

prediction / literature value

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

2.5

2.0

1.5

1.0

0.5

0.0

TCF-1

TCF-3

TCF-2

x

x

x

x

x

x

x

x

x

x

x

x

x

x

x

x

x

x