

prediction / literature value

7
6
5
4
3
2
1
0

230-b

- B3LYP
- M062X
- MP2
- PBE0
- cam-B3LYP
- wb97xd

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X