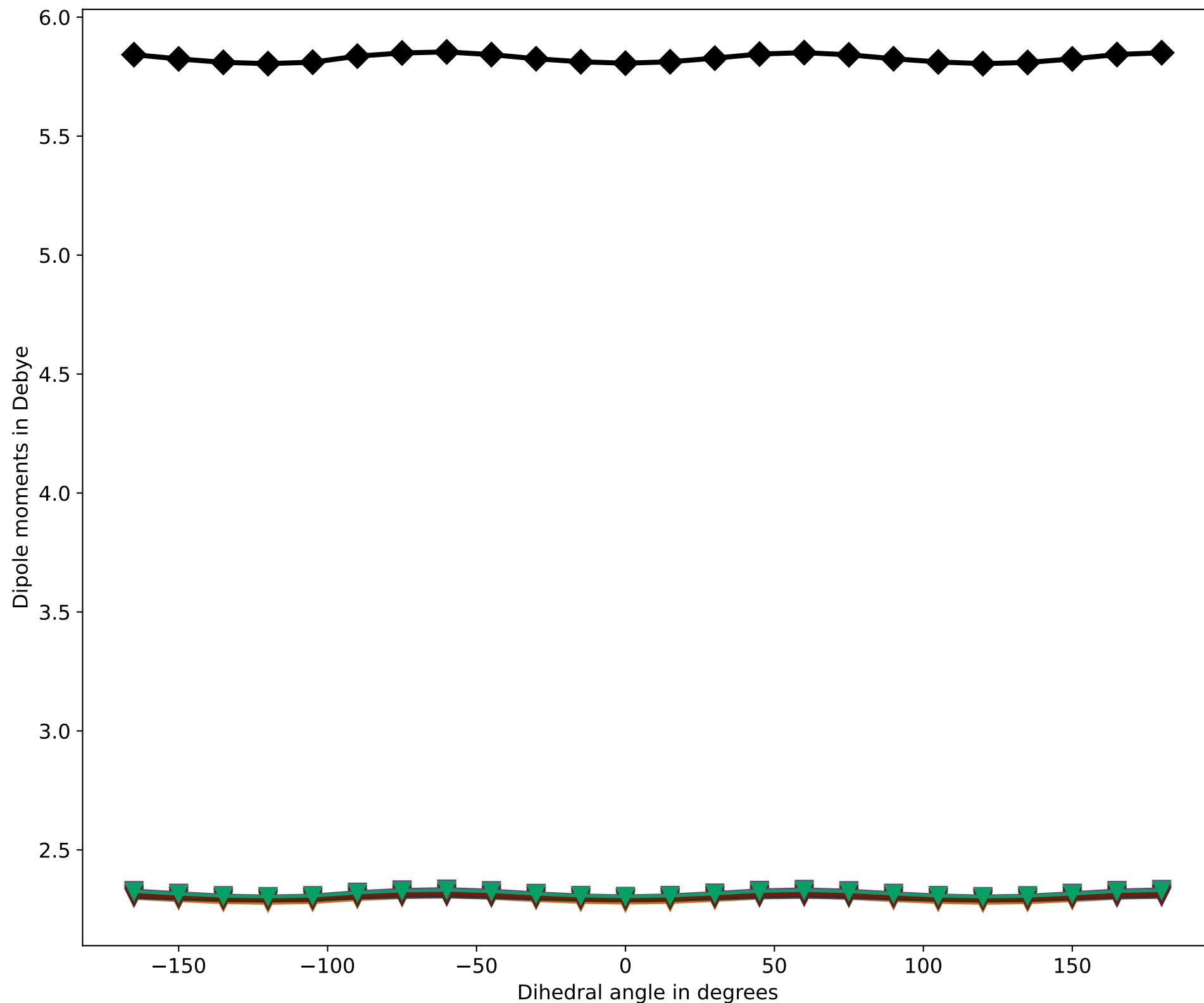
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp (red)
- ◆ b3lyp-d3bj/def2-tzvpd (orange)
- ◆ b3lyp-d3bj/def2-tzvpp (black)
- ◆ b3lyp-d3bj/def2-tzvppd (purple)
- ◆ b3lyp-d3bj/def2-qzvp (dark red)
- ◆ b3lyp-d3bj/6-31+g** (pink)
- ◆ b3lyp-d3bj/6-311+g** (green)

Charged molecule

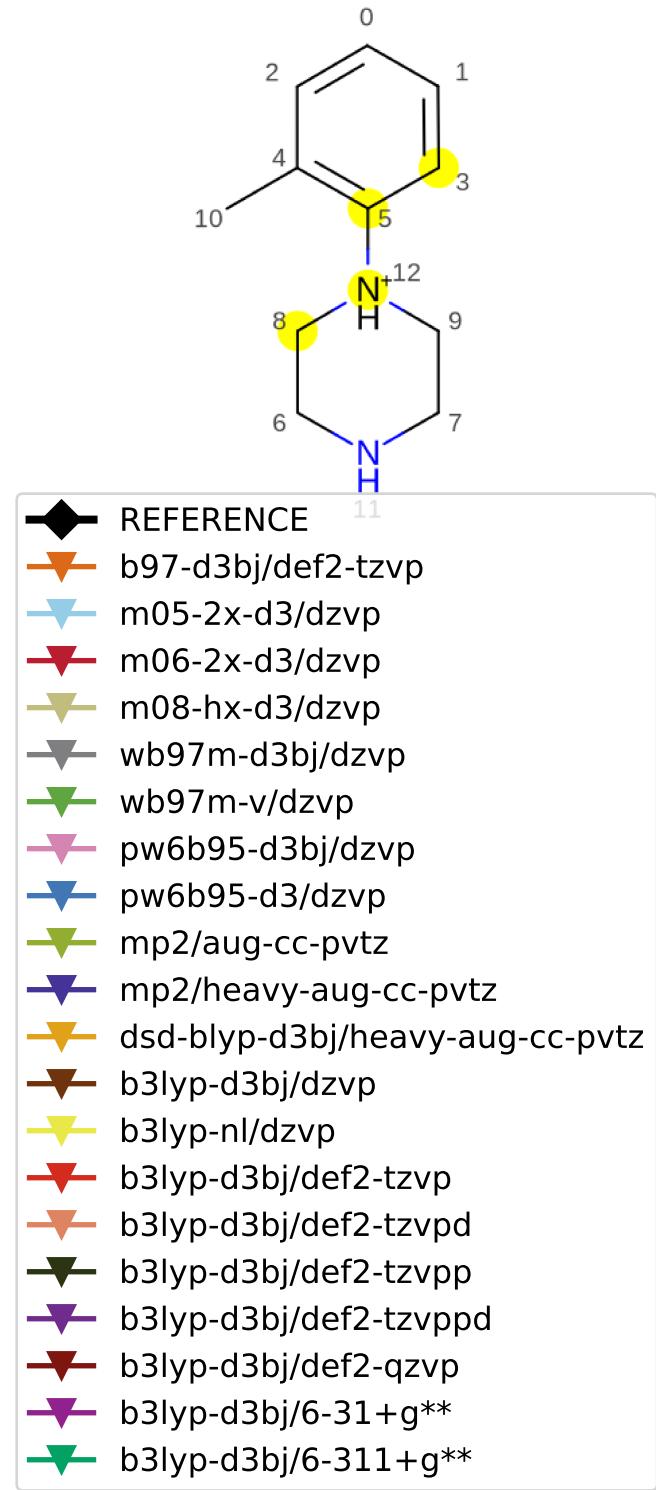
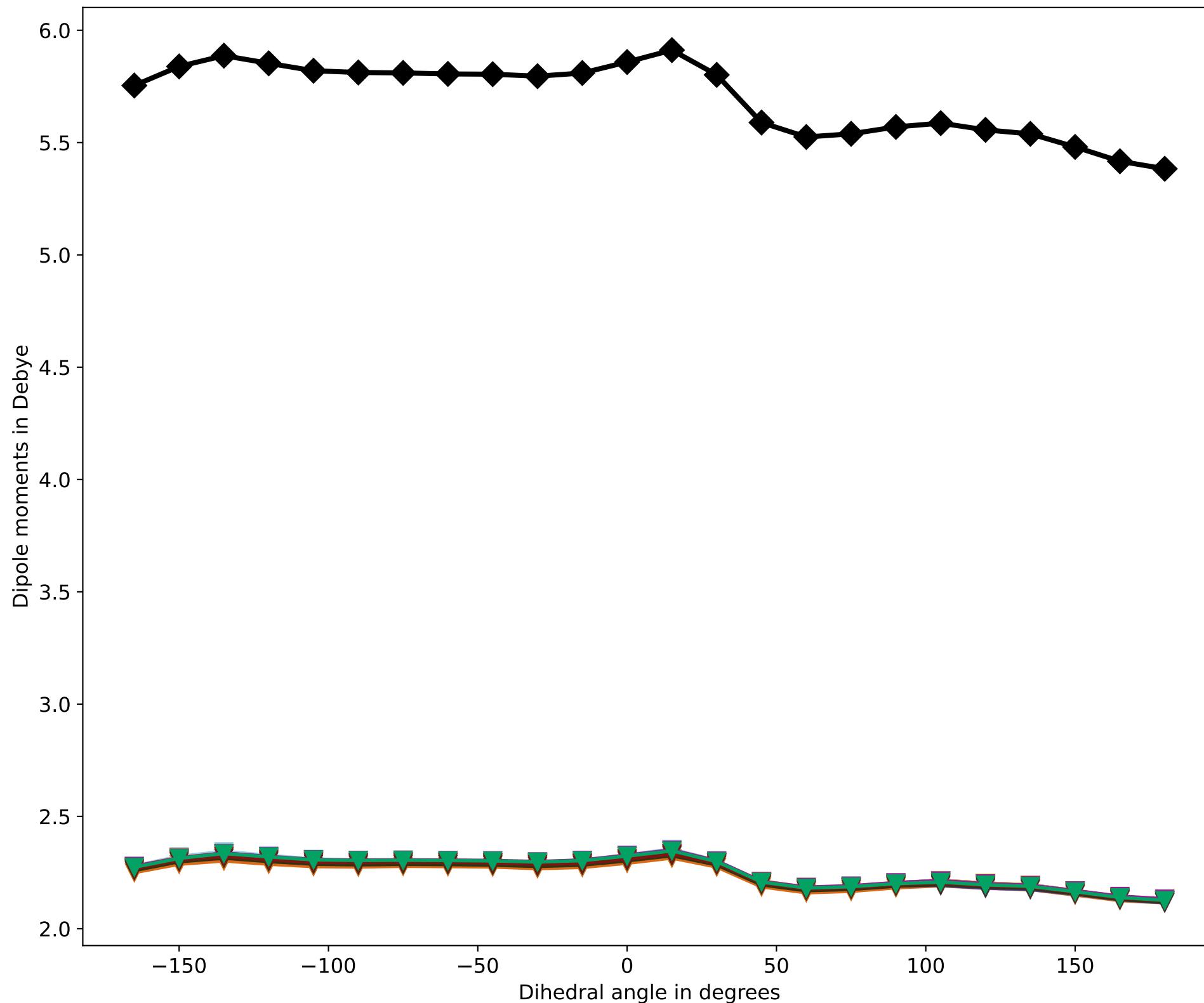


- REFERENCE**

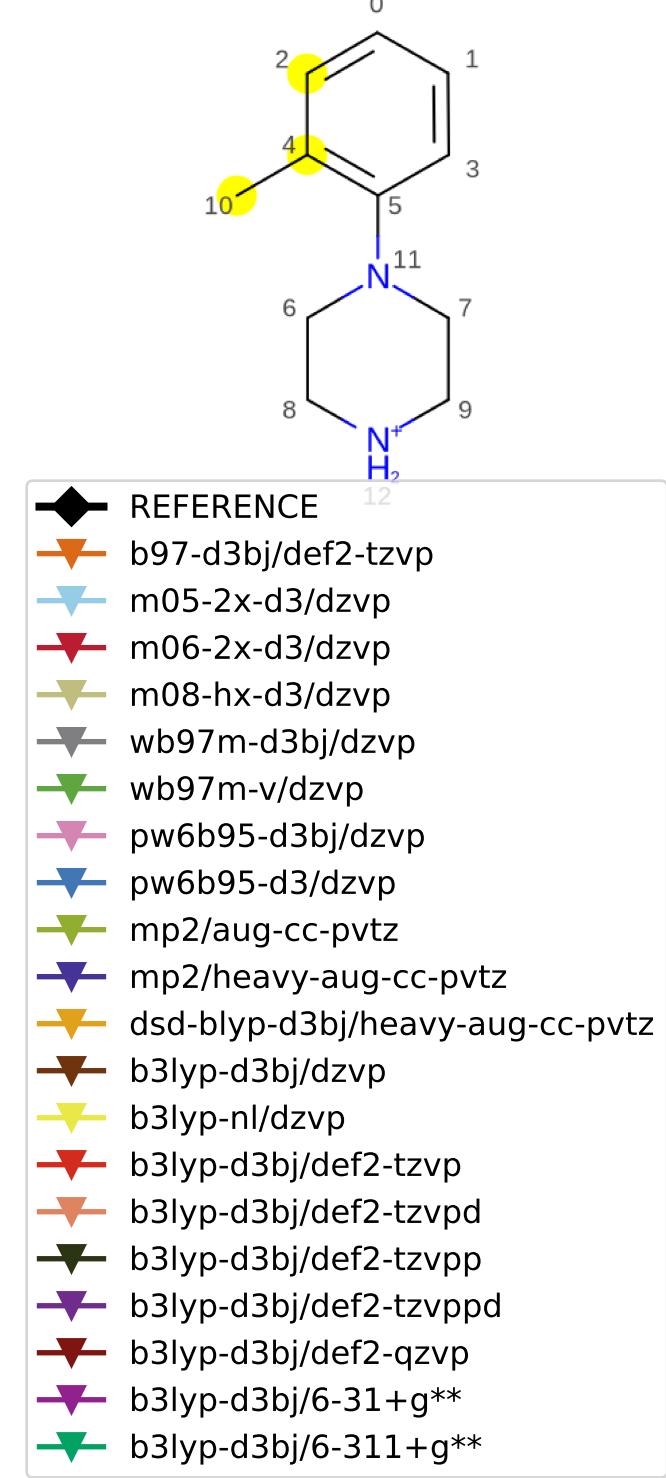
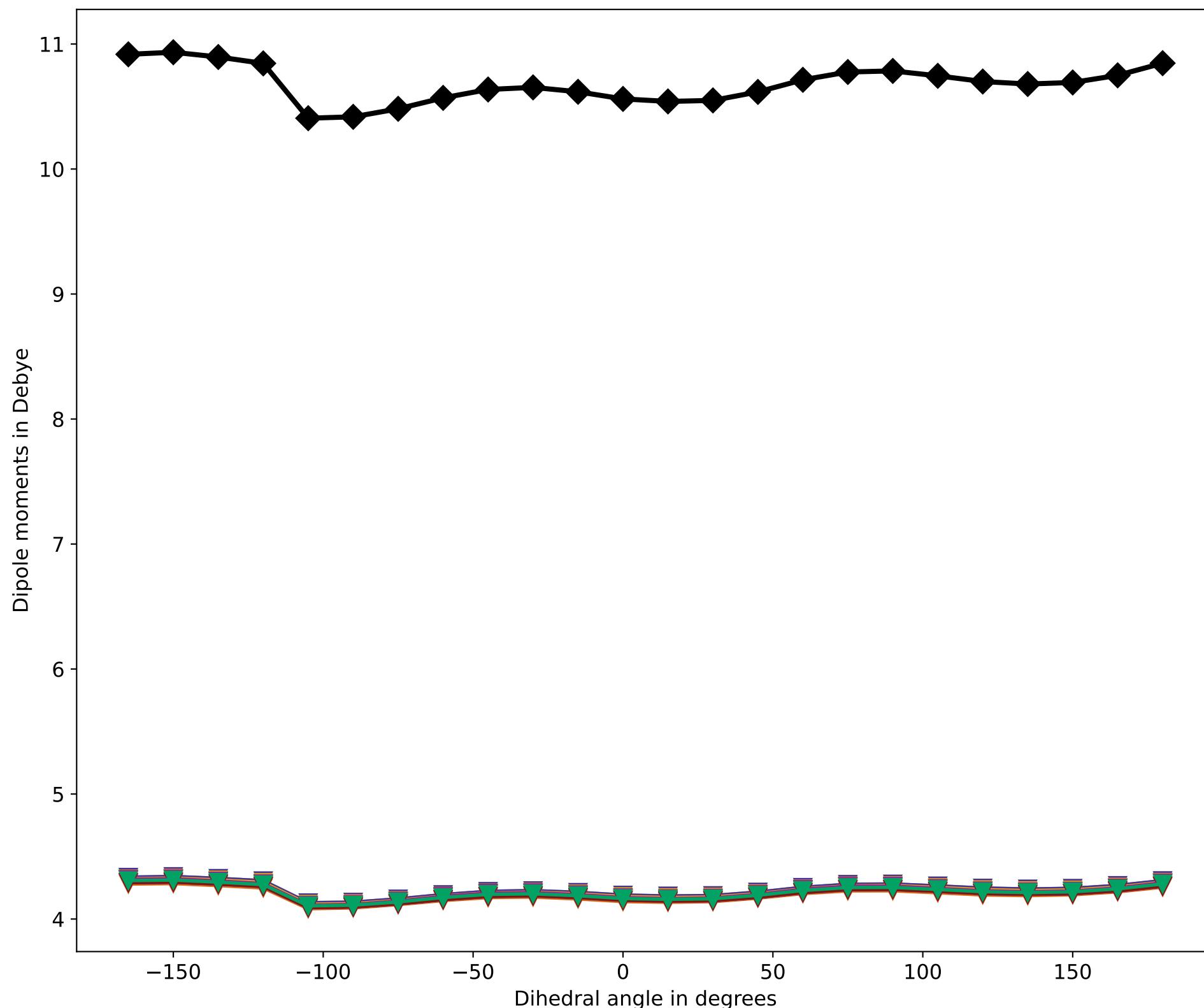
 - b97-d3bj/def2-tzvp
 - ▲ m05-2x-d3/dzvp
 - ▼ m06-2x-d3/dzvp
 - ▬ m08-hx-d3/dzvp
 - ▬ wb97m-d3bj/dzvp
 - ▬ wb97m-v/dzvp
 - ▬ pw6b95-d3bj/dzvp
 - ▬ pw6b95-d3/dzvp
 - ▬ mp2/aug-cc-pvtz
 - ▬ mp2/heavy-aug-cc-pvtz
 - ▬ dsd-blyp-d3bj/heavy-aug-cc-pvtz
 - ▬ b3lyp-d3bj/dzvp
 - ▬ b3lyp-nl/dzvp
 - ▬ b3lyp-d3bj/def2-tzvp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

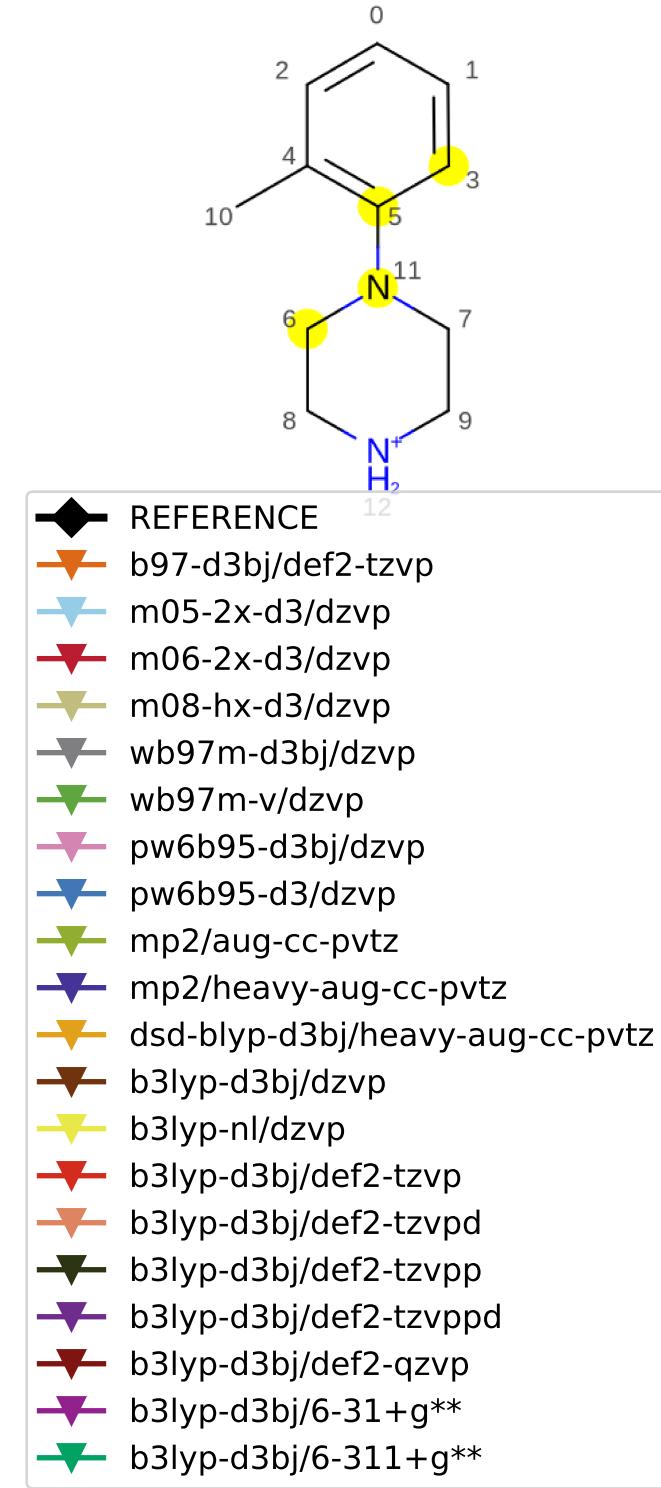
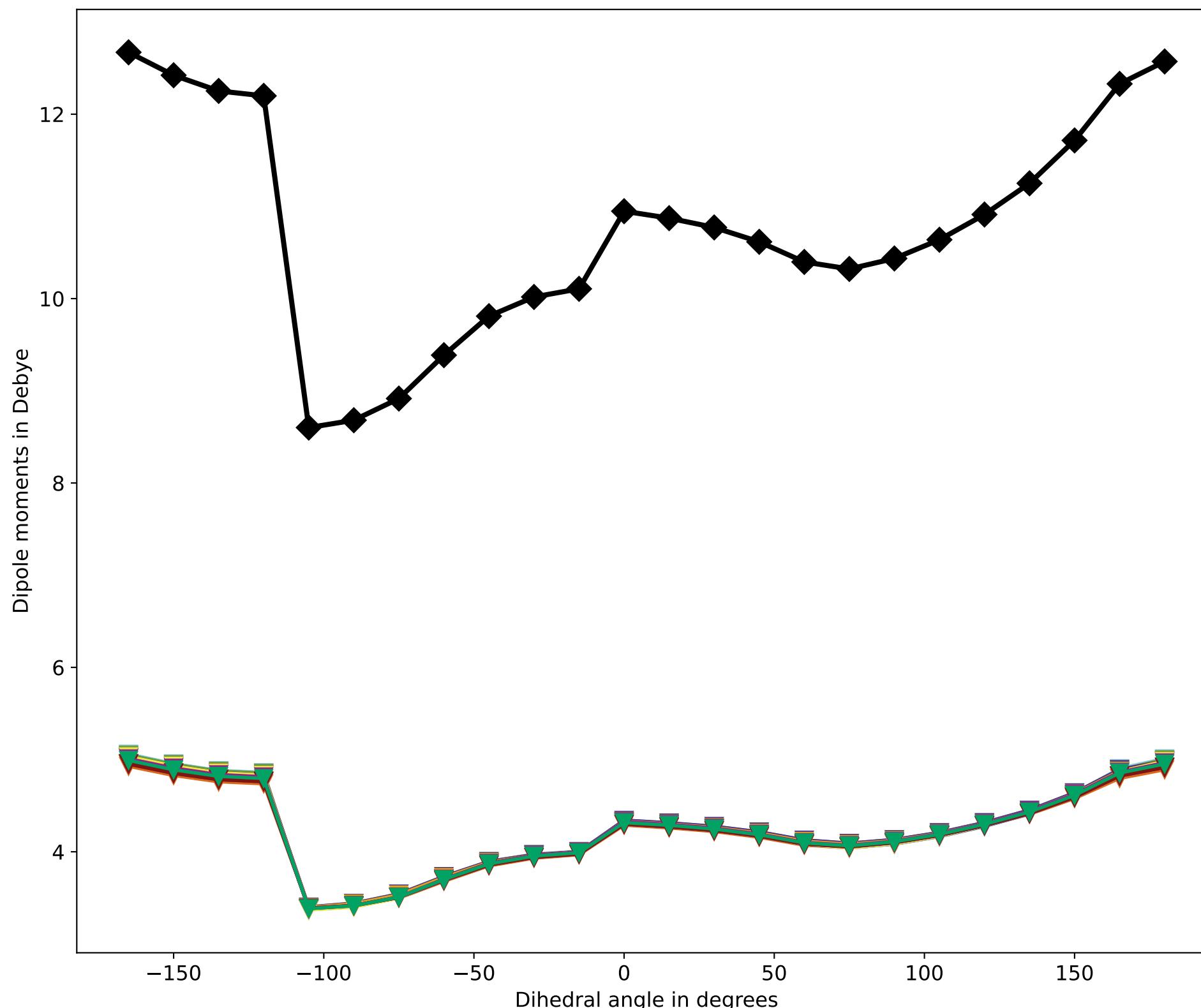


Charged molecule

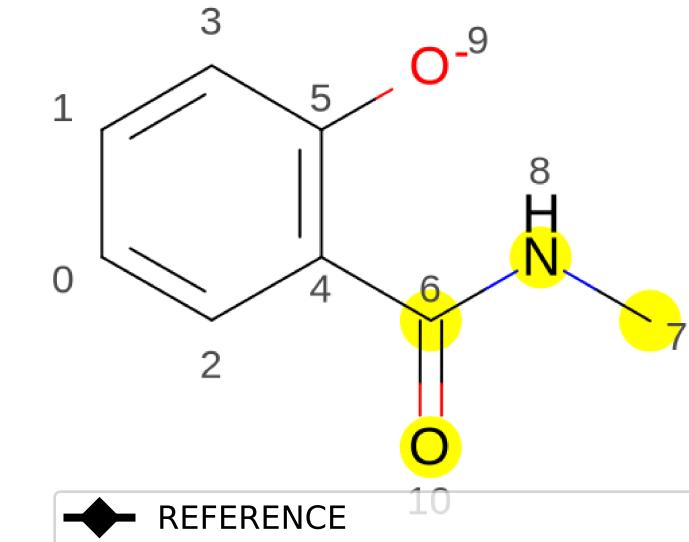
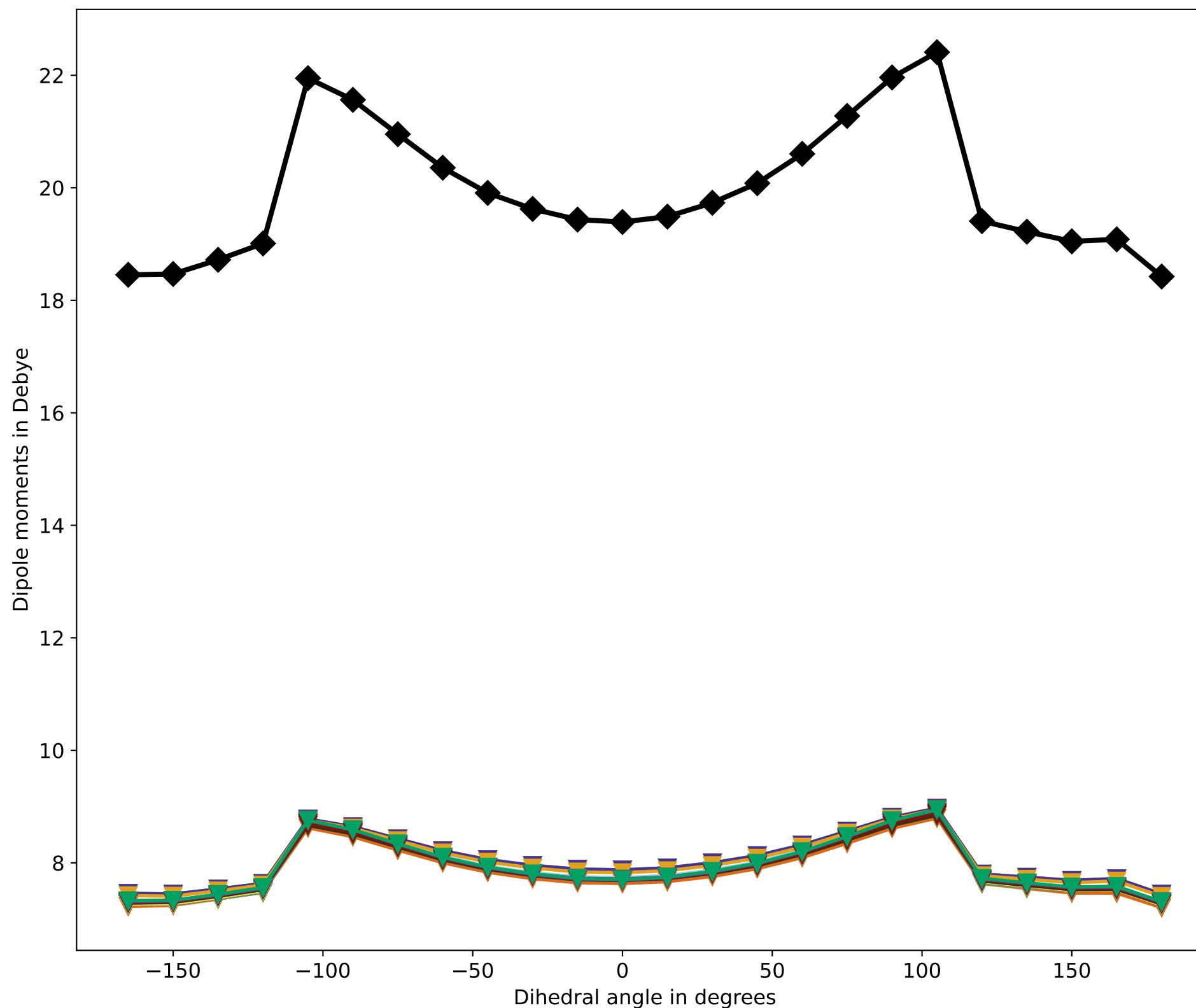


Charged molecule



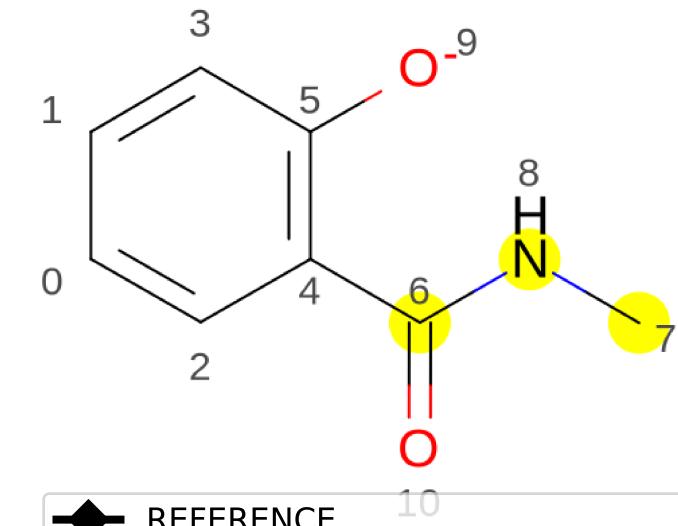
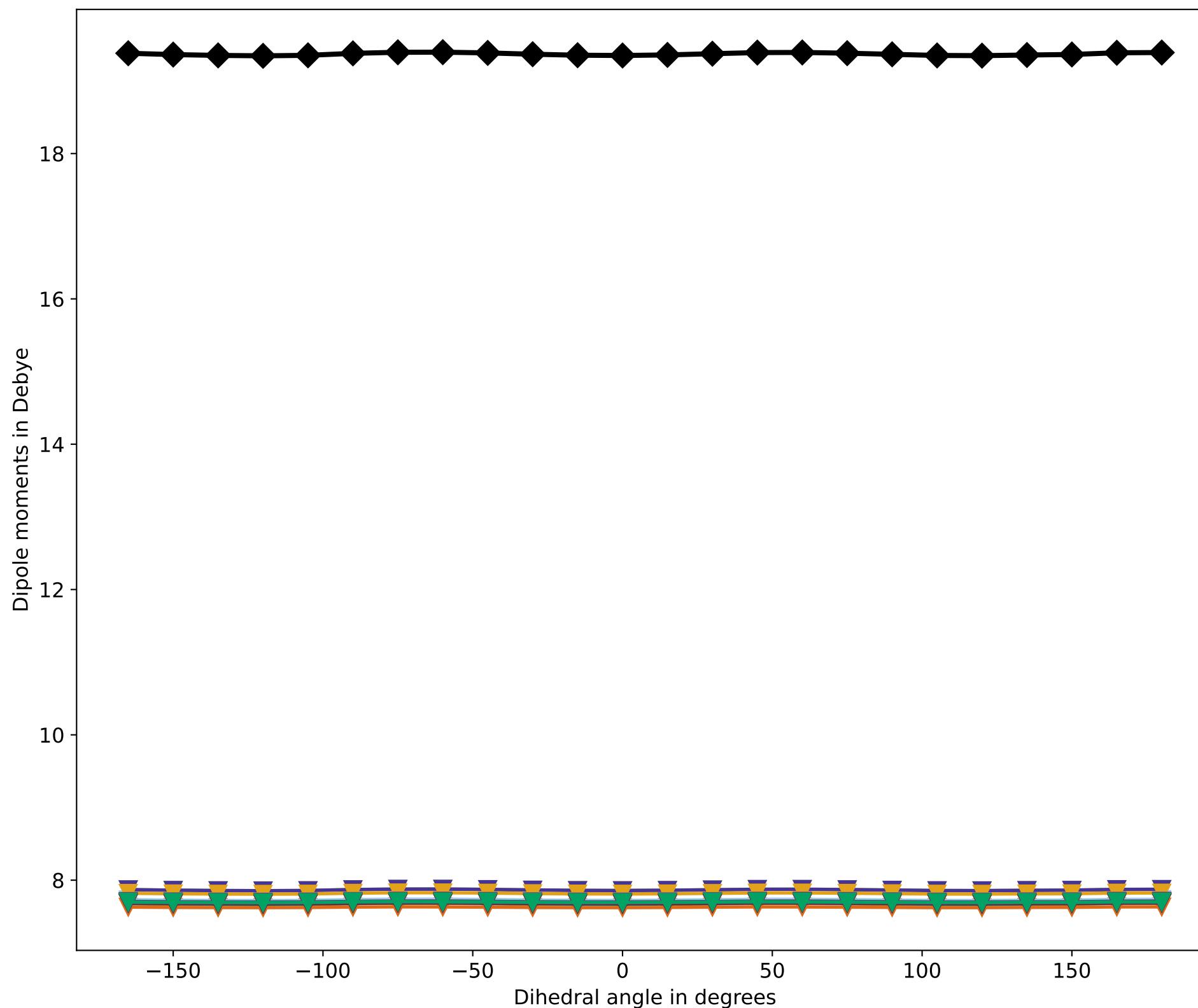


Charged molecule



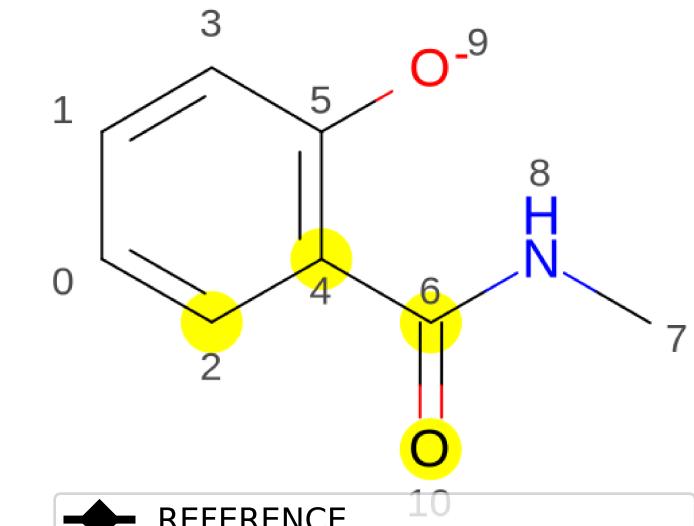
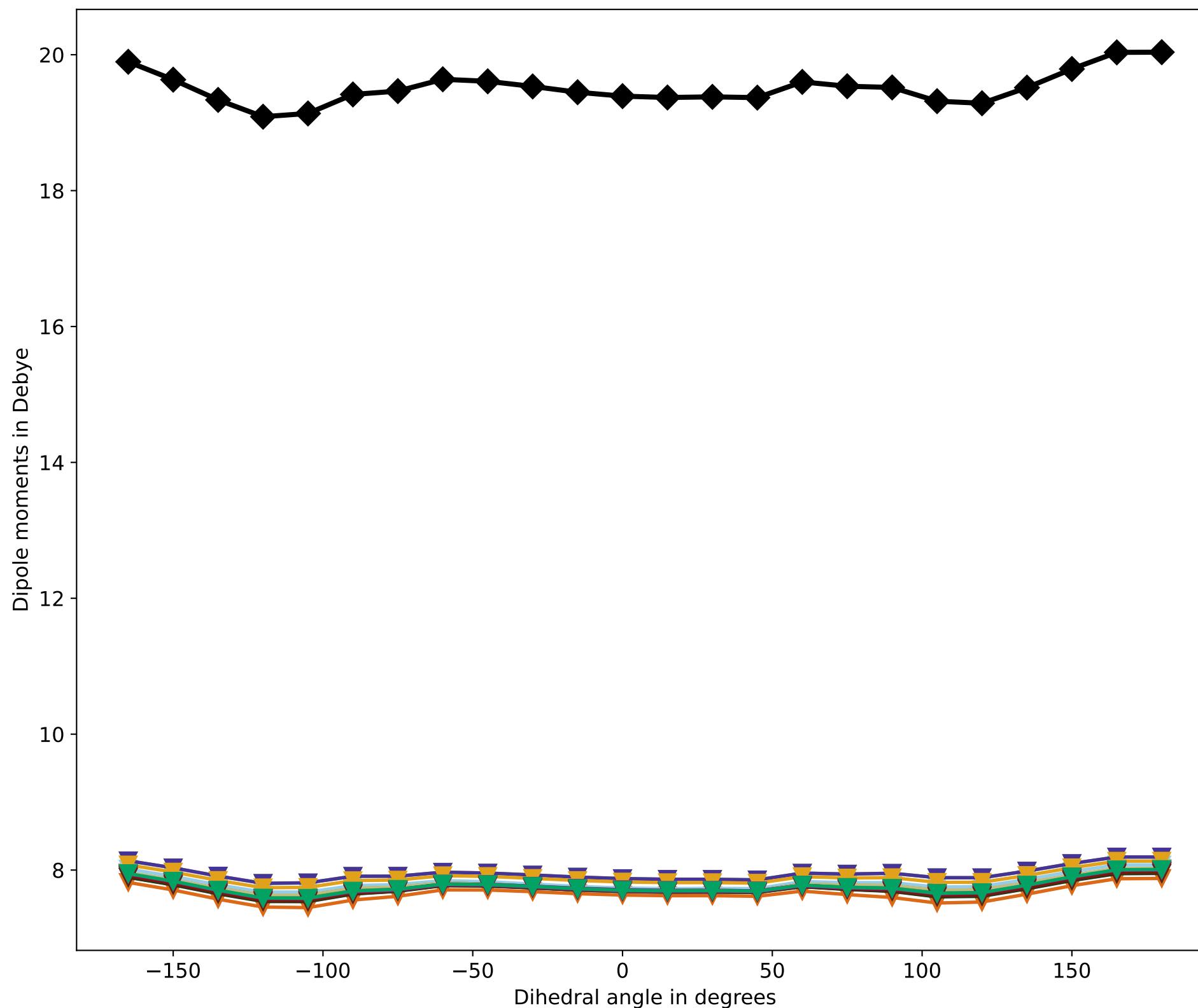
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

Charged molecule



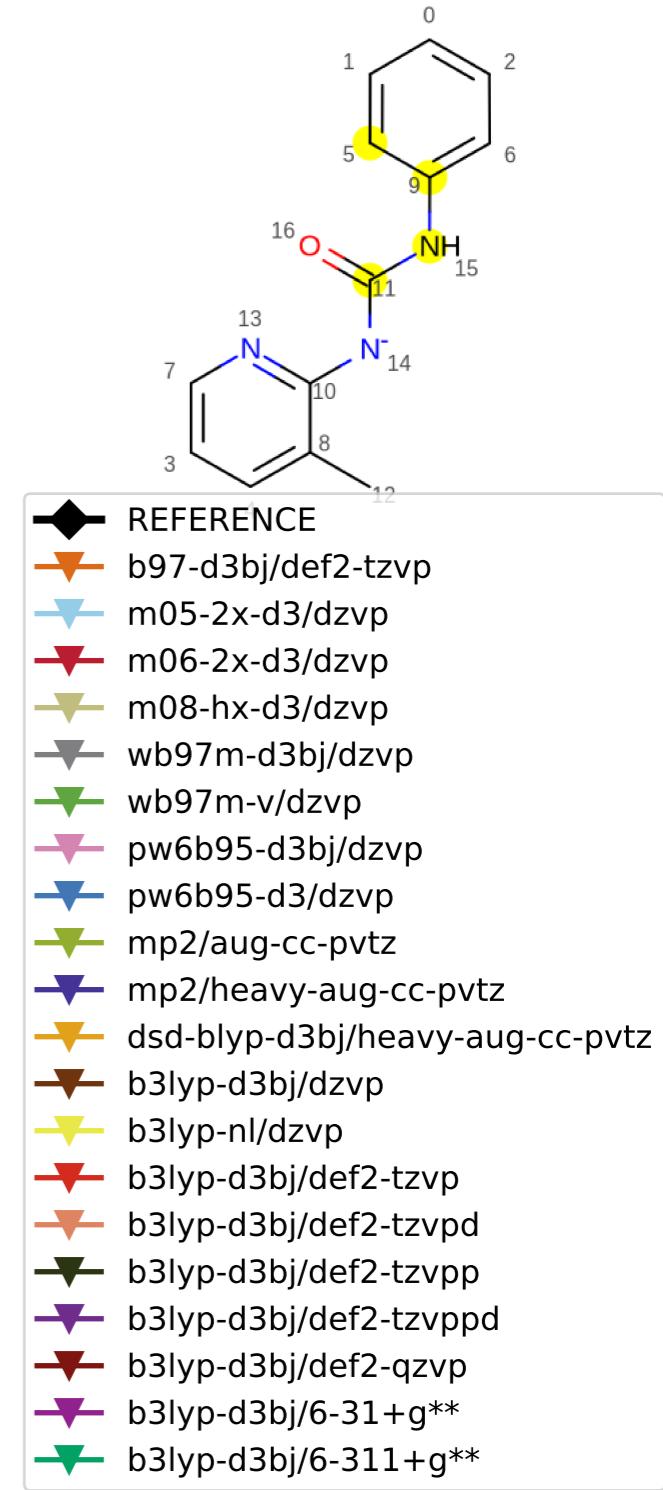
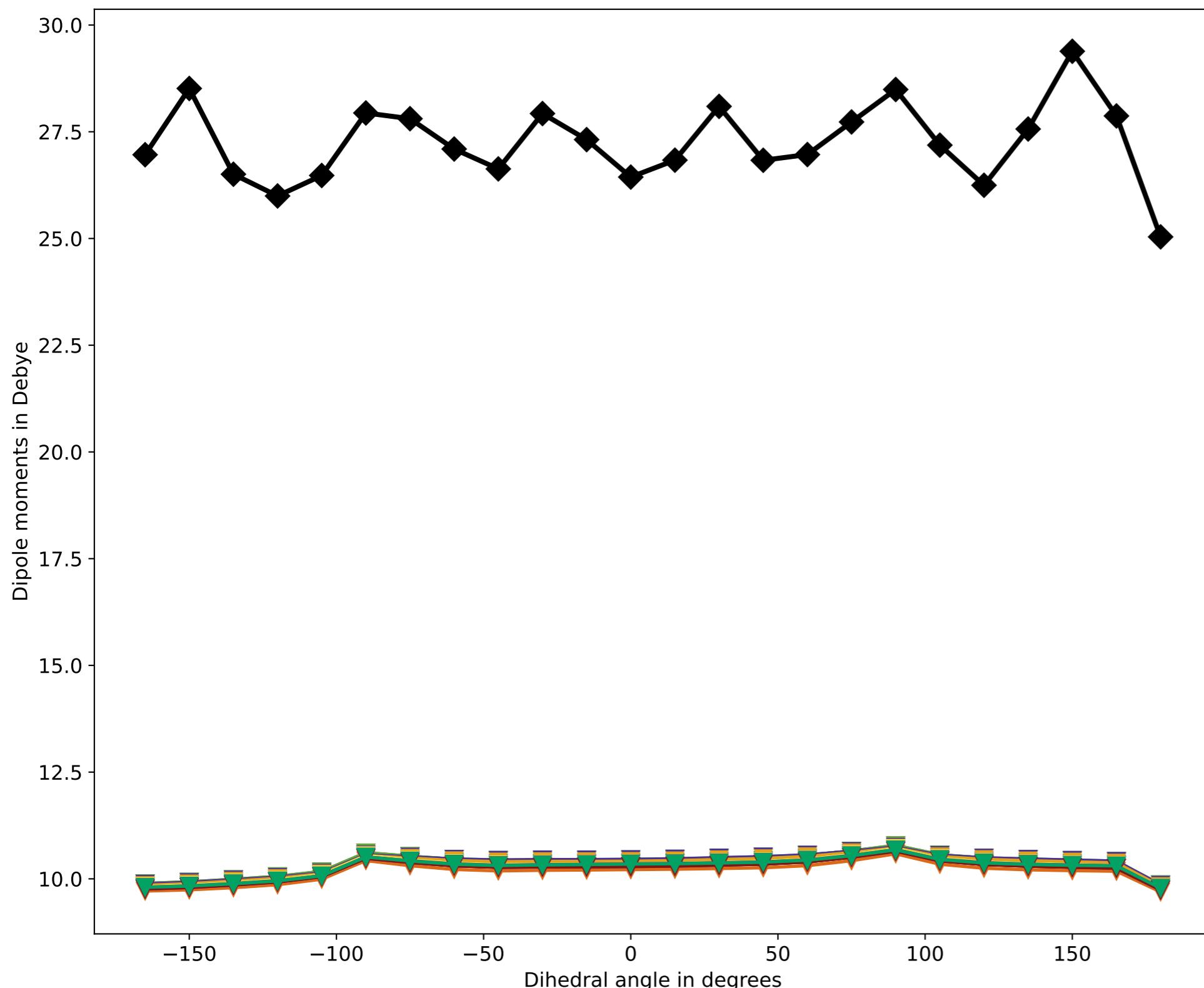
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

Charged molecule

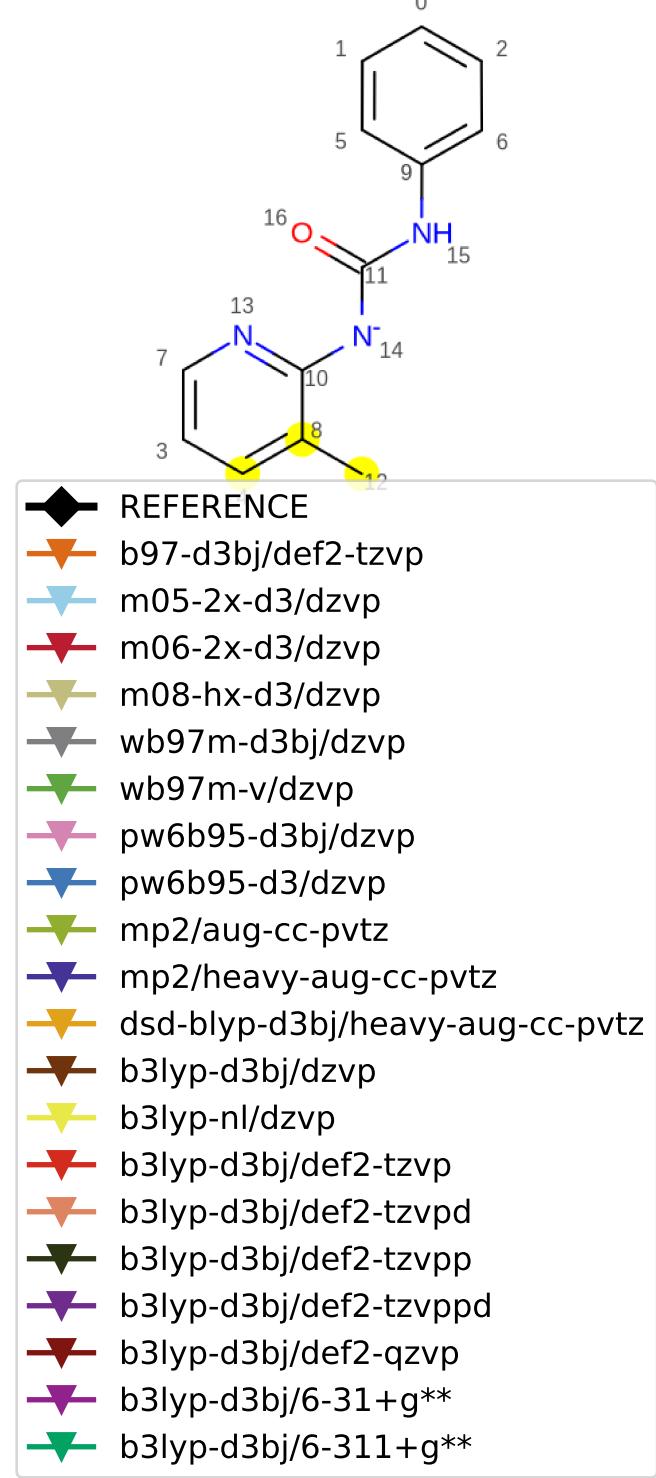
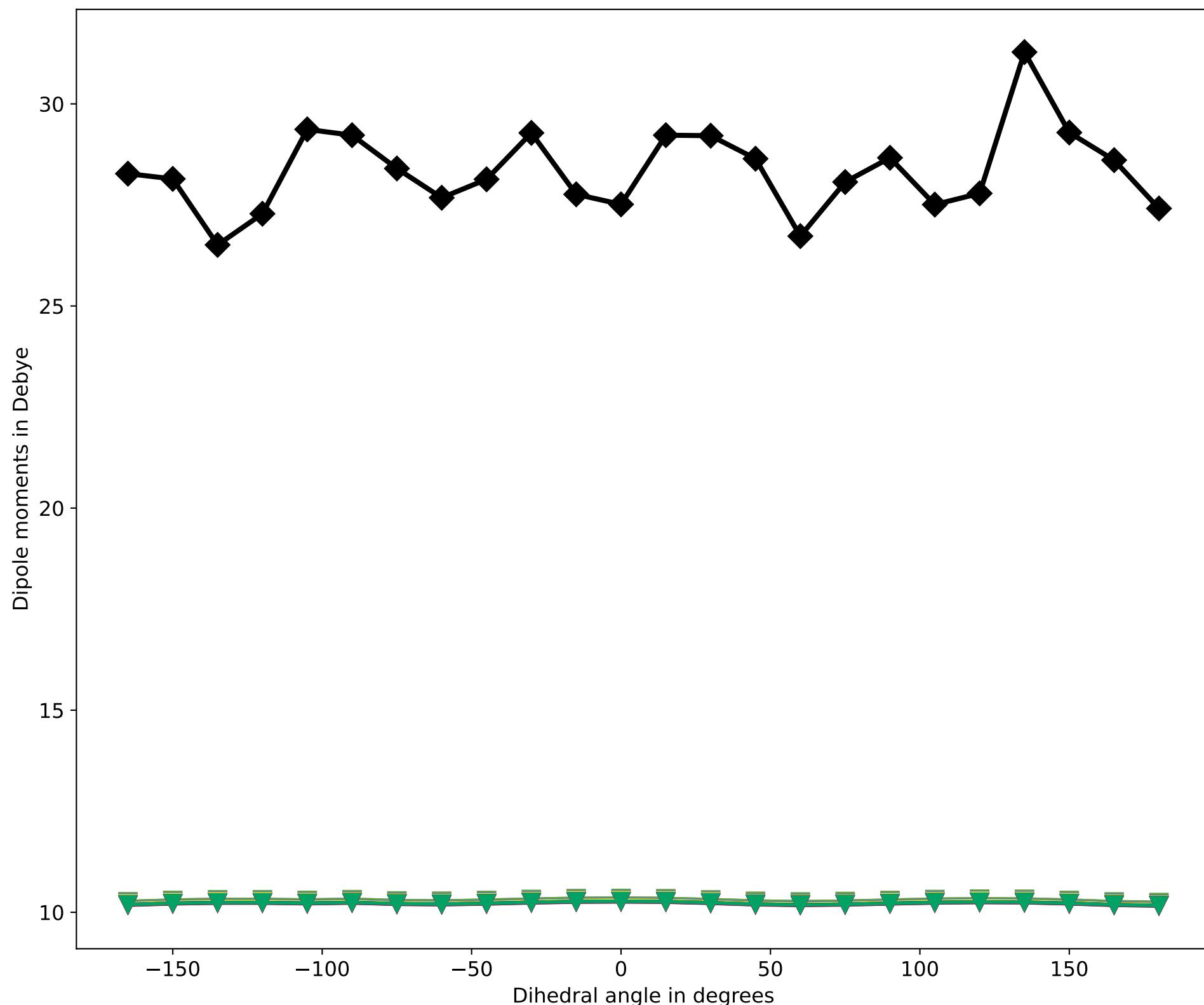


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

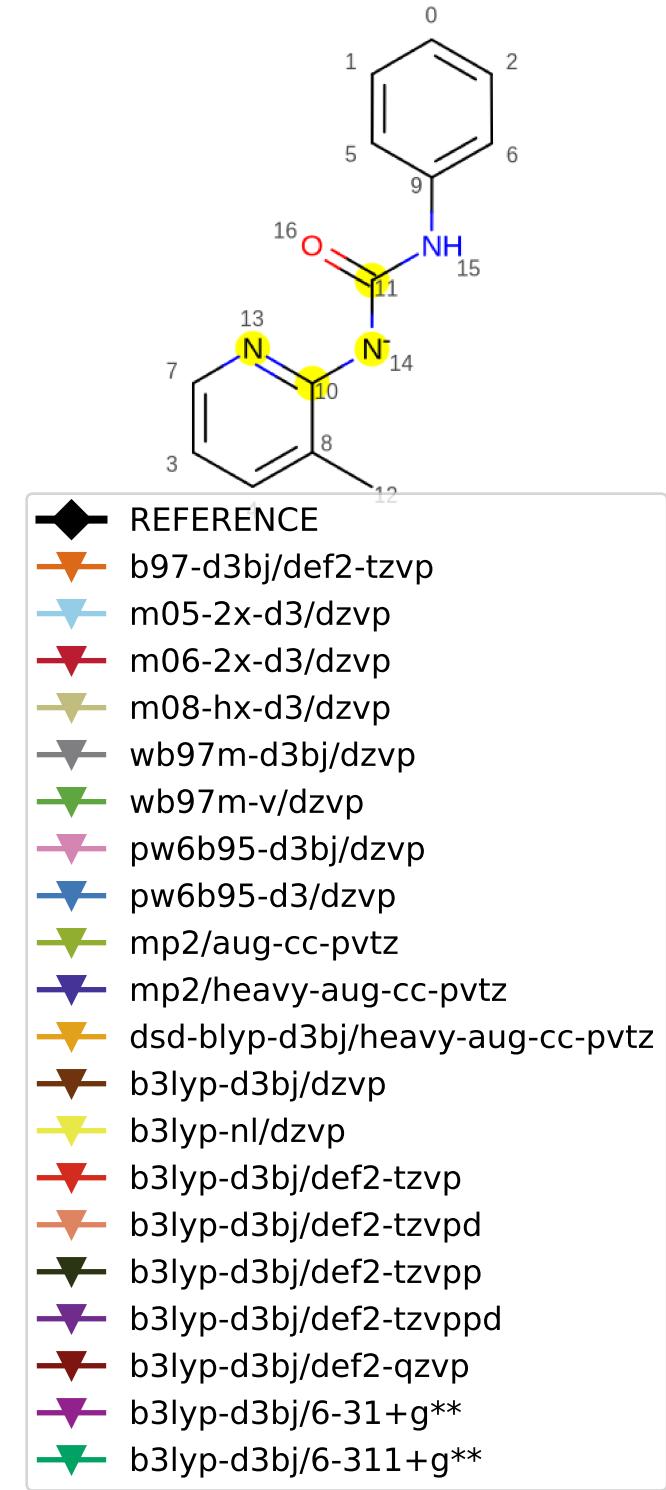
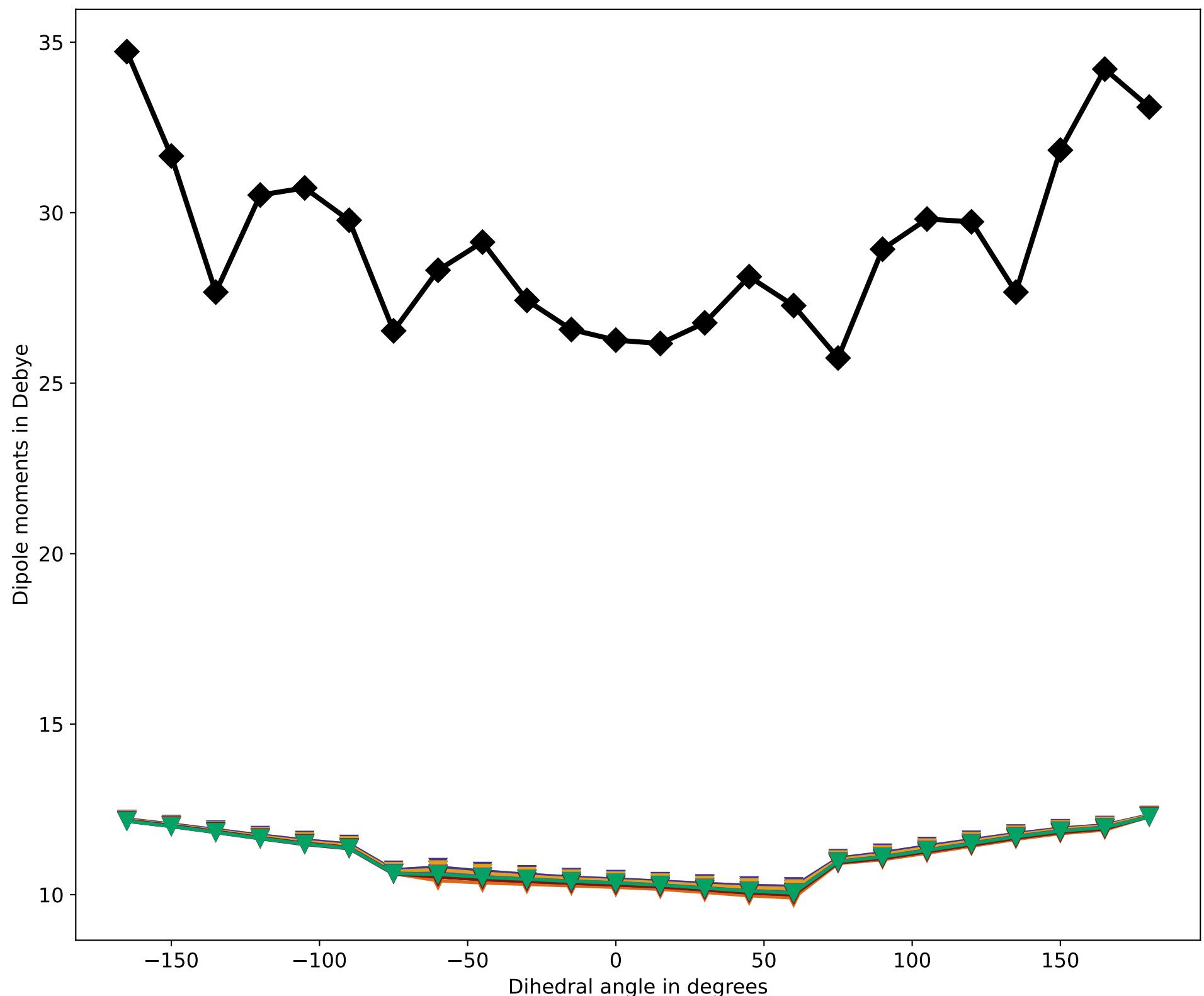
Charged molecule



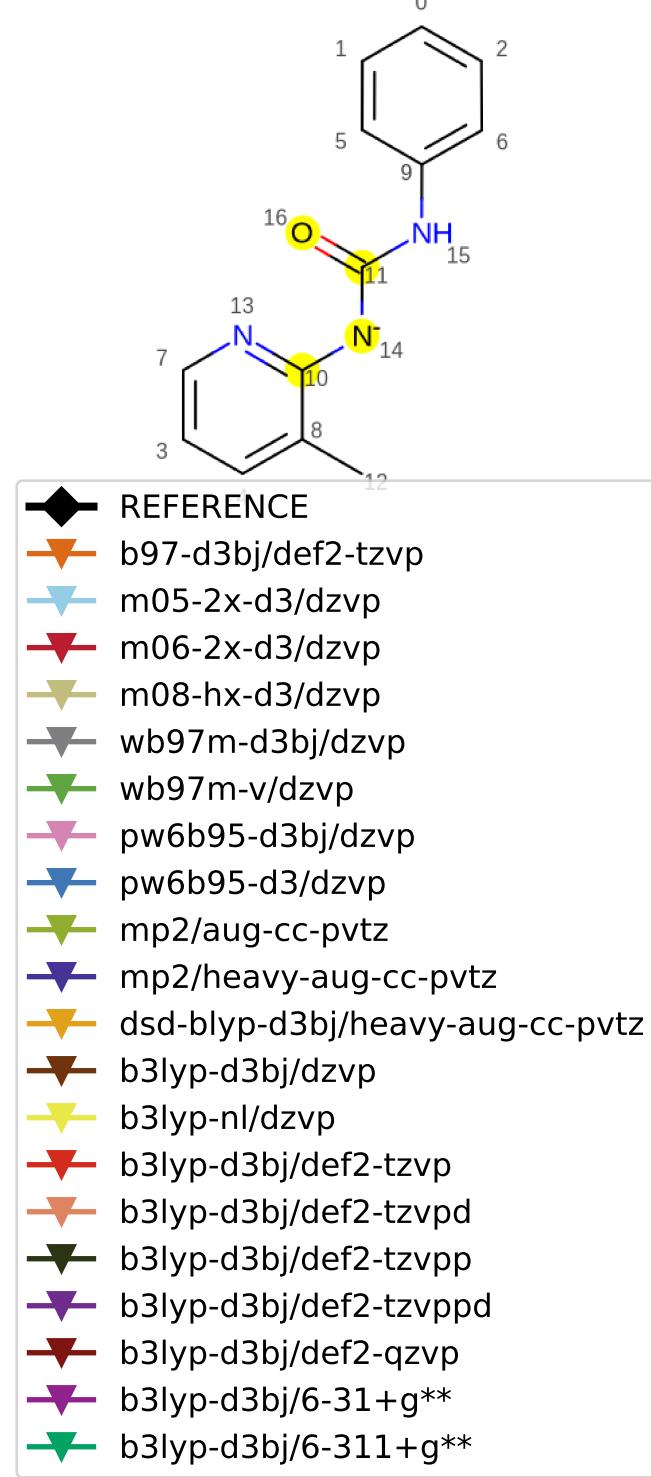
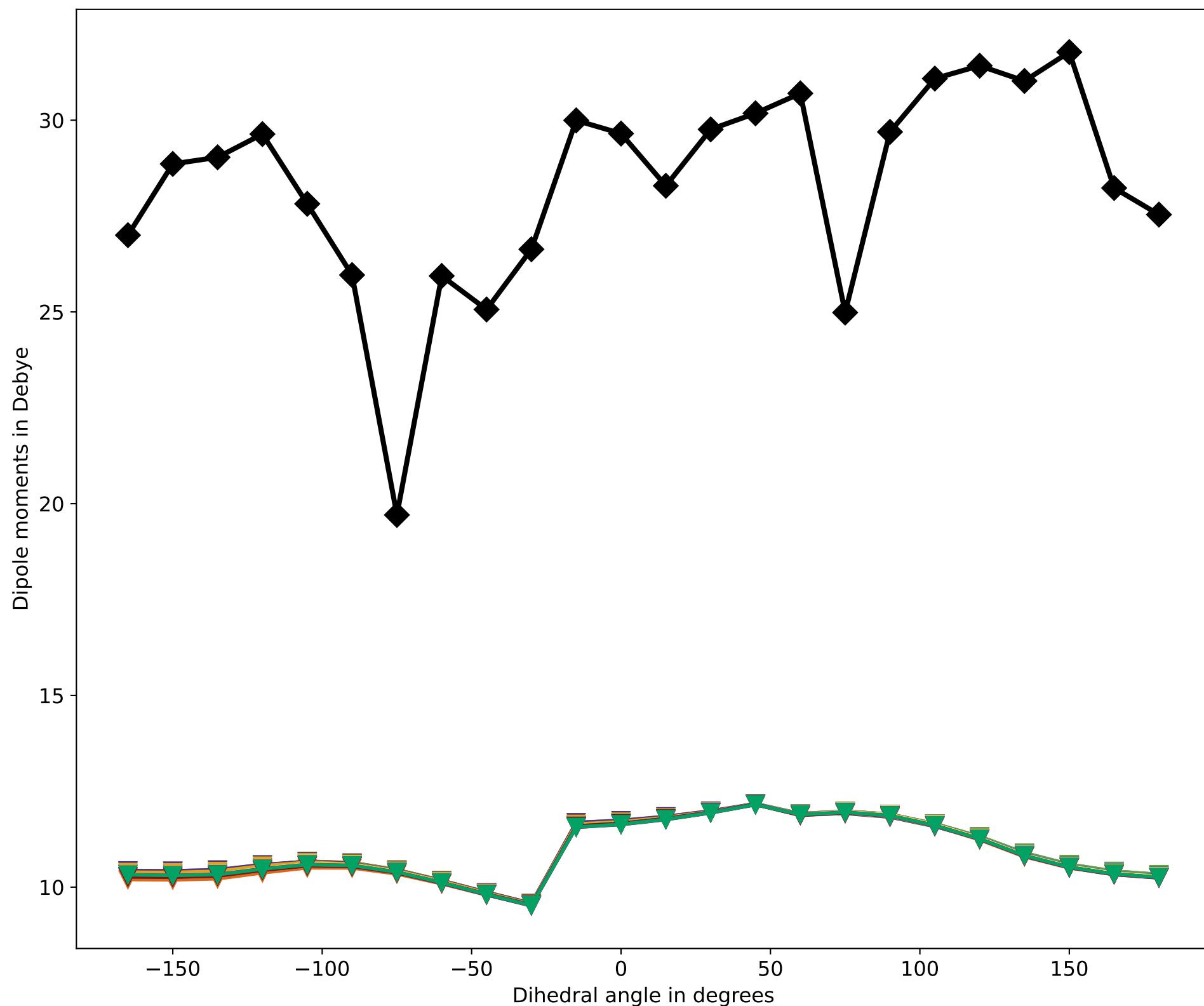
Charged molecule



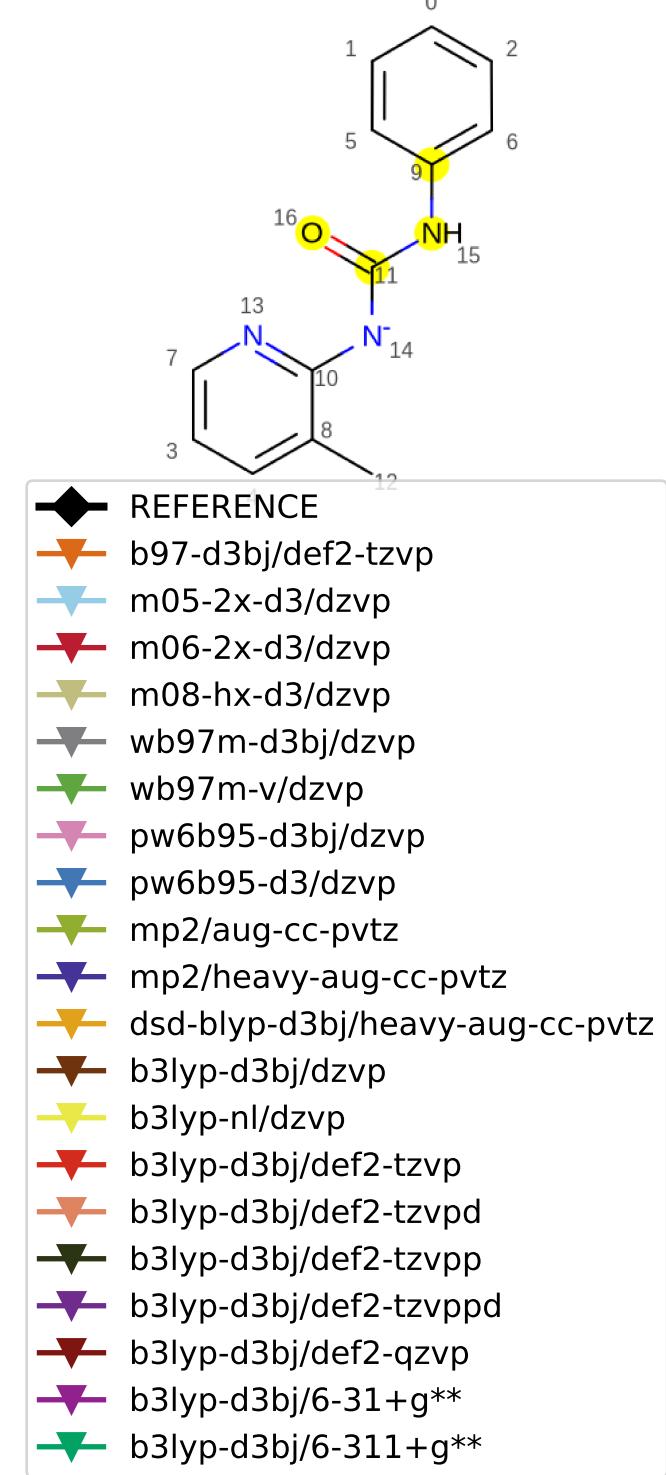
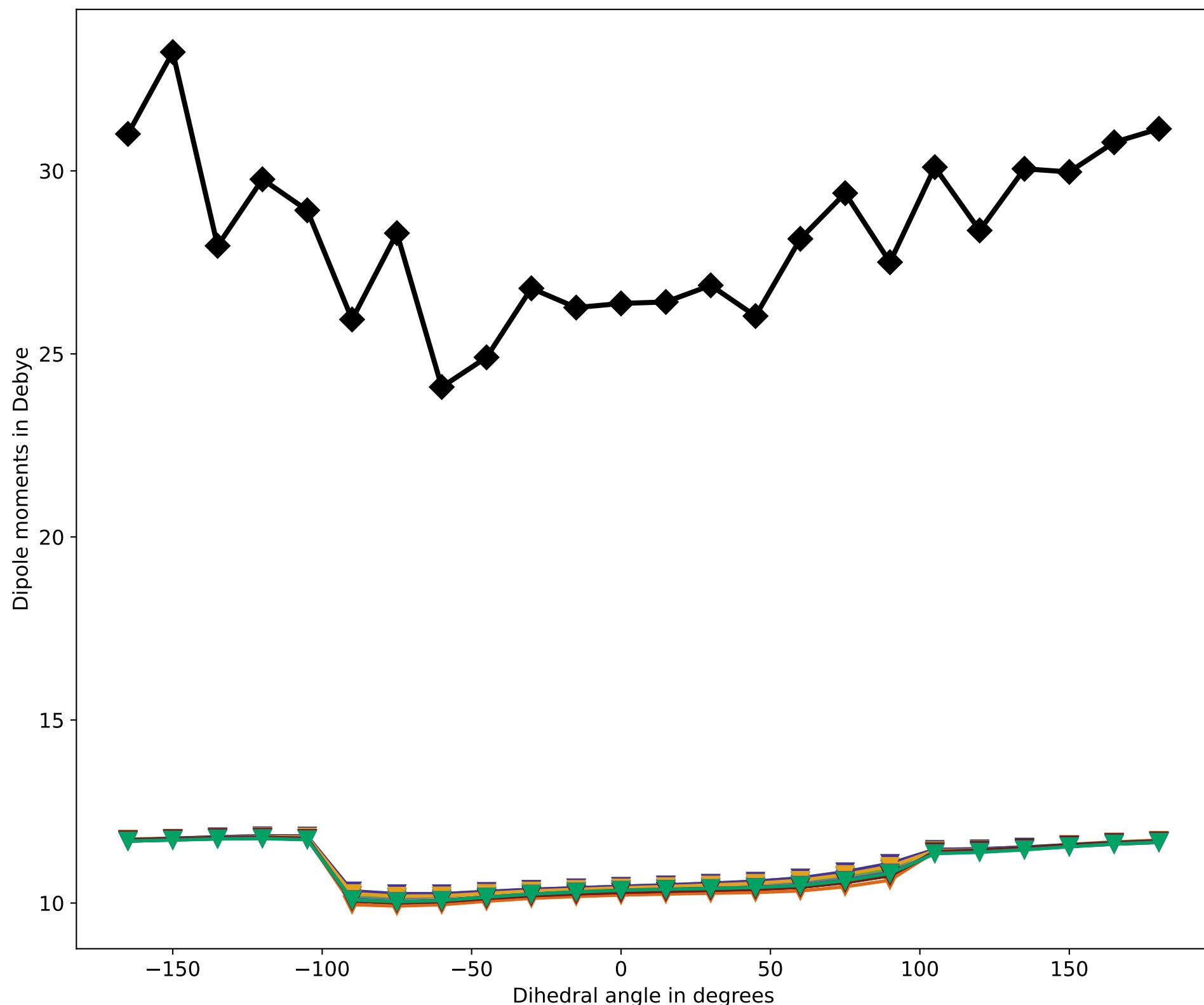
Charged molecule

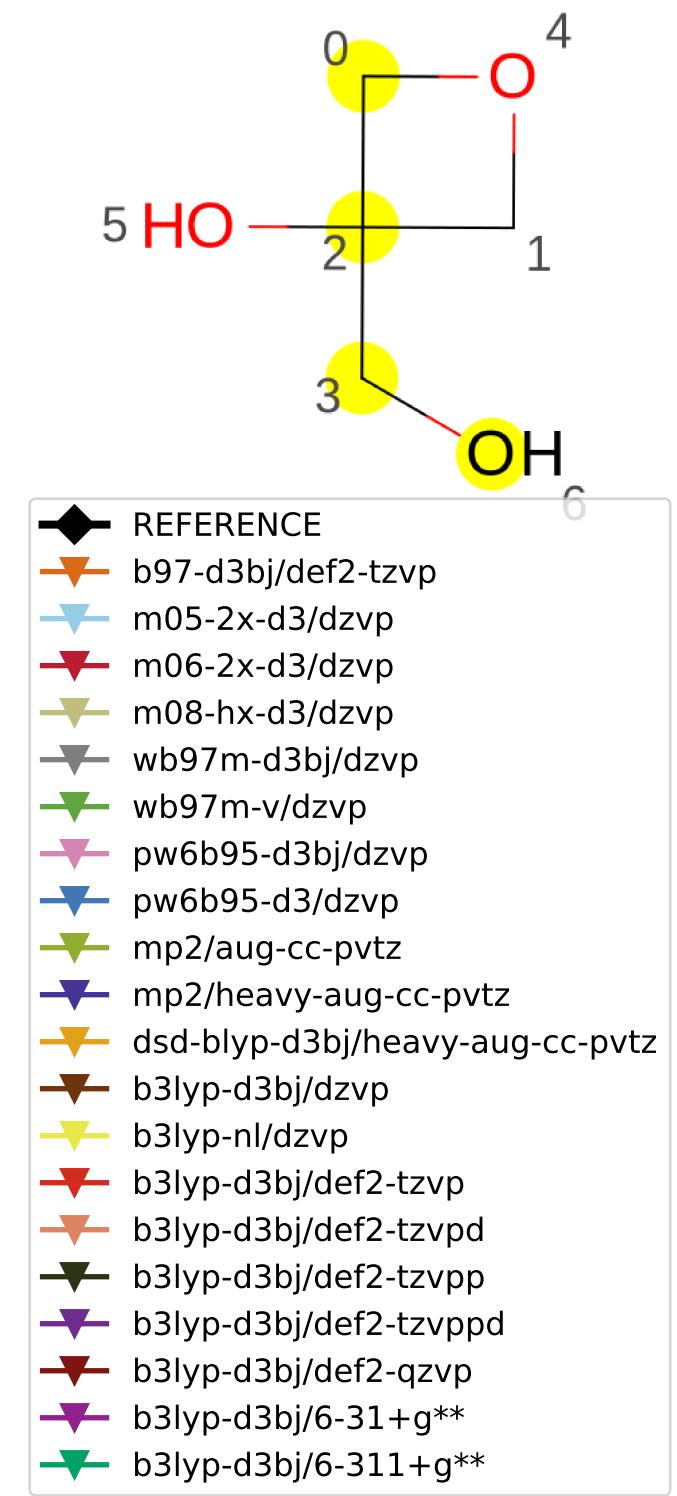
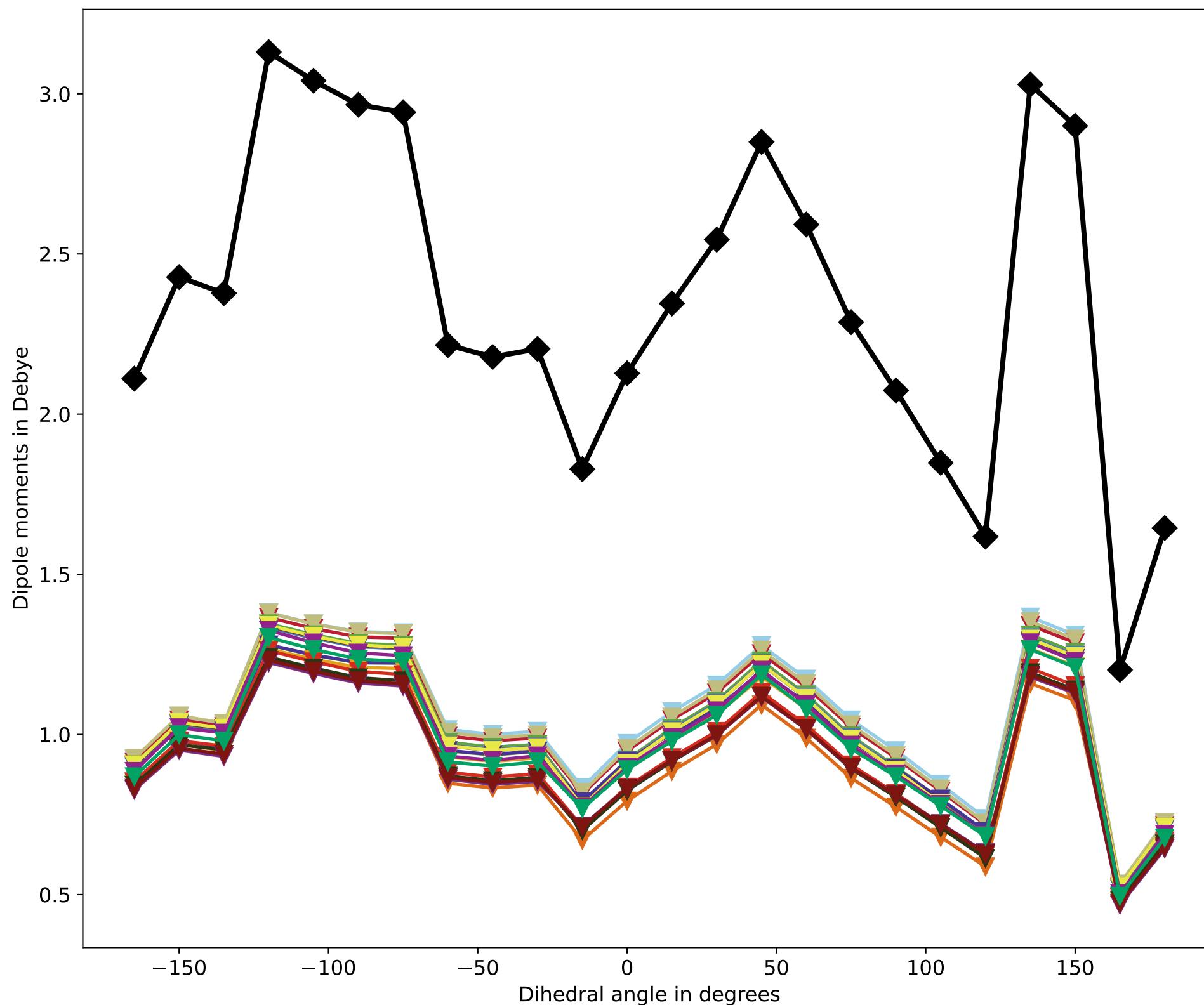


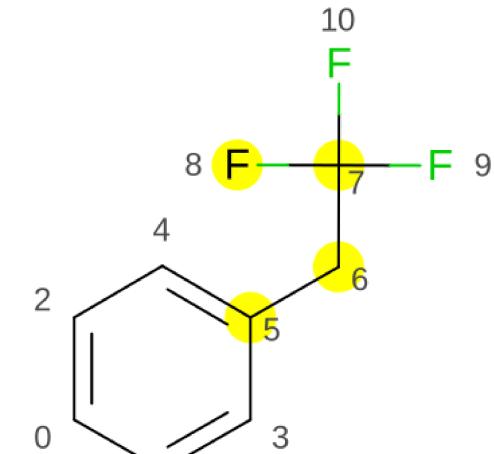
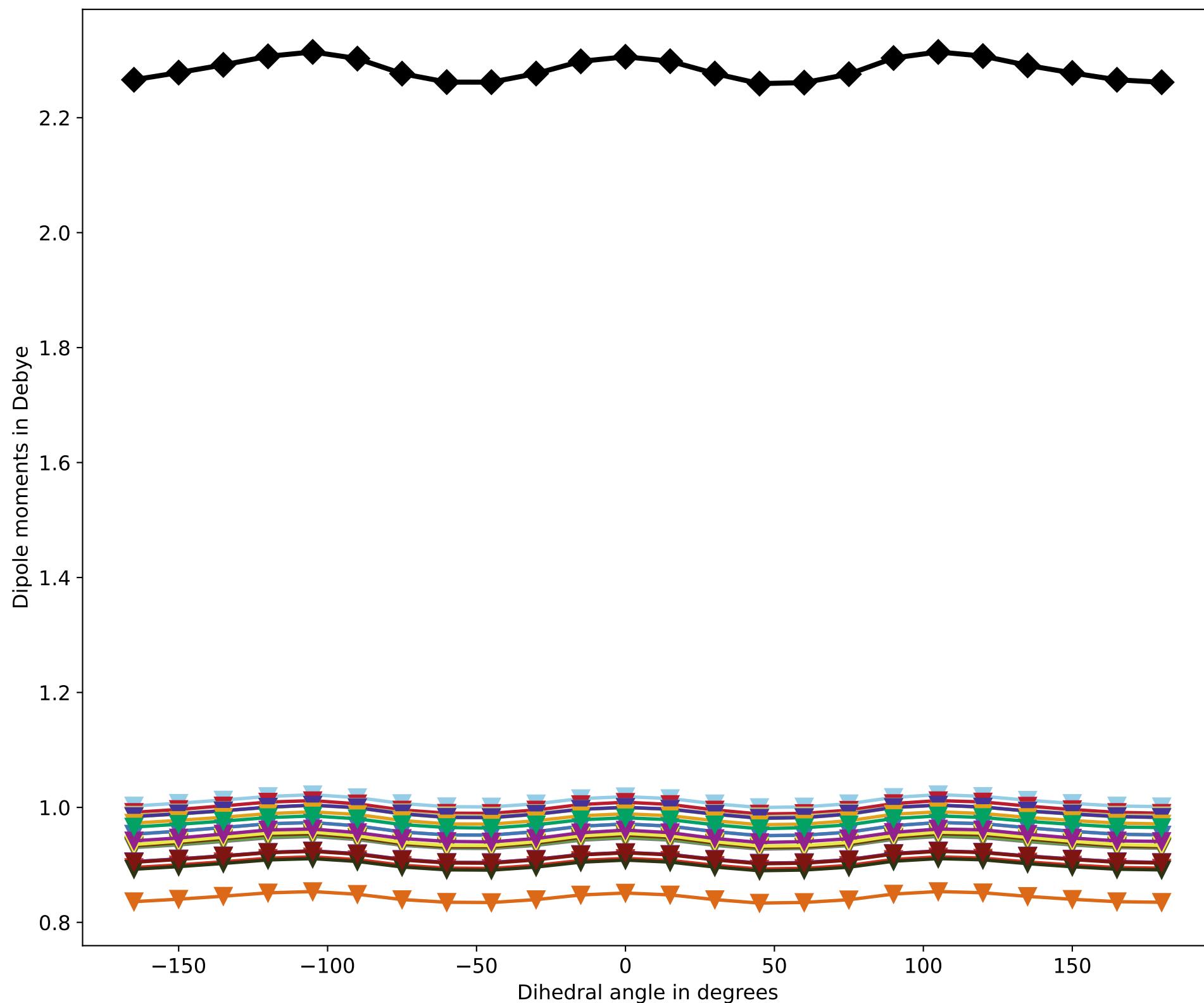
Charged molecule



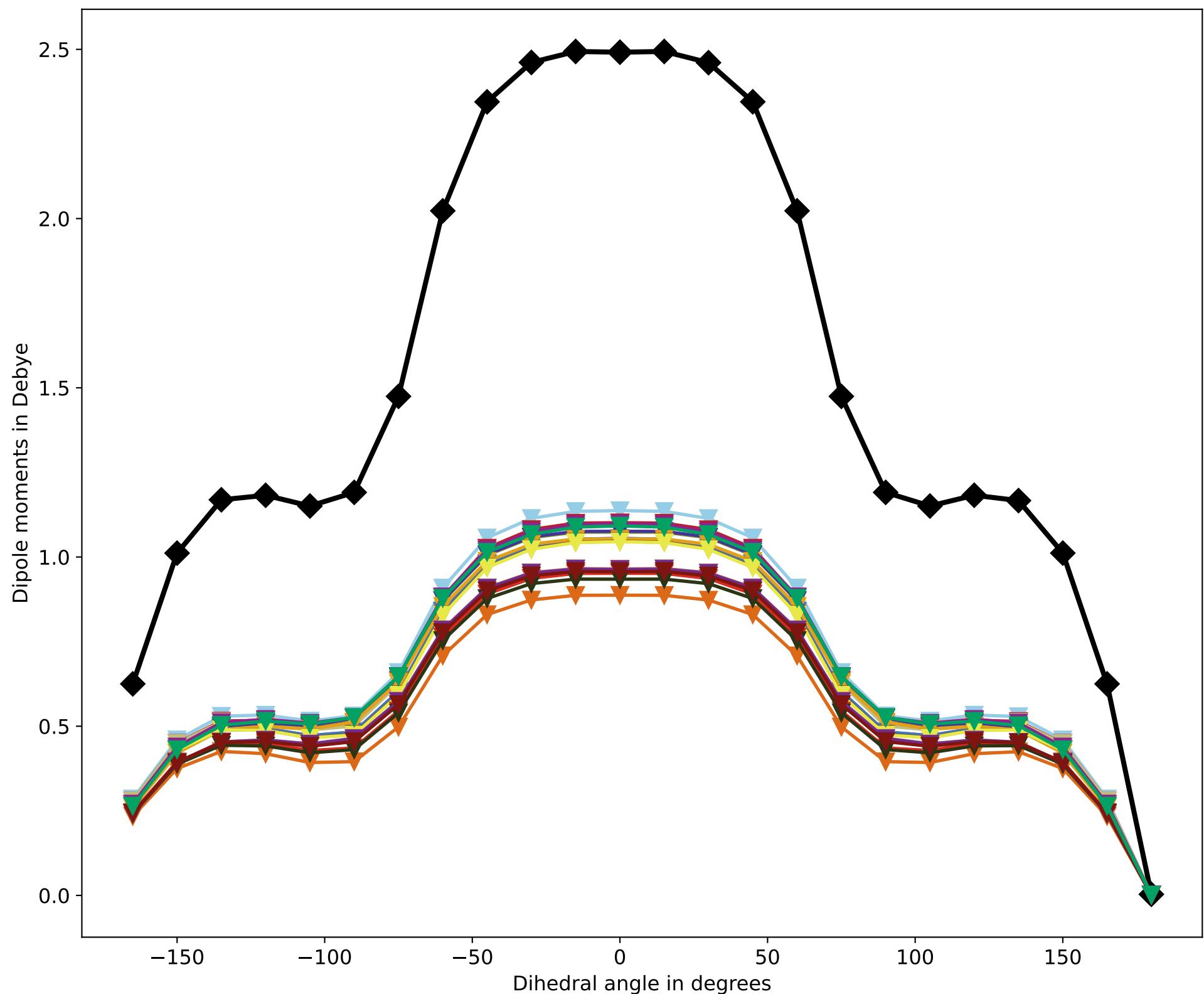
Charged molecule

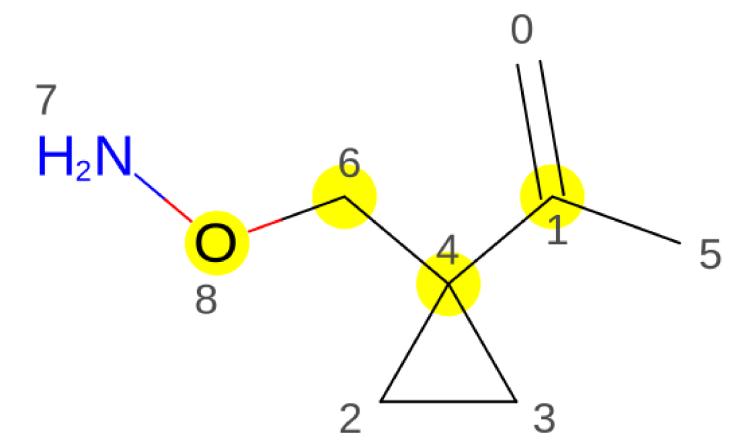
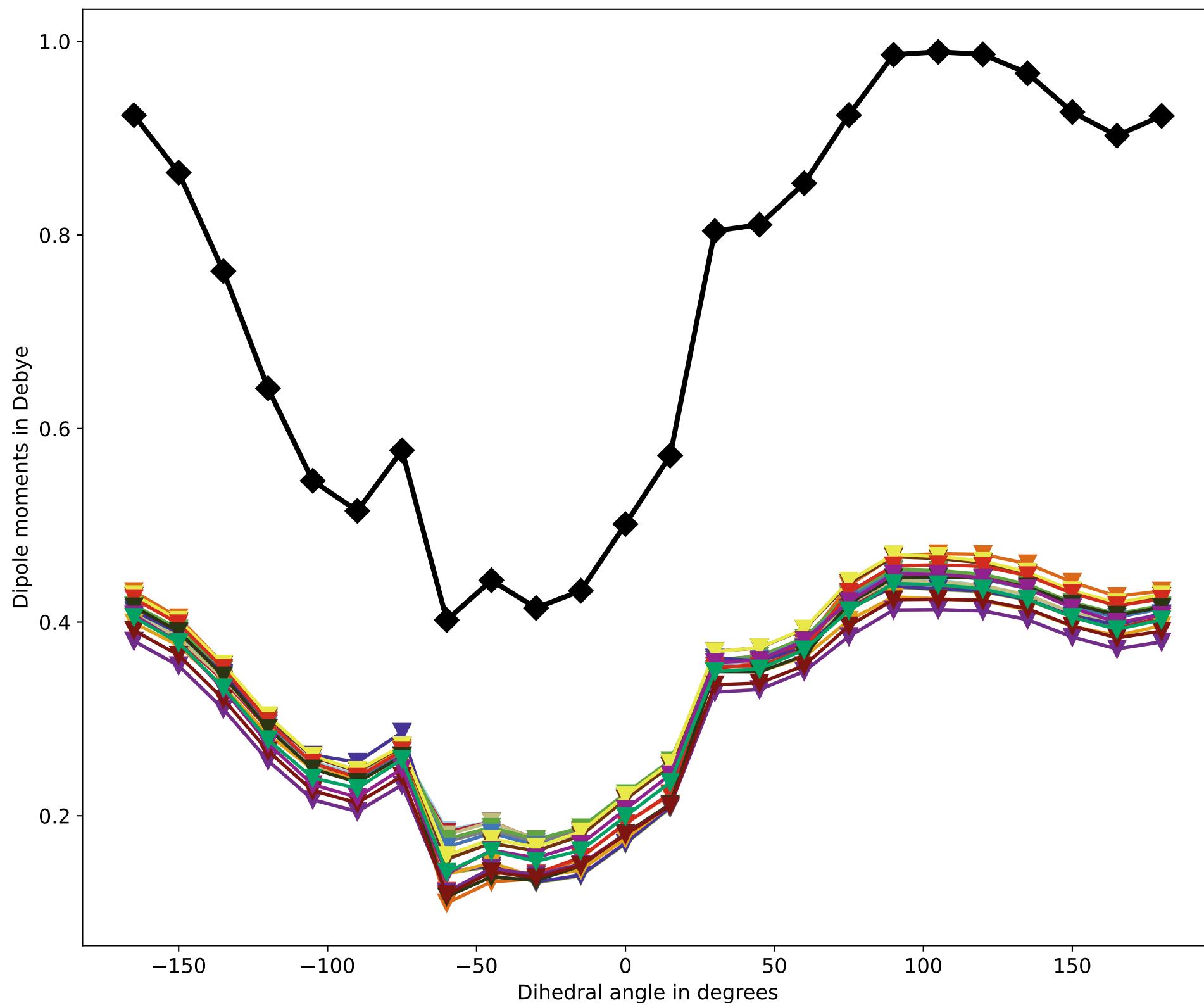




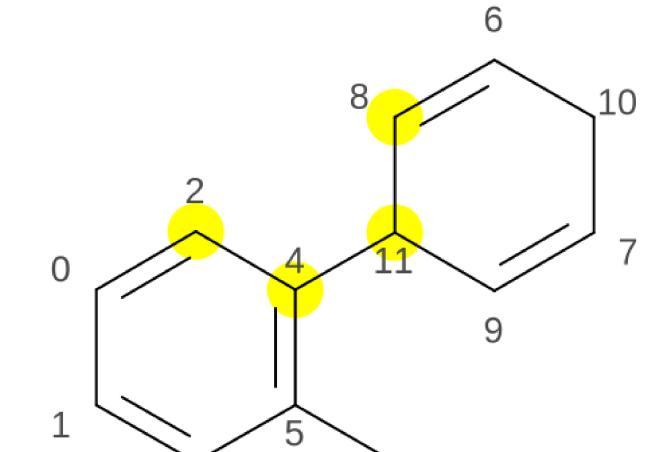
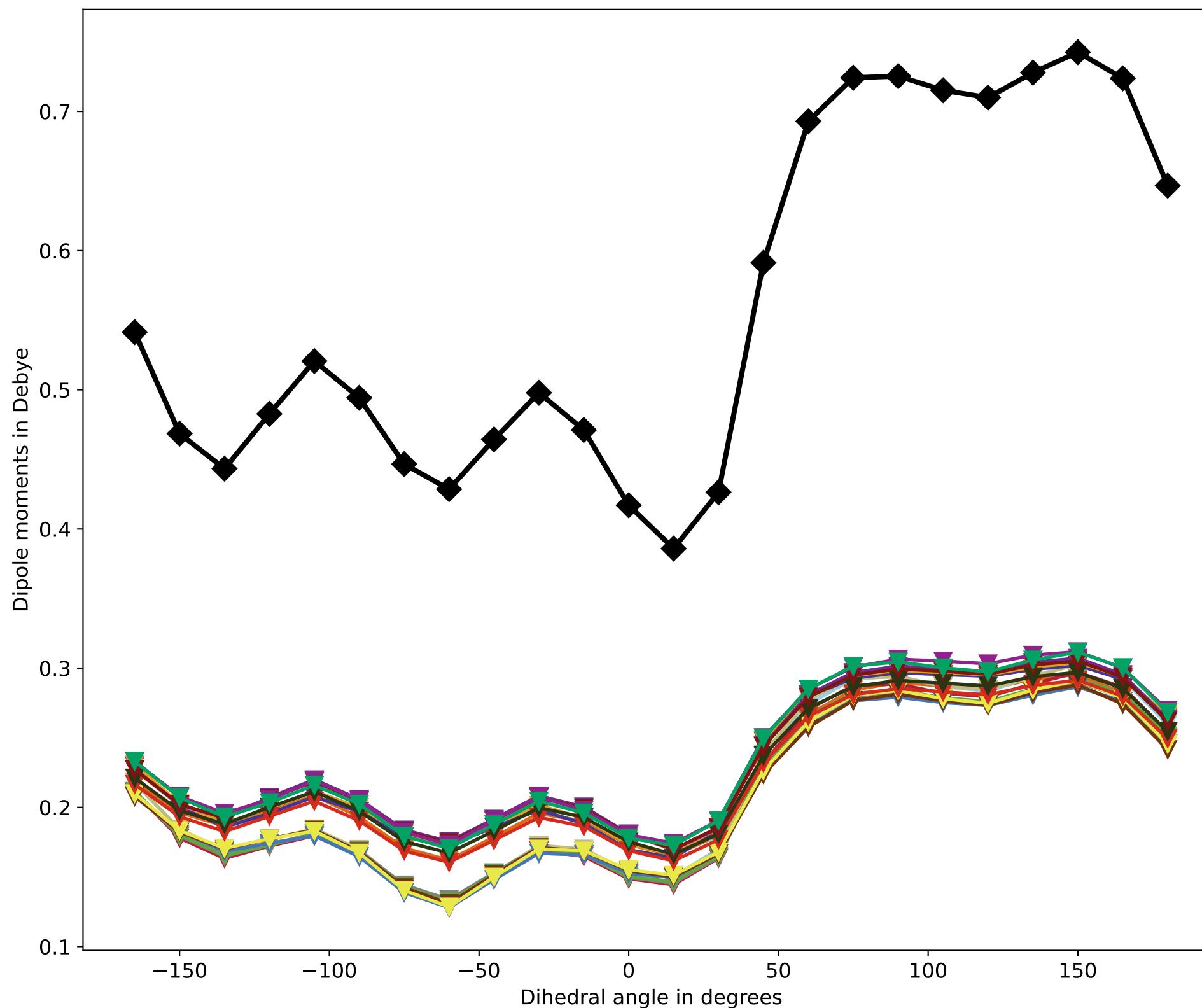


- ◆ REFERENCE
- ▼ b97-d3bj/def2-tzvp
- △ m05-2x-d3/dzvp
- ▲ m06-2x-d3/dzvp
- ▽ m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- ▲ wb97m-v/dzvp
- ▼ pw6b95-d3bj/dzvp
- ▲ pw6b95-d3/dzvp
- ▽ mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- ▲ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ▼ b3lyp-d3bj/dzvp
- ▲ b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp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



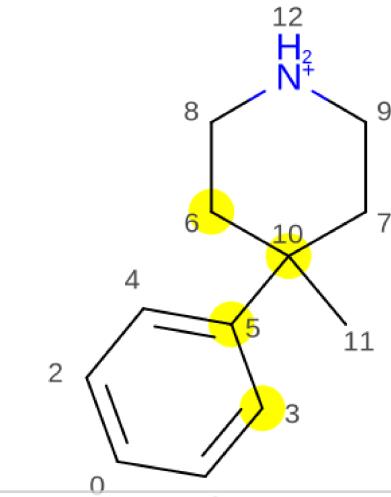
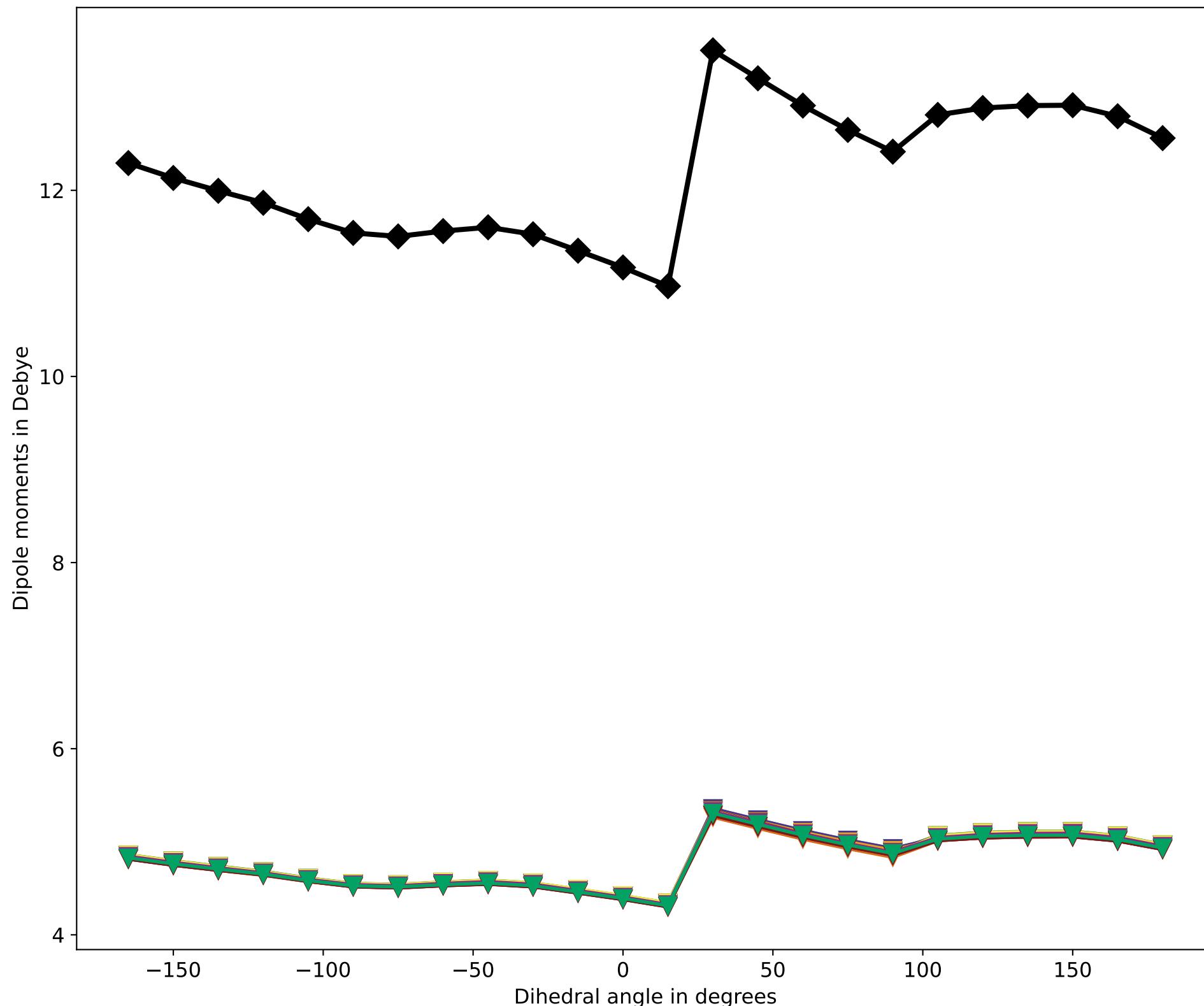


- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd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



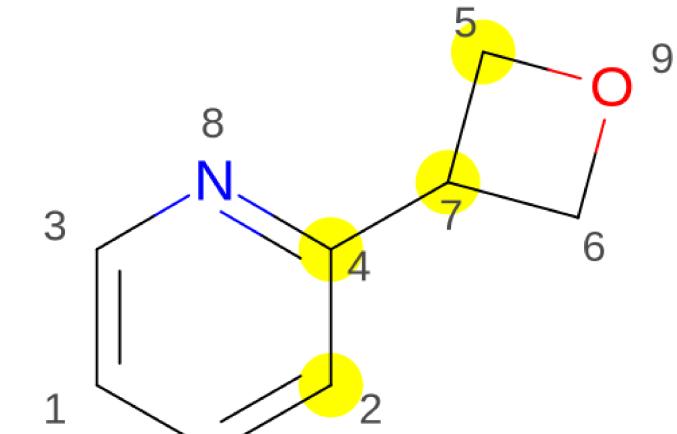
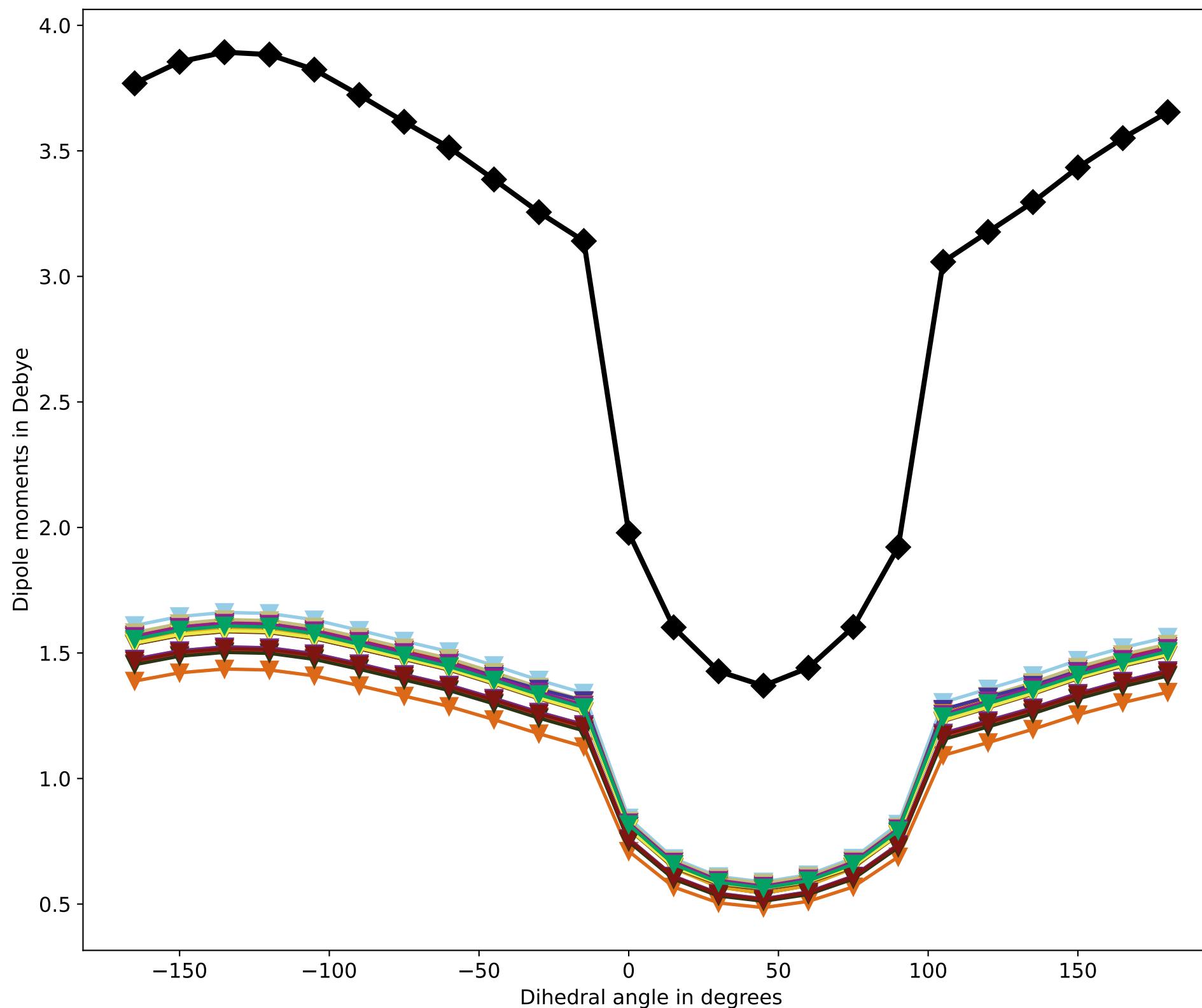
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

Charged molecule

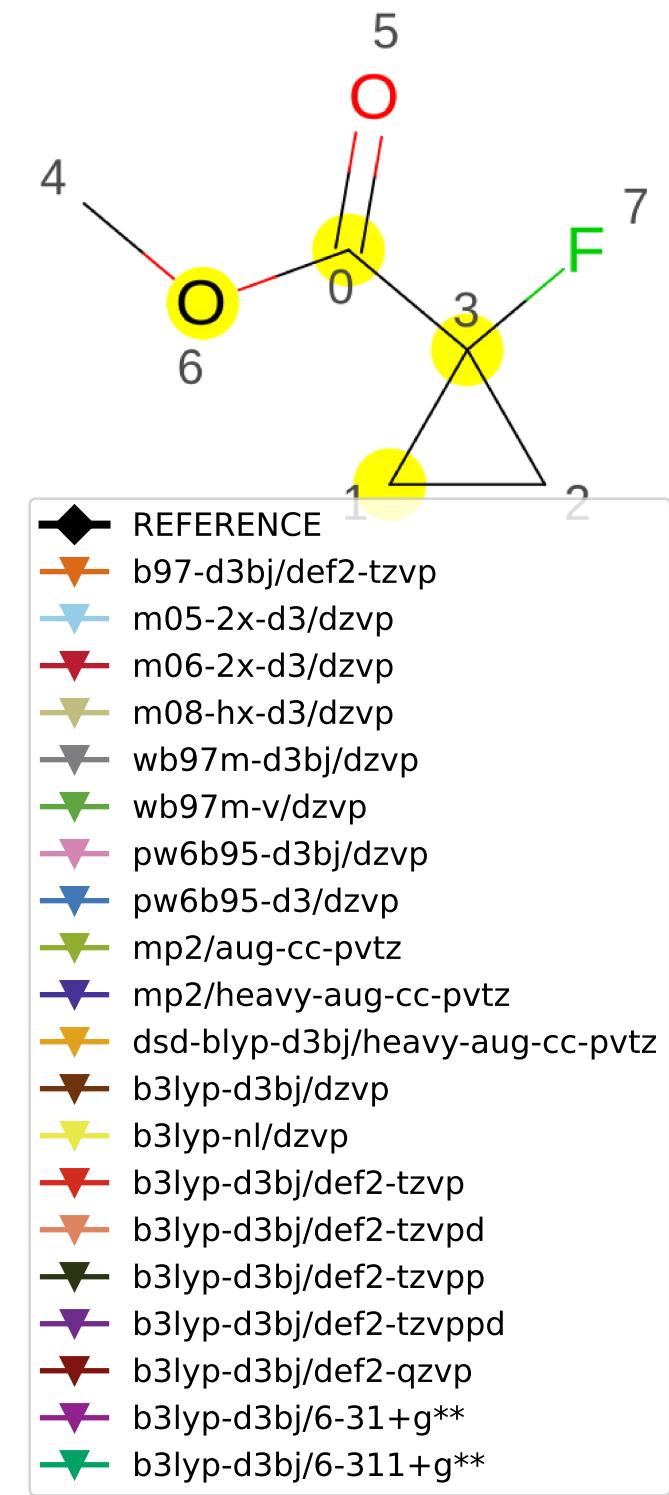
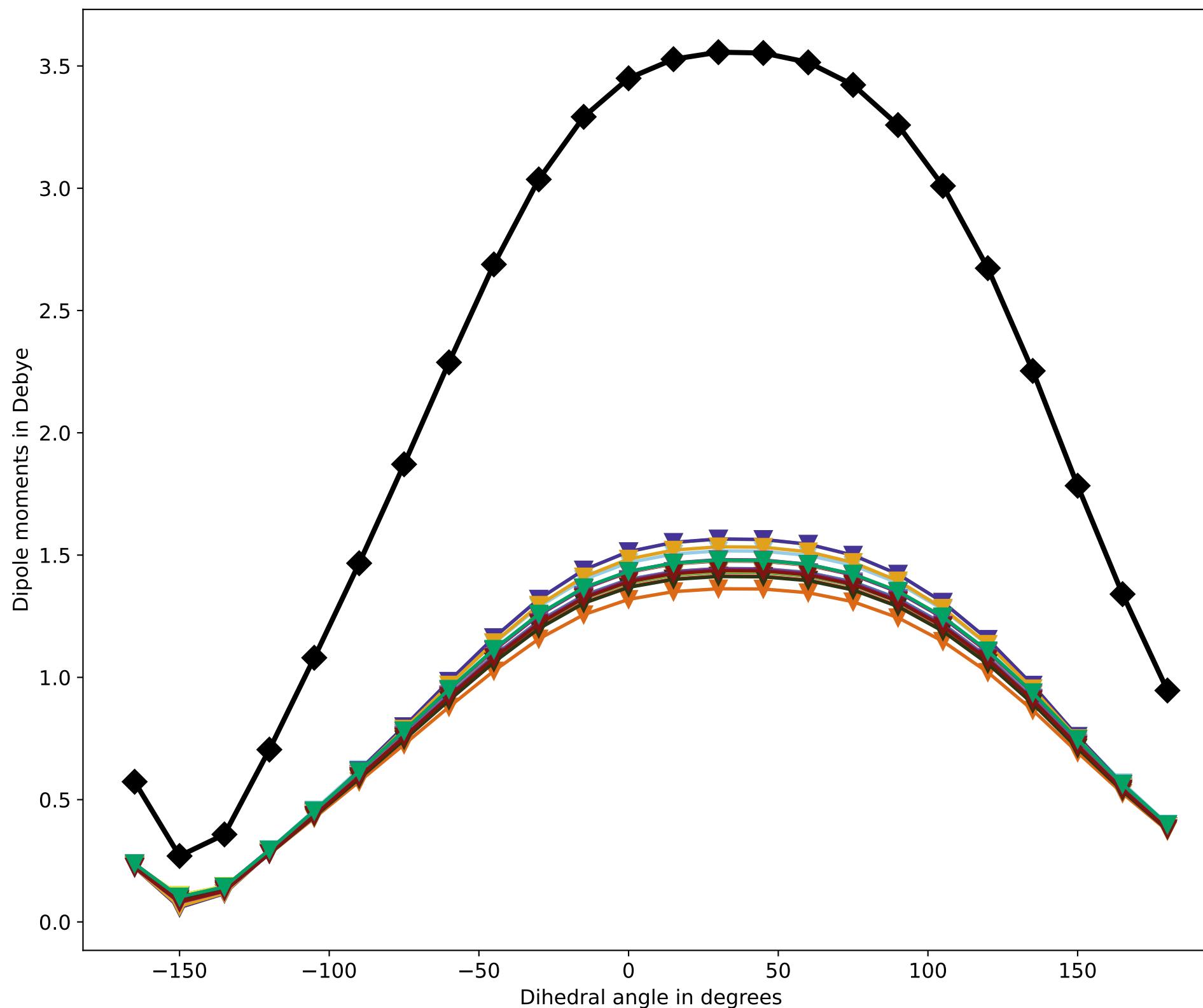


- REFERENCE 1

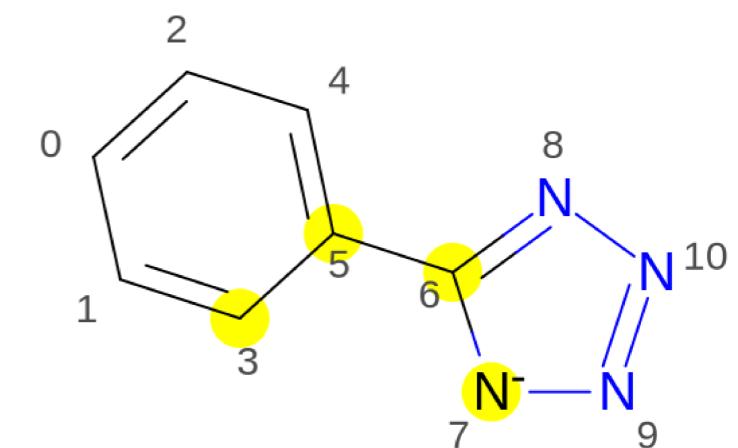
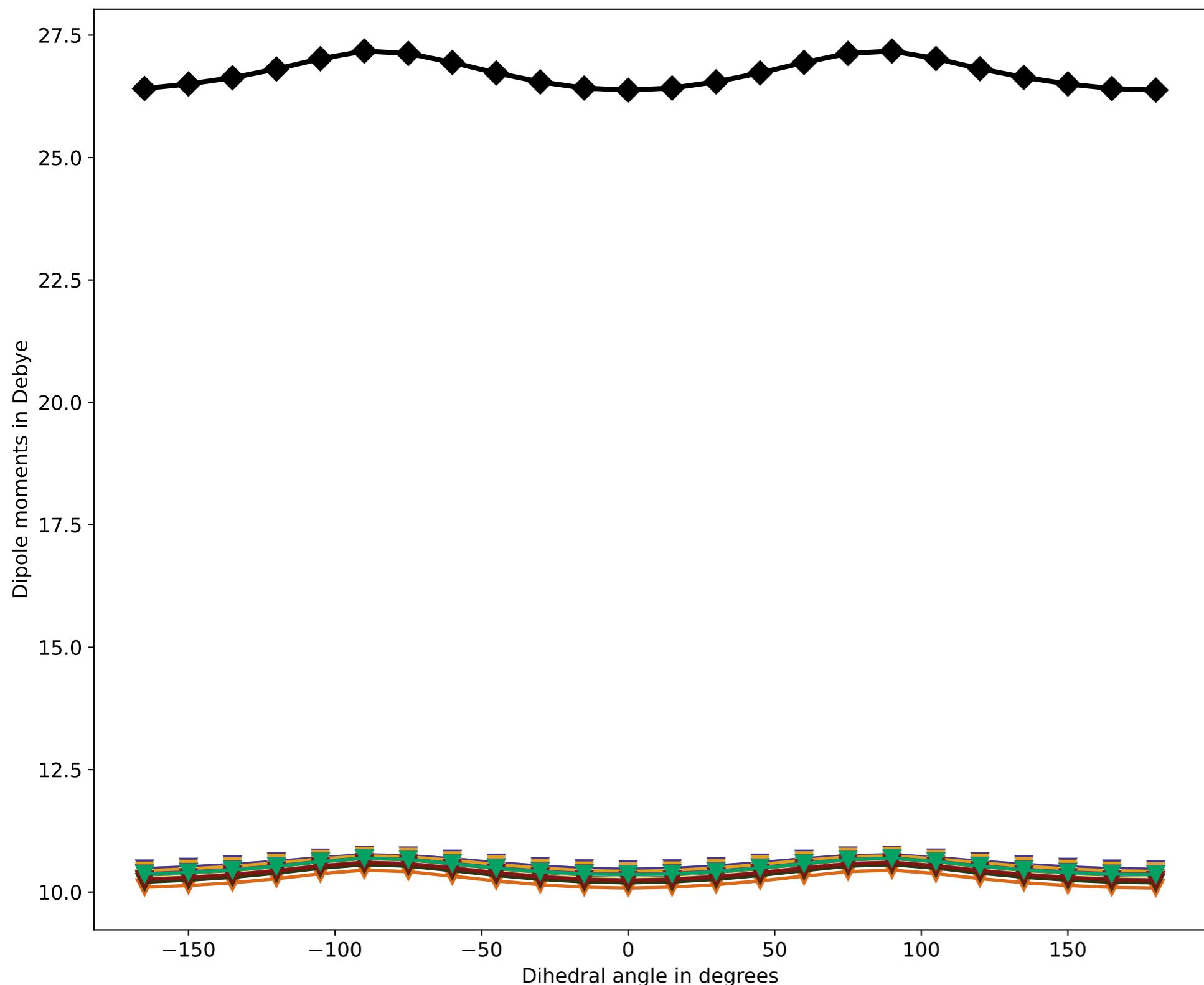
 -  b97-d3bj/def2-tzvp
 -  m05-2x-d3/dzvp
 -  m06-2x-d3/dzvp
 -  m08-hx-d3/dzvp
 -  wb97m-d3bj/dzvp
 -  wb97m-v/dzvp
 -  pw6b95-d3bj/dzvp
 -  pw6b95-d3/dzvp
 -  mp2/aug-cc-pvtz
 -  mp2/heavy-aug-cc-pvtz
 -  dsd-bllyp-d3bj/heavy-aug-cc-pvtz
 -  b3lyp-d3bj/dzvp
 -  b3lyp-nl/dzvp
 -  b3lyp-d3bj/def2-tzvp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



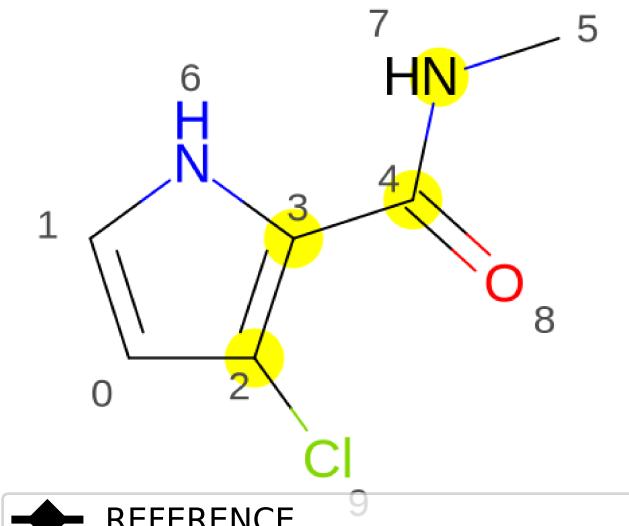
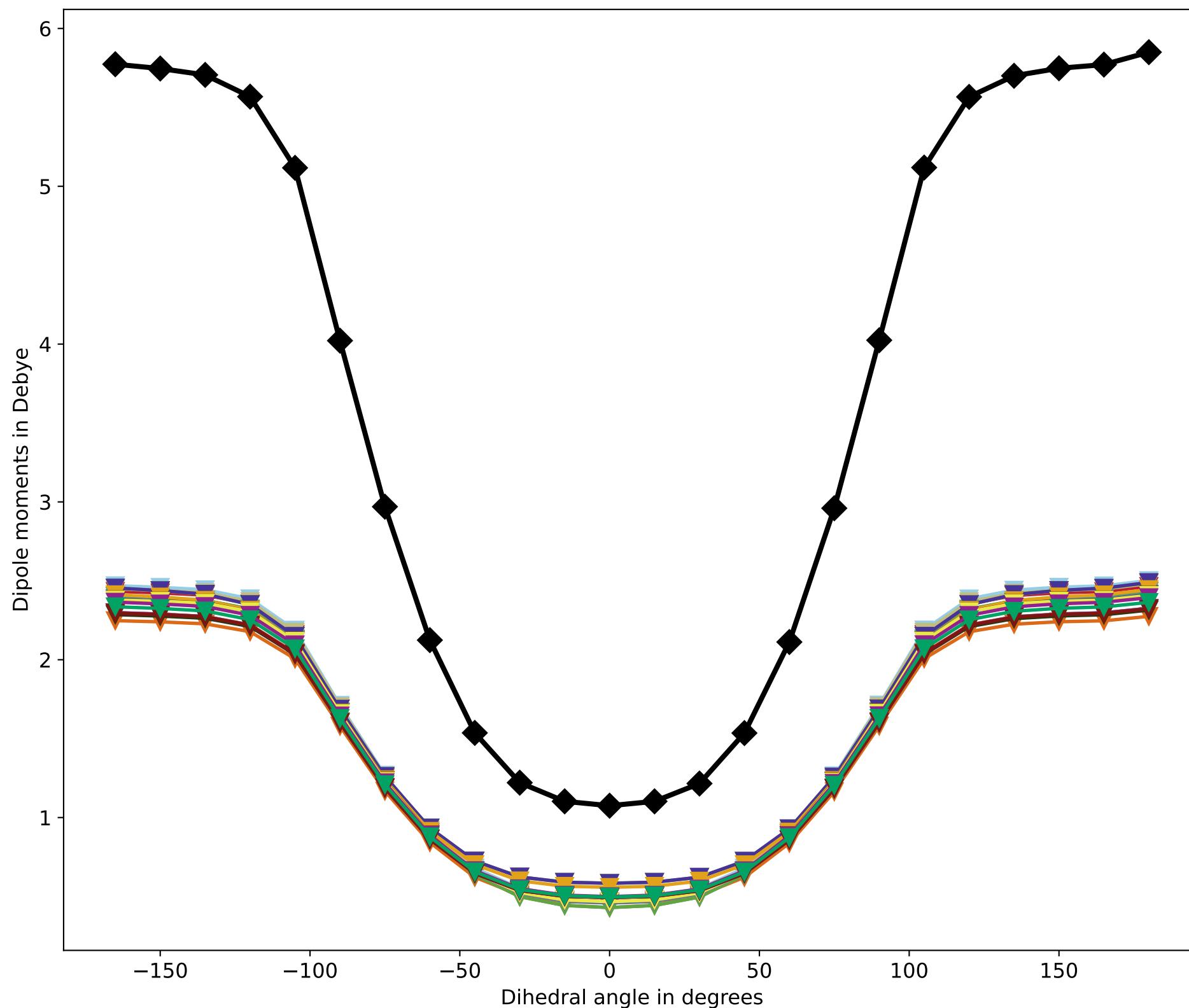
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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



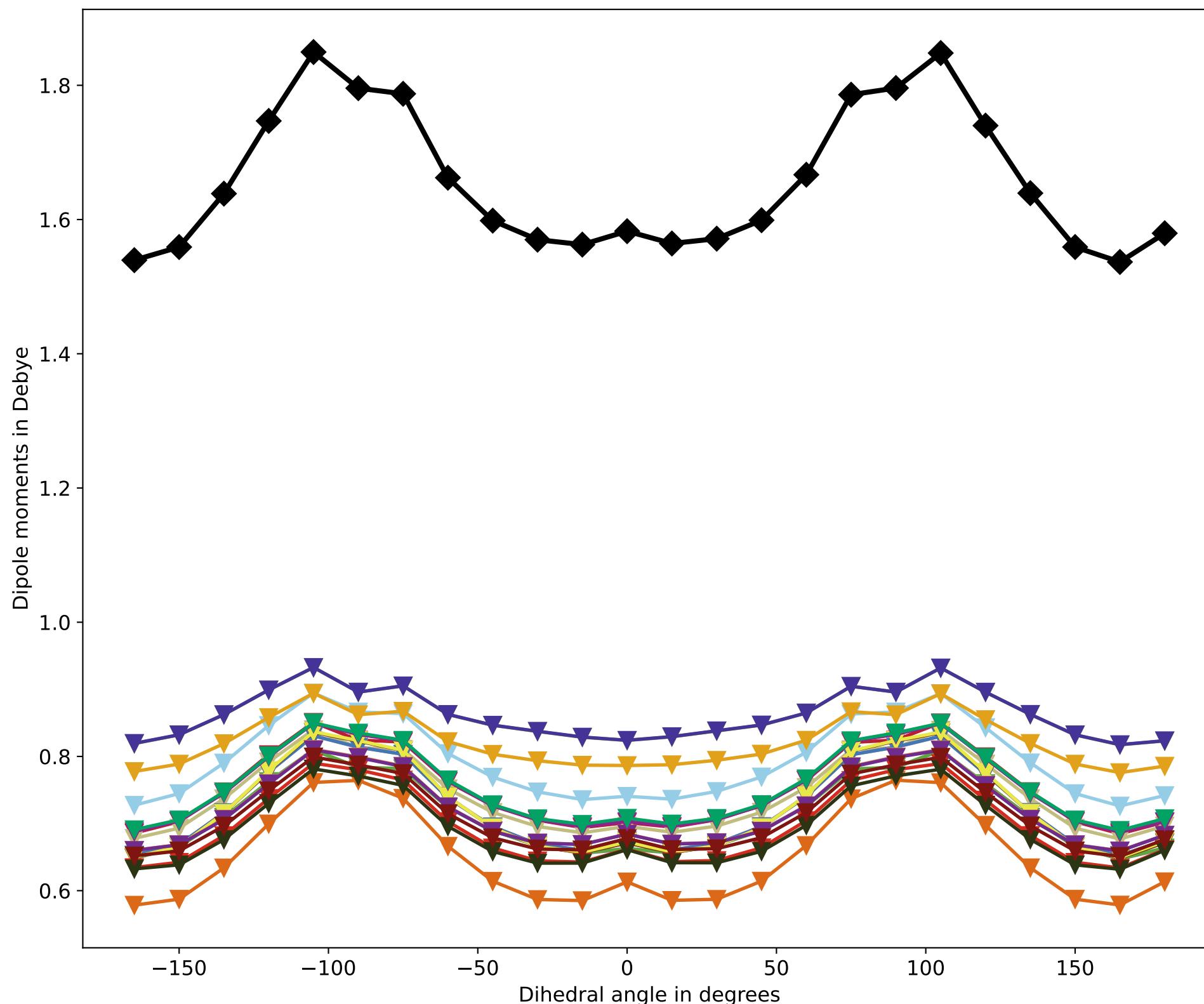
Charged molecule

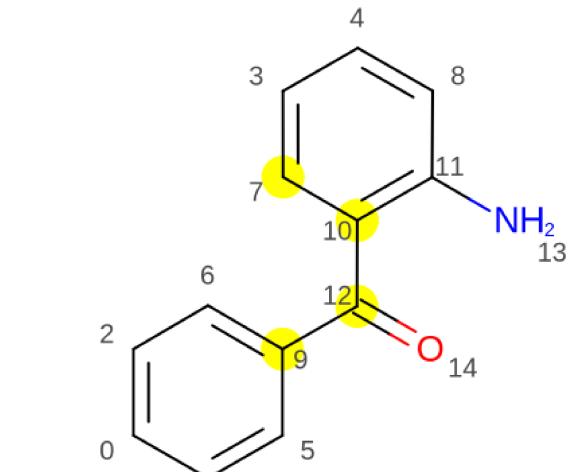
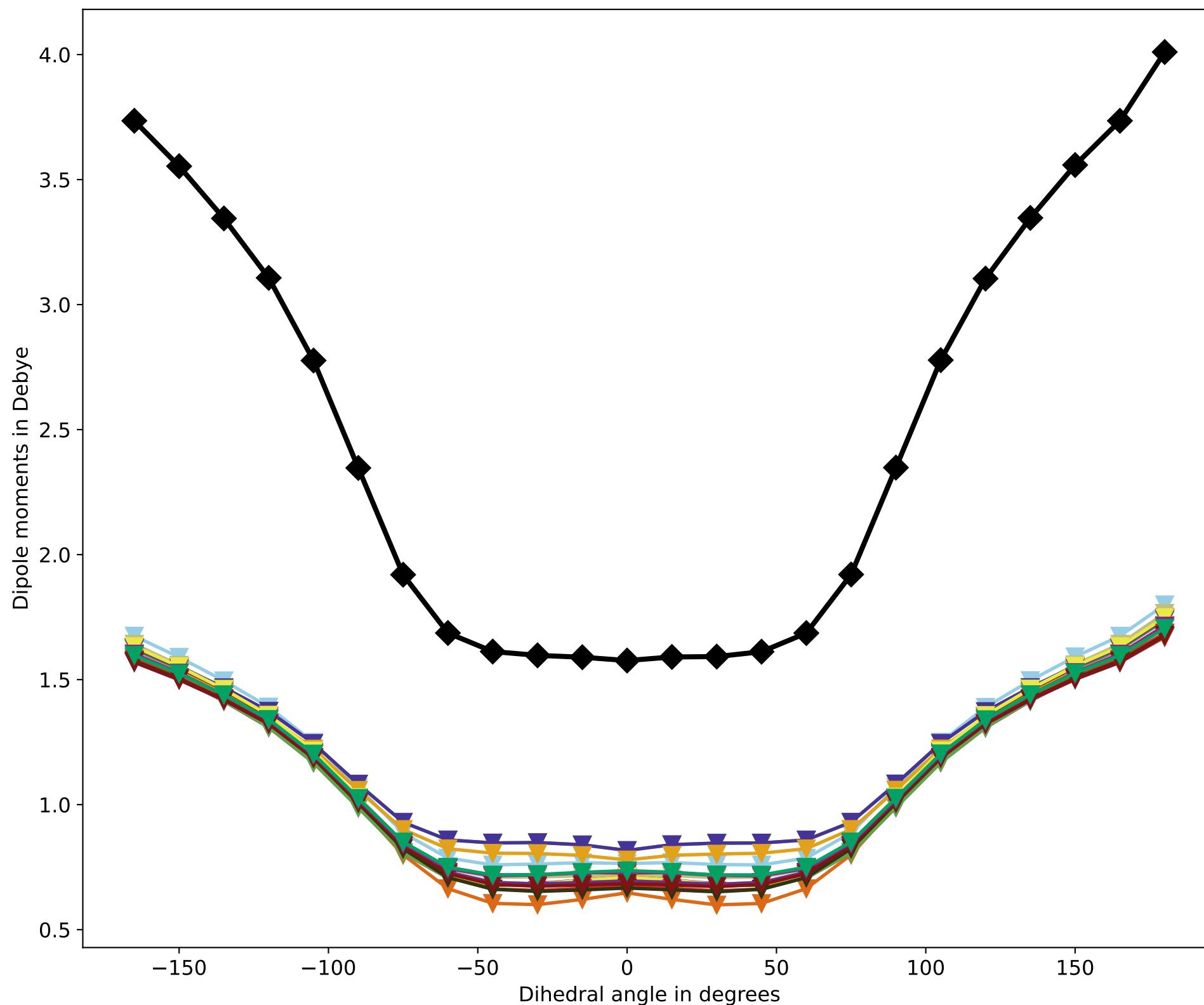


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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



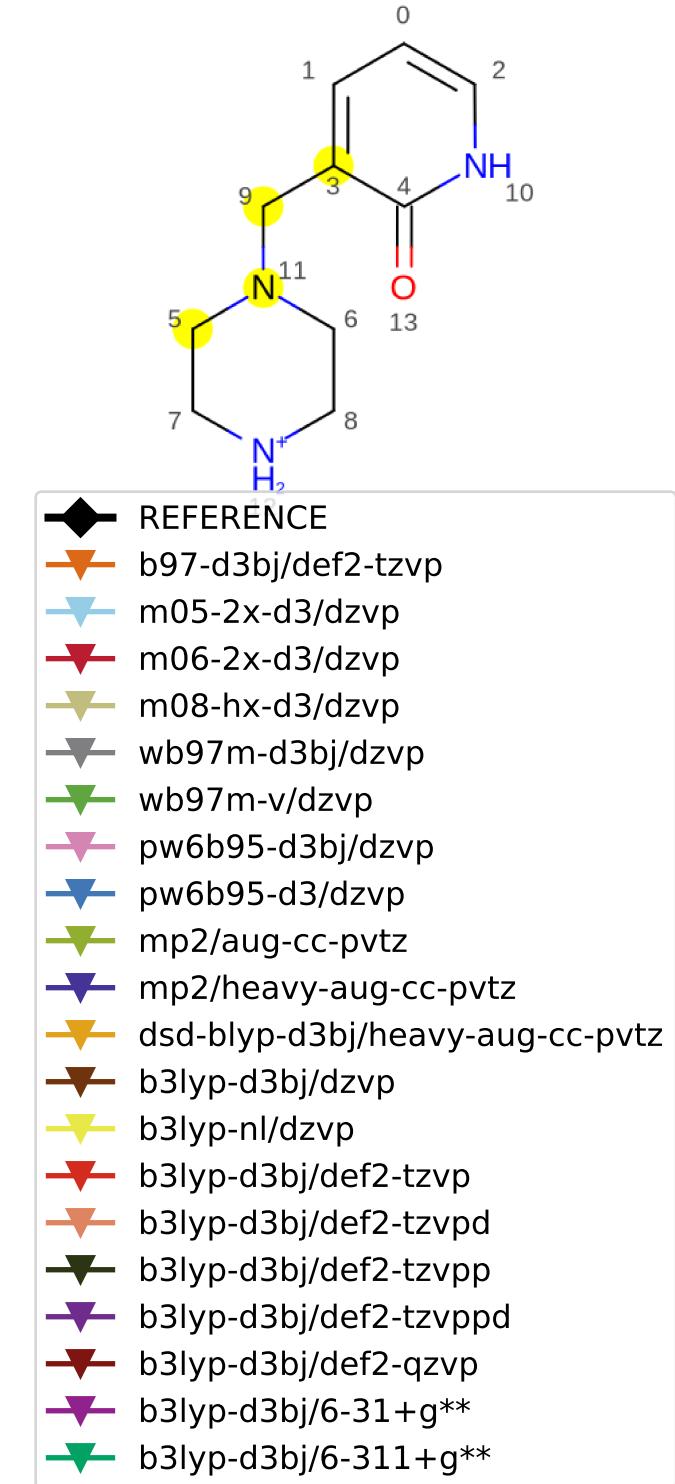
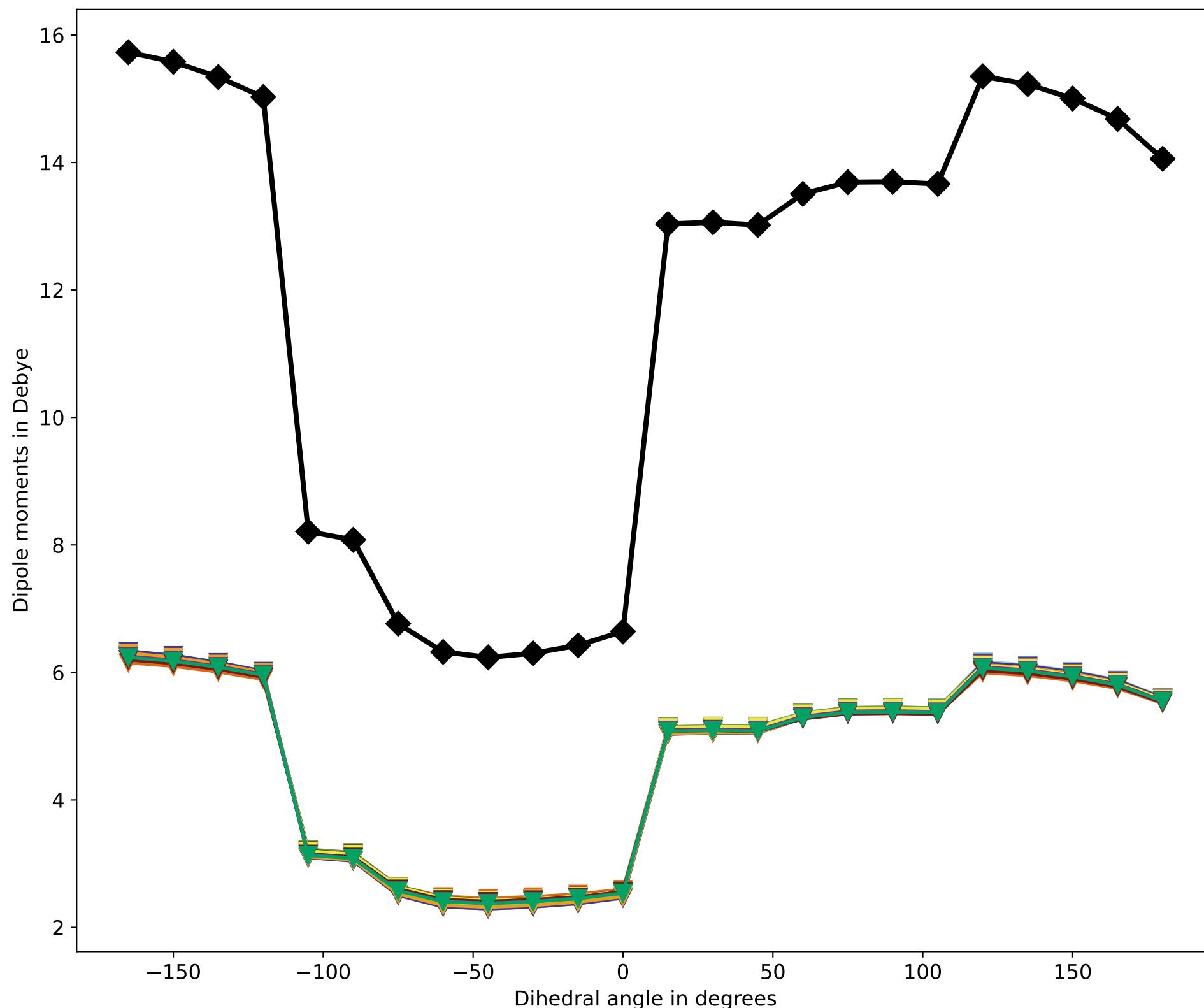
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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



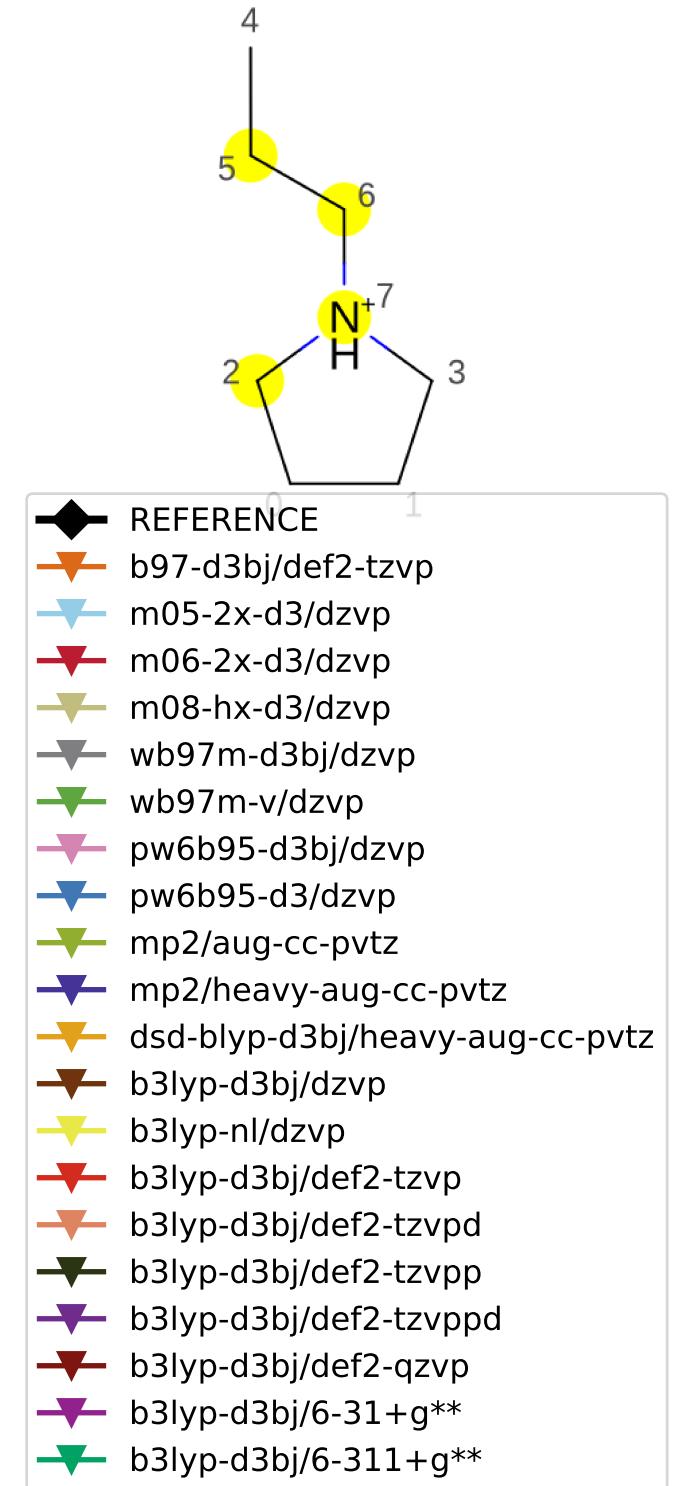
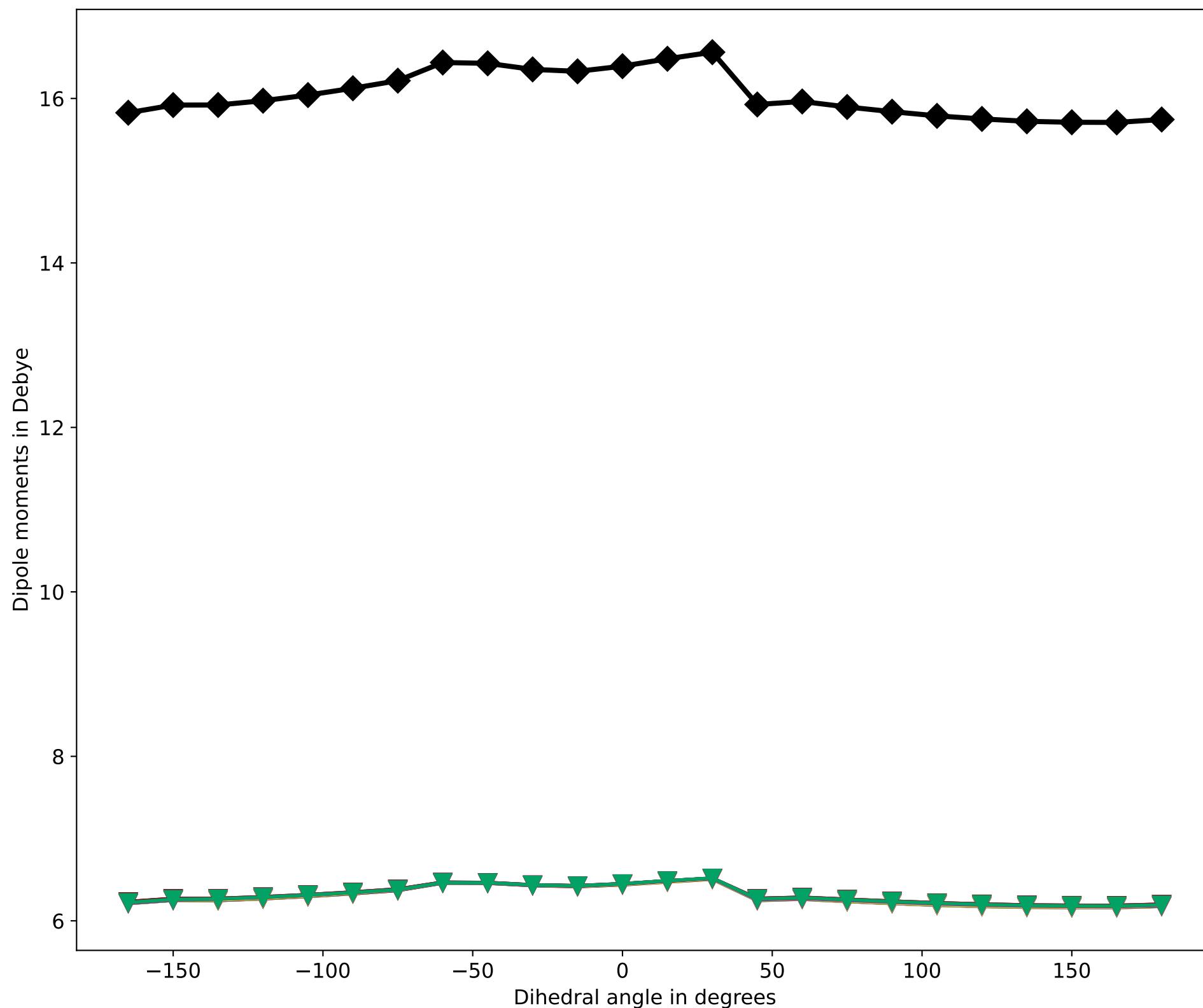


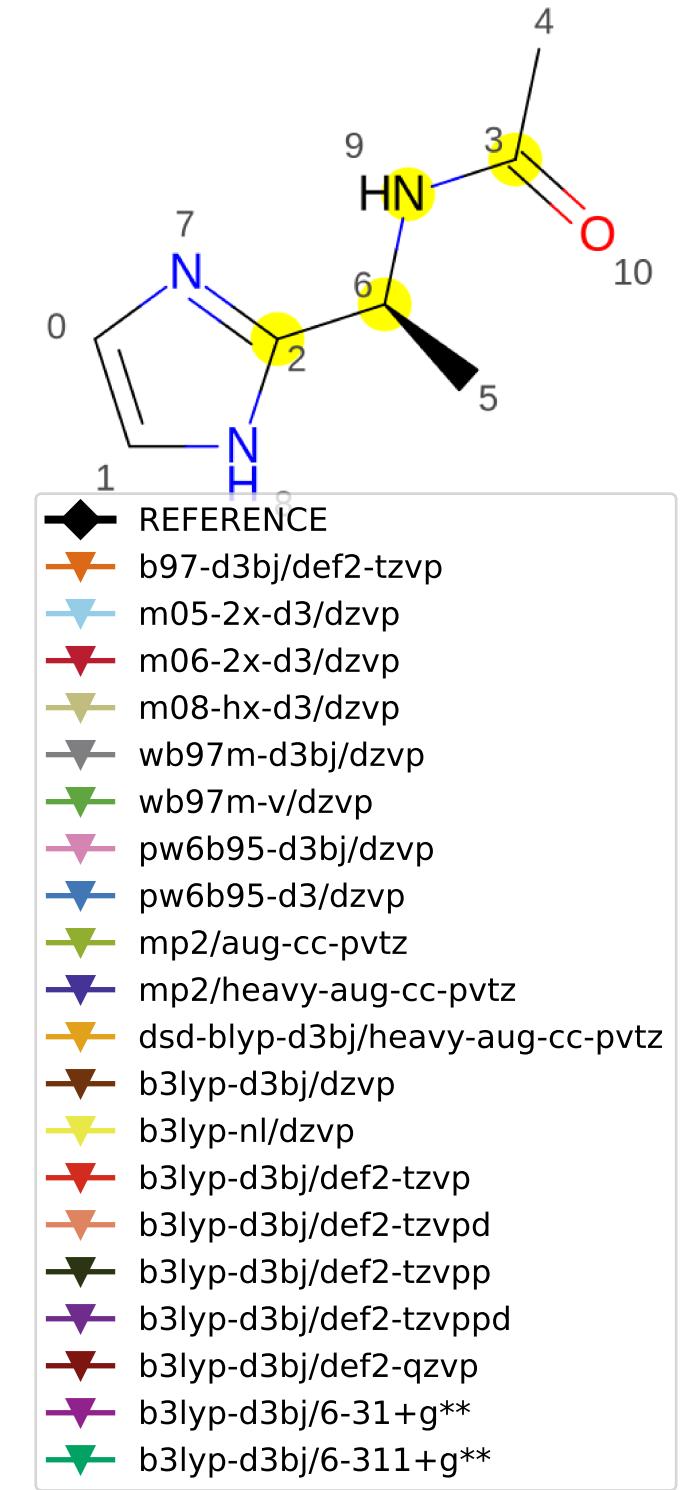
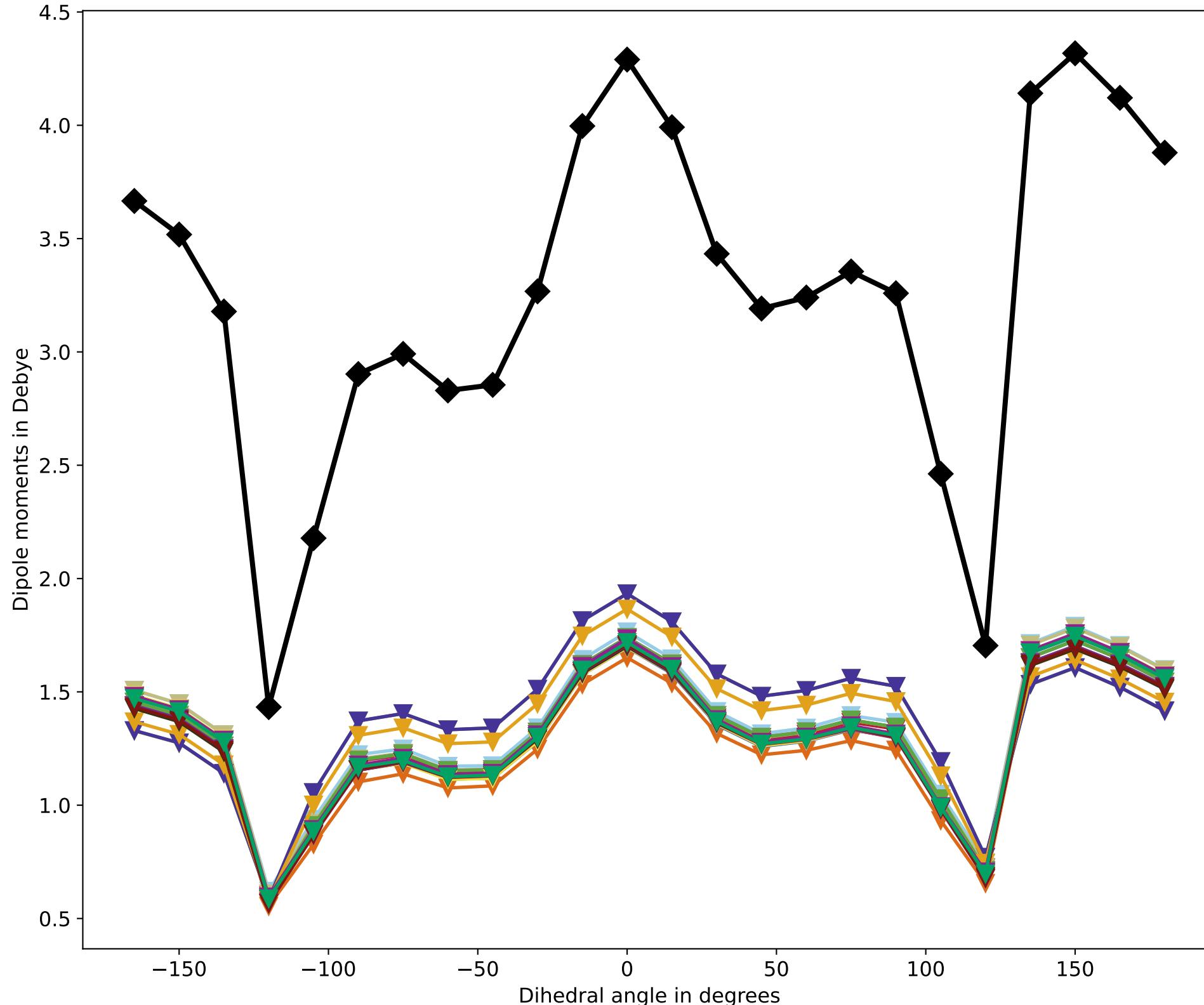
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

Charged molecule

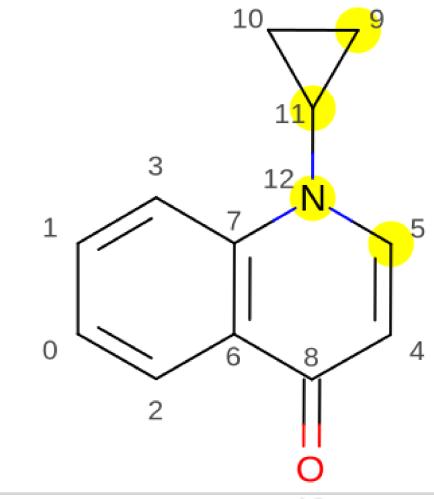
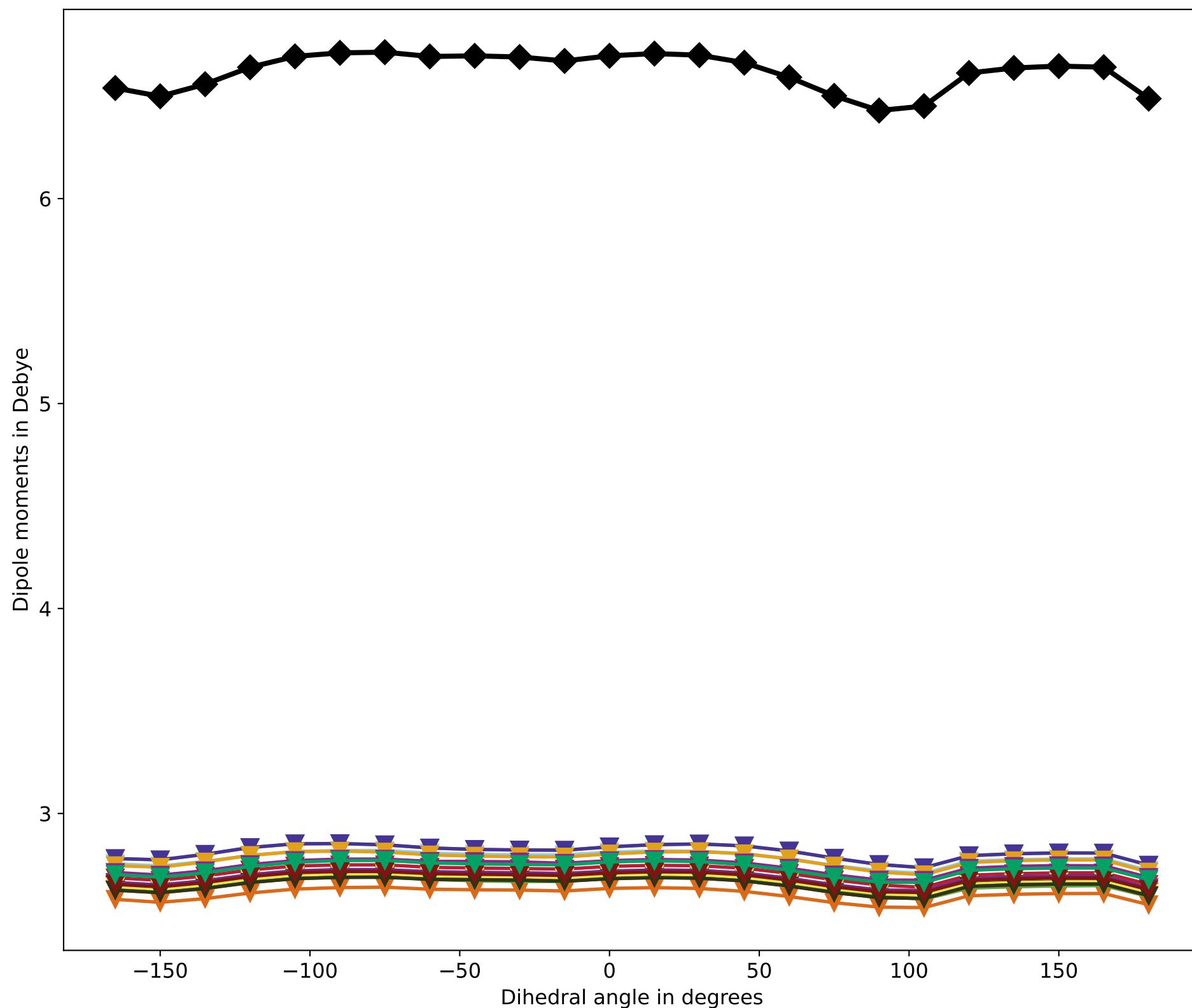


Charged molecule

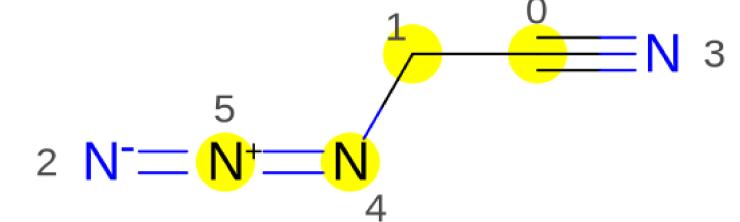
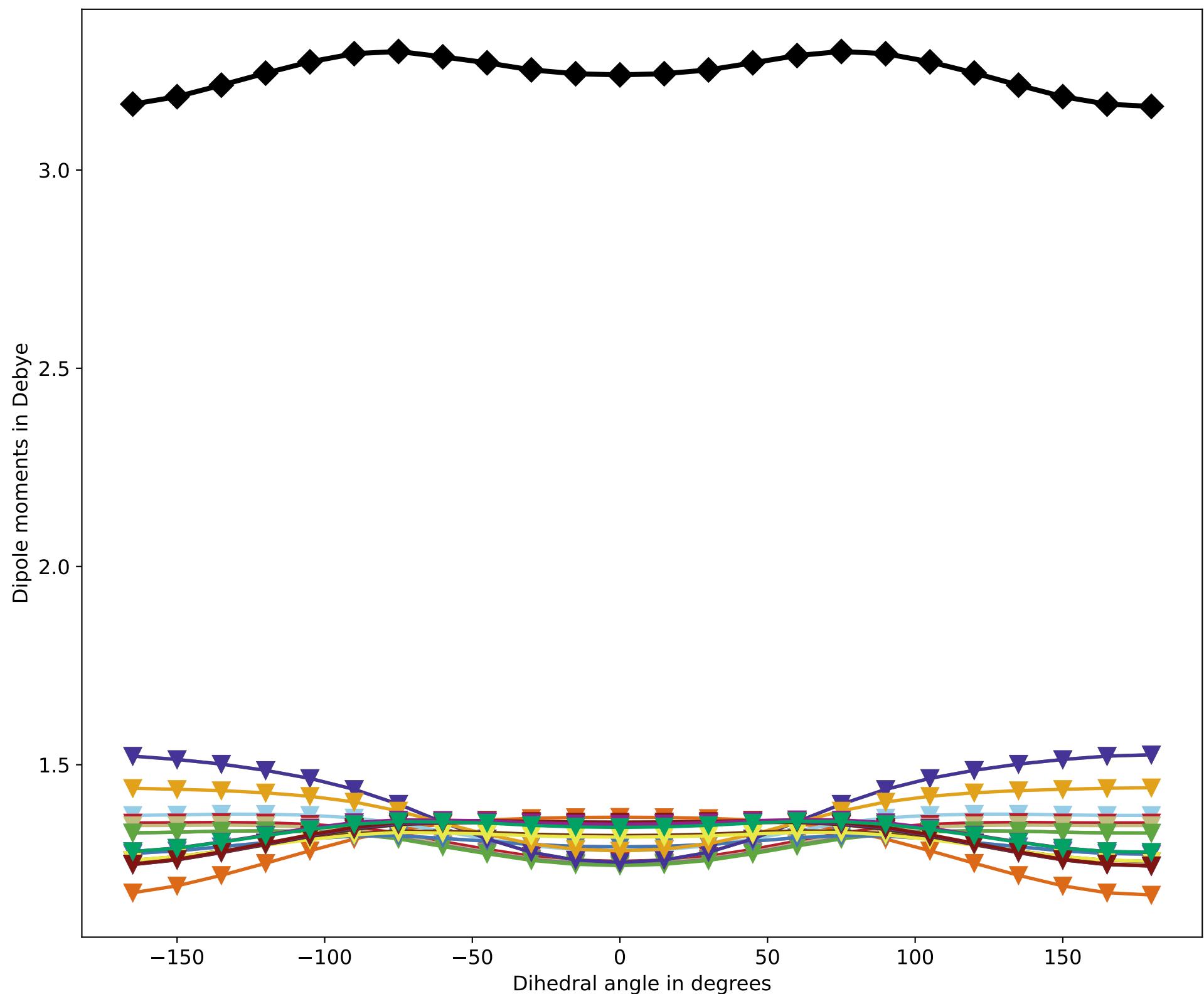




Neutral molecule

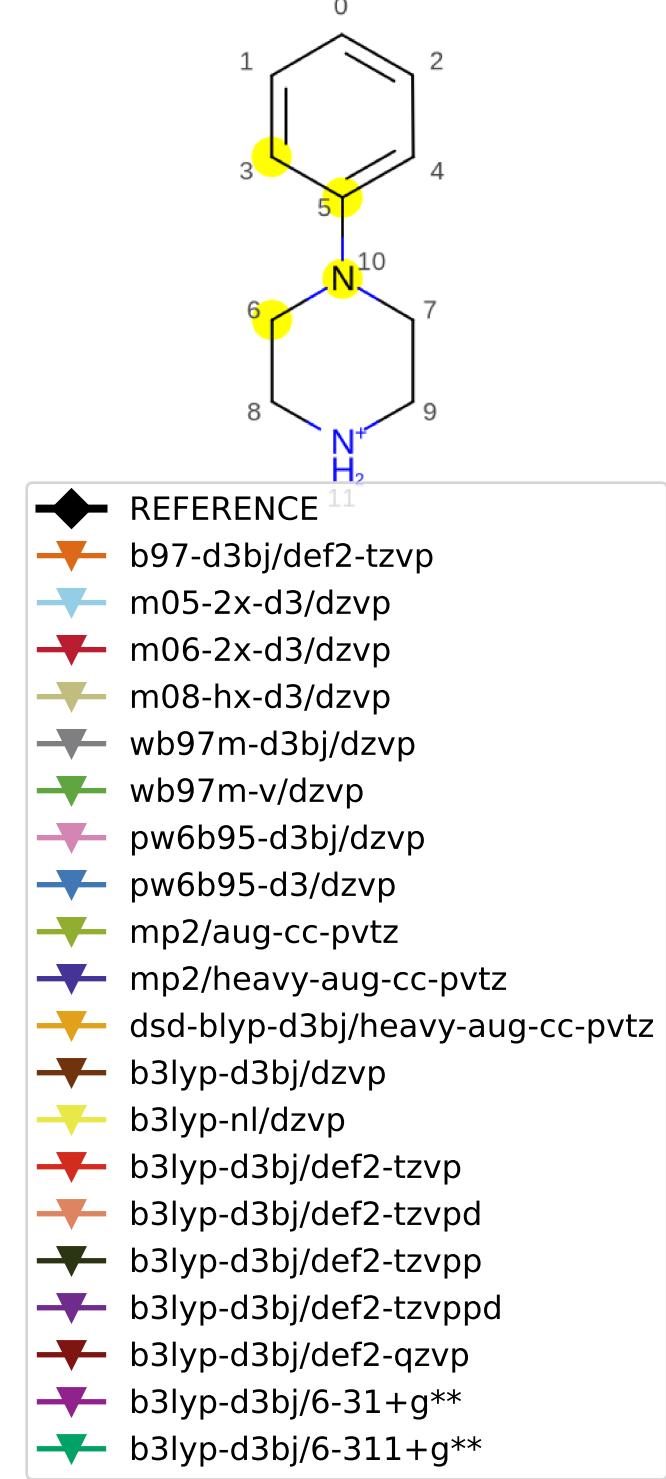
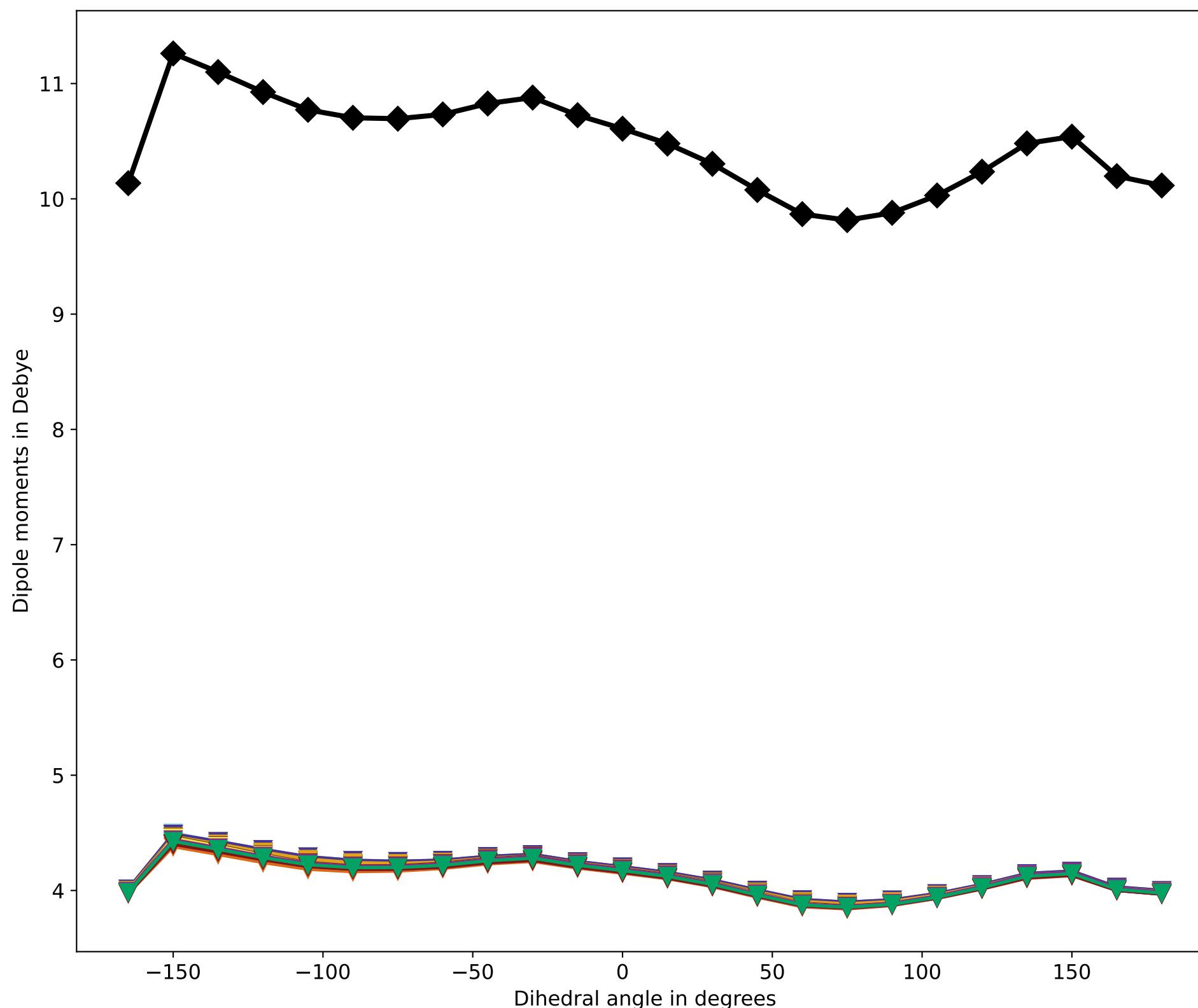


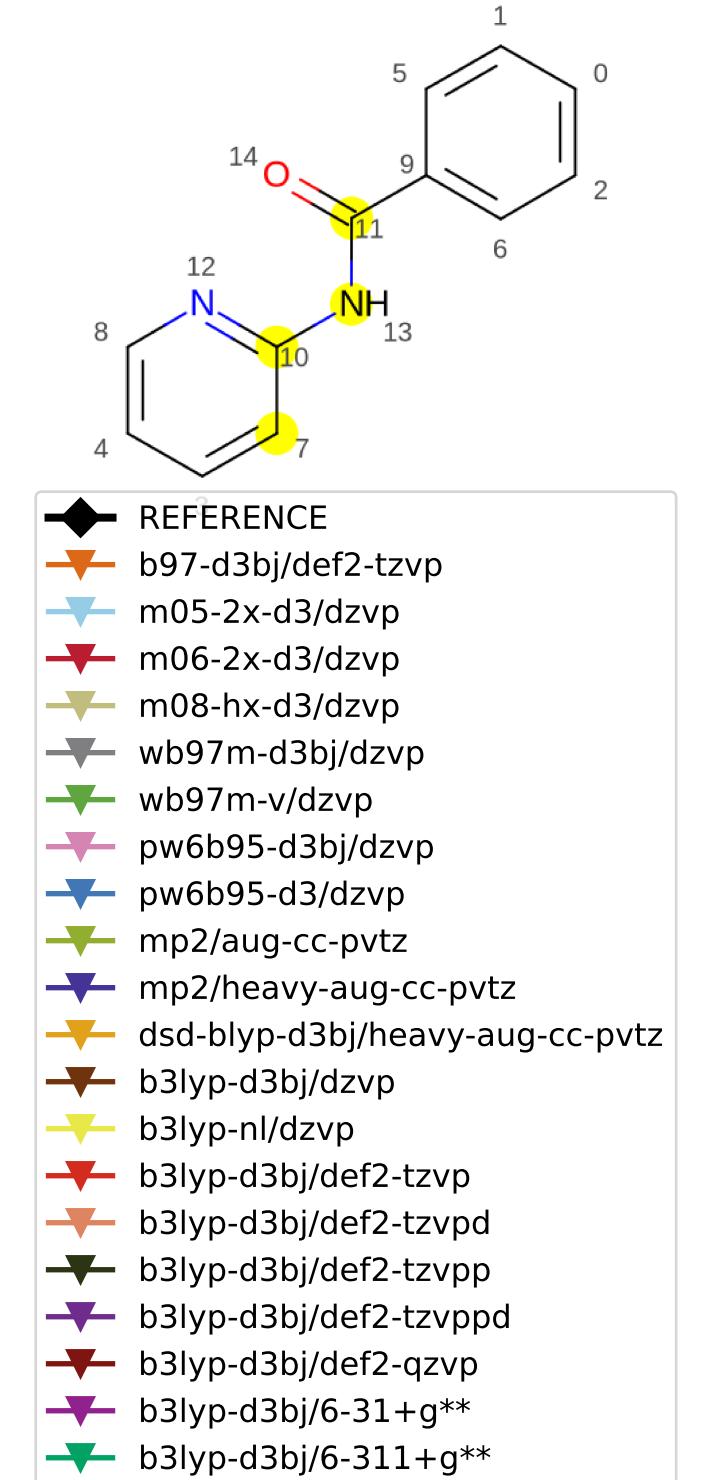
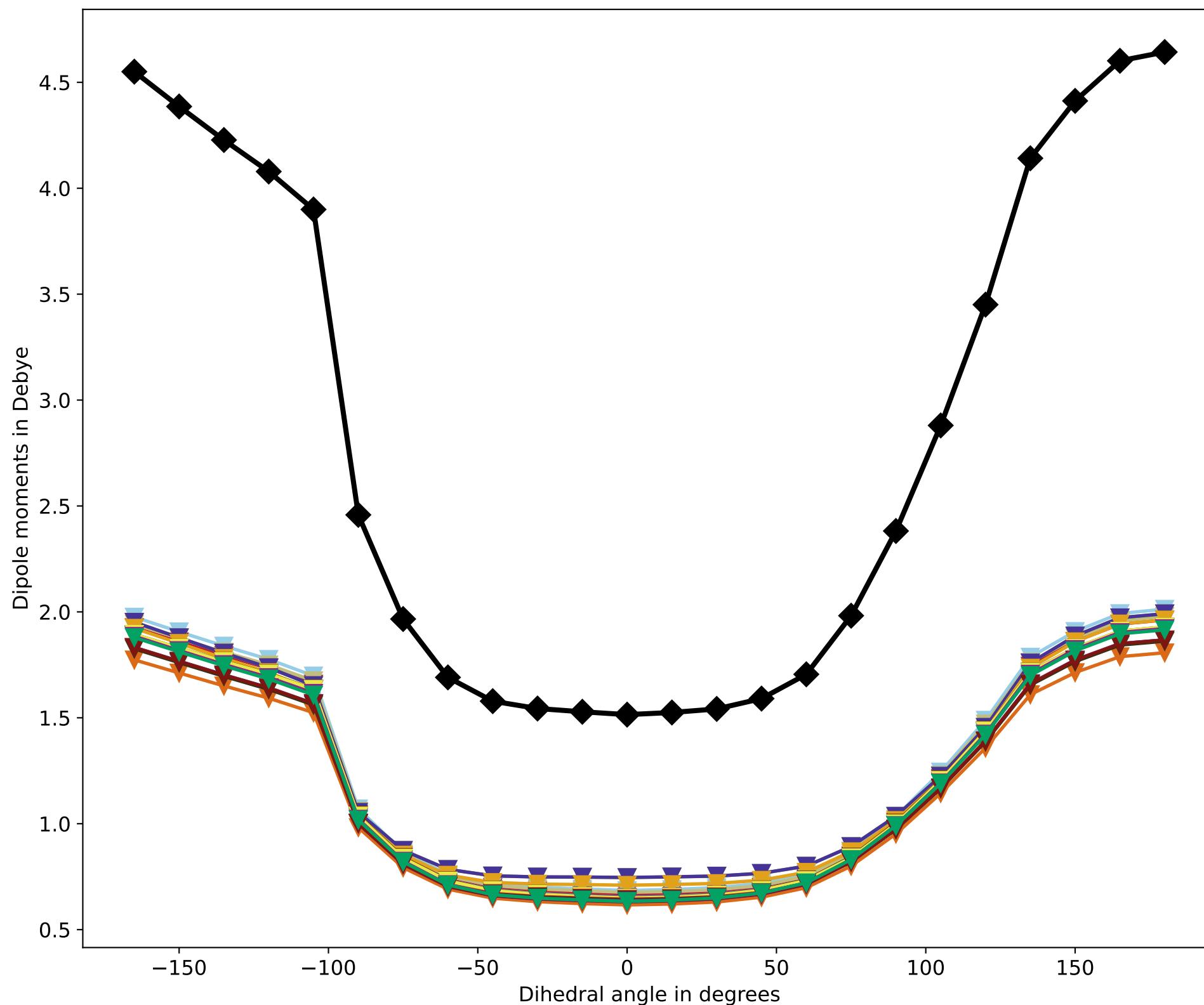
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

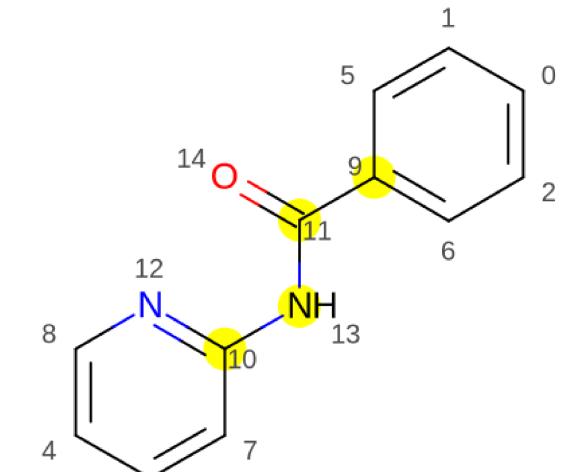
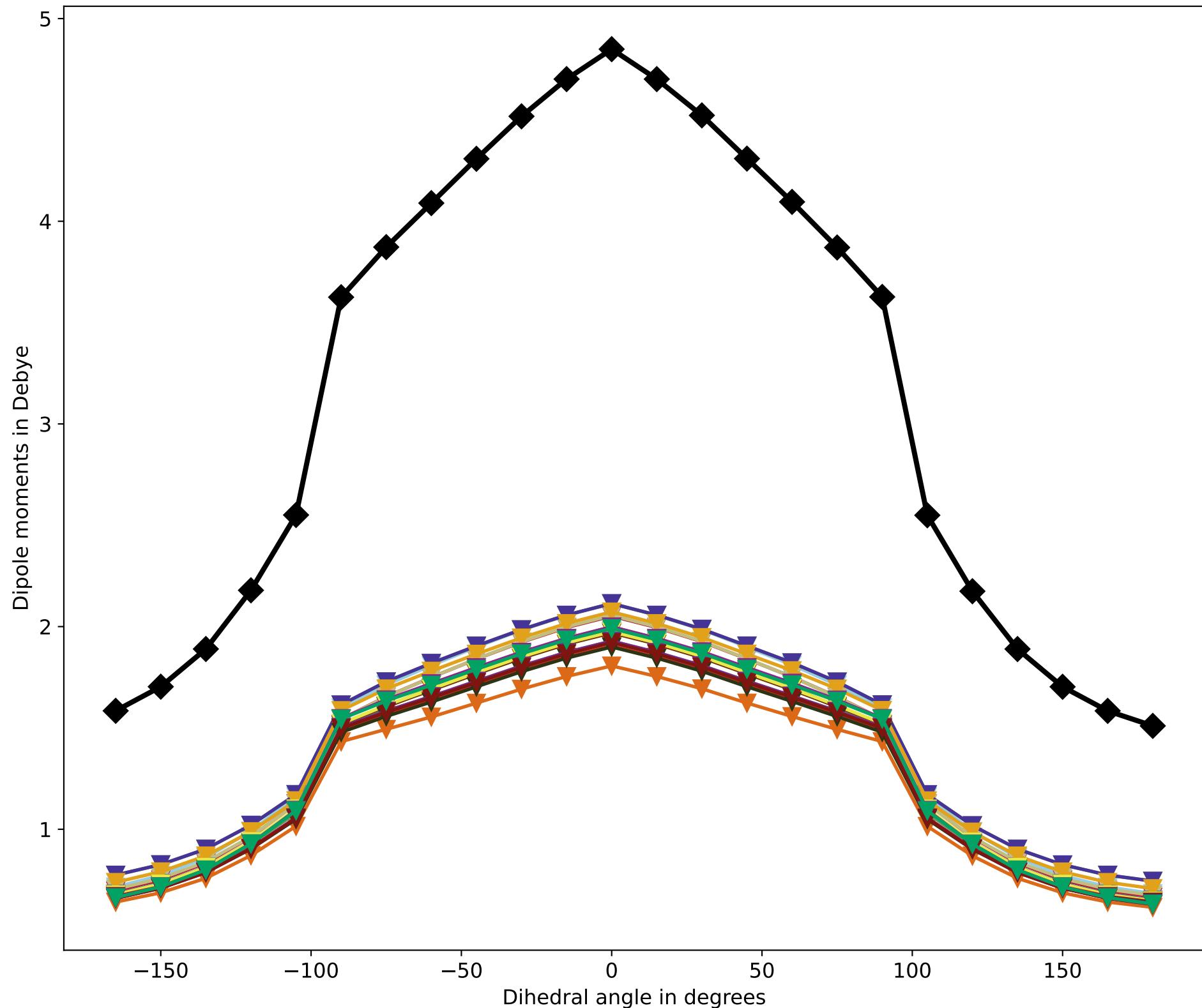


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

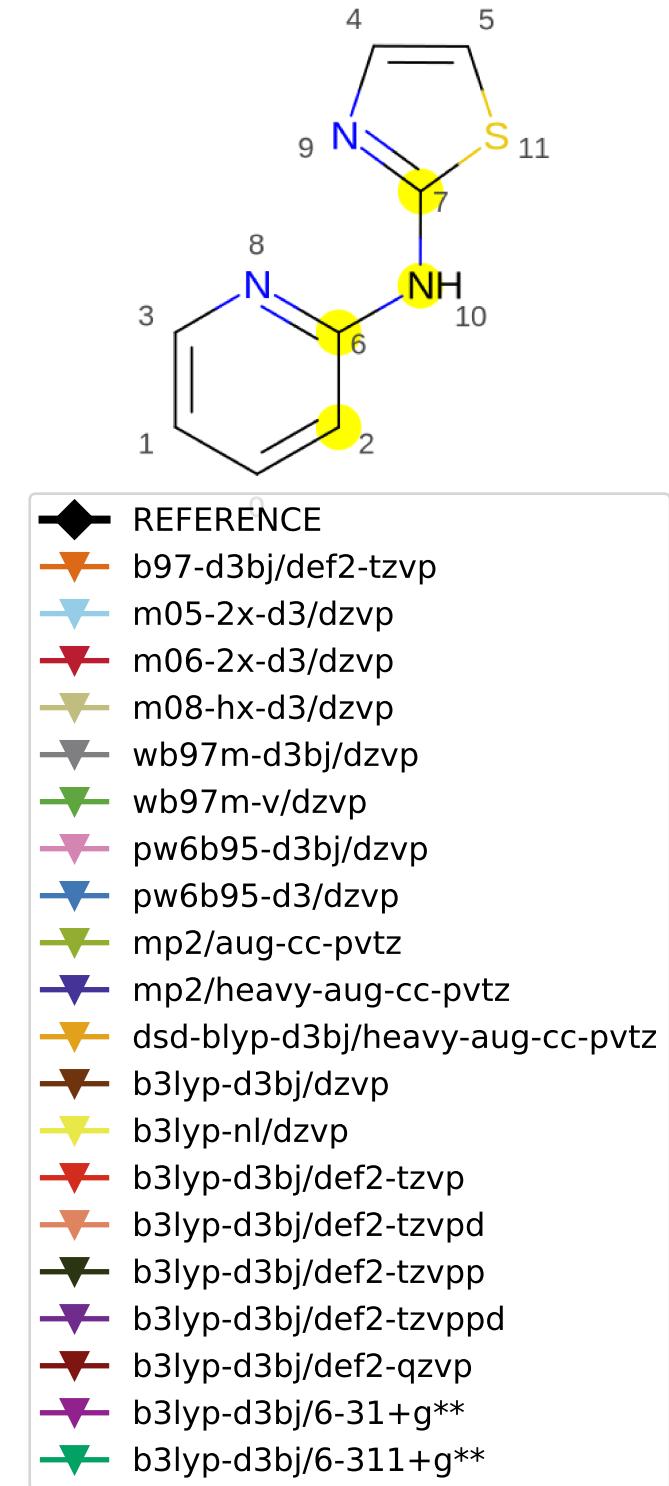
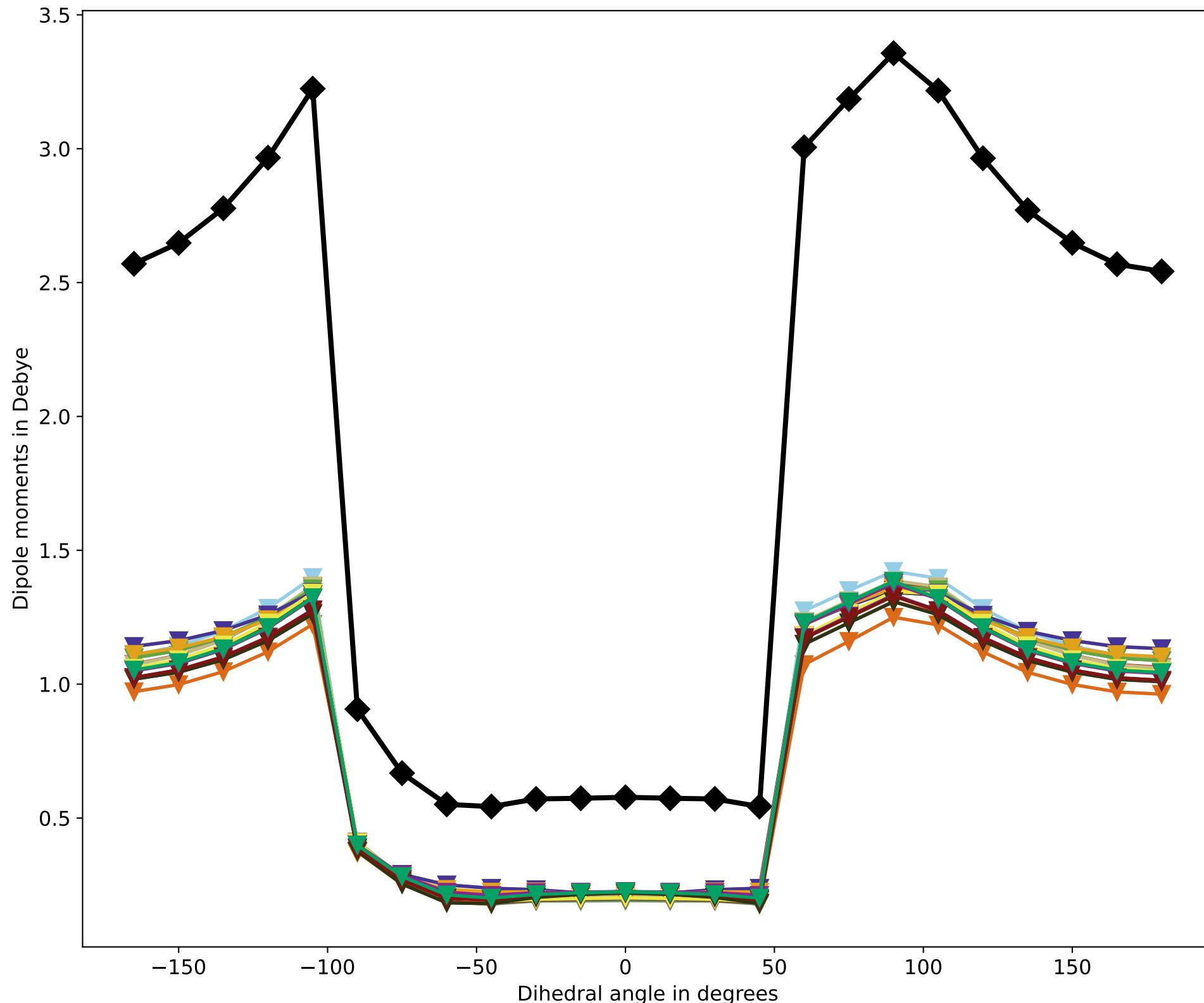
Charged molecule

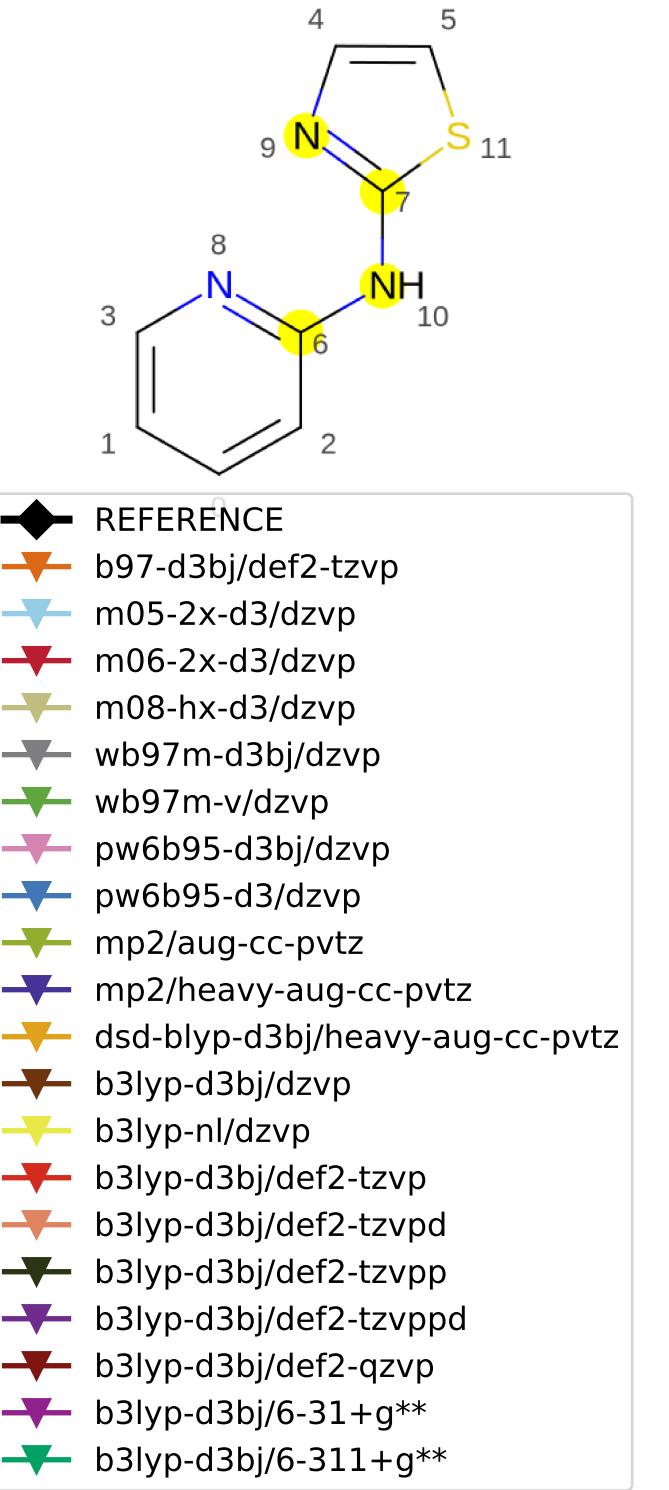
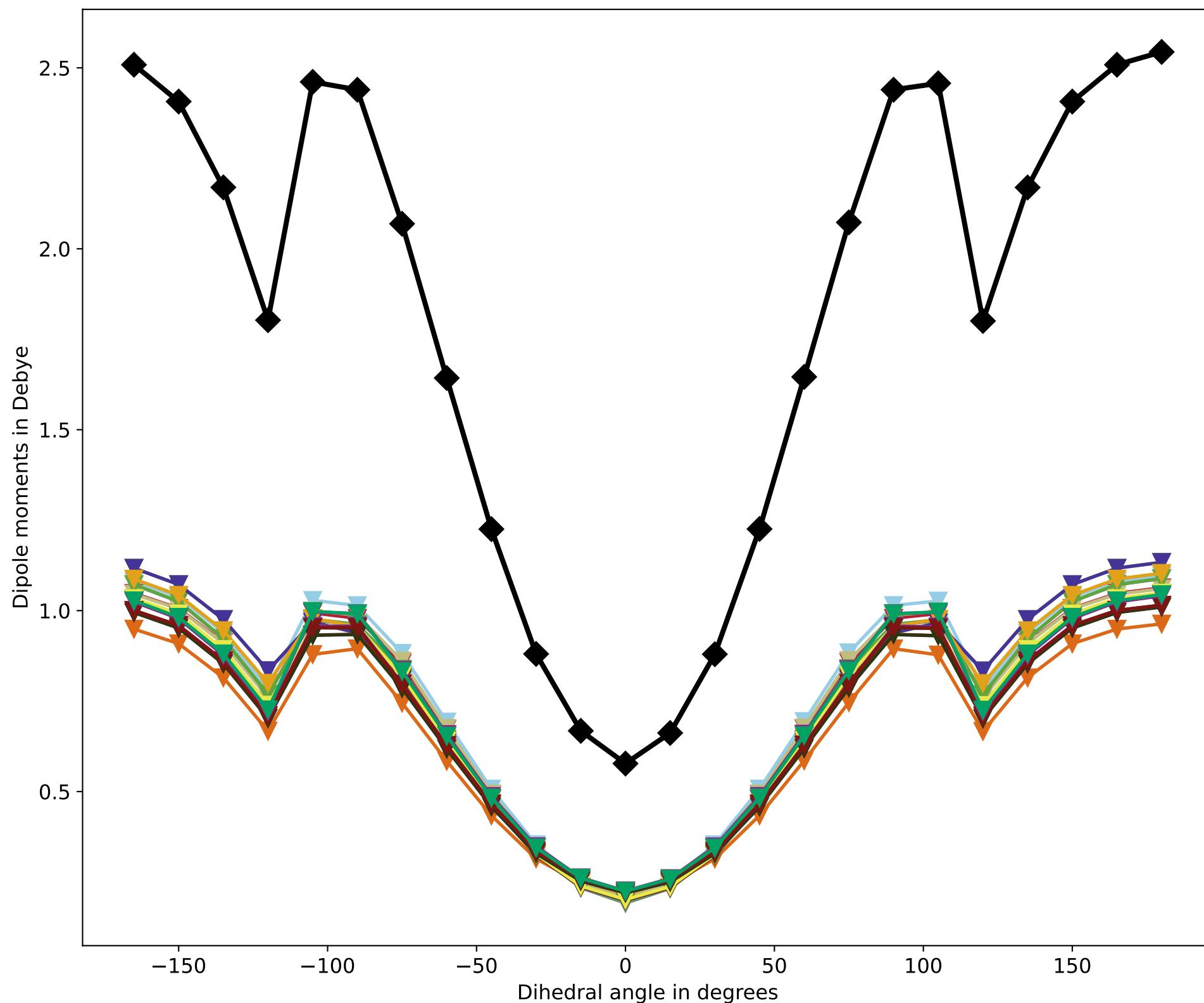


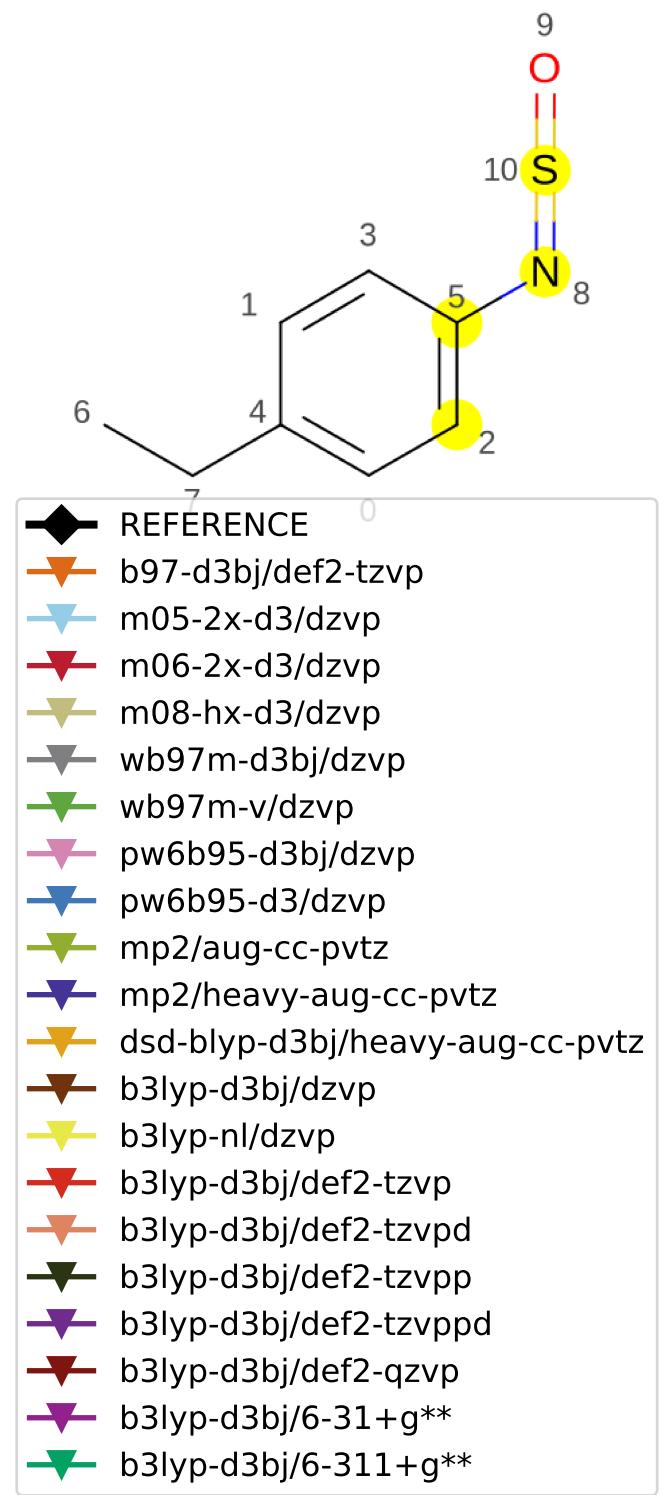
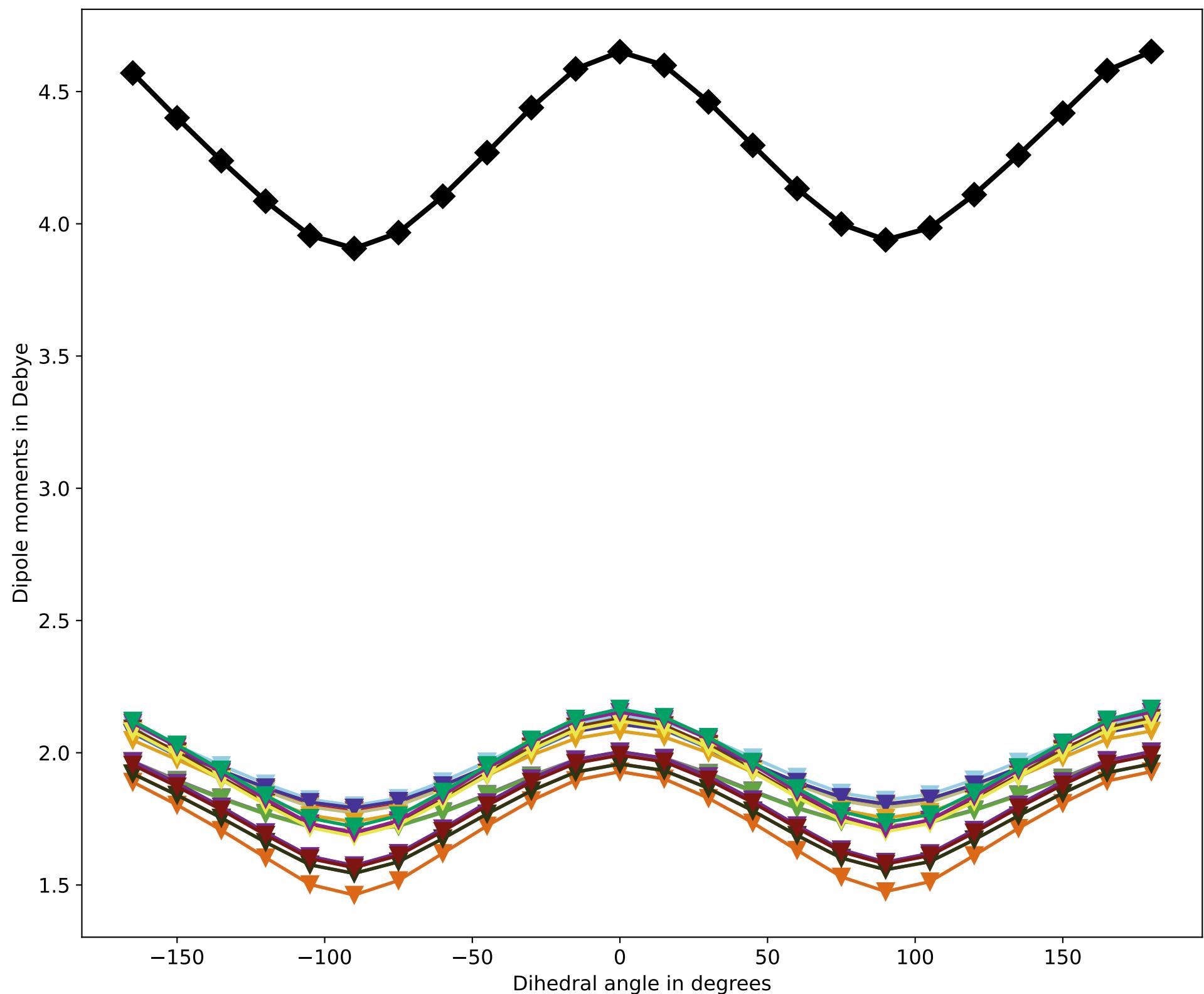


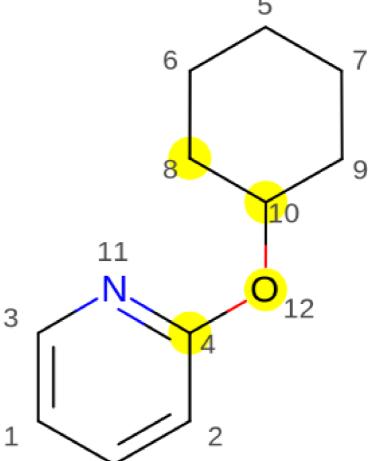
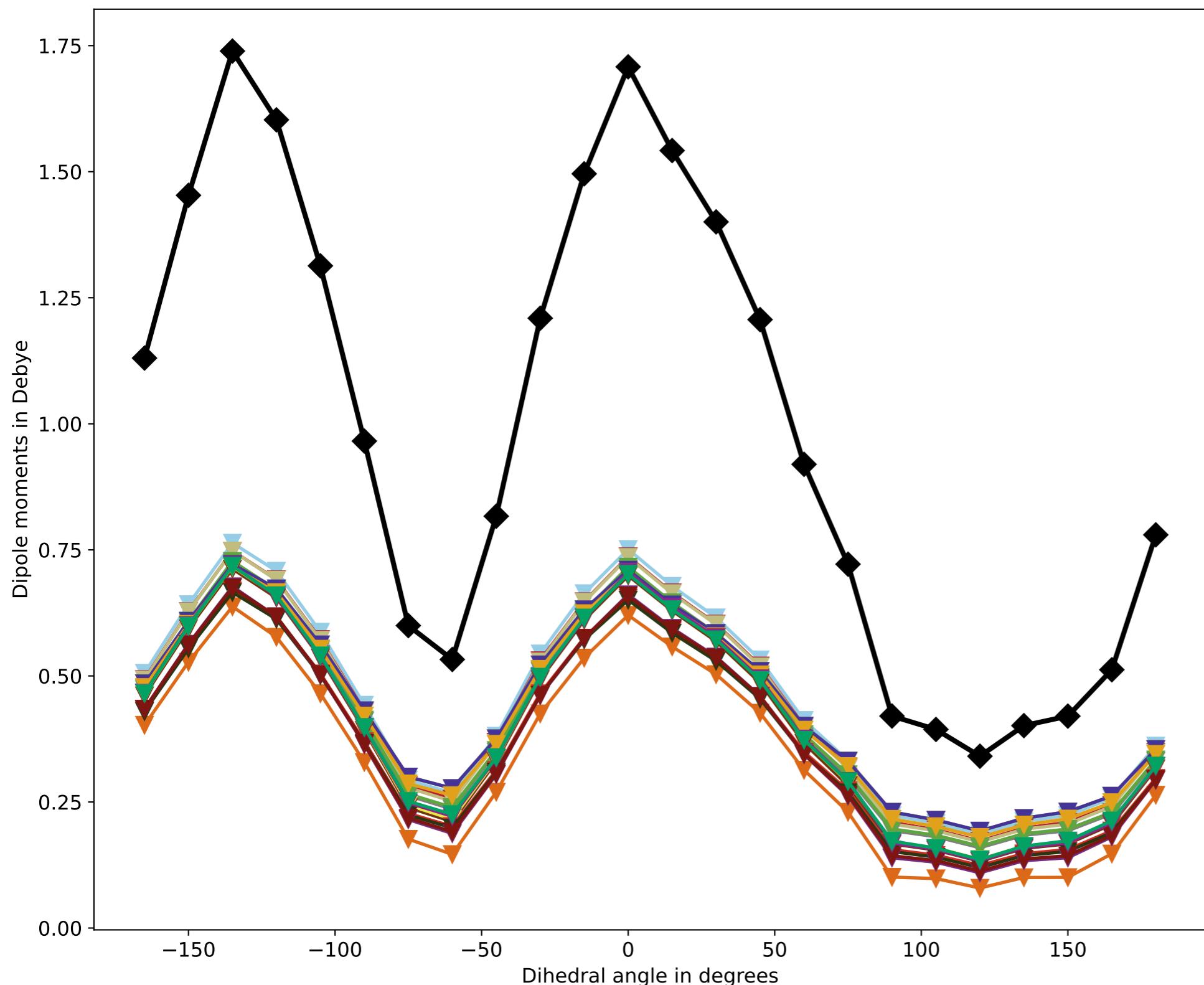


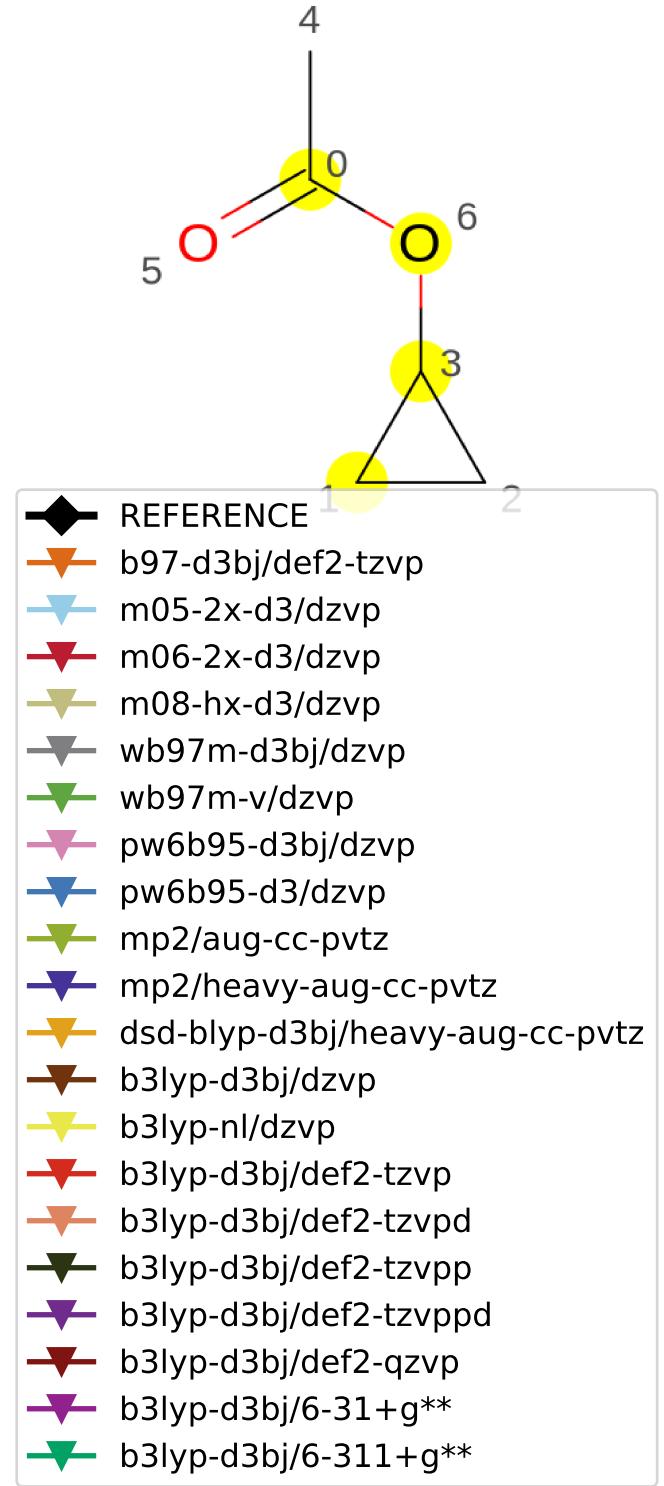
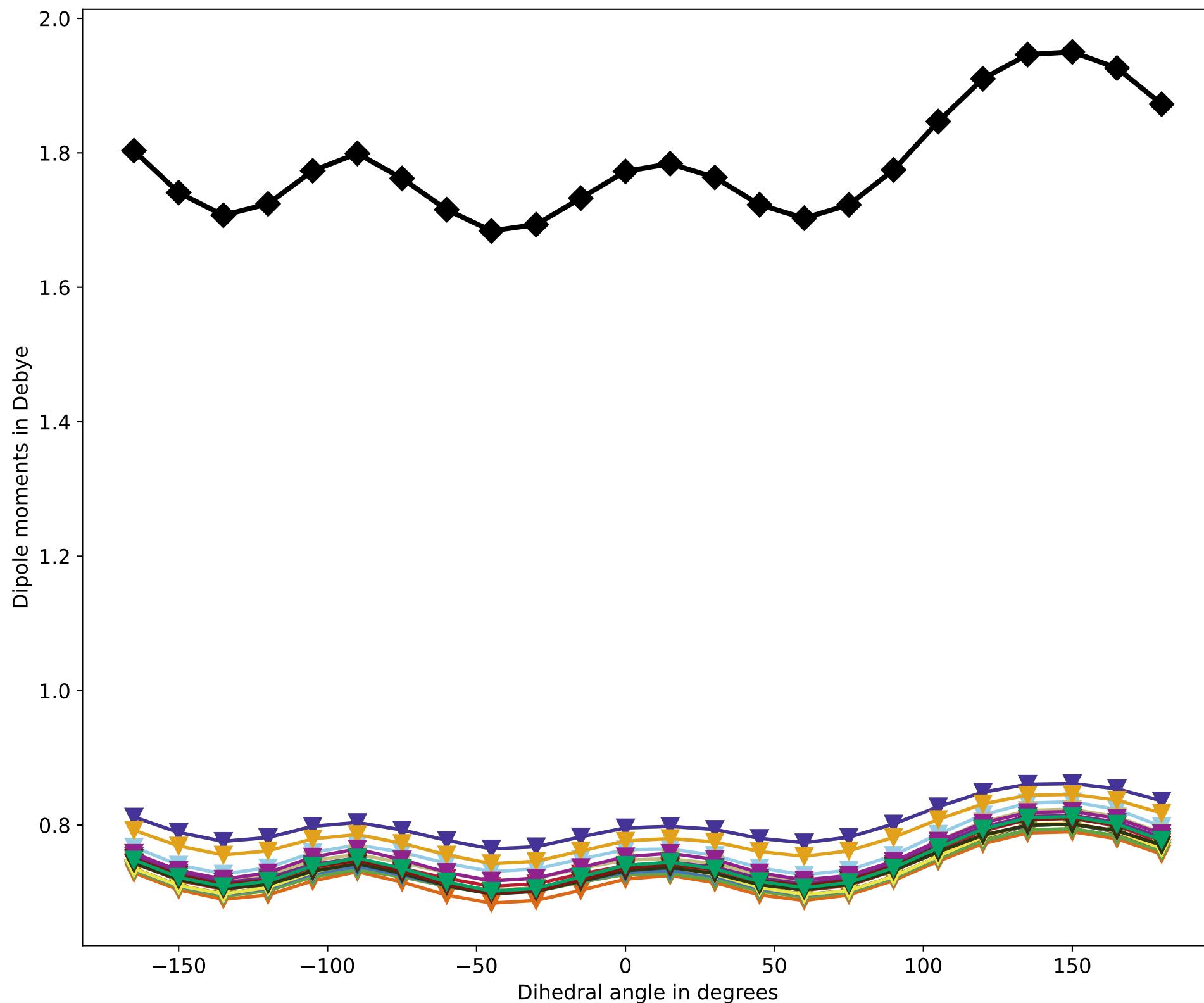
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp (red inverted triangle)
- ◆ b3lyp-d3bj/def2-tzvpd (orange triangle)
- ◆ b3lyp-d3bj/def2-tzvpp (black triangle)
- ◆ b3lyp-d3bj/def2-tzvppd (purple triangle)
- ◆ b3lyp-d3bj/def2-qzvp (dark red triangle)
- ◆ b3lyp-d3bj/6-31+g** (pink triangle)
- ◆ b3lyp-d3bj/6-311+g** (green triangle)

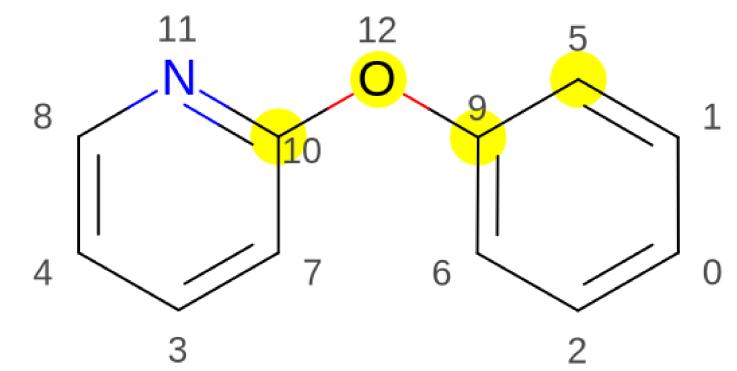
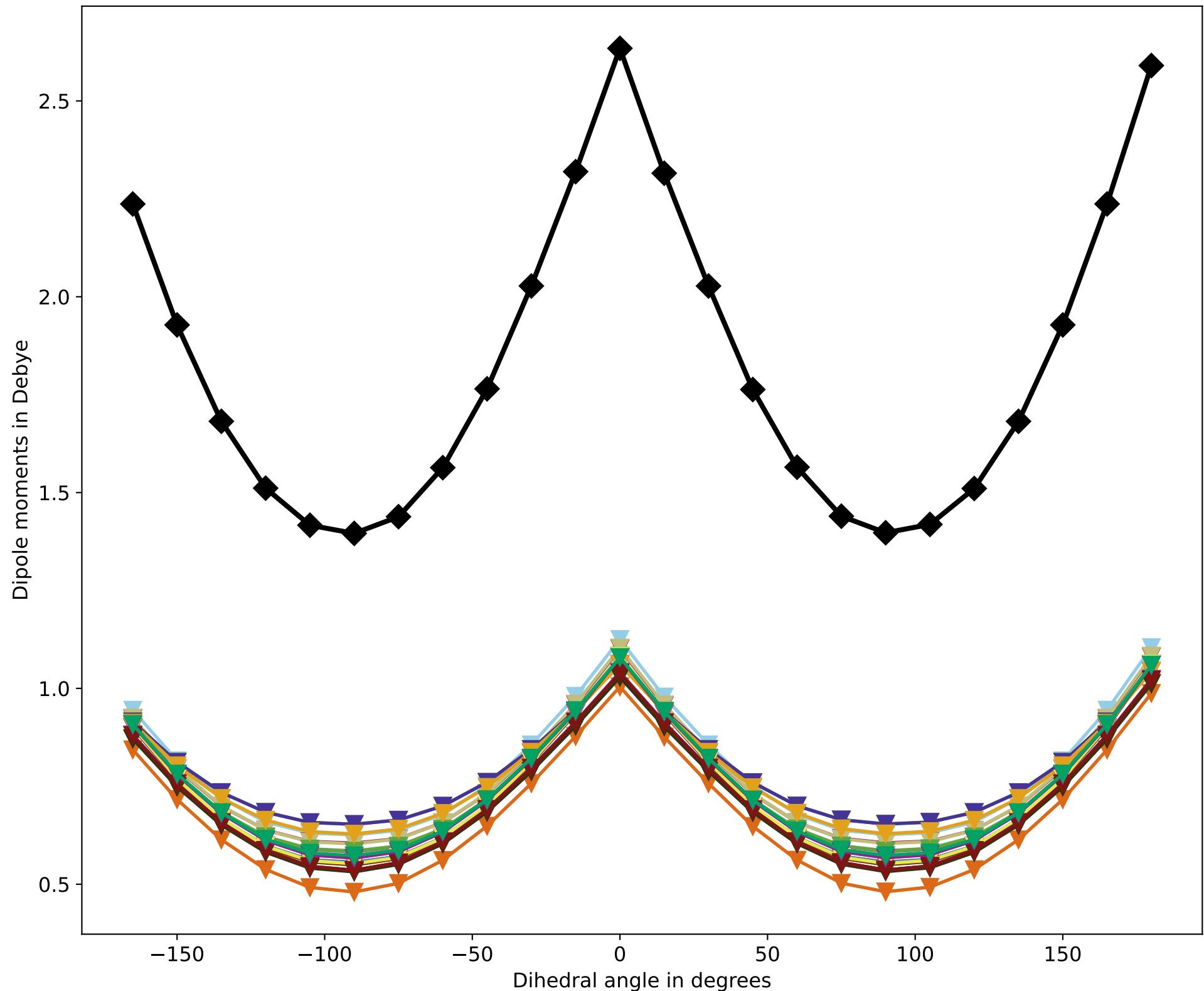




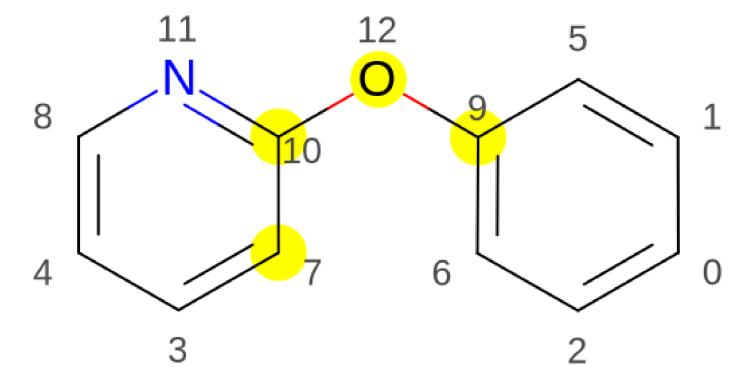
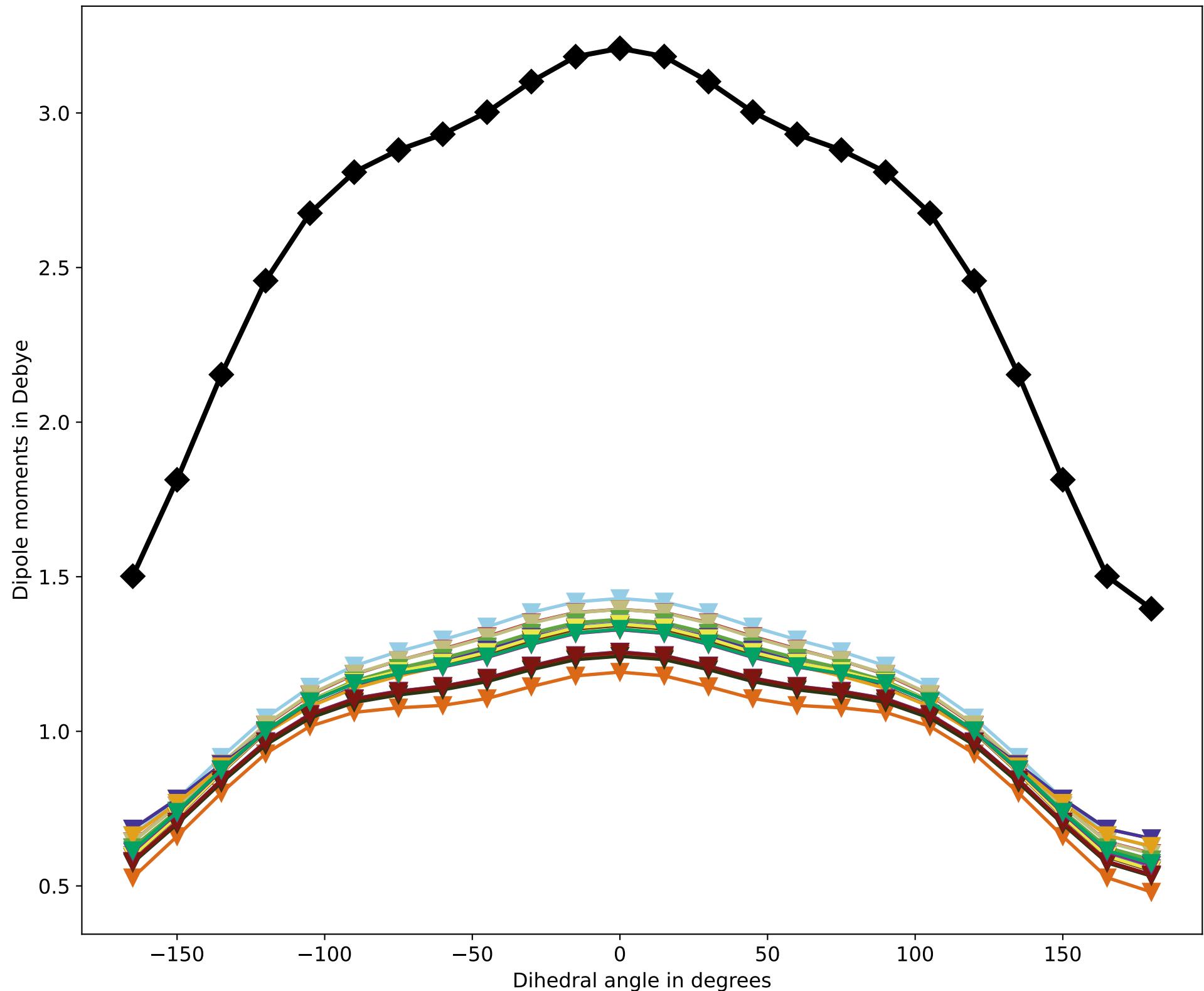




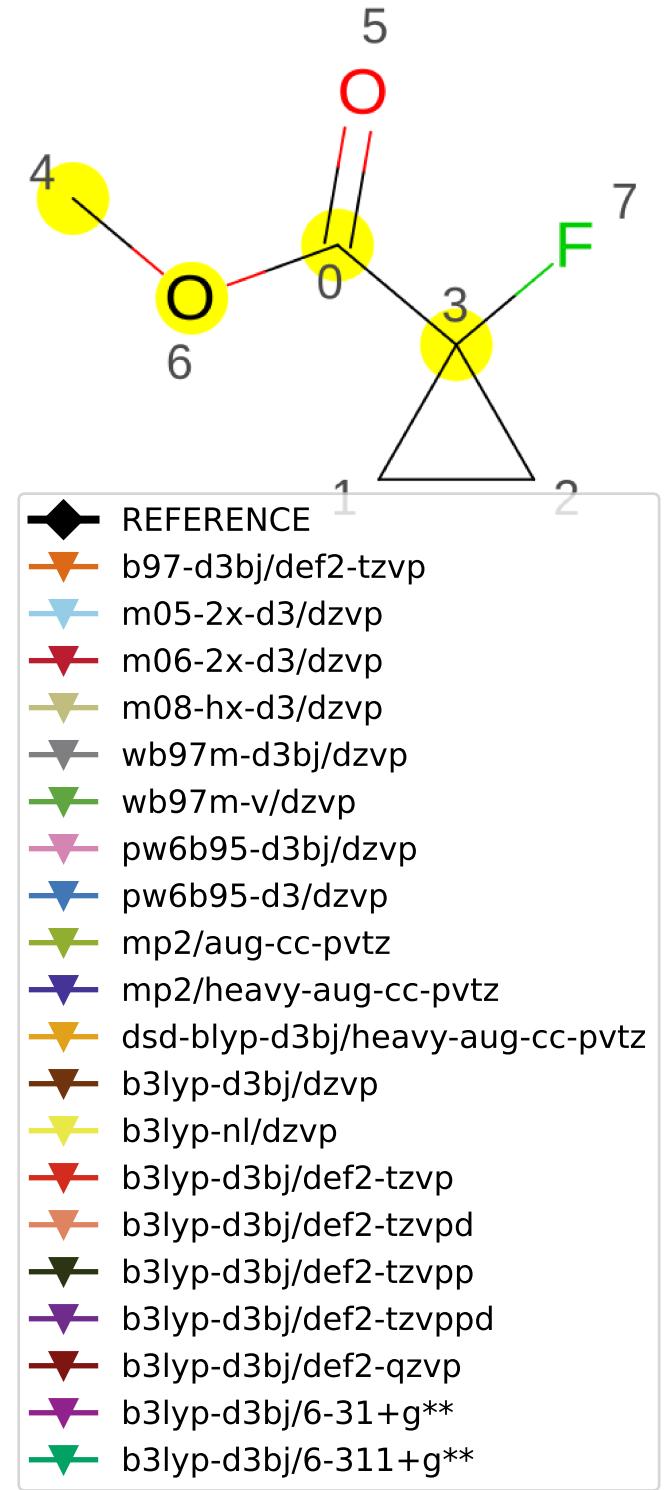
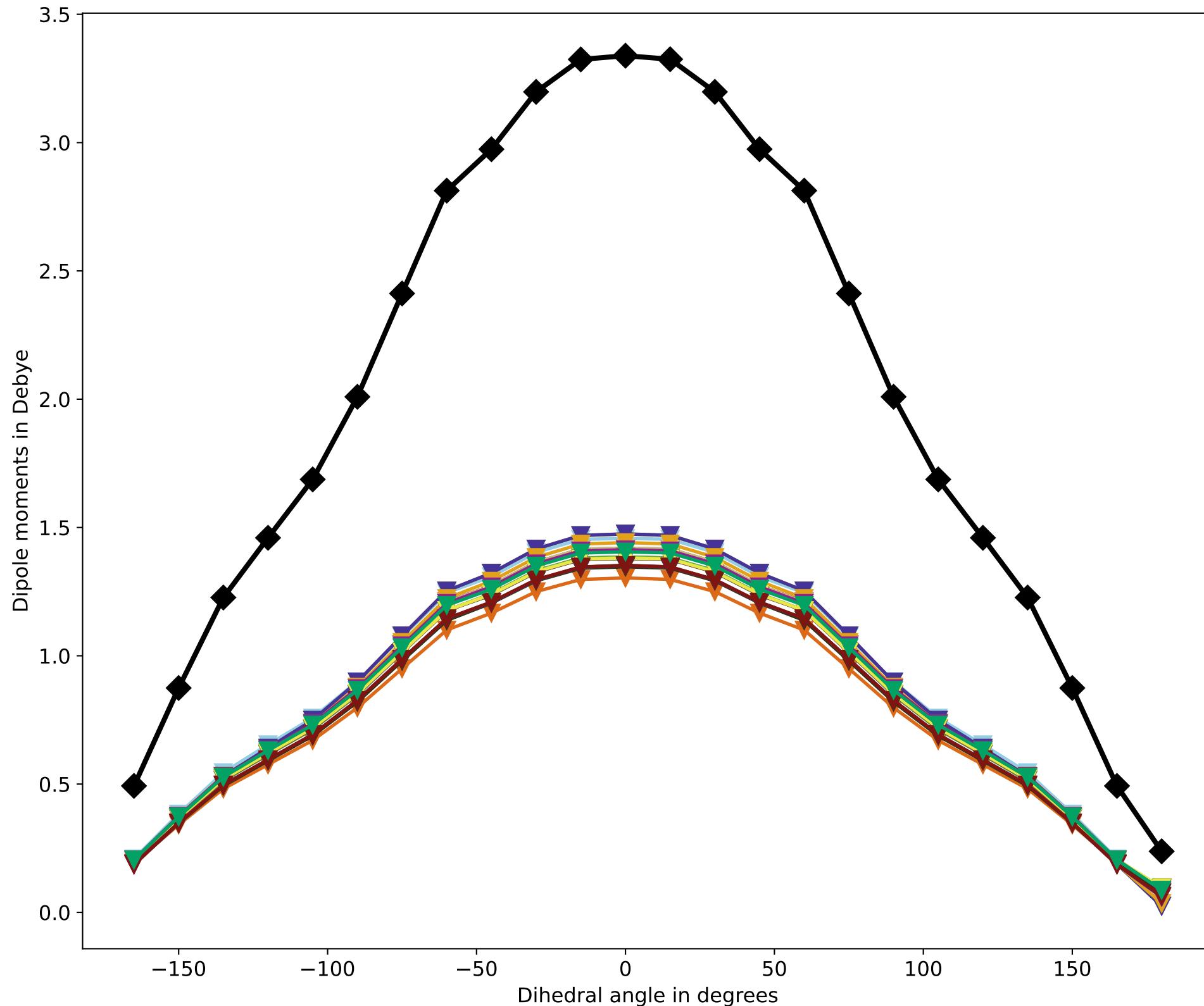


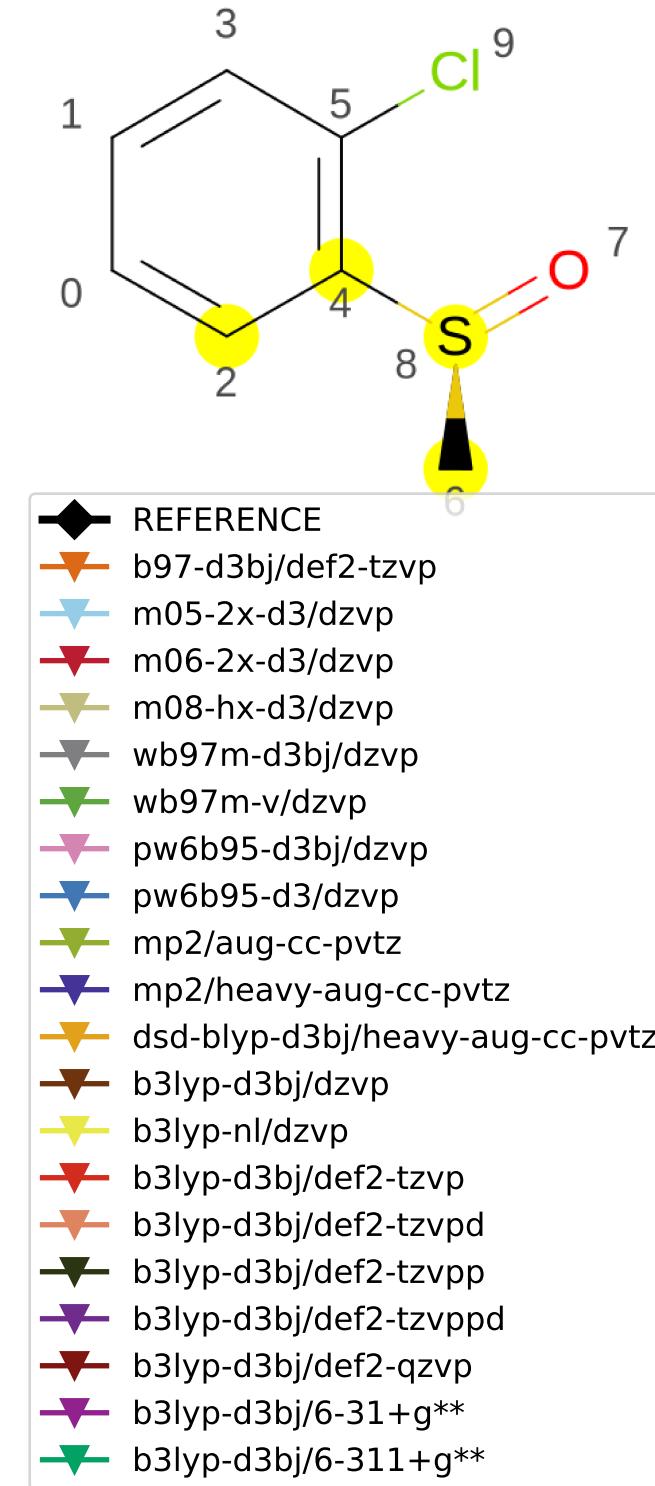
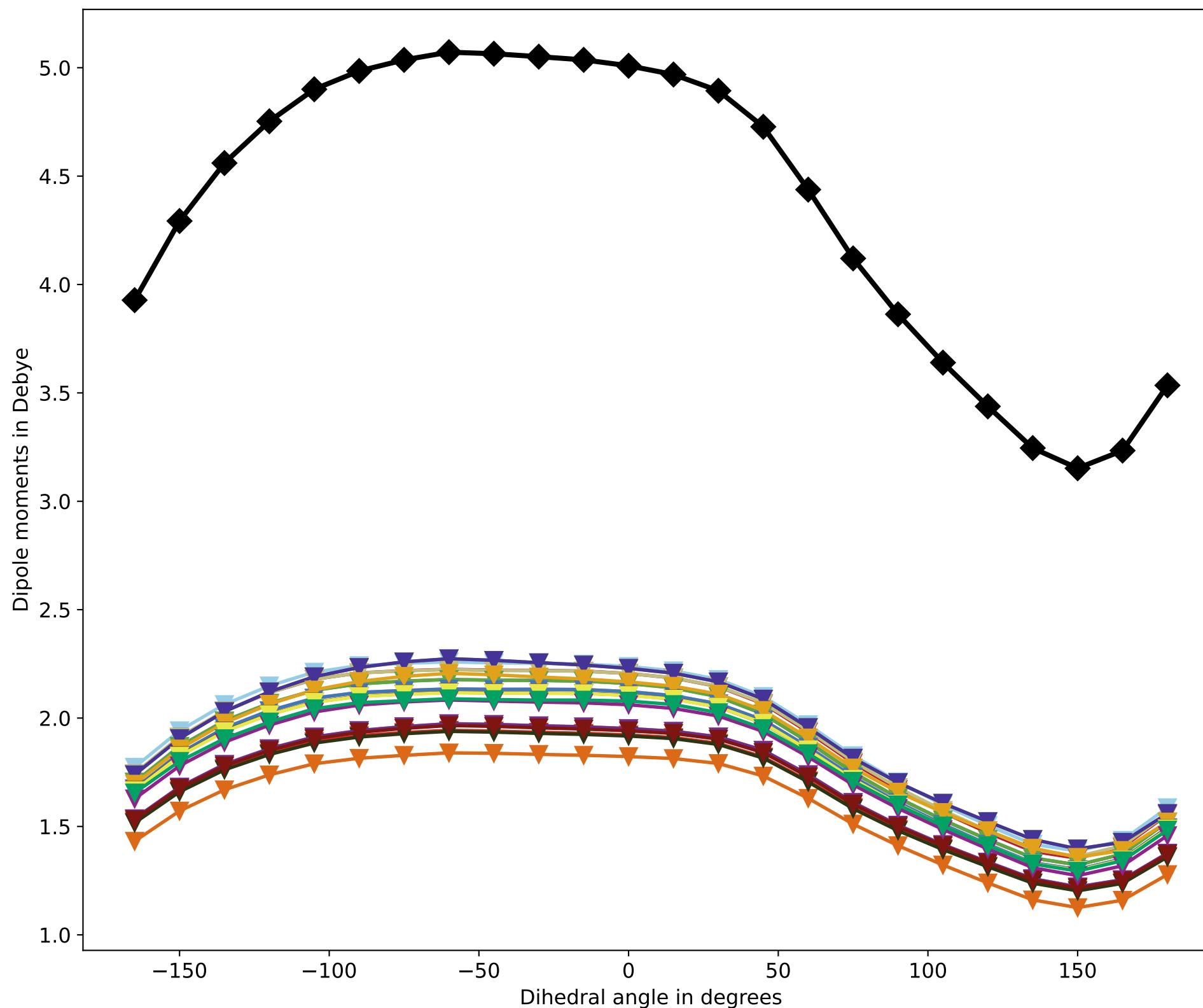


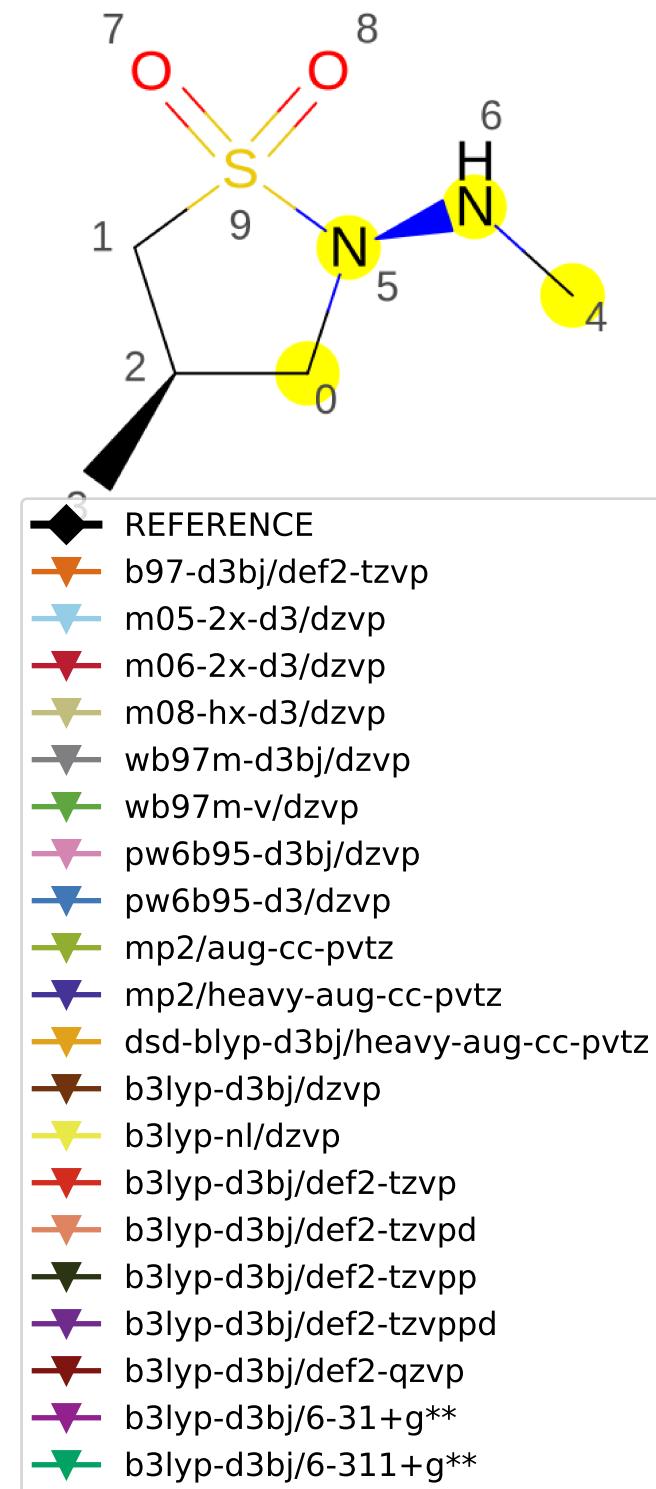
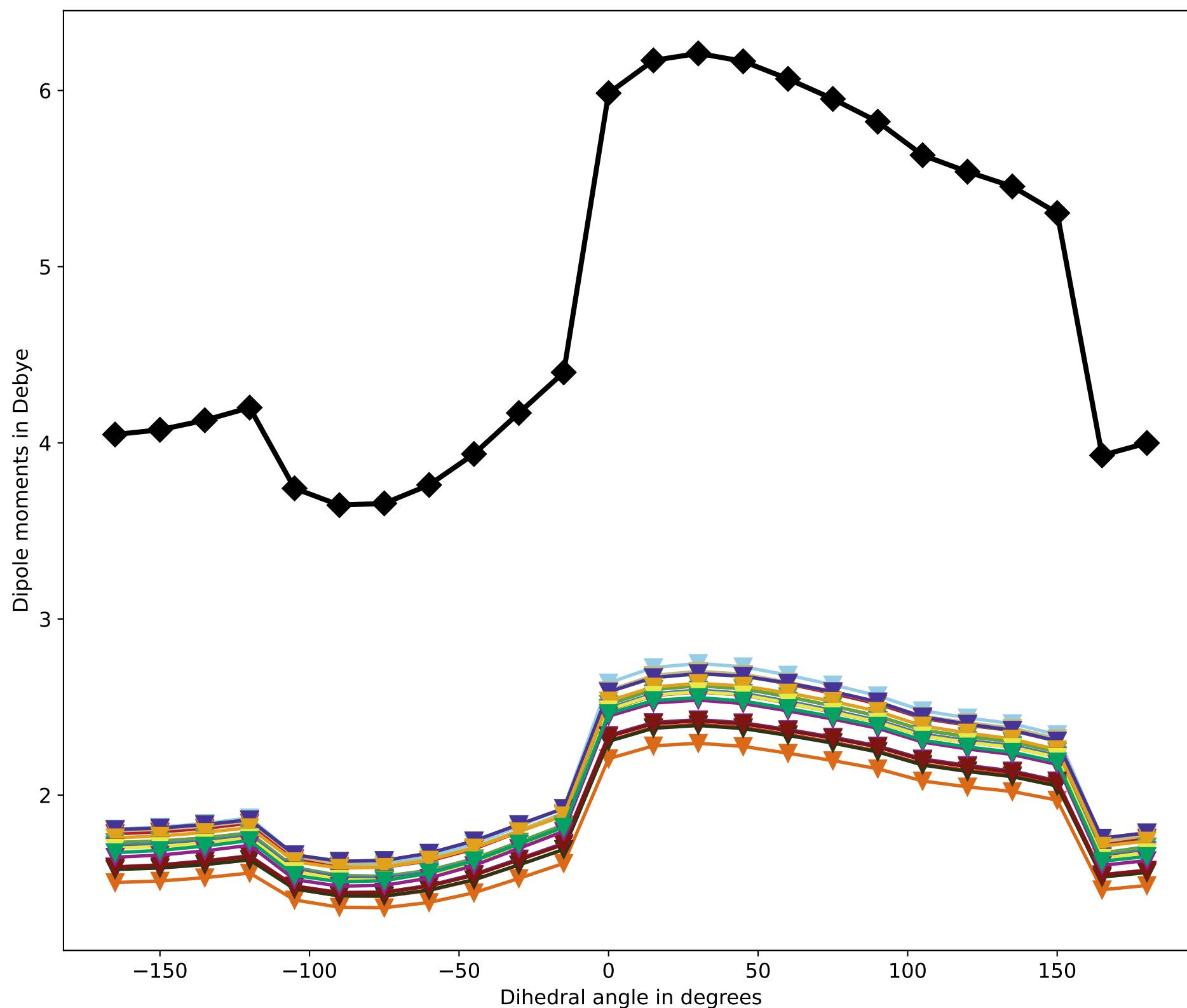
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

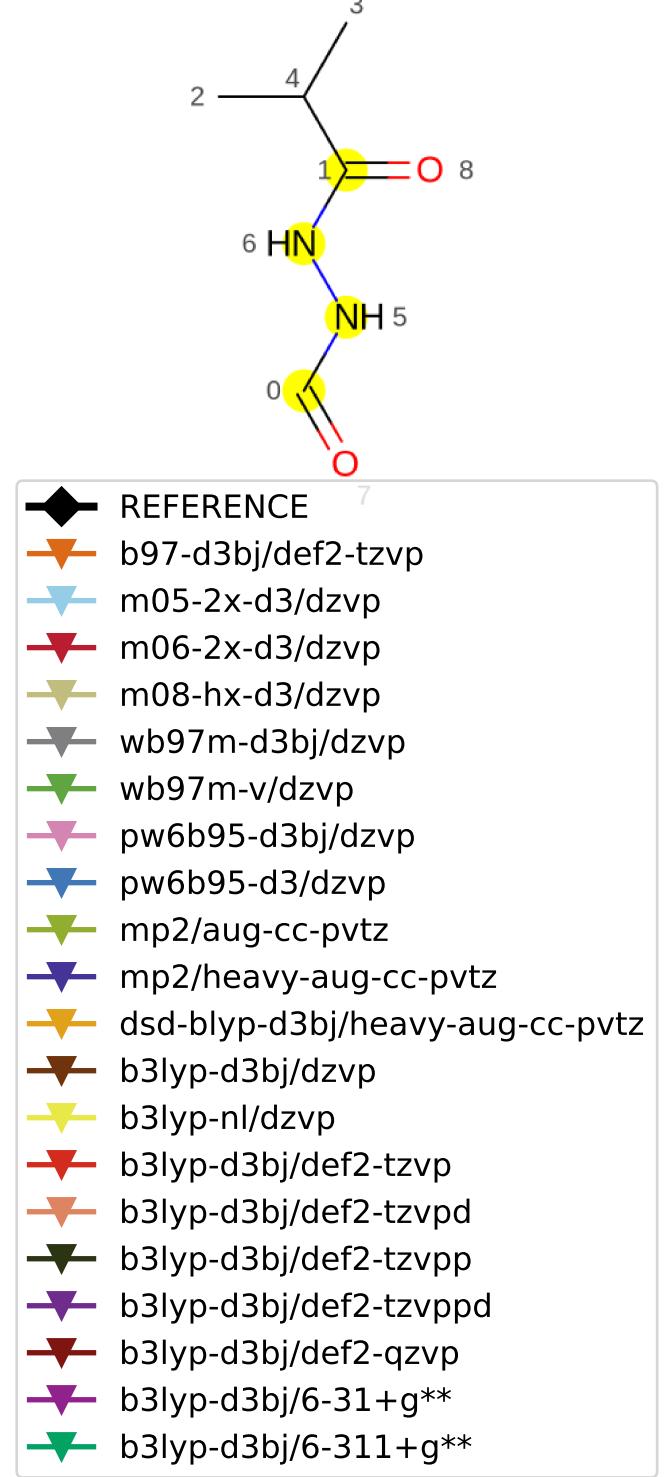
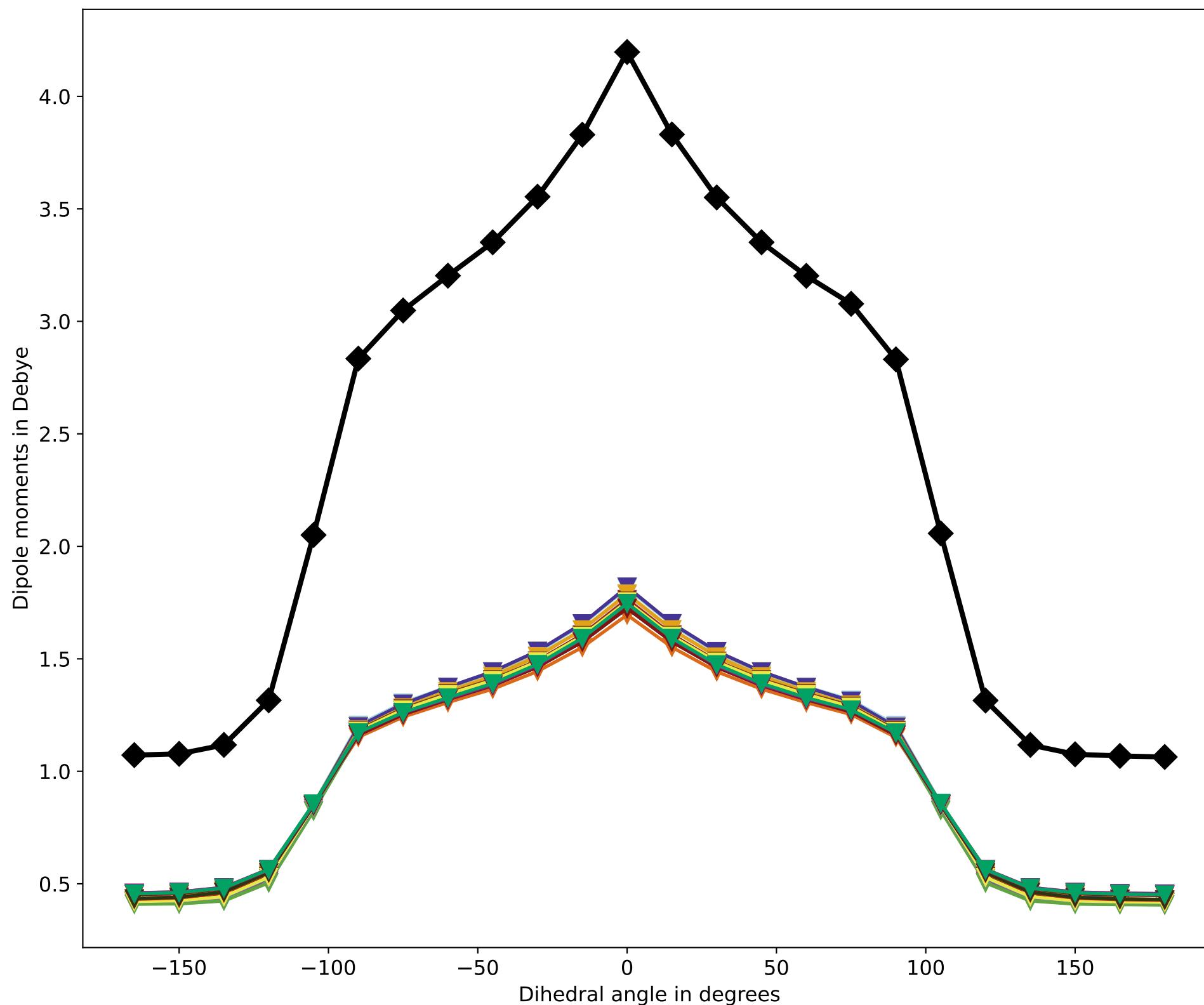


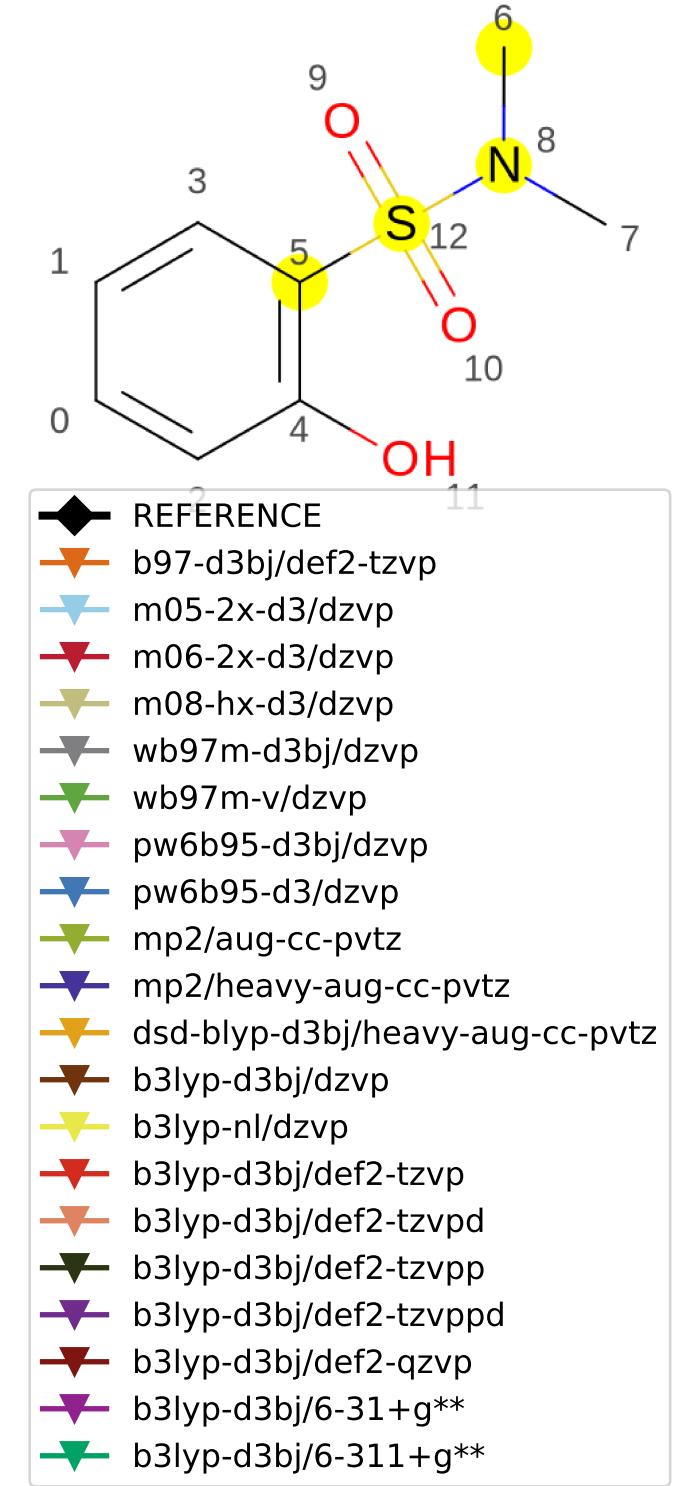
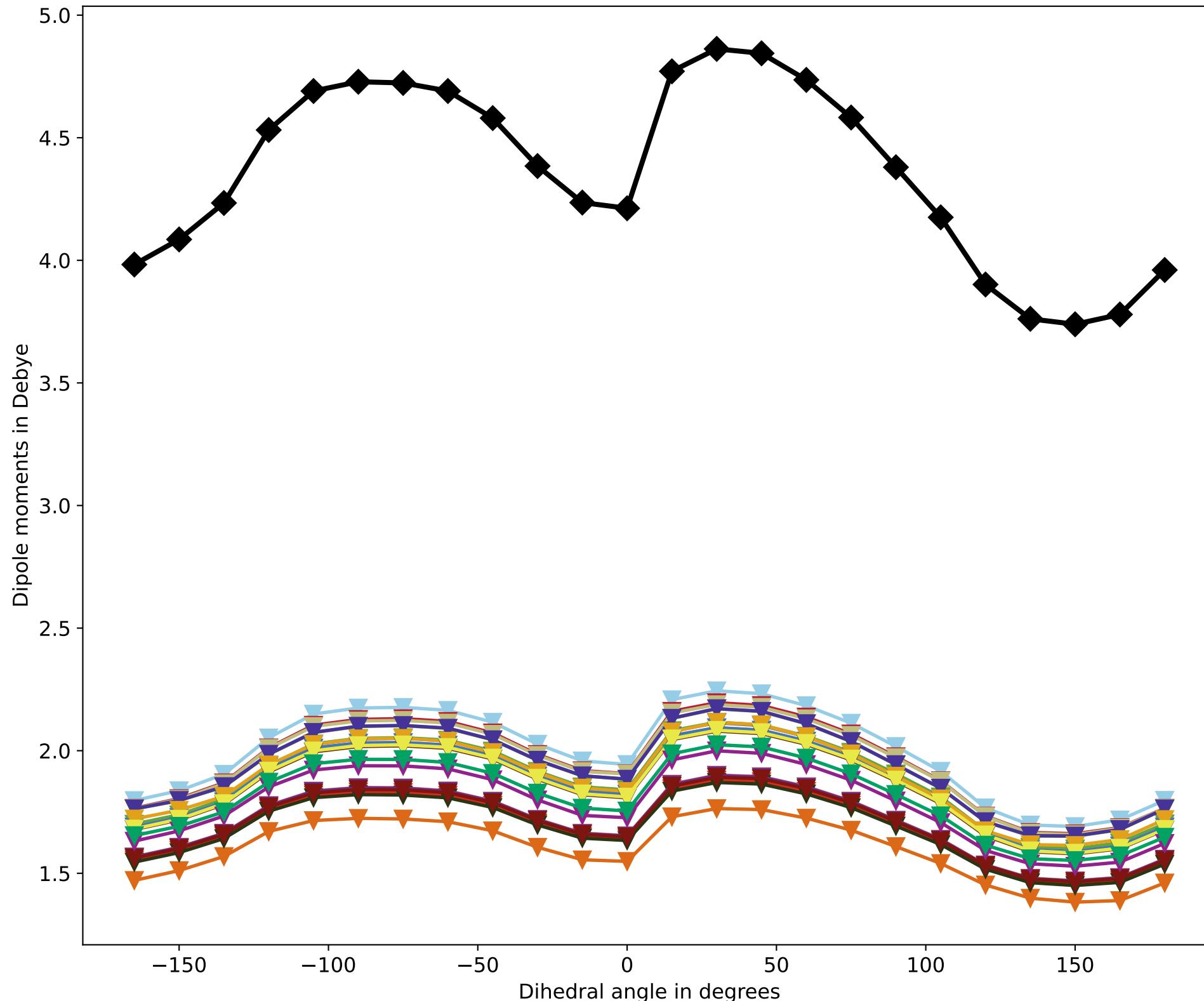
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

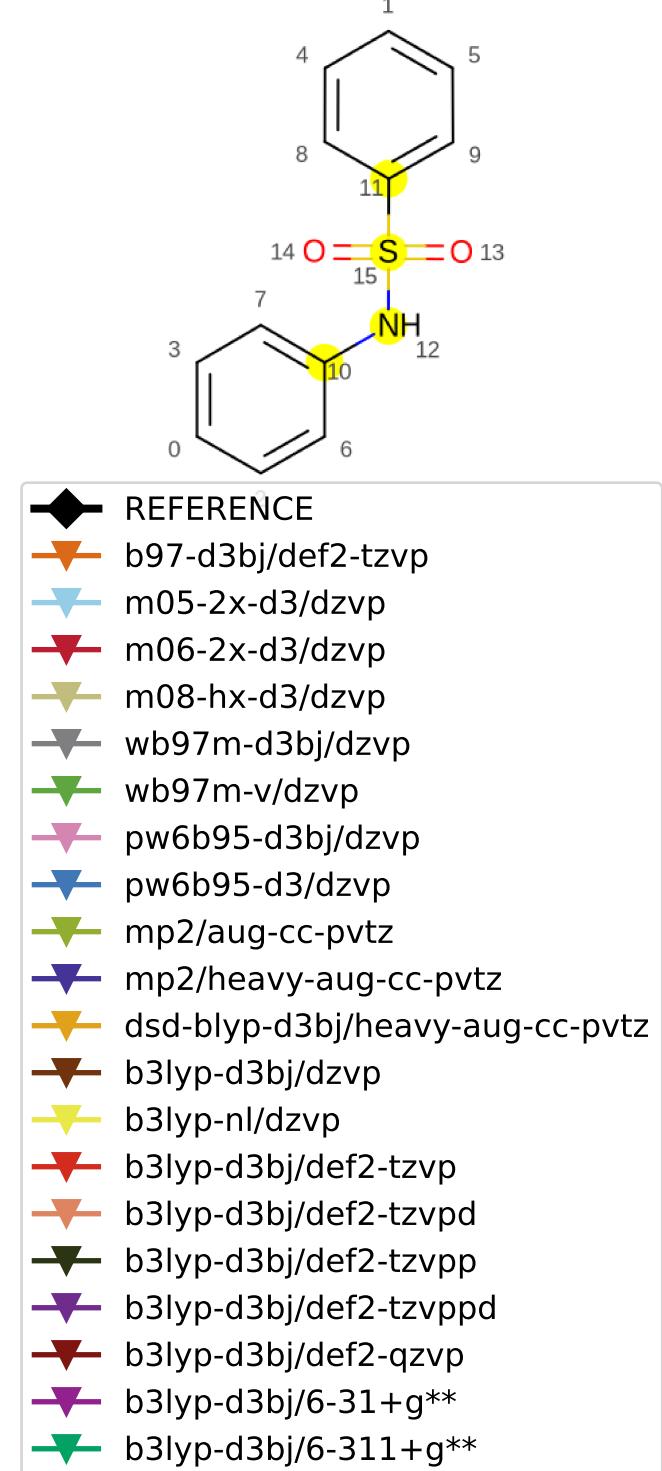
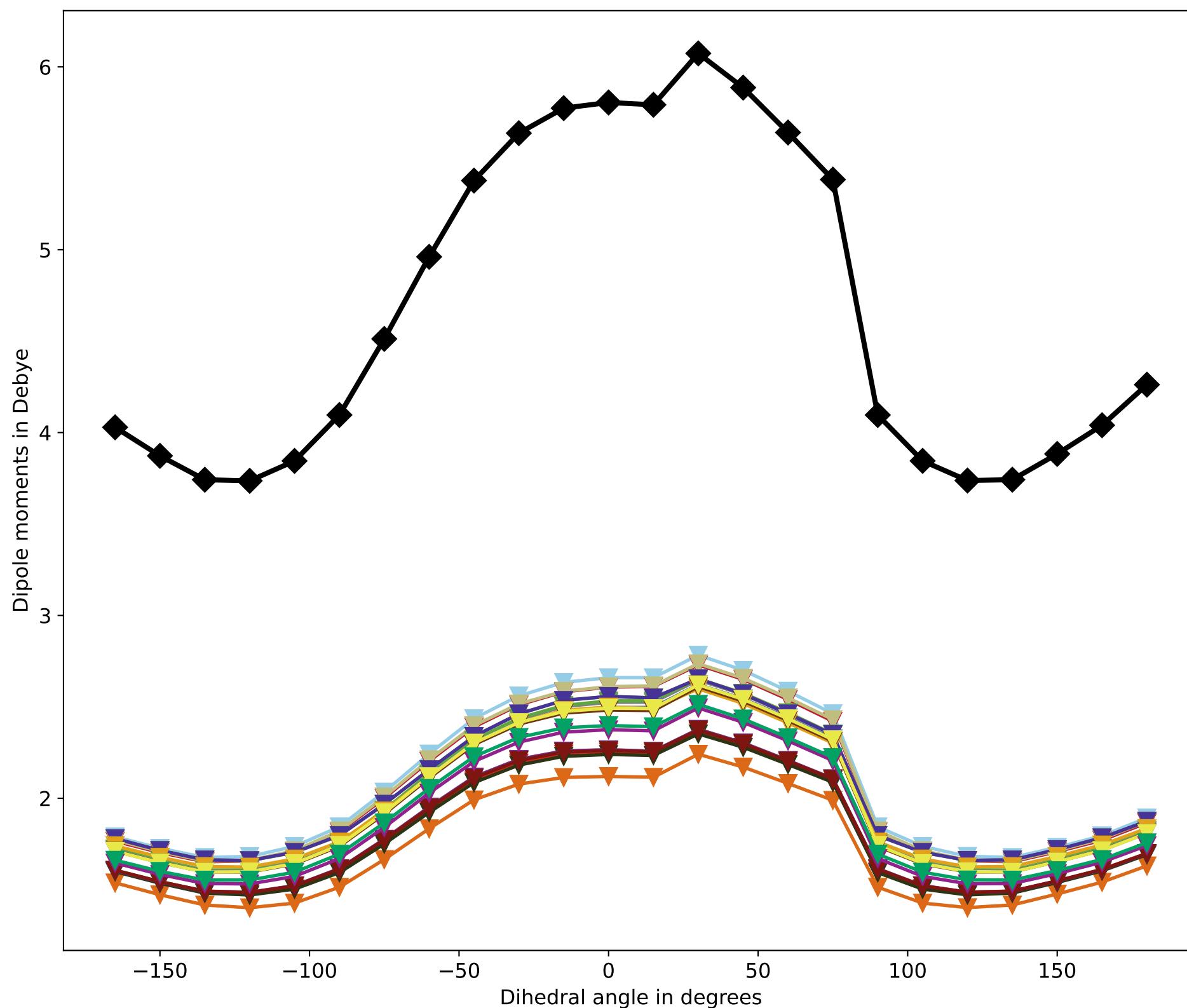


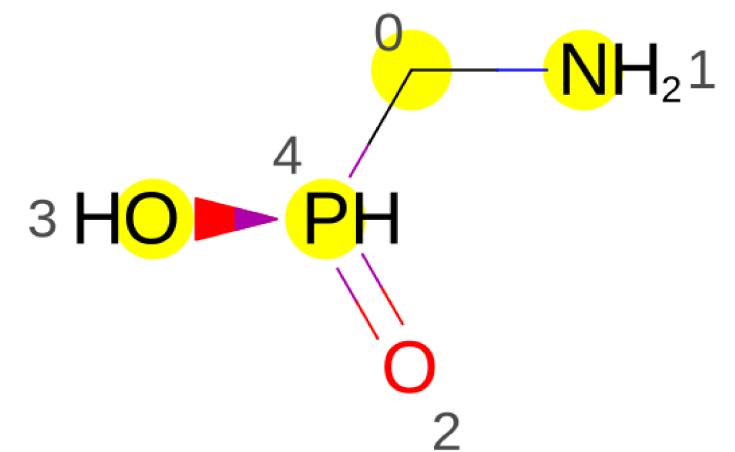
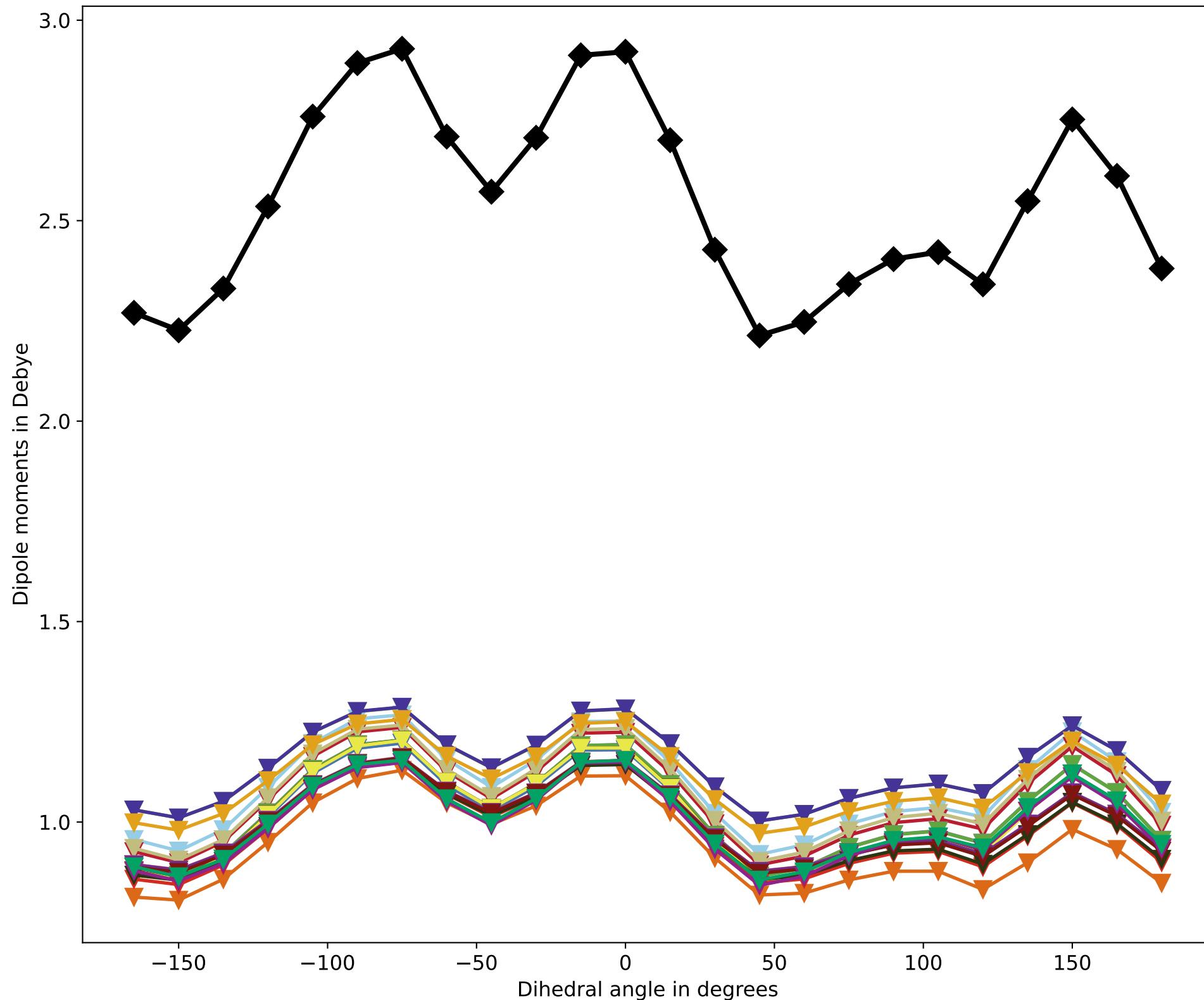




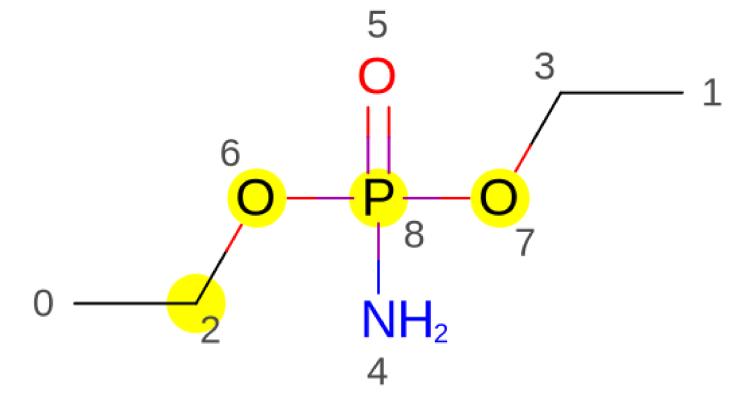
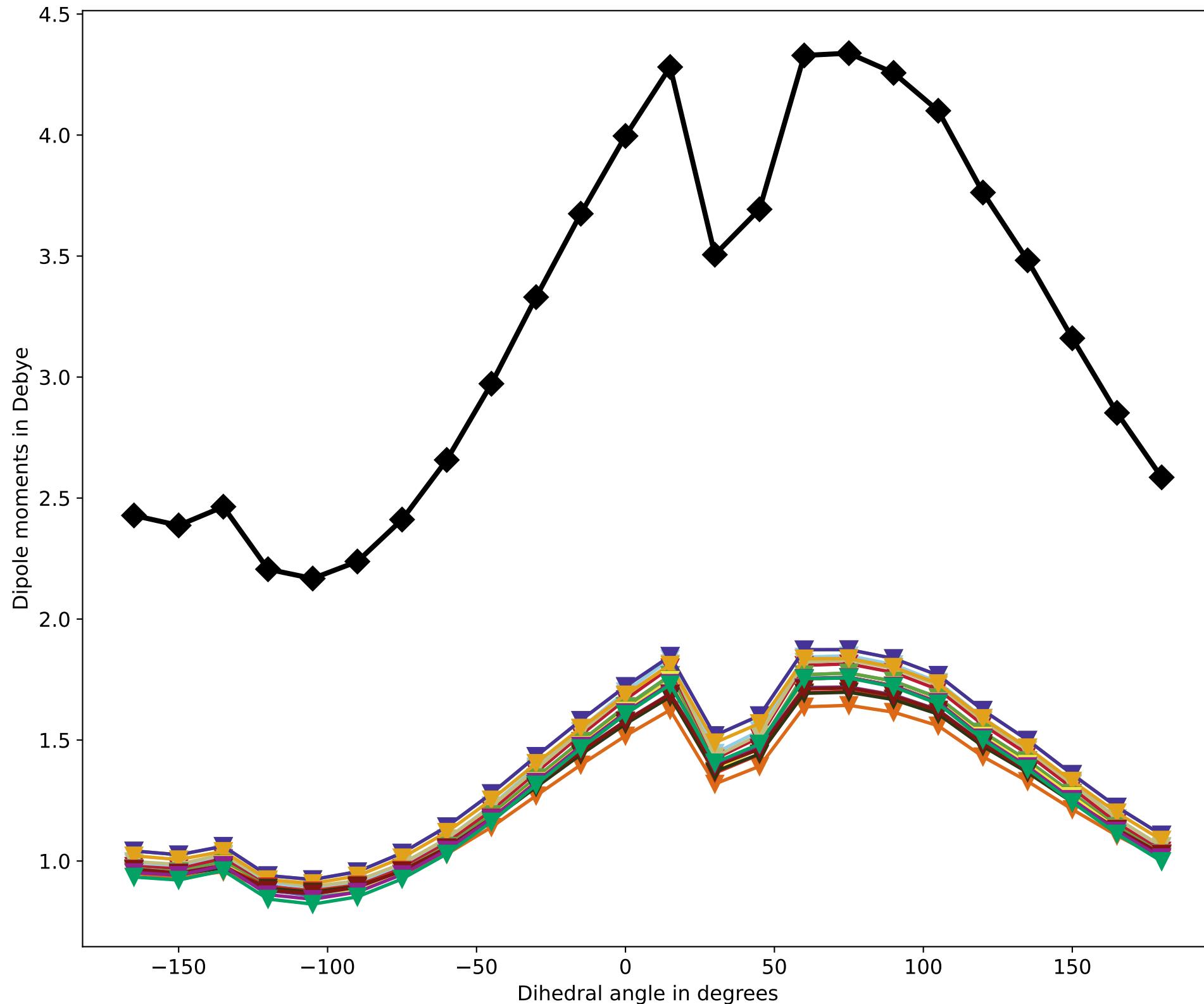




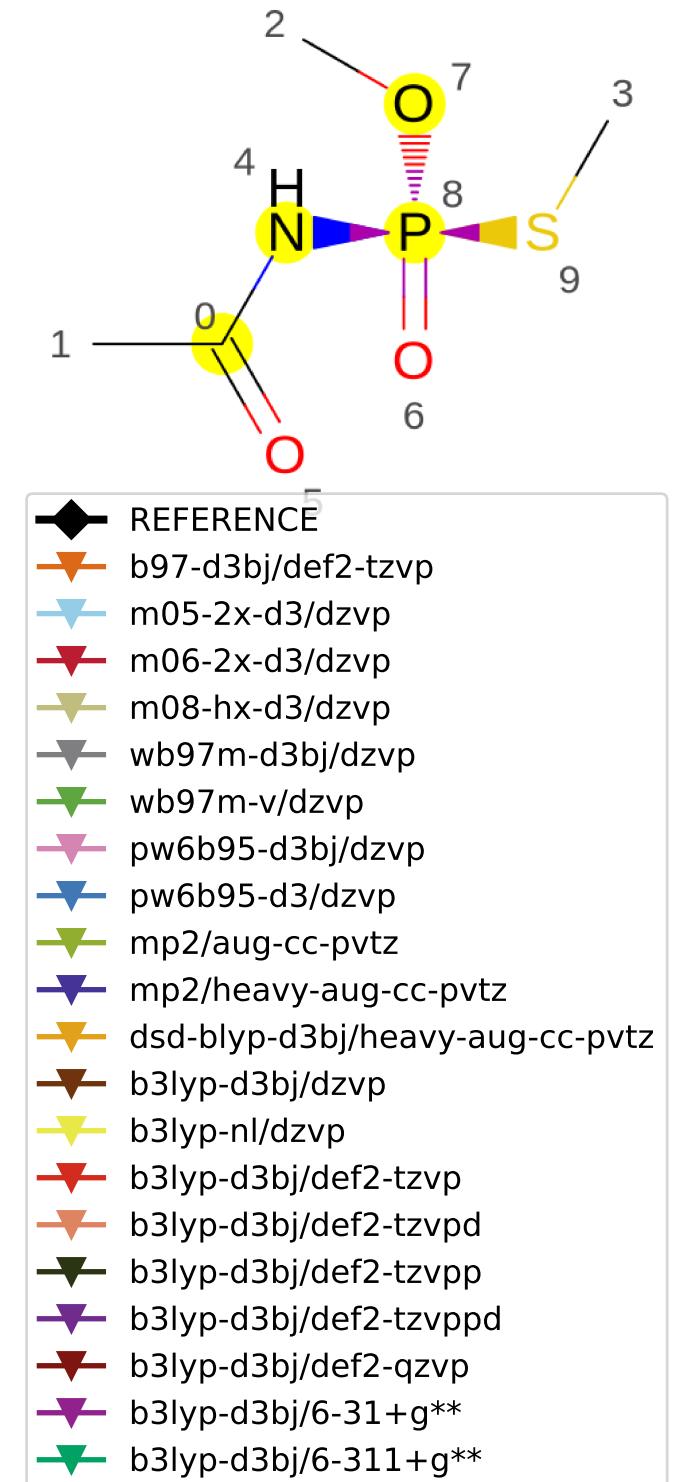
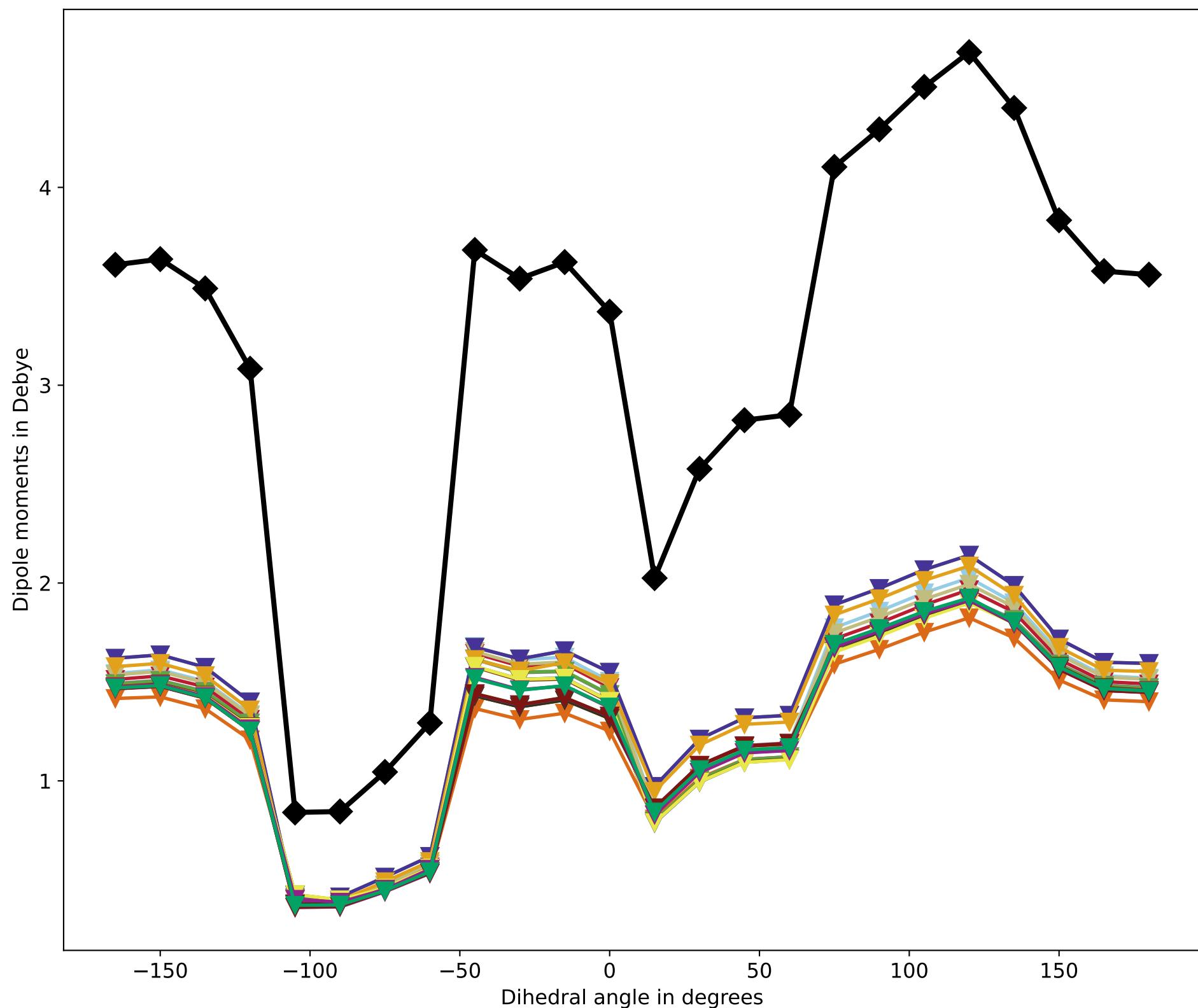




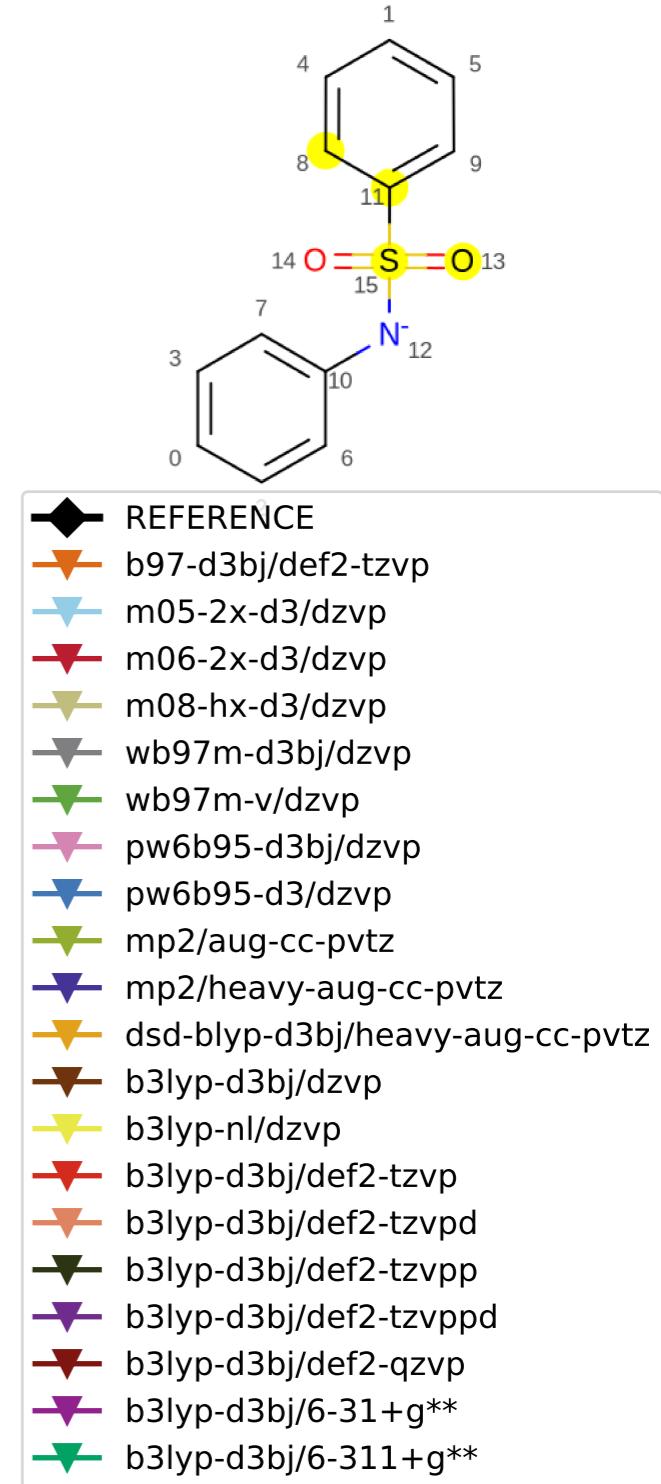
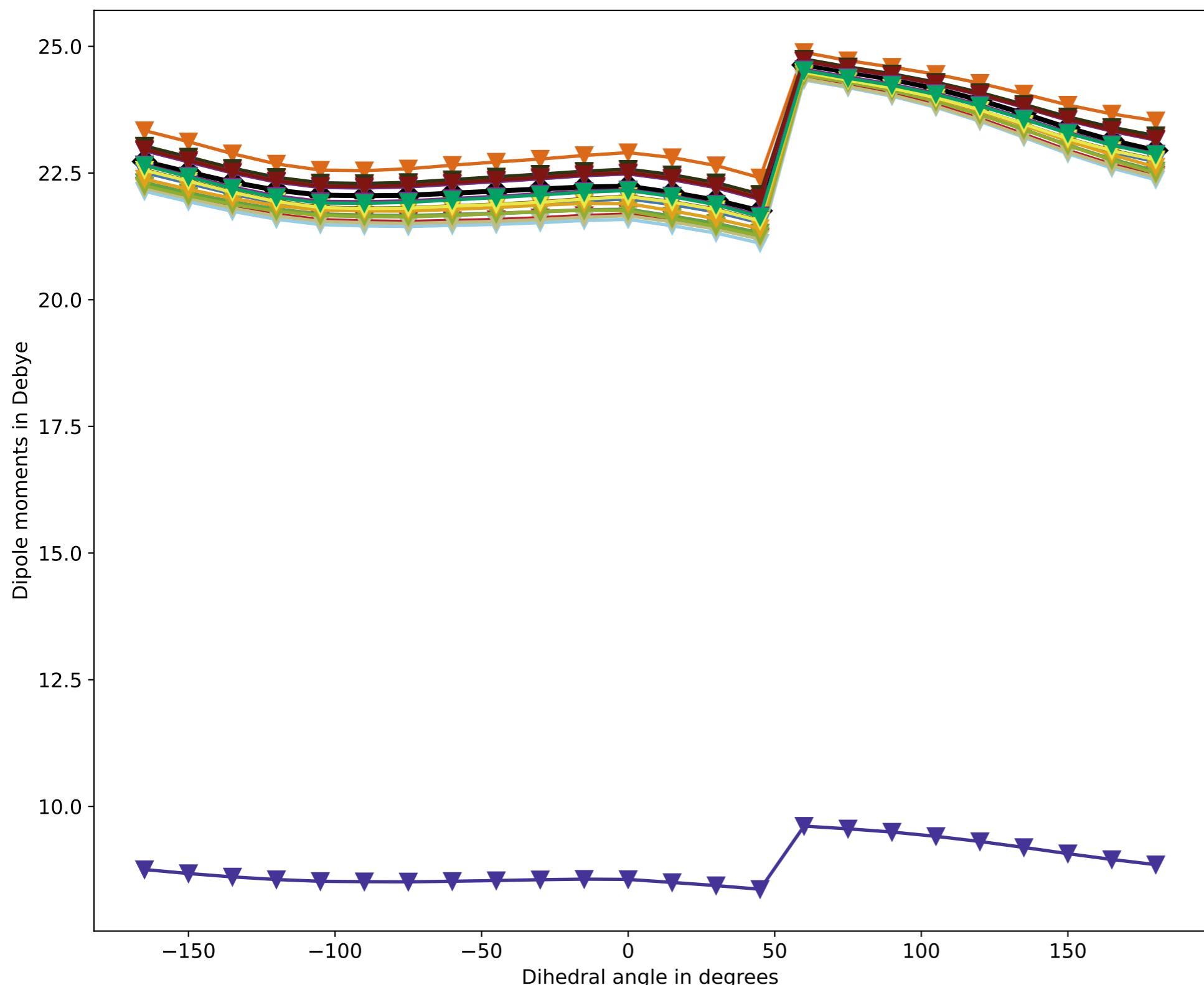
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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



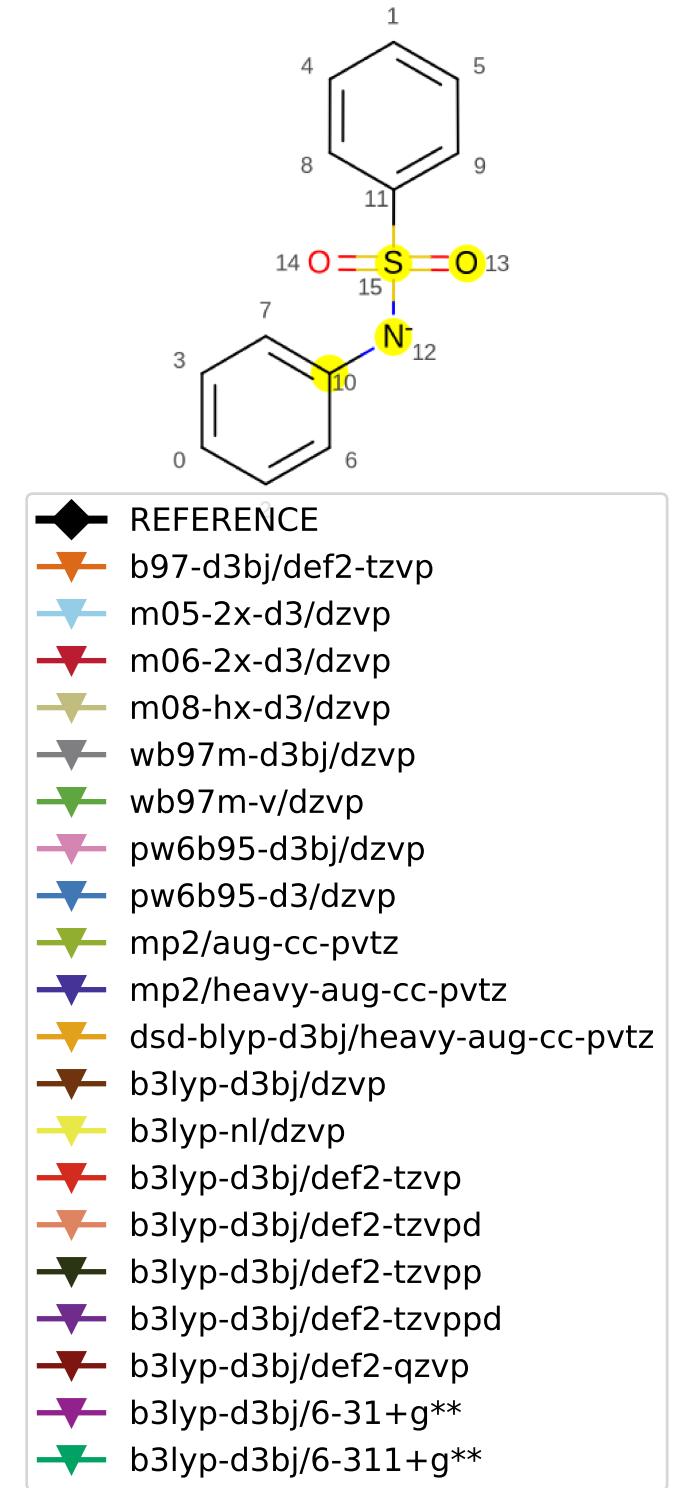
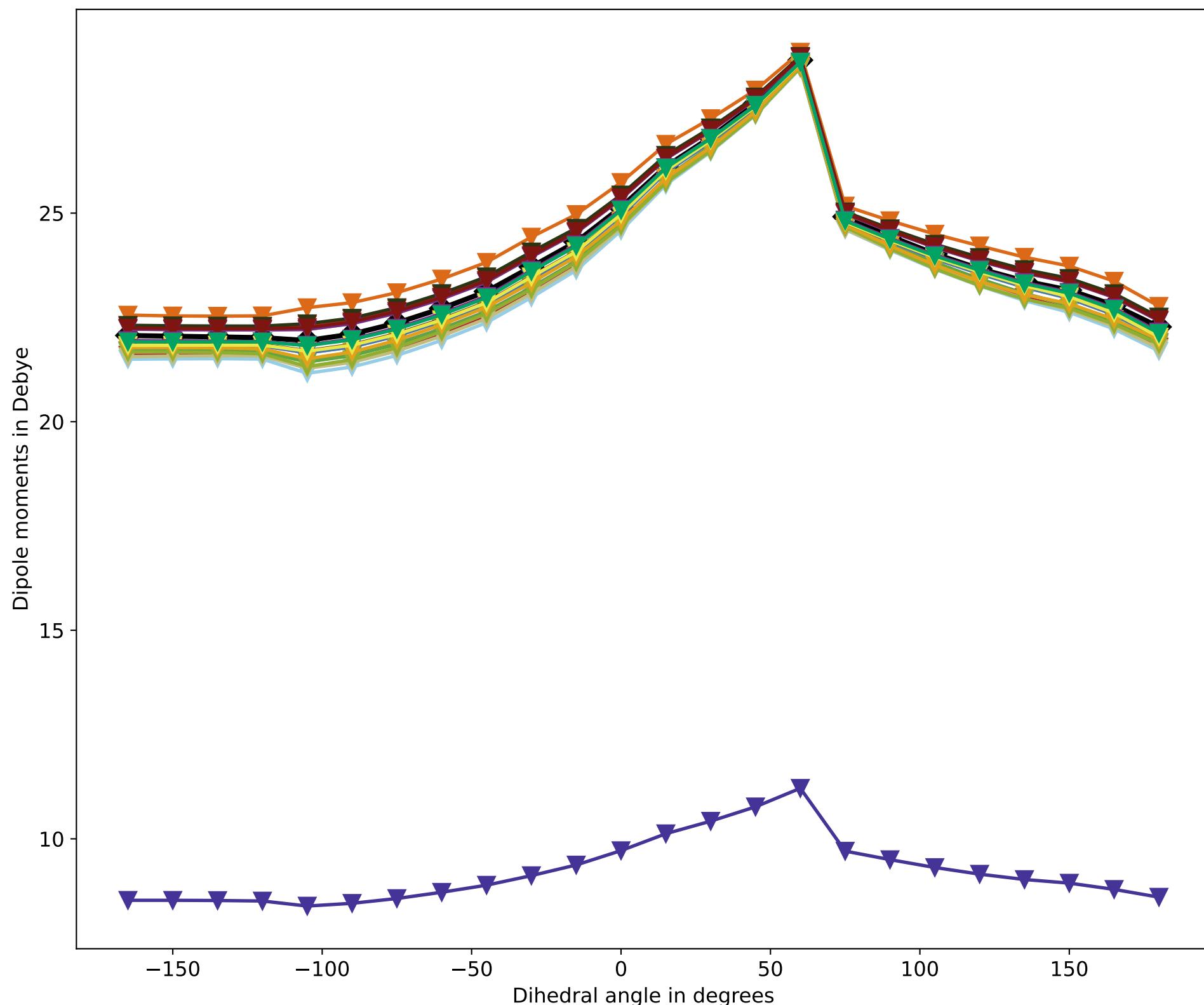
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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



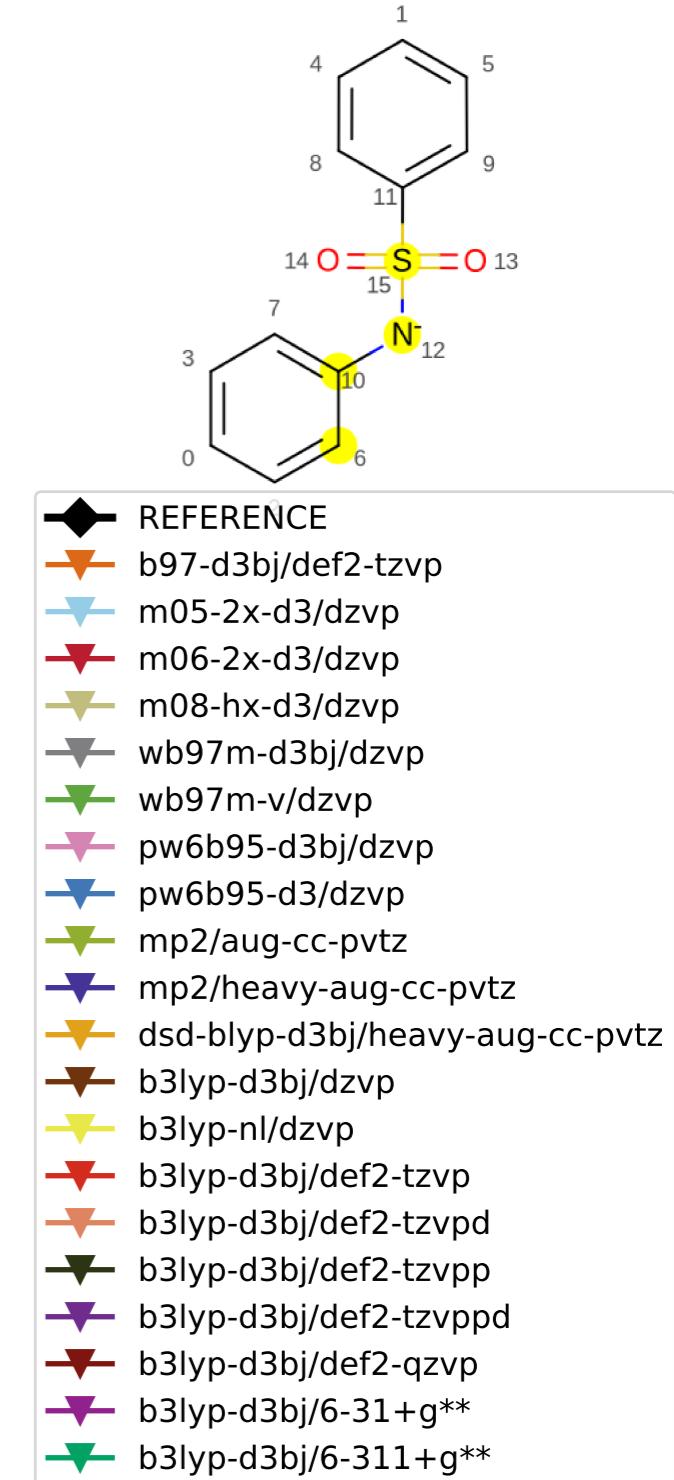
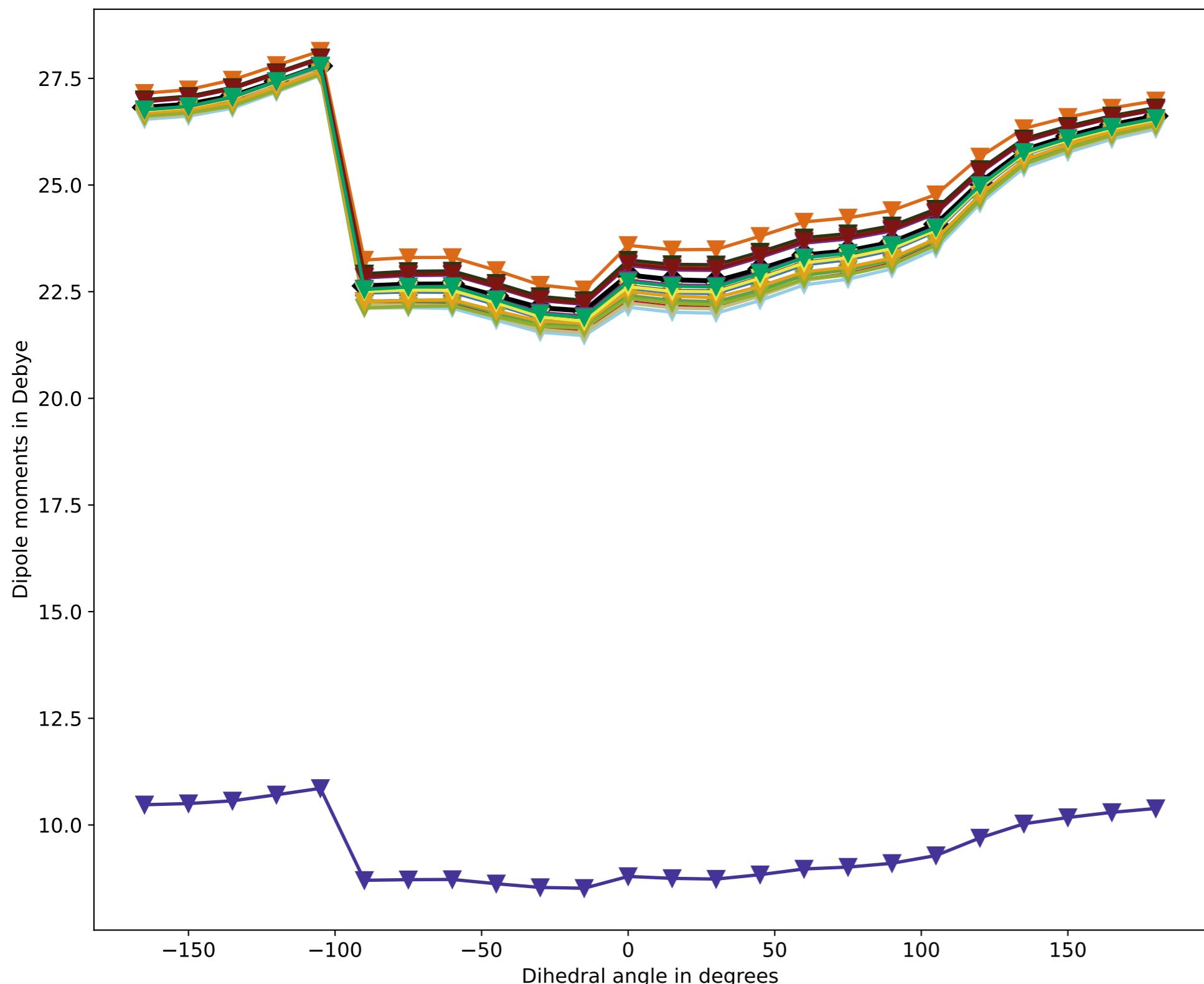
Charged molecule



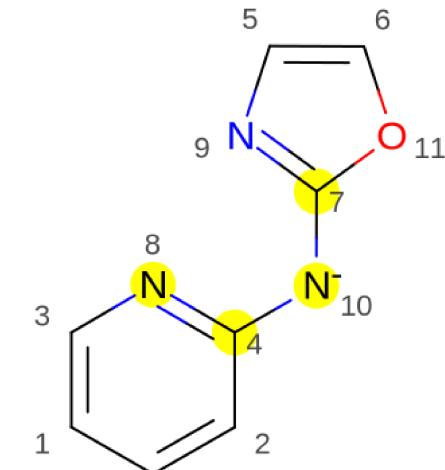
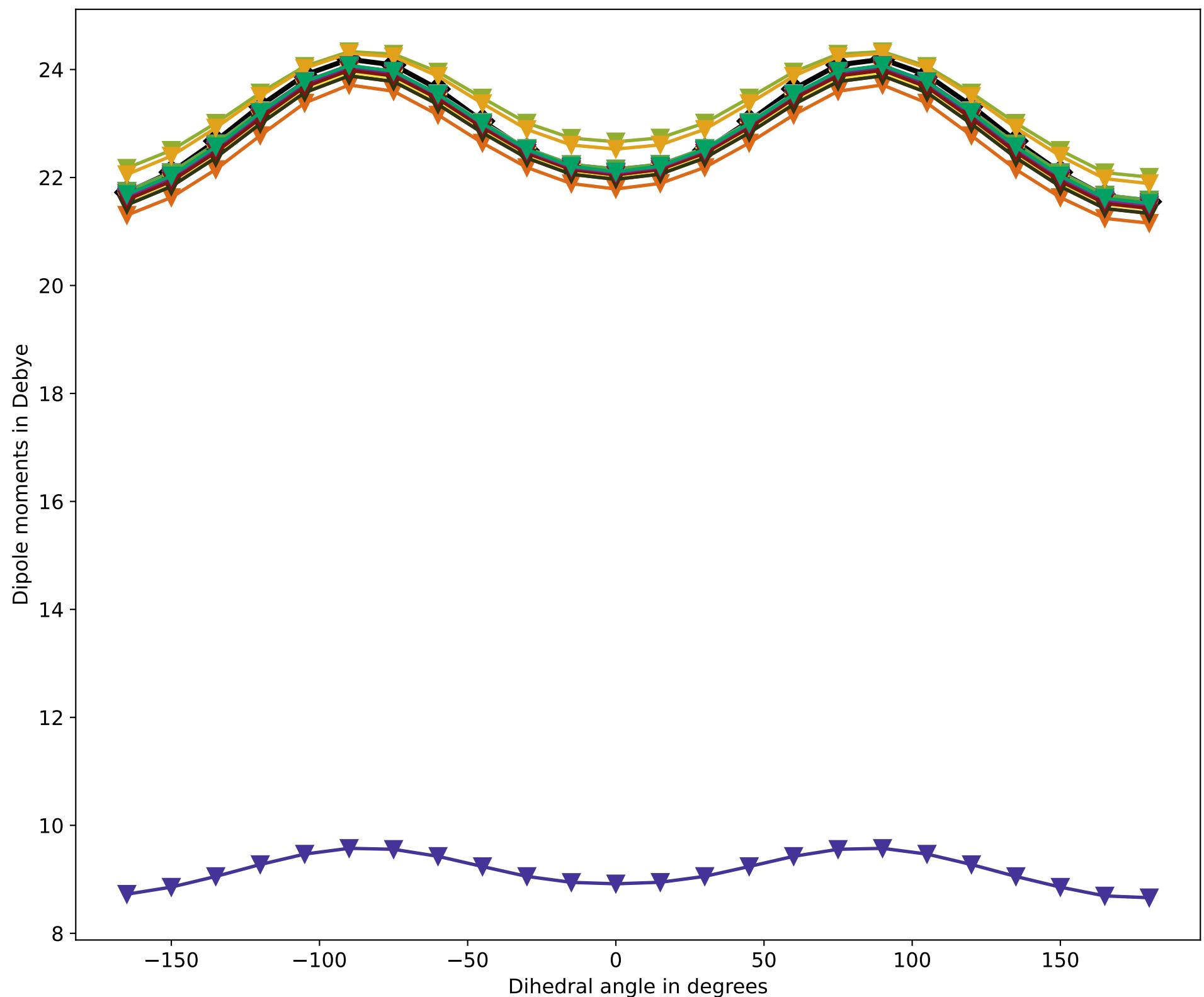
Charged molecule



Charged molecule

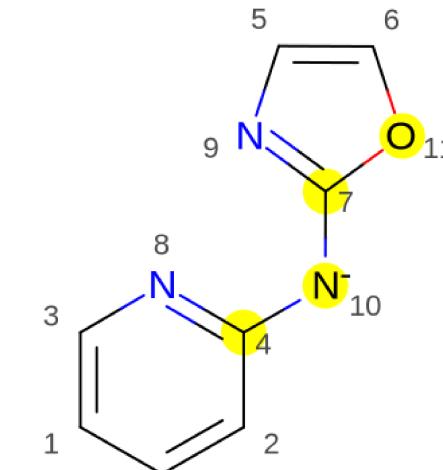
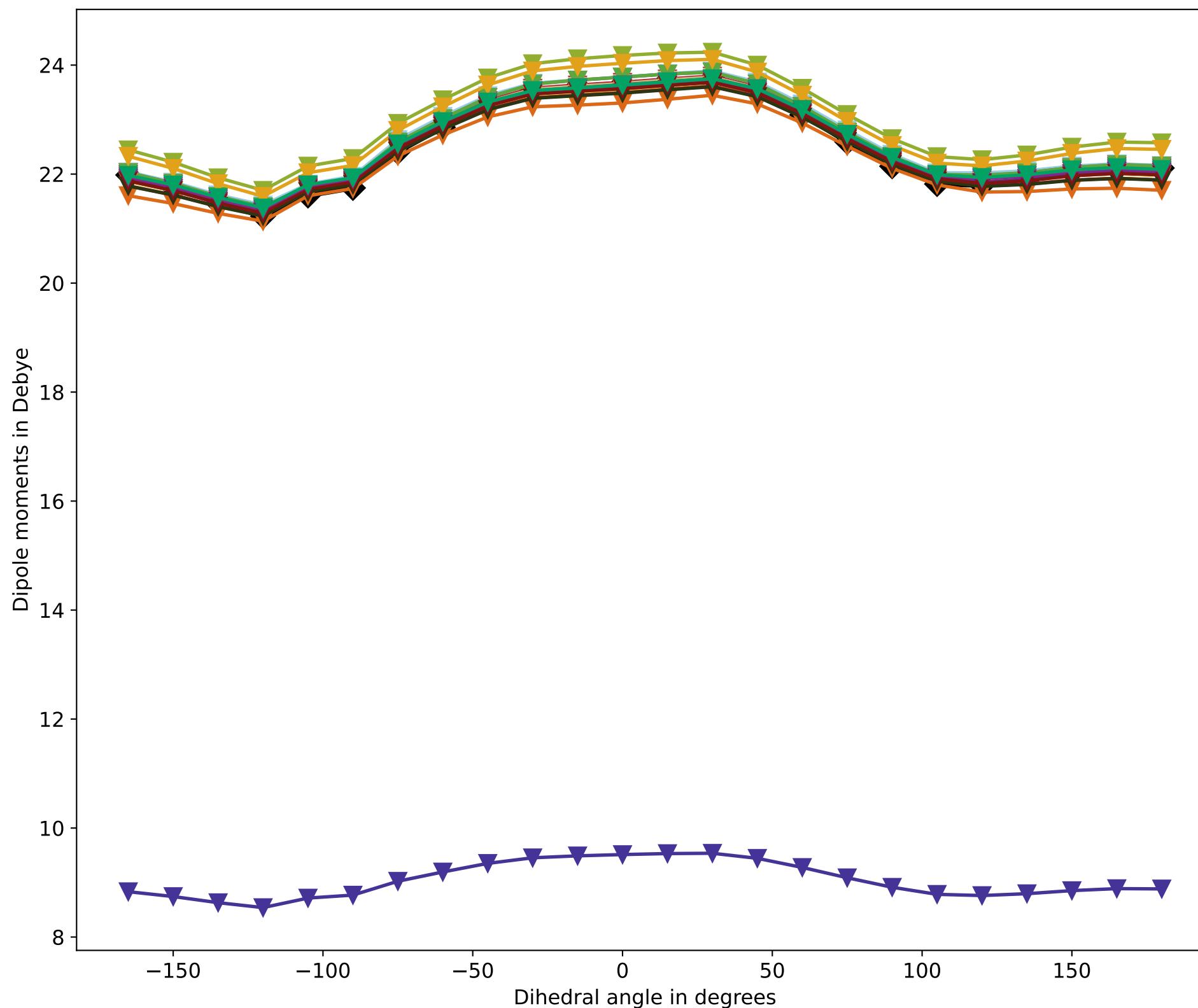


Charged molecule



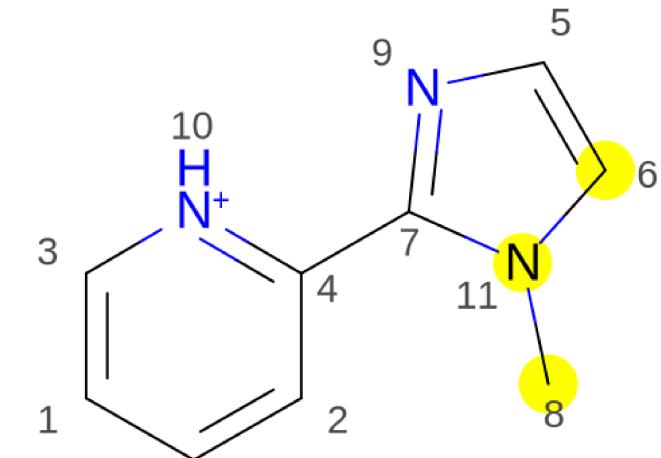
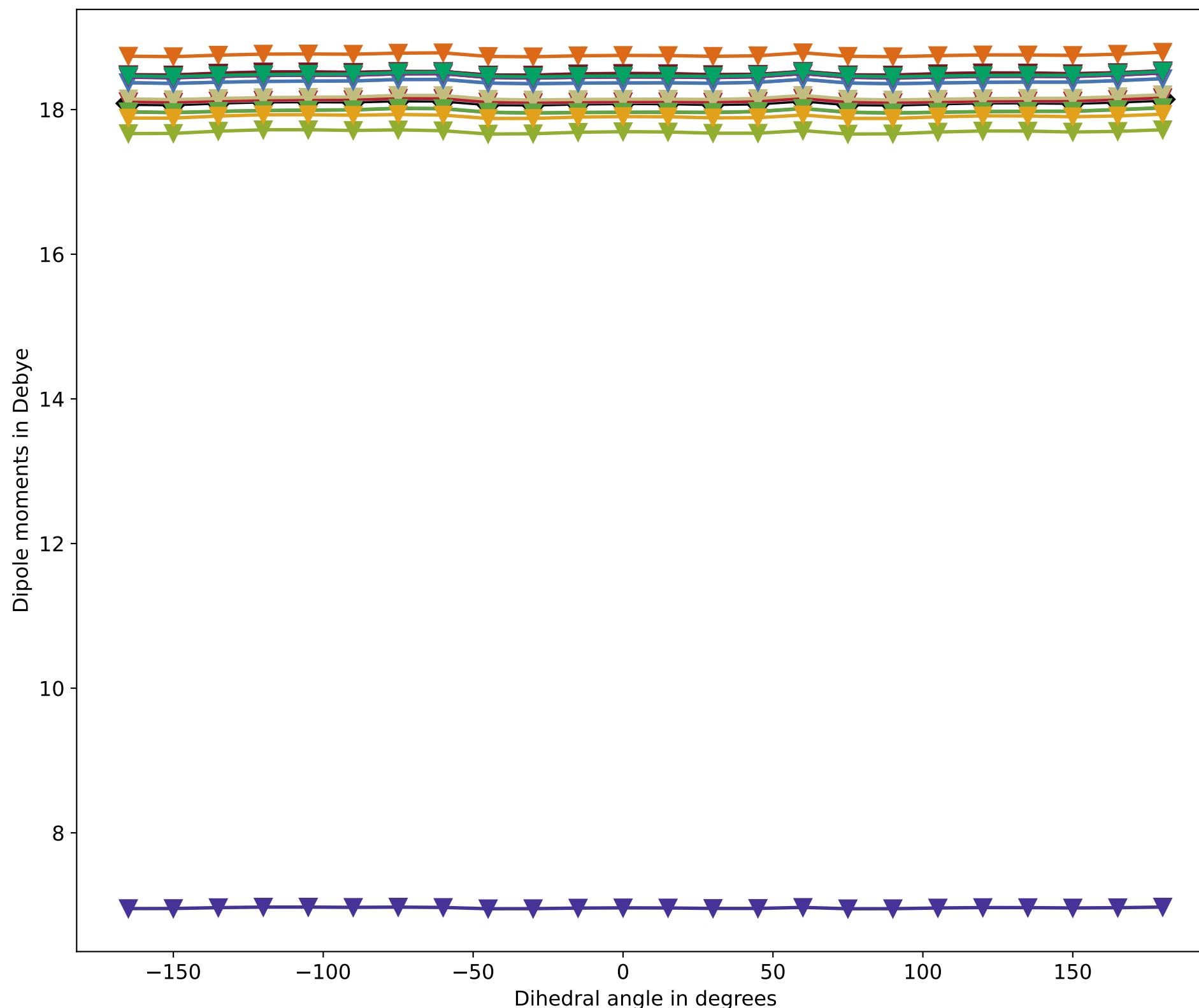
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

Charged molecule



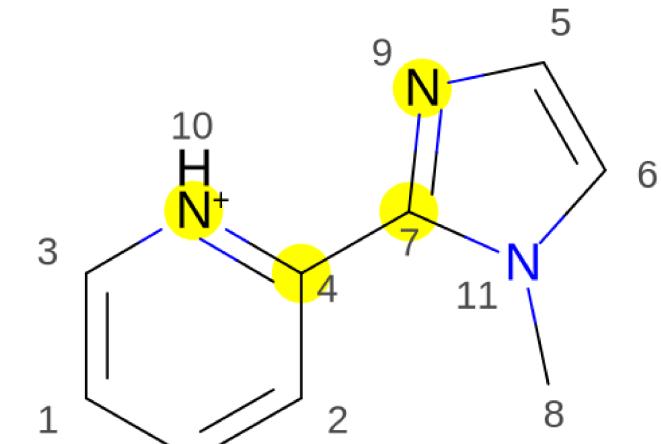
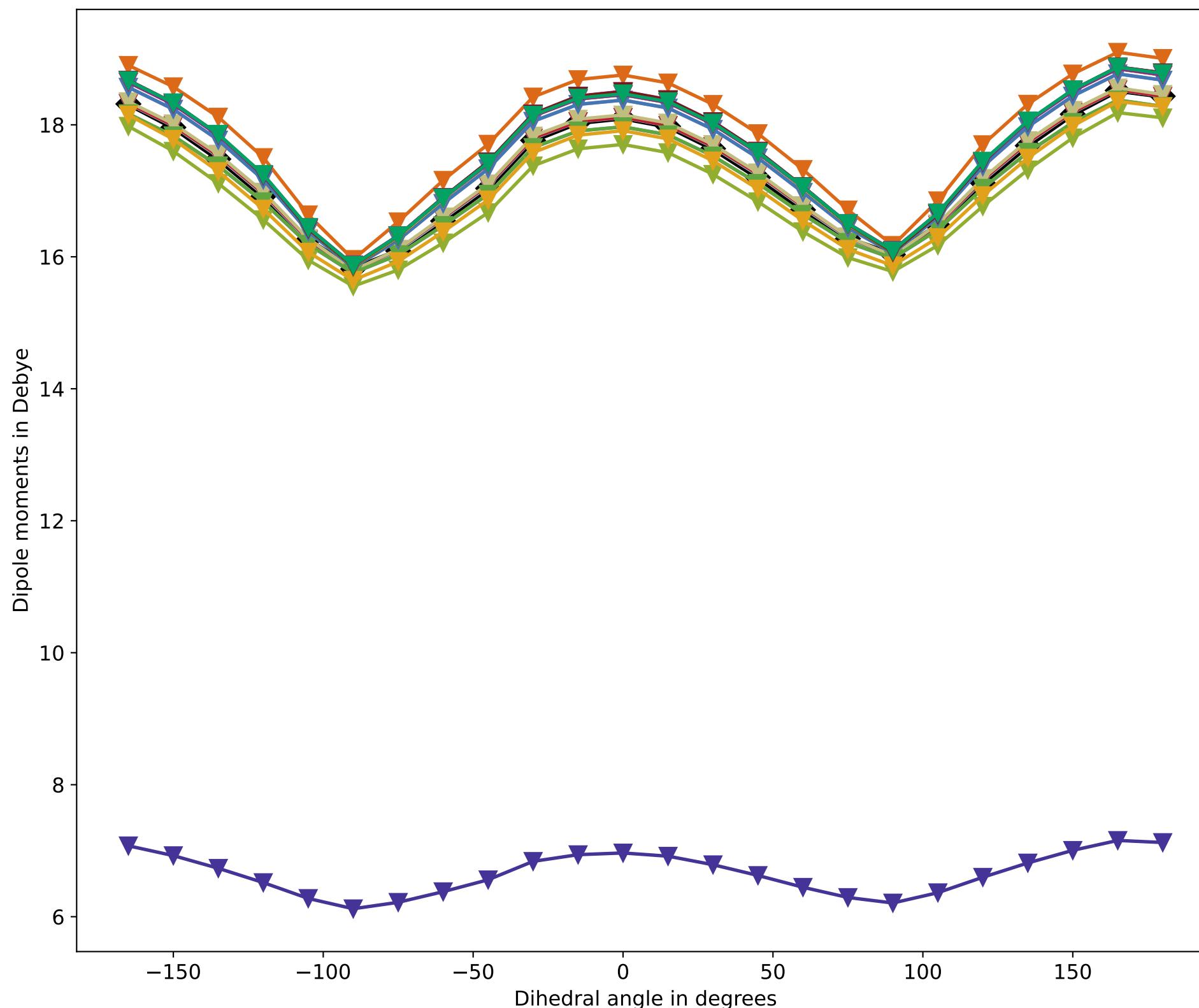
- | | |
|---|------------------------------|
| REFERENCE | Black diamond marker |
| b97-d3bj/def2-tzvp | Orange triangle marker |
| m05-2x-d3/dzvp | Light blue triangle marker |
| m06-2x-d3/dzvp | Red triangle marker |
| m08-hx-d3/dzvp | Yellow-green triangle marker |
| wb97m-d3bj/dzvp | Grey triangle marker |
| wb97m-v/dzvp | Green triangle marker |
| pw6b95-d3bj/dzvp | Magenta triangle marker |
| pw6b95-d3/dzvp | Blue triangle marker |
| mp2/aug-cc-pvtz | Dark green triangle marker |
| mp2/heavy-aug-cc-pvtz | Purple triangle marker |
| dsd-bllyp-d3bj/heavy-aug-cc-pvtz | Yellow triangle marker |
| b3lyp-d3bj/dzvp | Brown triangle marker |
| b3lyp-nl/dzvp | Yellow-green triangle marker |
| b3lyp-d3bj/def2-tzvp | Red triangle marker |
| b3lyp-d3bj/def2-tzvpd | Orange triangle marker |
| b3lyp-d3bj/def2-tzvpp | Black triangle marker |
| b3lyp-d3bj/def2-tzvppd | Purple triangle marker |
| b3lyp-d3bj/def2-qzvp | Maroon triangle marker |
| b3lyp-d3bj/6-31+g** | Magenta triangle marker |
| b3lyp-d3bj/6-311+g** | Green triangle marker |

Charged molecule



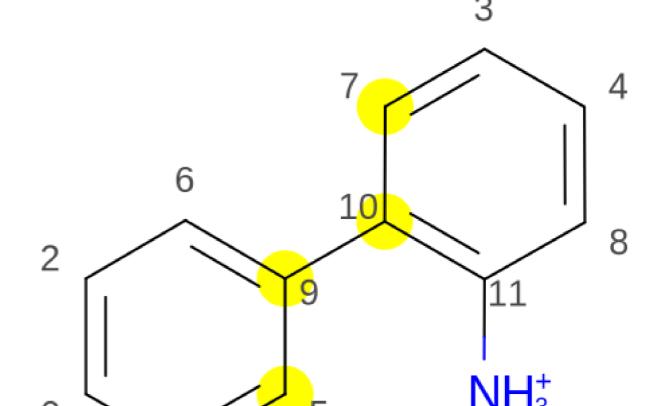
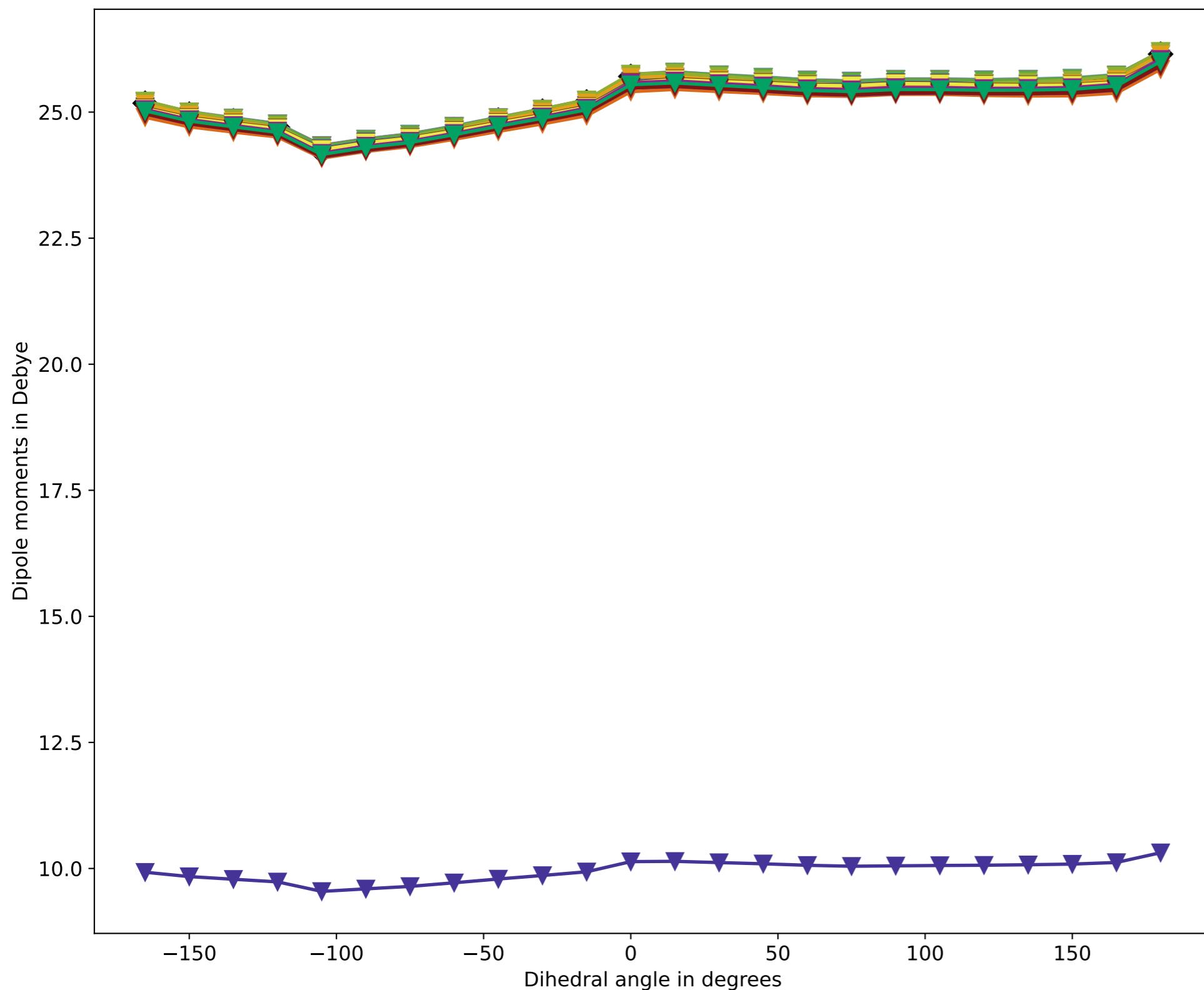
- ◆ REFERENCE
- b97-d3bj/def2-tzvp
- △ m05-2x-d3/dzvp
- ▼ m06-2x-d3/dzvp
- ◀ m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- ▲ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ▲ pw6b95-d3/dzvp
- ▼ mp2/aug-cc-pvtz
- ▶ mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ▼ b3lyp-d3bj/dzvp
- ▲ b3lyp-nl/dzvp
- ▼ b3lyp-d3bj/def2-tzvp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

Charged molecule



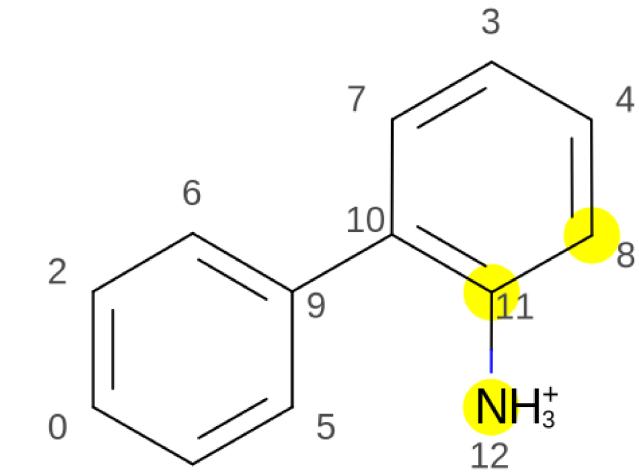
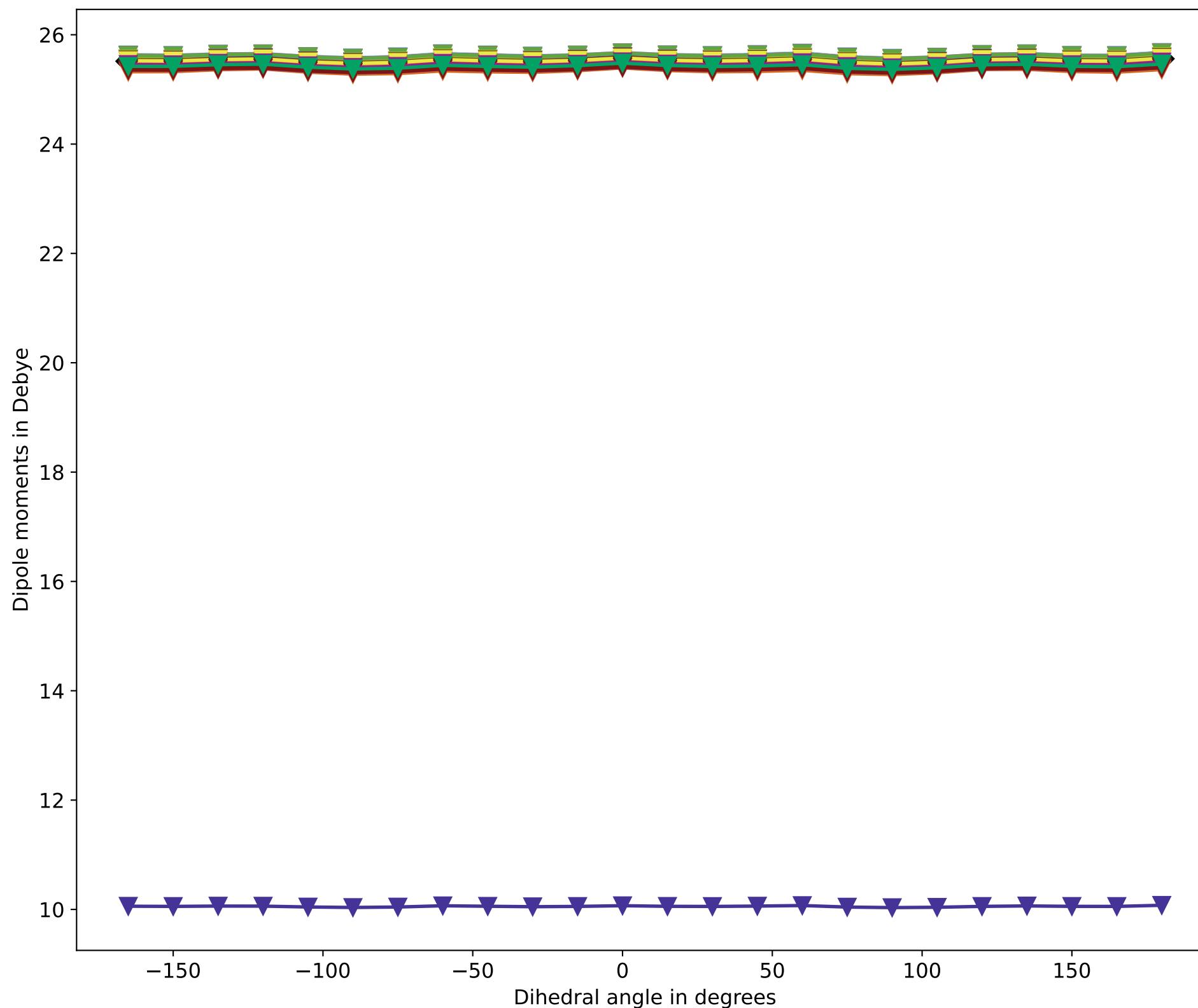
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd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

Charged molecule



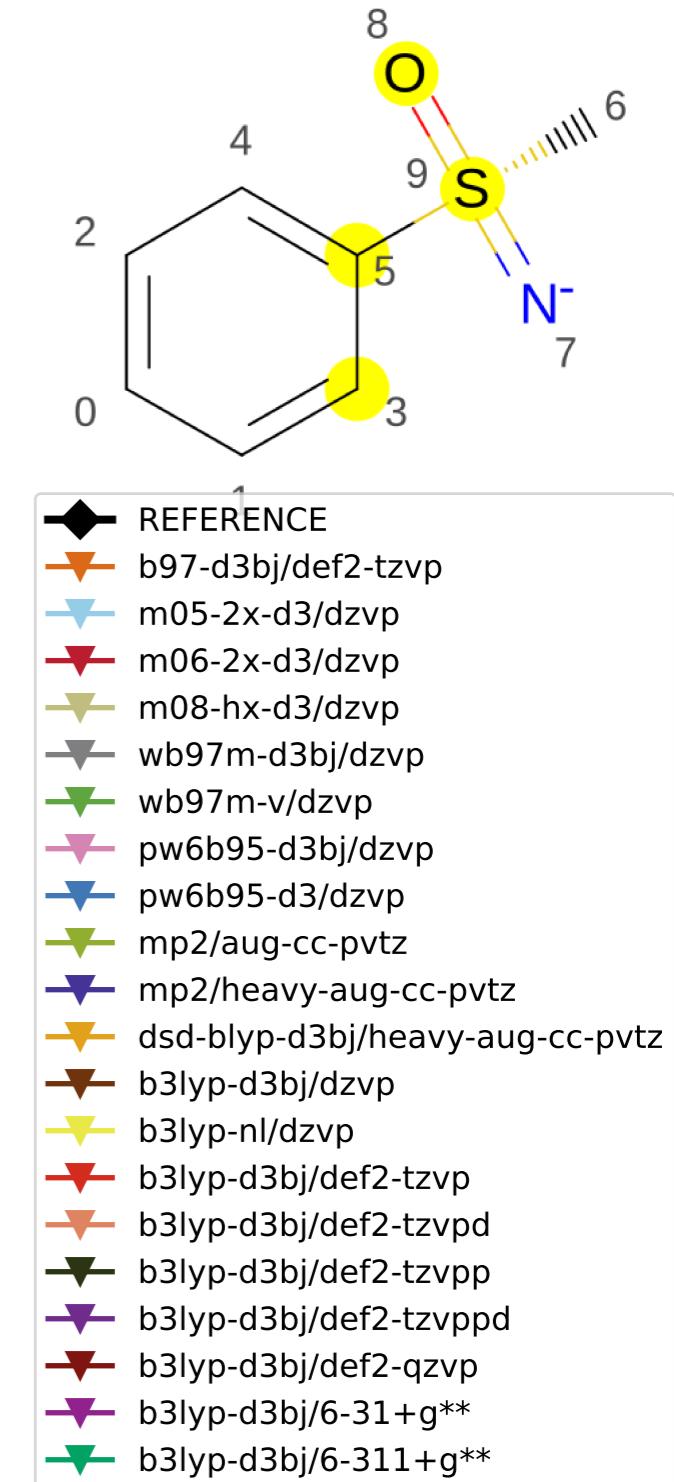
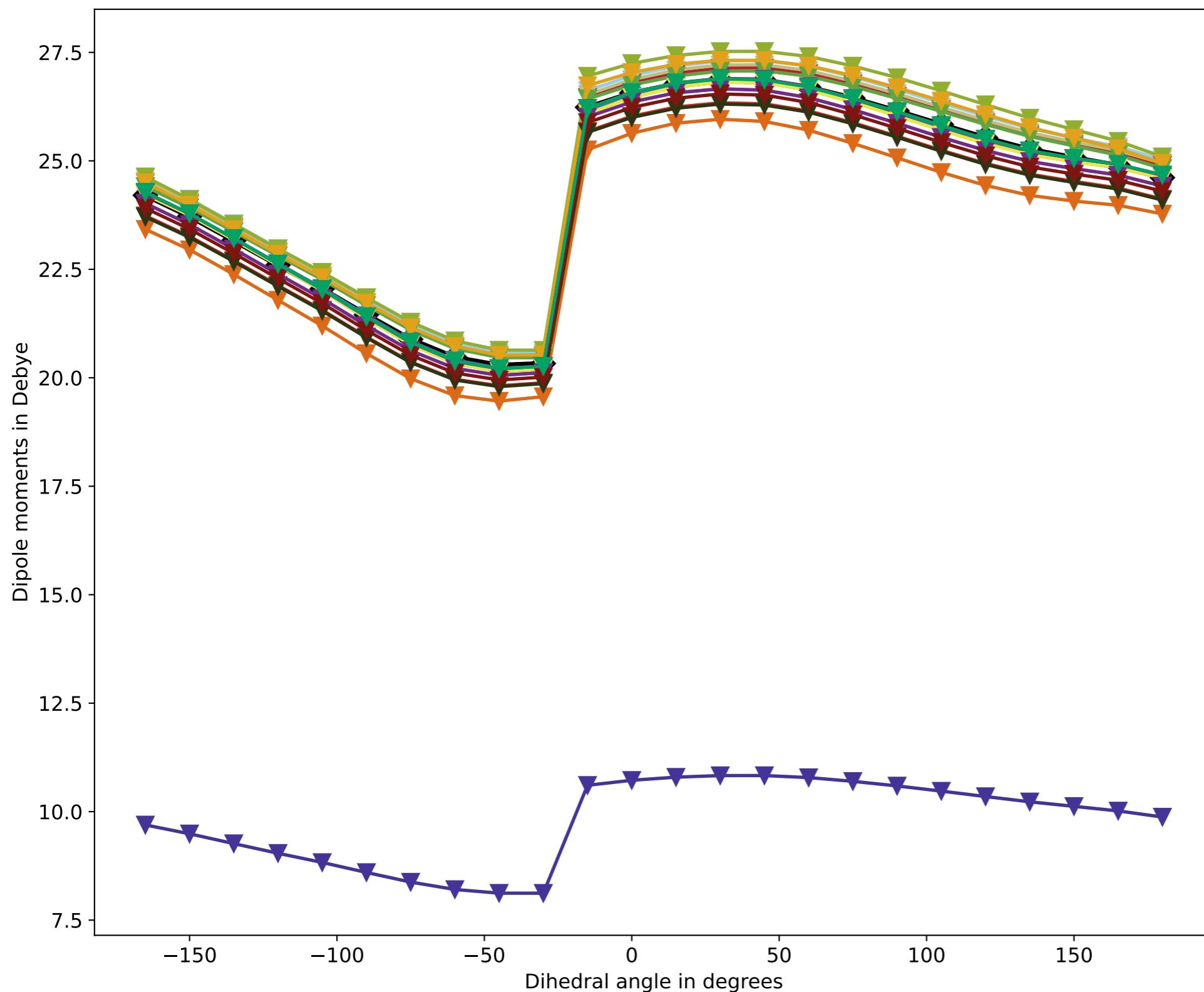
- REFERENCE
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd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

Charged molecule

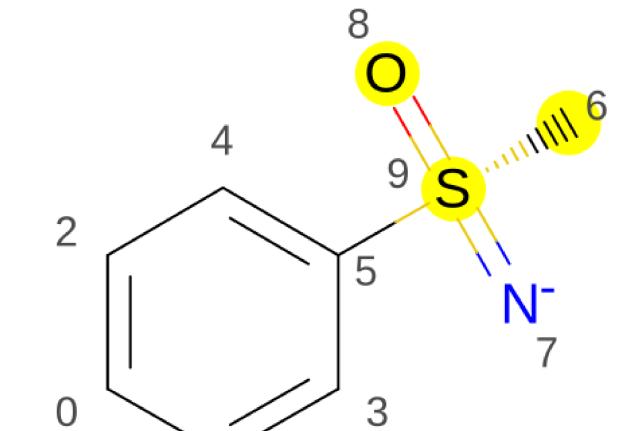
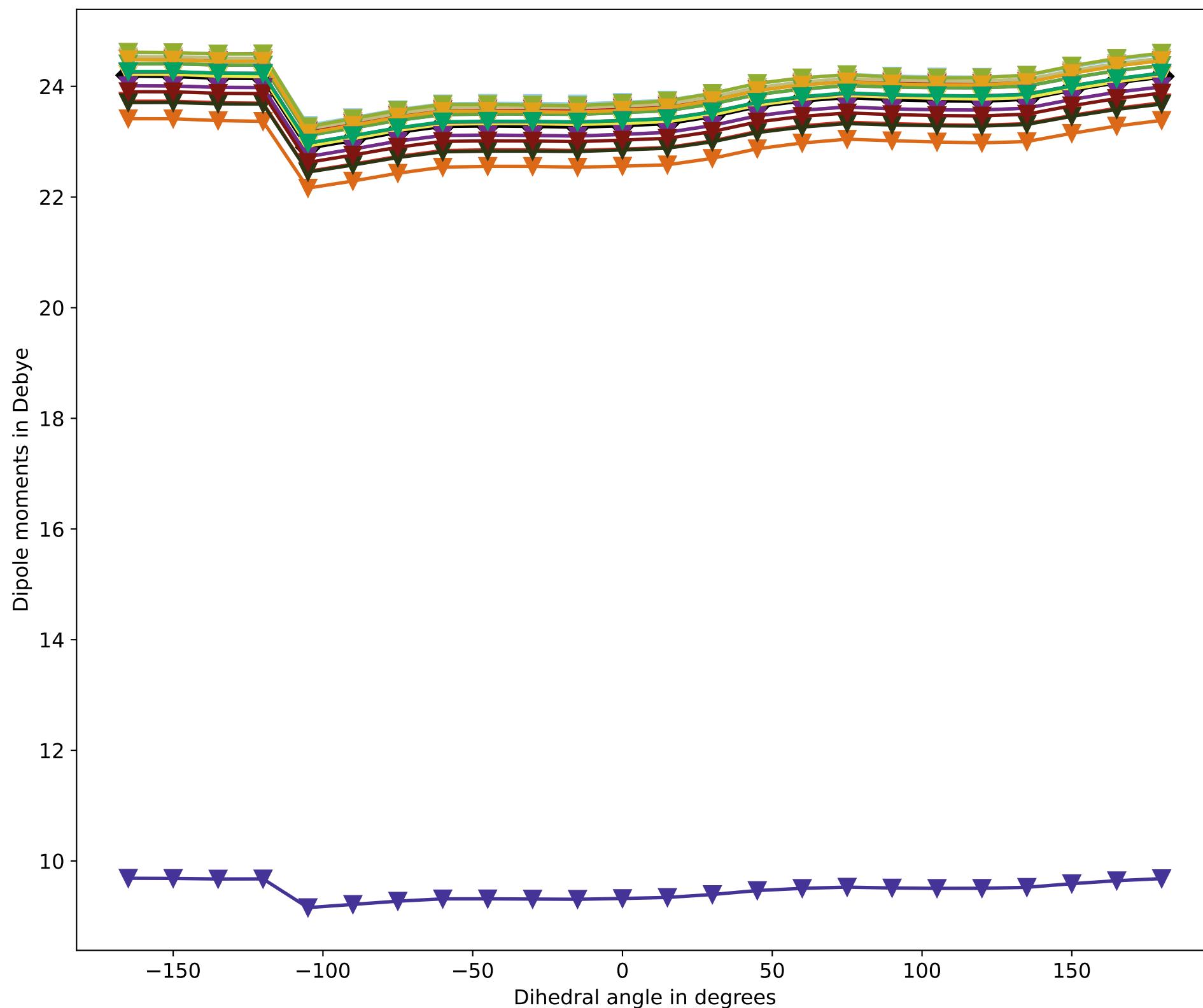


- ◆ REFERENCE
- b97-d3bj/def2-tzvp
- △ m05-2x-d3/dzvp
- ▼ m06-2x-d3/dzvp
- ◀ m08-hx-d3/dzvp
- ▬ wb97m-d3bj/dzvp
- ▲ wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- ▬ pw6b95-d3/dzvp
- ▲ mp2/aug-cc-pvtz
- ▼ mp2/heavy-aug-cc-pvtz
- ▬ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ▬ b3lyp-d3bj/dzvp
- ▬ b3lyp-nl/dzvp
- ▼ b3lyp-d3bj/def2-tzvp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

Charged molecule

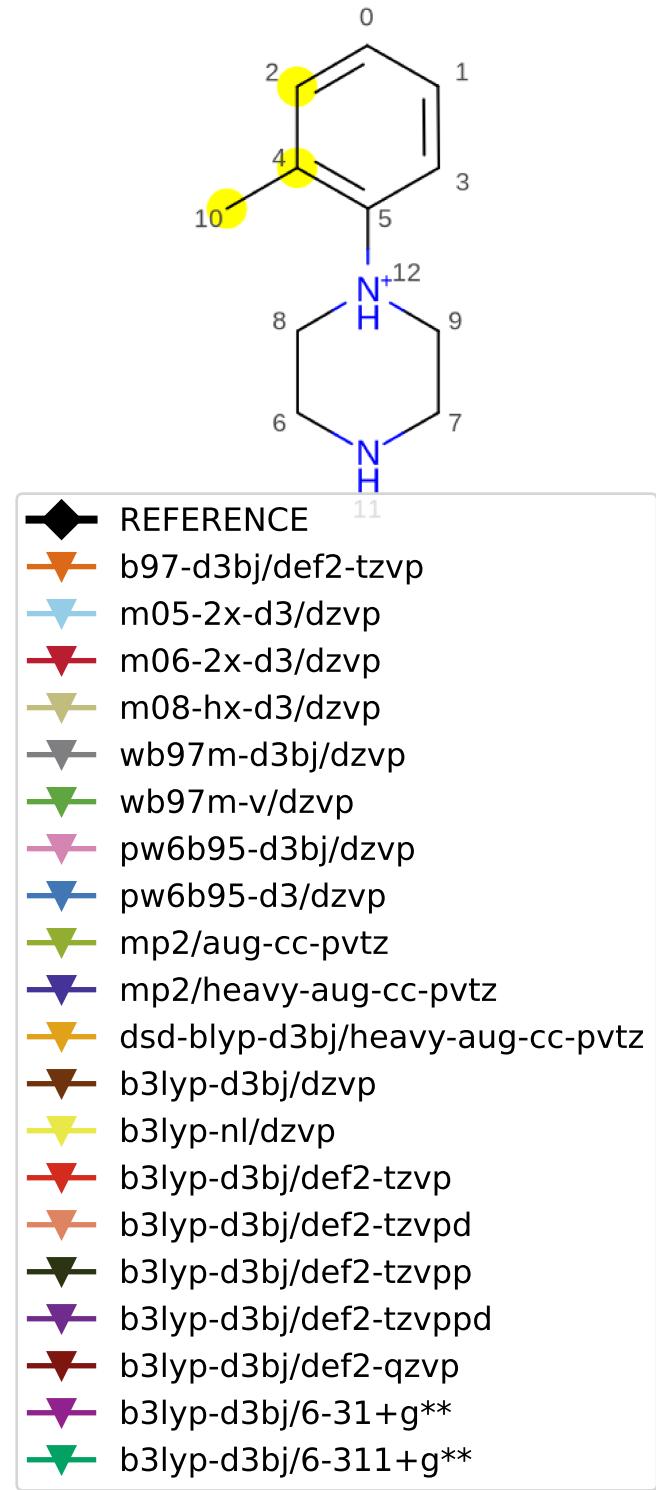
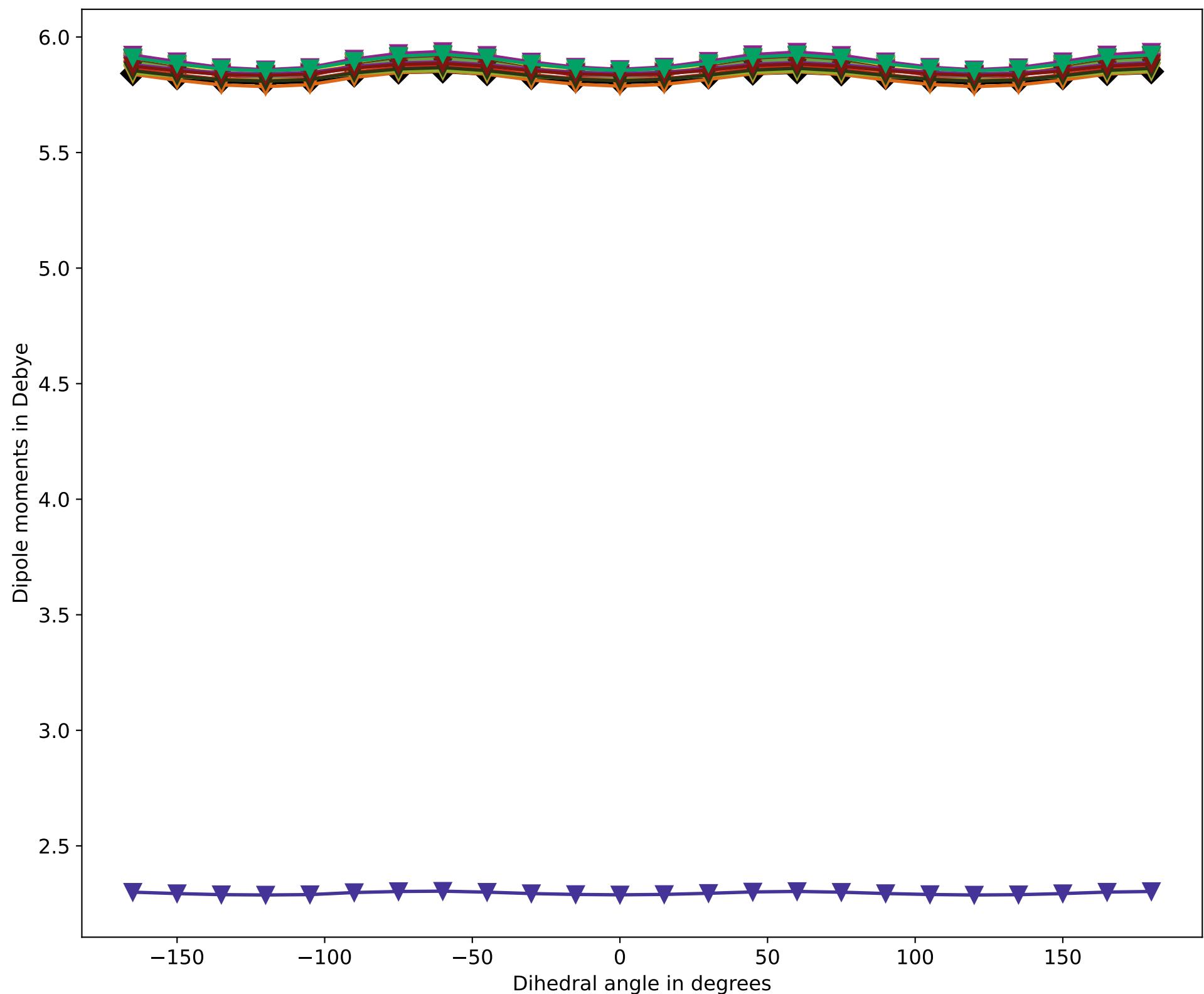


Charged molecule

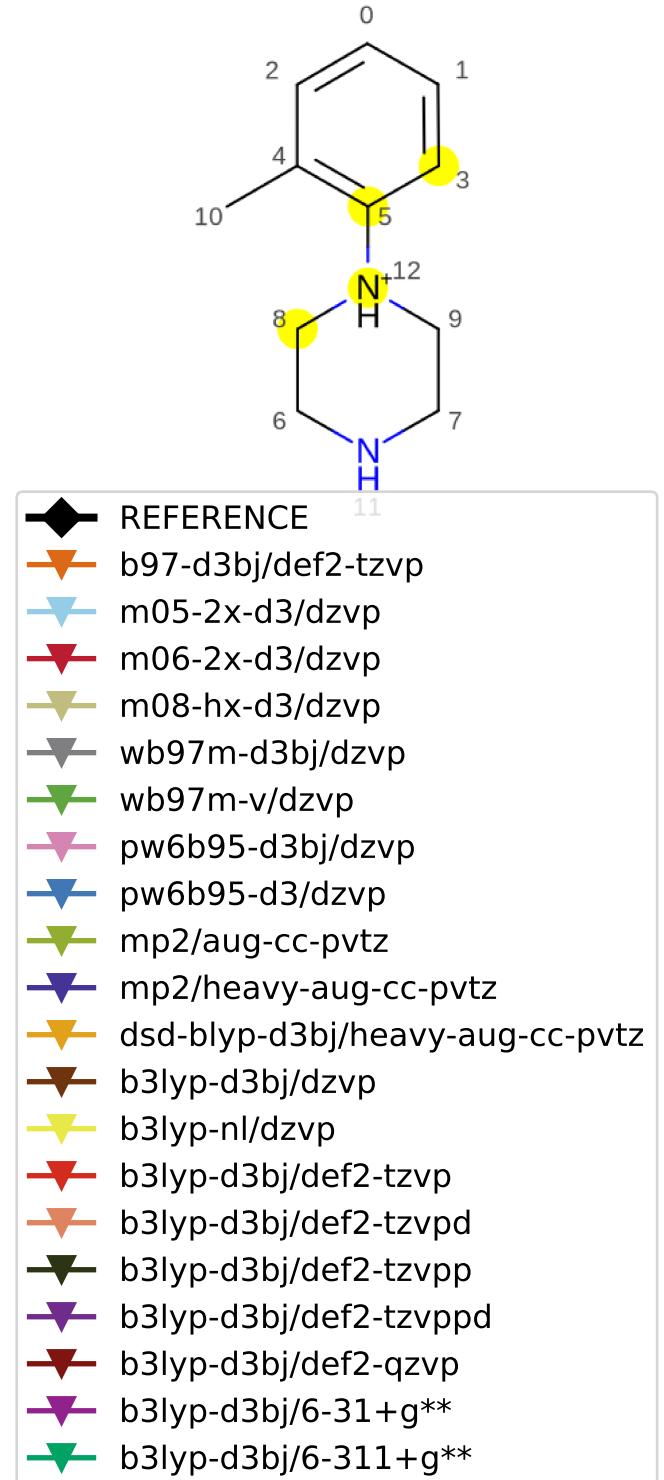
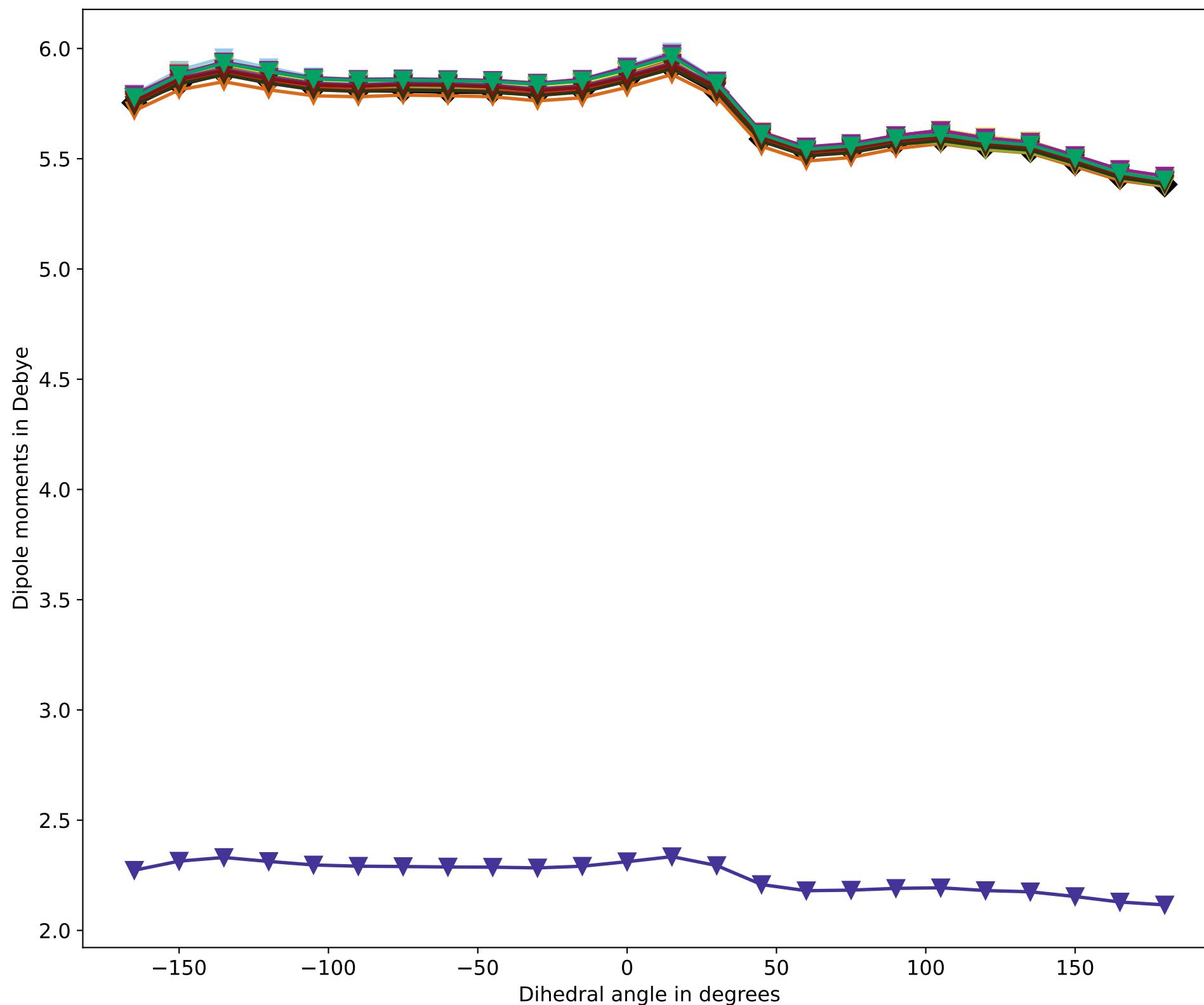


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

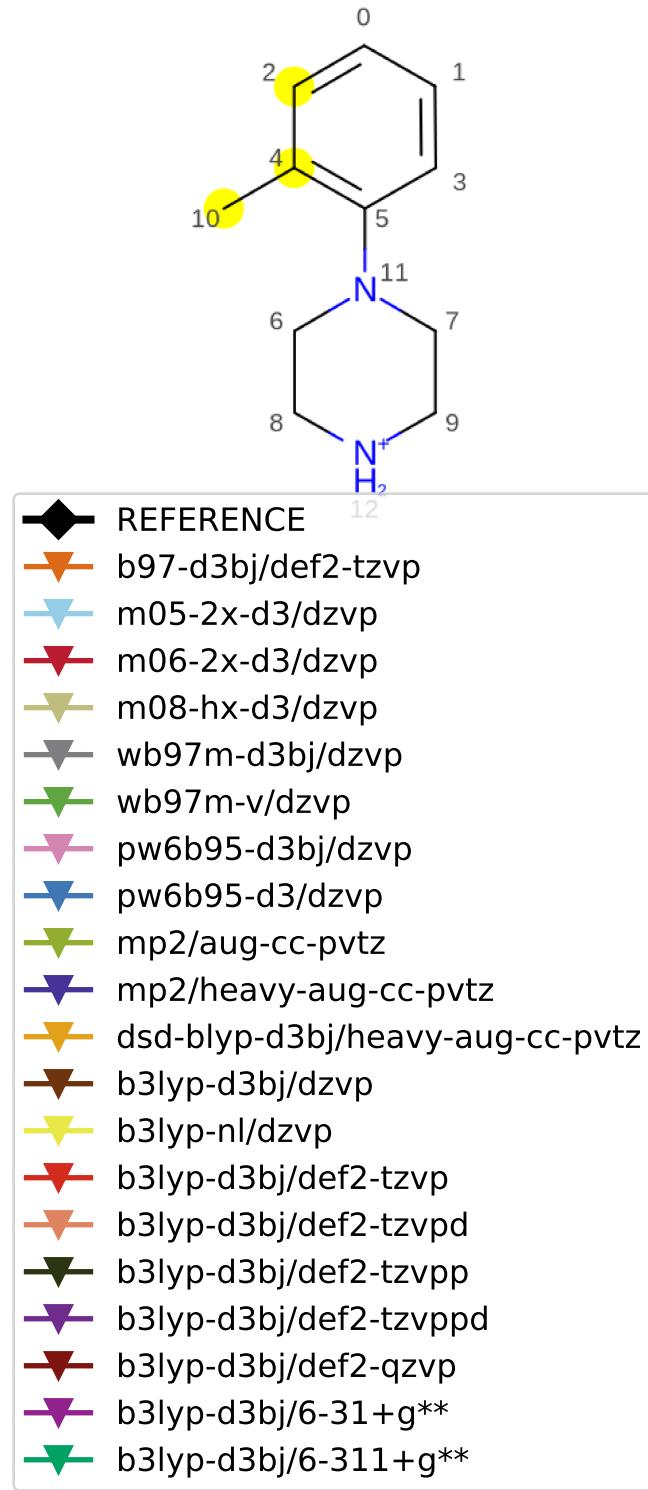
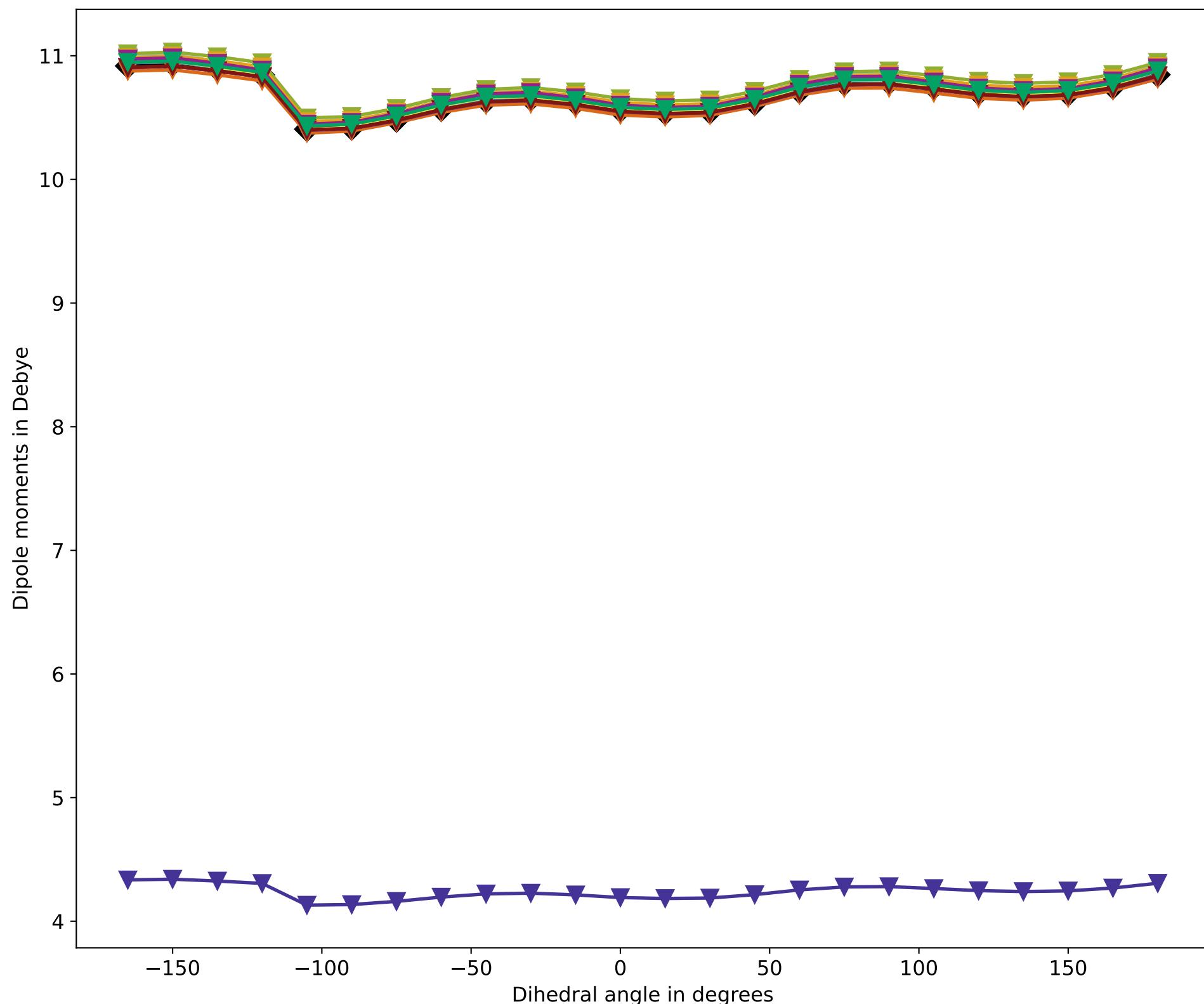
Charged molecule

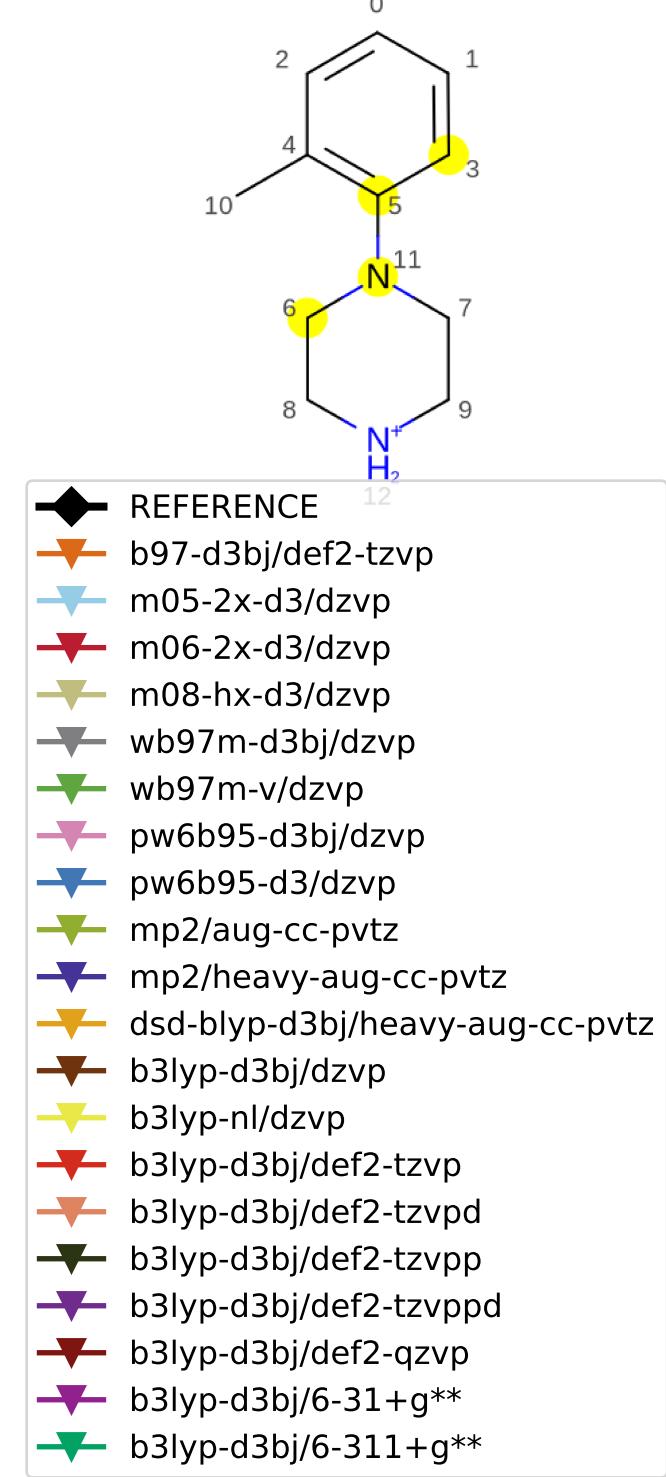
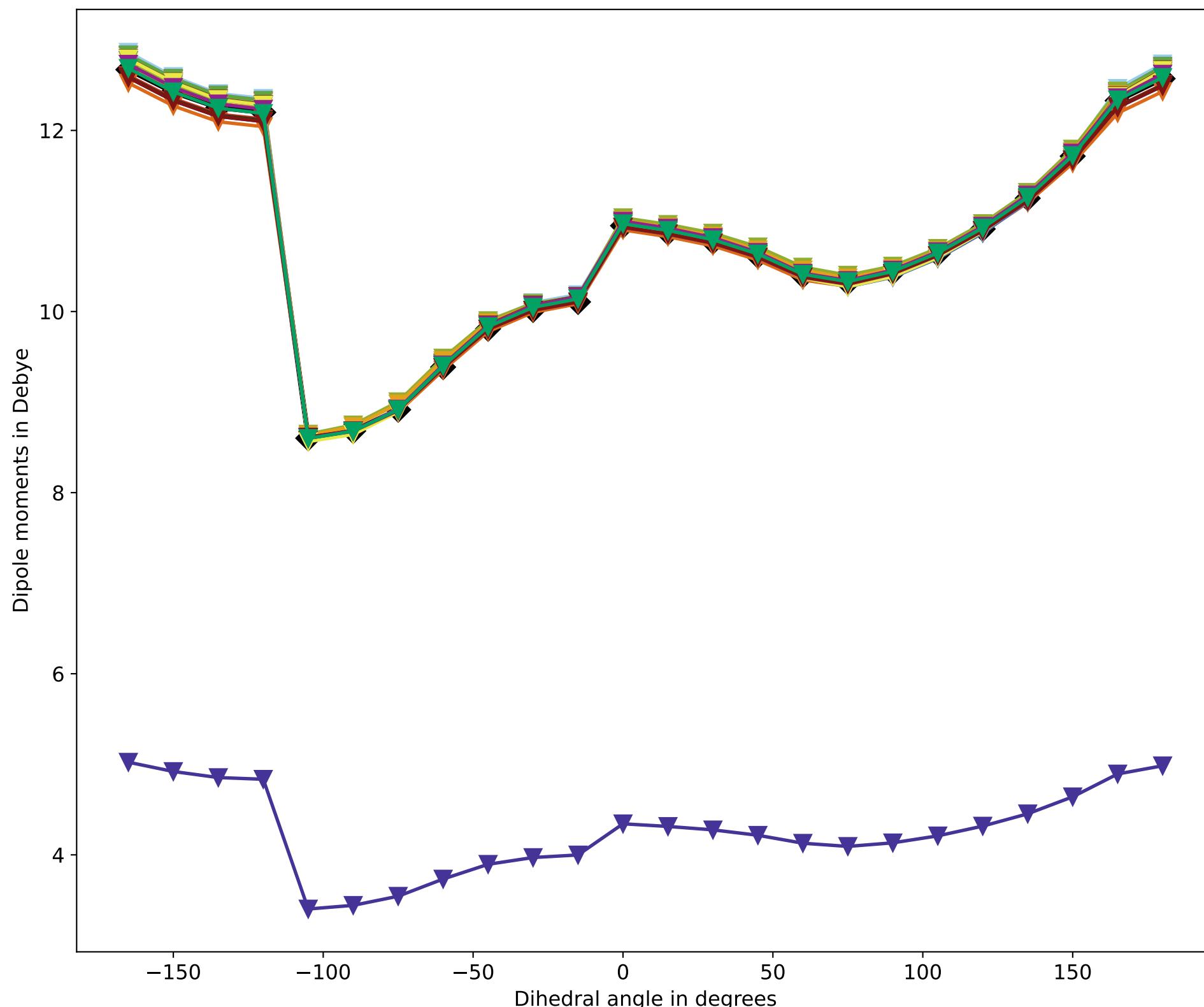


Charged molecule

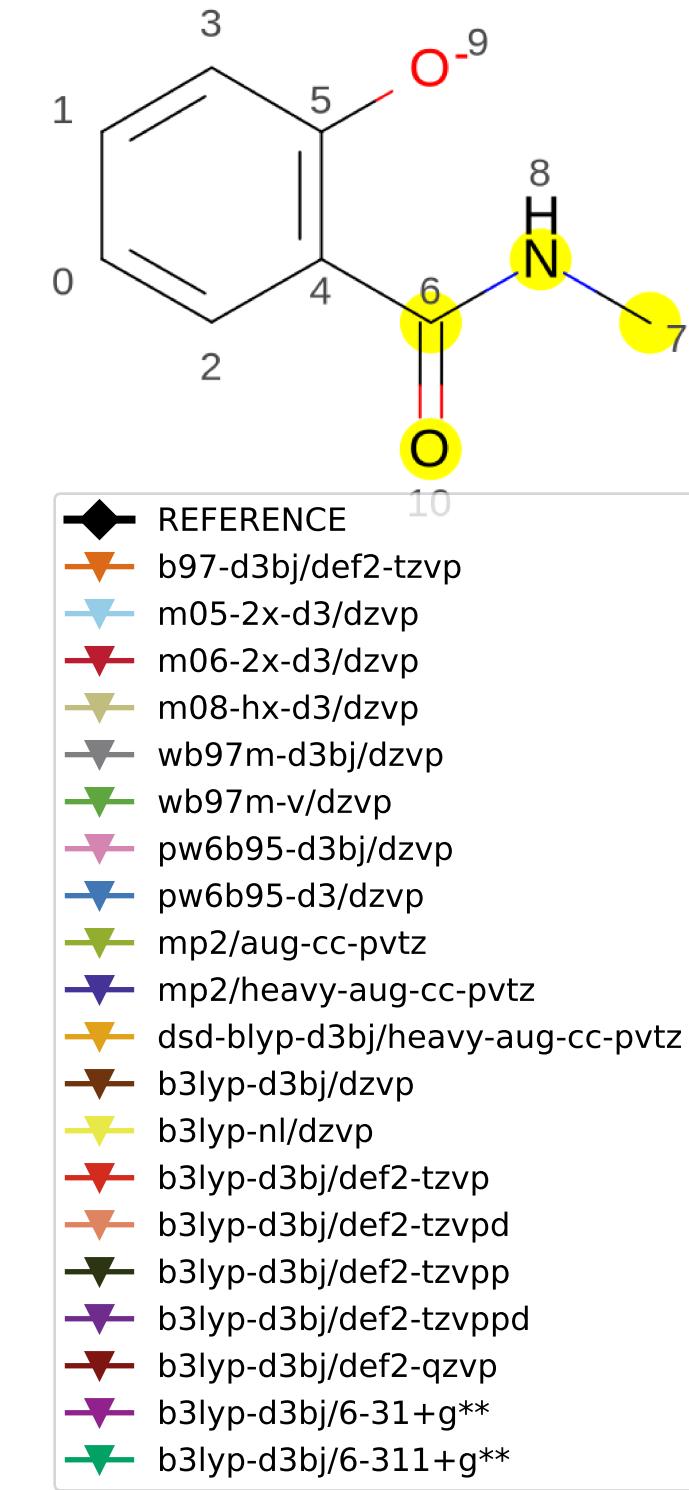
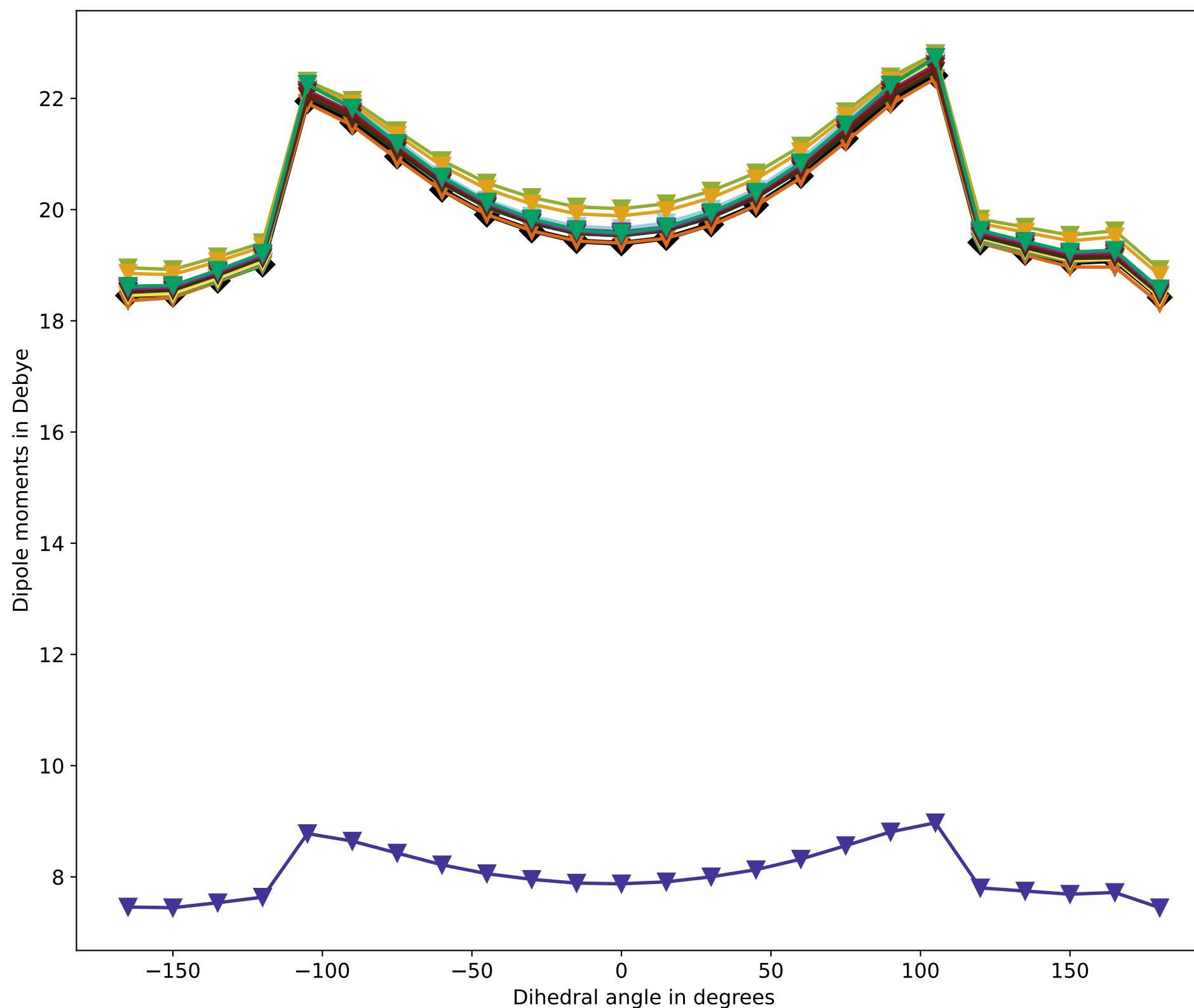


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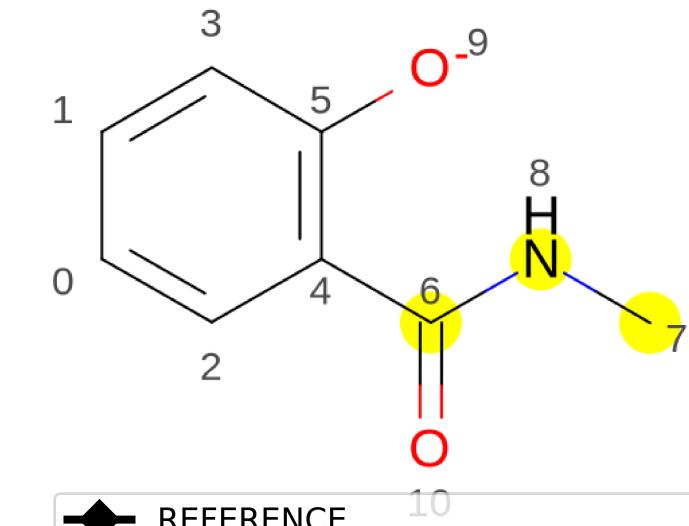
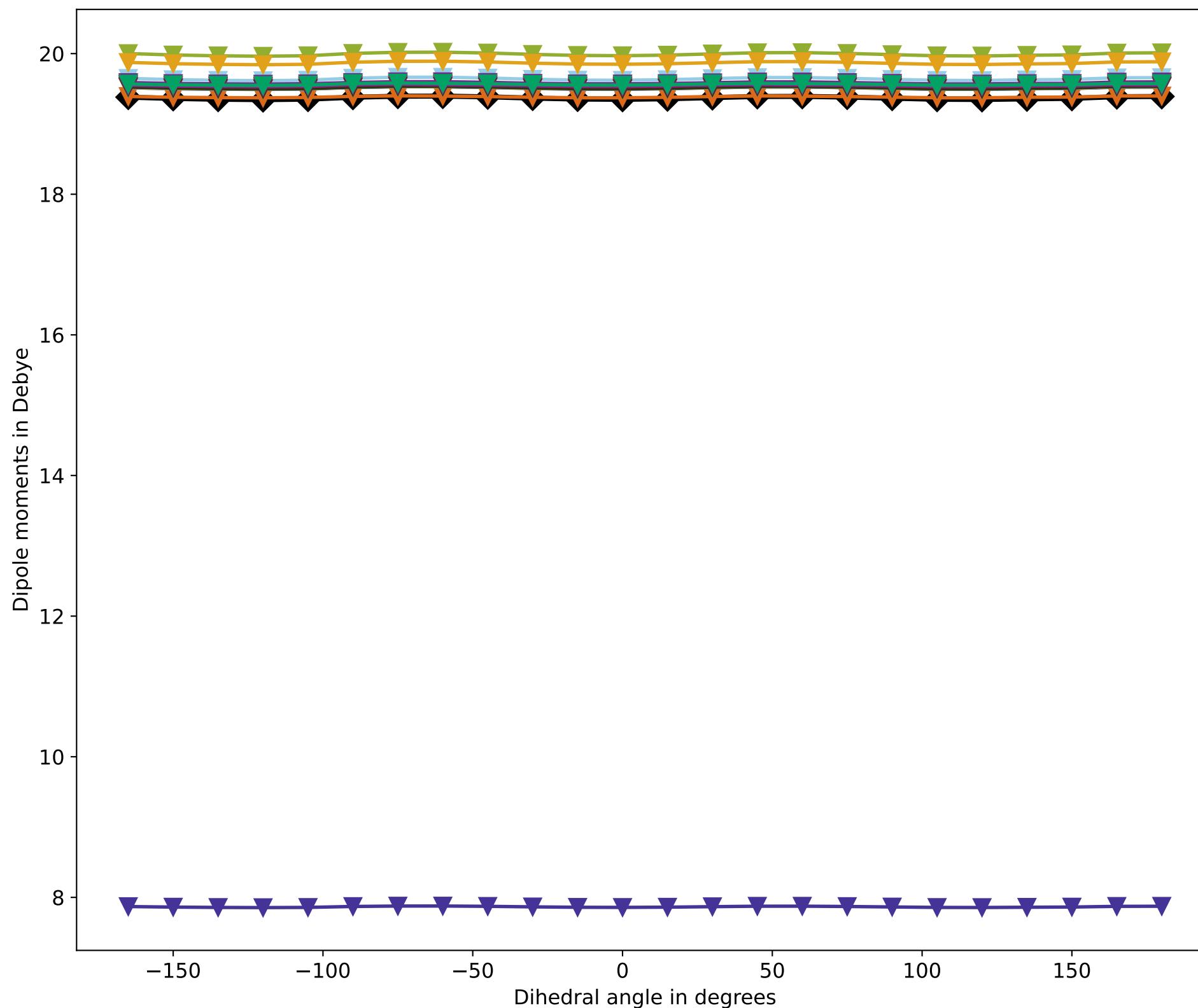




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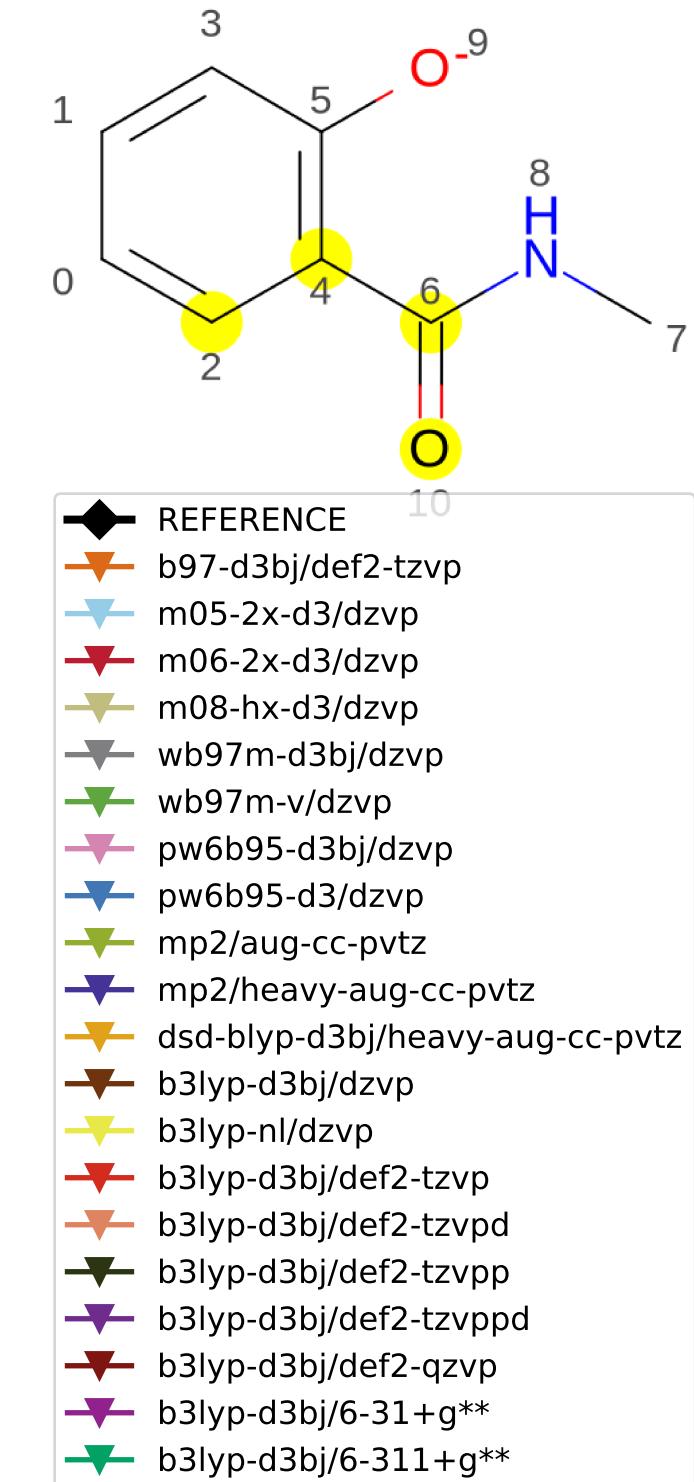
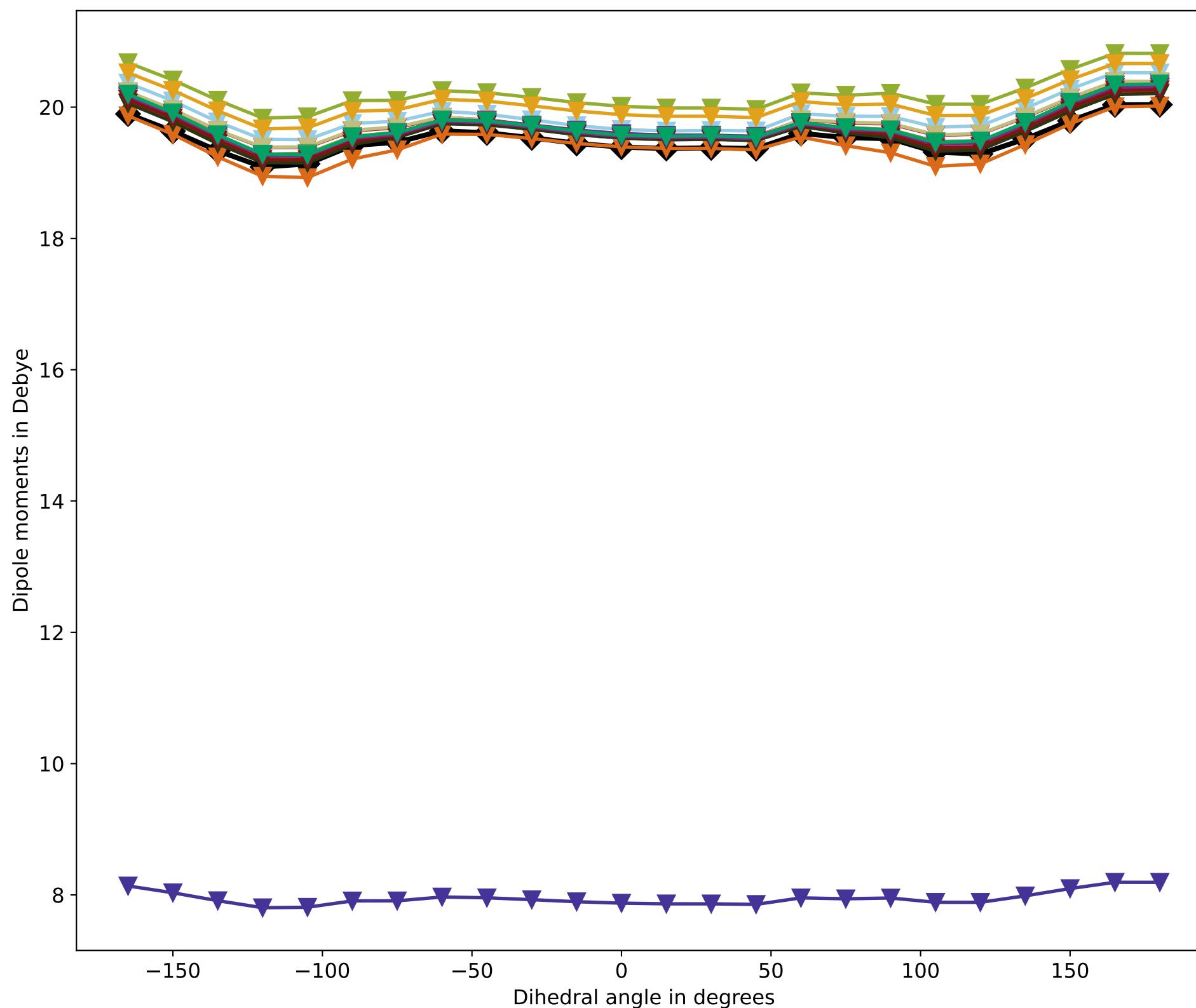


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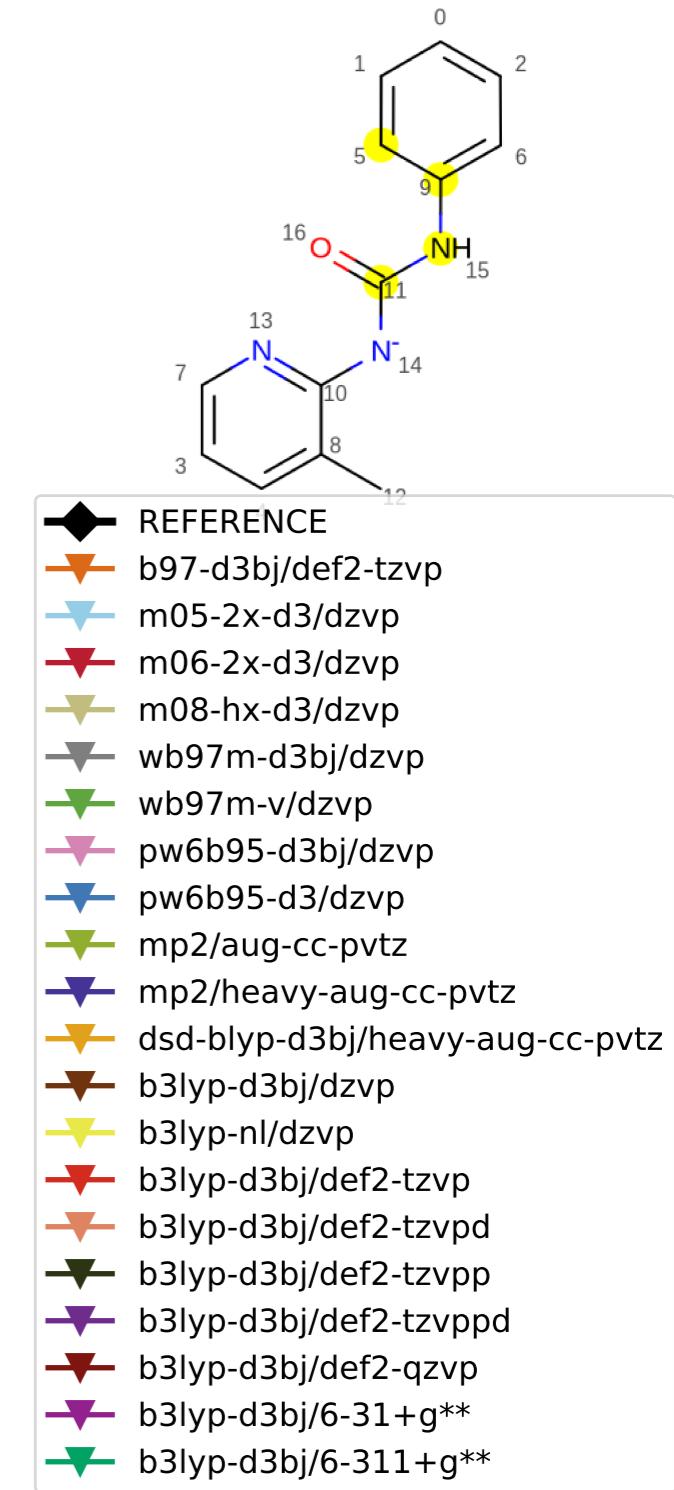
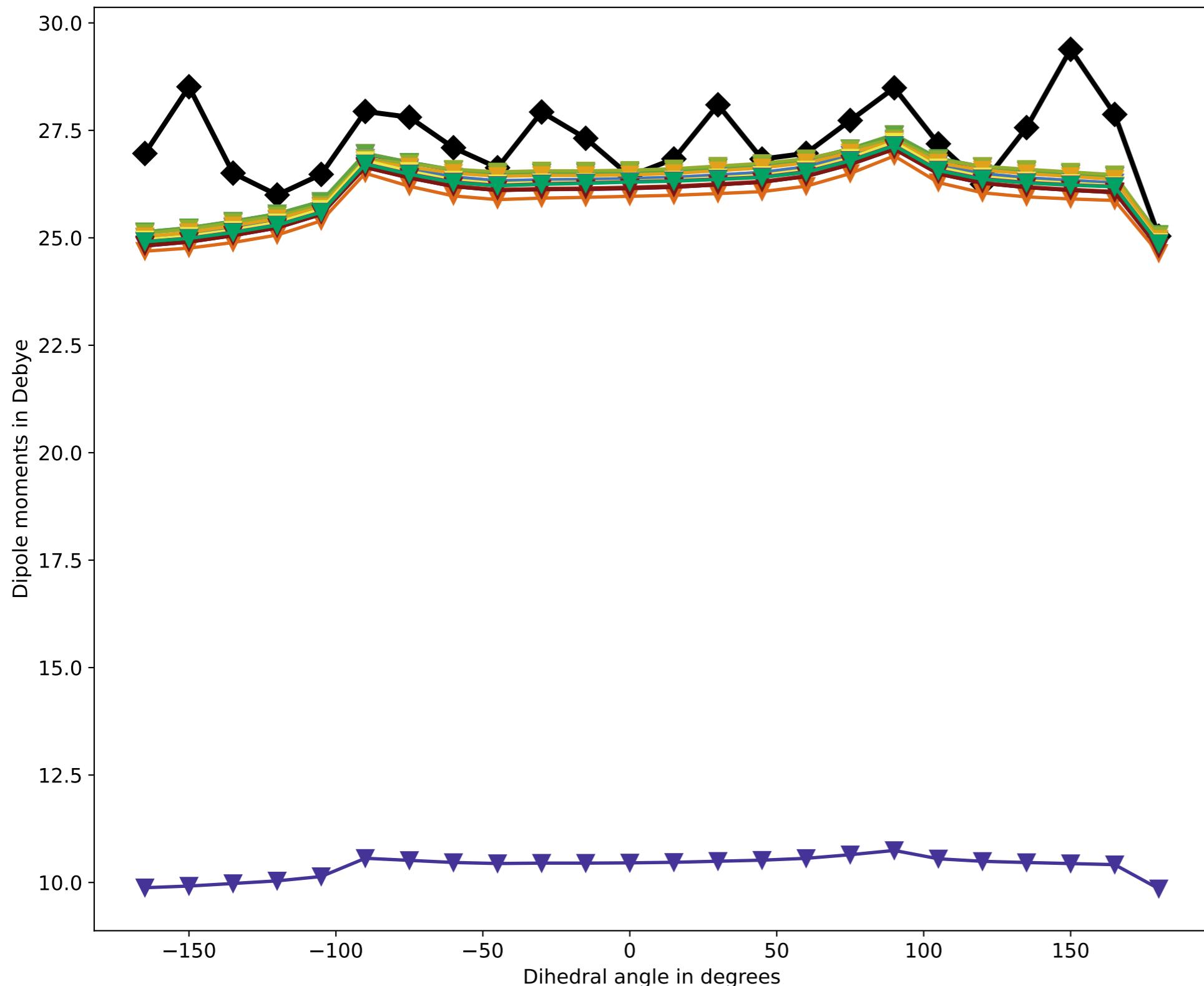


- ◆ REFERENCE
- ▼ b97-d3bj/def2-tzvp
- ▲ m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- ▲ m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- ▲ wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- ▲ pw6b95-d3/dzvp
- ▲ mp2/aug-cc-pvtz
- ▲ mp2/heavy-aug-cc-pvtz
- ▲ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ▲ b3lyp-d3bj/dzvp
- ▲ b3lyp-nl/dzvp
- ▲ b3lyp-d3bj/def2-tzvp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

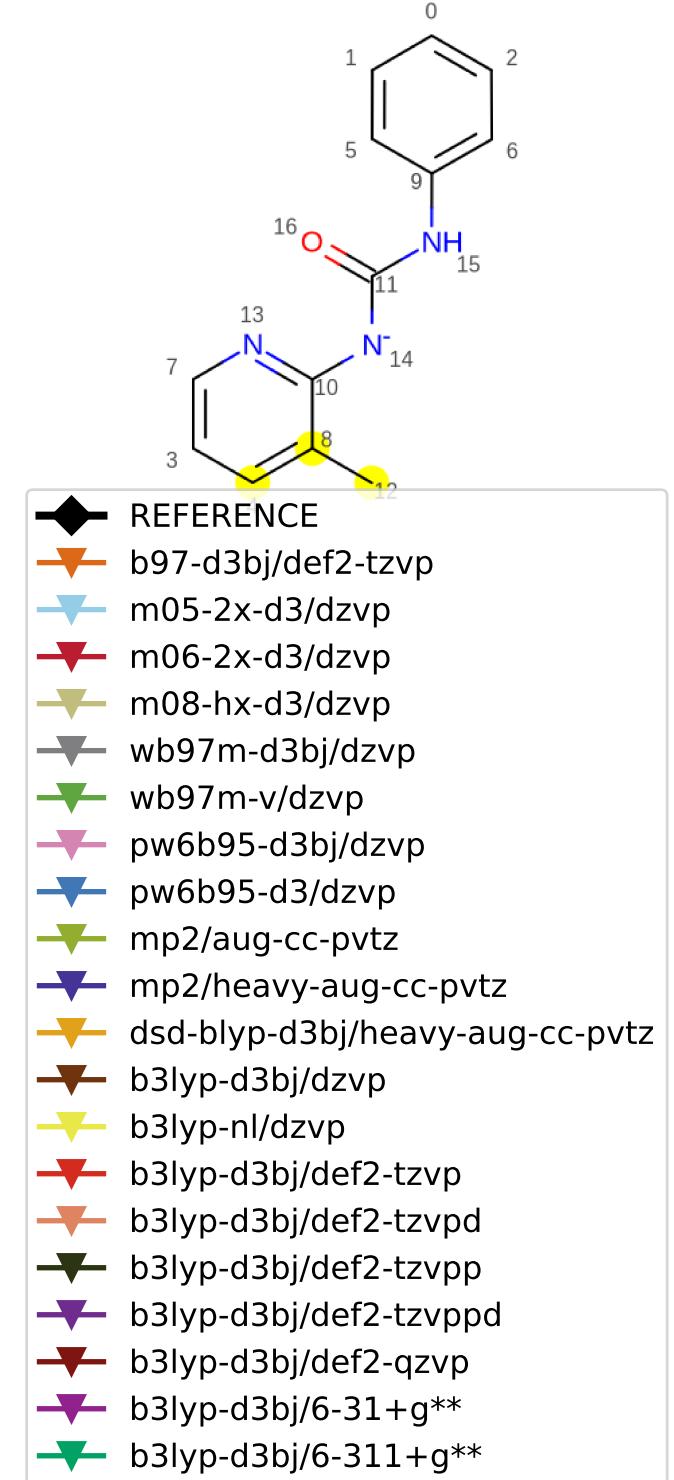
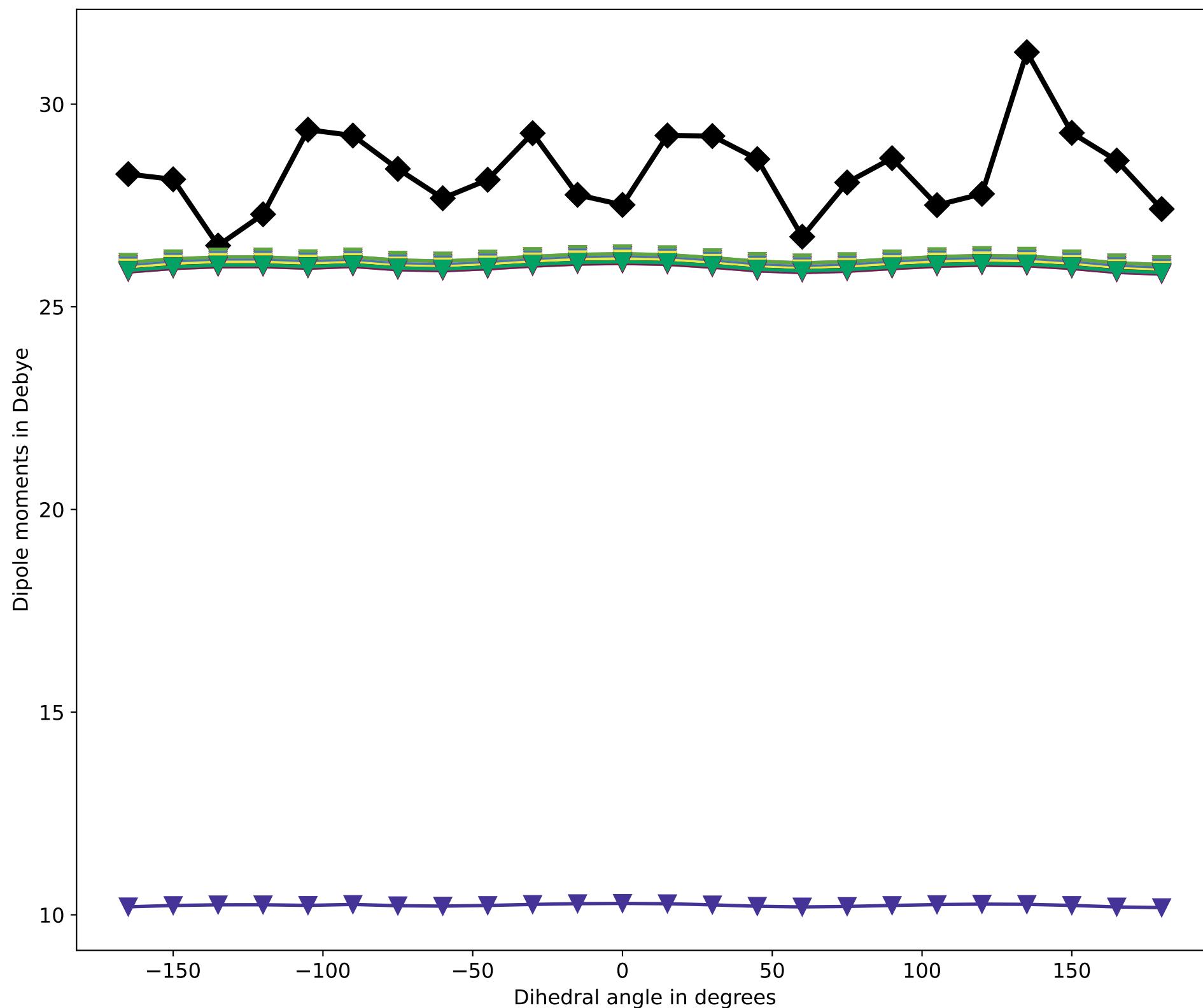
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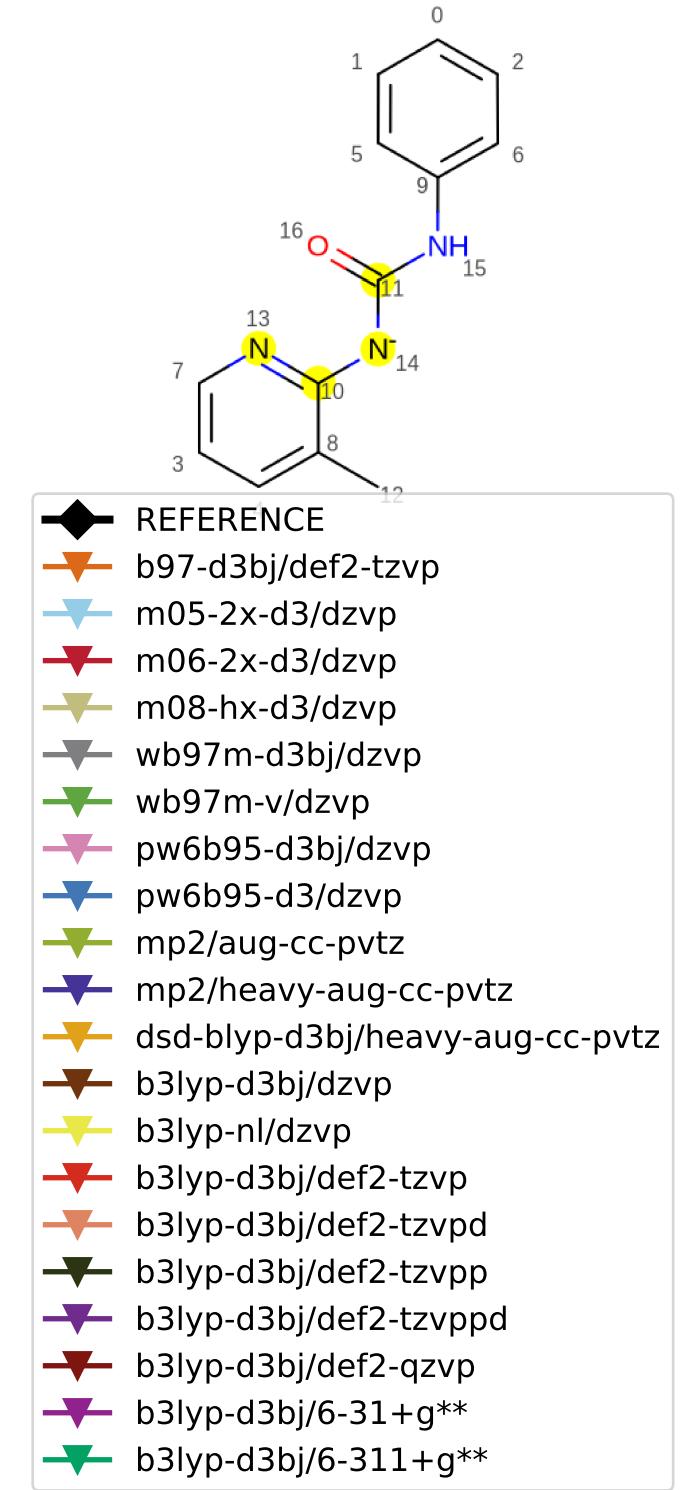
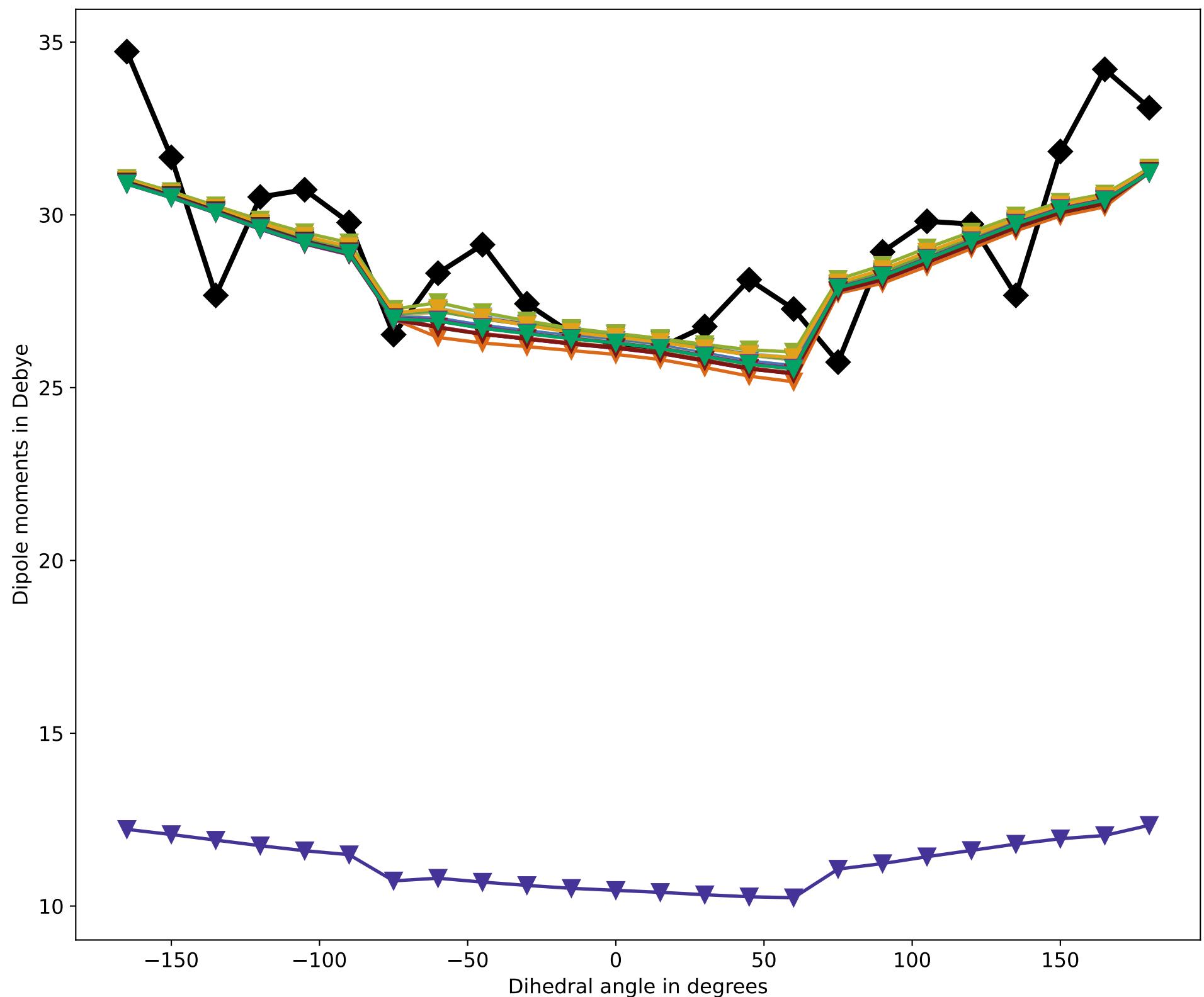
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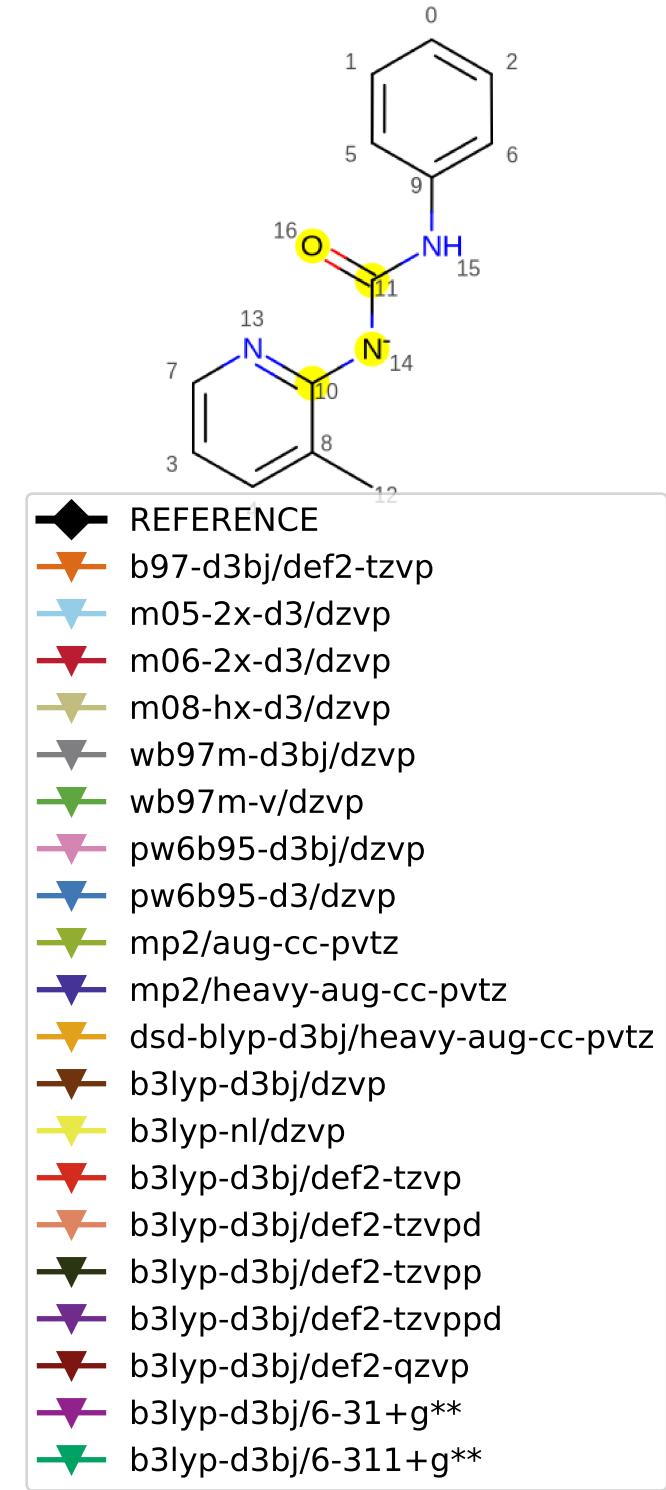
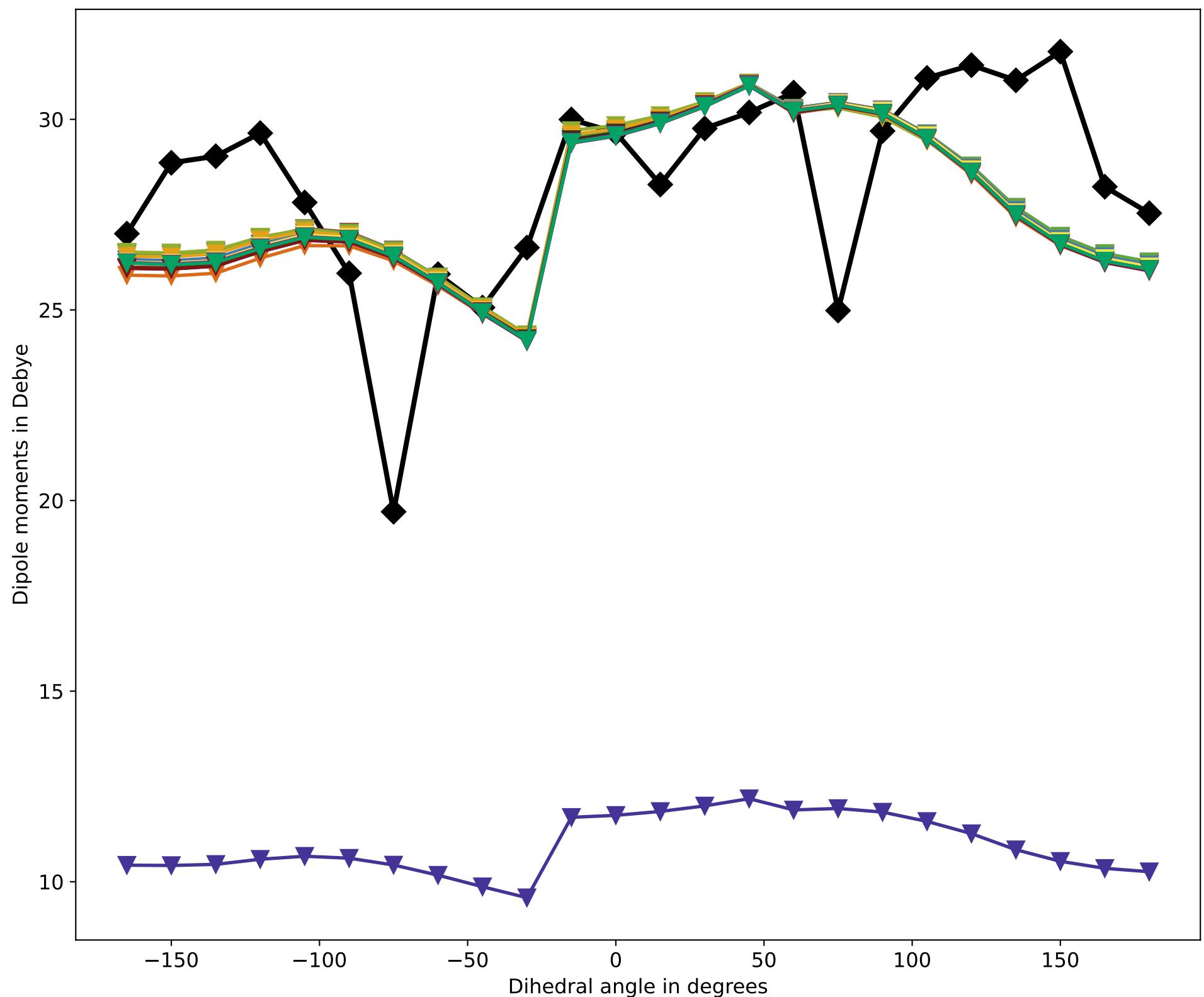
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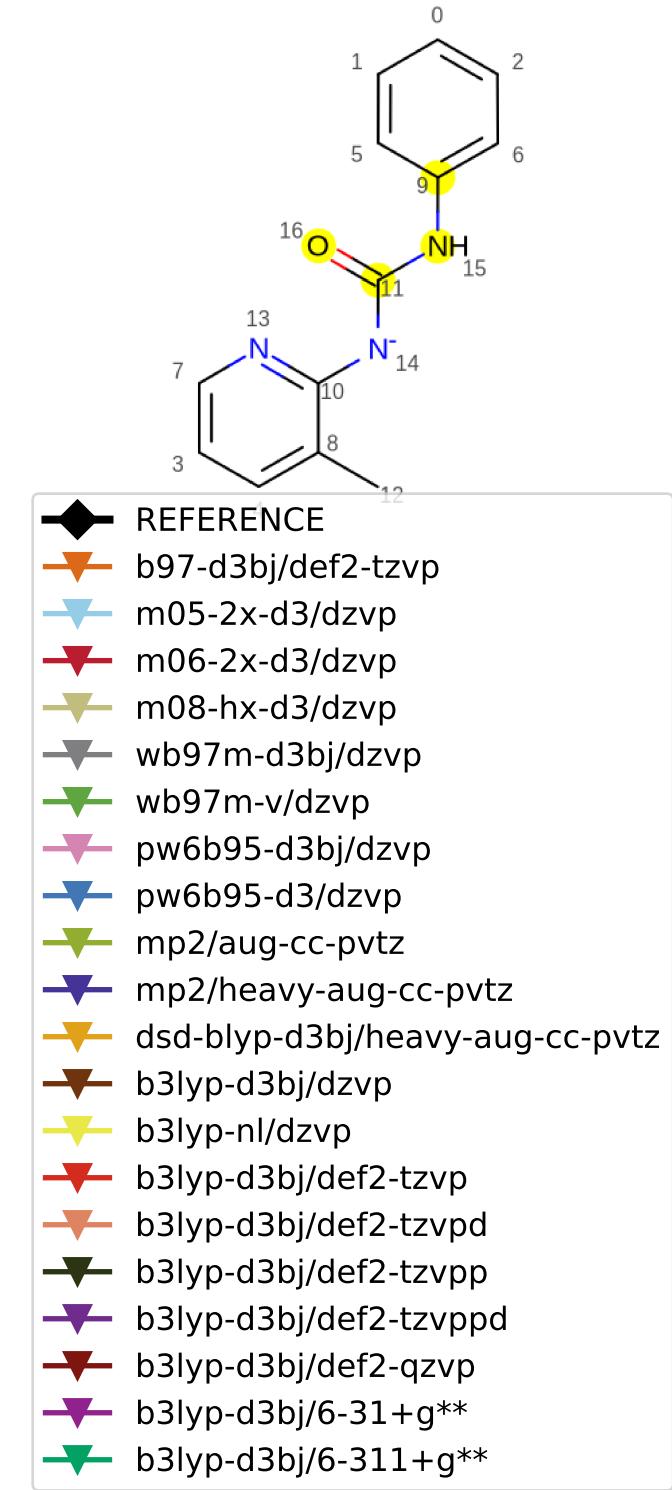
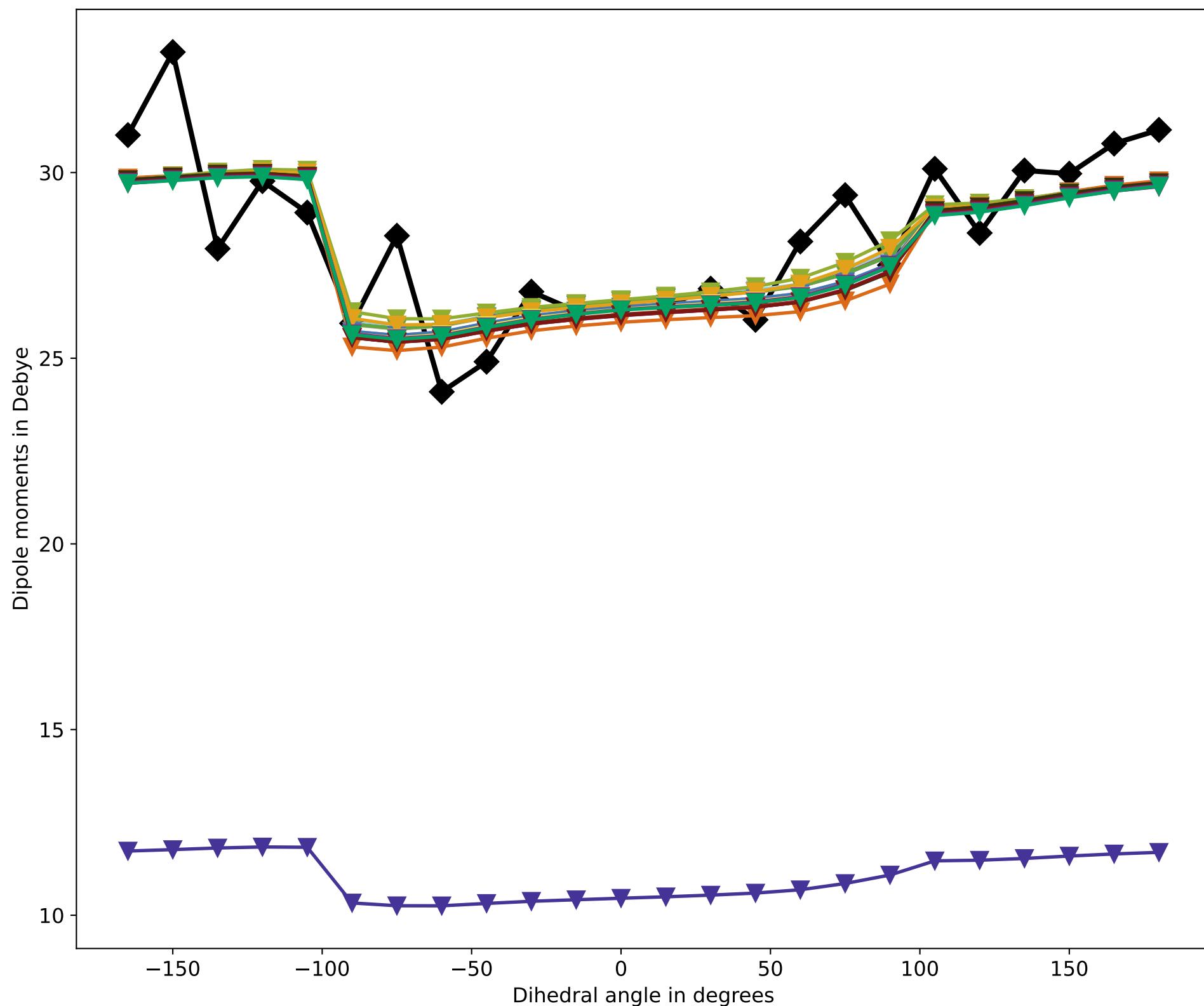
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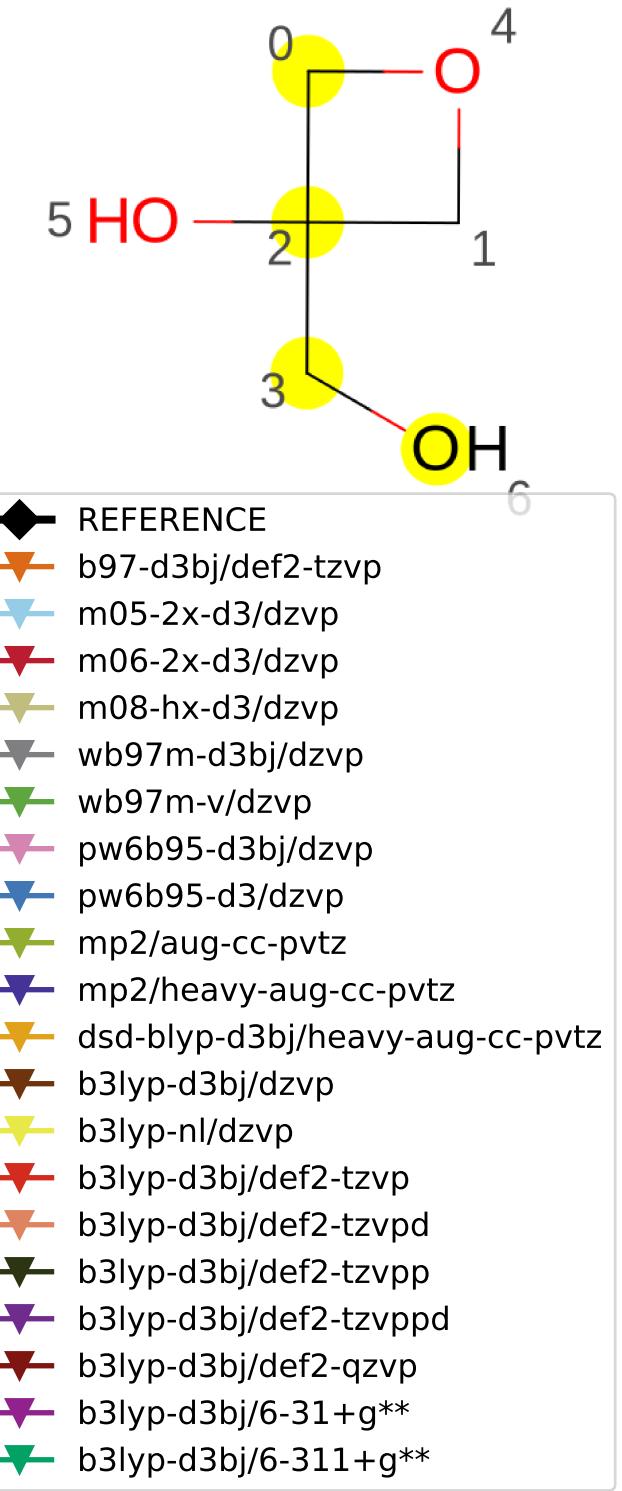
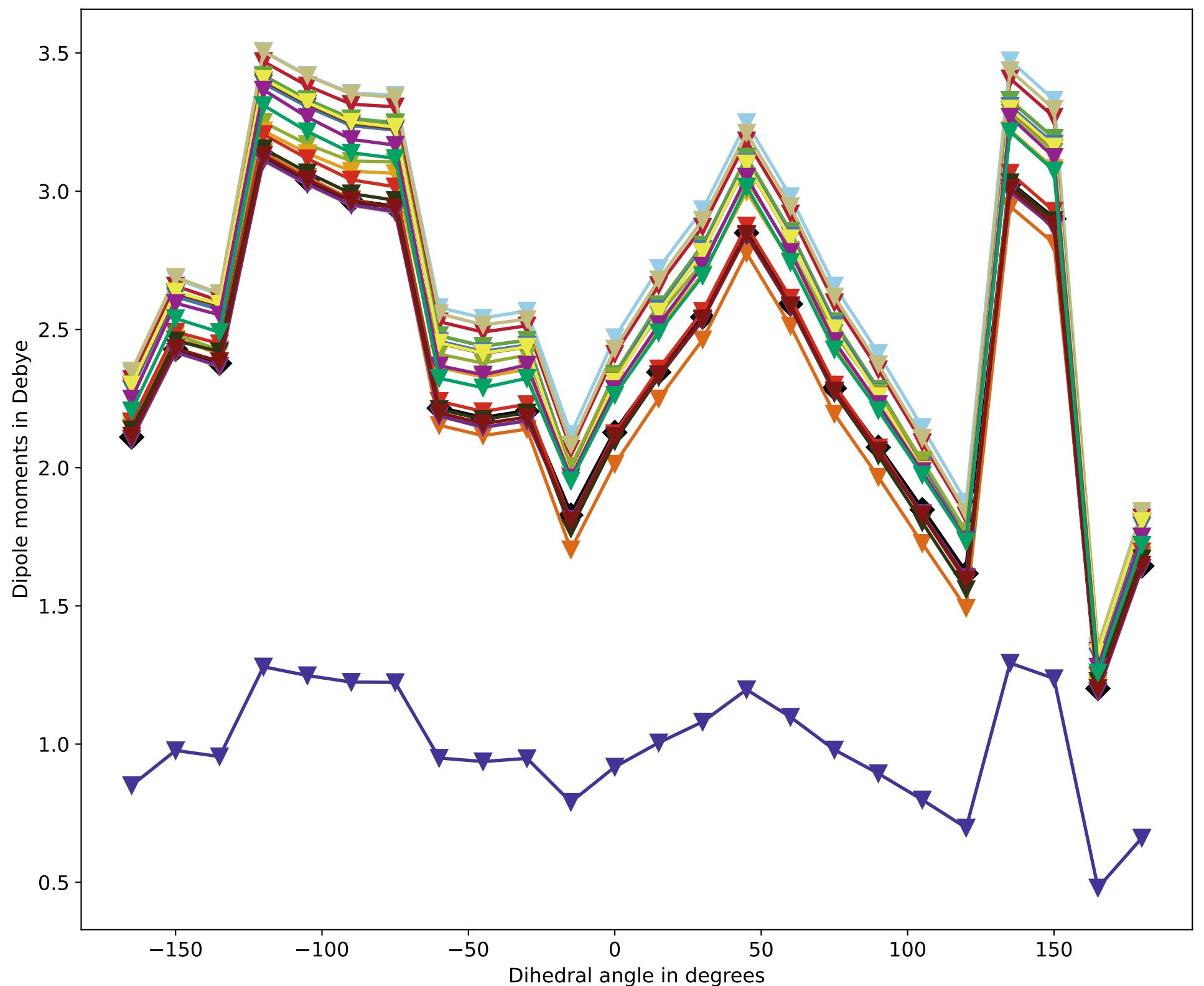


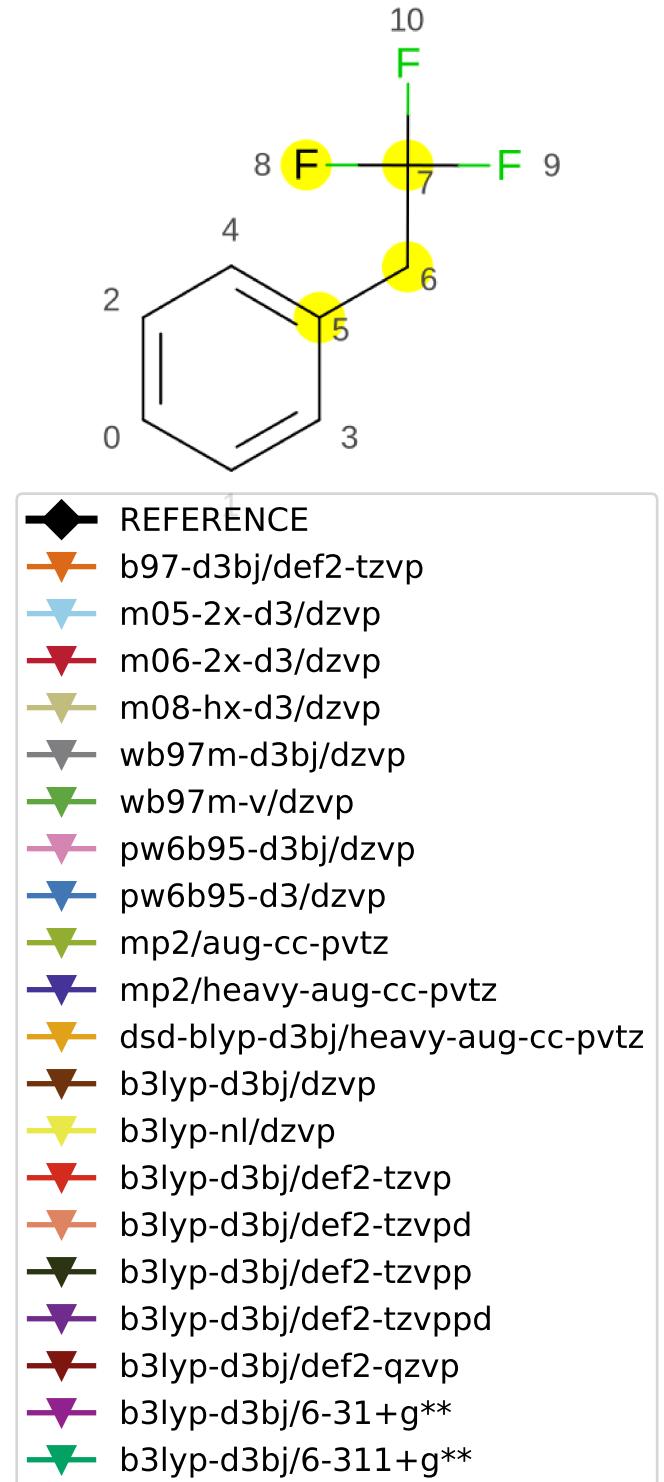
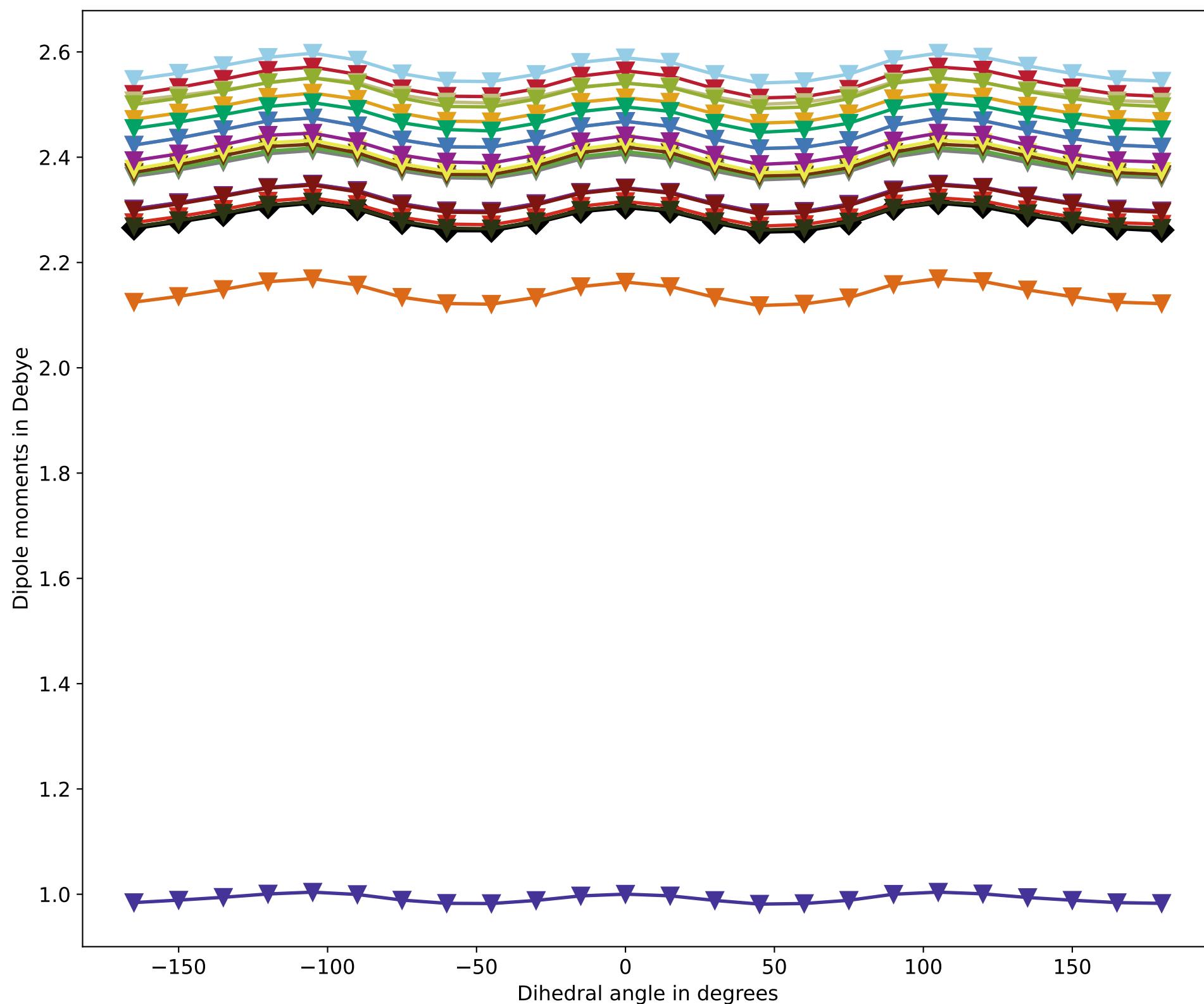
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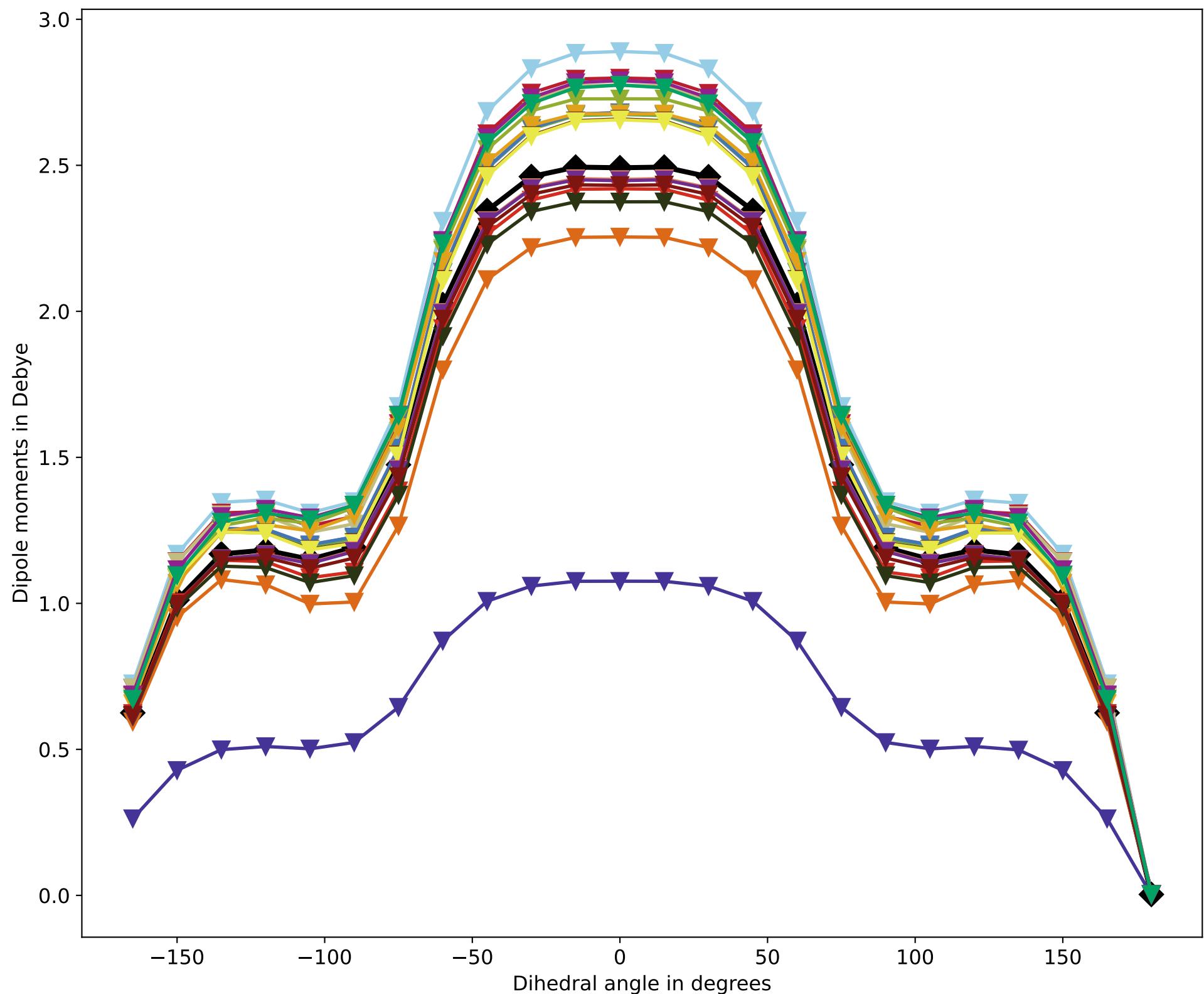


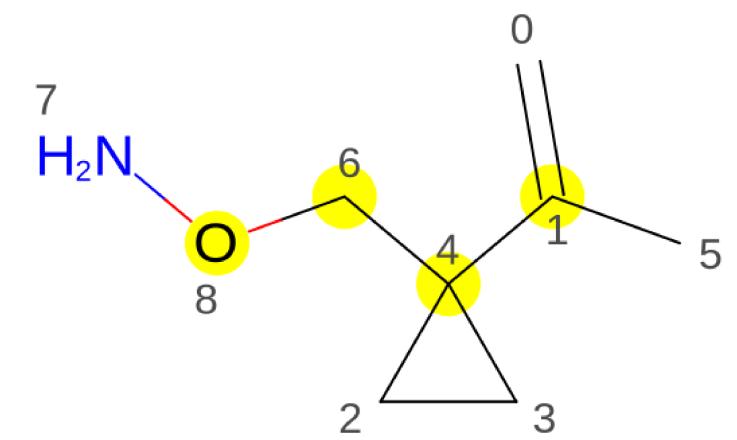
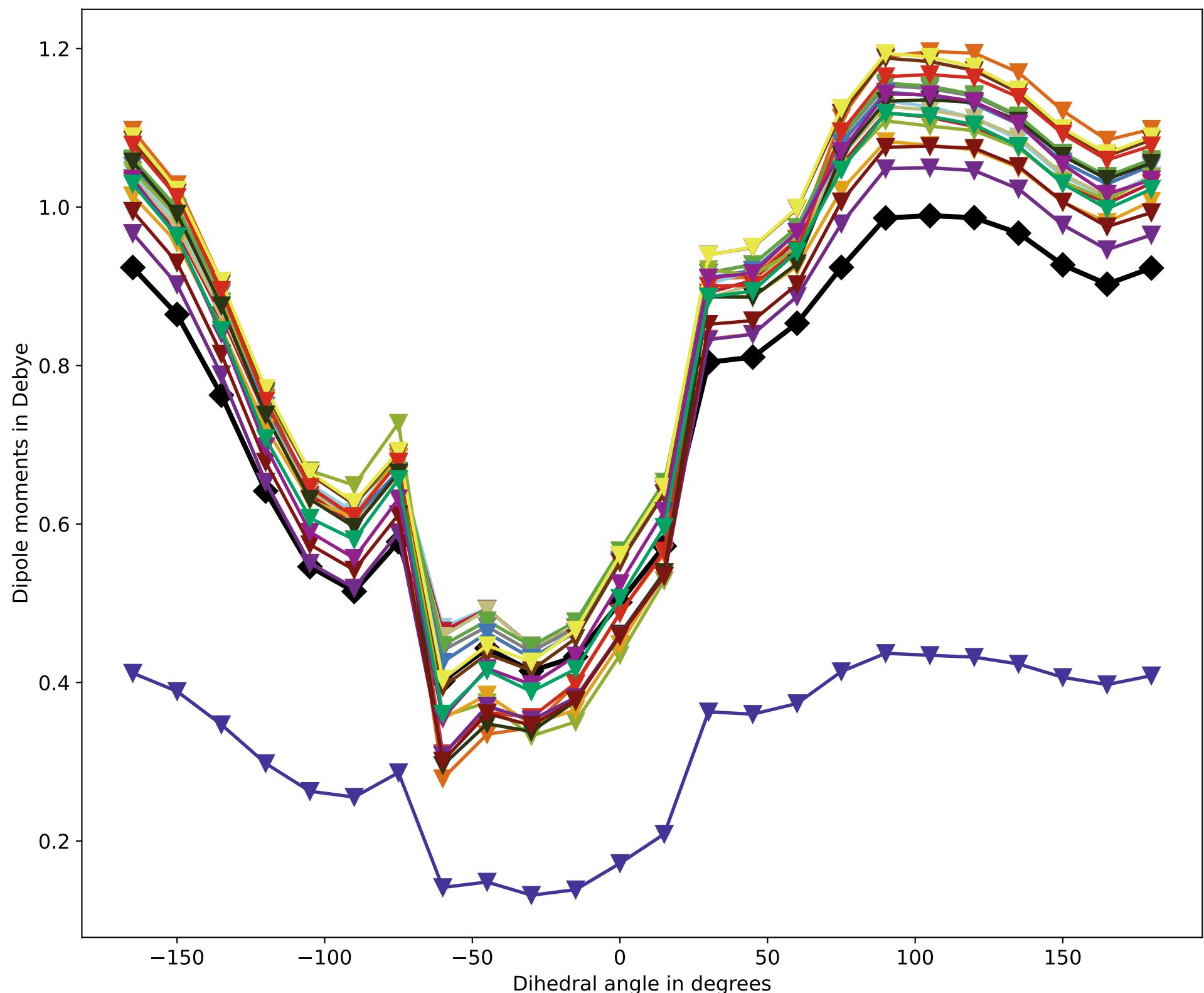
Charged molecule





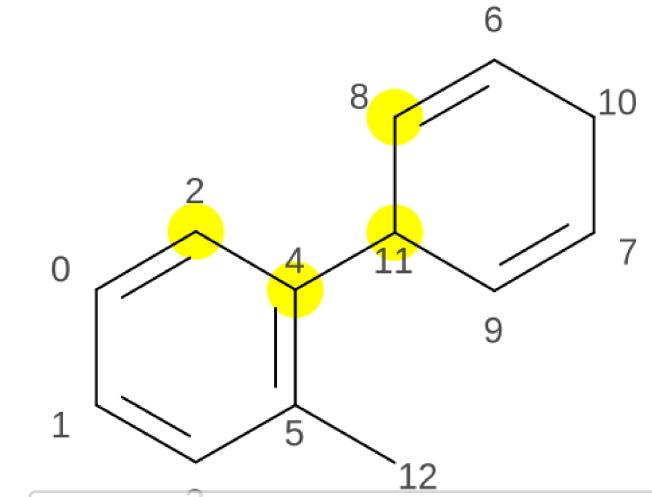
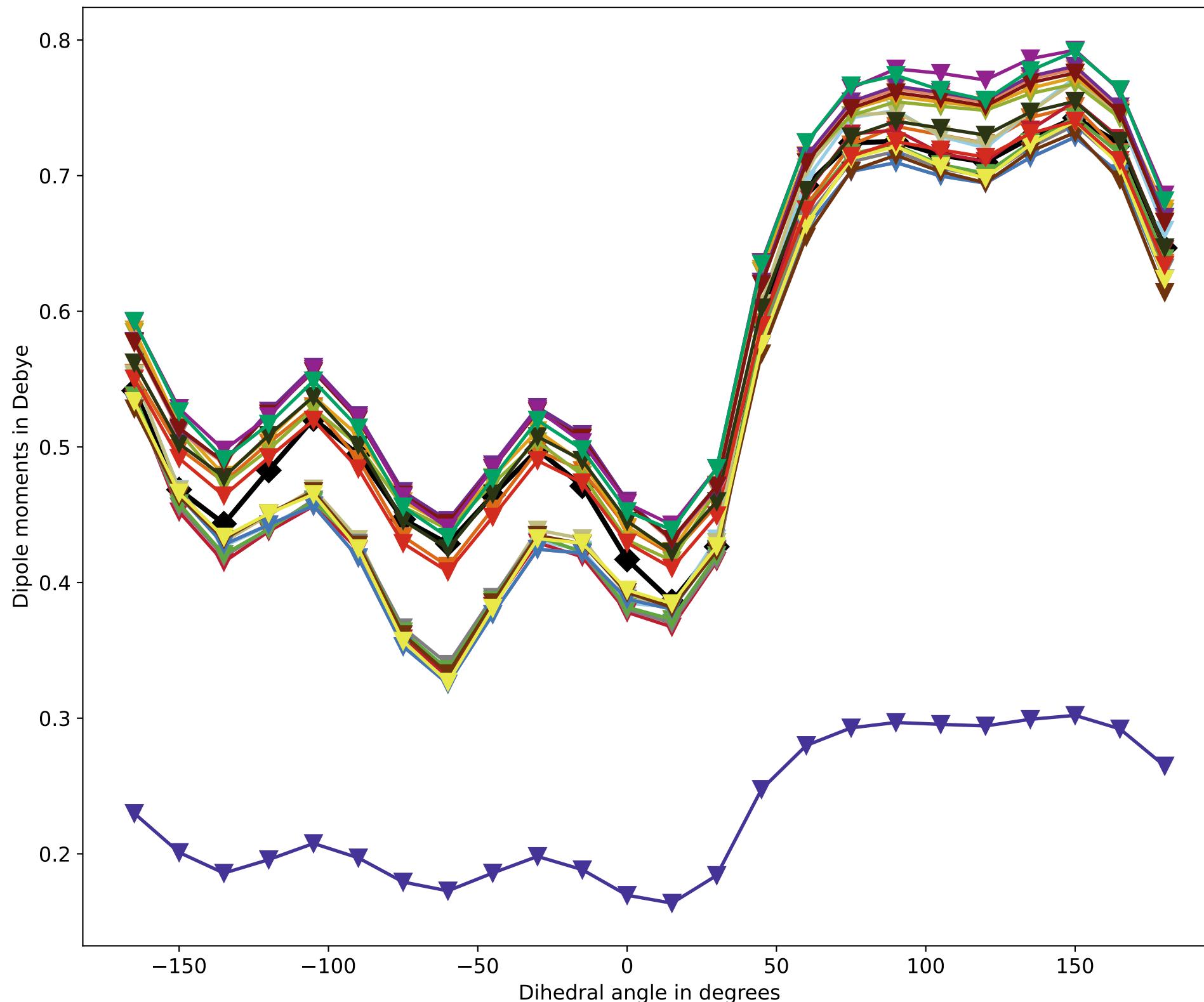






- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

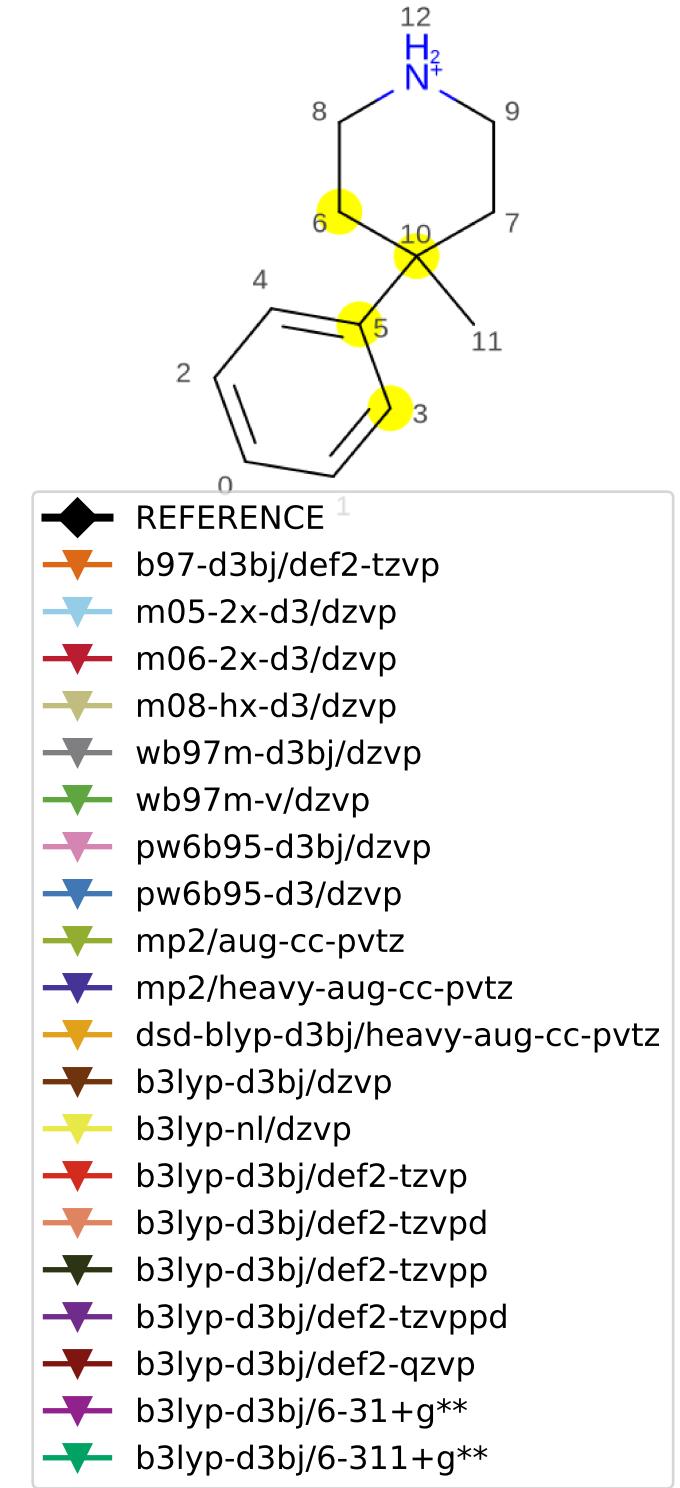
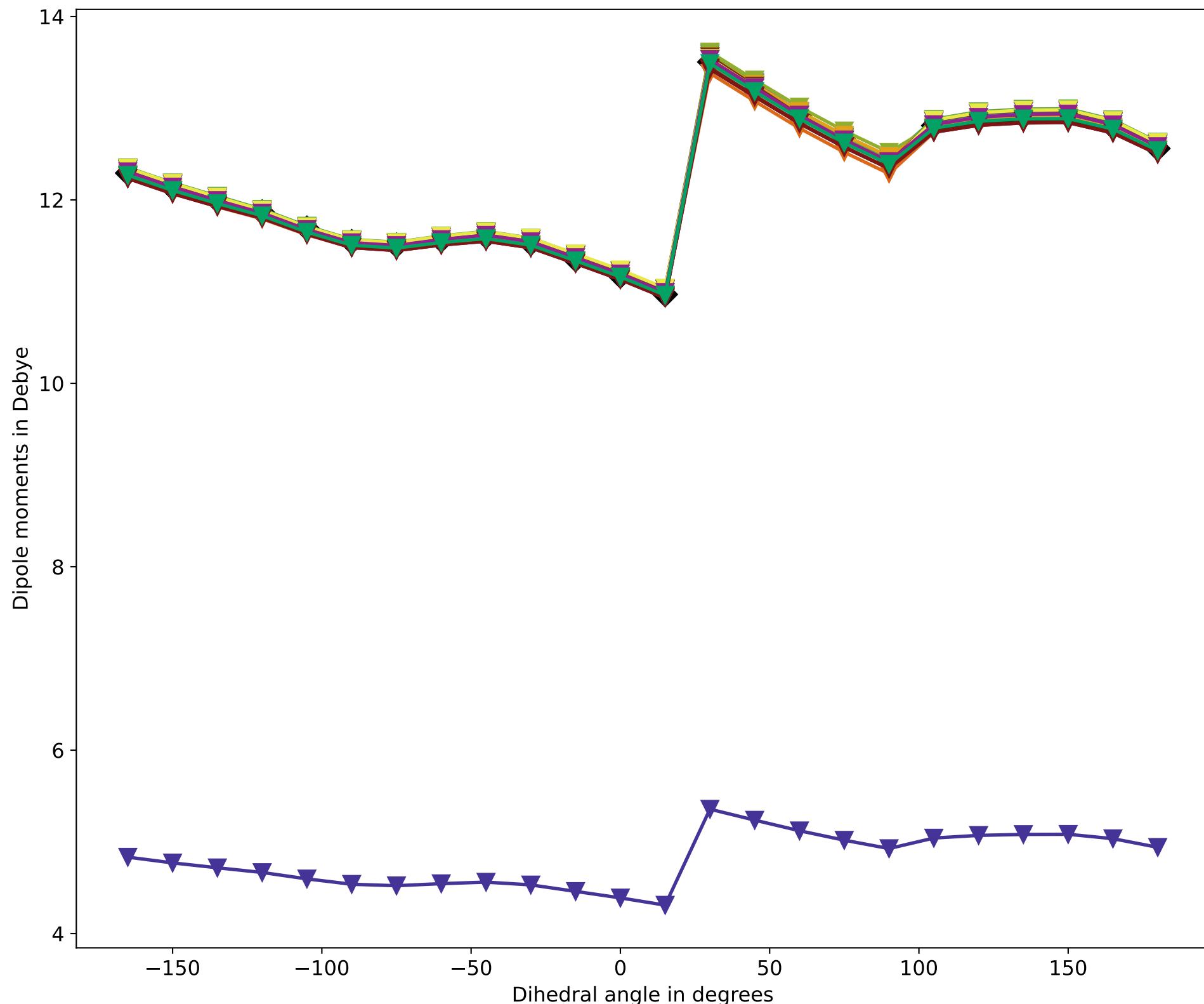
Neutral molecule

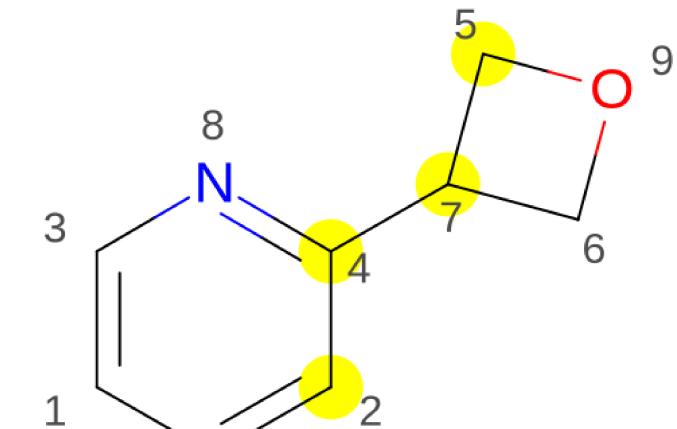
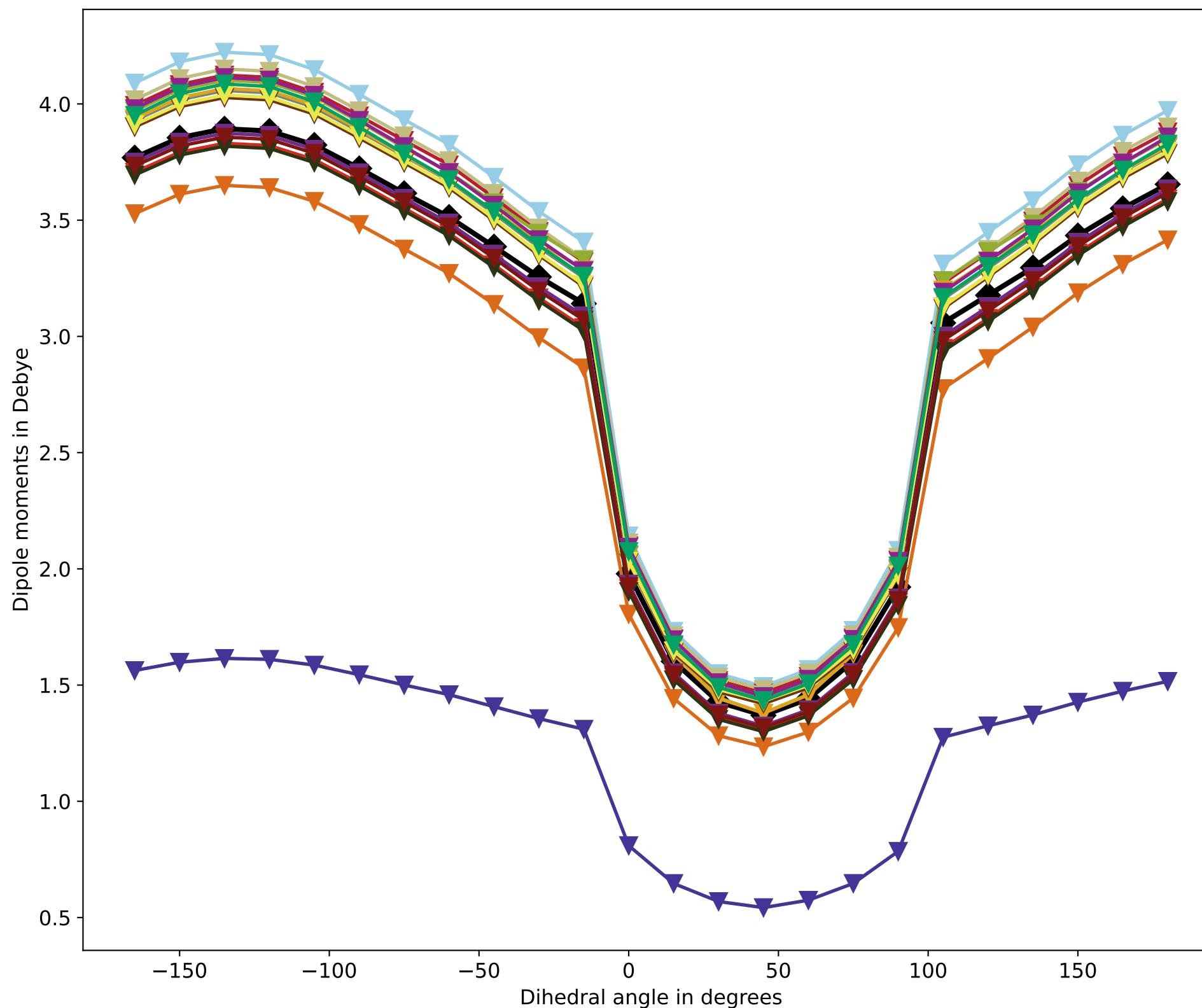


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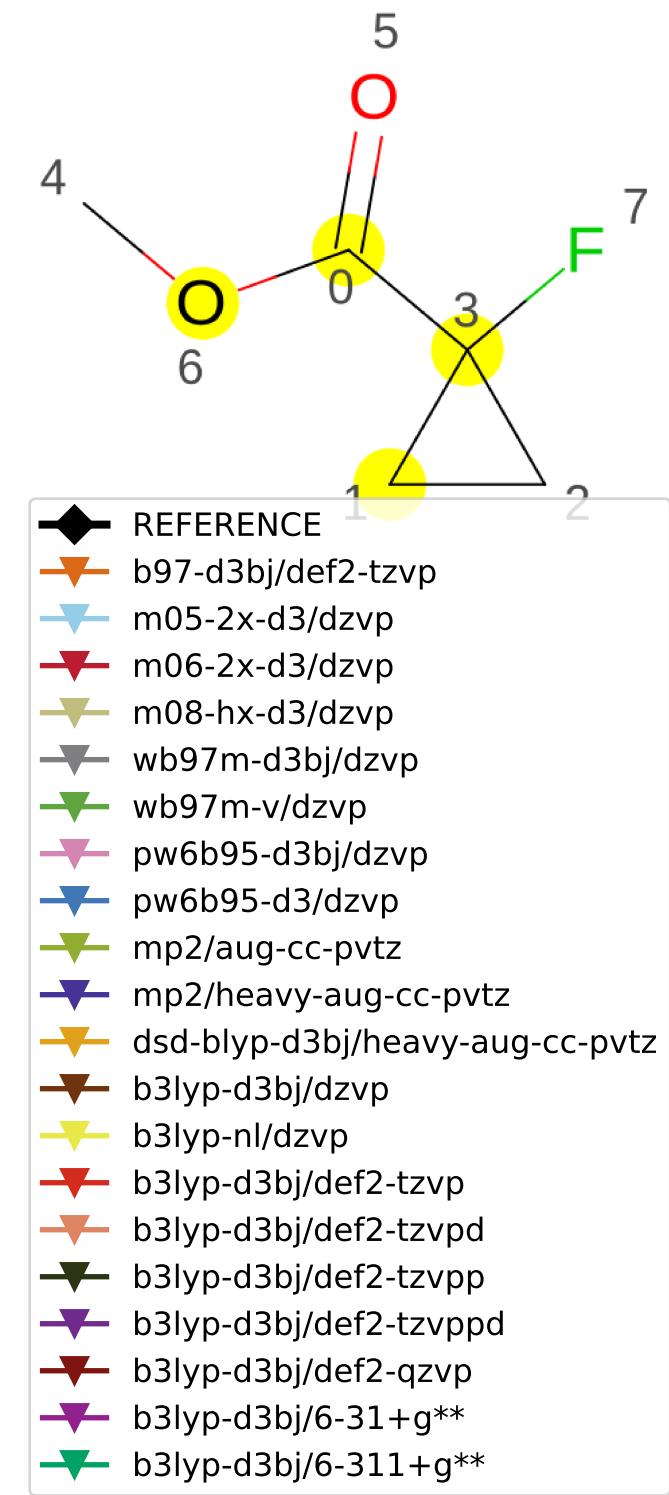
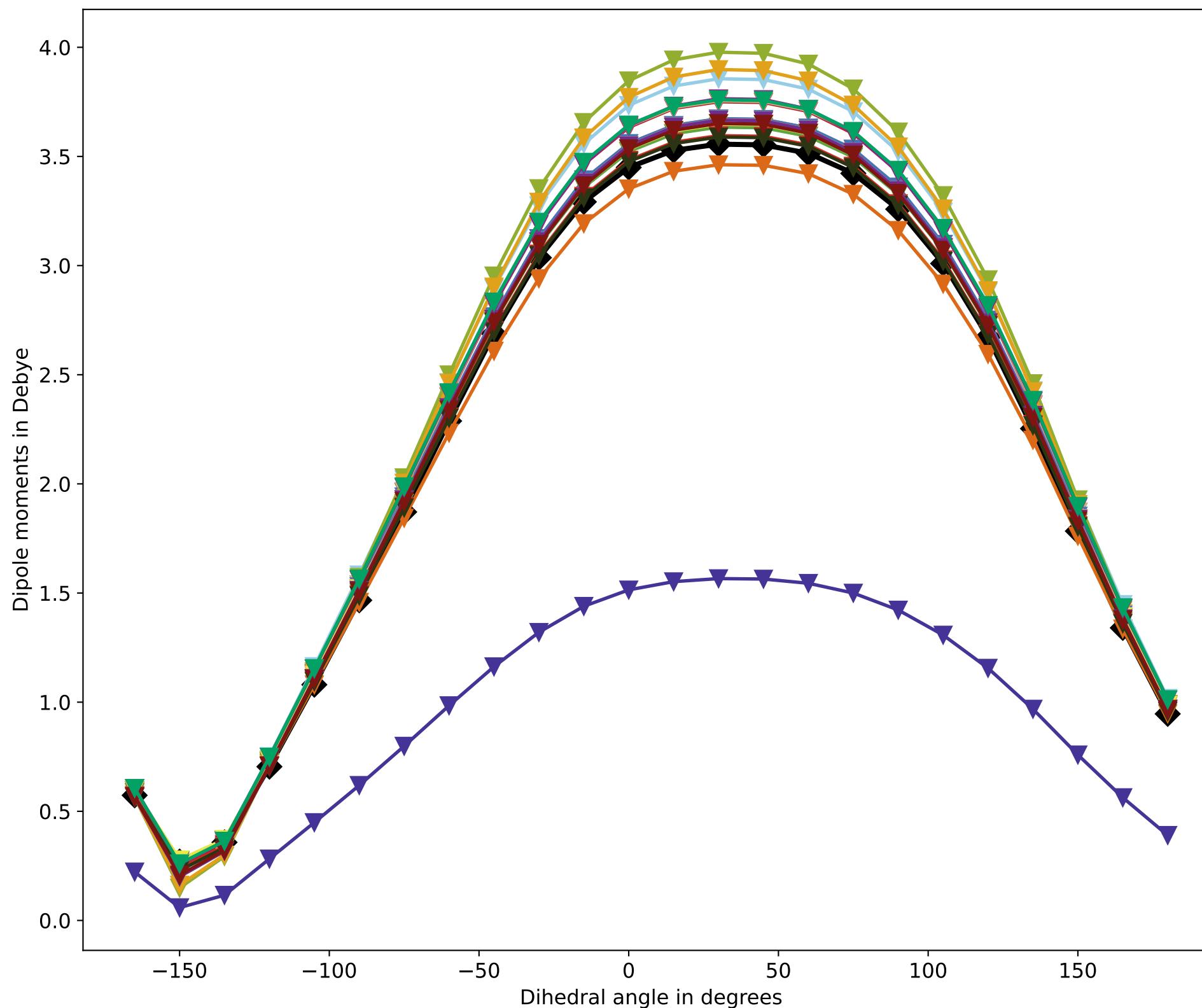
- ▶ b97-d3bj/def2-tzvp
- ◀ m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- ◀ m08-hx-d3/dzvp
- ◀ wb97m-d3bj/dzvp
- ◀ wb97m-v/dzvp
- ◀ pw6b95-d3bj/dzvp
- ◀ pw6b95-d3/dzvp
- ◀ mp2/aug-cc-pvtz
- ◀ mp2/heavy-aug-cc-pvtz
- ◀ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◀ b3lyp-d3bj/dzvp
- ◀ b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- ◀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

Charged molecule

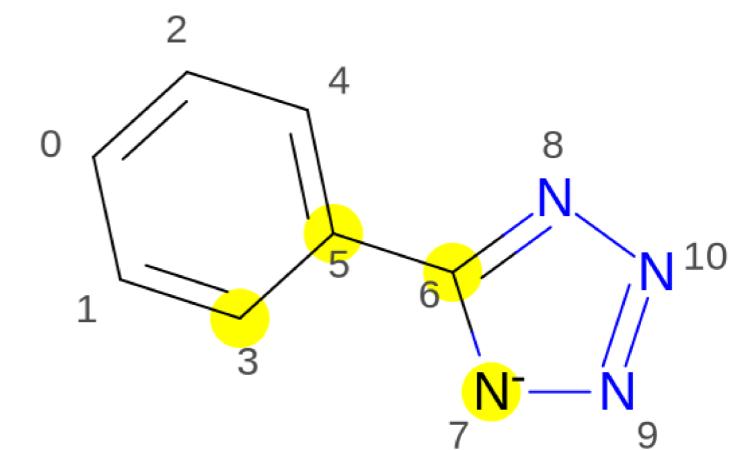
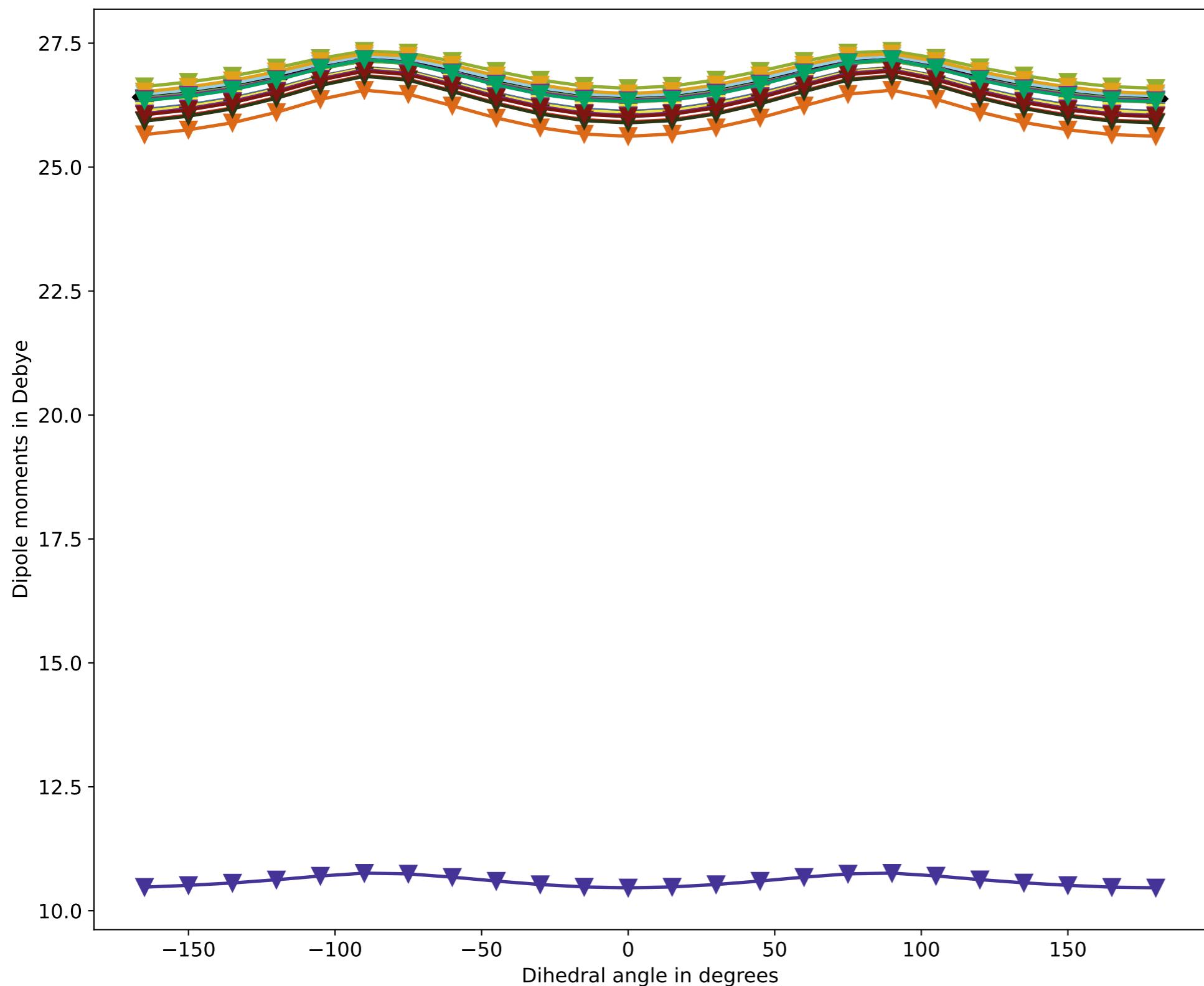




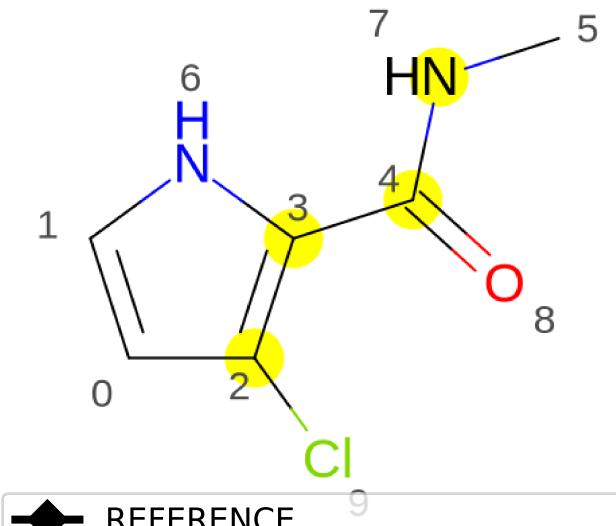
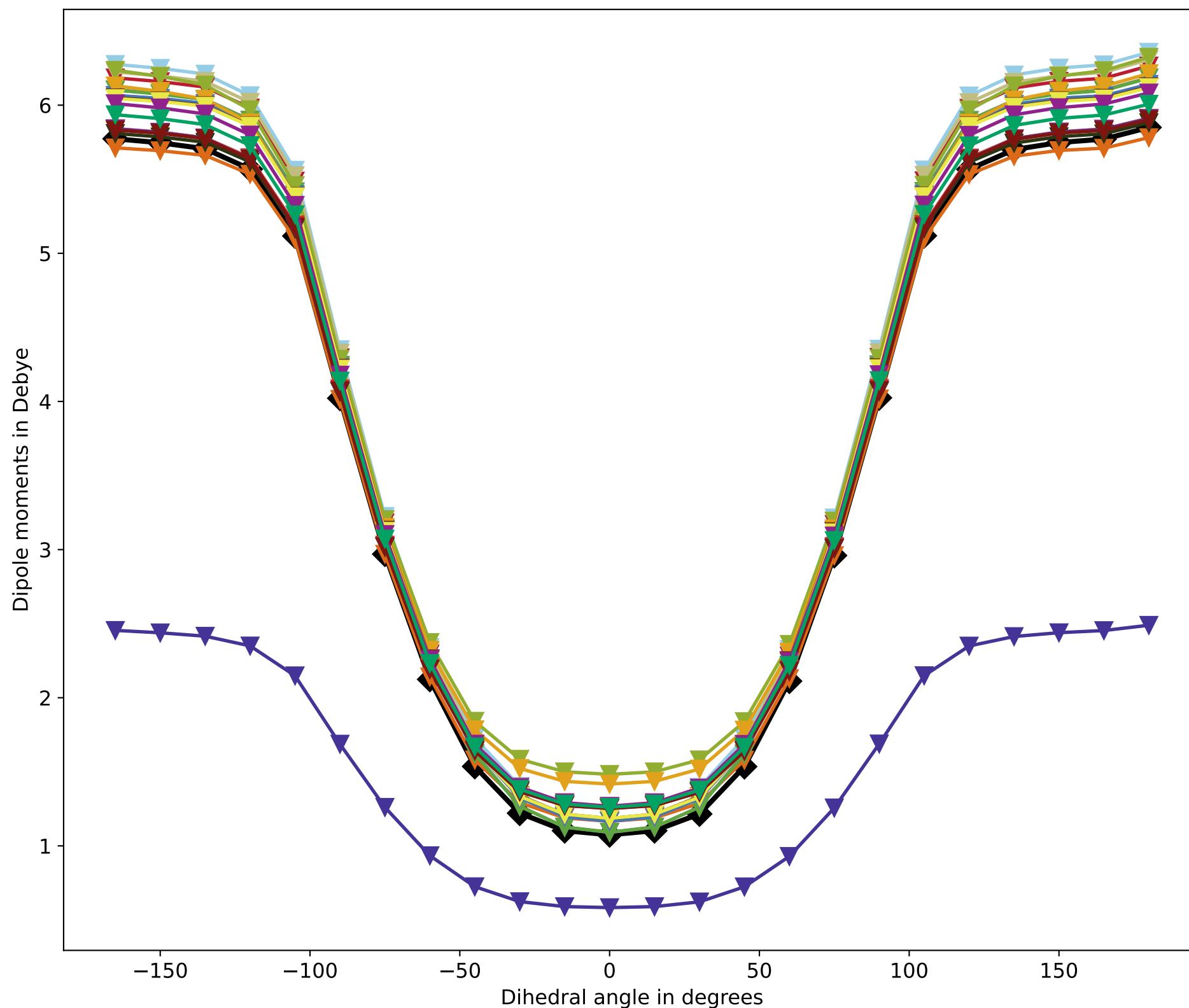
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|--|--|
| ◆ REFERENCE | |
| ◆ b97-d3bj/def2-tzvp | |
| ◆ m05-2x-d3/dzvp | |
| ◆ m06-2x-d3/dzvp | |
| ◆ m08-hx-d3/dzvp | |
| ◆ wb97m-d3bj/dzvp | |
| ◆ wb97m-v/dzvp | |
| ◆ pw6b95-d3bj/dzvp | |
| ◆ pw6b95-d3/dzvp | |
| ◆ mp2/aug-cc-pvtz | |
| ◆ mp2/heavy-aug-cc-pvtz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



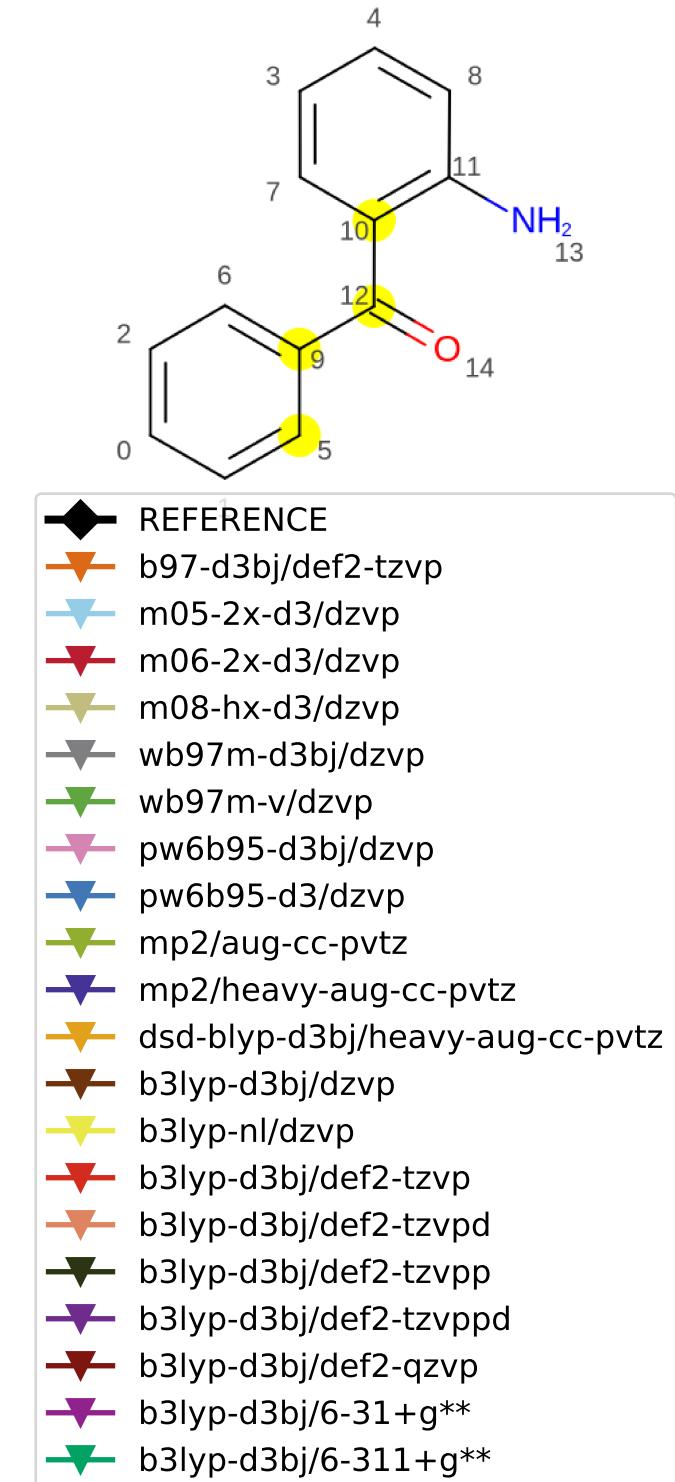
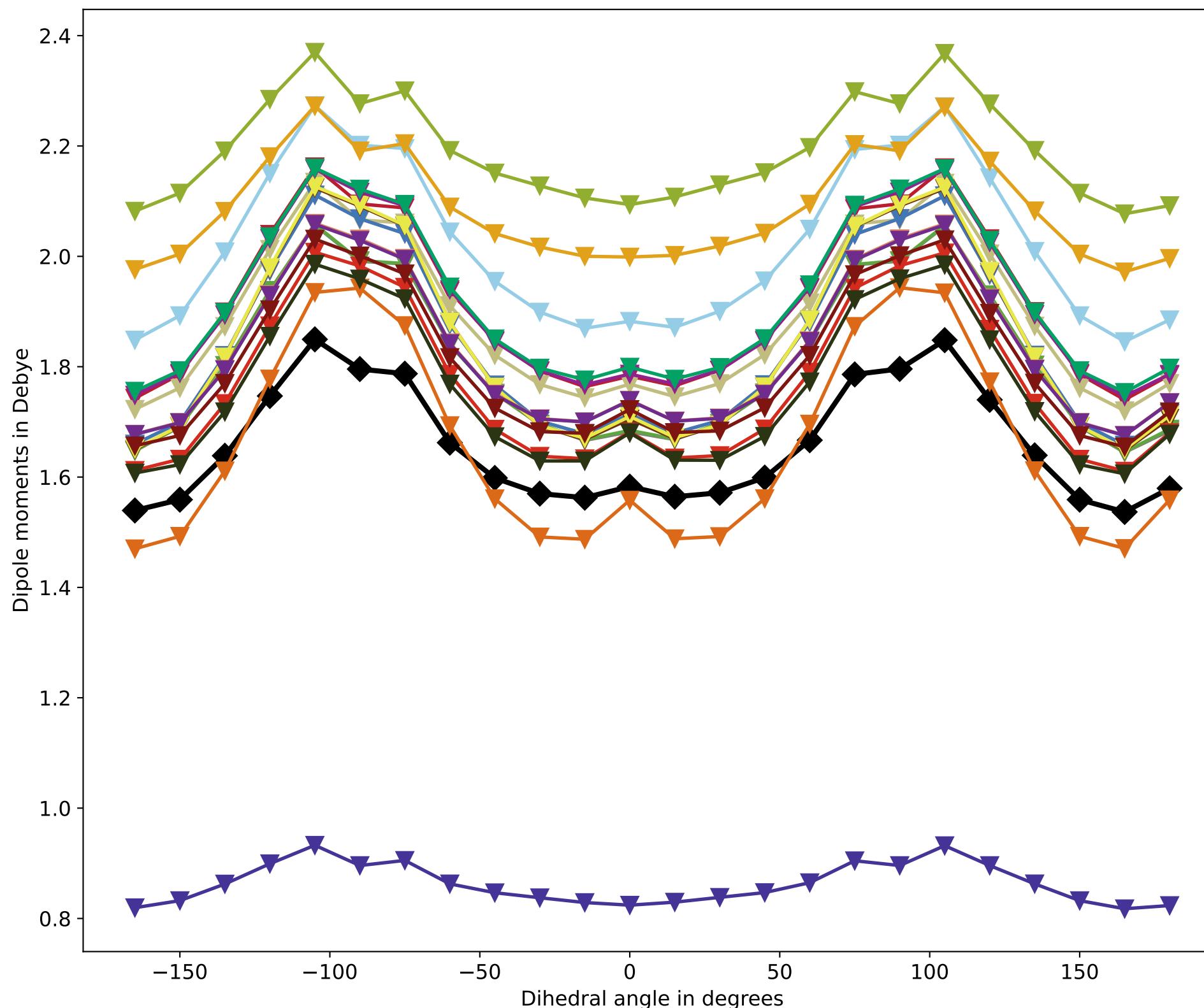
Charged molecule

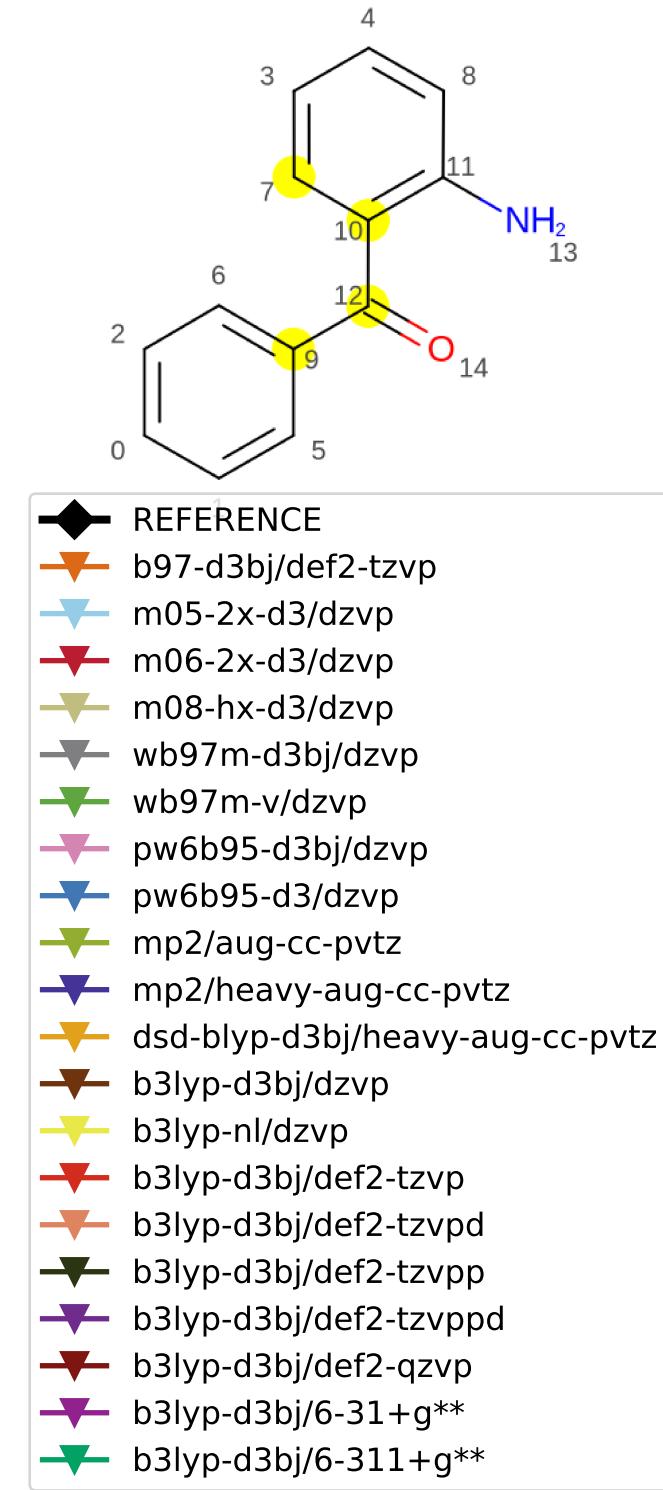
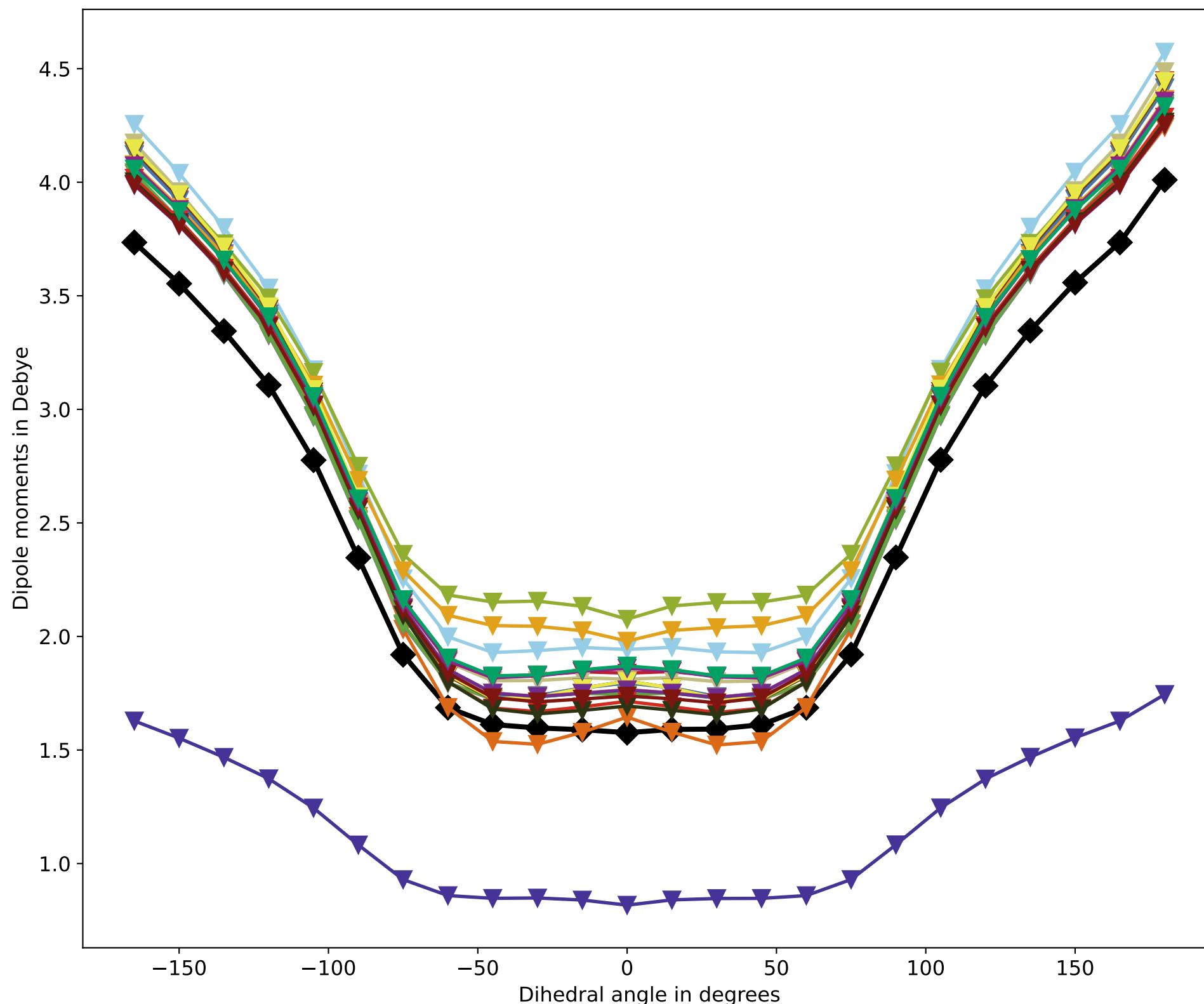


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

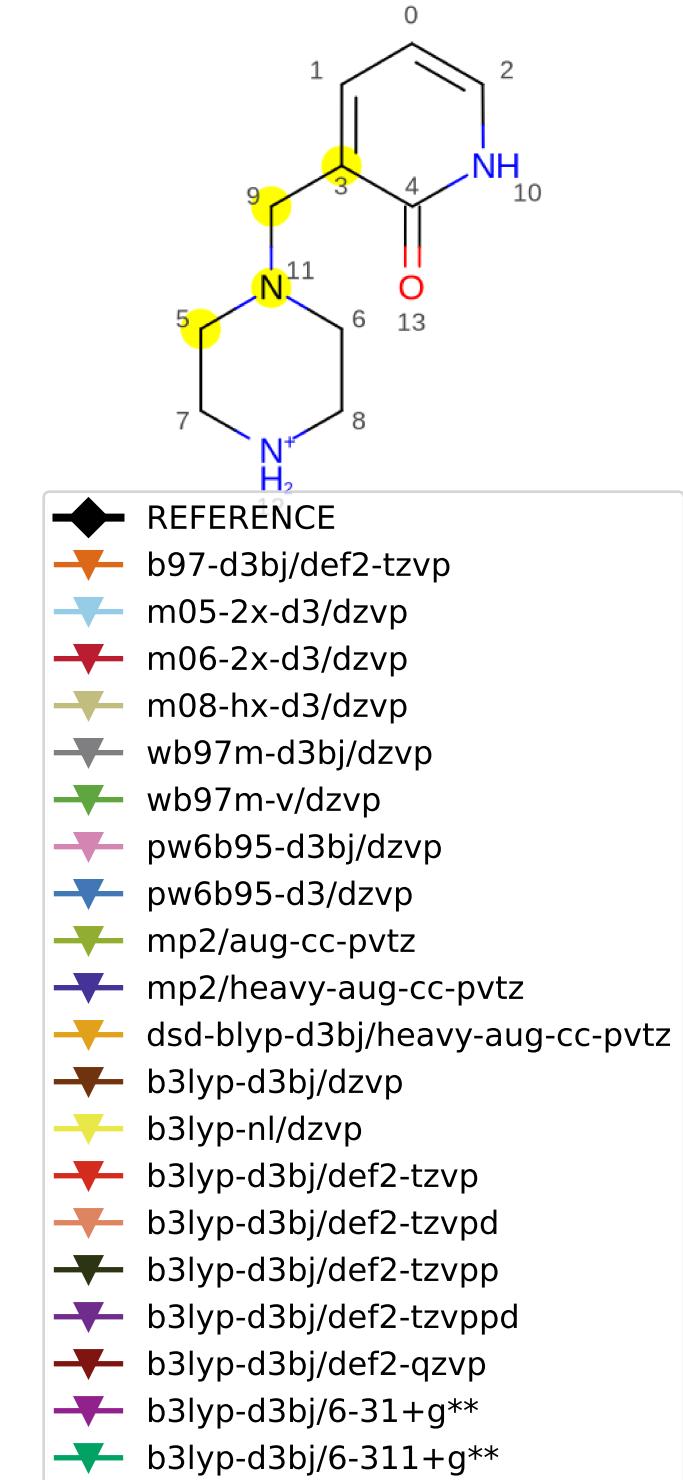
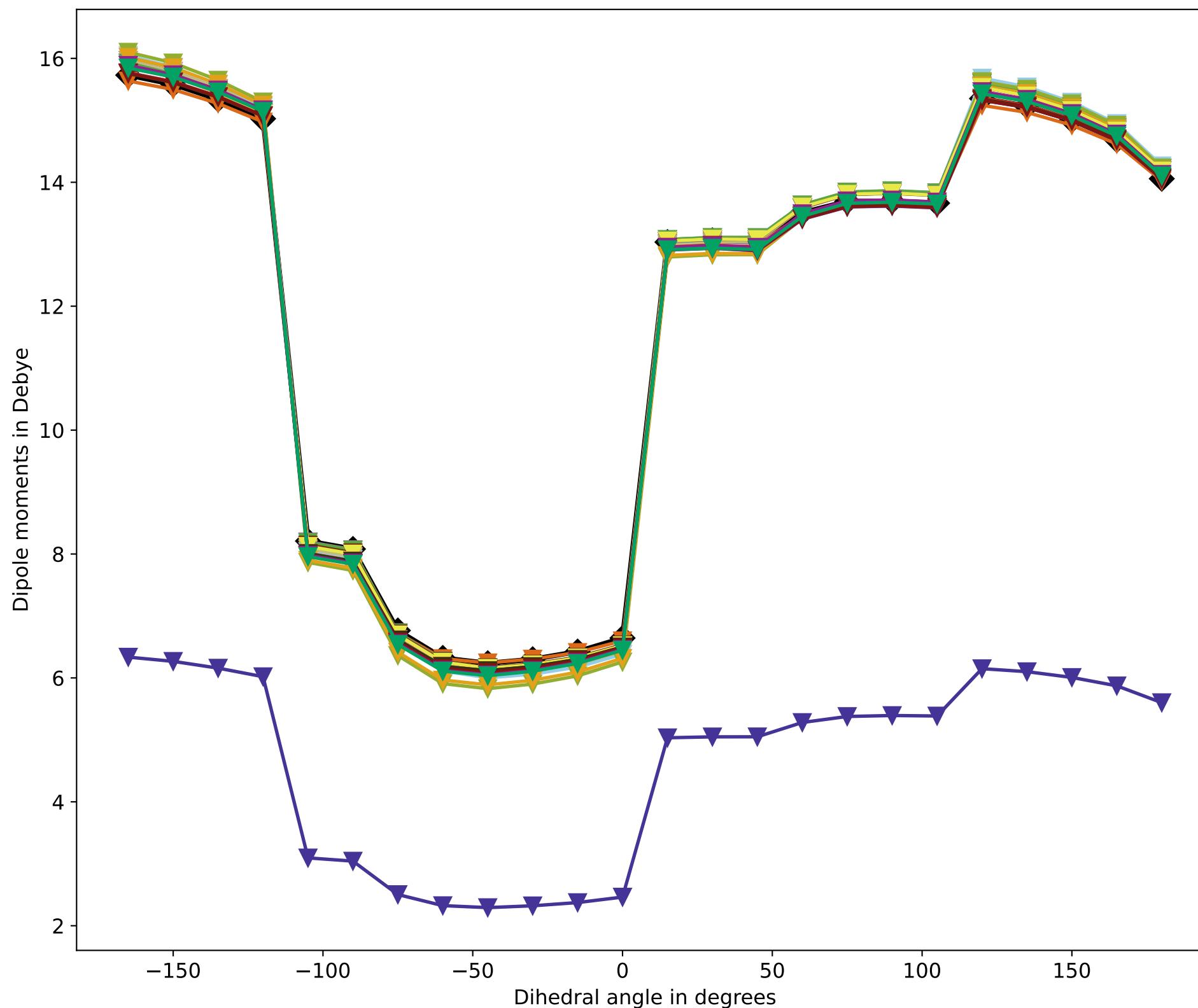


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

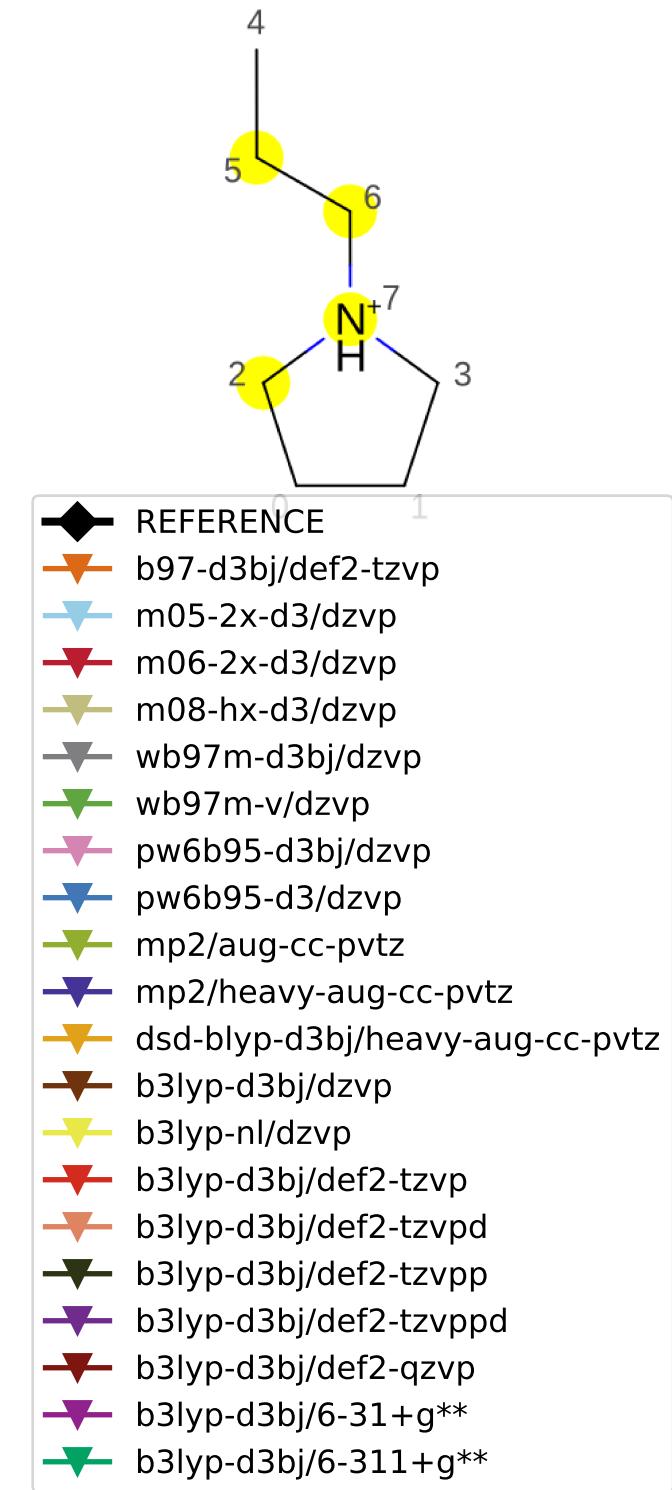
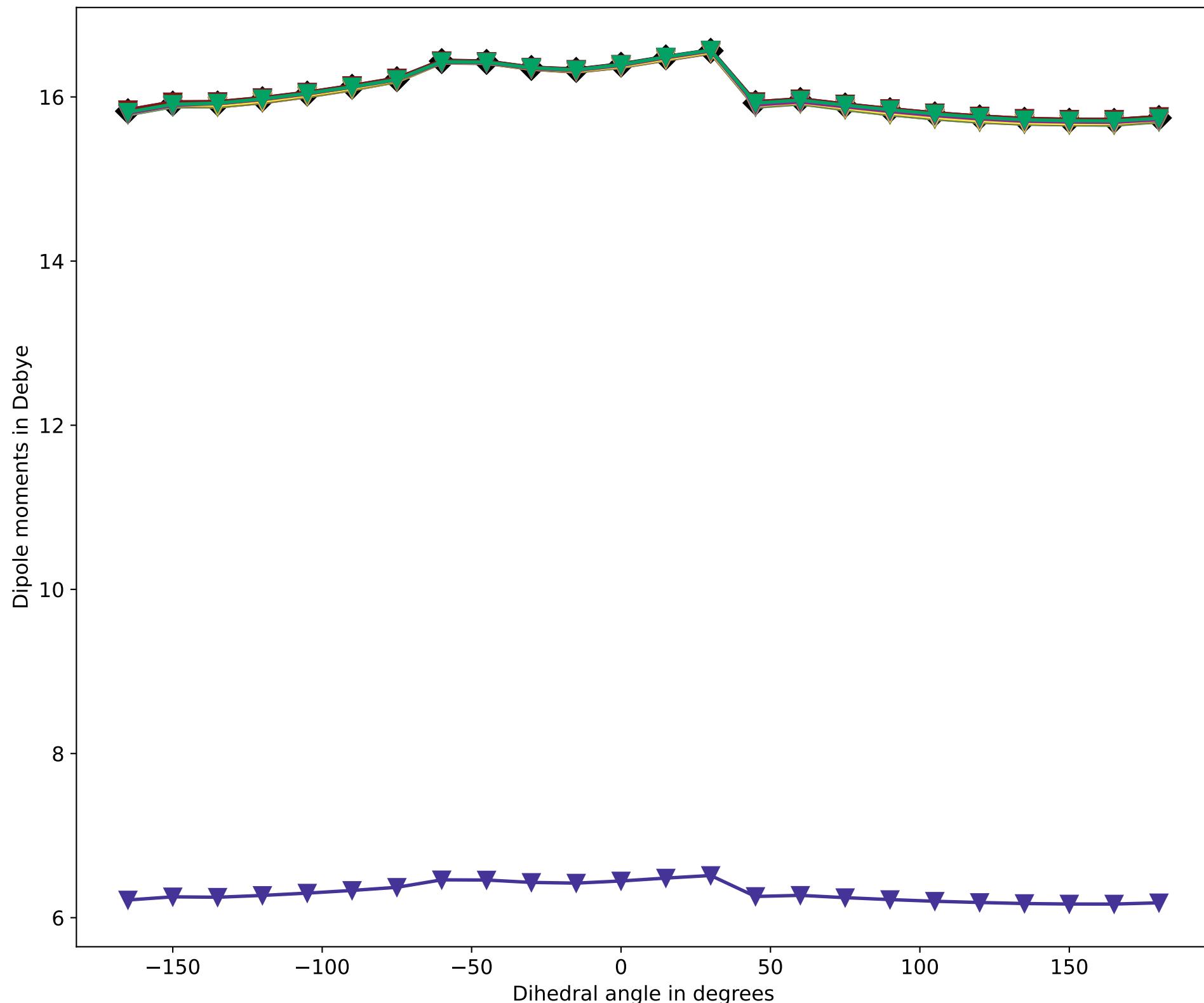


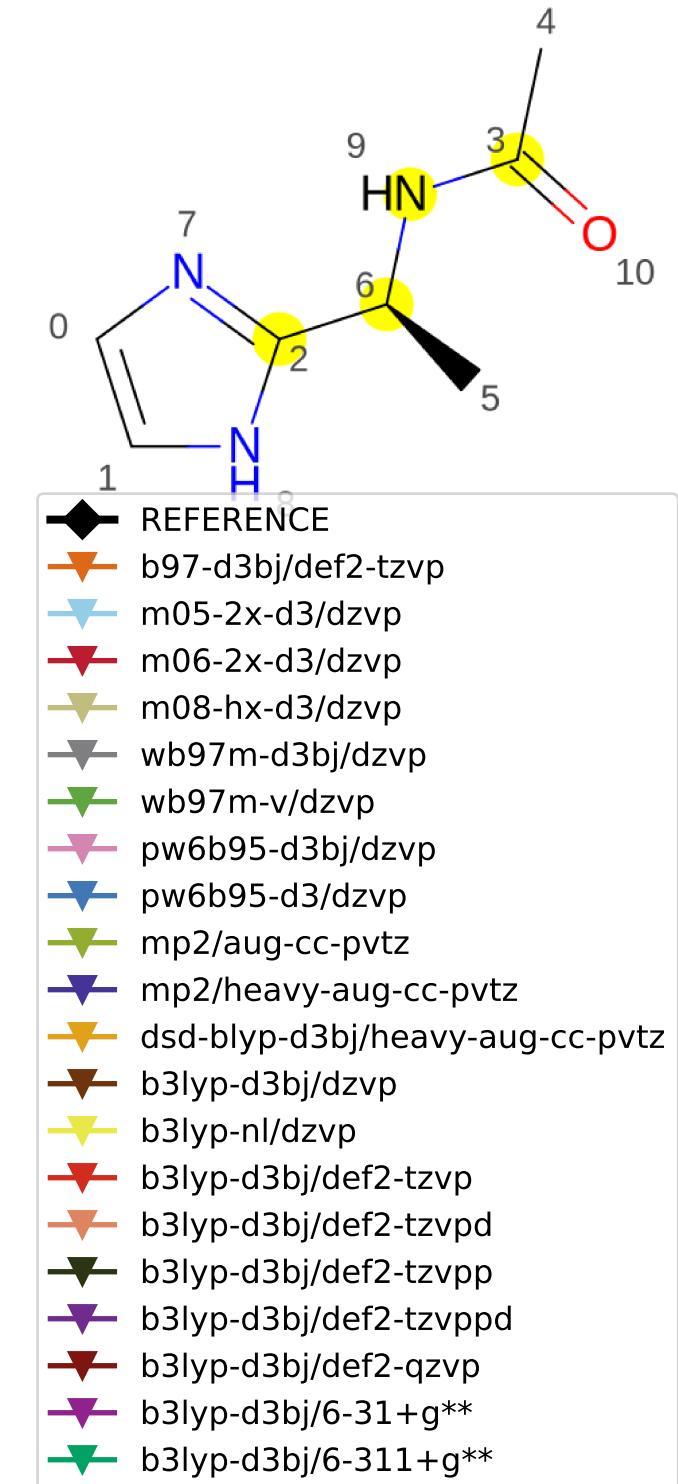
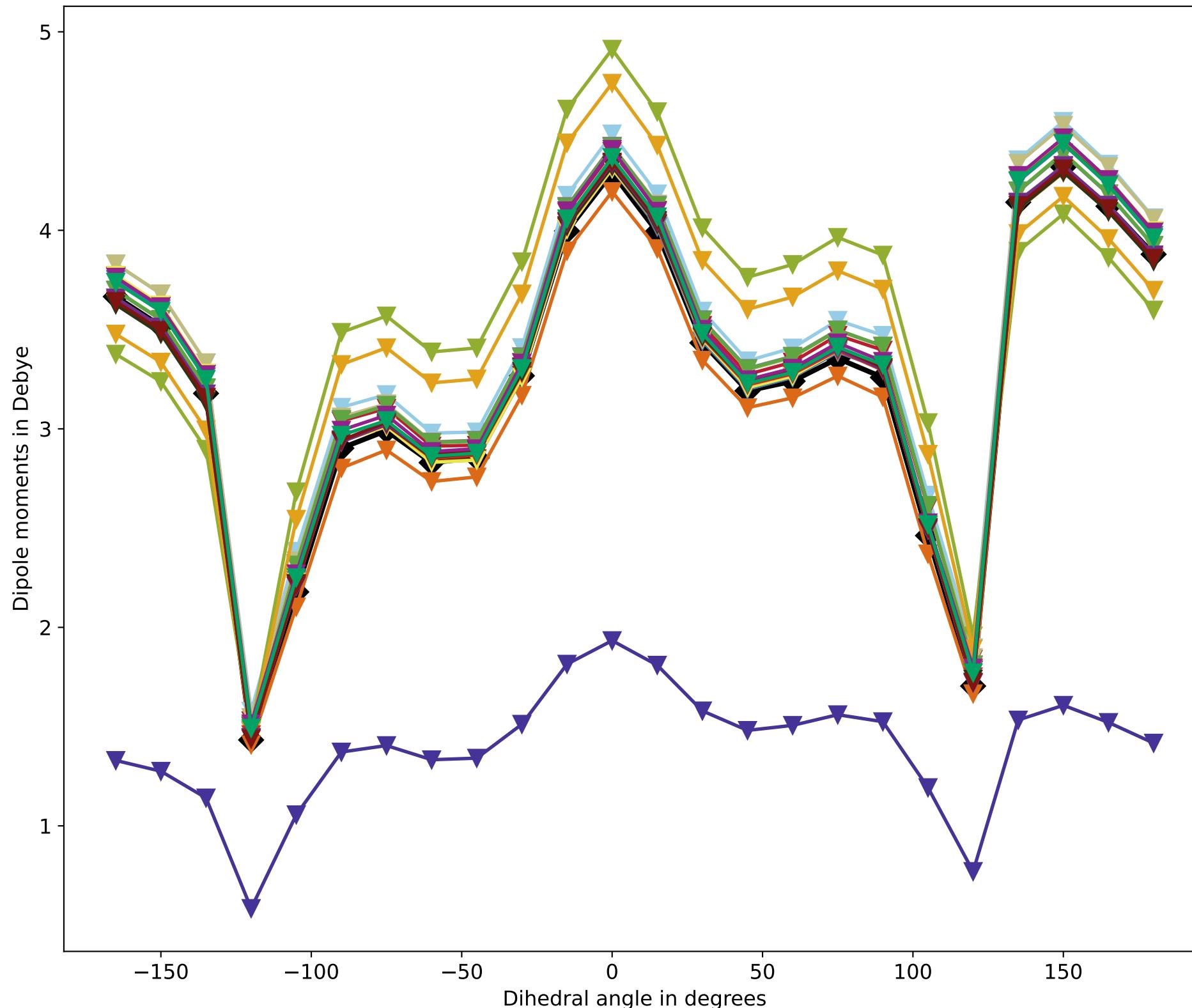


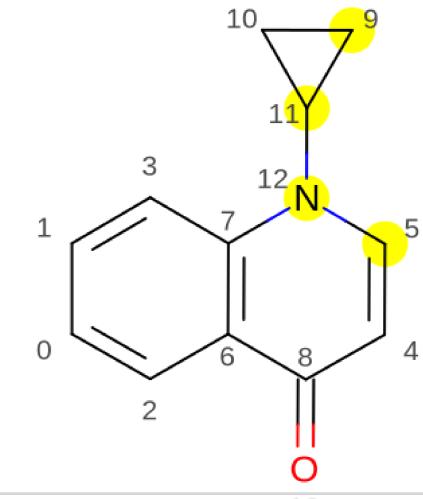
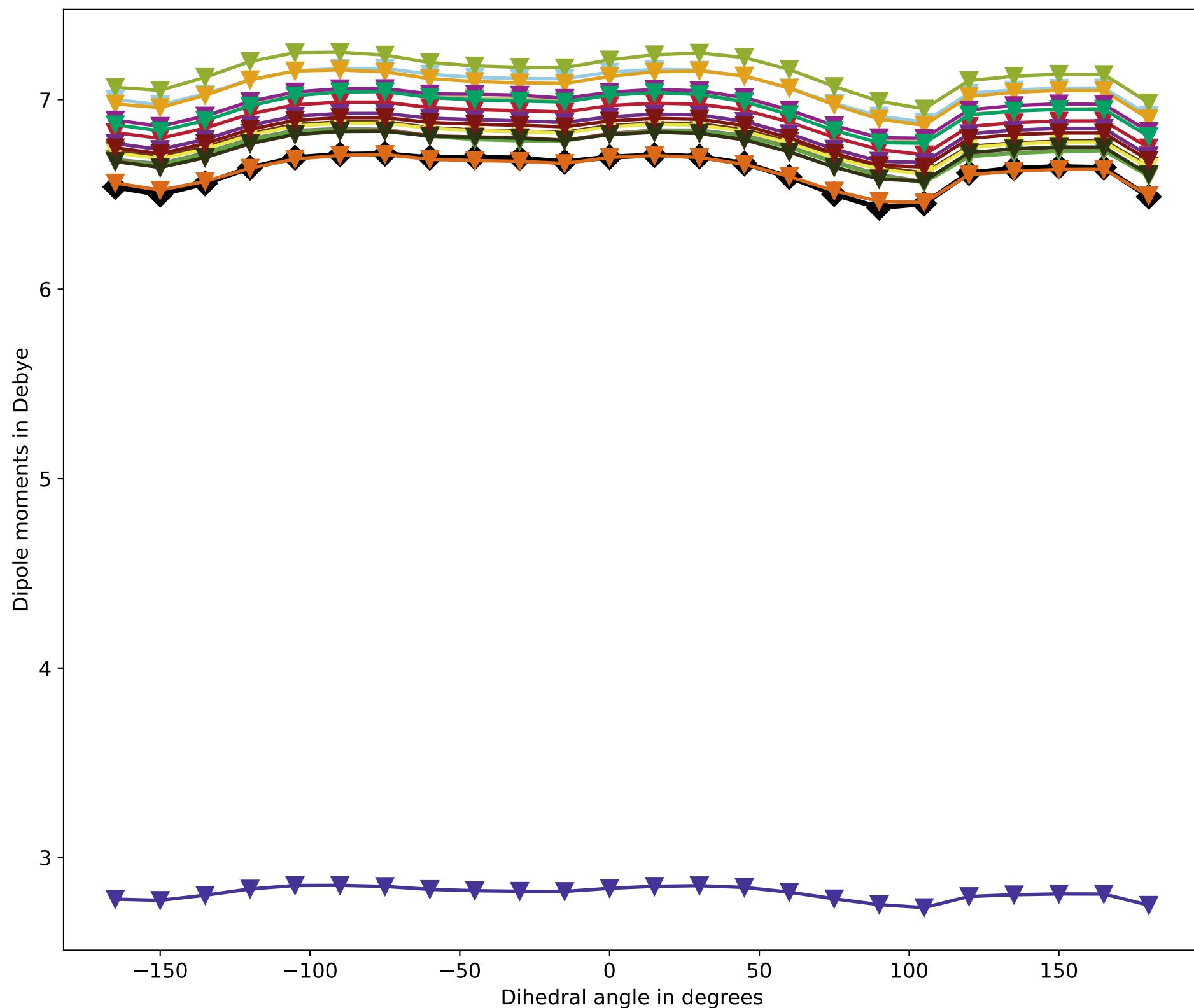
Charged molecule



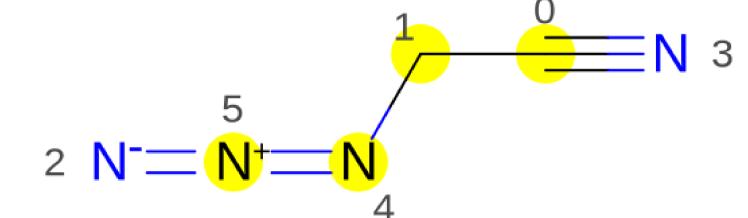
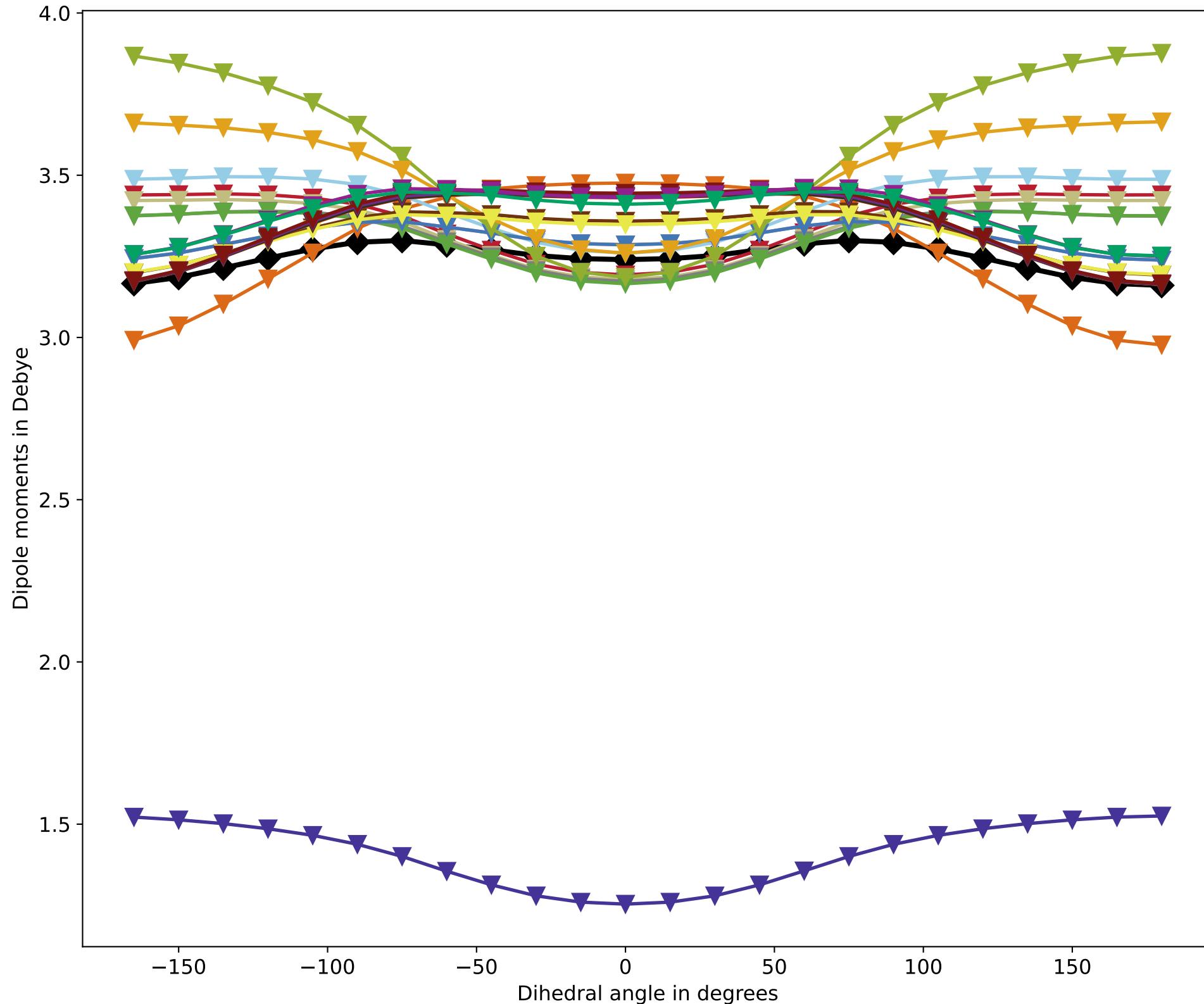
Charged molecule





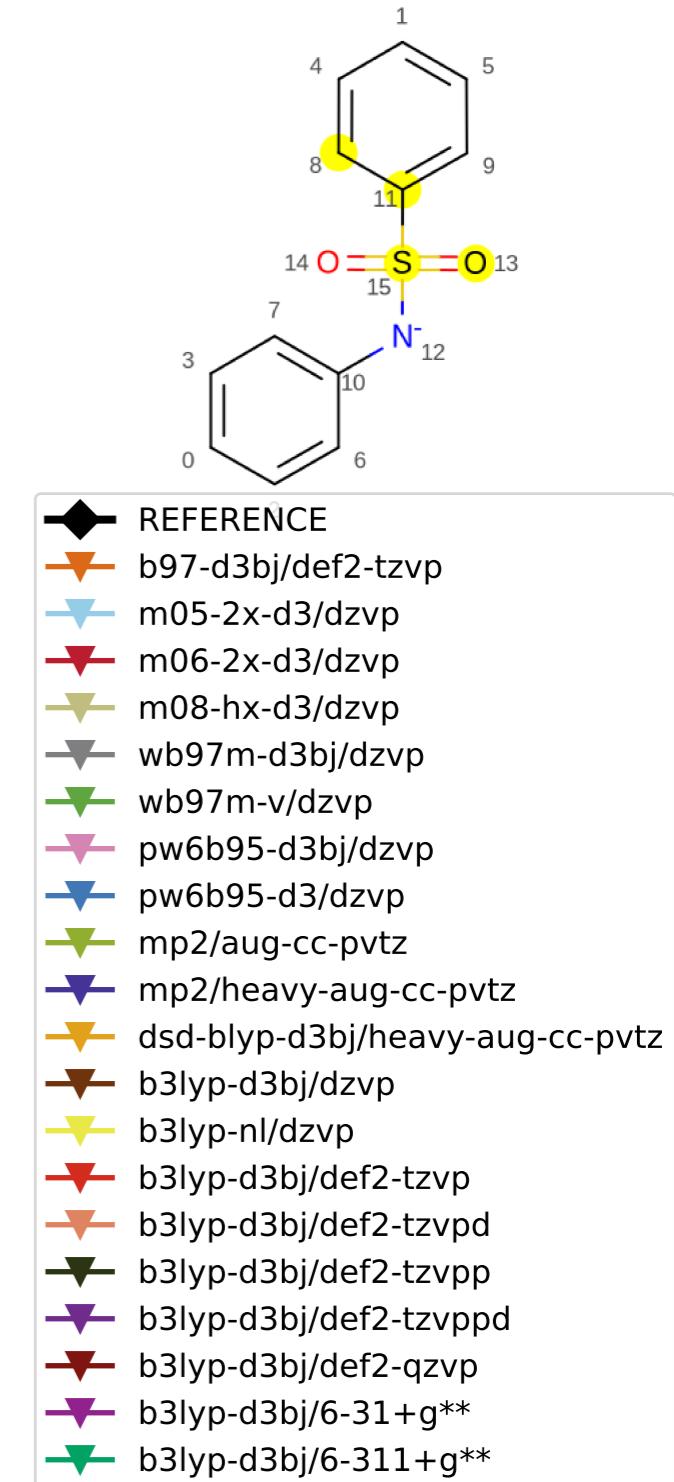
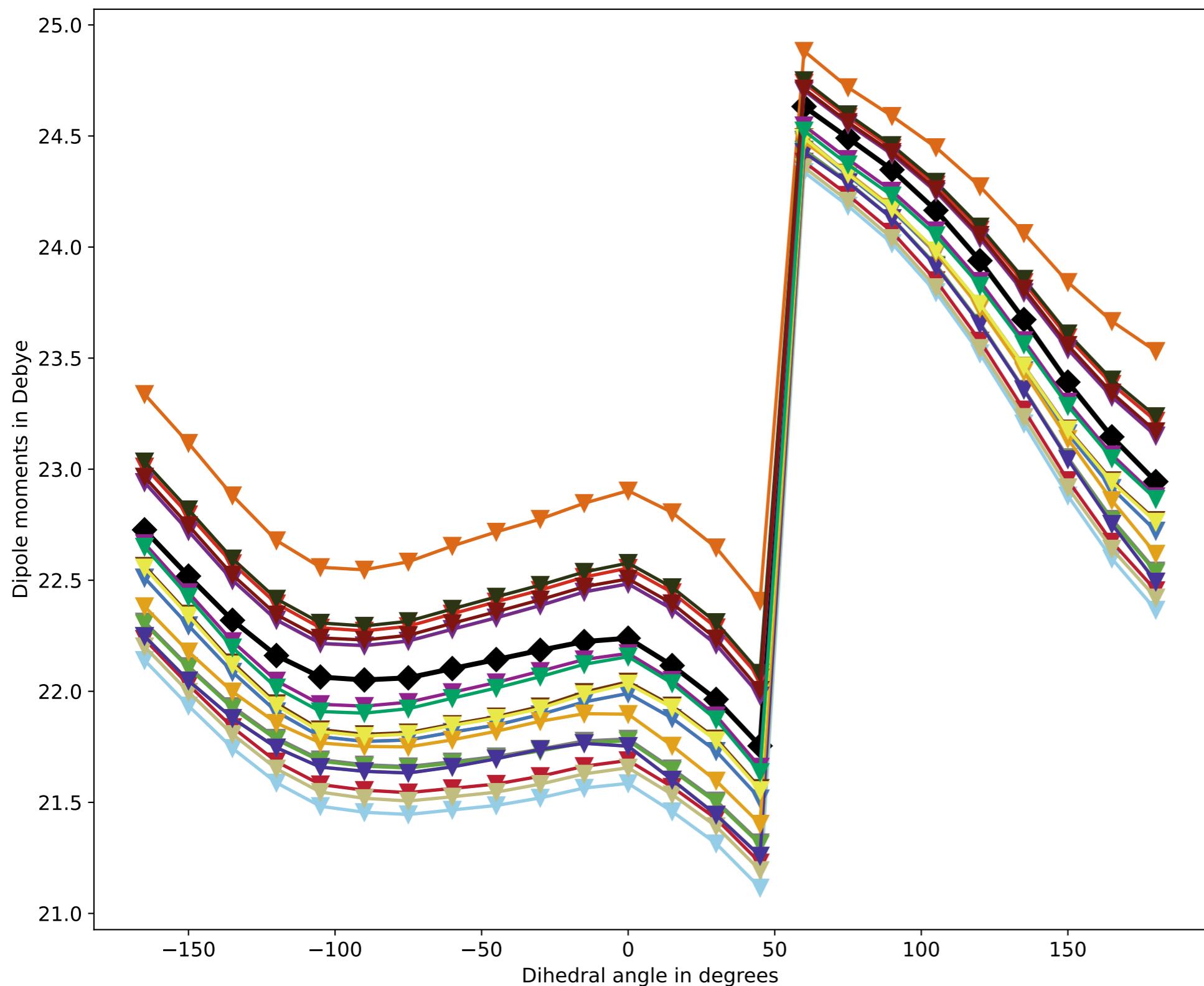


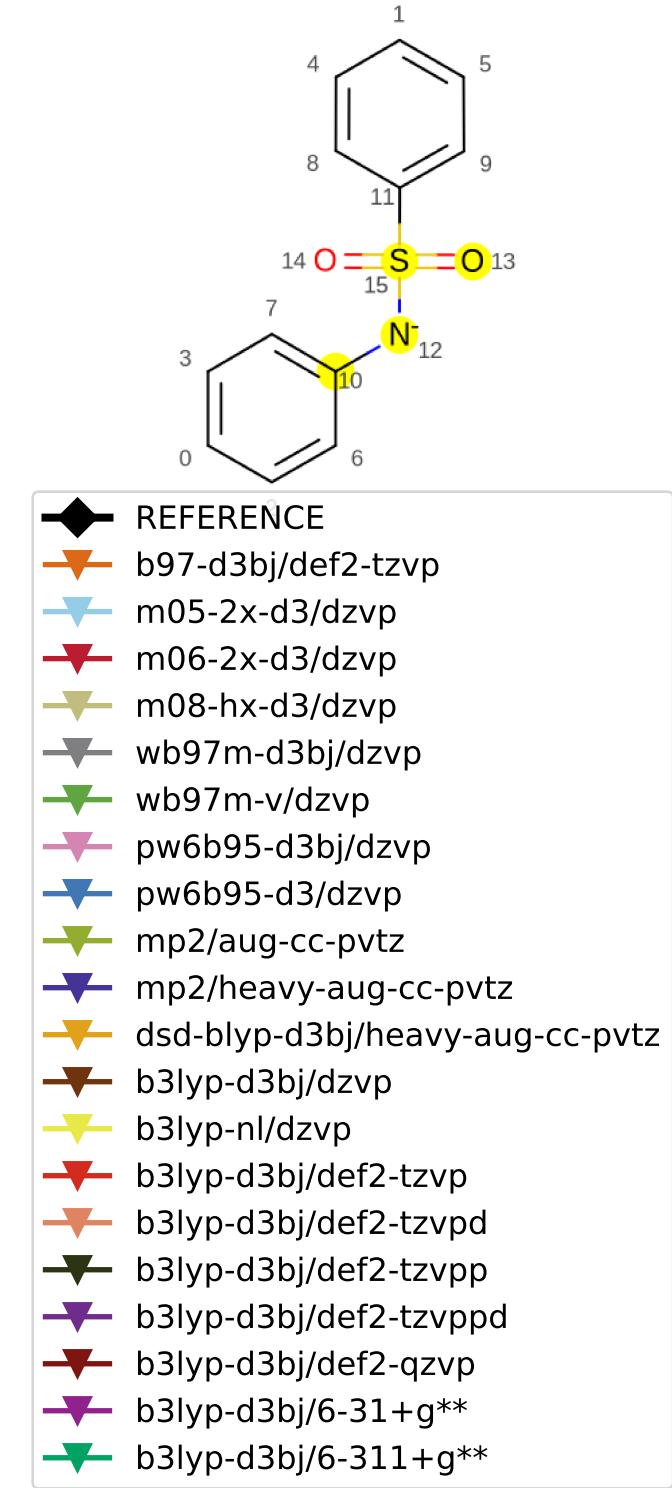
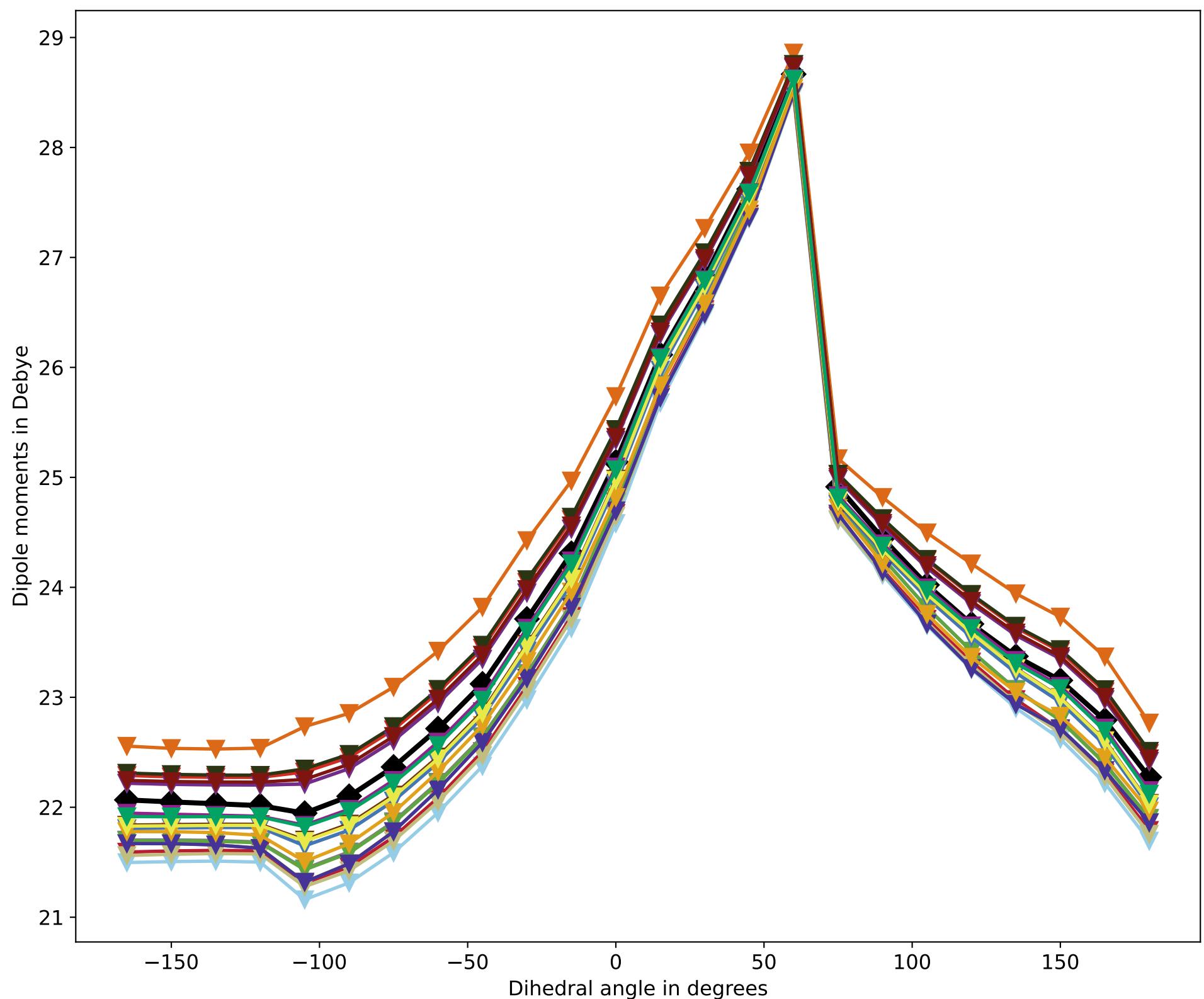
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|---|---------------------------------|
| ◆ | REFERENCE |
| ◆ | b97-d3bj/def2-tzvp |
| ◆ | m05-2x-d3/dzvp |
| ◆ | m06-2x-d3/dzvp |
| ◆ | m08-hx-d3/dzvp |
| ◆ | wb97m-d3bj/dzvp |
| ◆ | wb97m-v/dzvp |
| ◆ | pw6b95-d3bj/dzvp |
| ◆ | pw6b95-d3/dzvp |
| ◆ | 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-tzvpd |
| ◆ | b3lyp-d3bj/def2-tzvpp |
| ◆ | b3lyp-d3bj/def2-tzvppd |
| ◆ | b3lyp-d3bj/def2-qzvp |
| ◆ | b3lyp-d3bj/6-31+g** |
| ◆ | b3lyp-d3bj/6-311+g** |

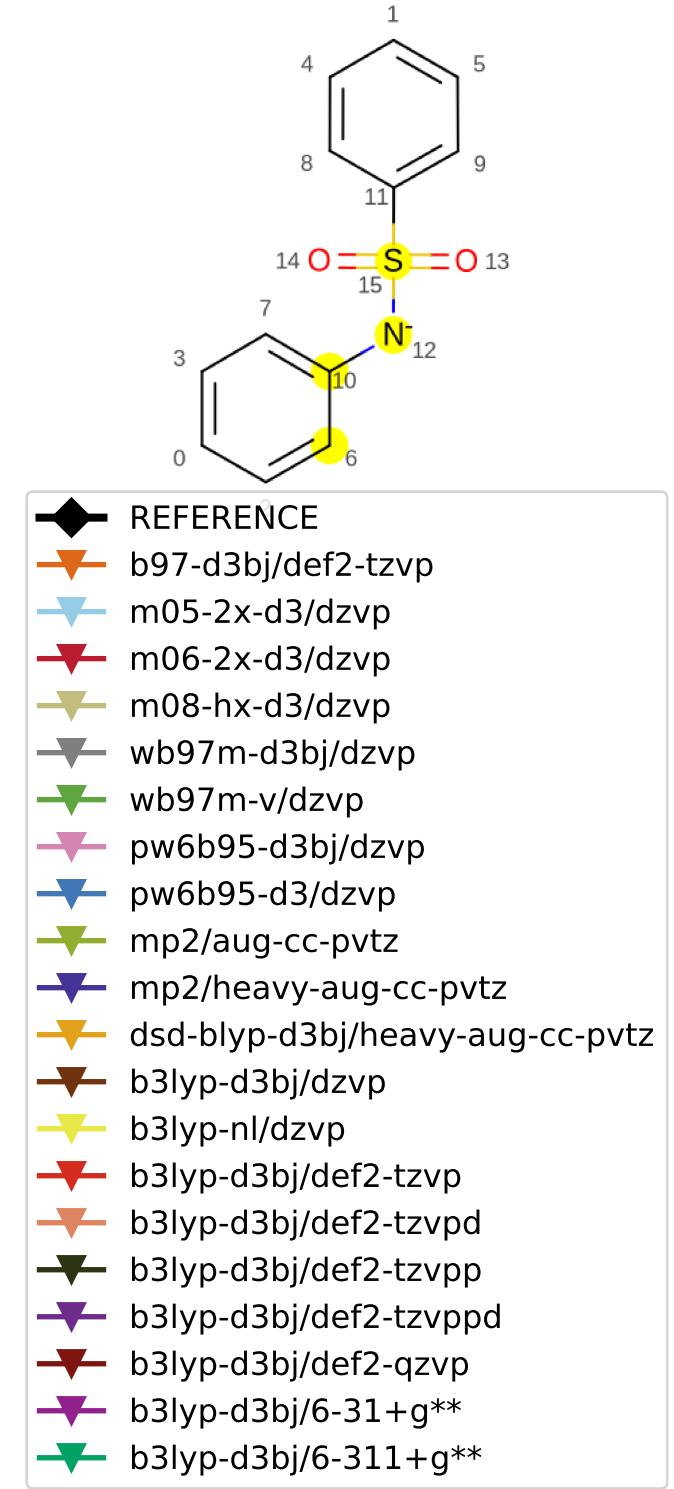
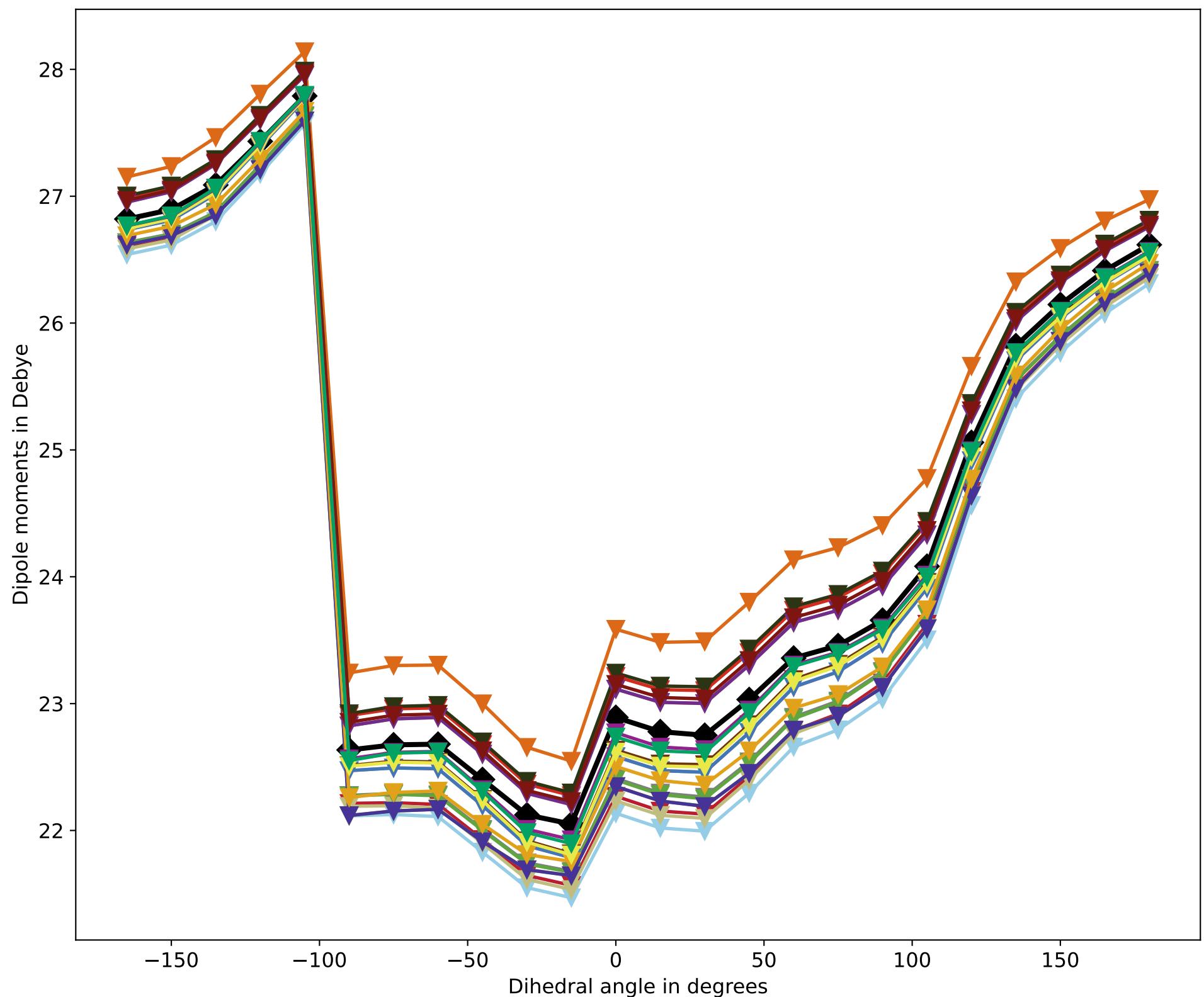


- | | |
|---|---------------------------------|
| ◆ | REFERENCE |
| ◆ | b97-d3bj/def2-tzvp |
| ◆ | m05-2x-d3/dzvp |
| ◆ | m06-2x-d3/dzvp |
| ◆ | m08-hx-d3/dzvp |
| ◆ | wb97m-d3bj/dzvp |
| ◆ | wb97m-v/dzvp |
| ◆ | pw6b95-d3bj/dzvp |
| ◆ | pw6b95-d3/dzvp |
| ◆ | mp2/aug-cc-pvtz |
| ◆ | mp2/heavy-aug-cc-pvtz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

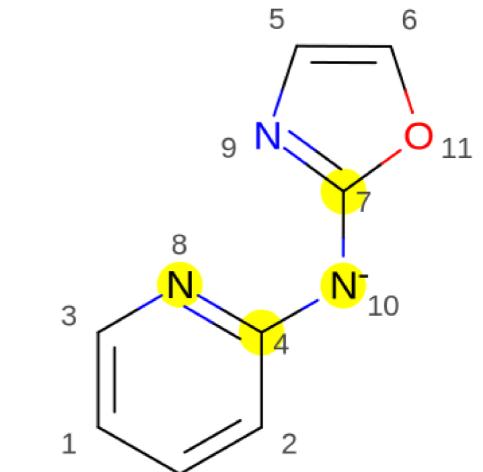
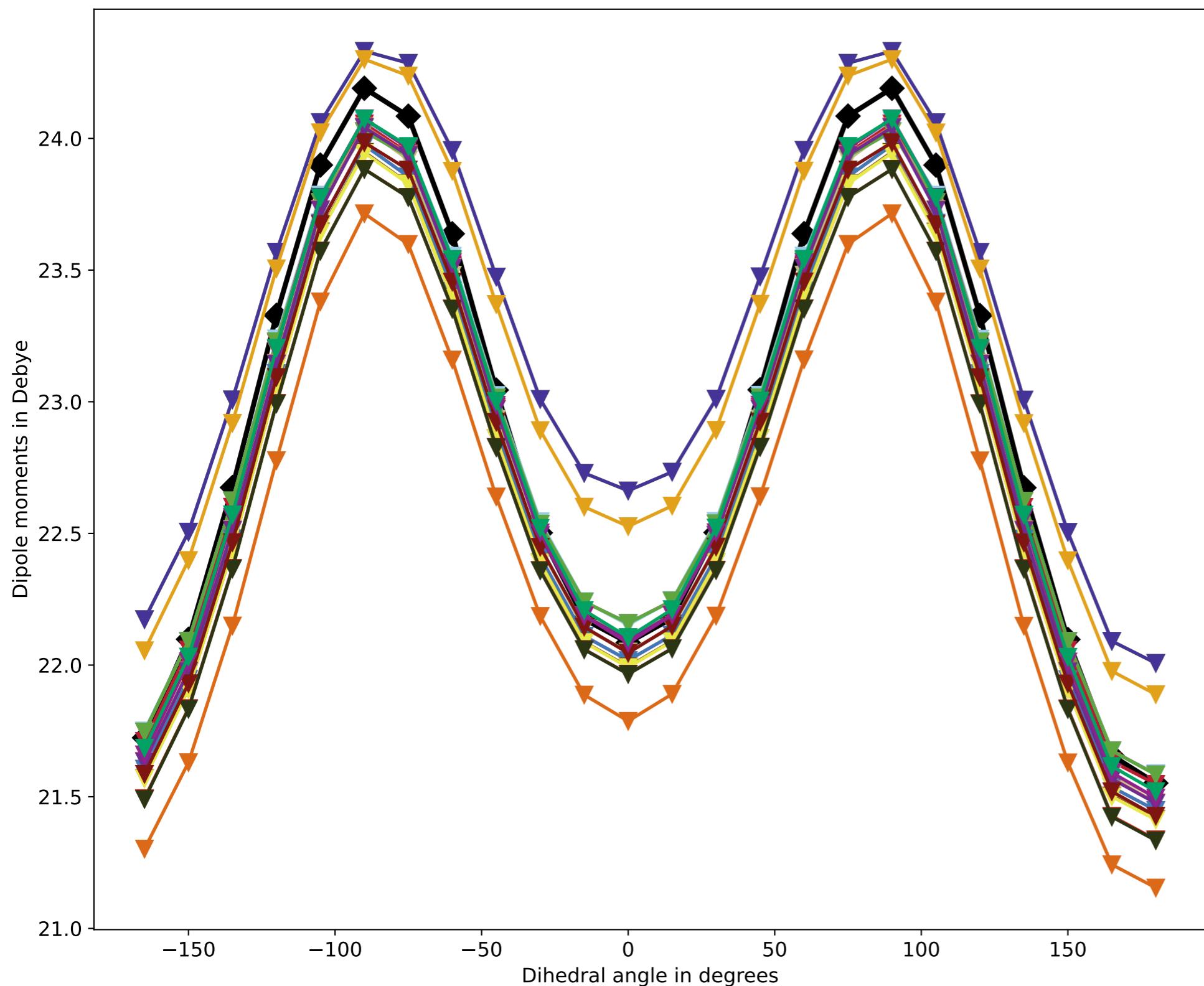
Charged molecule





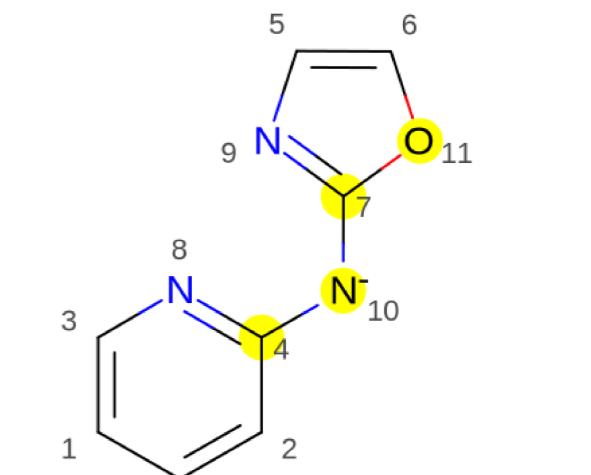
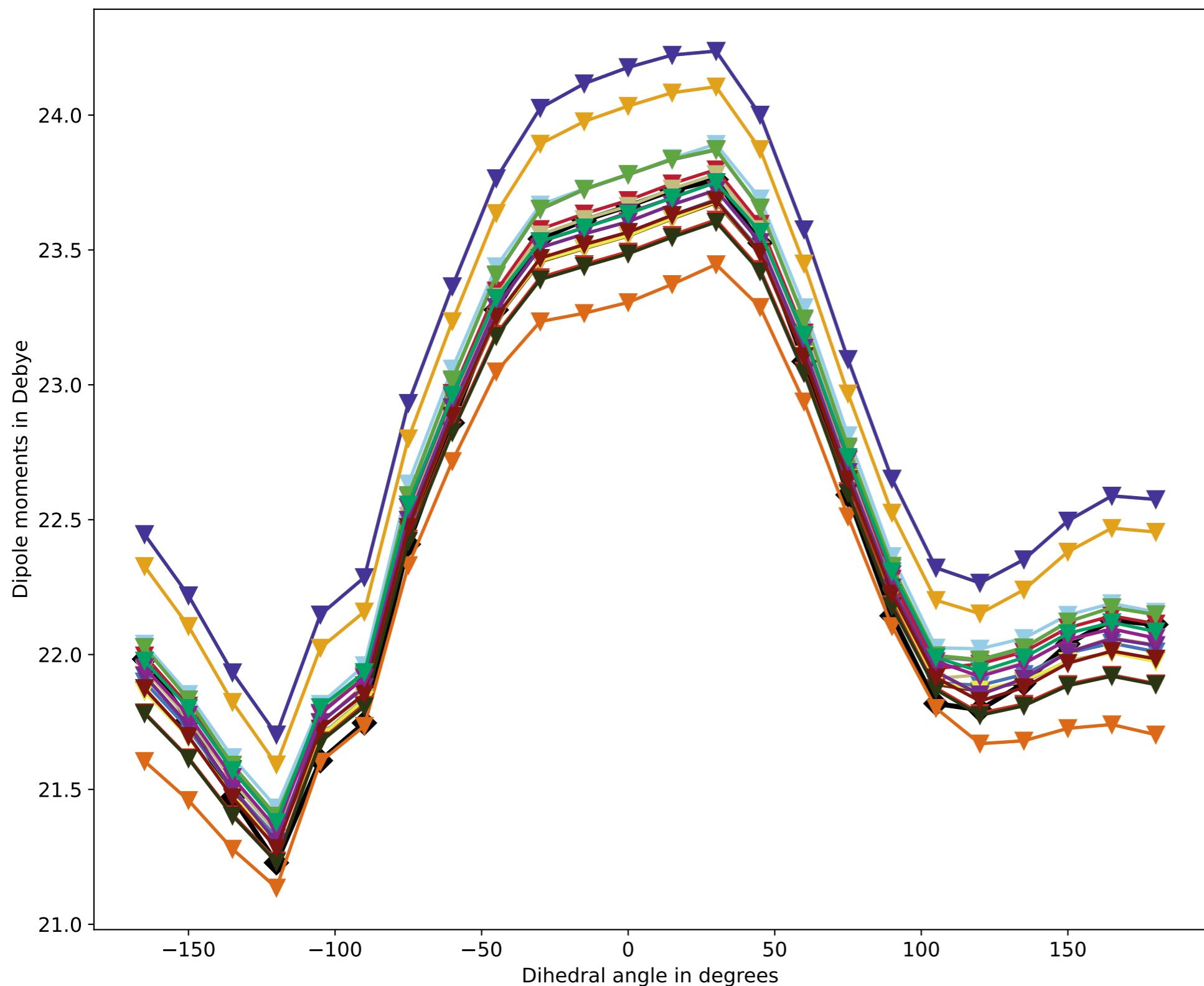


Charged molecule



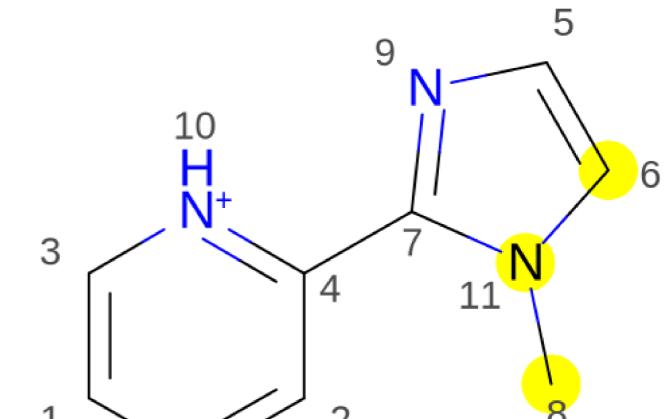
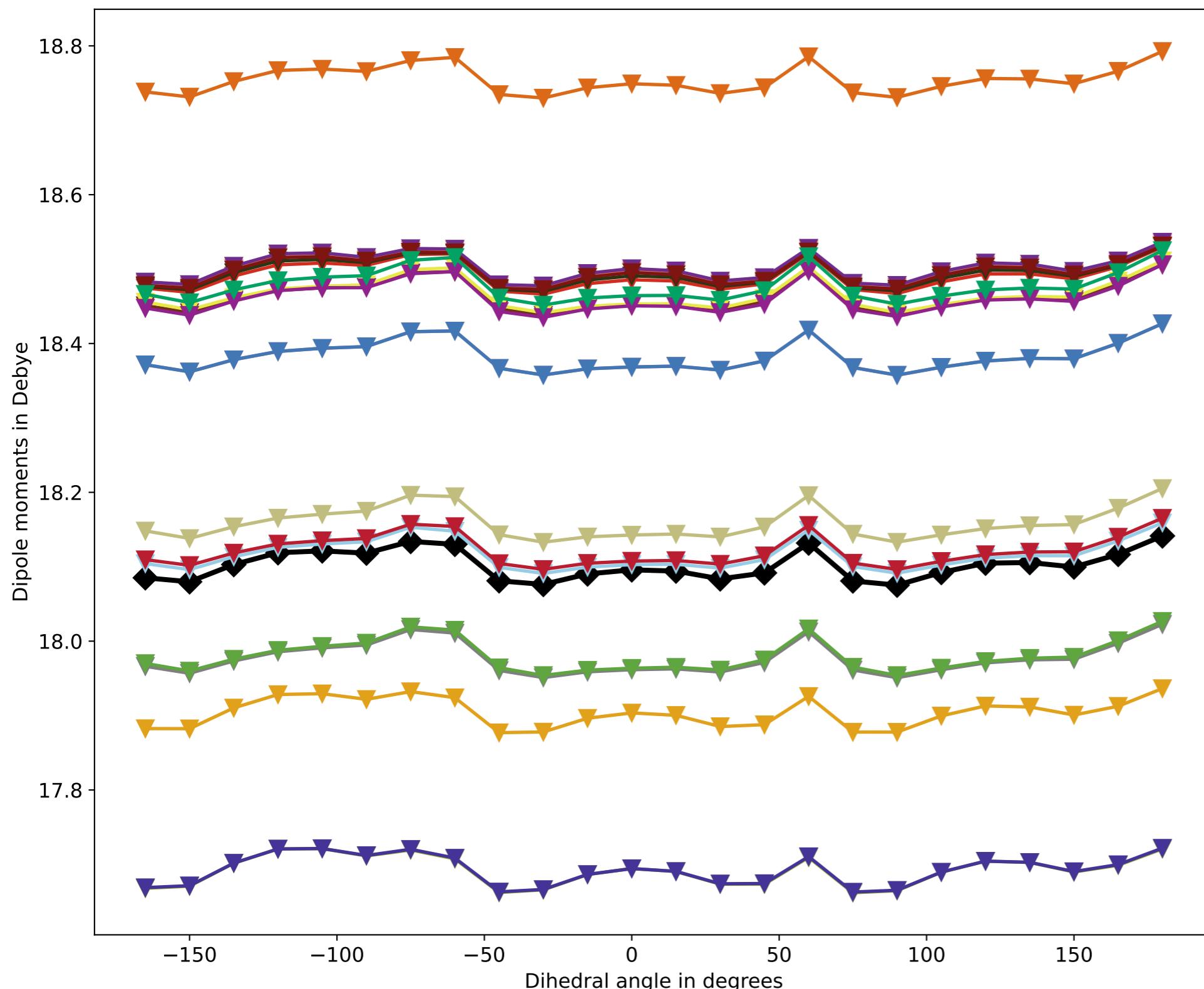
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- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp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

Charged molecule



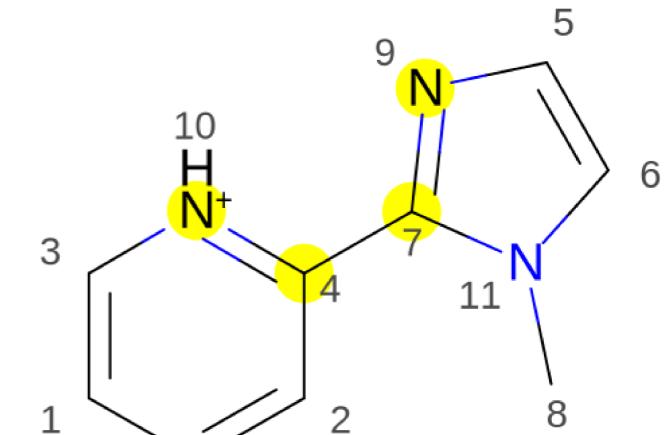
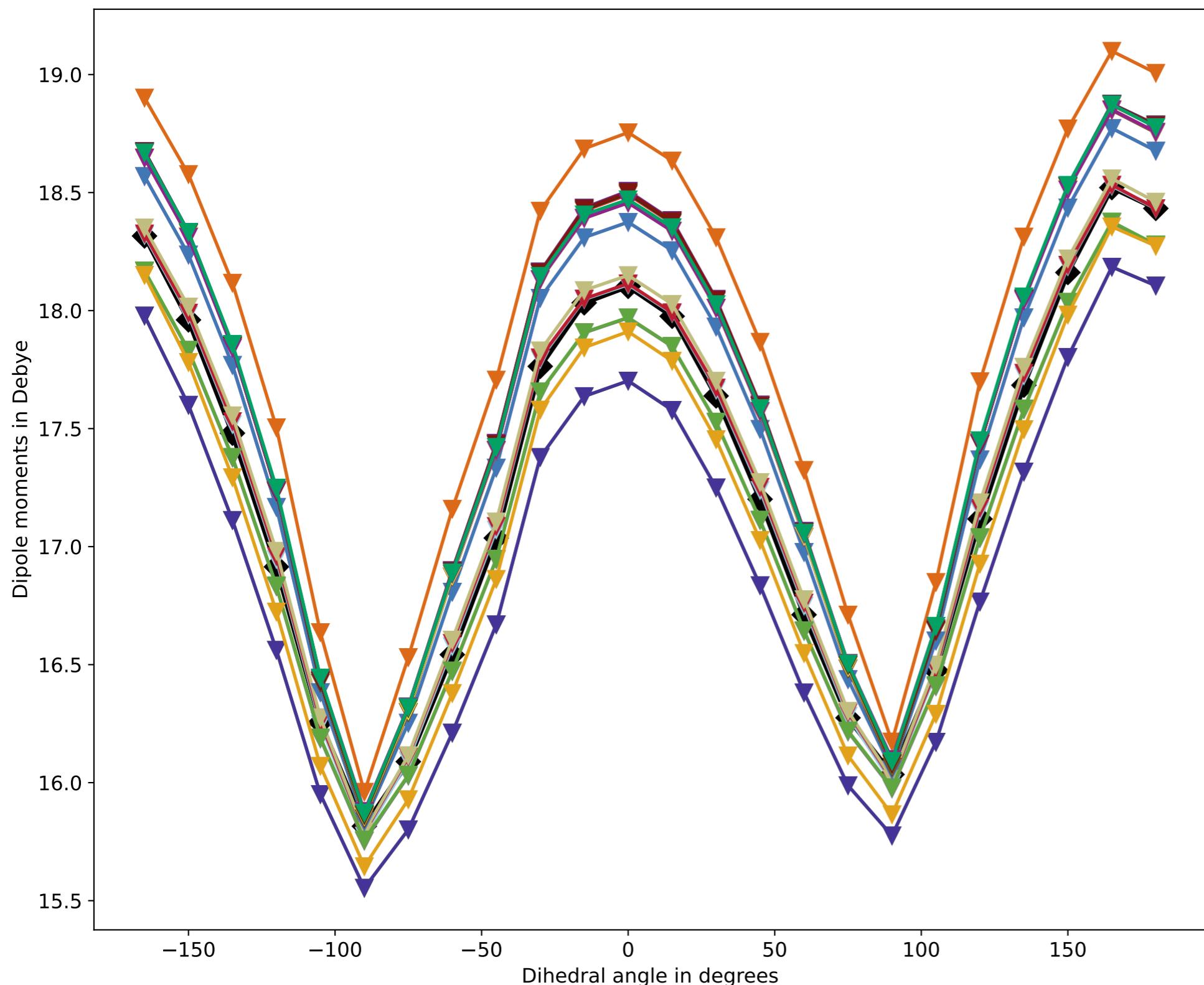
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- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

Charged molecule



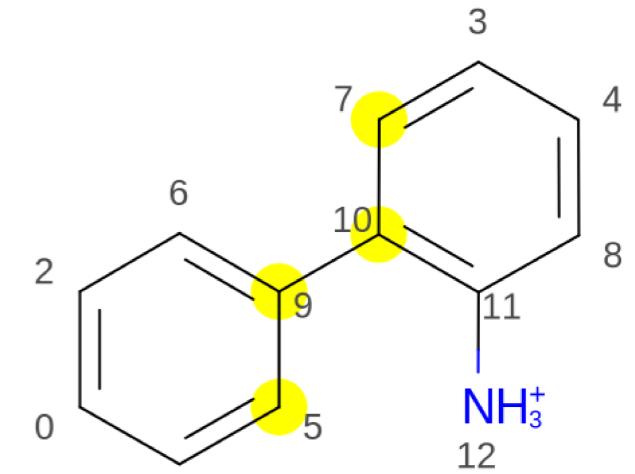
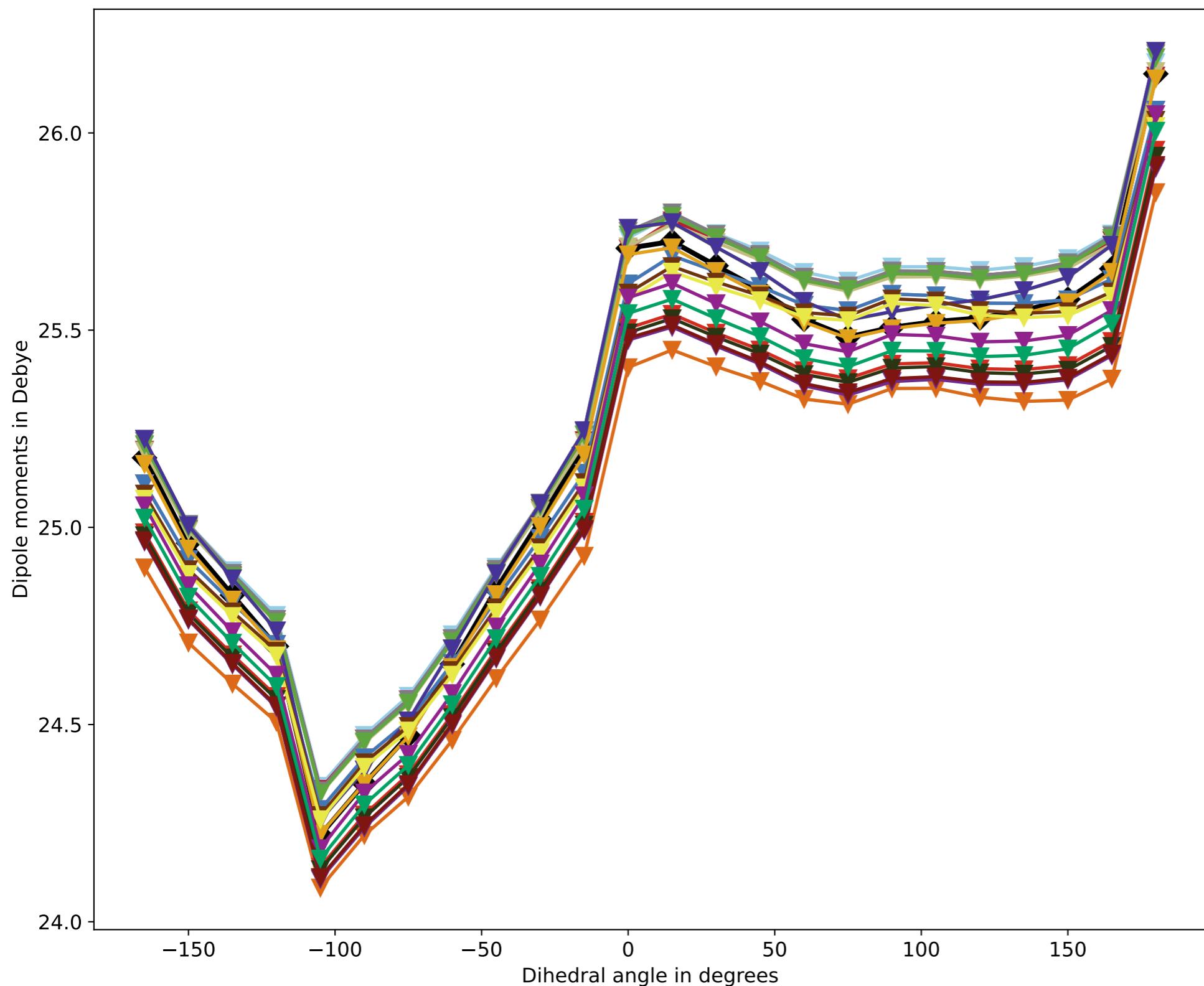
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- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp
- ◆ b3lyp-d3bj/def2-tzvpd
- ◆ b3lyp-d3bj/def2-tzvpp
- ◆ b3lyp-d3bj/def2-tzvppd
- ◆ b3lyp-d3bj/def2-qzvp
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Charged molecule

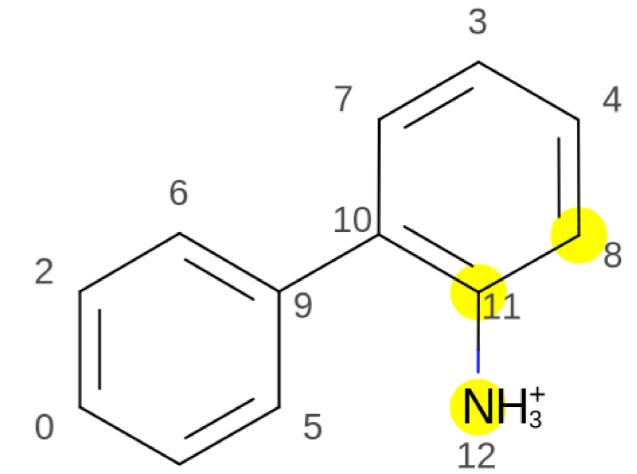
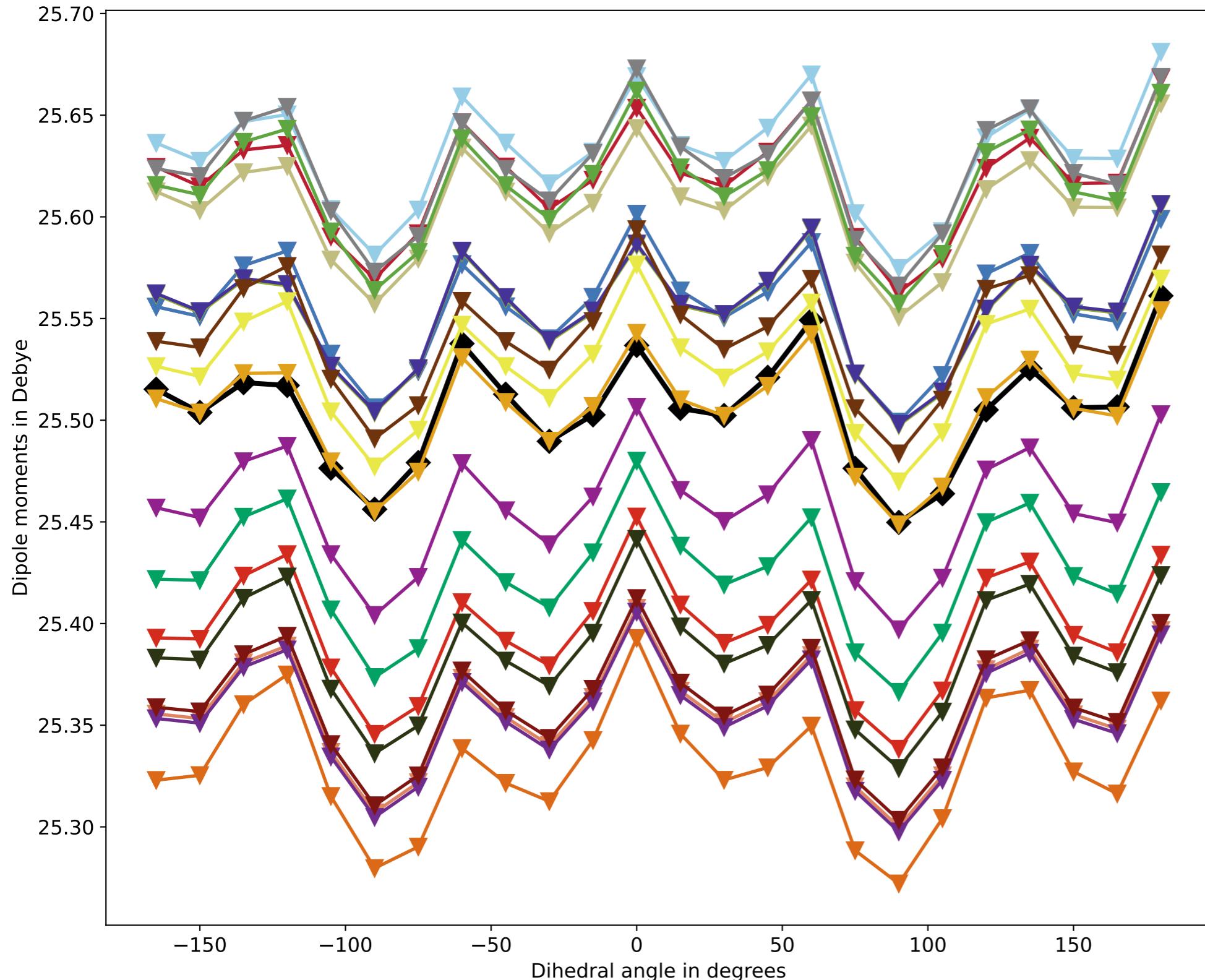


- ◆ REFERENCE
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- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp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

Charged molecule

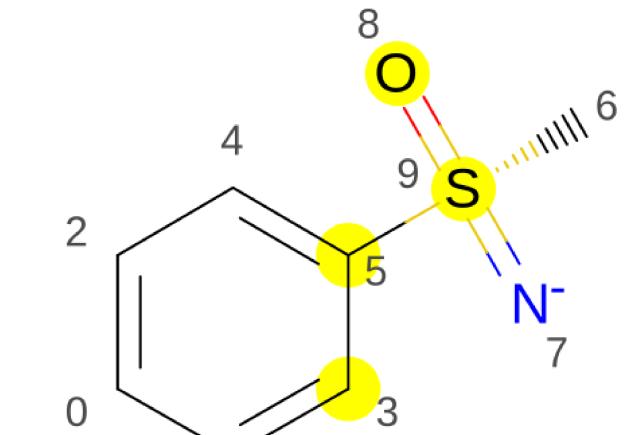
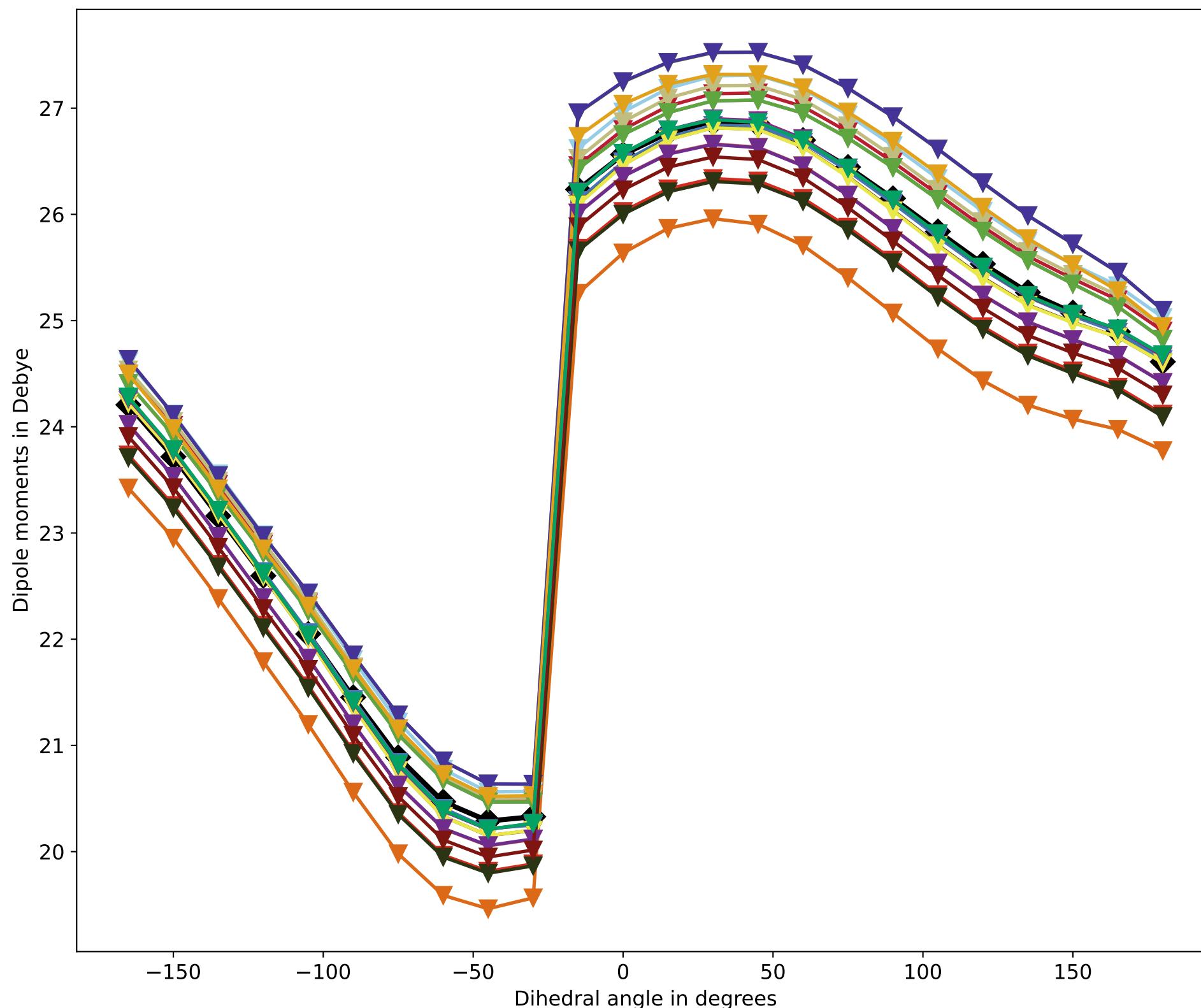


- ◆ REFERENCE
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- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp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



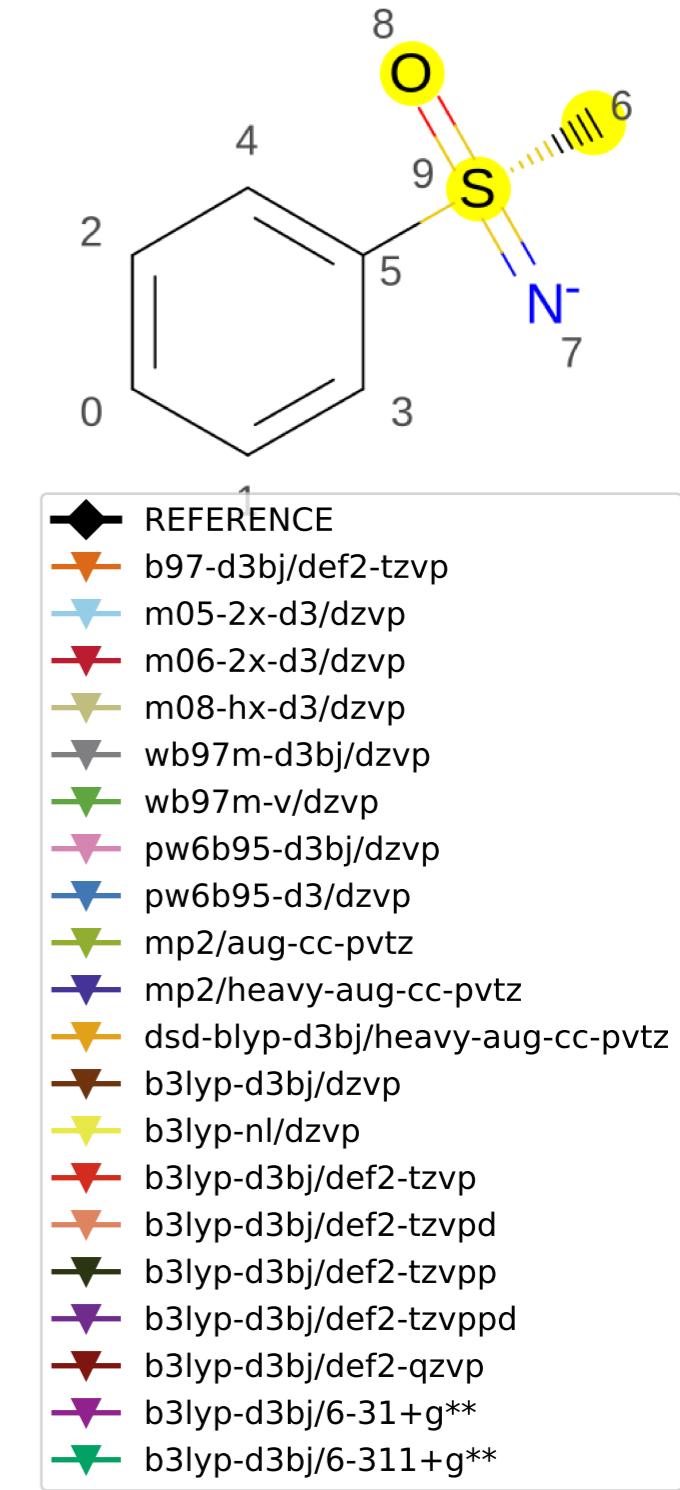
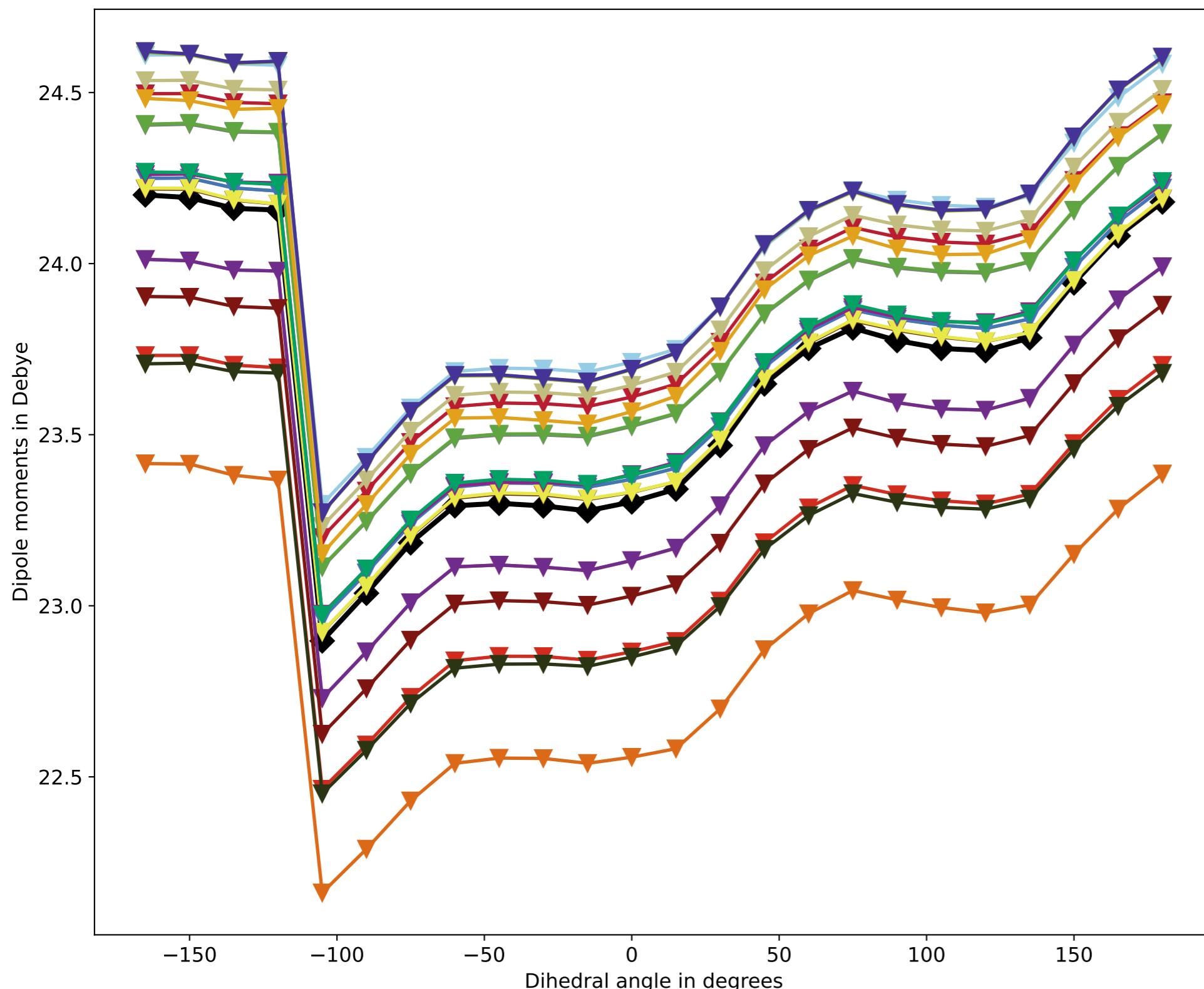
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- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd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

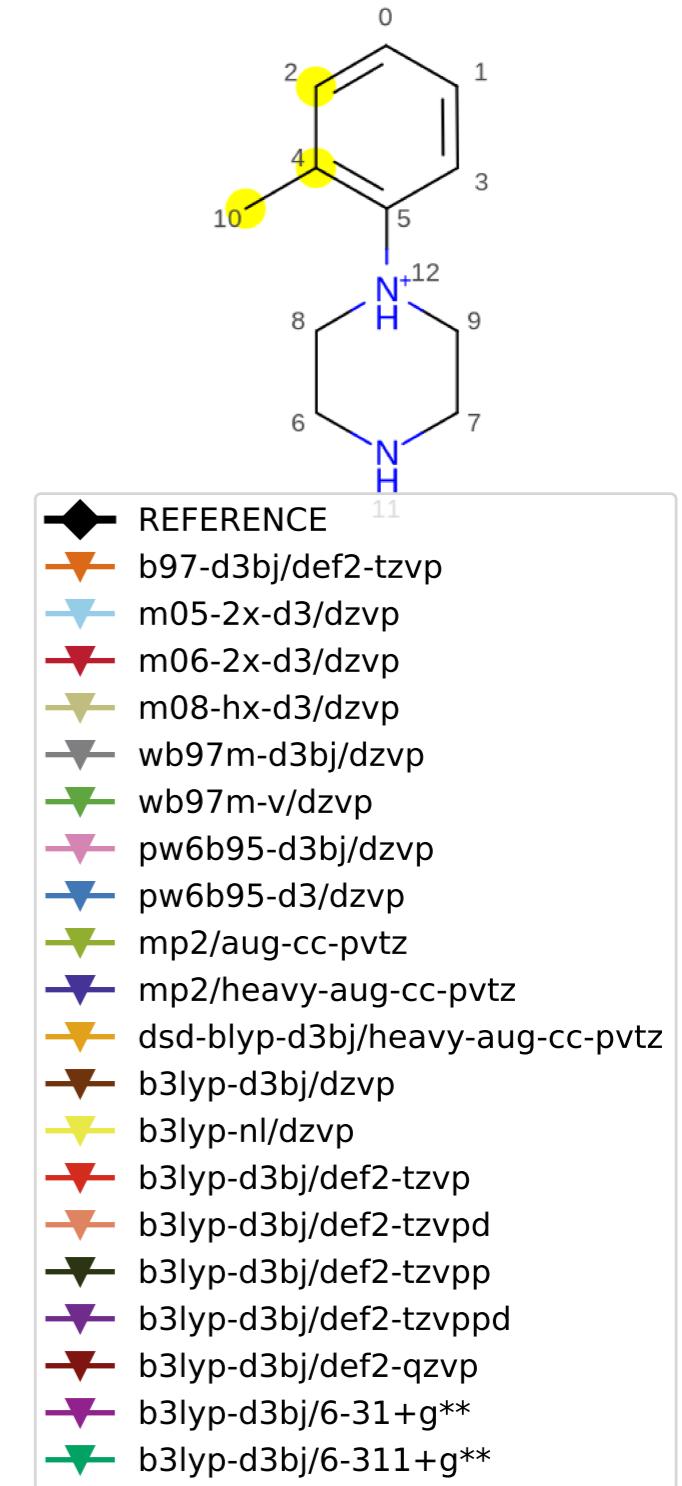
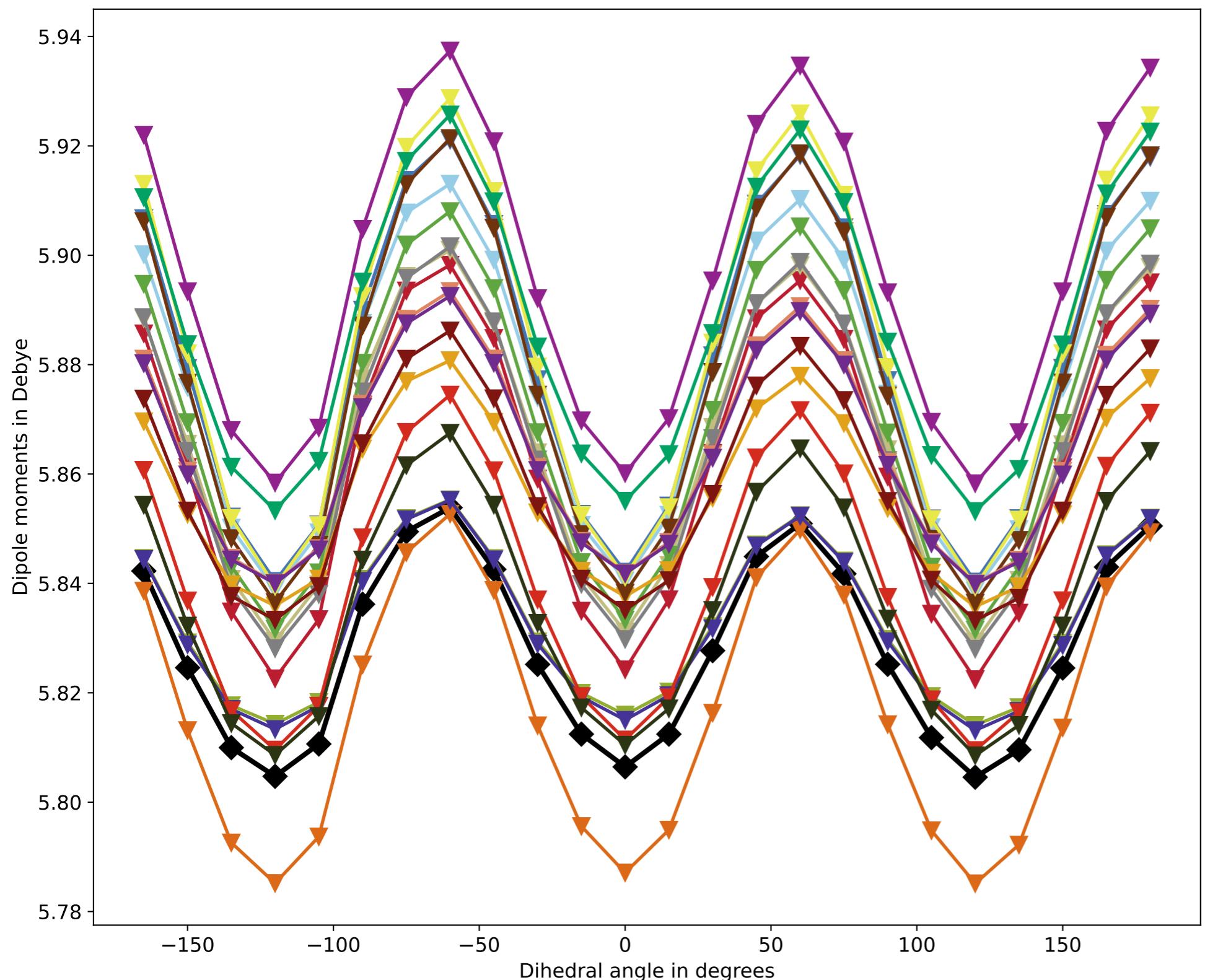
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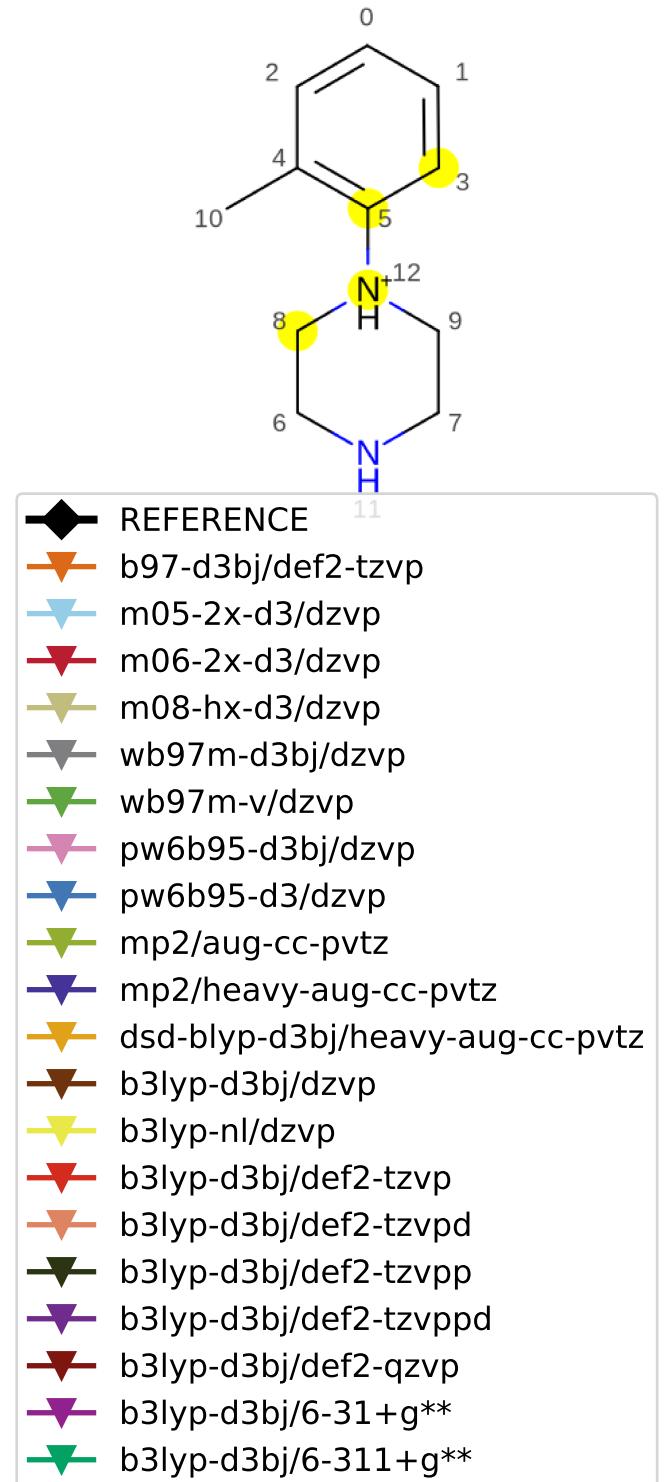
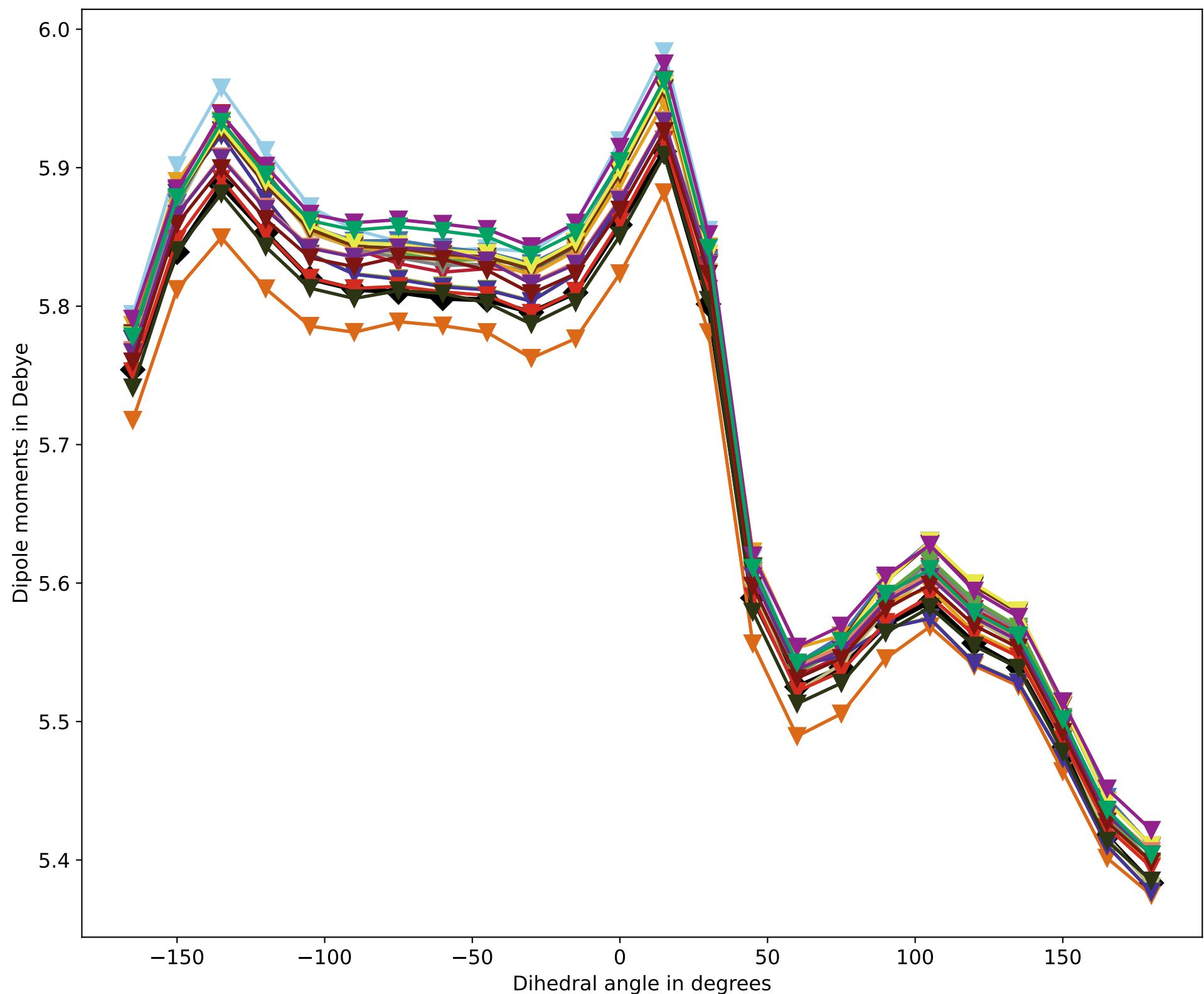


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

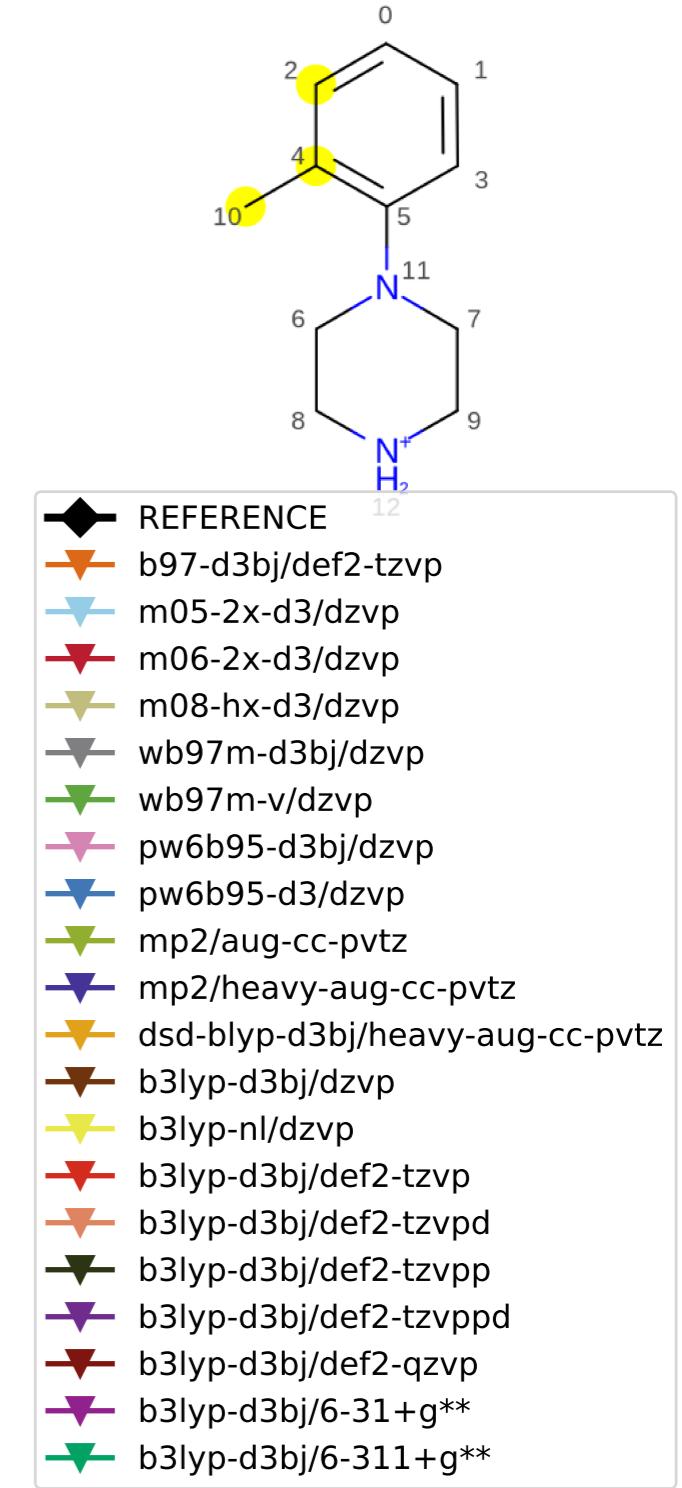
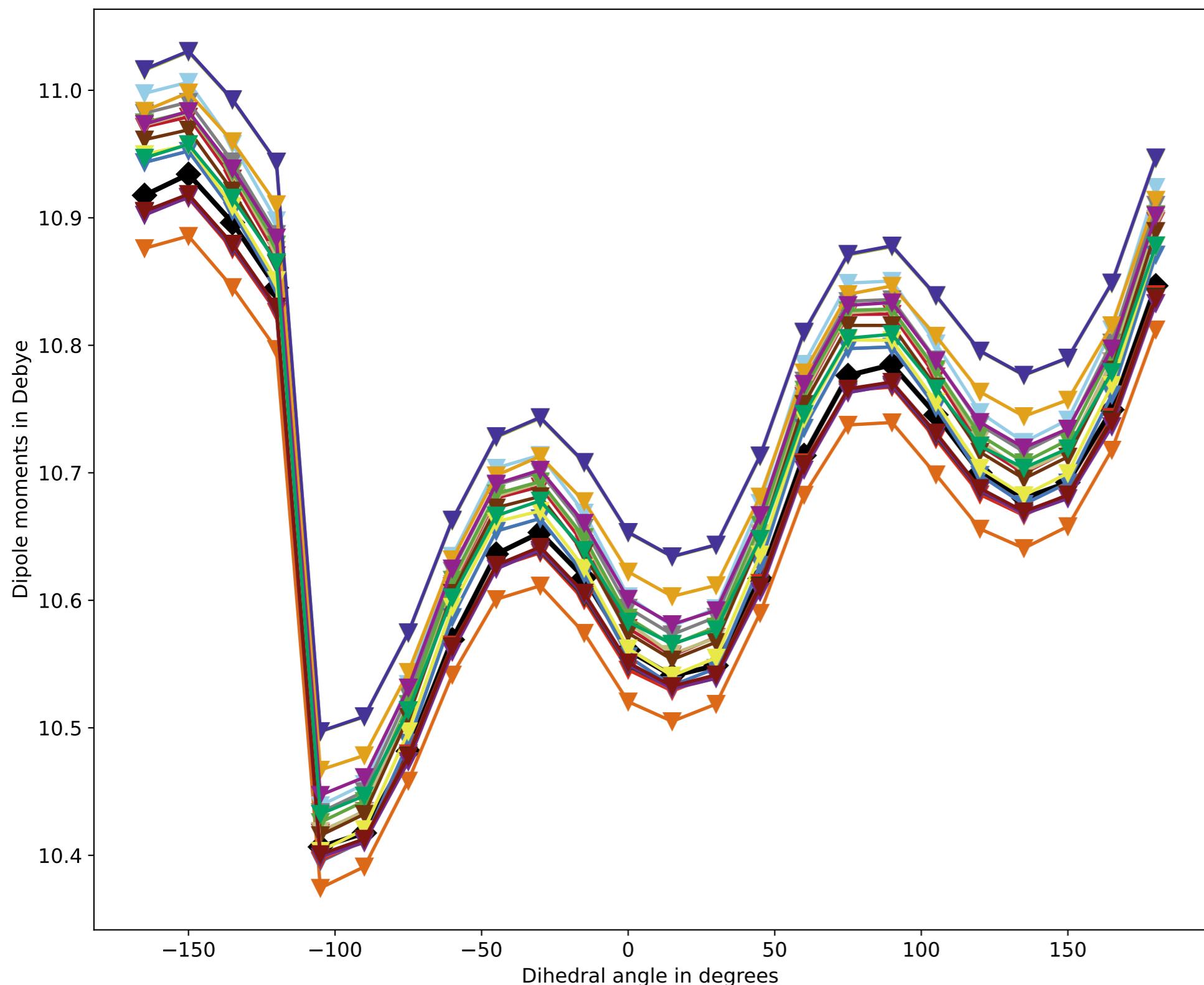
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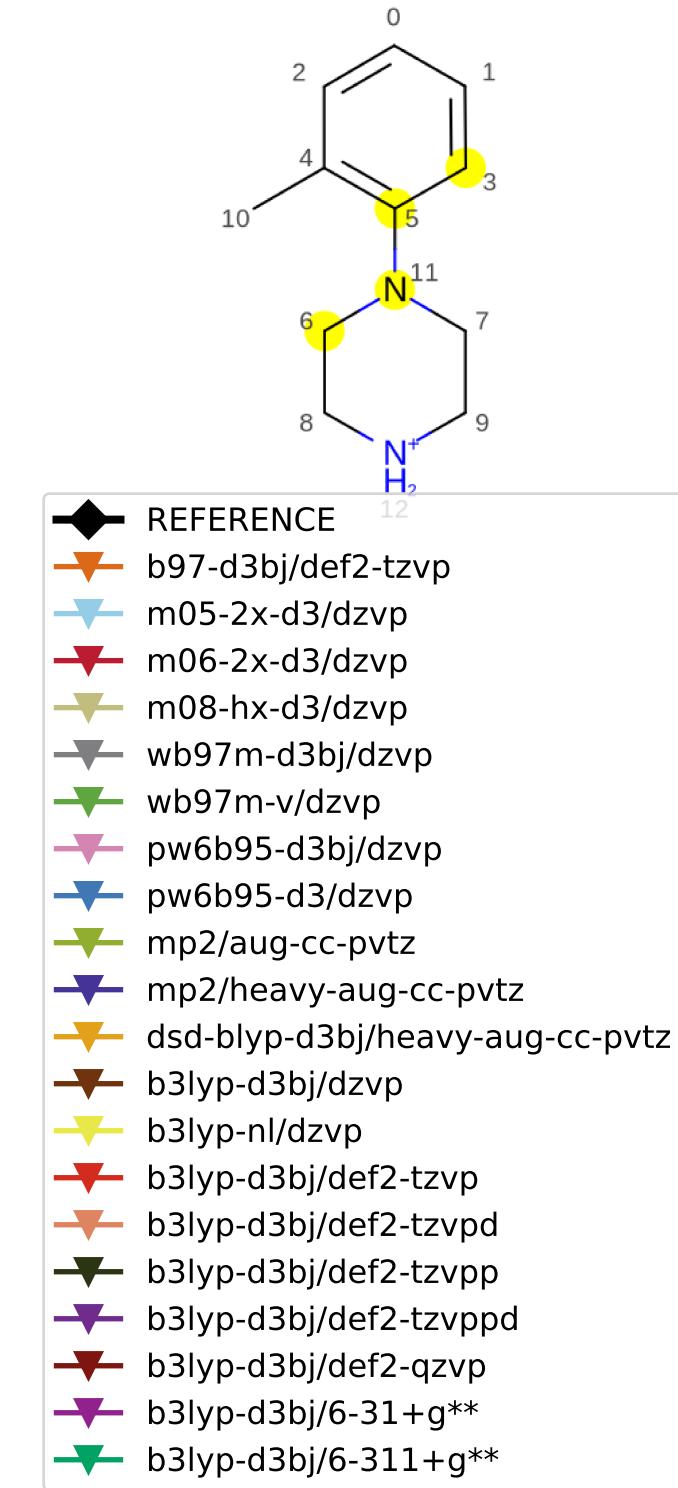
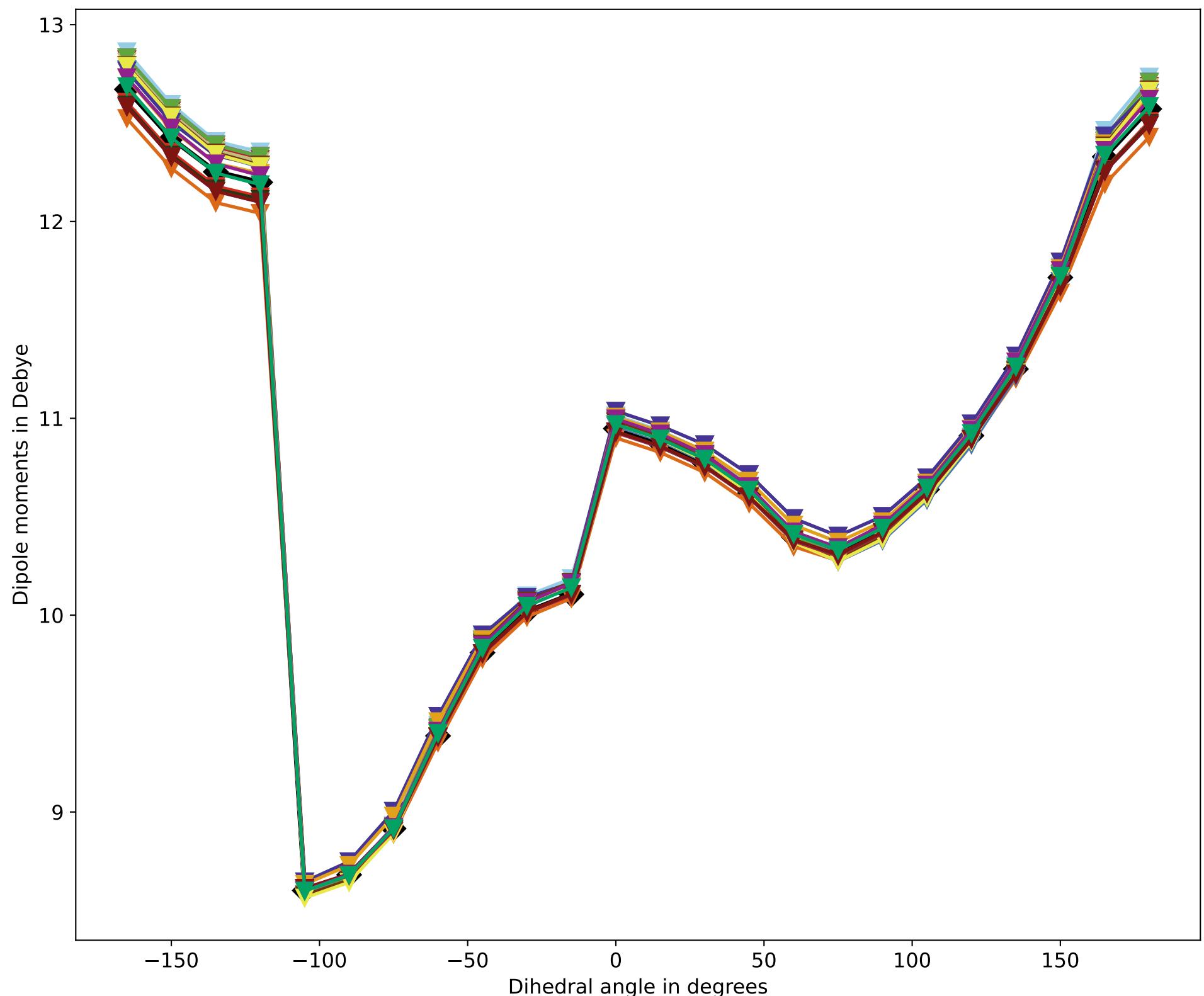




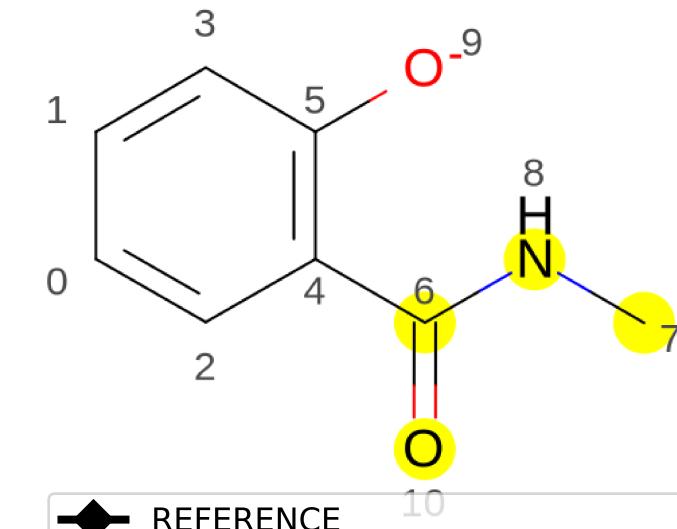
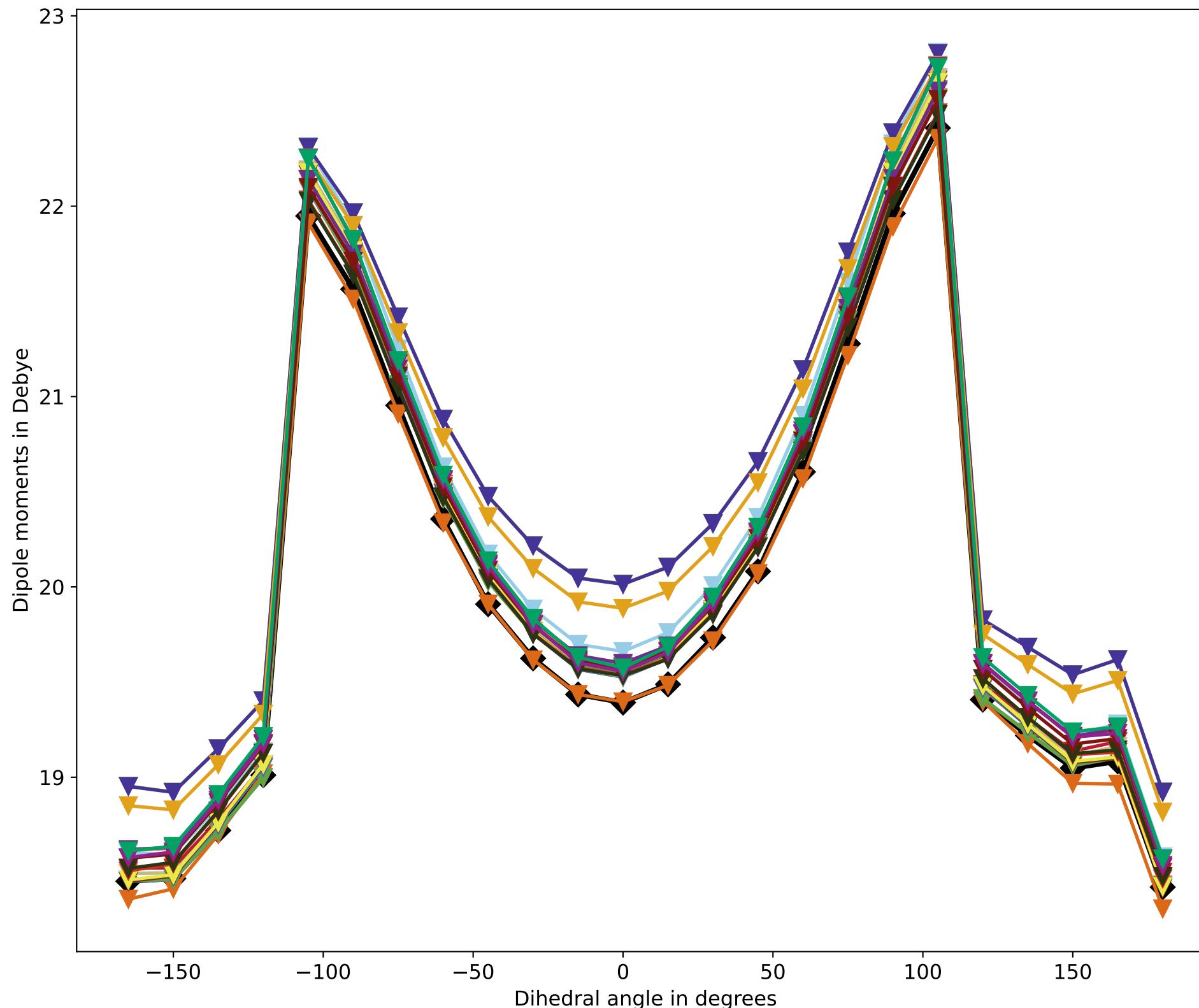


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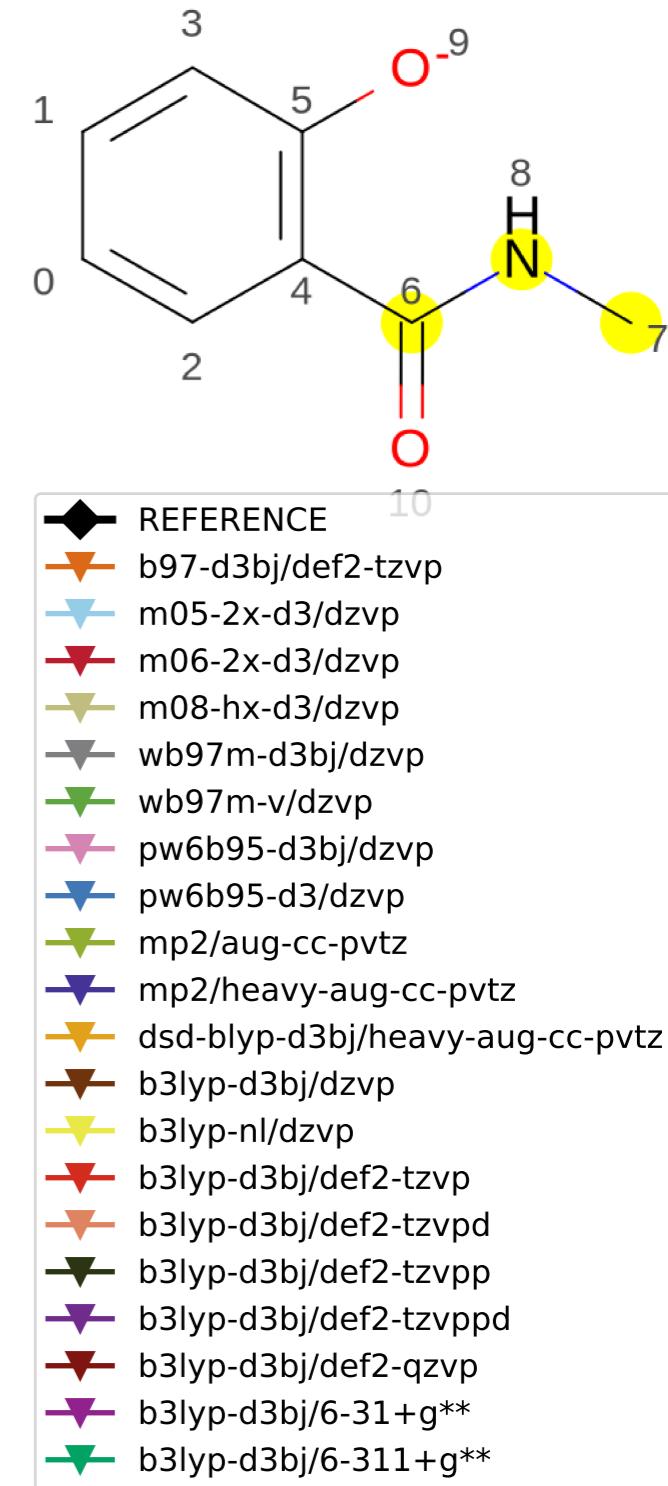
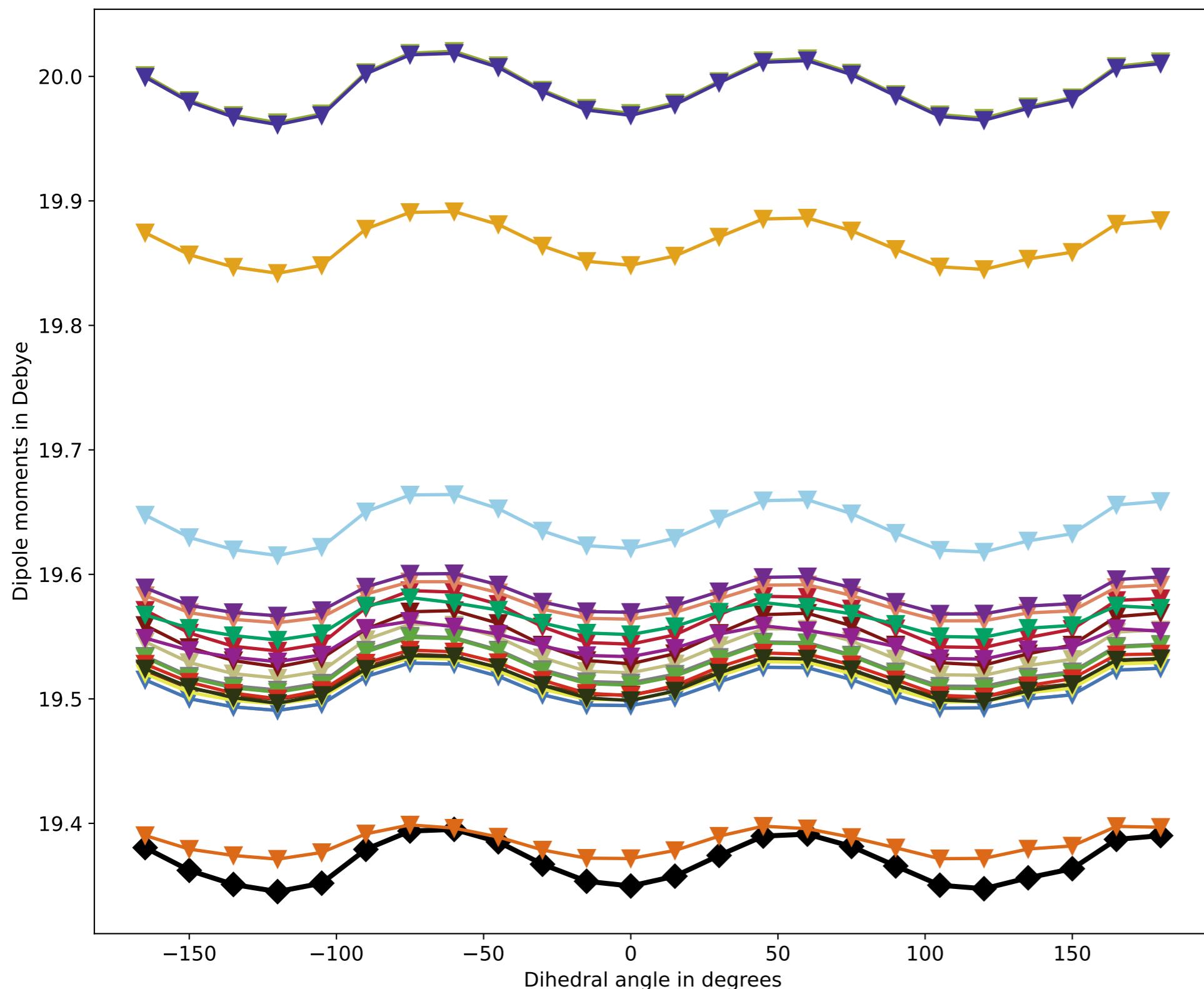


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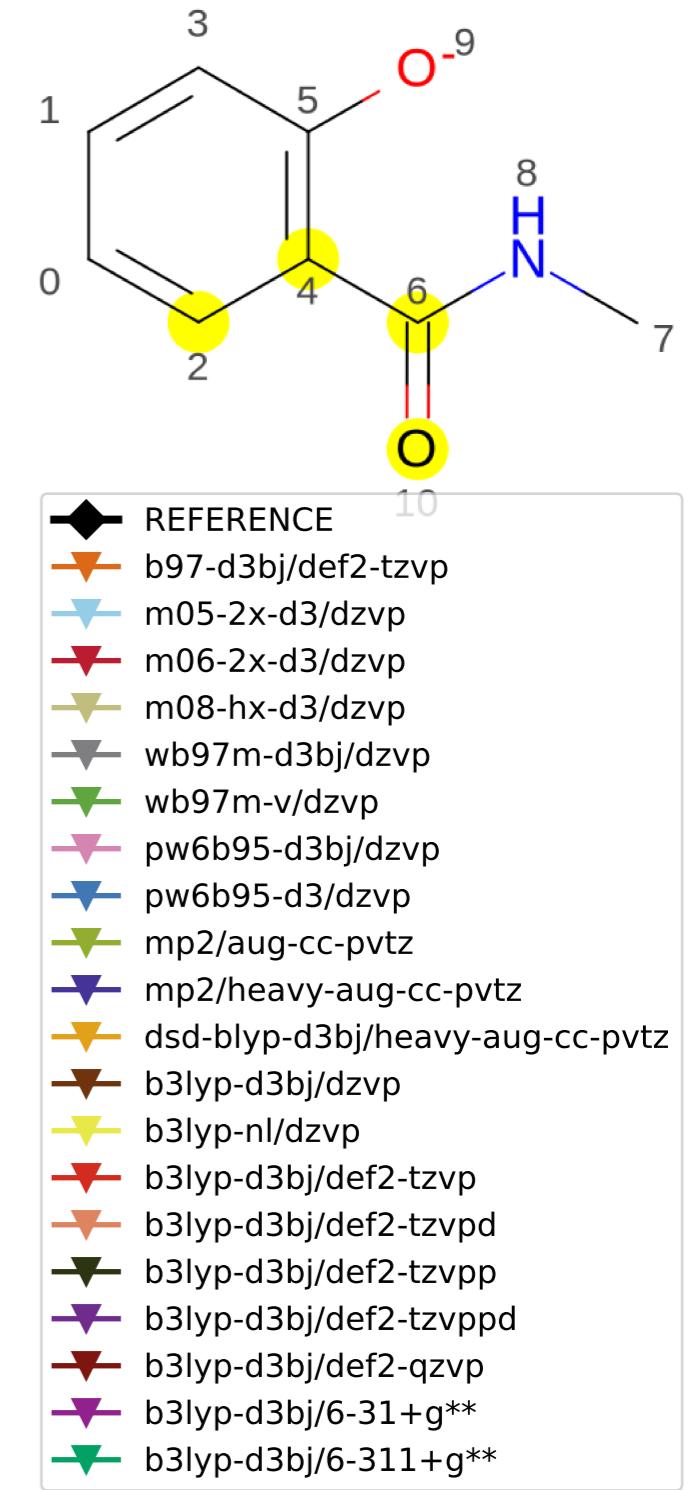
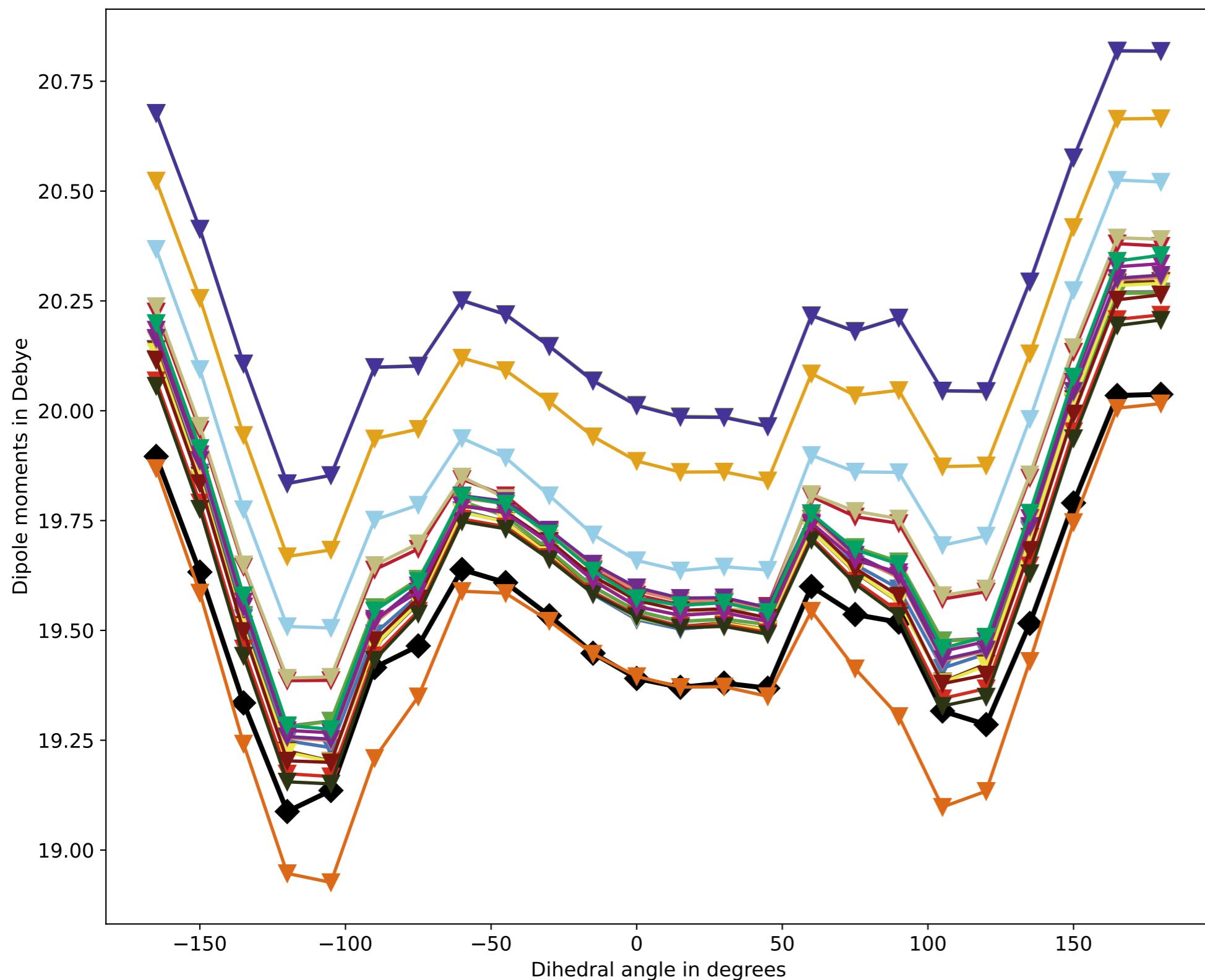


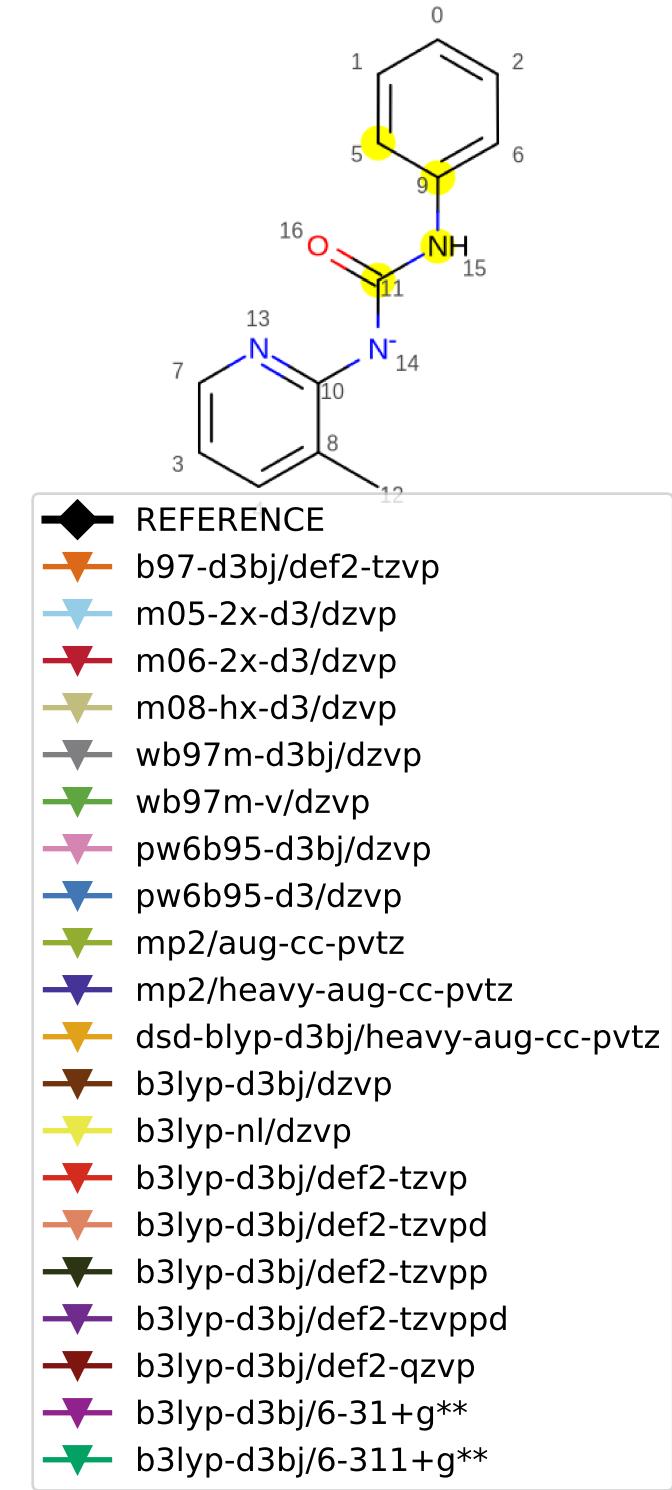
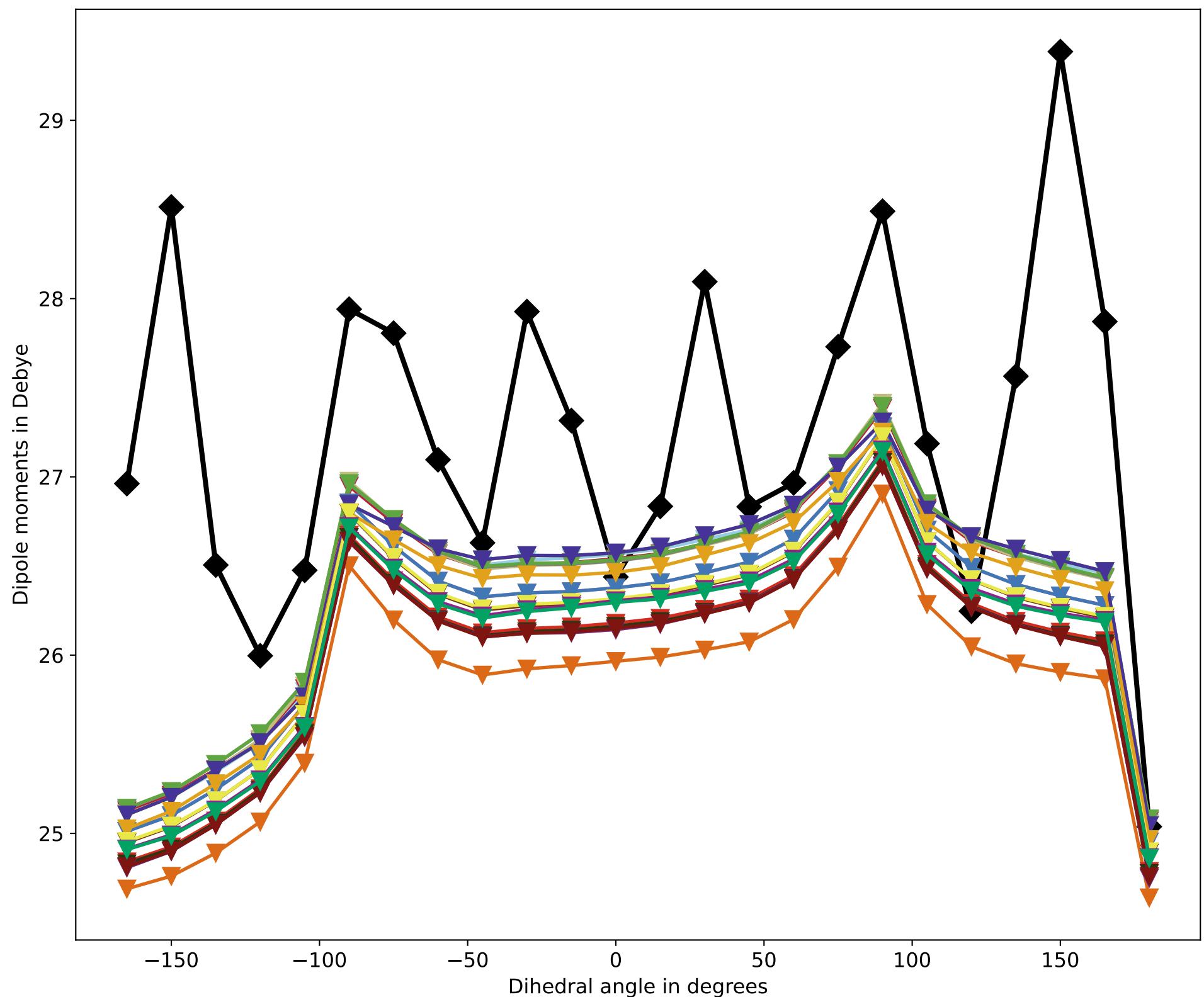
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- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-bllyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp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

Charged molecule

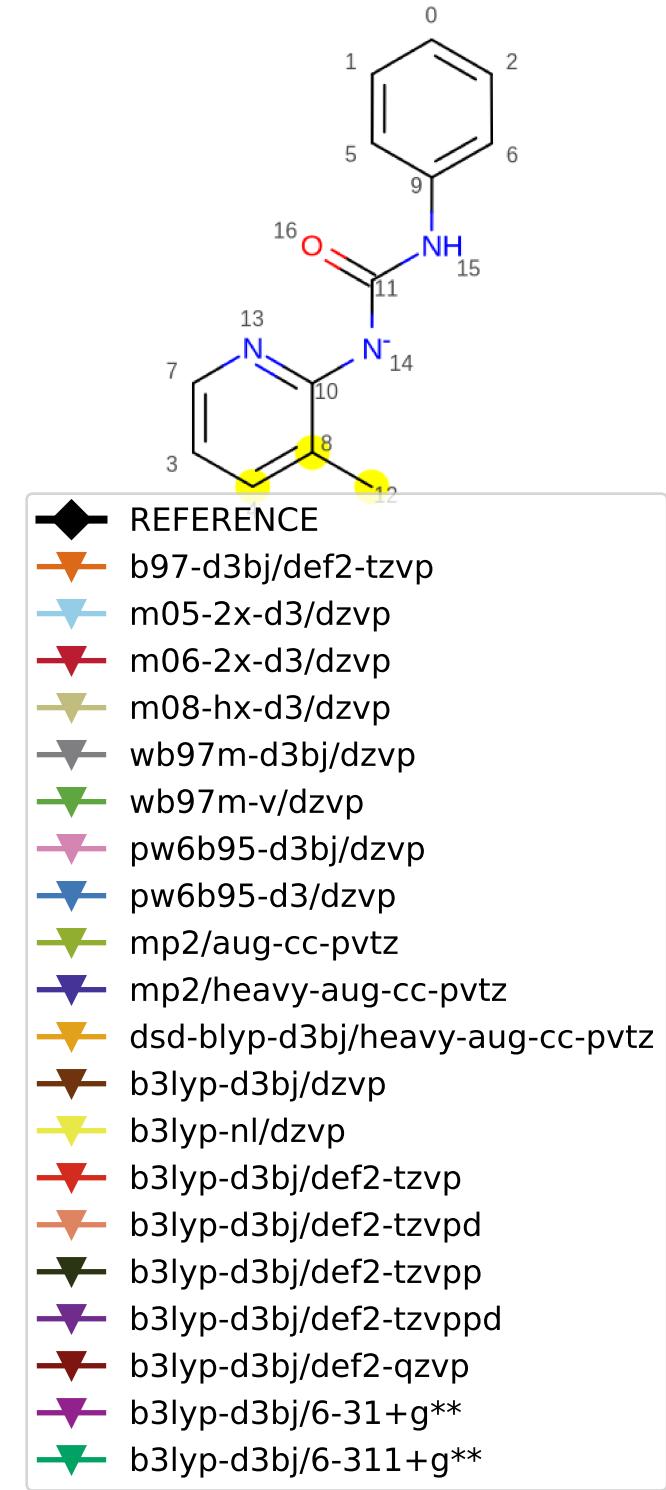
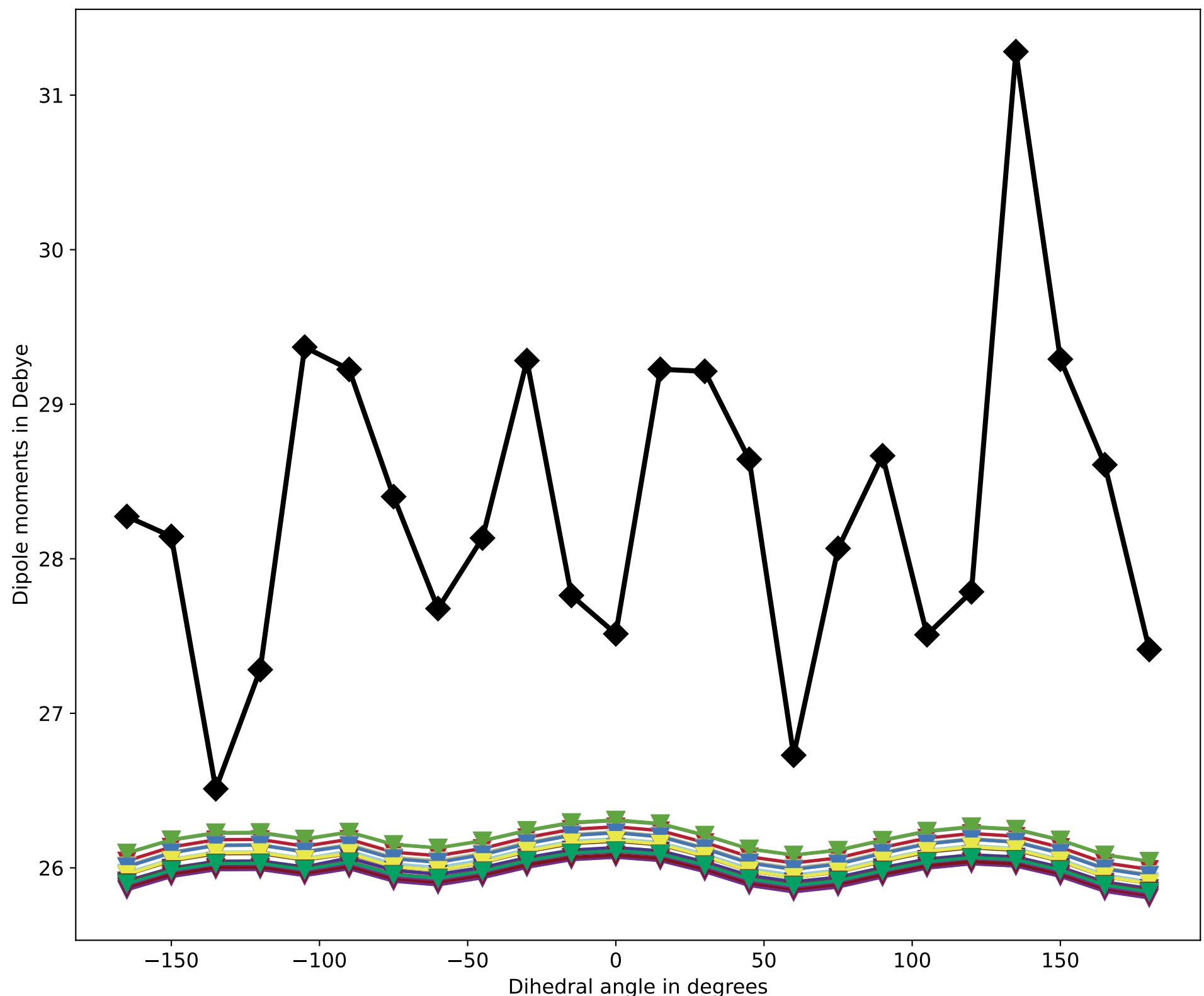


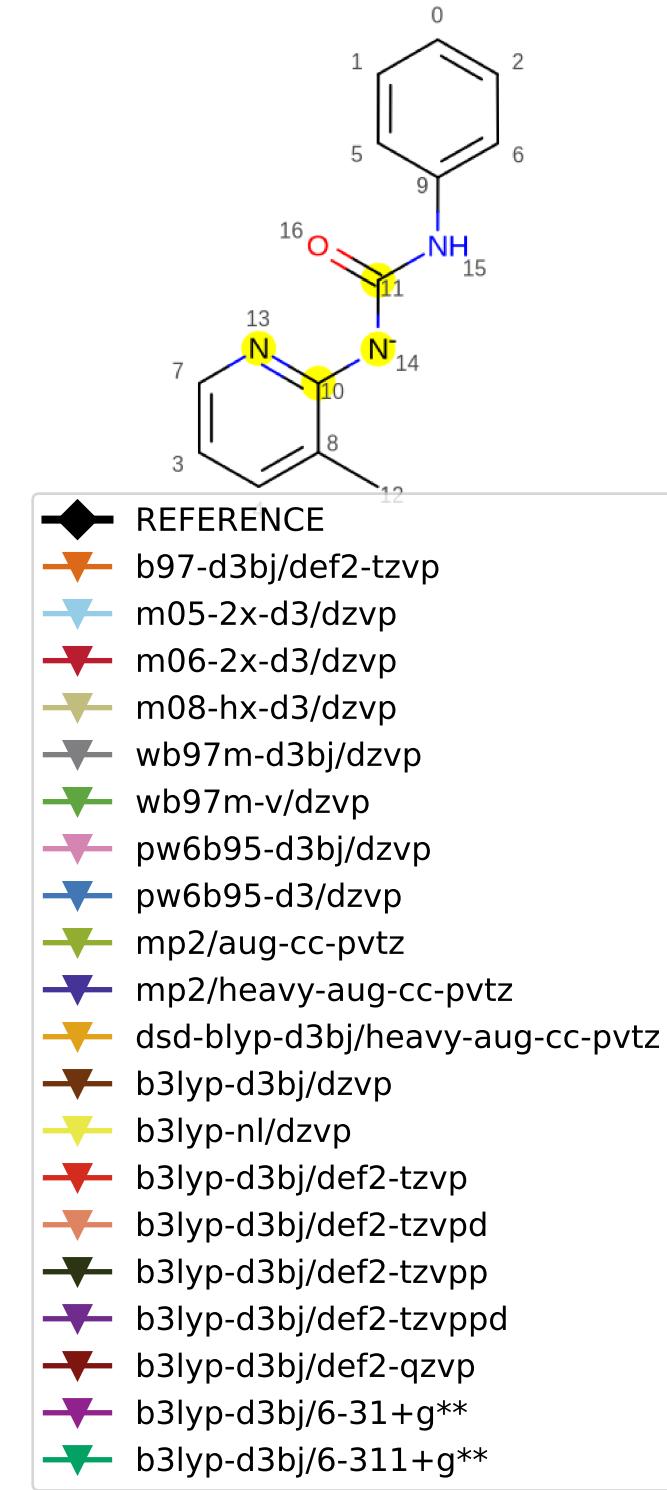
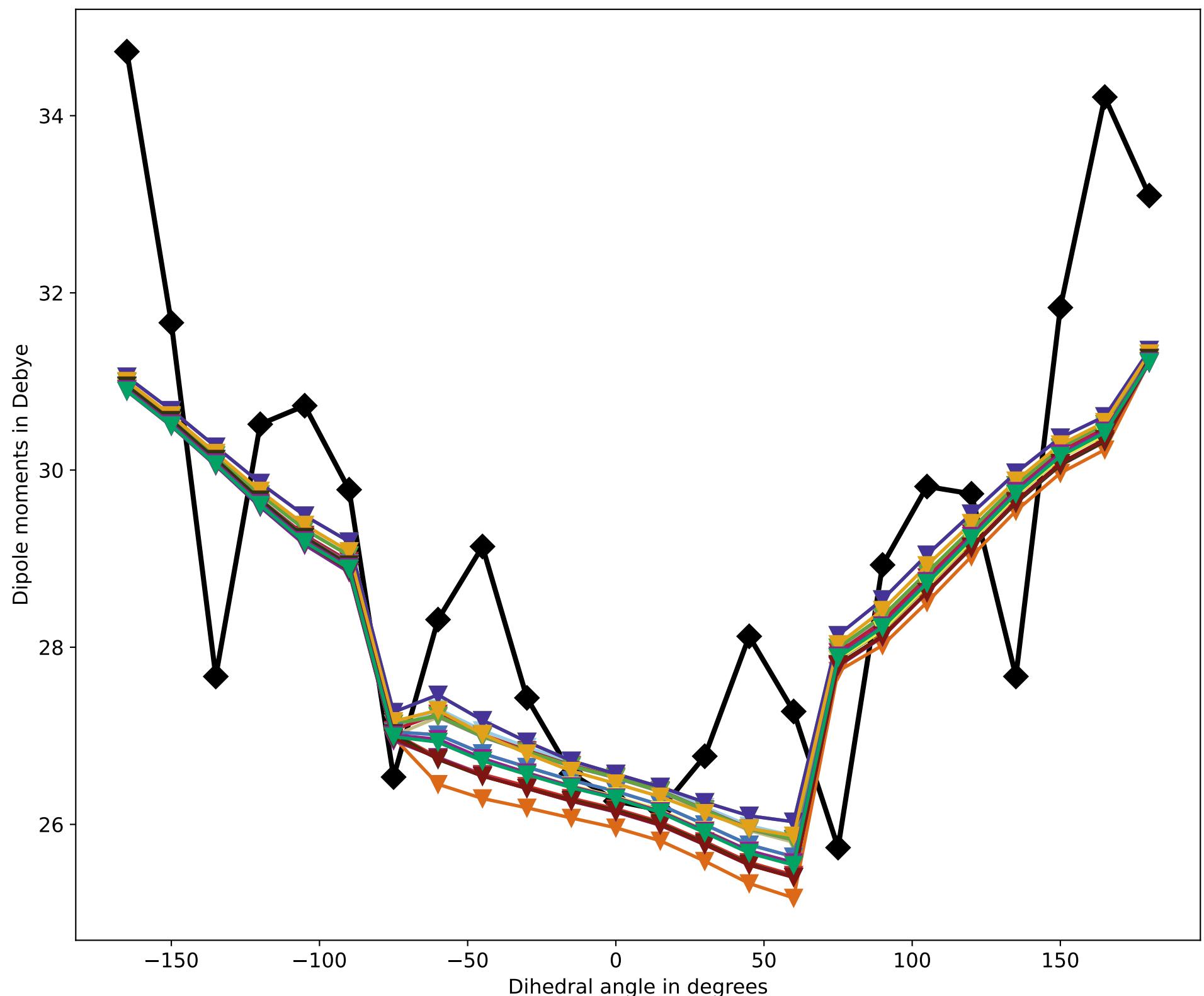
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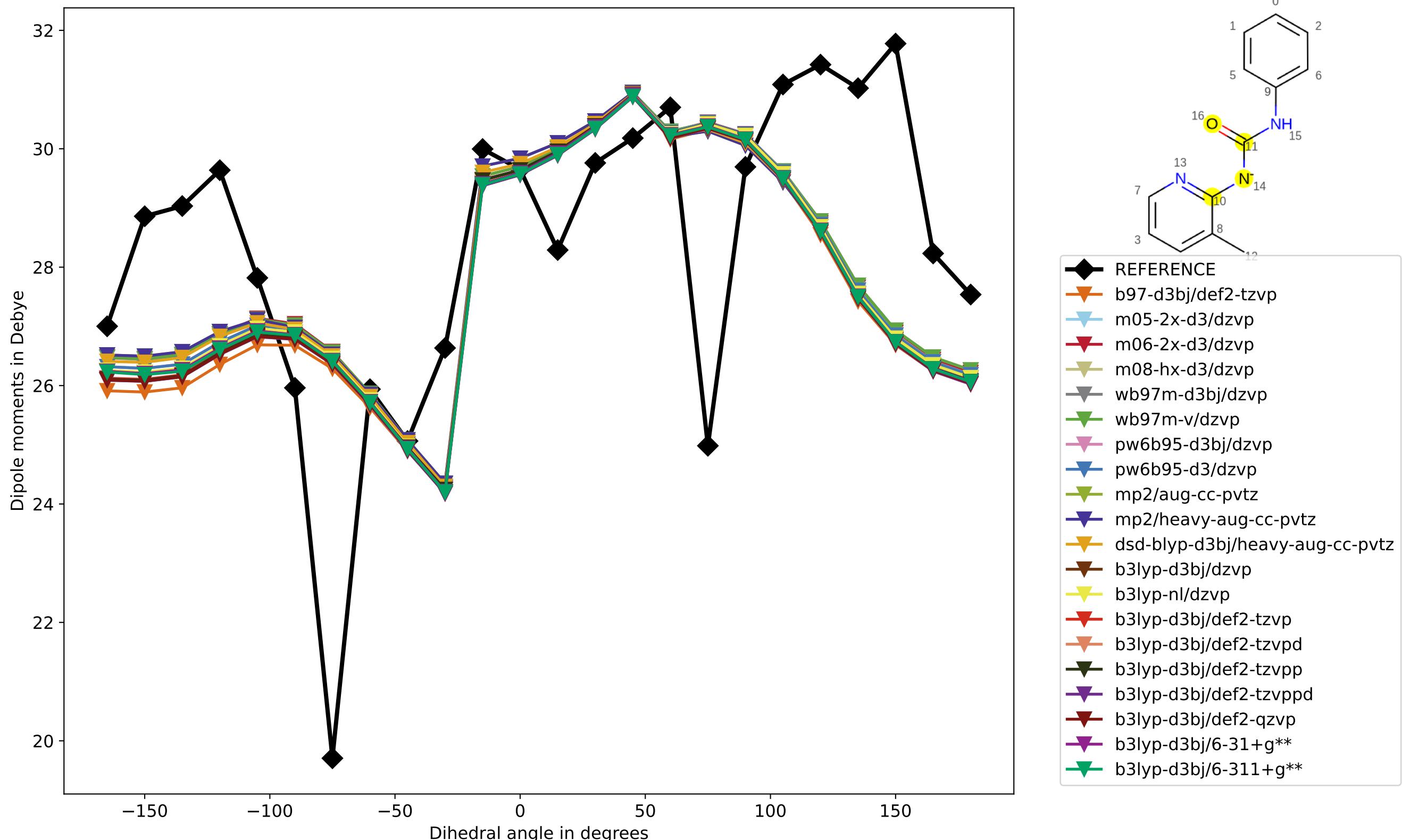


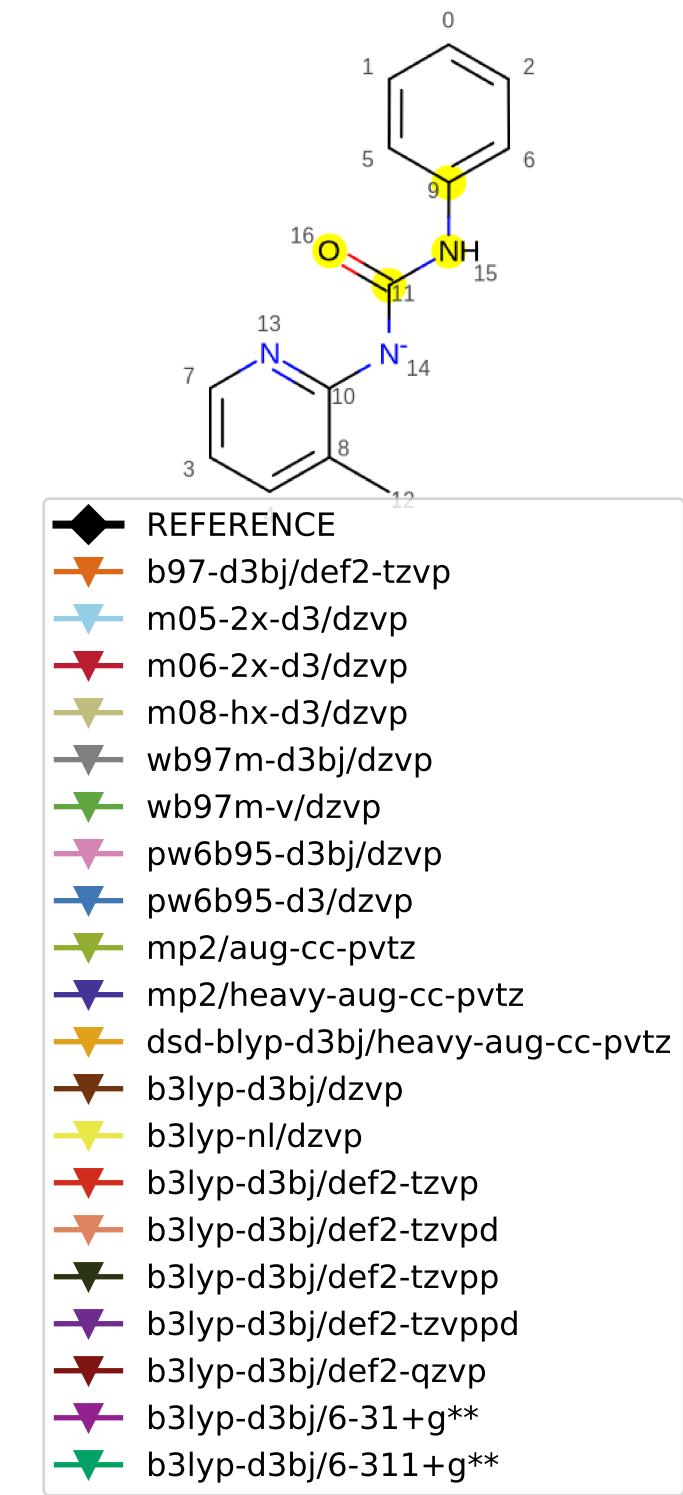
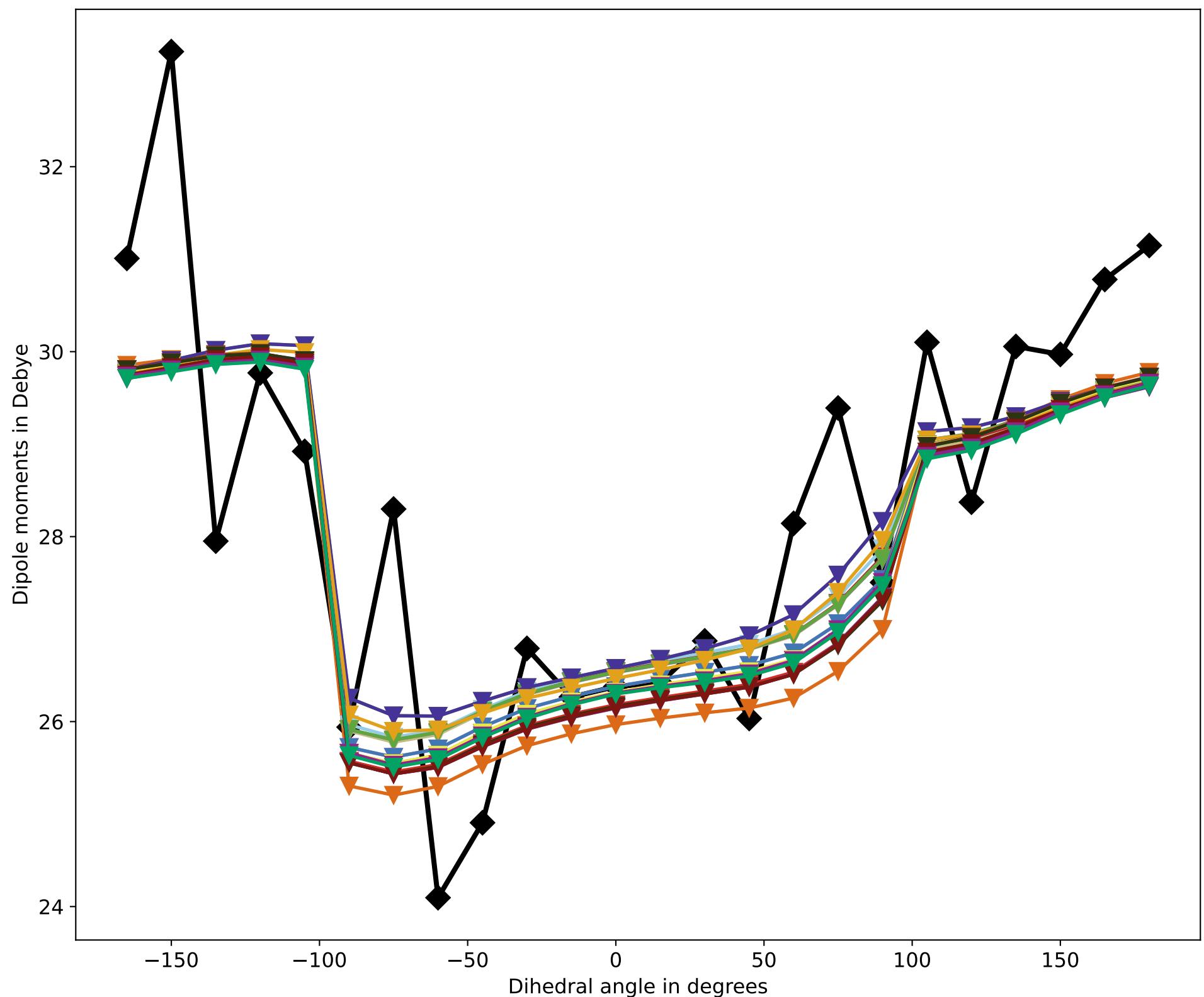
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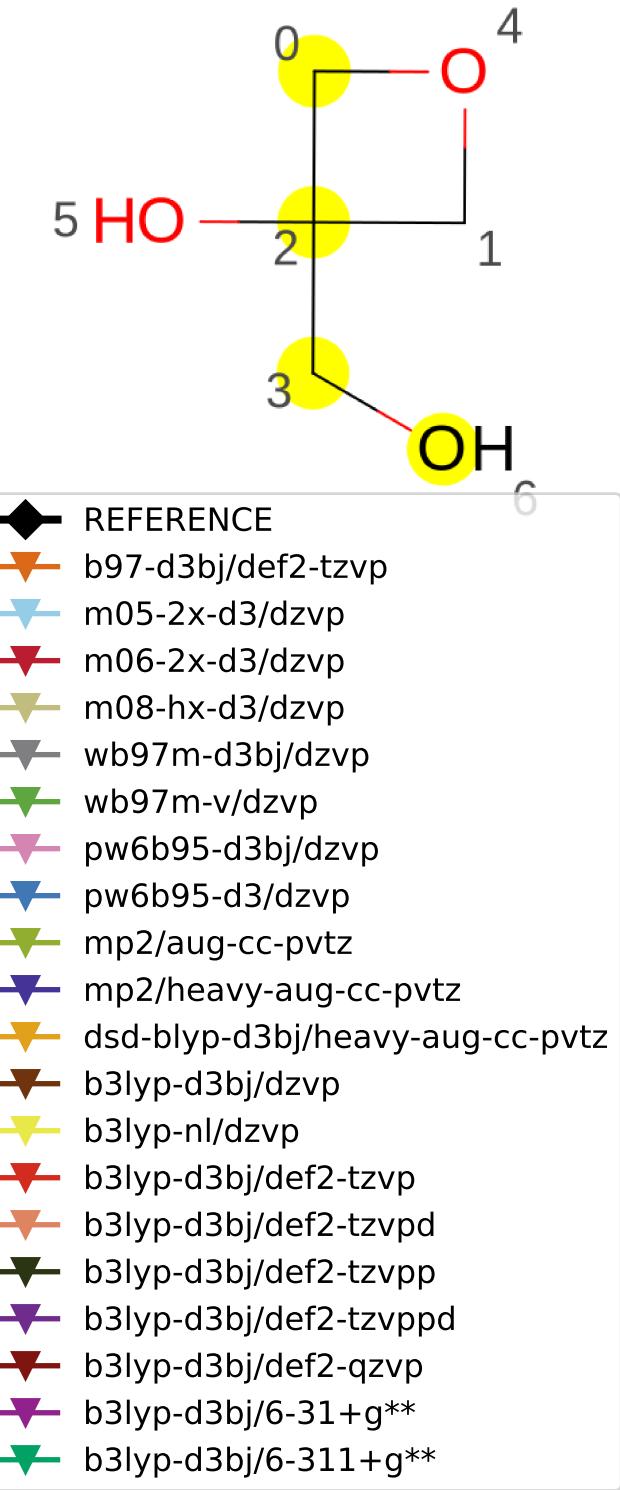
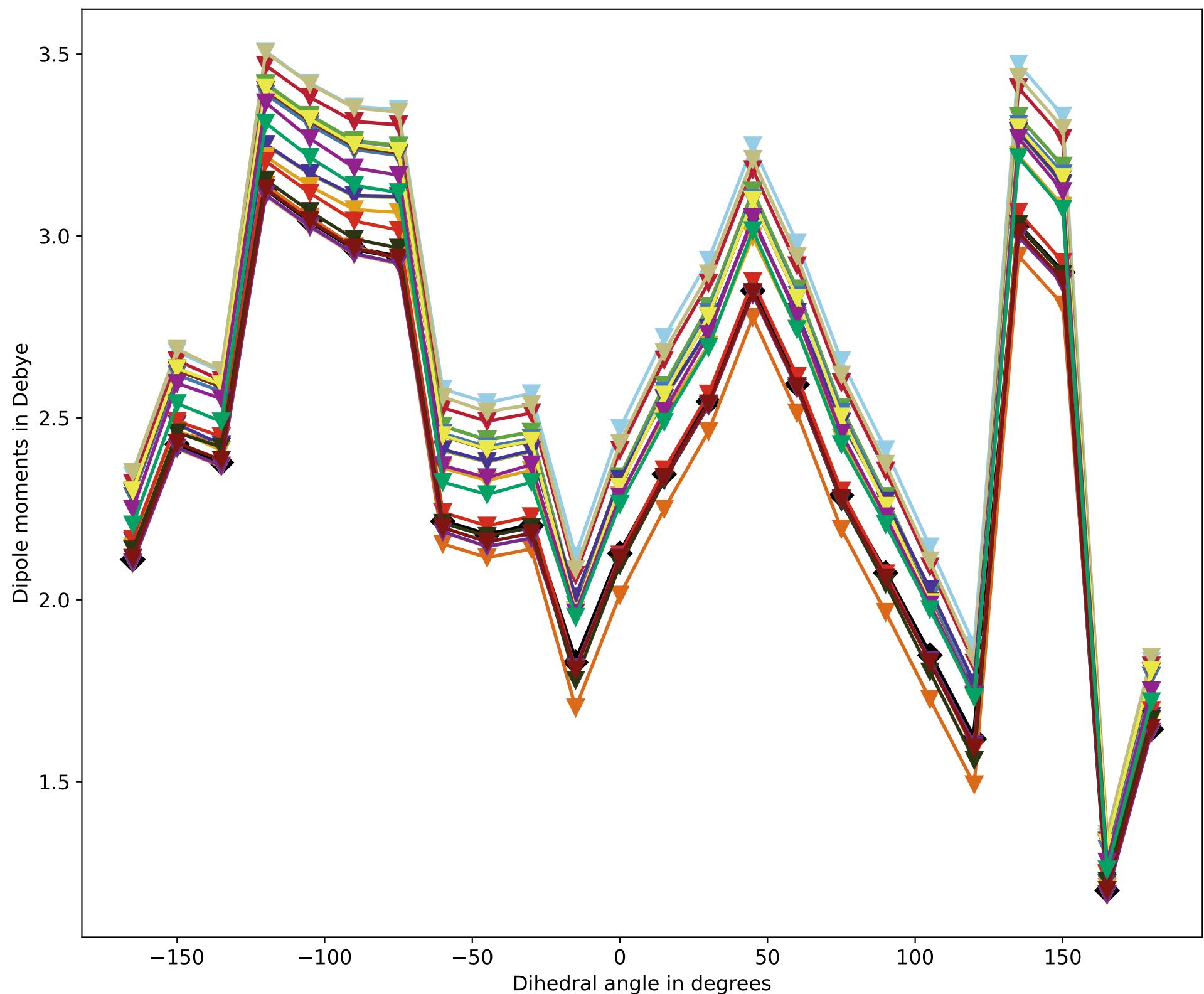


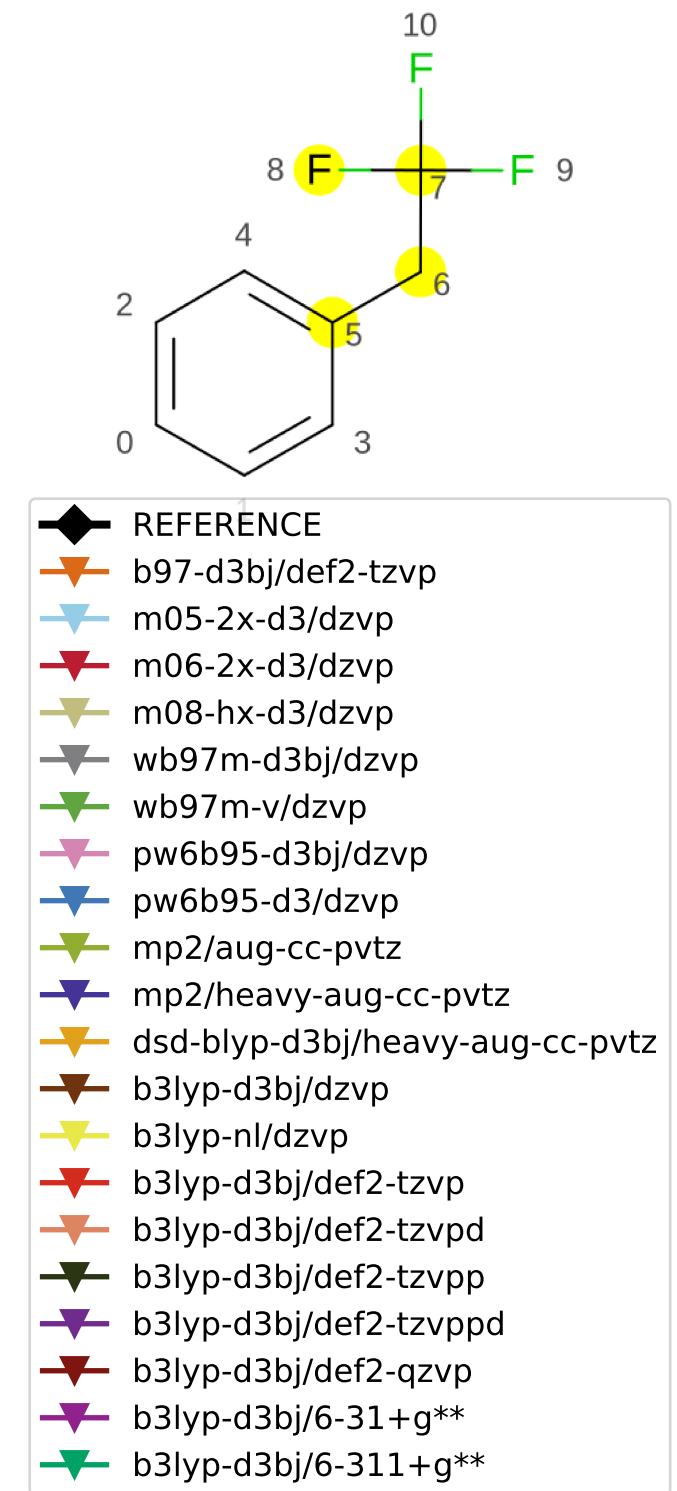
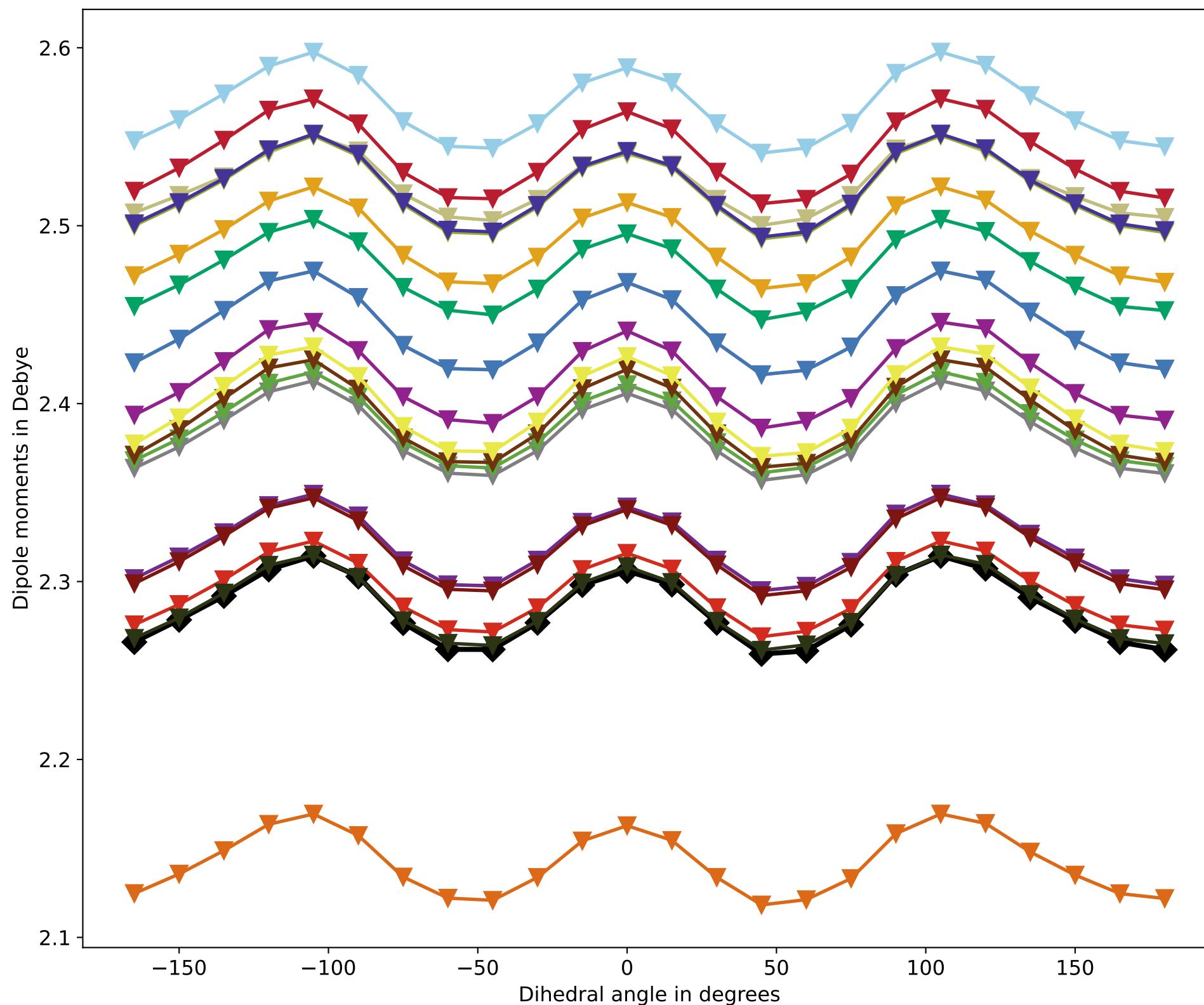


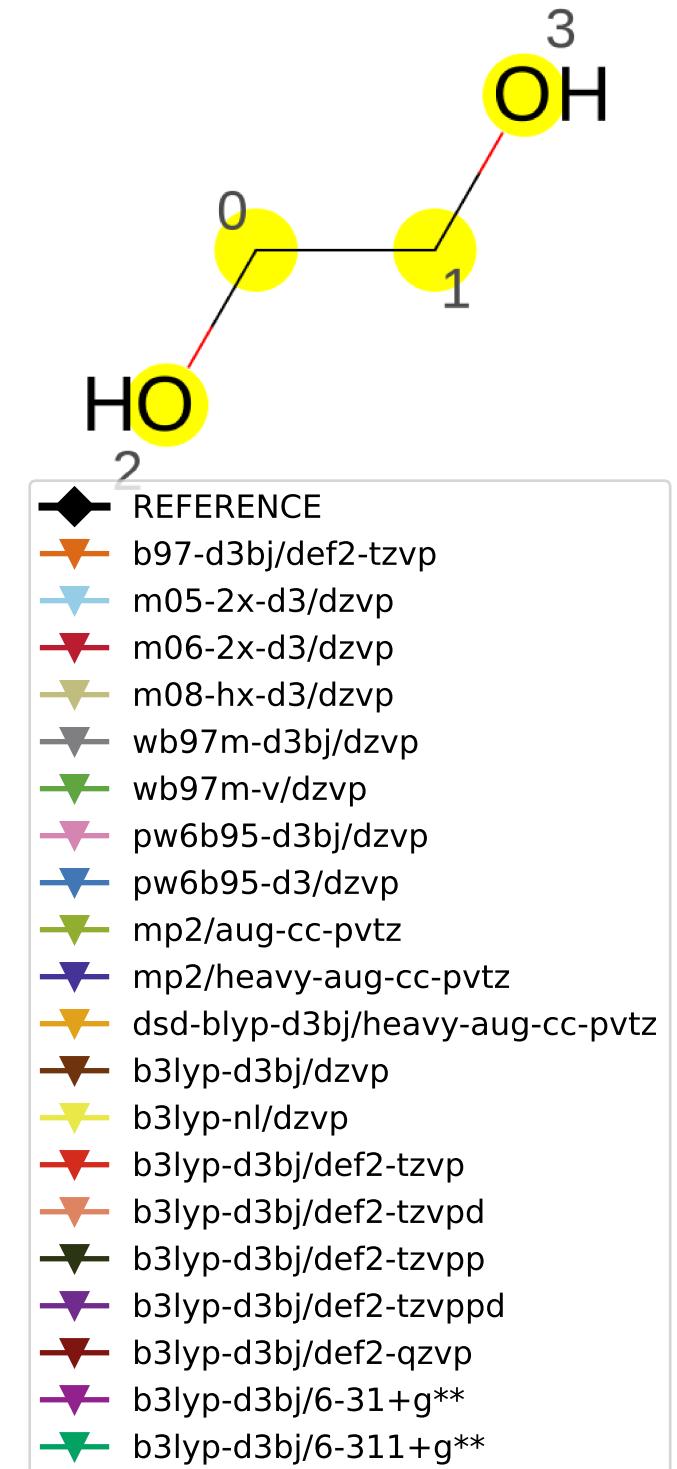
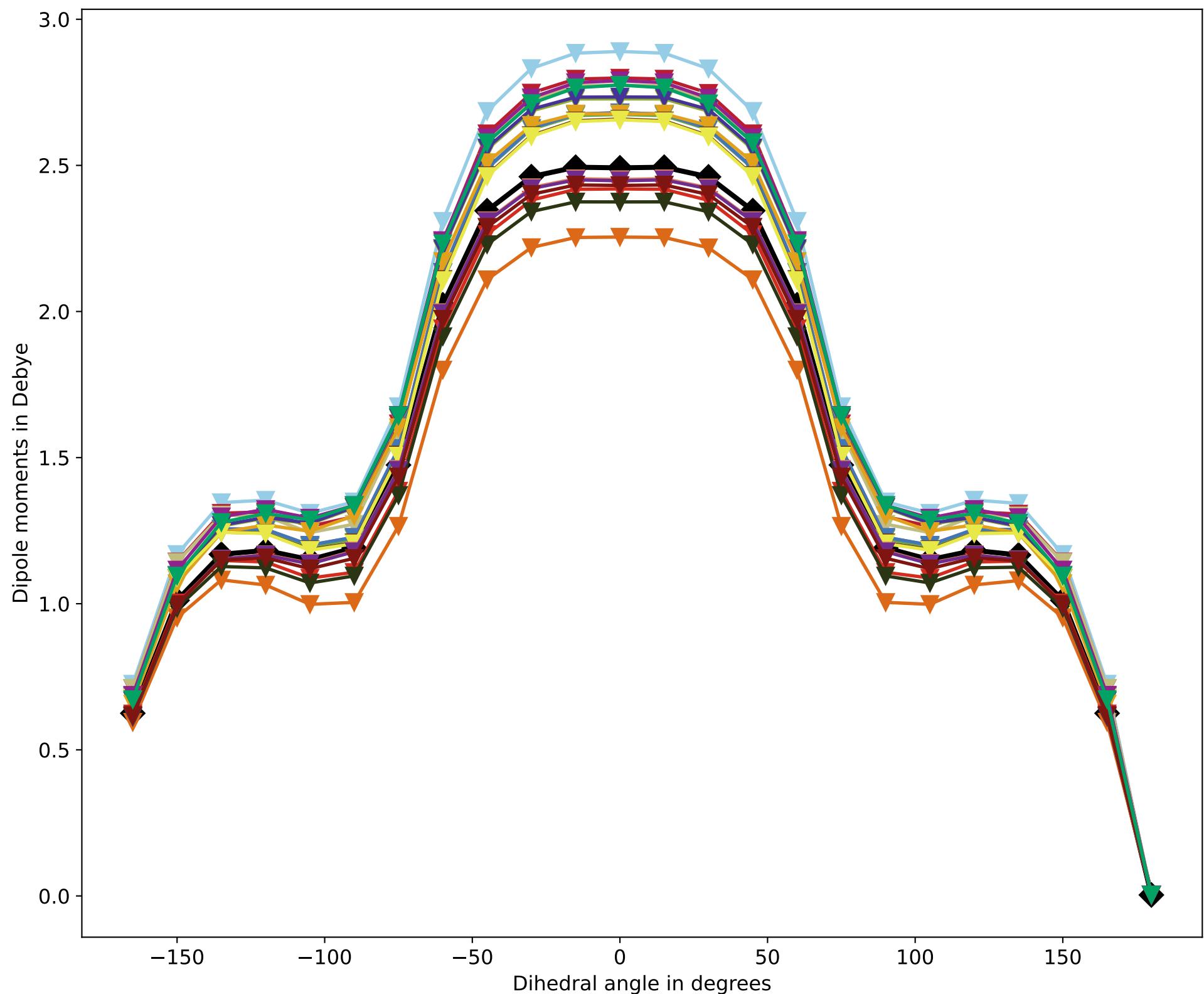
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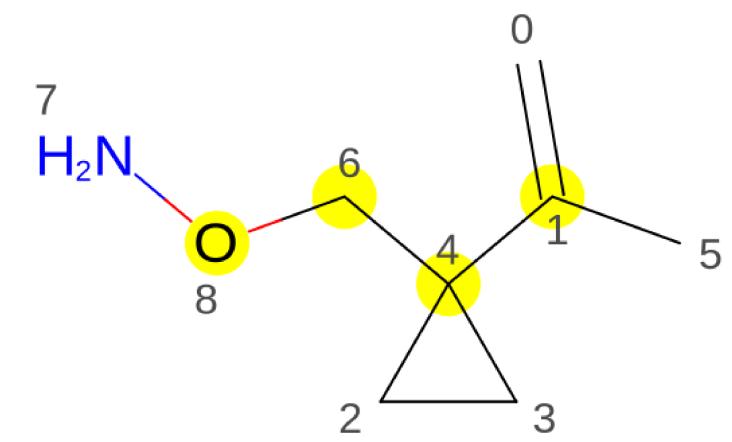
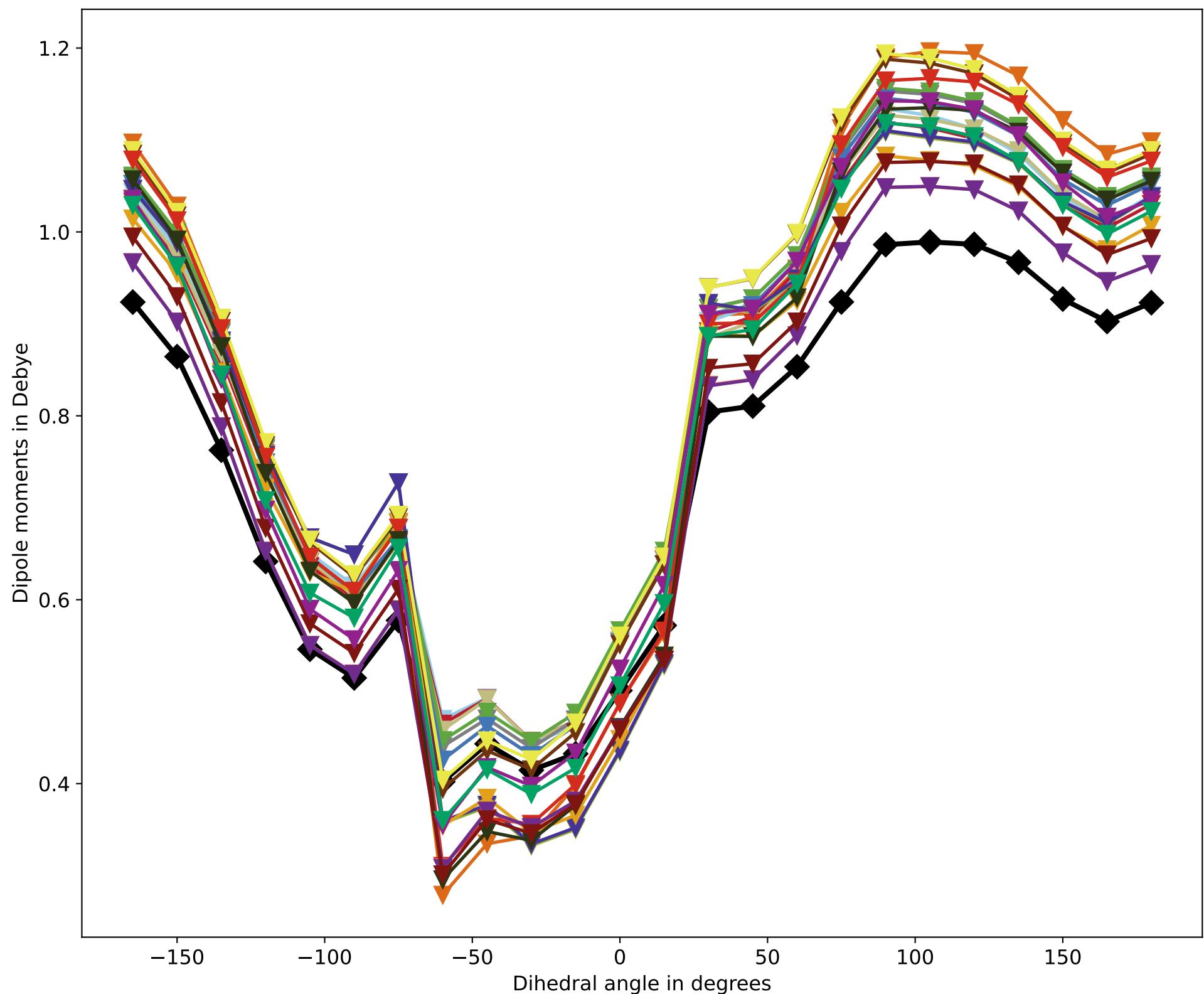




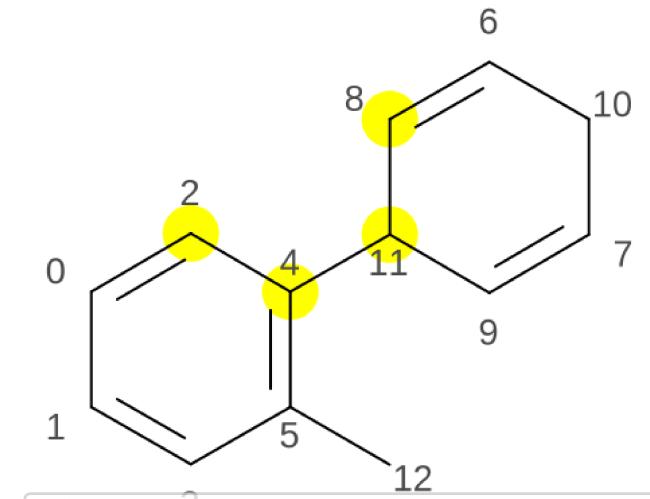
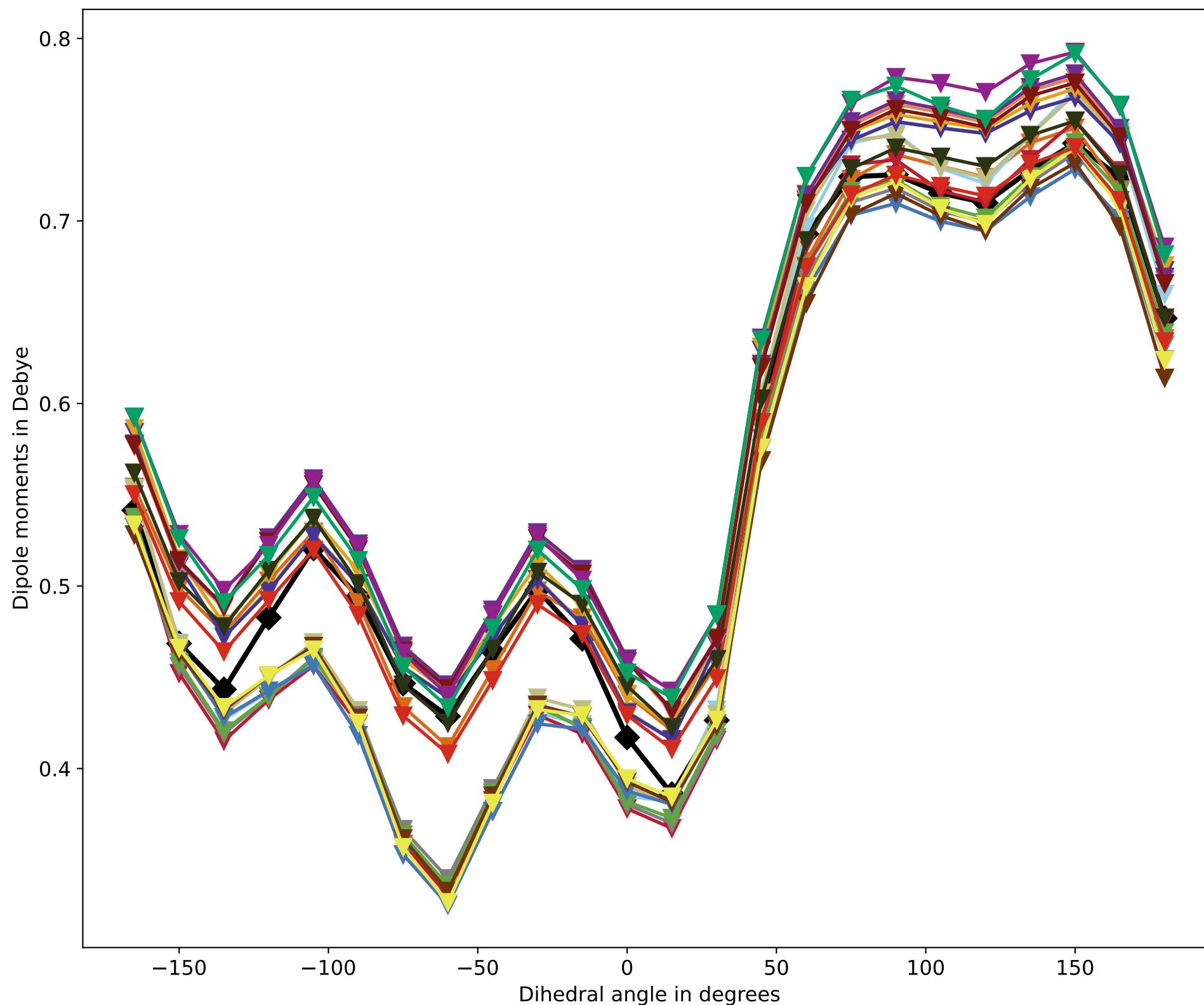






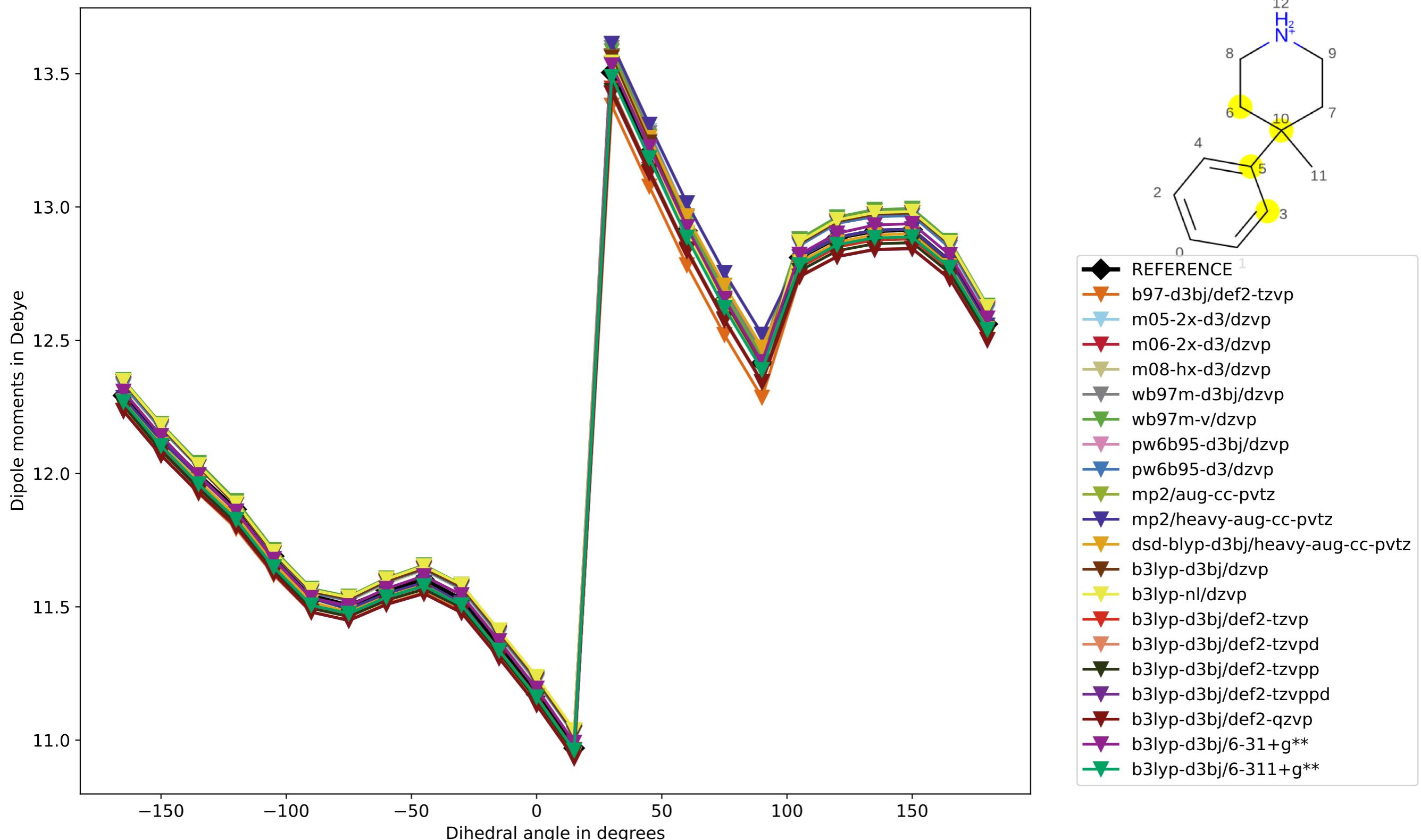


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

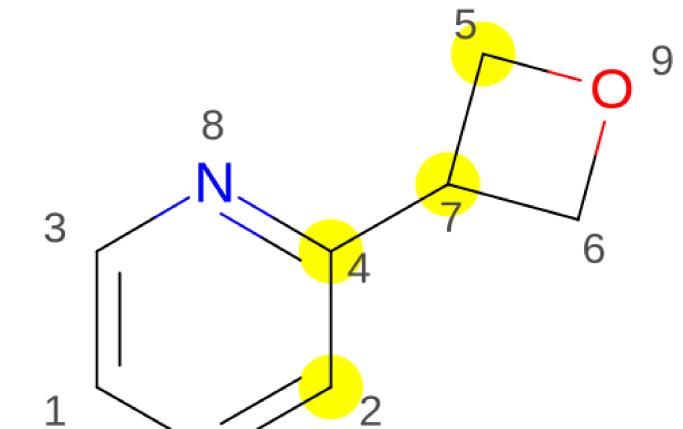
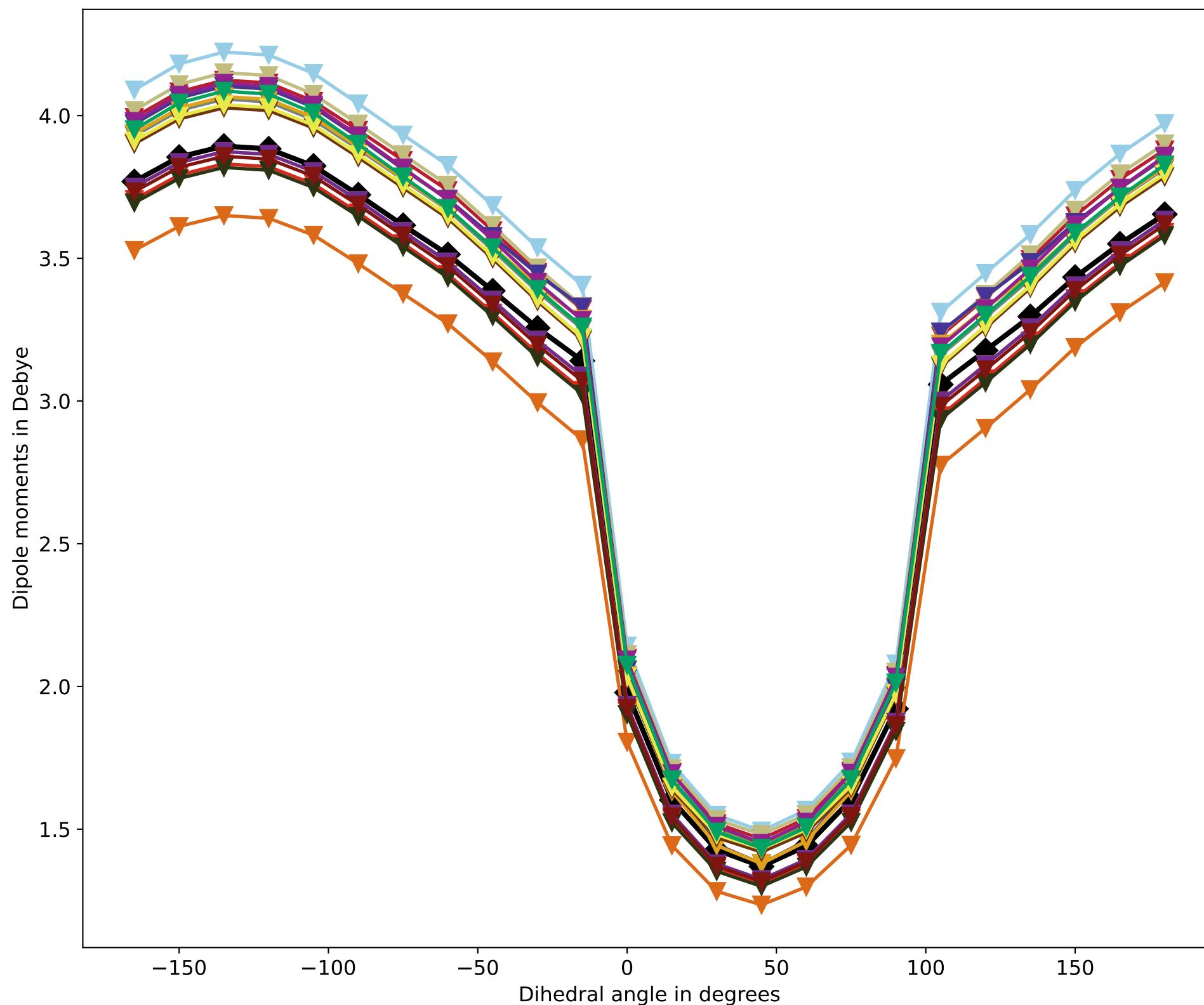


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- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvpd
- ◆ b3lyp-d3bj/def2-tzvpp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

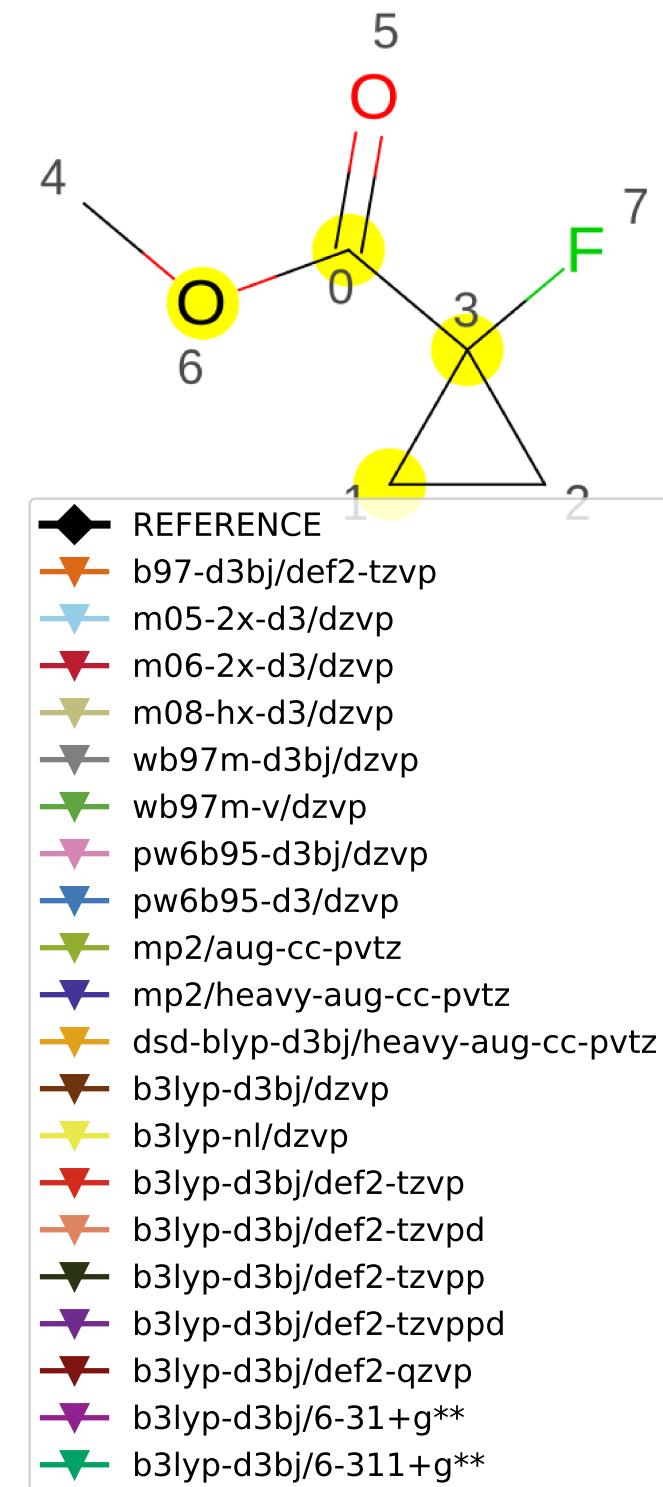
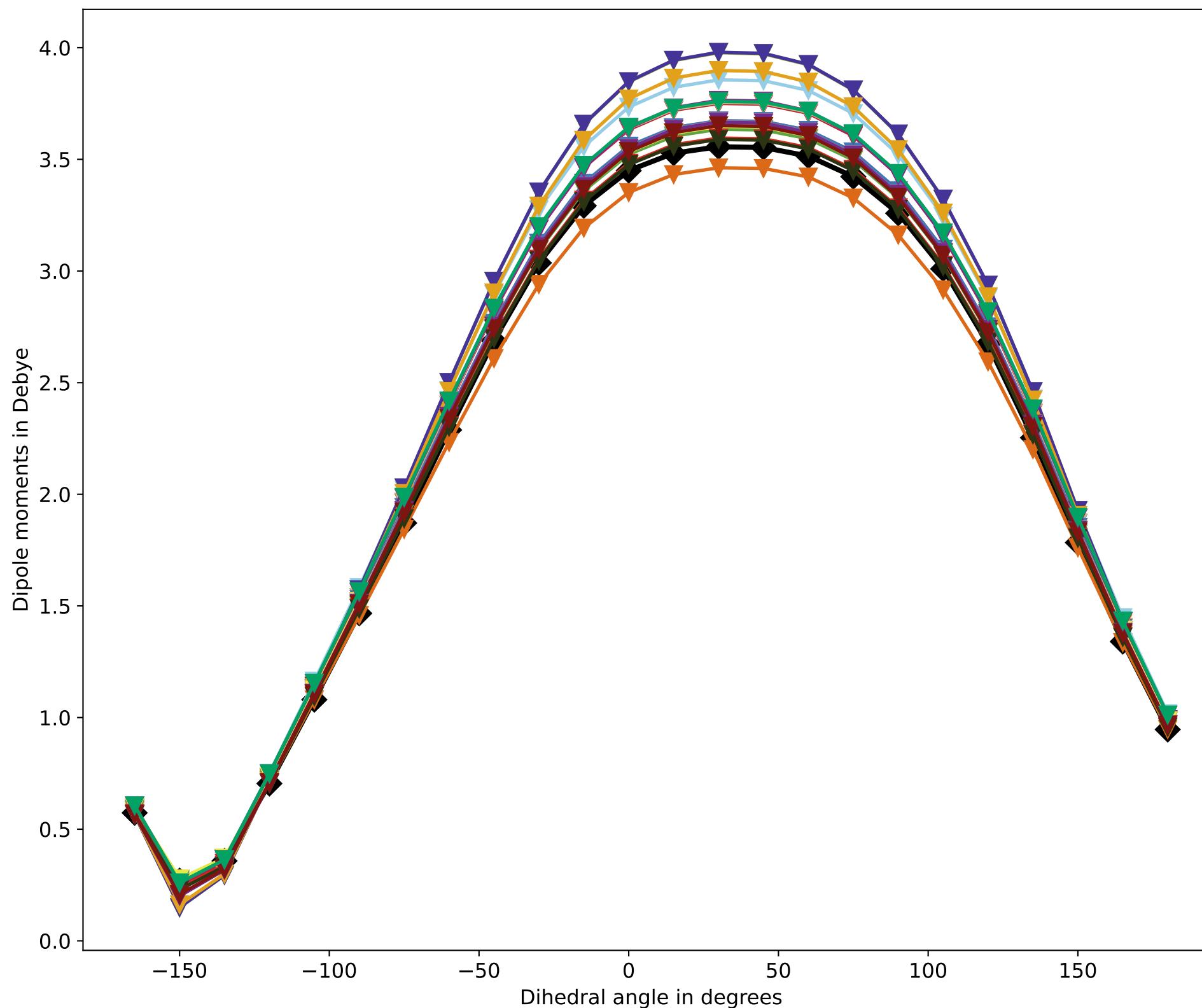
Charged molecule

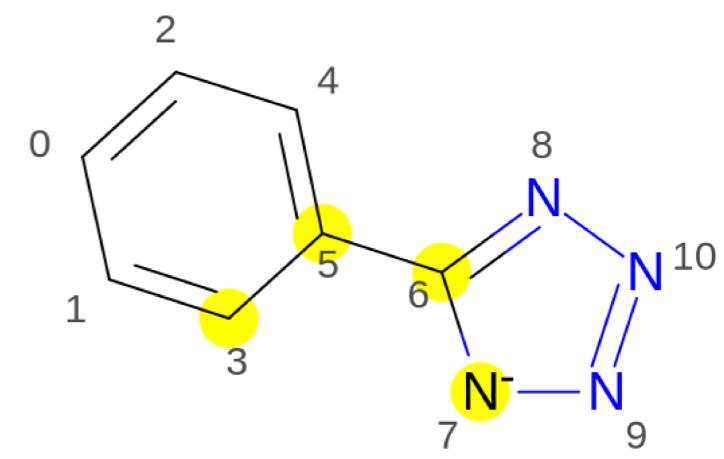
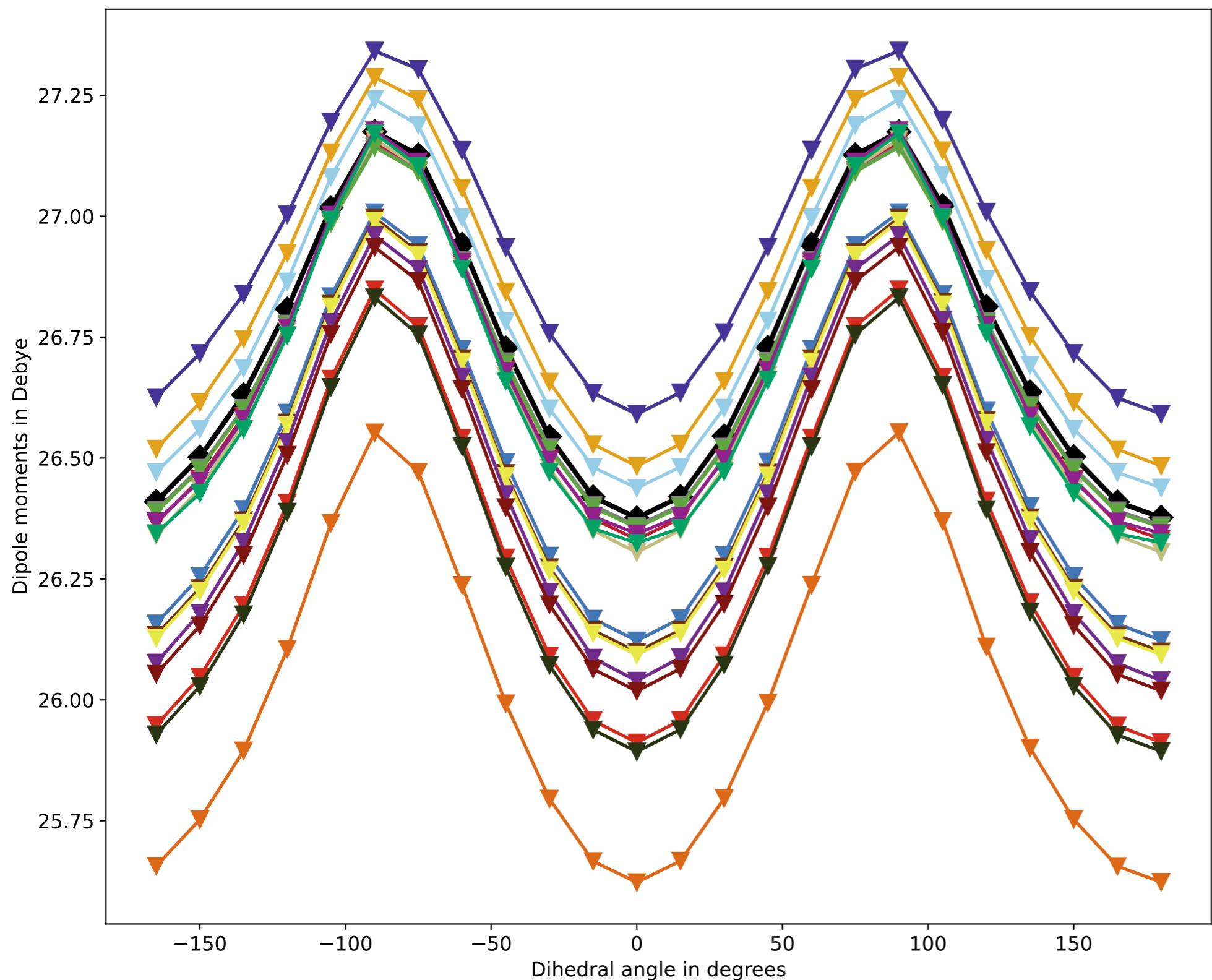


Neutral molecule

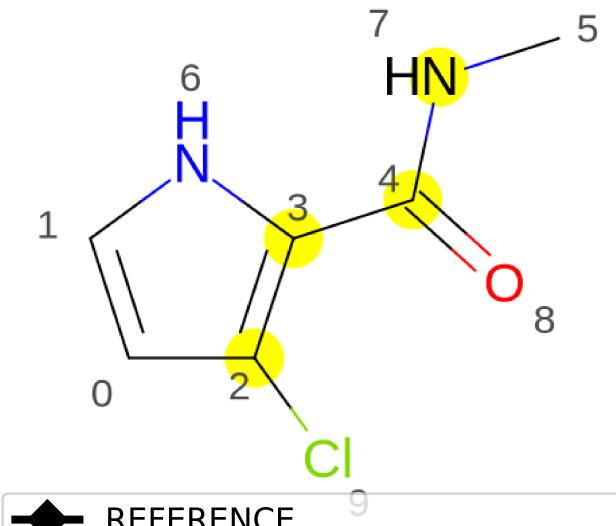
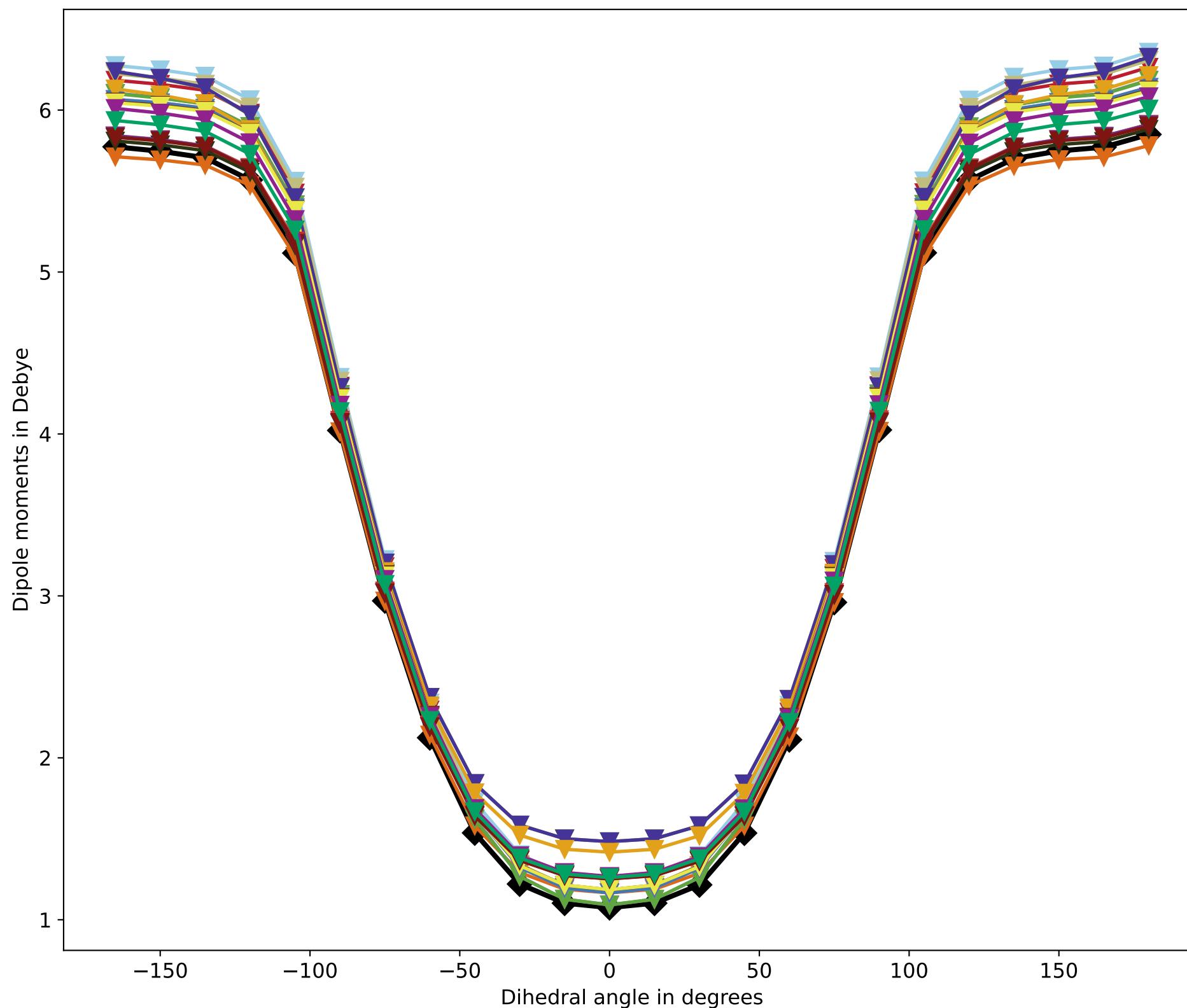


- Legend:
- REFERENCE
 - b97-d3bj/def2-tzvp
 - m05-2x-d3/dzvp
 - m06-2x-d3/dzvp
 - m08-hx-d3/dzvp
 - wb97m-d3bj/dzvp
 - wb97m-v/dzvp
 - pw6b95-d3bj/dzvp
 - pw6b95-d3/dzvp
 - mp2/aug-cc-pvtz
 - mp2/heavy-aug-cc-pvtz
 - dsd-blyp-d3bj/heavy-aug-cc-pvtz
 - b3lyp-d3bj/dzvp
 - b3lyp-nl/dzvp
 - b3lyp-d3bj/def2-tzvp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

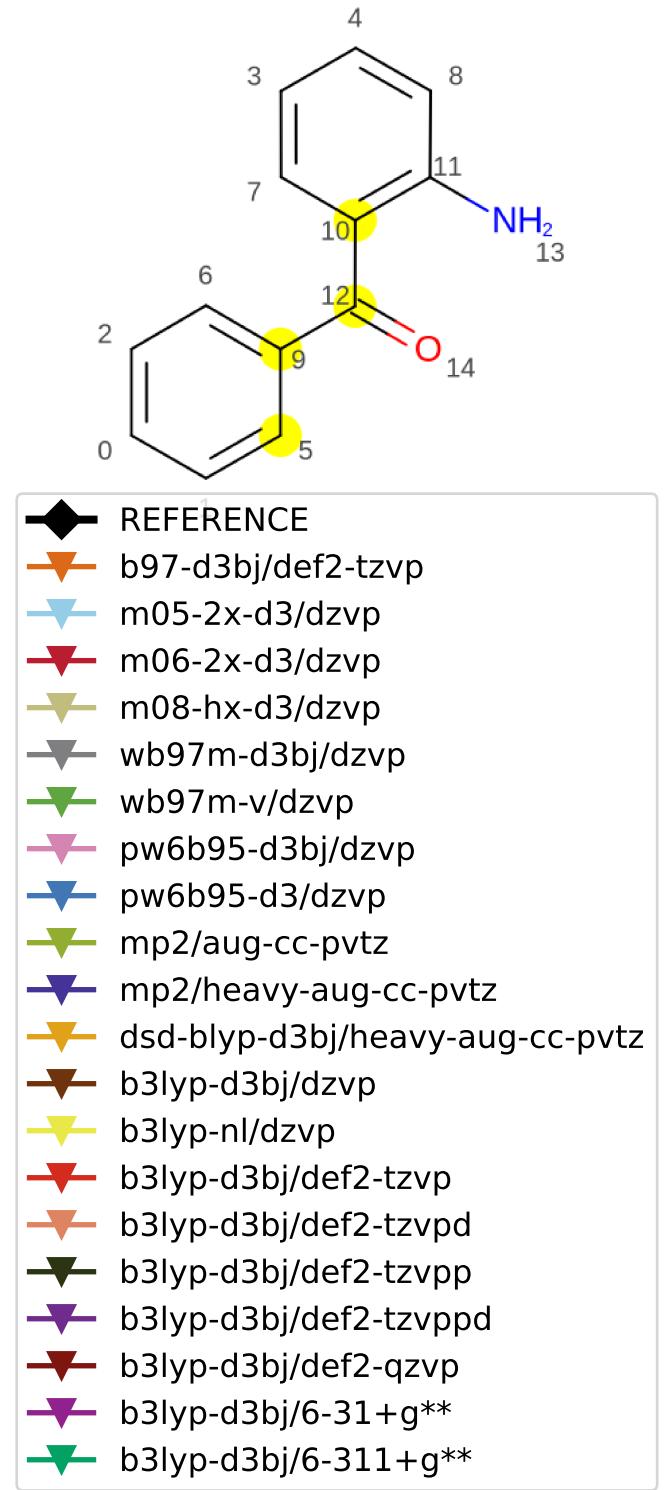
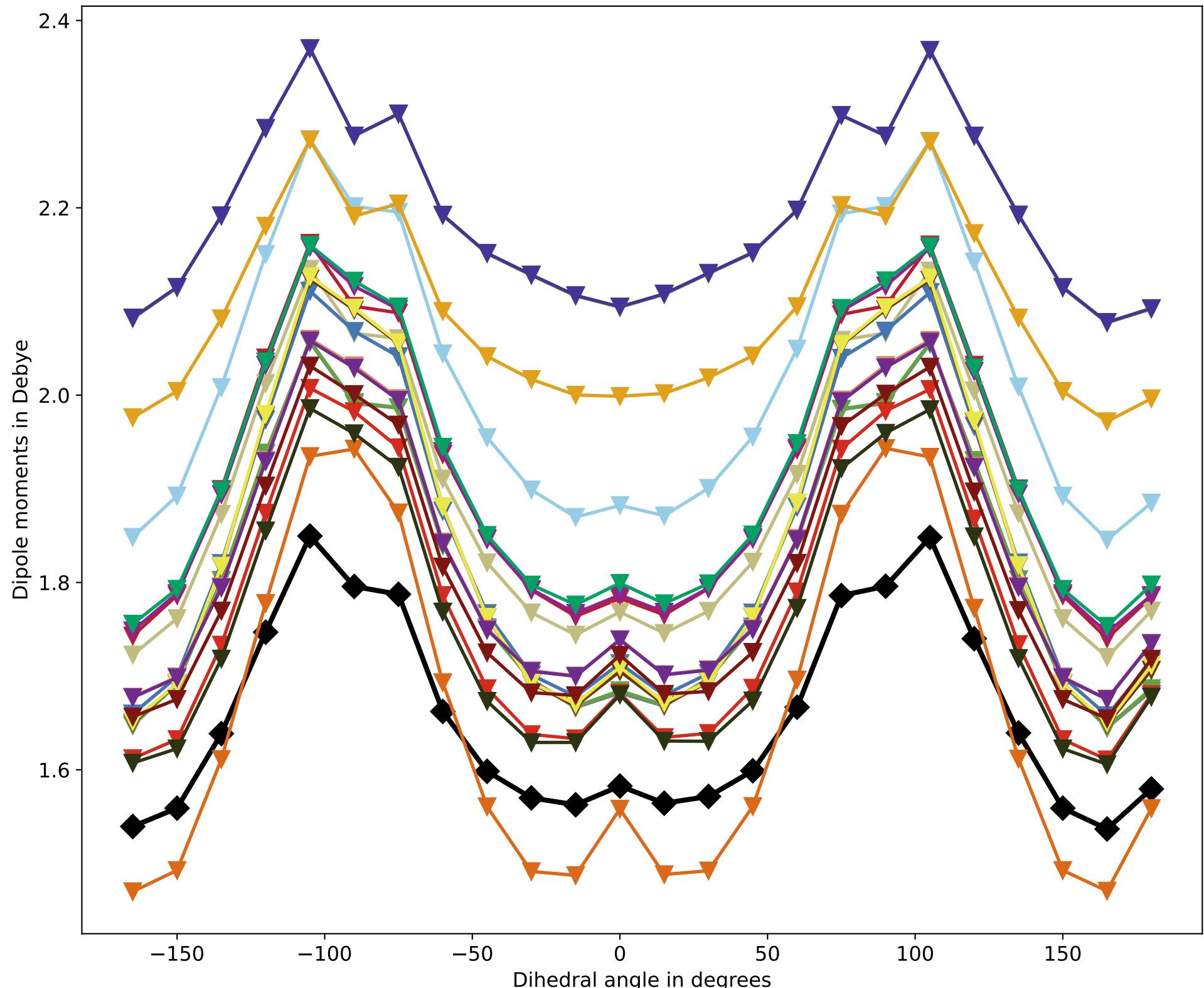


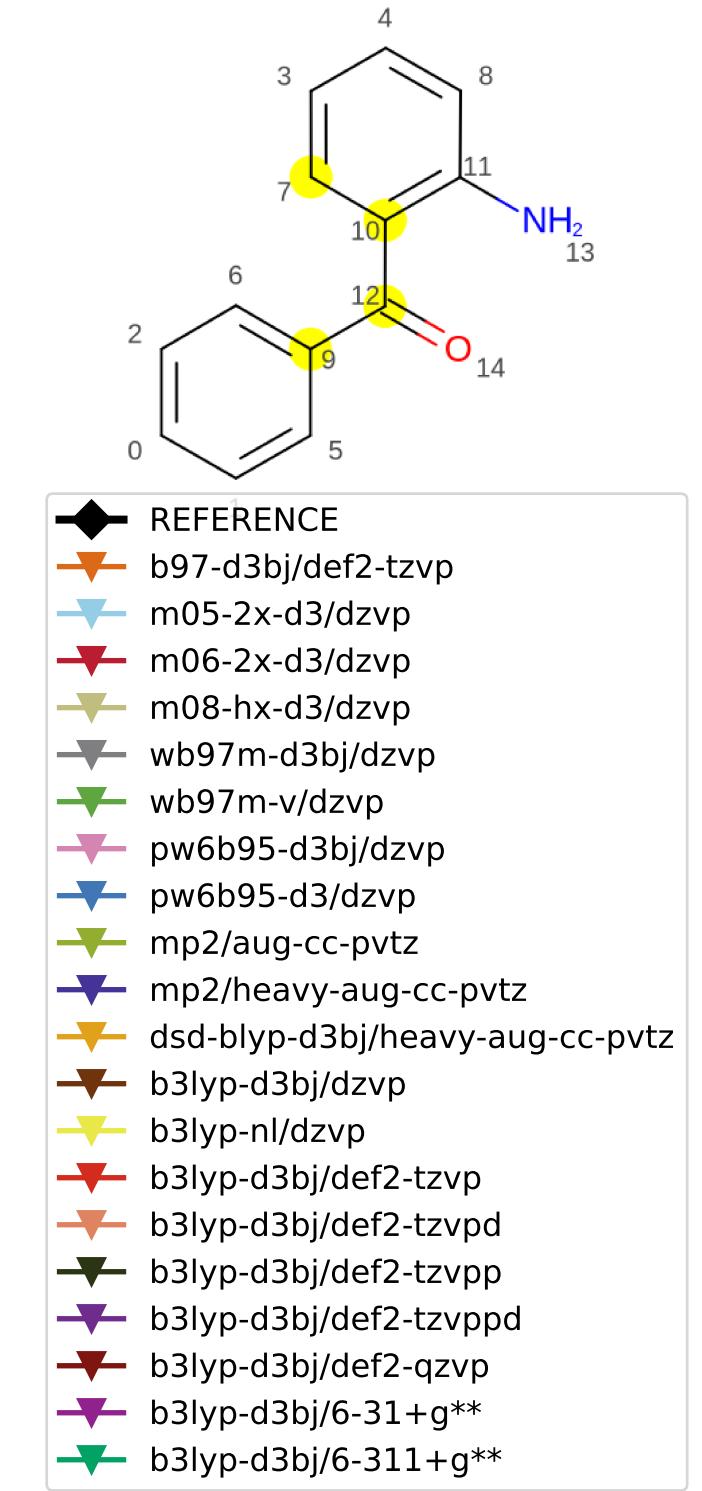
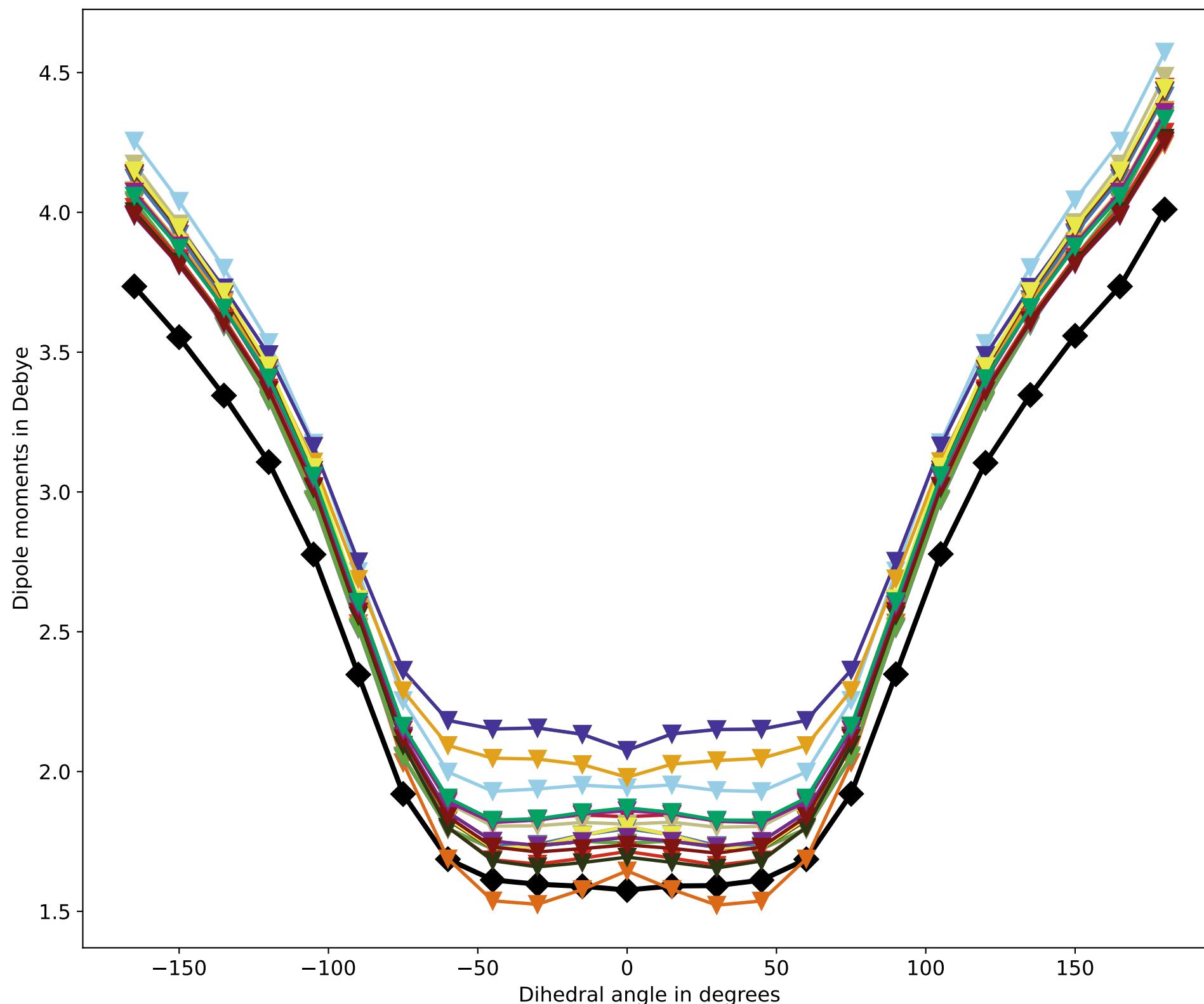


- | | |
|--|---------------------------------|
| | REFERENCE |
| | b97-d3bj/def2-tzvp |
| | m05-2x-d3/dzvp |
| | m06-2x-d3/dzvp |
| | m08-hx-d3/dzvp |
| | wb97m-d3bj/dzvp |
| | wb97m-v/dzvp |
| | pw6b95-d3bj/dzvp |
| | pw6b95-d3/dzvp |
| | mp2/aug-cc-pvtz |
| | mp2/heavy-aug-cc-pvtz |
| | dsd-blyp-d3bj/heavy-aug-cc-pvtz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

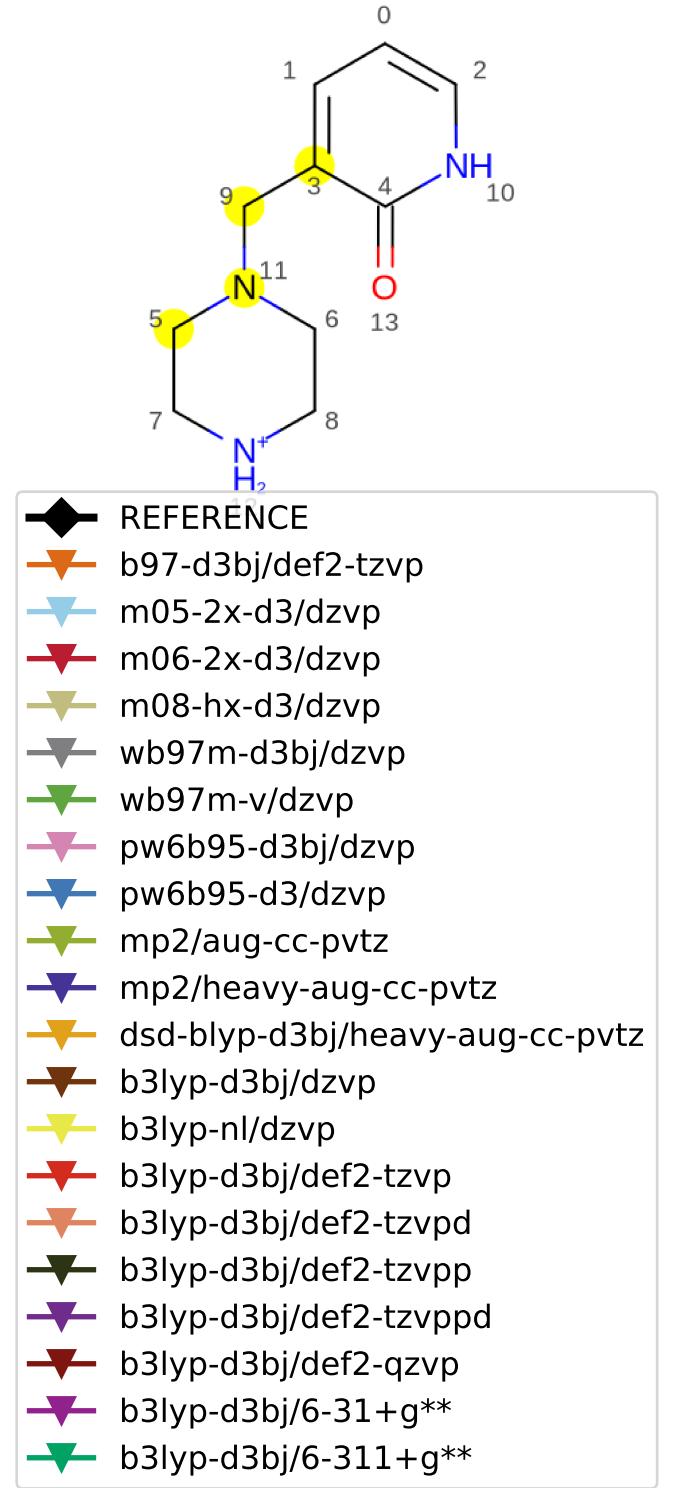
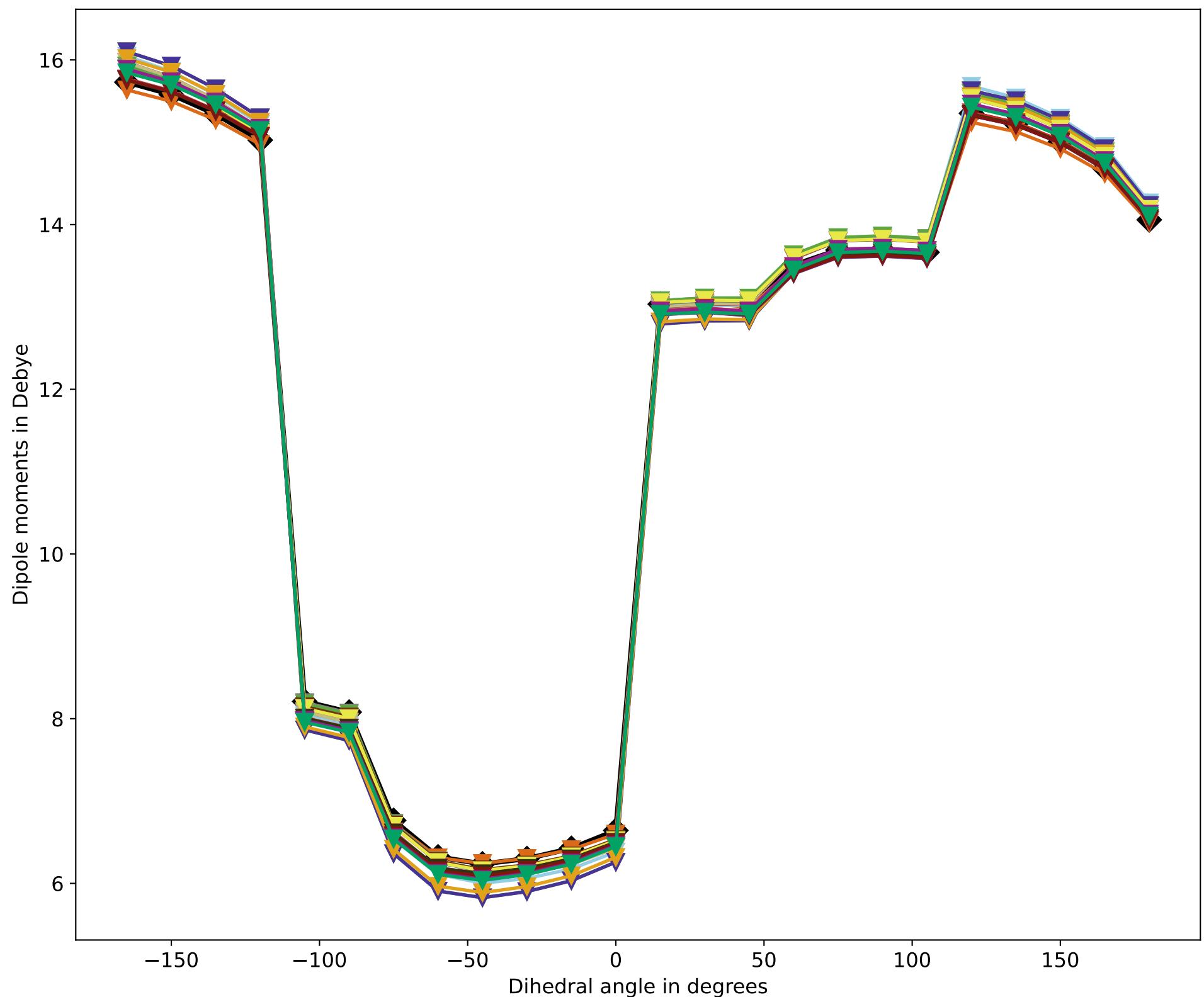


- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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

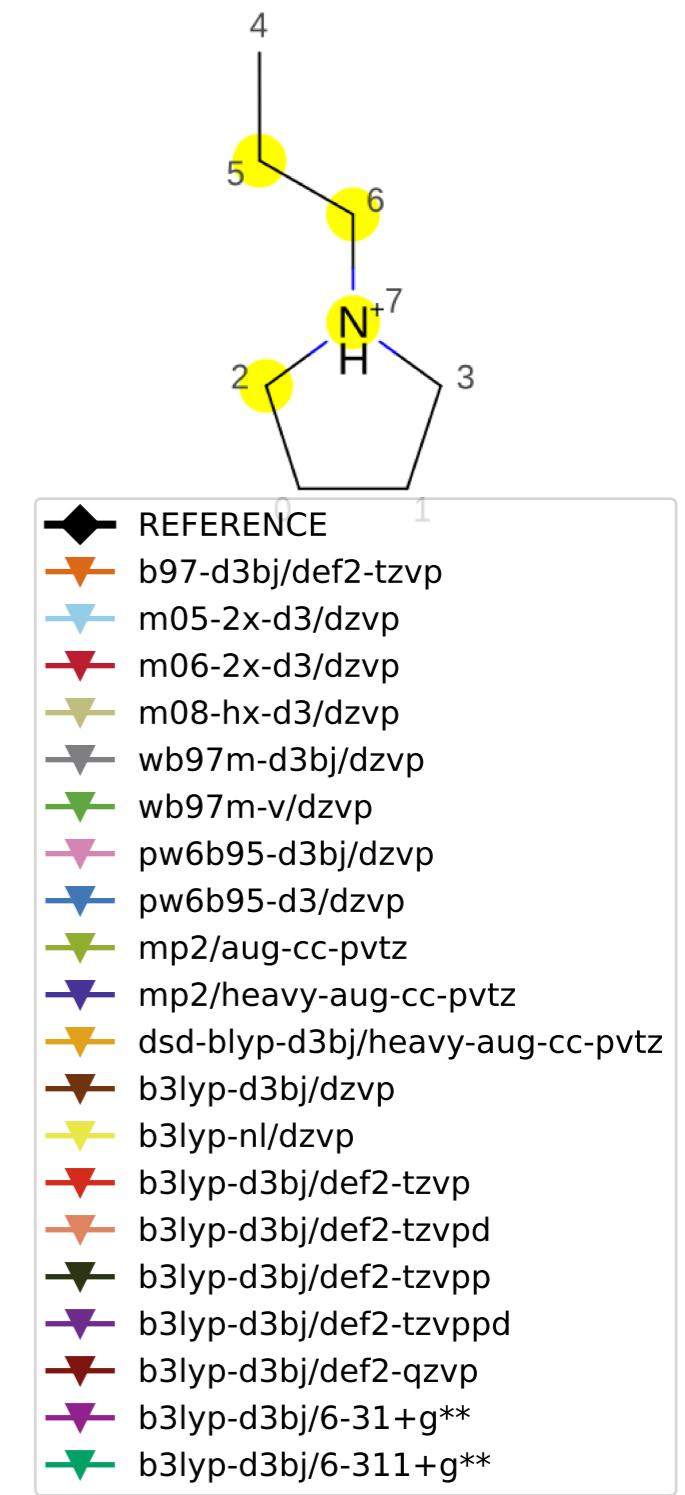
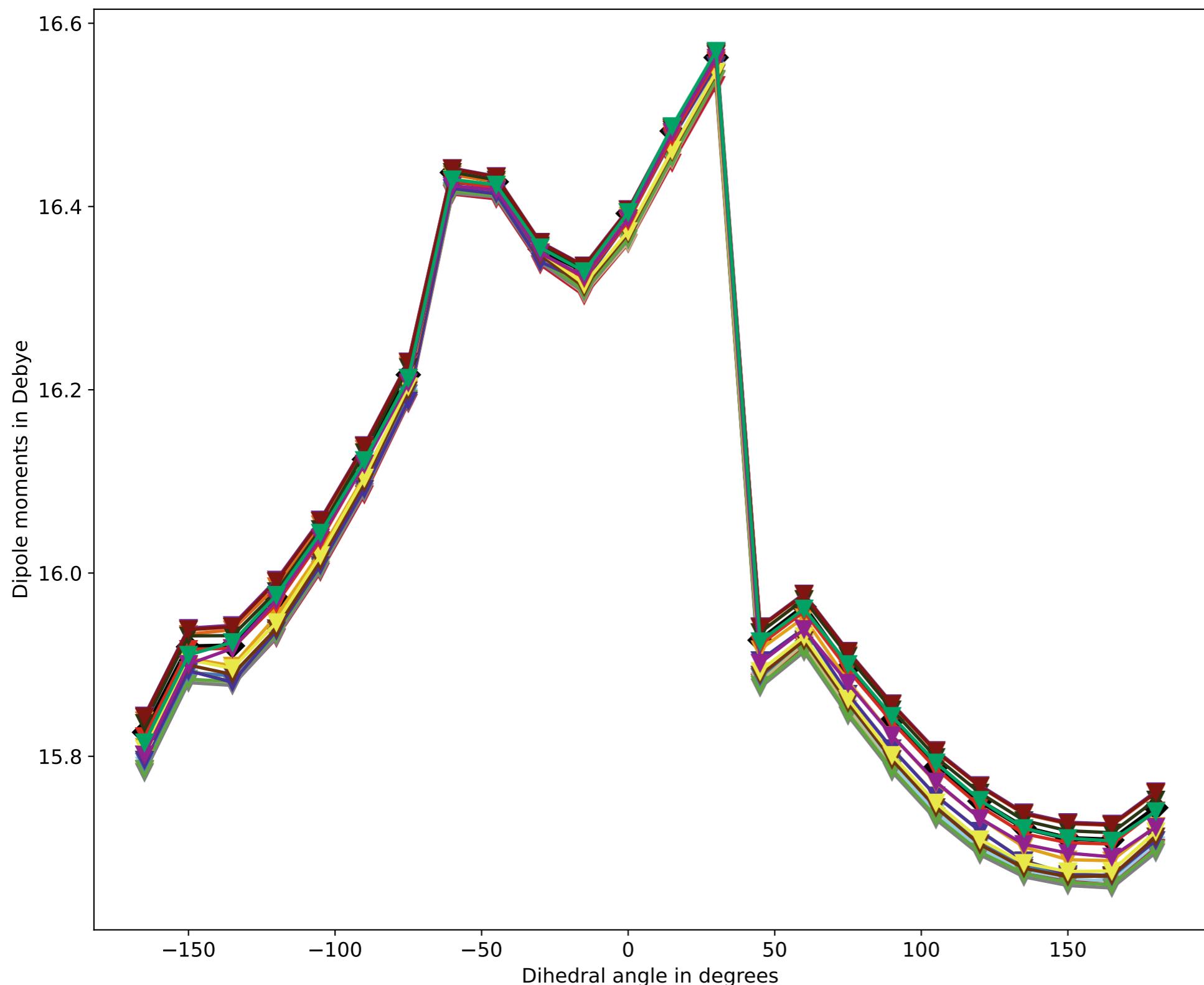


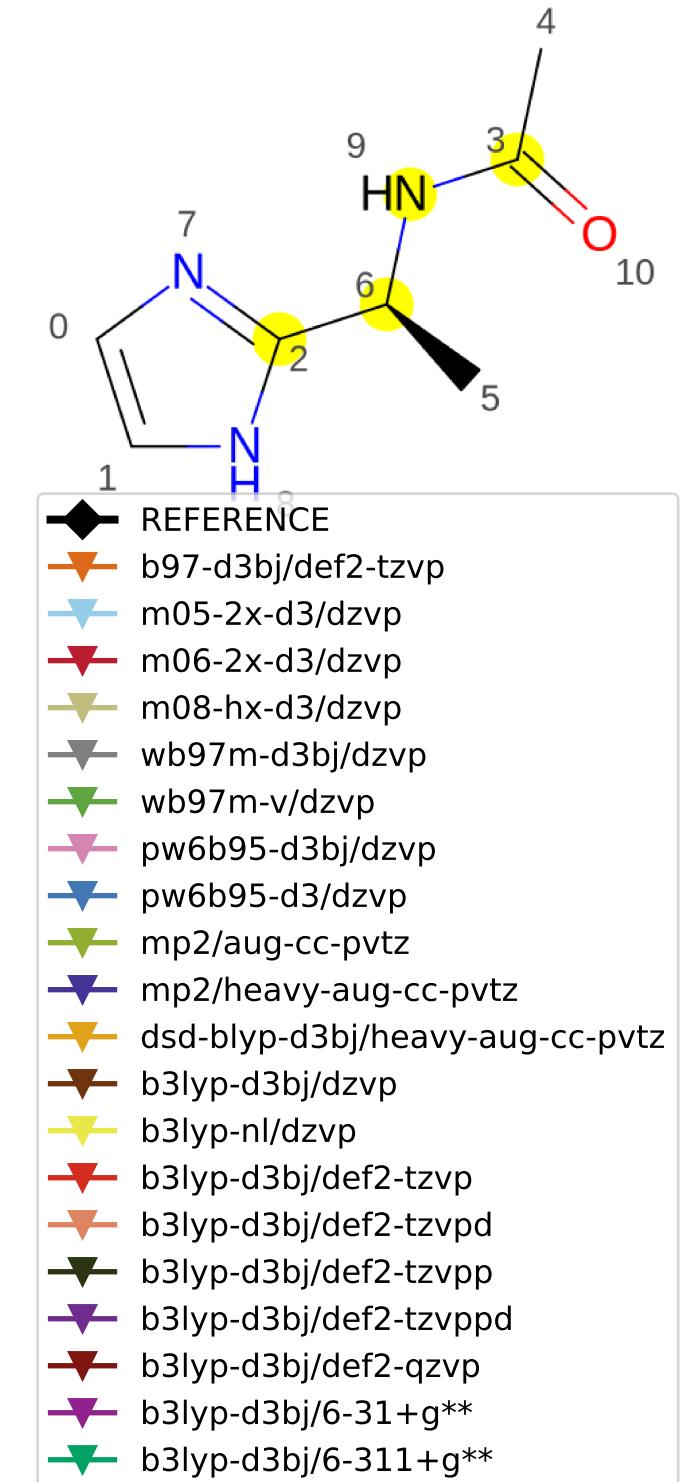
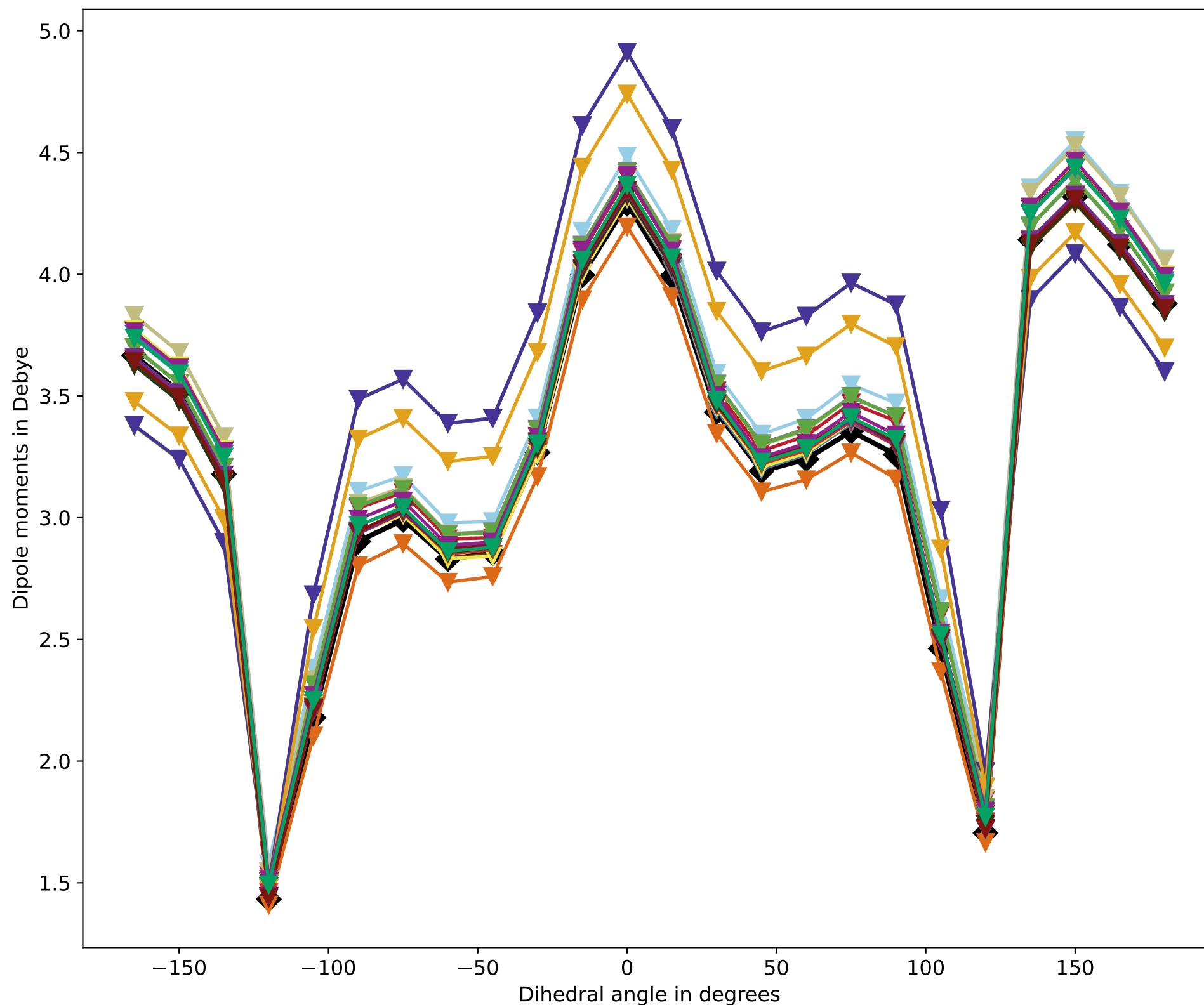


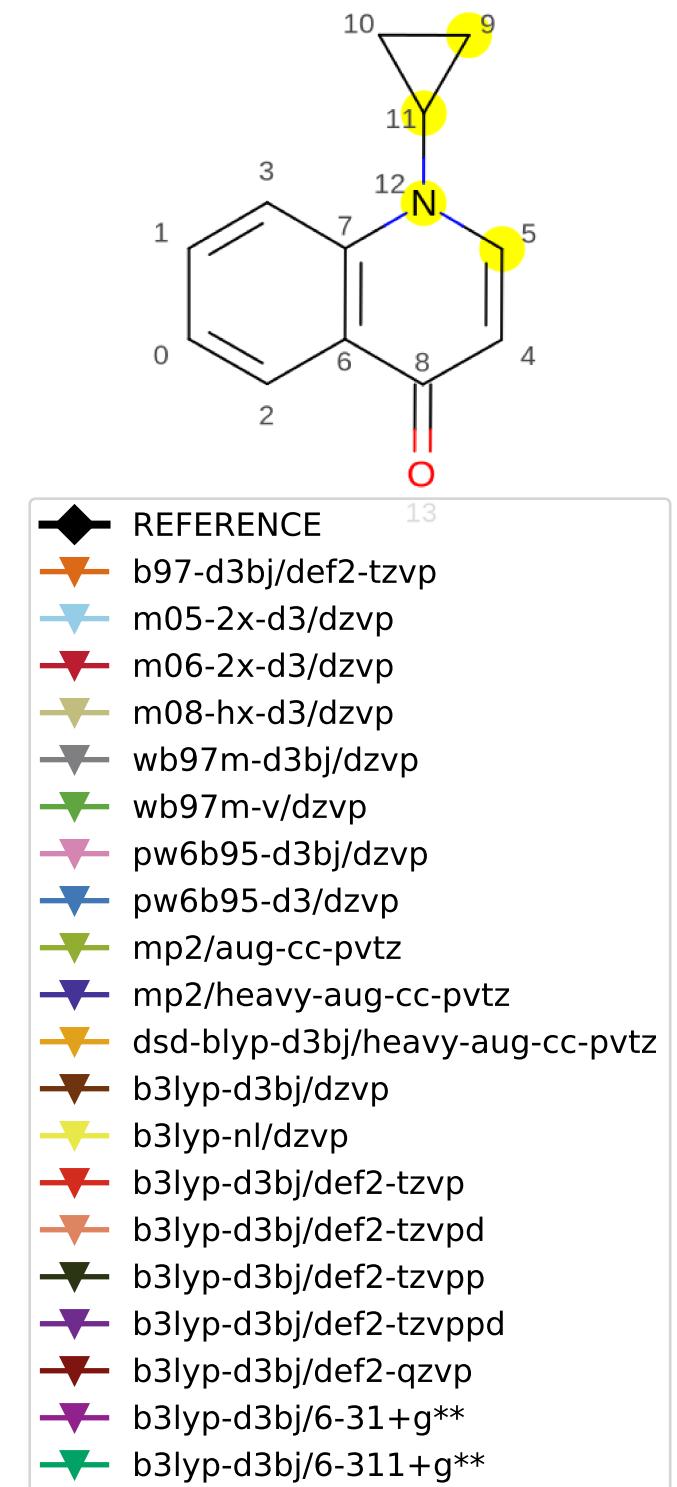
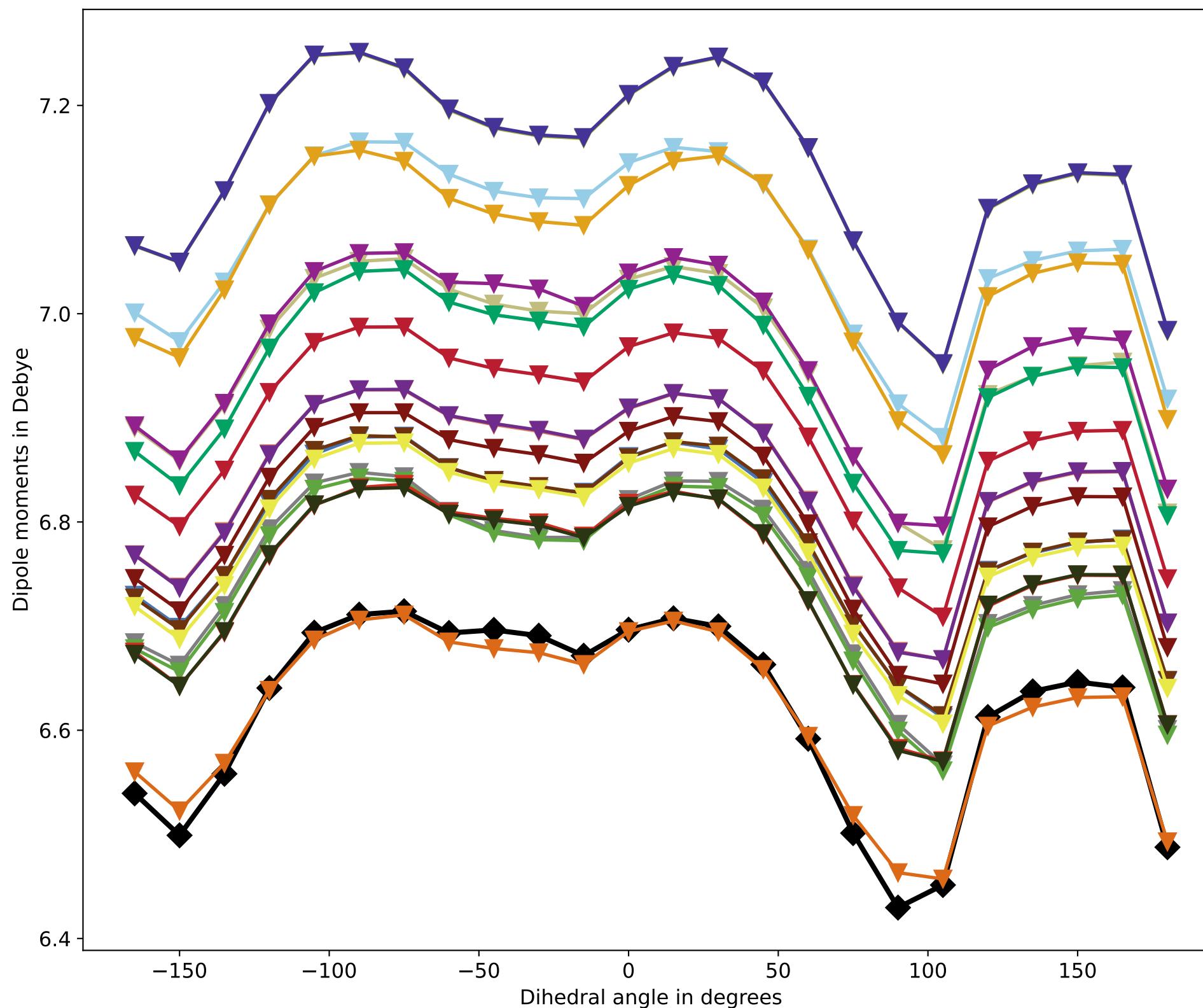
Charged molecule

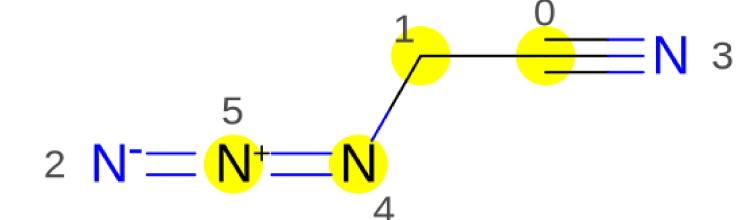
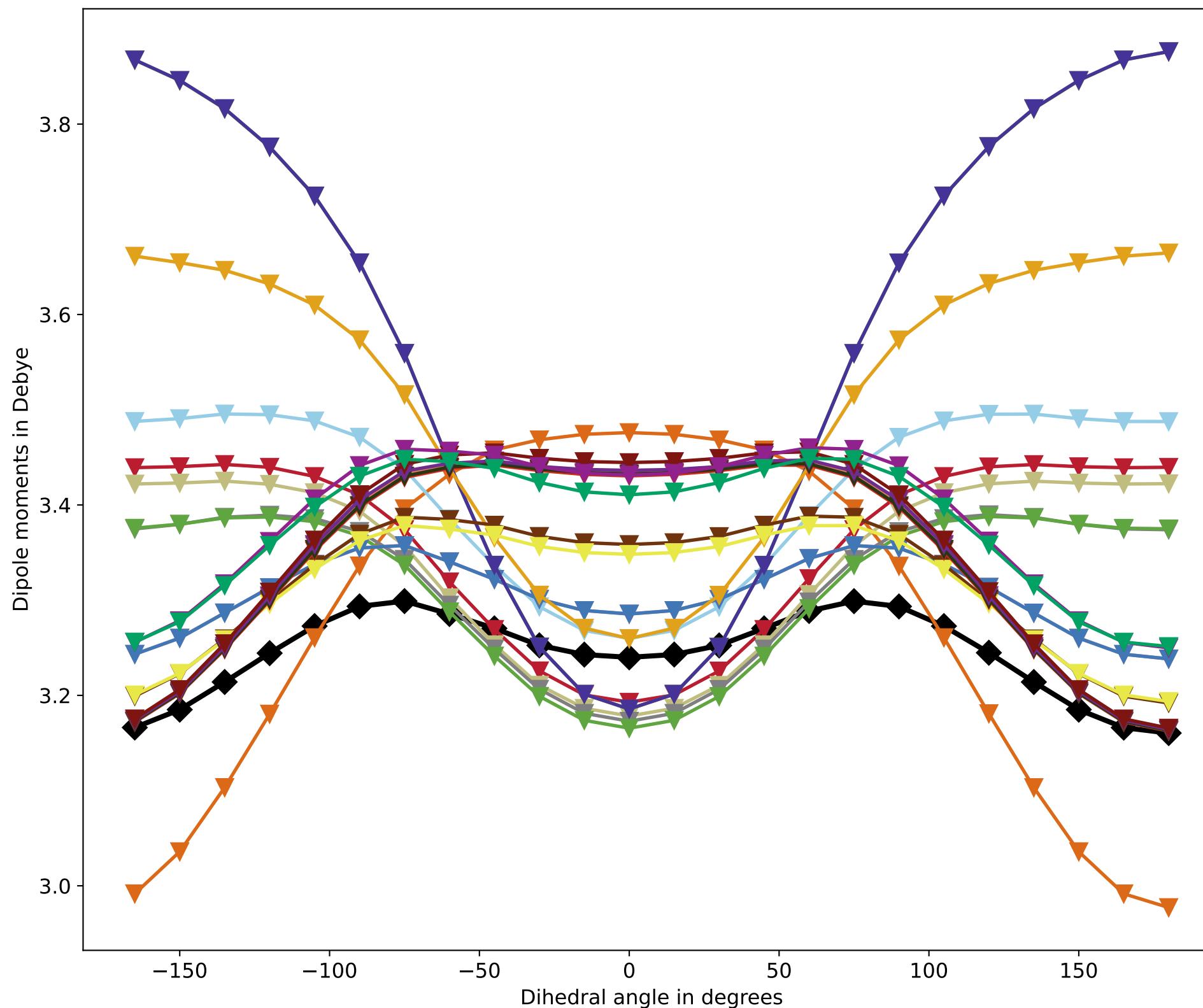


Charged molecule



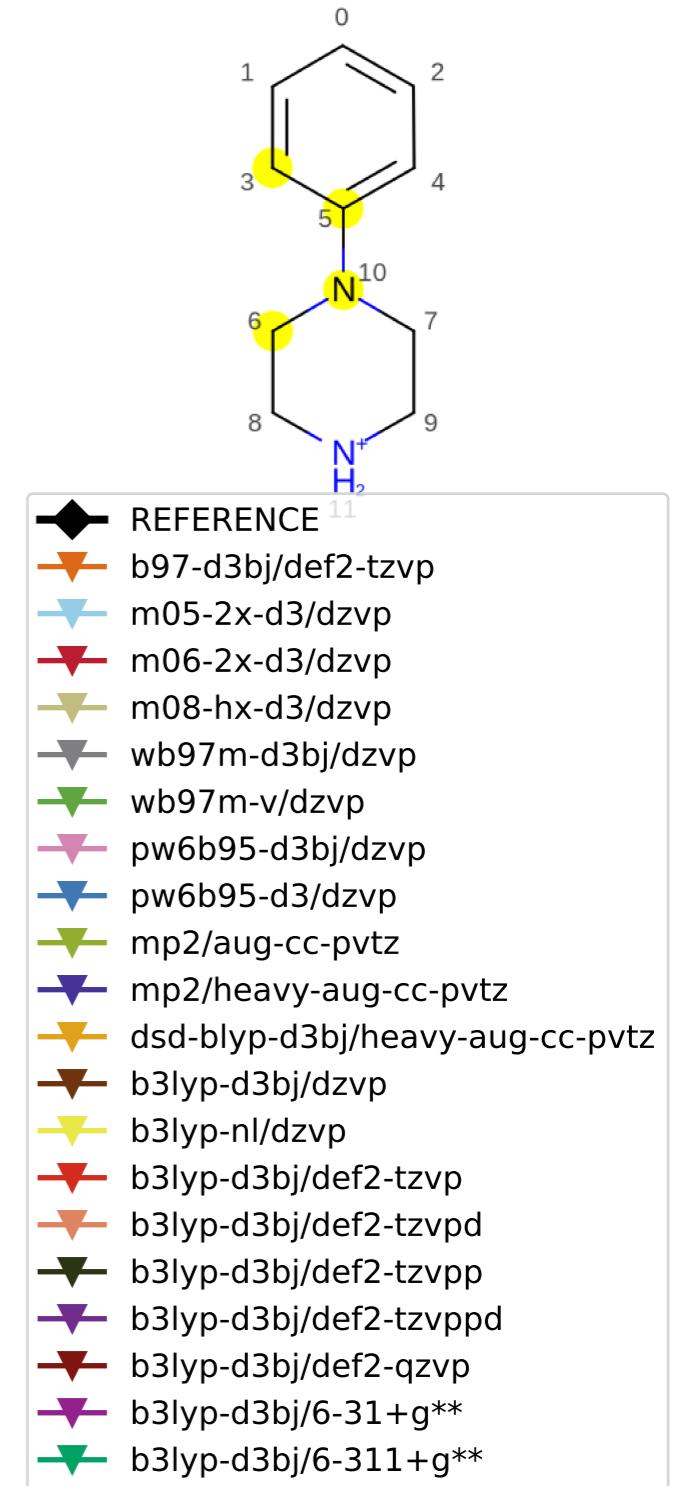
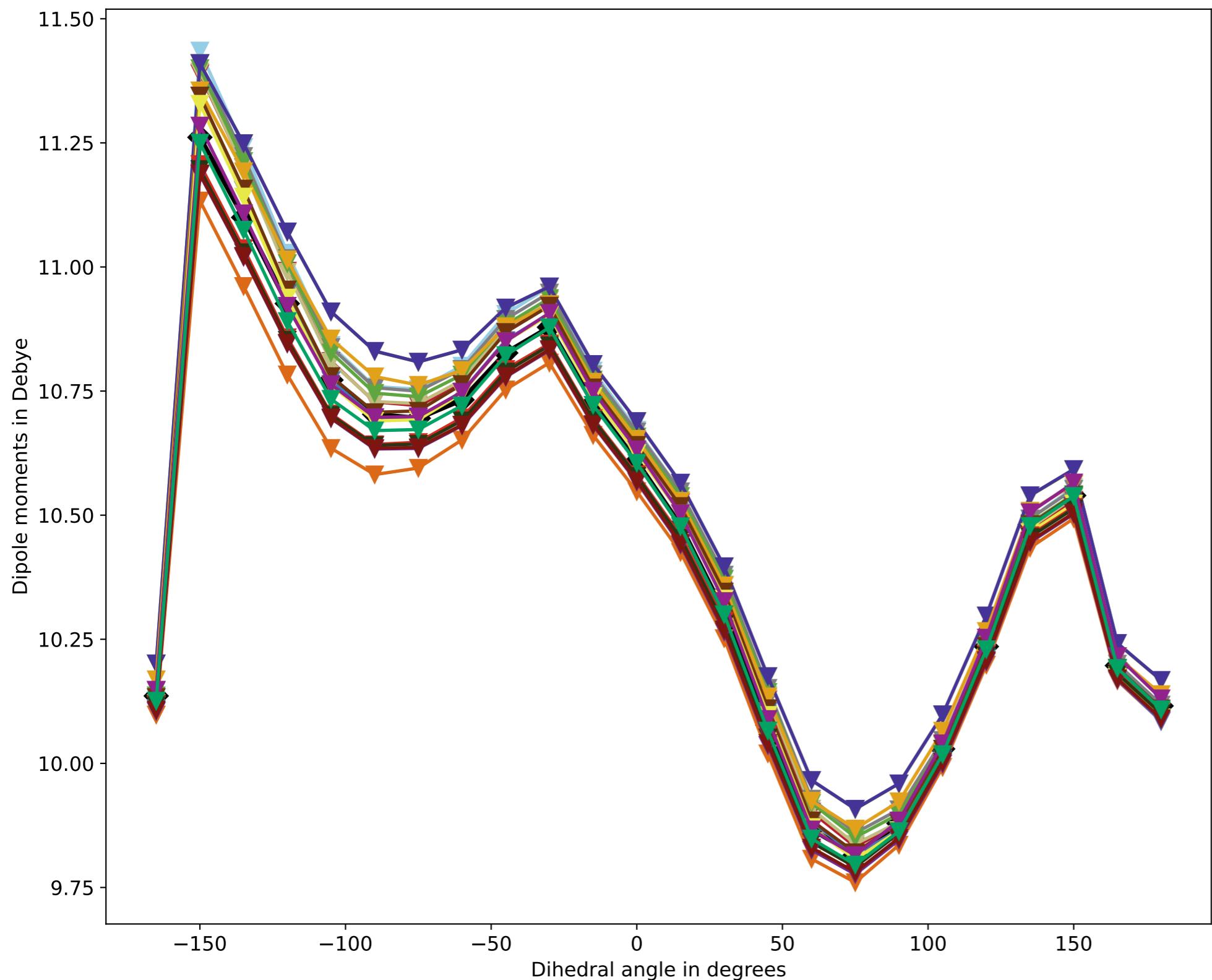


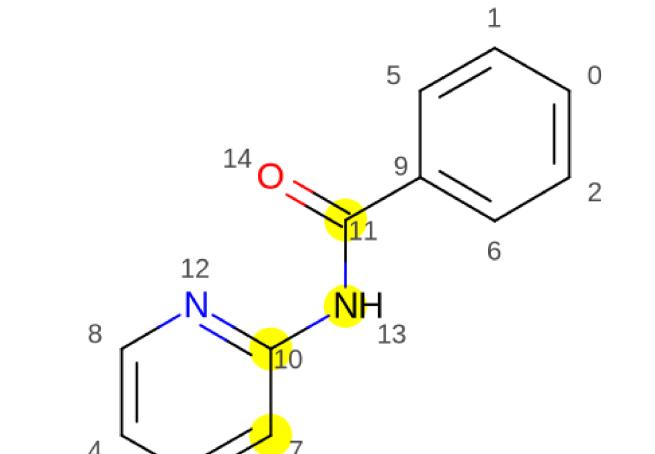
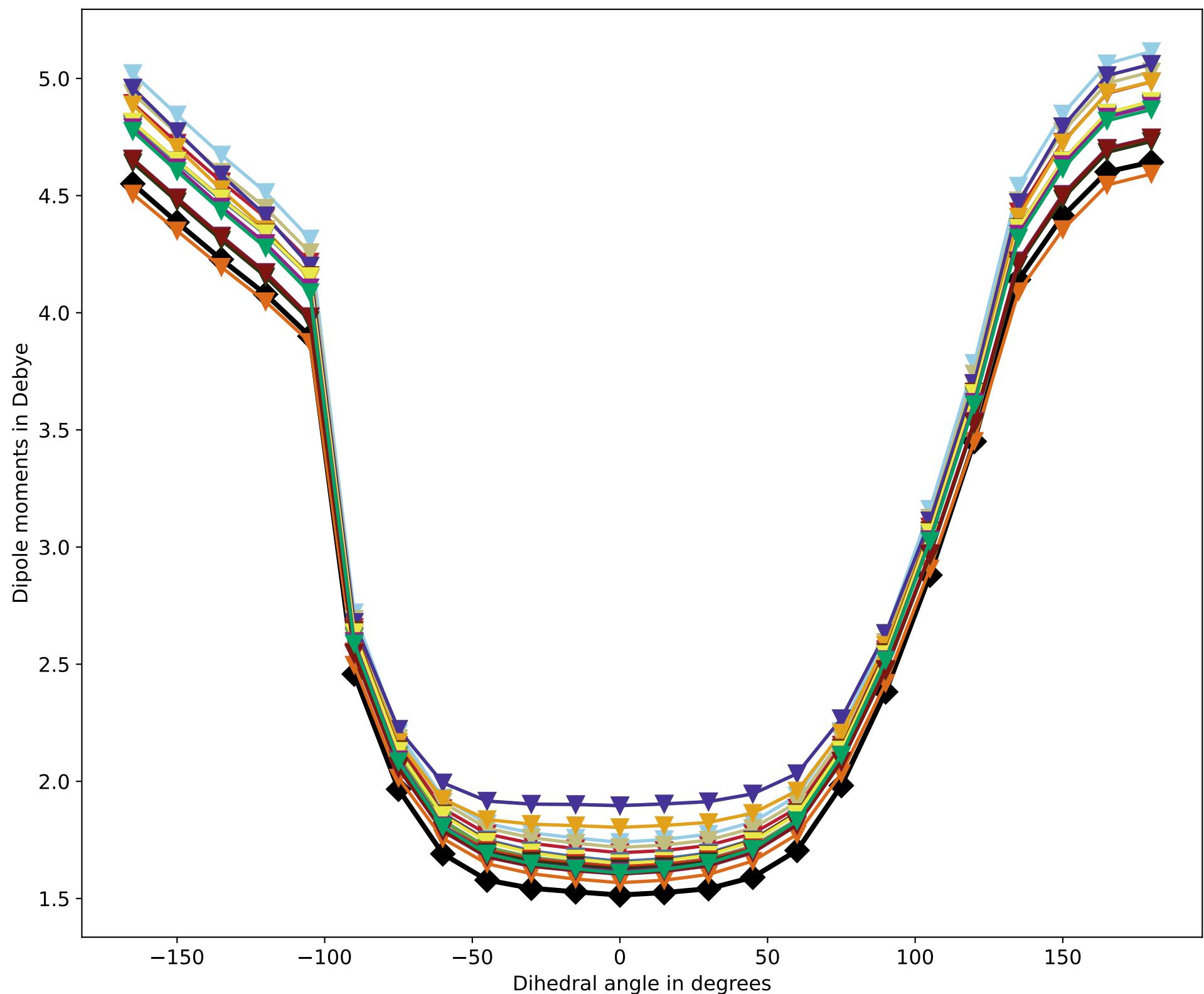




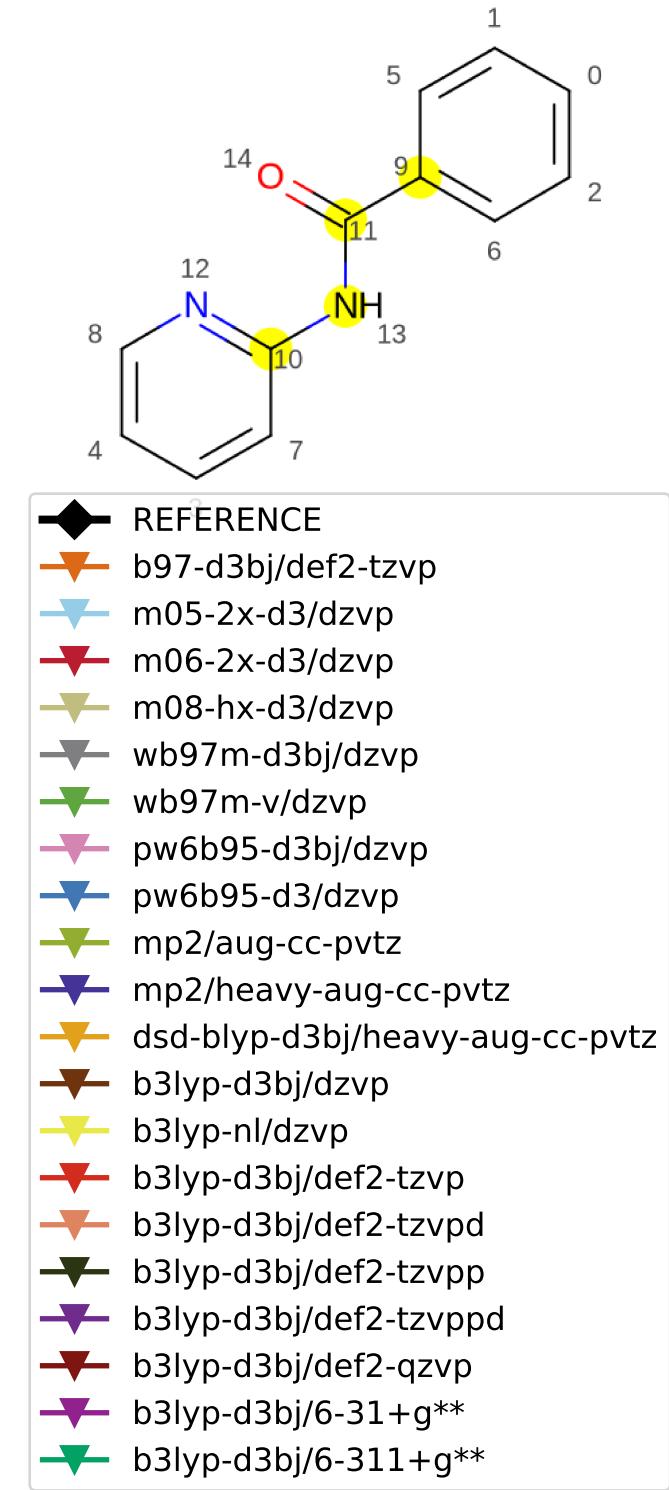
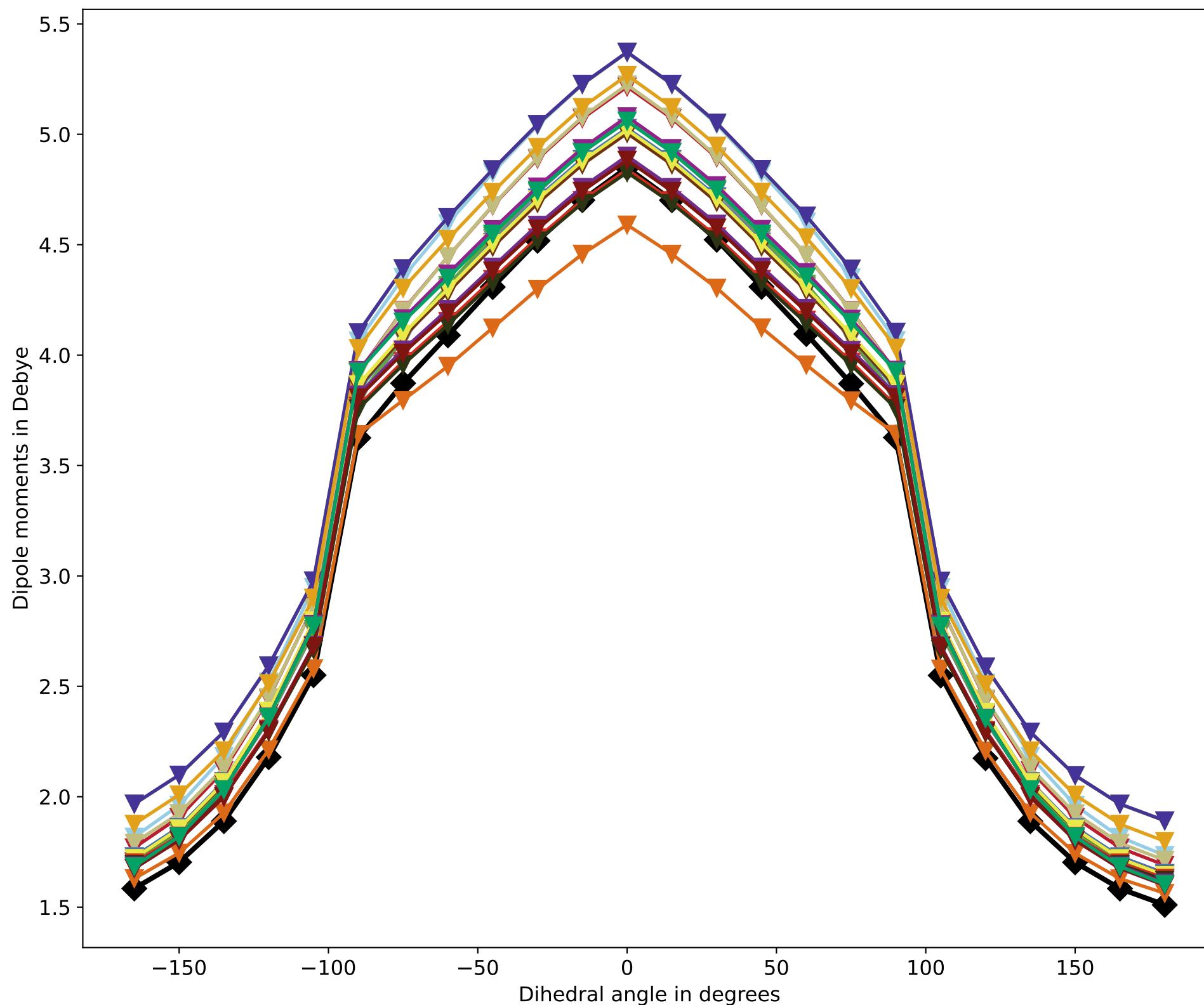
- REFERENCE**
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd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

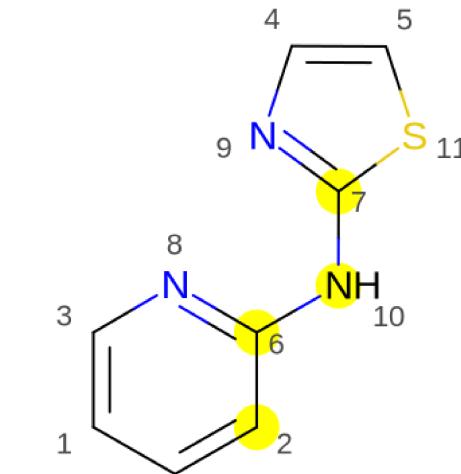
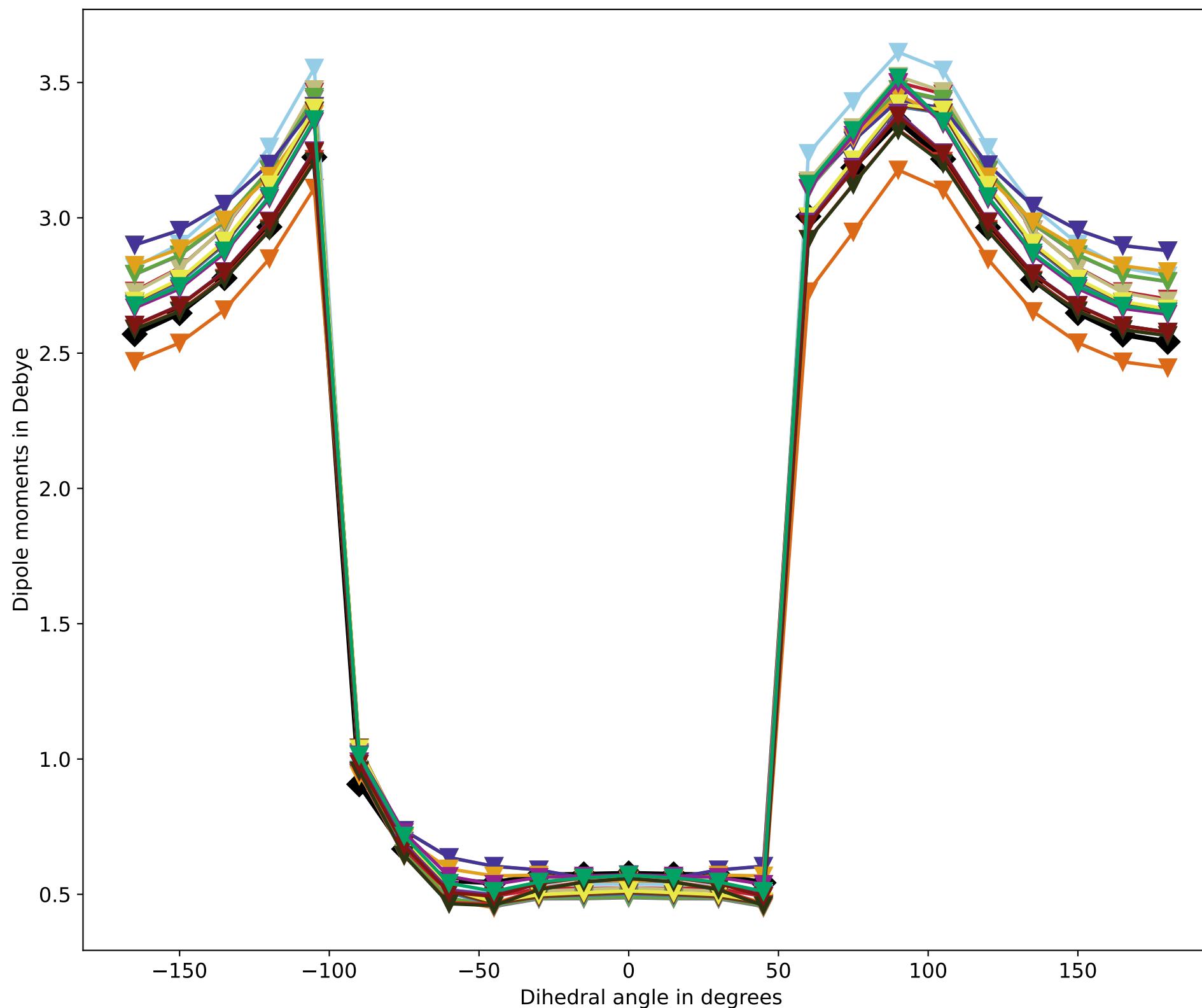
Charged molecule



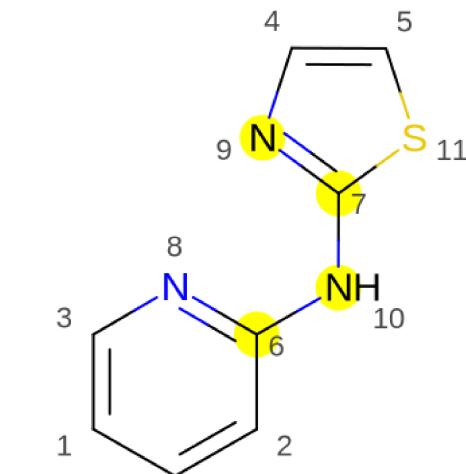
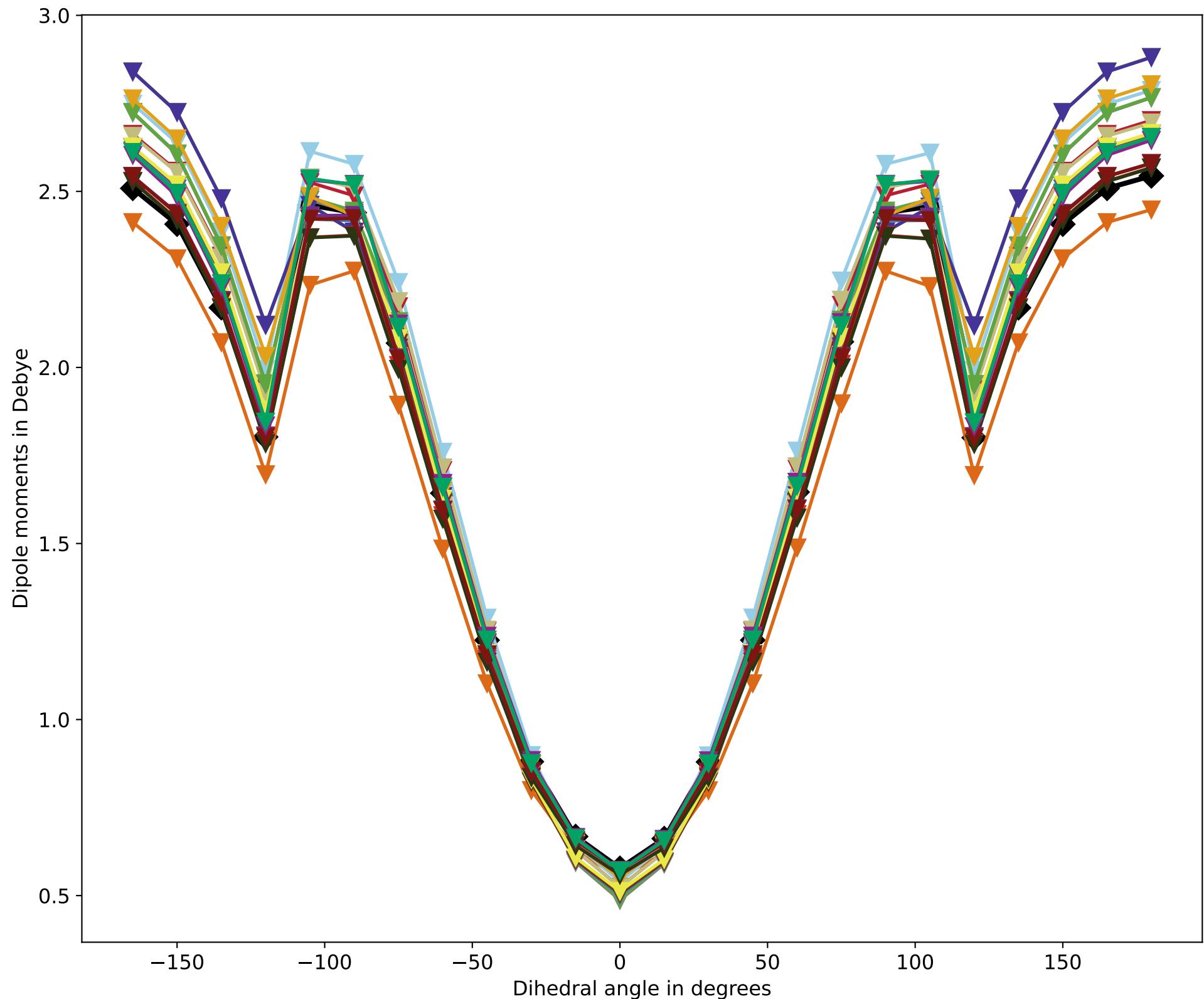


- REFERENCE**
- b97-d3bj/def2-tzvp
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-d3bj/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- mp2/aug-cc-pvtz
- mp2/heavy-aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- b3lyp-d3bj/dzvp
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvpd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



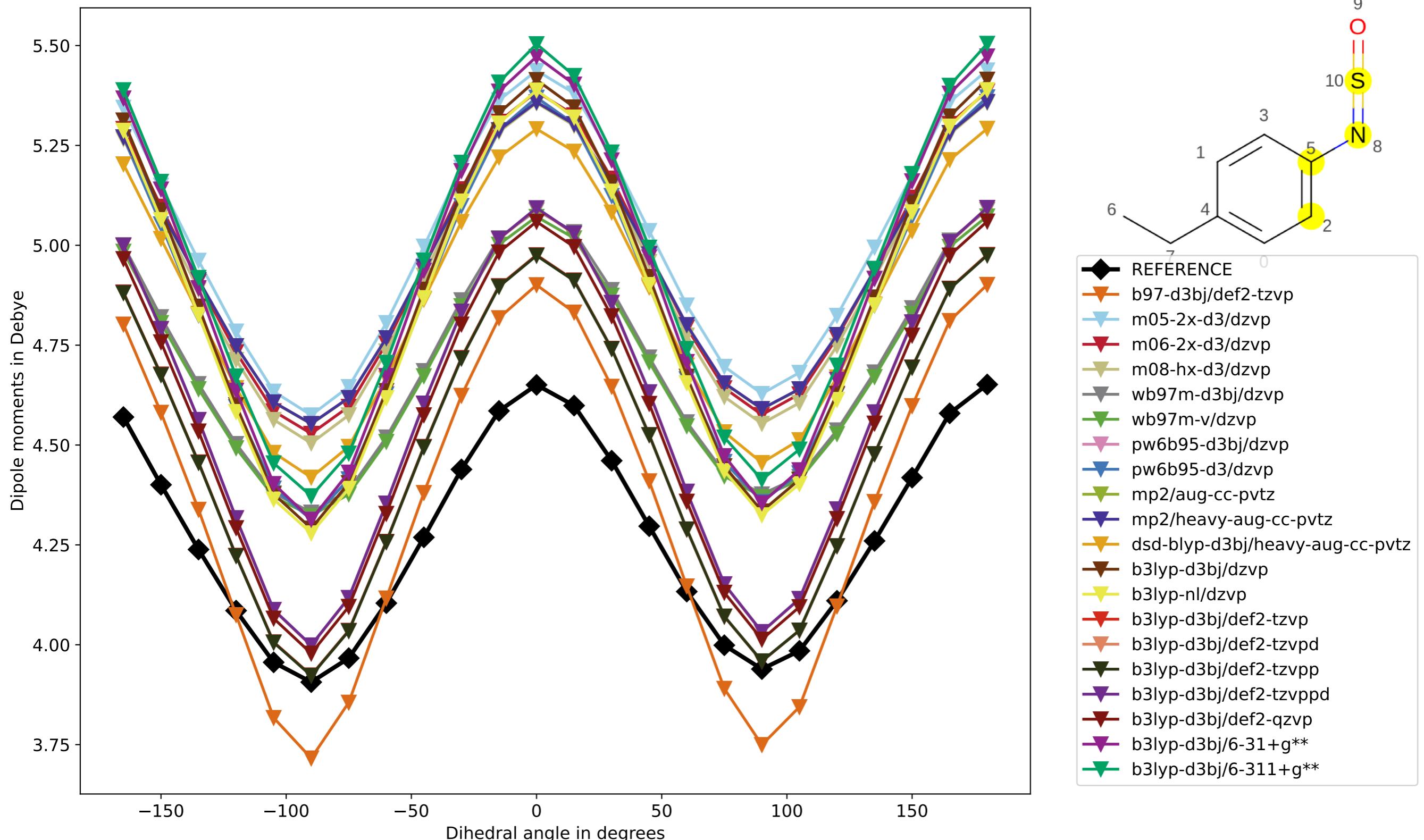


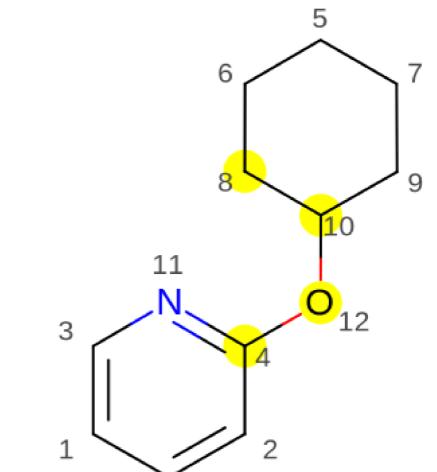
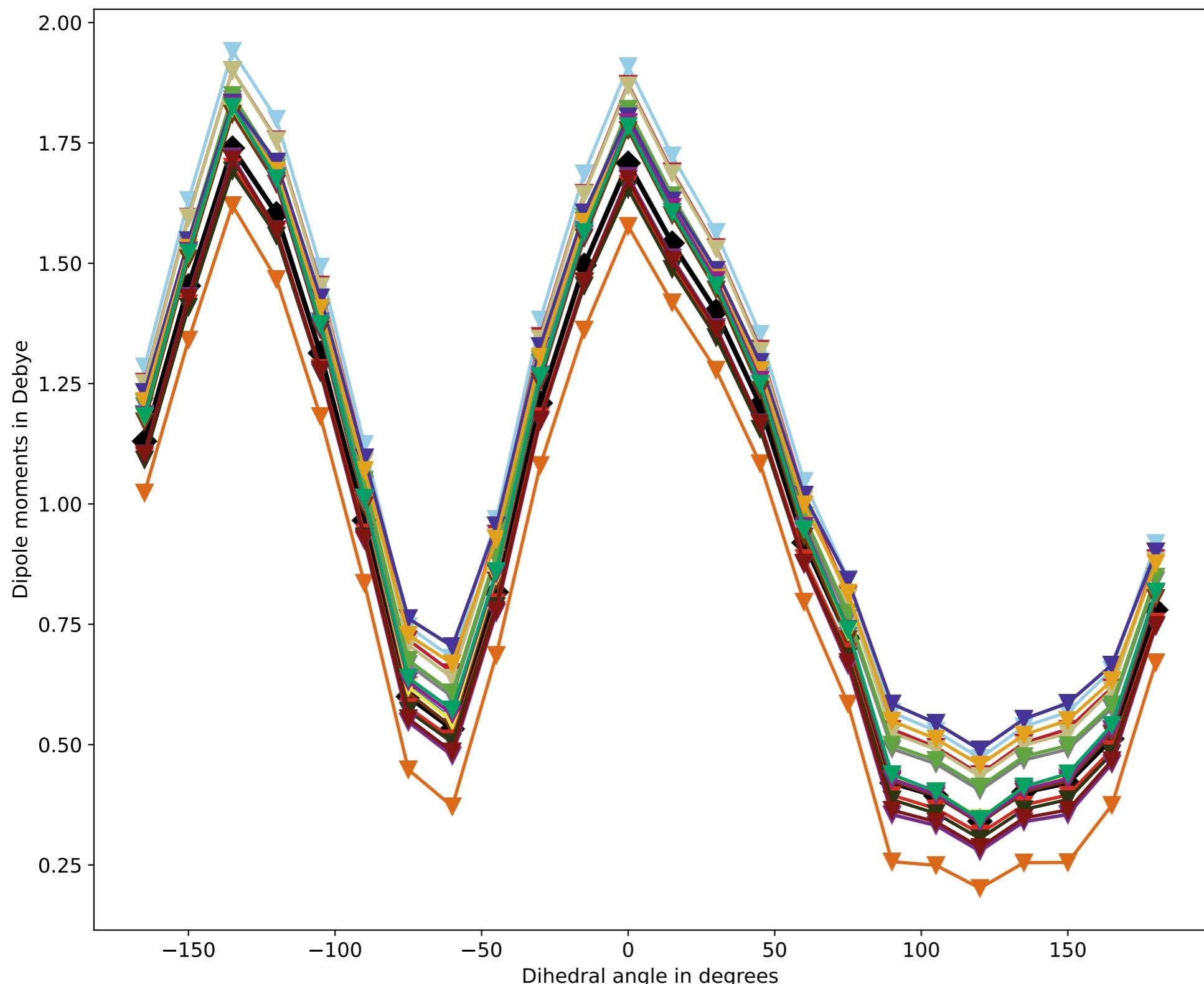
- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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



- ◆ 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-tzvpd
- ◆ b3lyp-d3bj/def2-tzvpp
- ◆ b3lyp-d3bj/def2-tzvppd
- ◆ b3lyp-d3bj/def2-qzvp
- ◆ b3lyp-d3bj/6-31+g**
- ◆ b3lyp-d3bj/6-311+g**

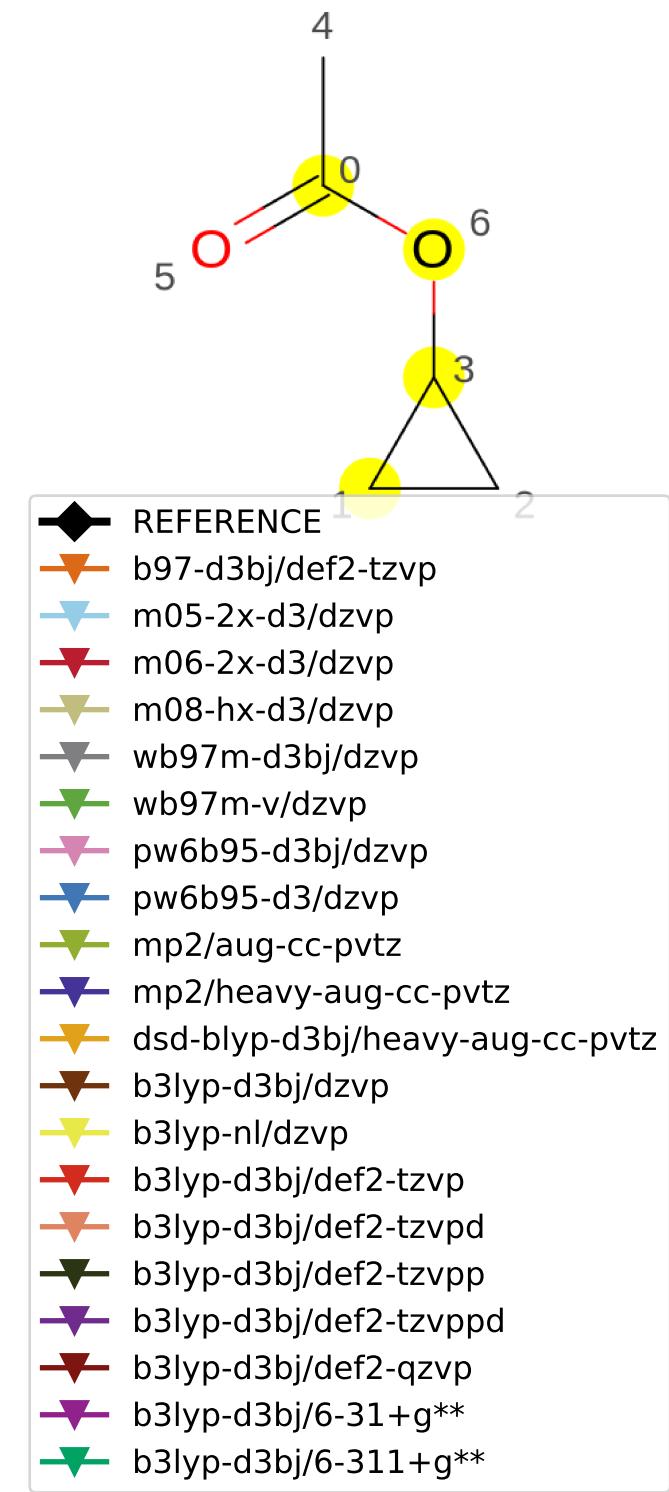
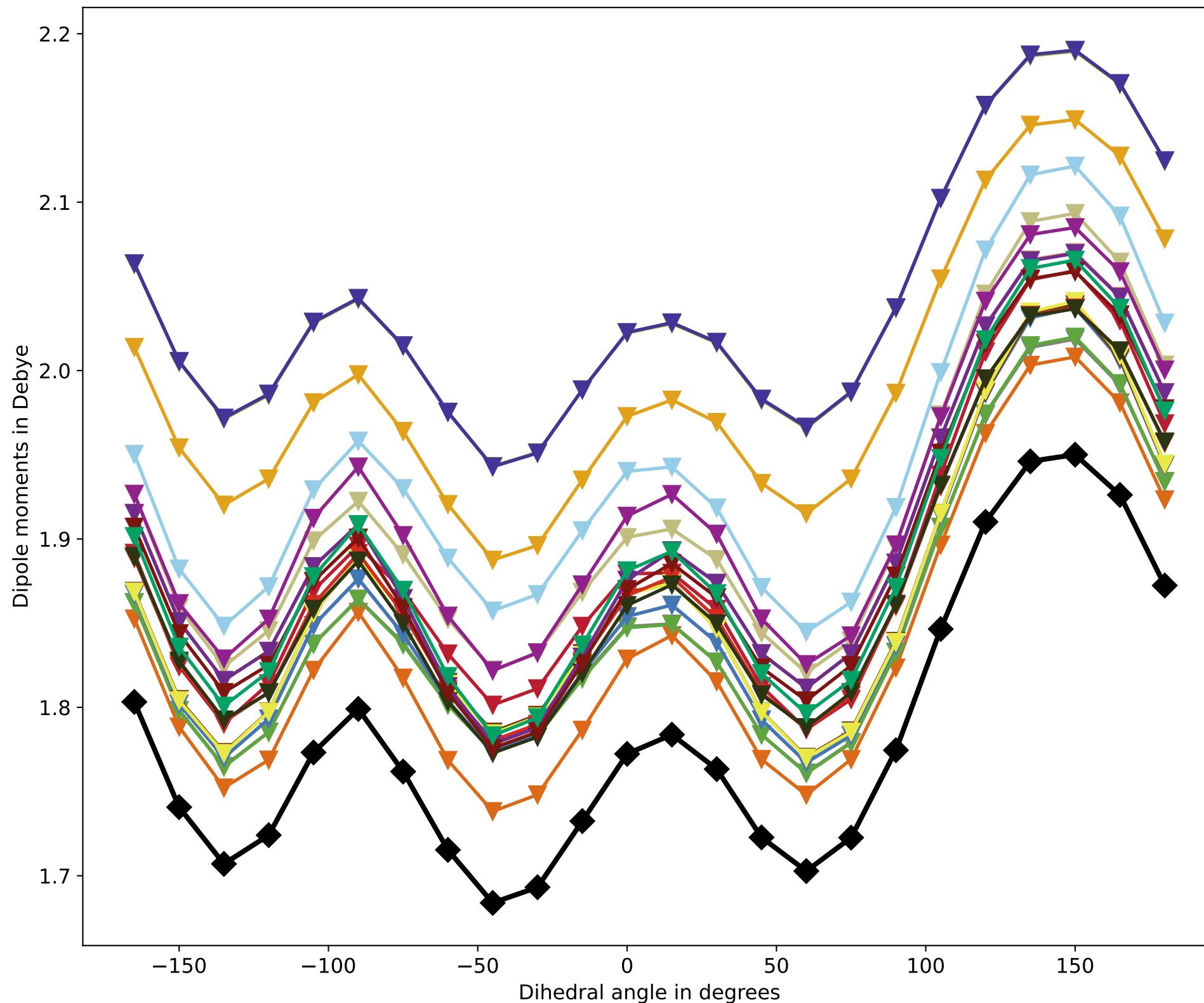
Dihedral angle in degrees

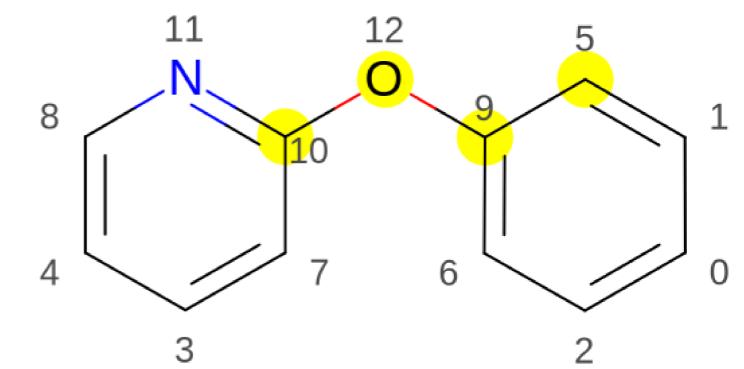
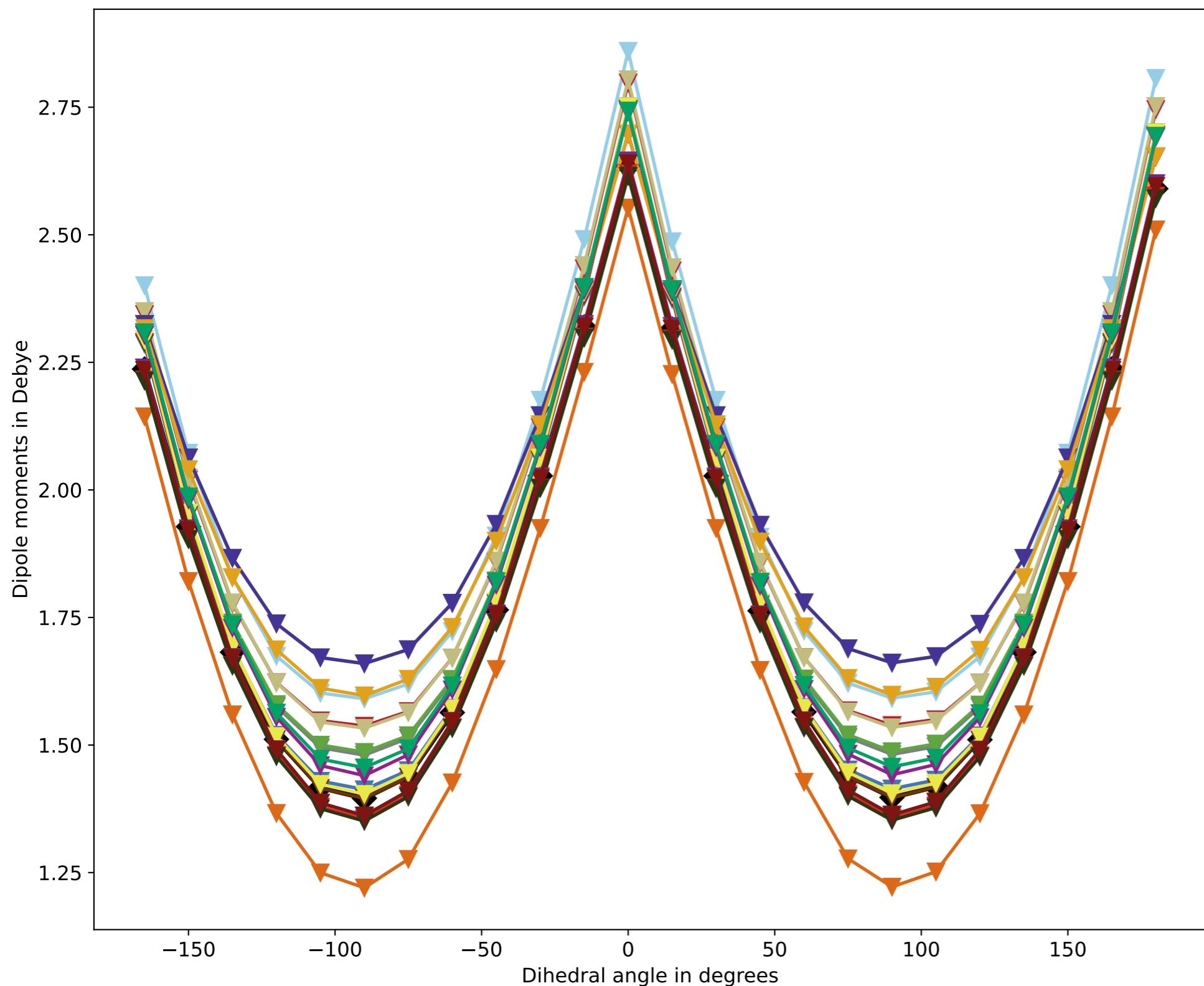


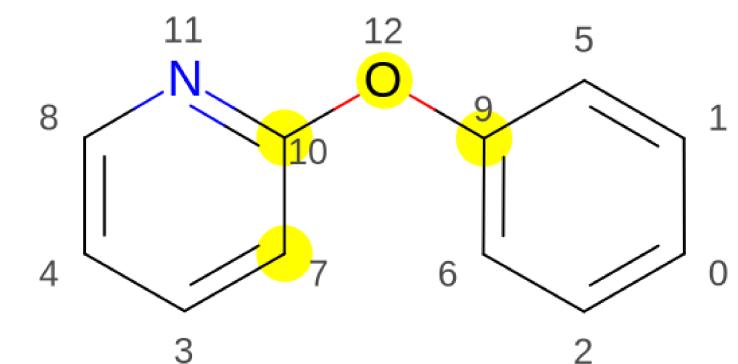
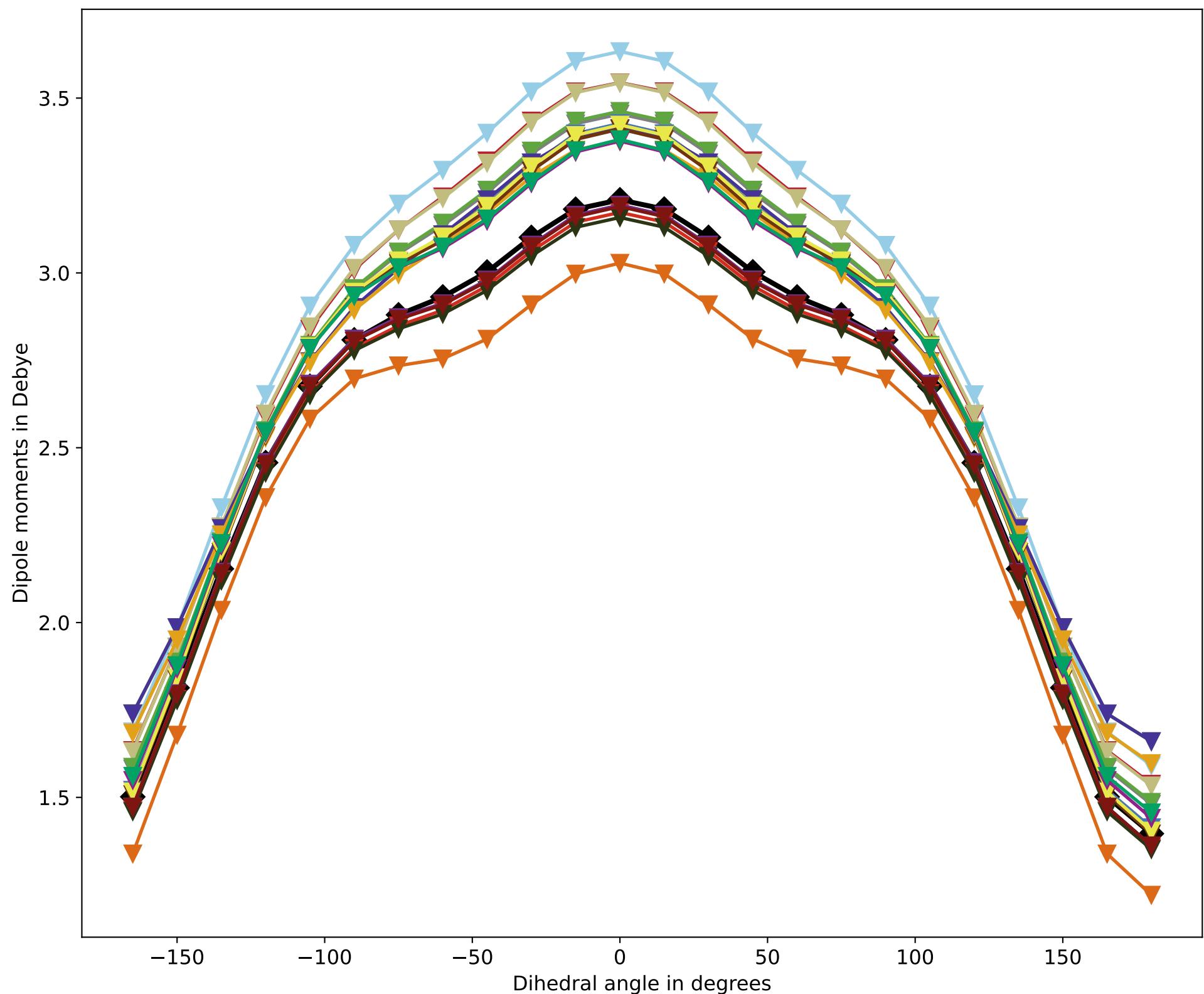


- | Method |
|---------------------------------|
| REFERENCE |
| b97-d3bj/def2-tzvp |
| m05-2x-d3/dzvp |
| m06-2x-d3/dzvp |
| m08-hx-d3/dzvp |
| wb97m-d3bj/dzvp |
| wb97m-v/dzvp |
| pw6b95-d3bj/dzvp |
| pw6b95-d3/dzvp |
| mp2/aug-cc-pvtz |
| mp2/heavy-aug-cc-pvtz |
| dsd-blyp-d3bj/heavy-aug-cc-pvtz |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

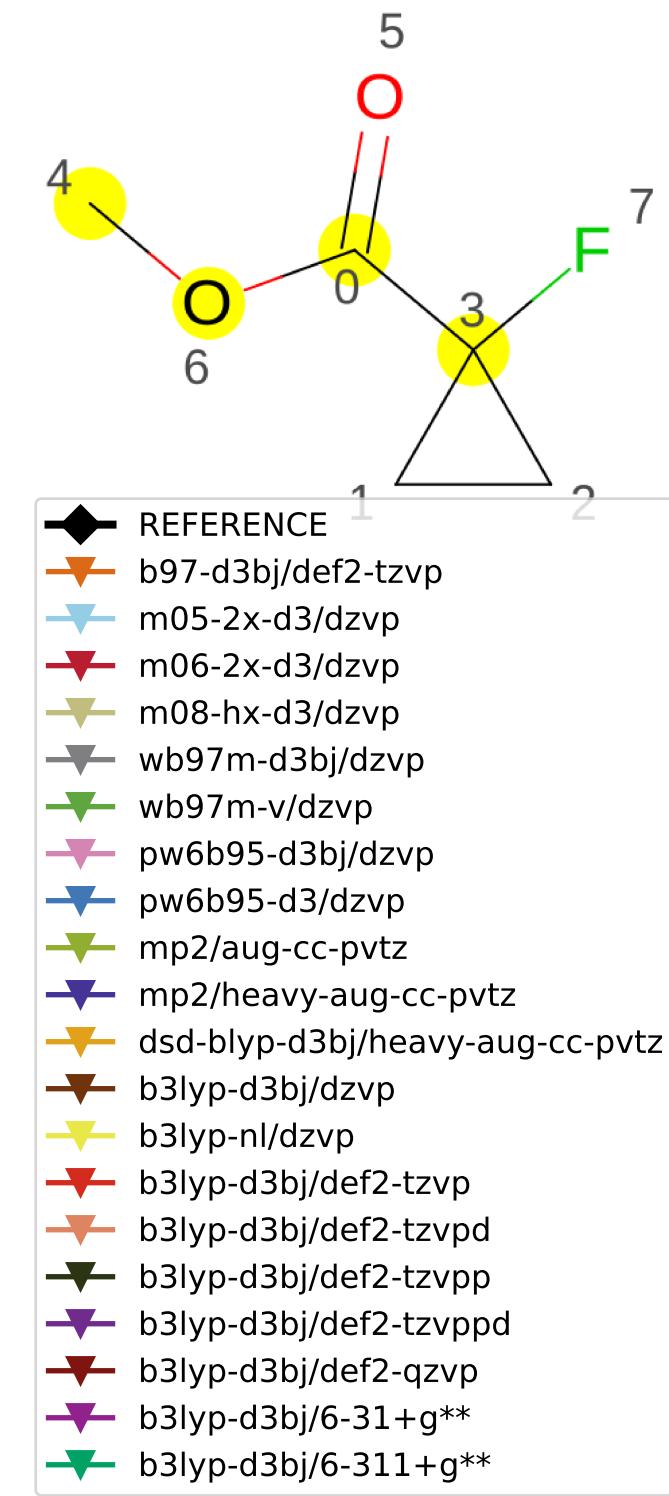
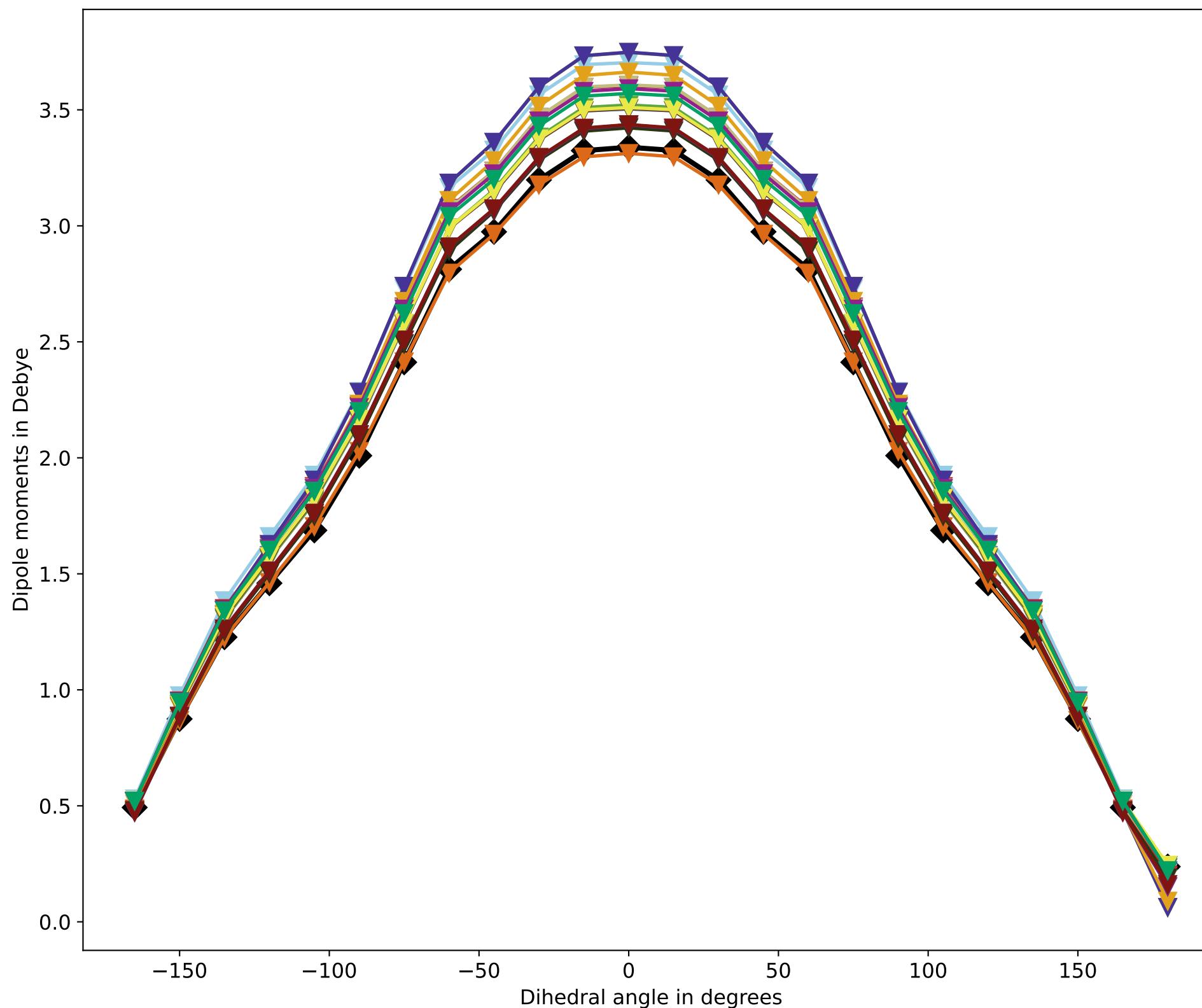
Neutral molecule

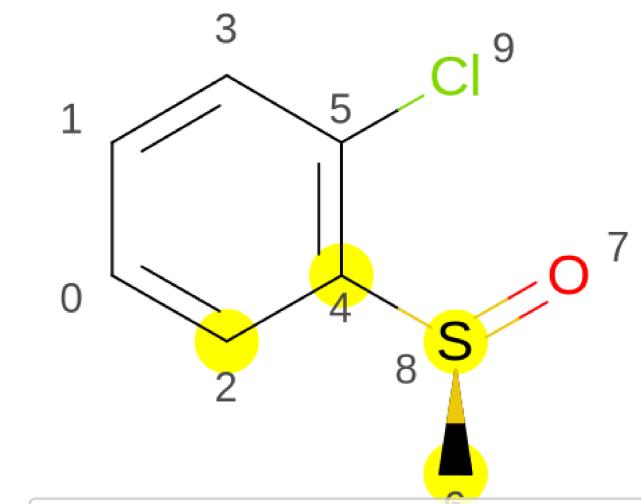
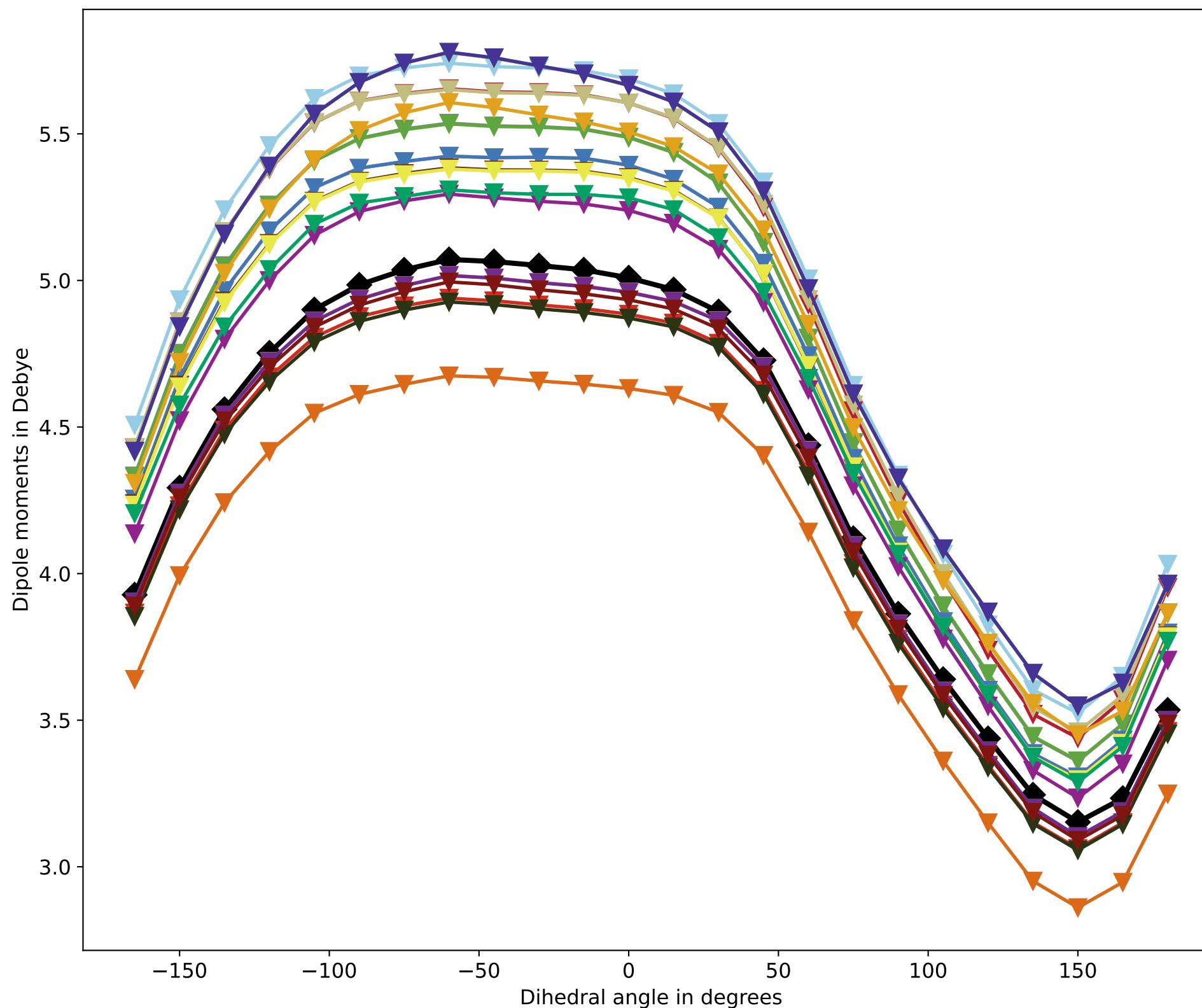




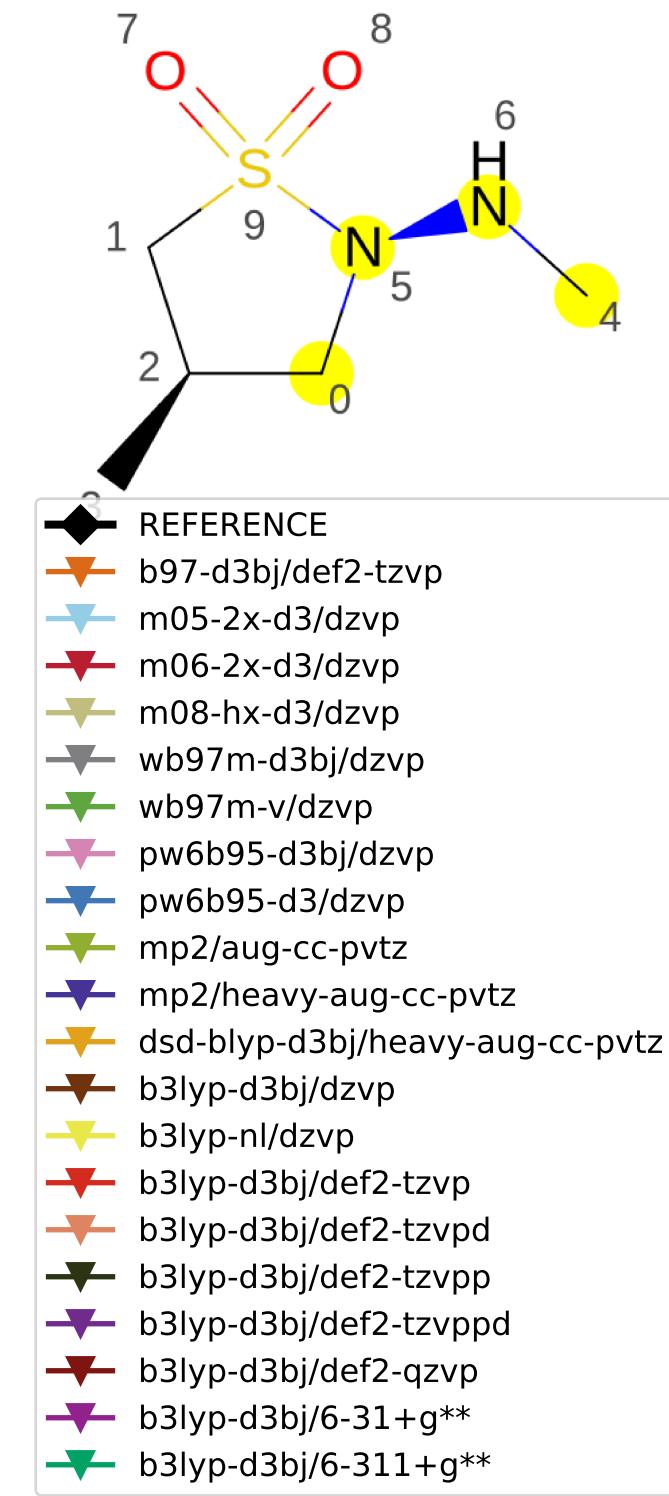
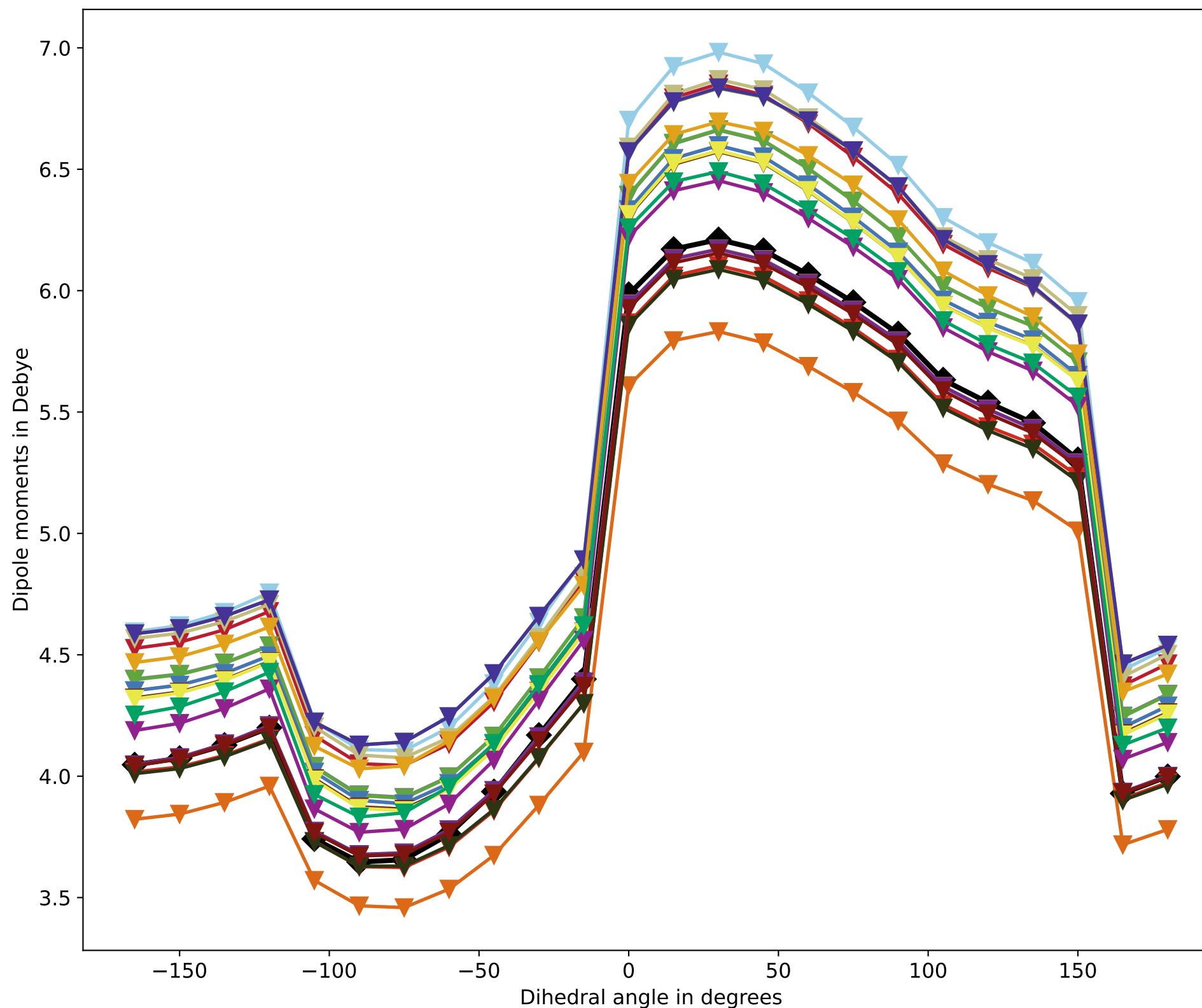


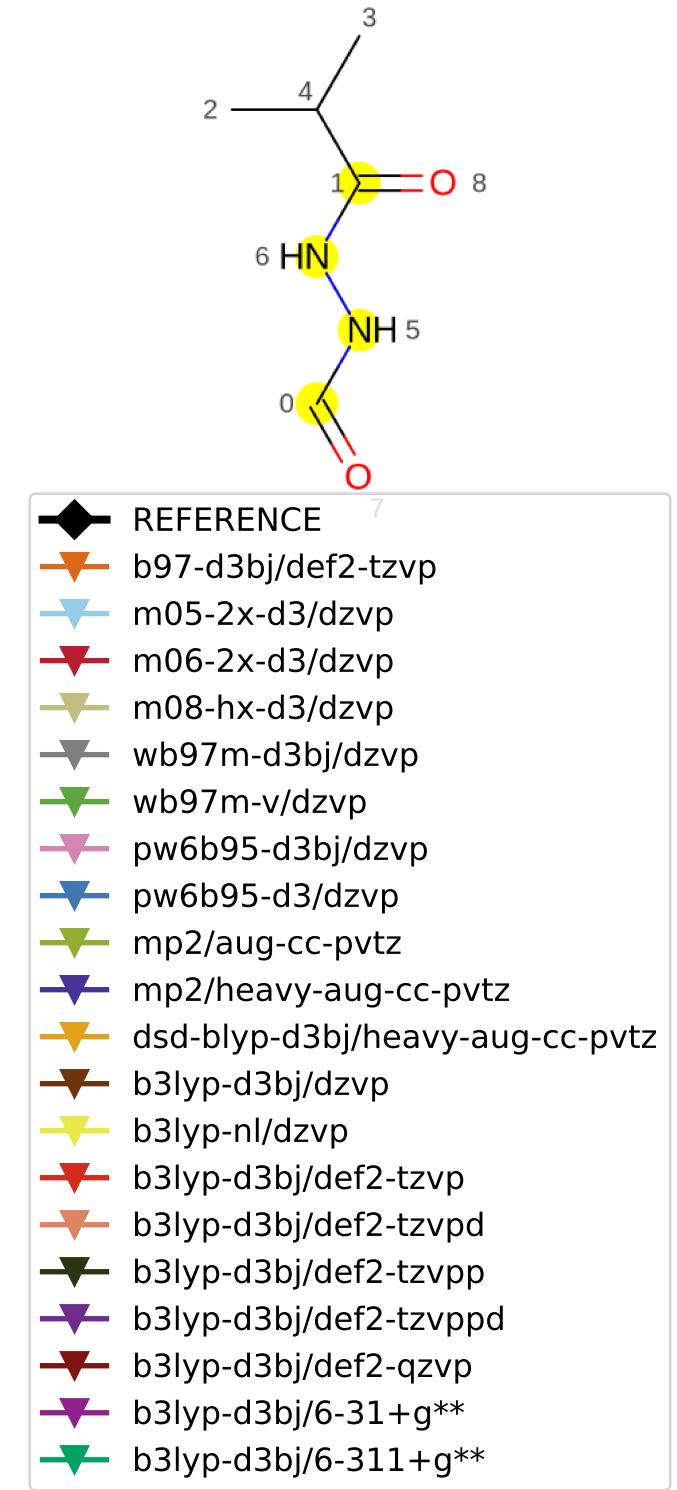
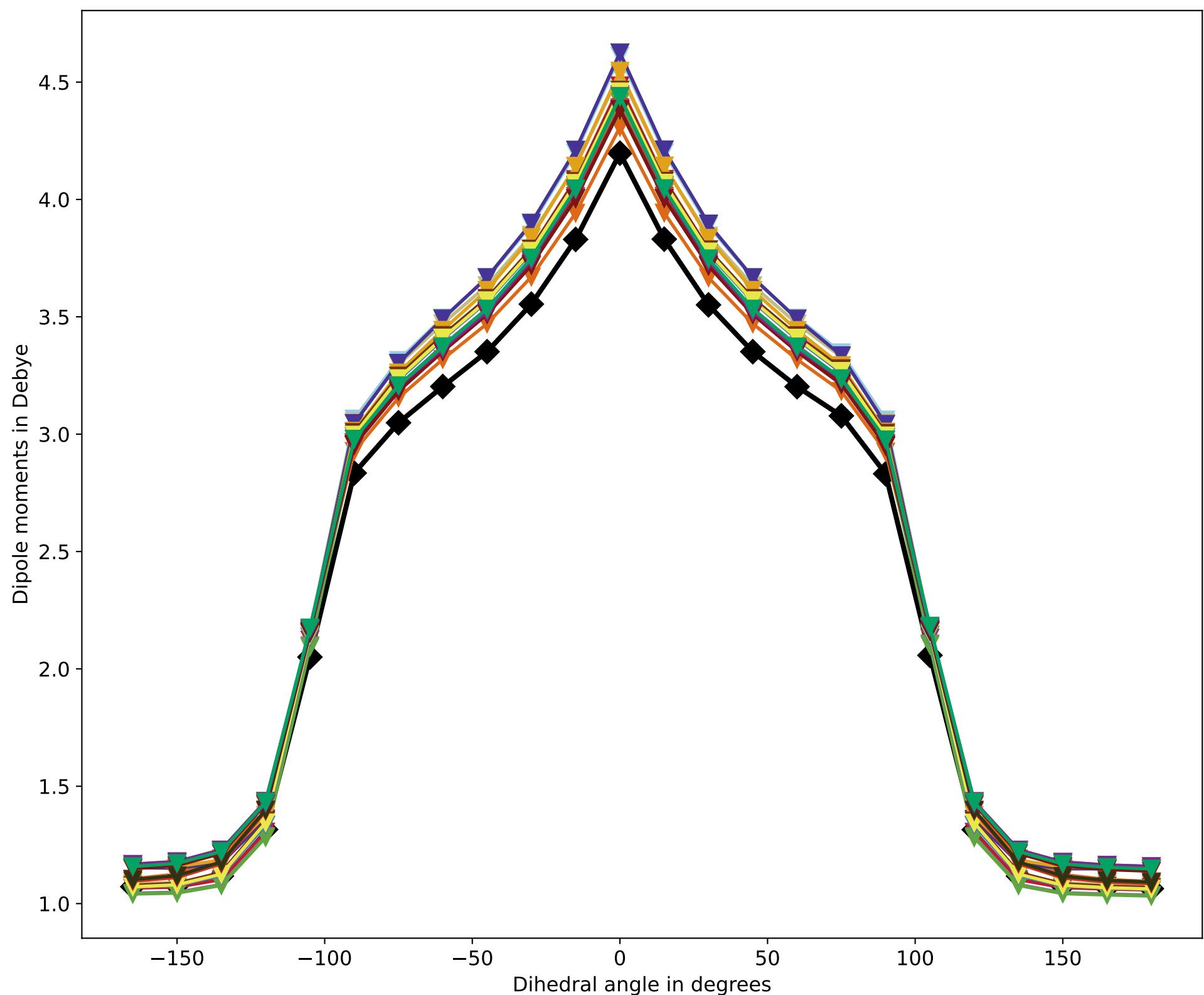
- ◆ REFERENCE
- ▼ b97-d3bj/def2-tzvp
- ▲ m05-2x-d3/dzvp
- ▼ m06-2x-d3/dzvp
- ▼ m08-hx-d3/dzvp
- ▼ wb97m-d3bj/dzvp
- ▼ wb97m-v/dzvp
- ▼ pw6b95-d3bj/dzvp
- ▼ pw6b95-d3/dzvp
- ▼ mp2/aug-cc-pvtz
- ▼ mp2/heavy-aug-cc-pvtz
- ▼ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ▼ b3lyp-d3bj/dzvp
- ▼ b3lyp-nl/dzvp
- ▼ b3lyp-d3bj/def2-tzvp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

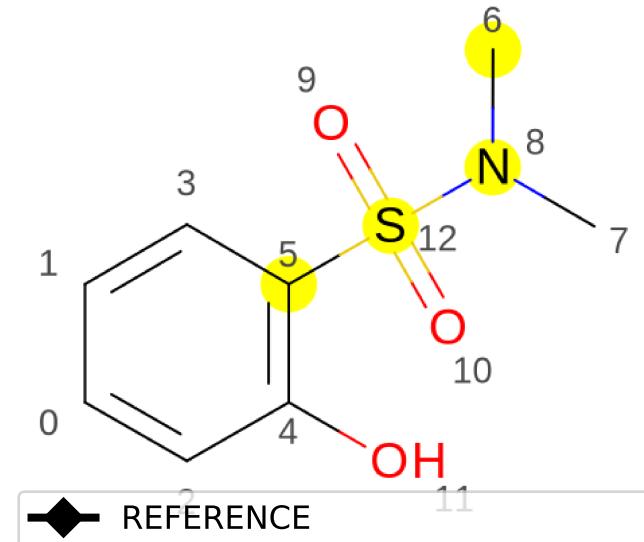
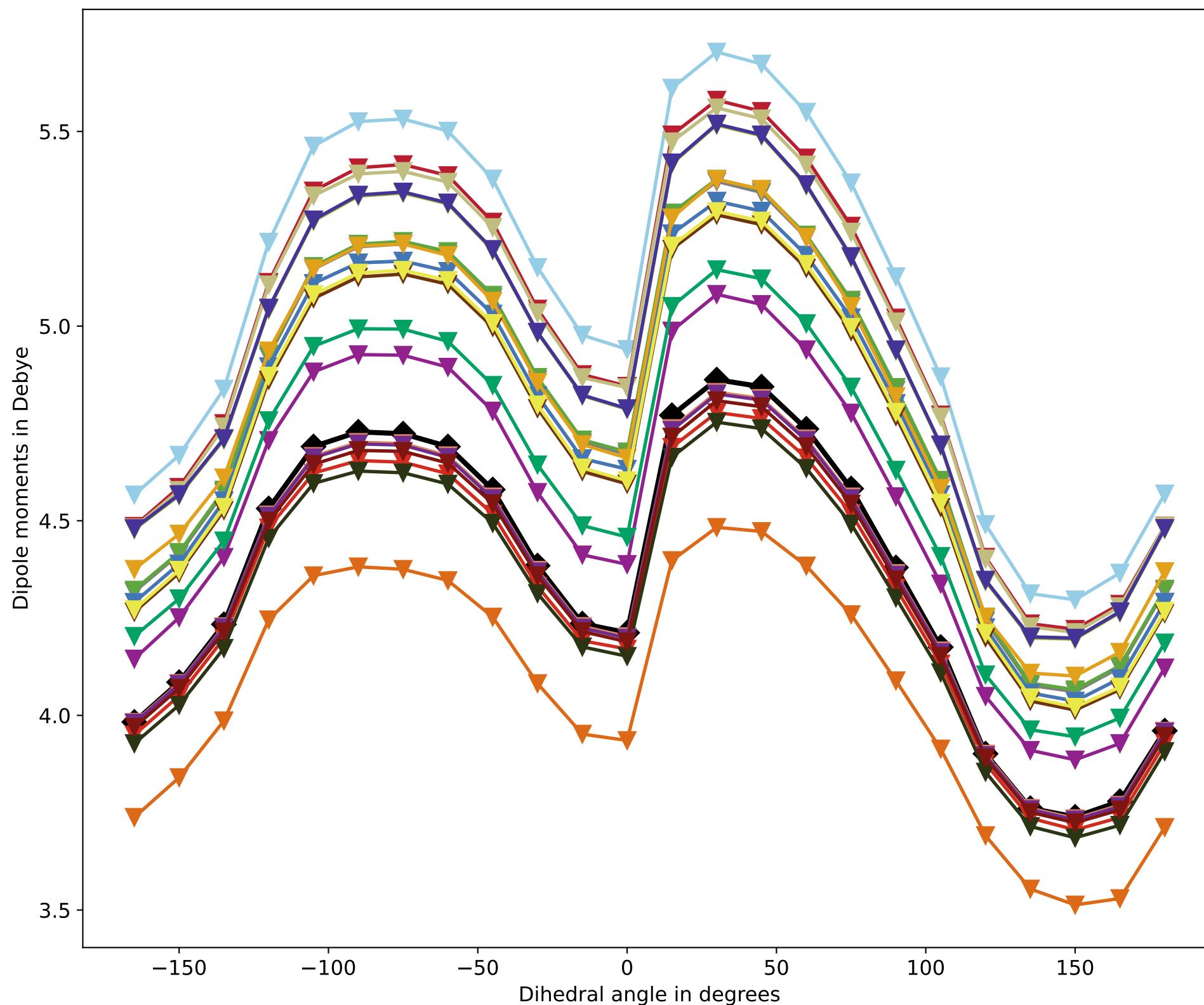




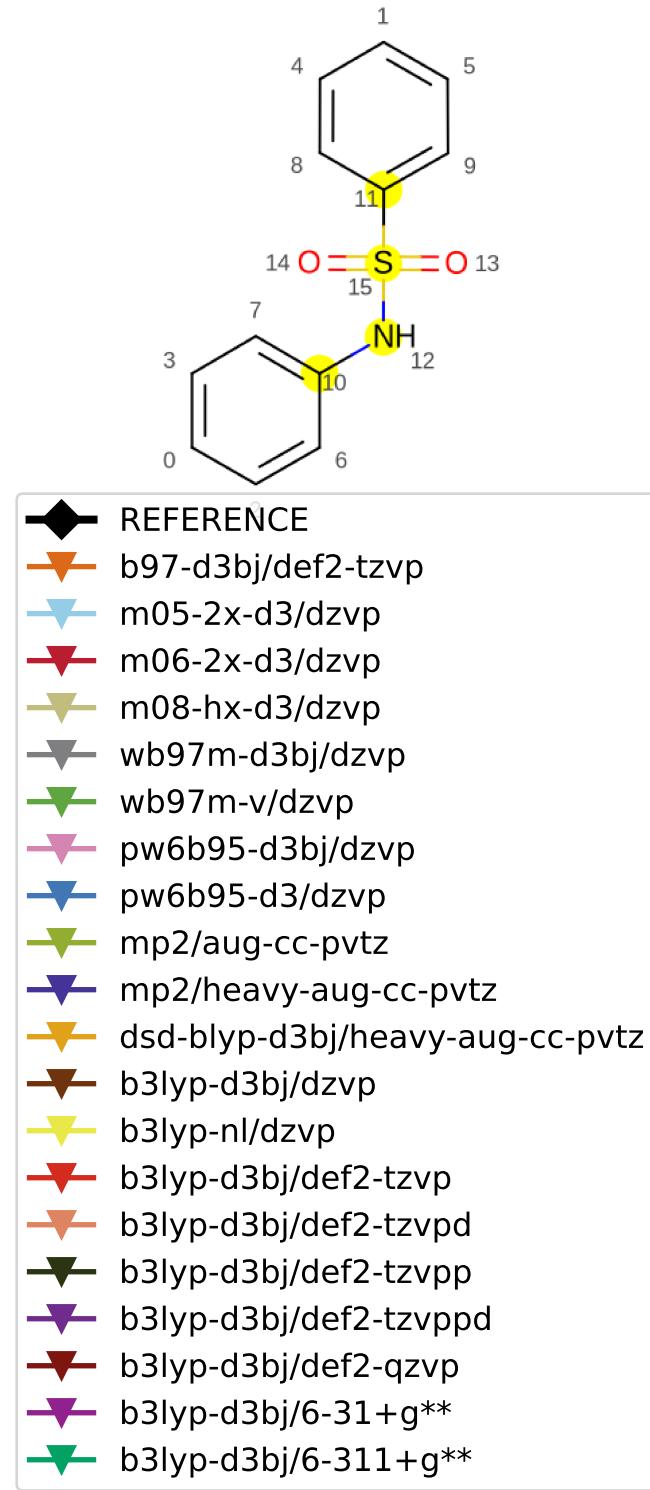
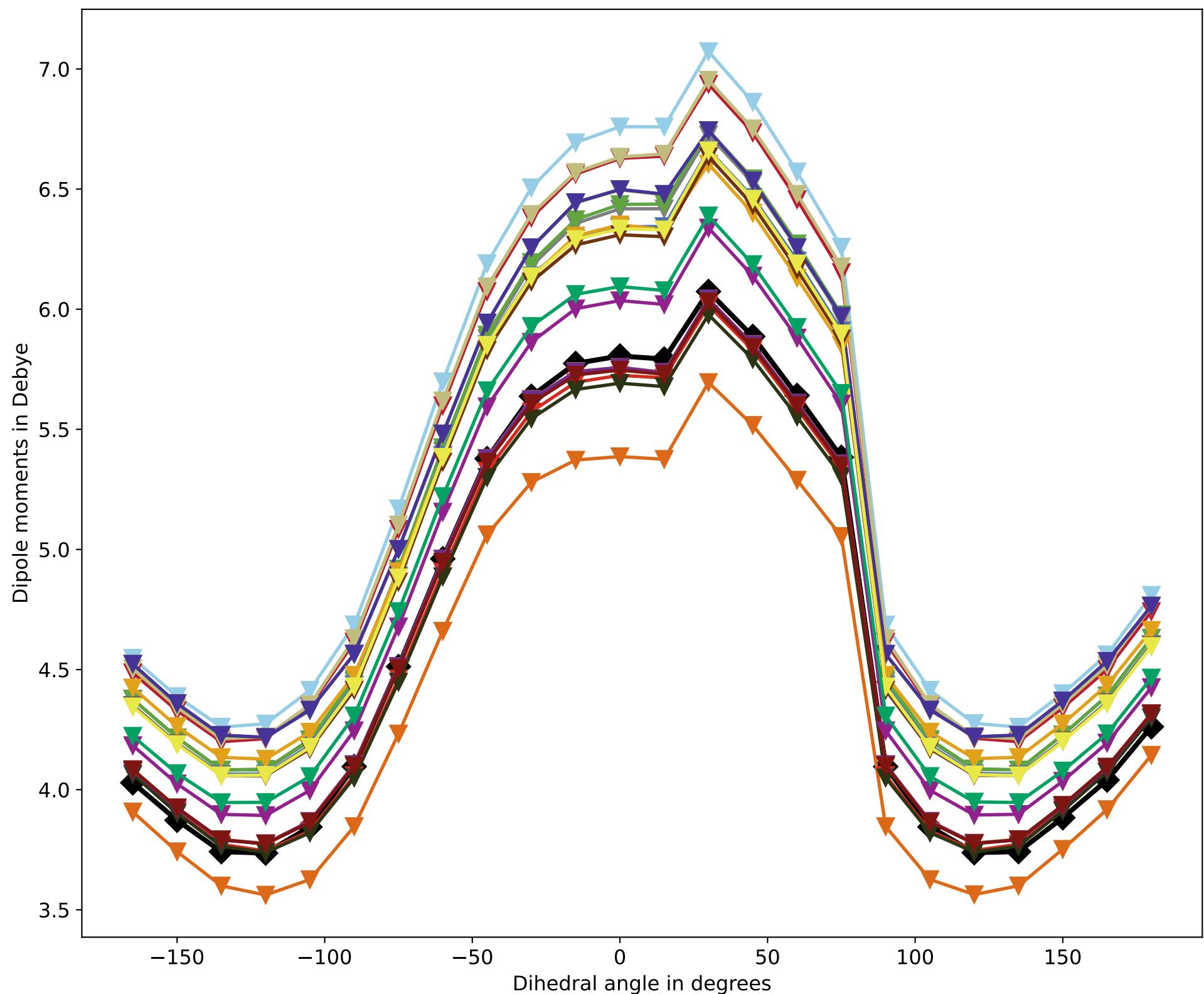
- | | |
|---|---------------------------------|
| ◆ | REFERENCE |
| ▼ | b97-d3bj/def2-tzvp |
| △ | m05-2x-d3/dzvp |
| ▲ | m06-2x-d3/dzvp |
| ◆ | m08-hx-d3/dzvp |
| ◆ | wb97m-d3bj/dzvp |
| ◆ | wb97m-v/dzvp |
| ◆ | pw6b95-d3bj/dzvp |
| ◆ | pw6b95-d3/dzvp |
| ◆ | mp2/aug-cc-pvtz |
| ◆ | mp2/heavy-aug-cc-pvtz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

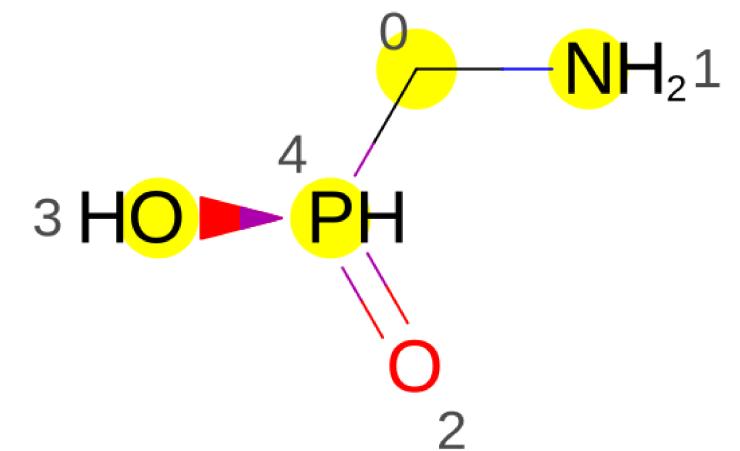
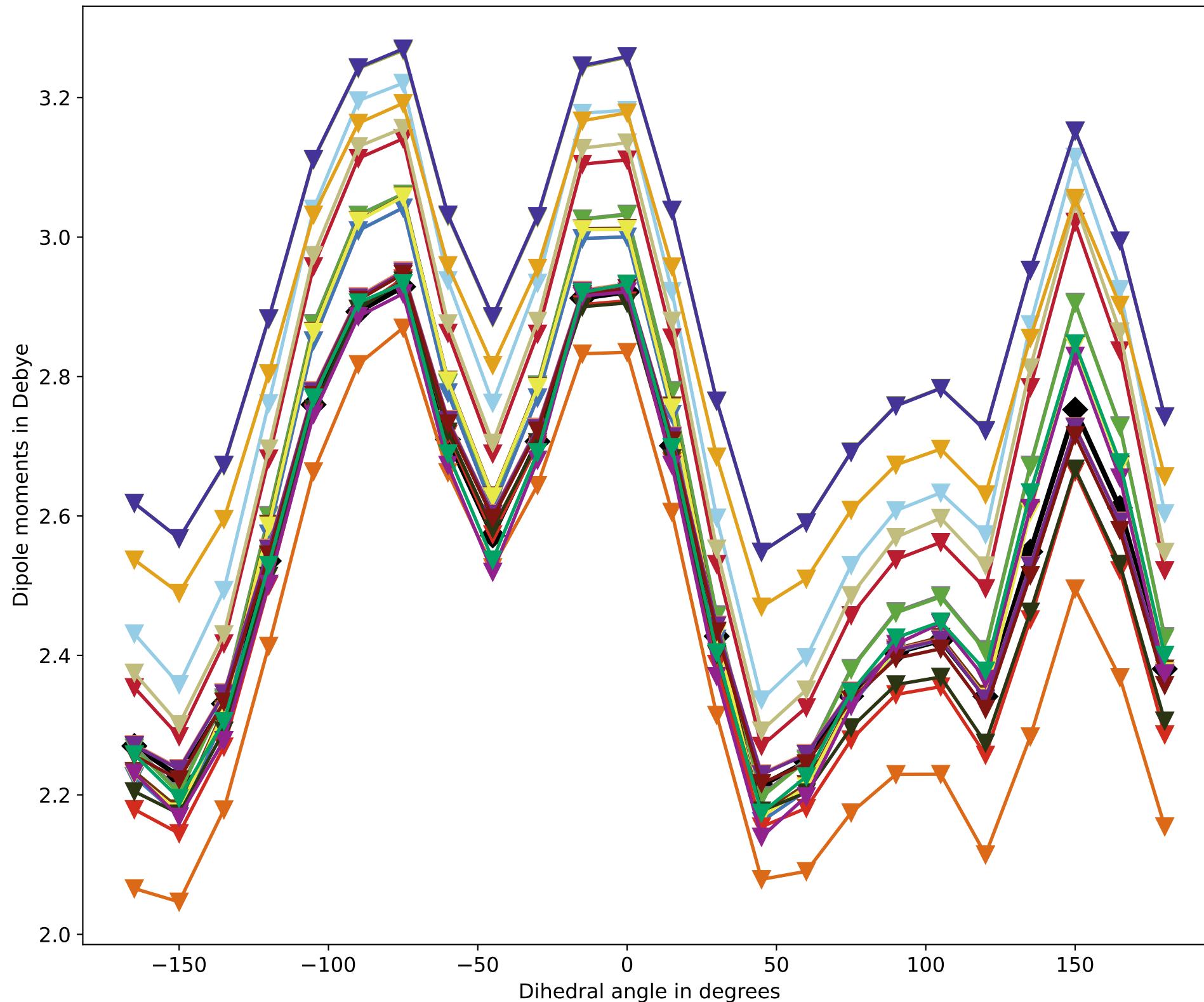




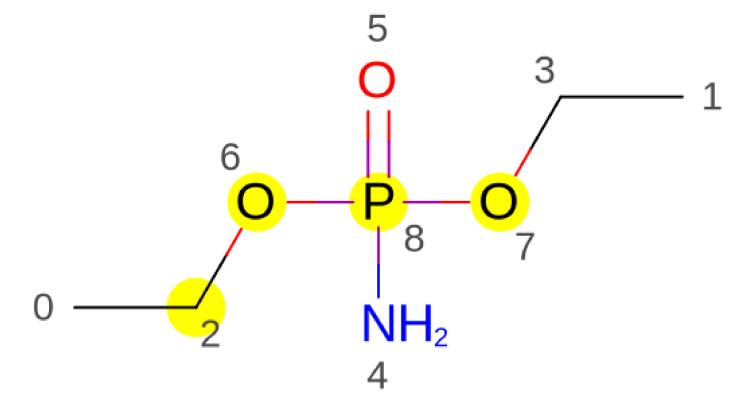
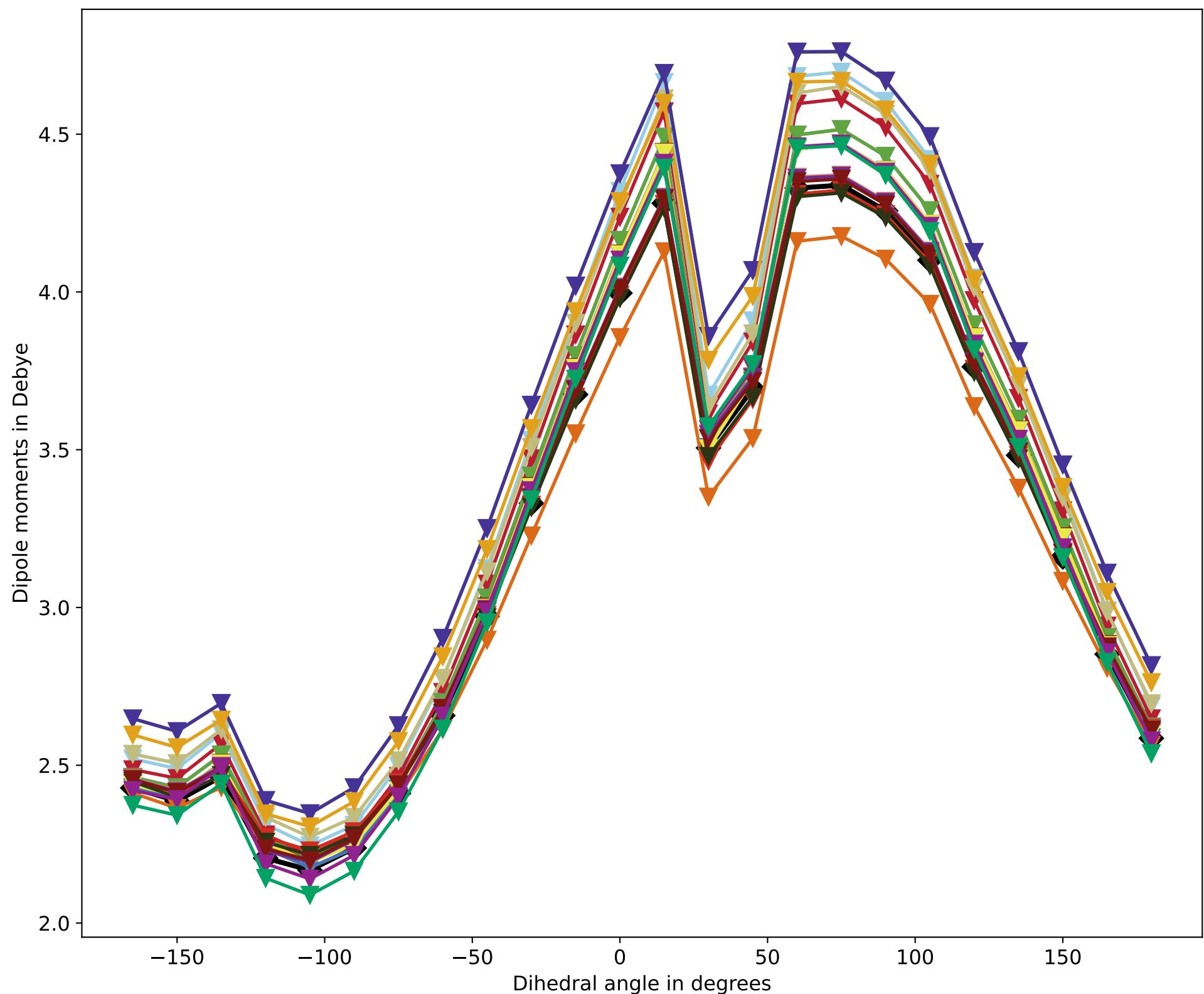


- Legend:
- REFERENCE
 - b97-d3bj/def2-tzvp
 - m05-2x-d3/dzvp
 - m06-2x-d3/dzvp
 - m08-hx-d3/dzvp
 - wb97m-d3bj/dzvp
 - wb97m-v/dzvp
 - pw6b95-d3bj/dzvp
 - pw6b95-d3/dzvp
 - mp2/aug-cc-pvtz
 - mp2/heavy-aug-cc-pvtz
 - dsd-blyp-d3bj/heavy-aug-cc-pvtz
 - b3lyp-d3bj/dzvp
 - b3lyp-nl/dzvp
 - b3lyp-d3bj/def2-tzvp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

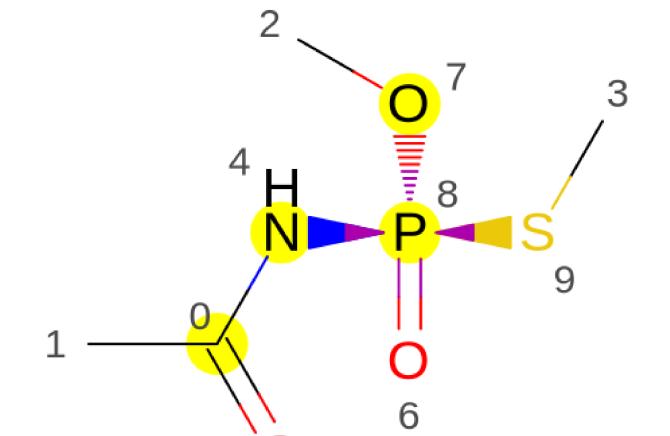
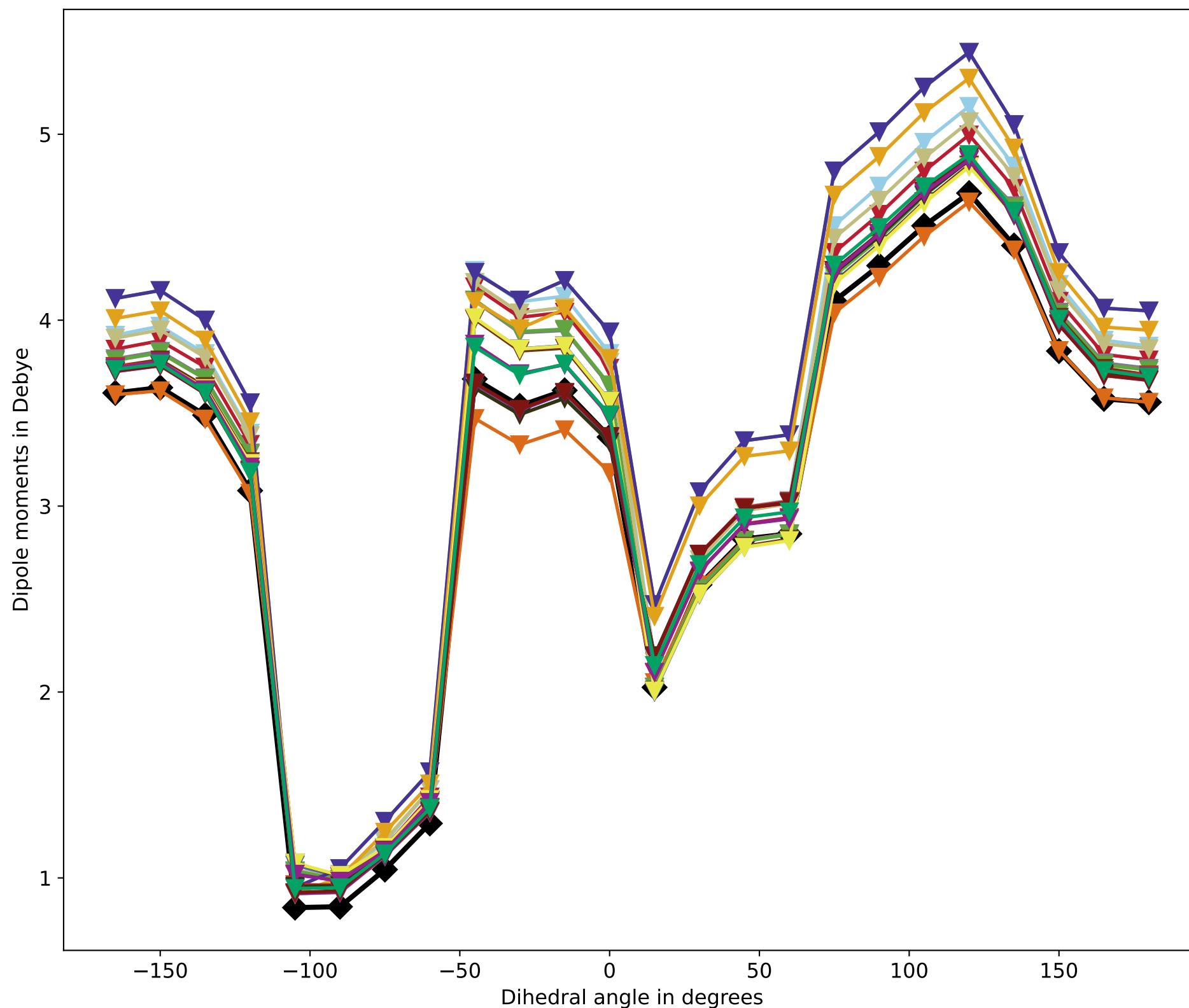




- ◆ REFERENCE
- ◆ b97-d3bj/def2-tzvp
- ◆ m05-2x-d3/dzvp
- ◆ m06-2x-d3/dzvp
- ◆ m08-hx-d3/dzvp
- ◆ wb97m-d3bj/dzvp
- ◆ wb97m-v/dzvp
- ◆ pw6b95-d3bj/dzvp
- ◆ pw6b95-d3/dzvp
- ◆ mp2/aug-cc-pvtz
- ◆ mp2/heavy-aug-cc-pvtz
- ◆ dsd-blyp-d3bj/heavy-aug-cc-pvtz
- ◆ b3lyp-d3bj/dzvp
- ◆ b3lyp-nl/dzvp
- ◆ b3lyp-d3bj/def2-tzvp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



- ◆ 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-tzvpd
- ◆ b3lyp-d3bj/def2-tzvpp
- ◆ b3lyp-d3bj/def2-tzvppd
- ◆ b3lyp-d3bj/def2-qzvp
- ◆ b3lyp-d3bj/6-31+g**
- ◆ b3lyp-d3bj/6-311+g**



- ◆ 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-tzvpd
- ◆ b3lyp-d3bj/def2-tzvpp
- ◆ b3lyp-d3bj/def2-tzvppd
- ◆ b3lyp-d3bj/def2-qzvp
- ◆ b3lyp-d3bj/6-31+g**
- ◆ b3lyp-d3bj/6-311+g**

Dihedral angle in degrees

