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Transition states of helicenes

IOCB Prague - Ivo Starý group

Emma Tekulová

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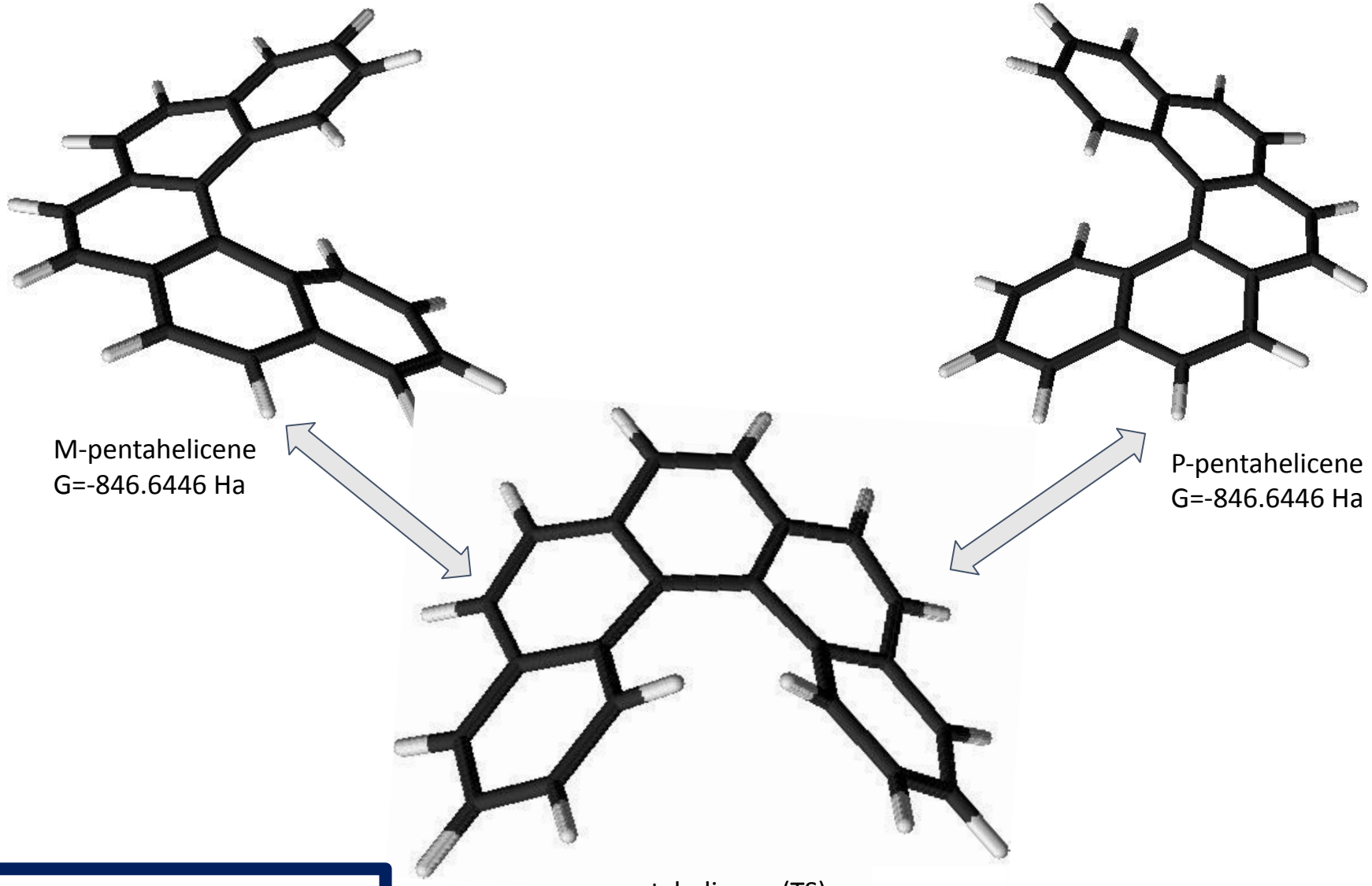
Pentahelicene



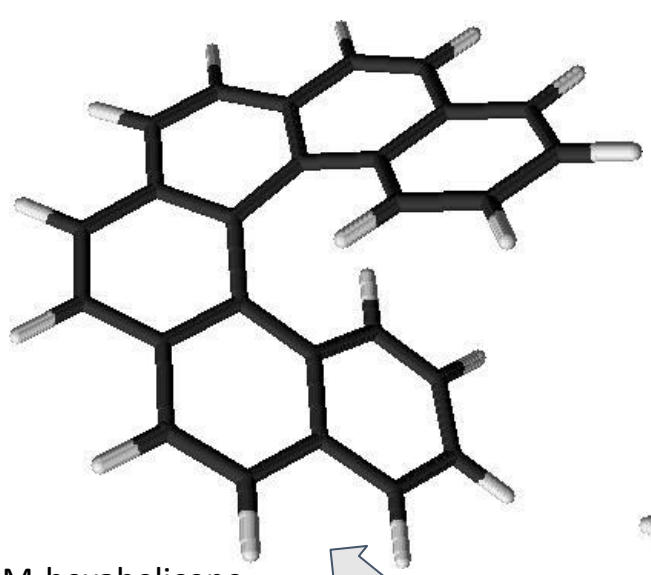
M-pentahelicene
G=-846.6446 Ha

P-pentahelicene
G=-846.6446 Ha

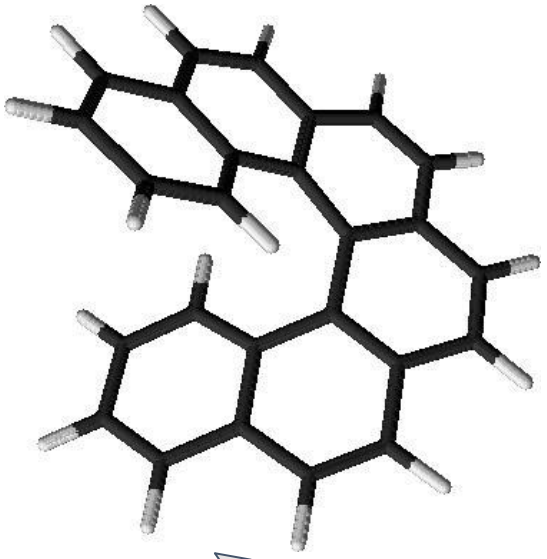
pentahelicene (TS)
G=-846.605407 Ha

B3LYP/cc-pVDZ
EmpiricalDispersion=GD3

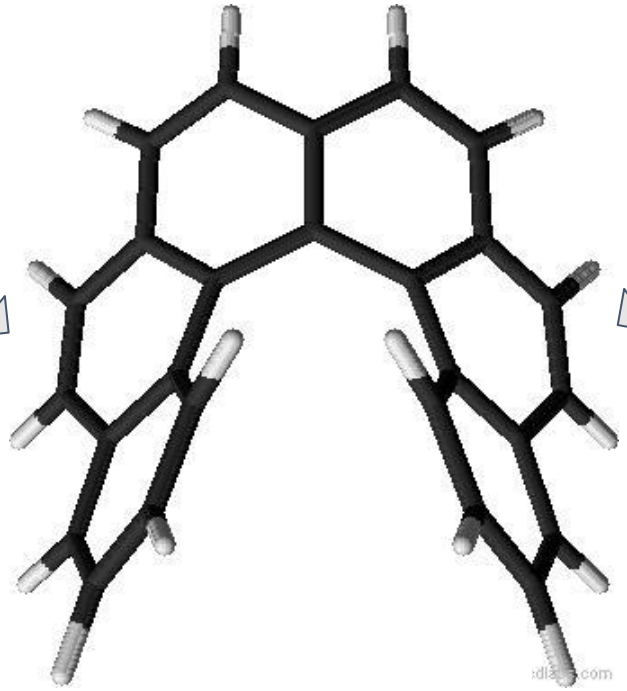
Hexahelicene



M-hexahelicene
G=-1000.256851 Ha



P-hexahelicene
G=-1000.256851Ha:w



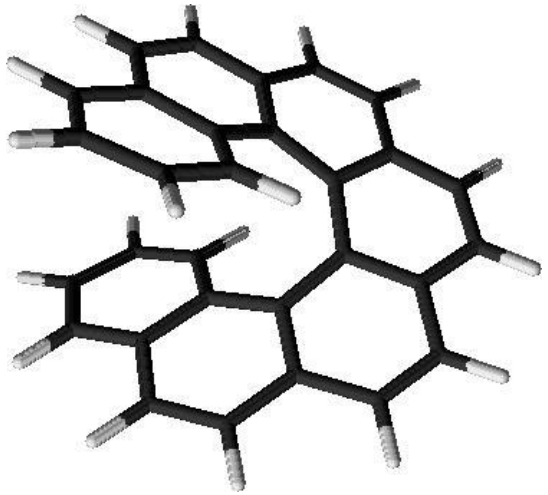
hexahelicene (TS)
G=-1000.196774 Ha

B3LYP/cc-pVDZ
EmpiricalDispersion=GD3

Heptahelicene

M-heptahelicene
G=-1153.869096 Ha

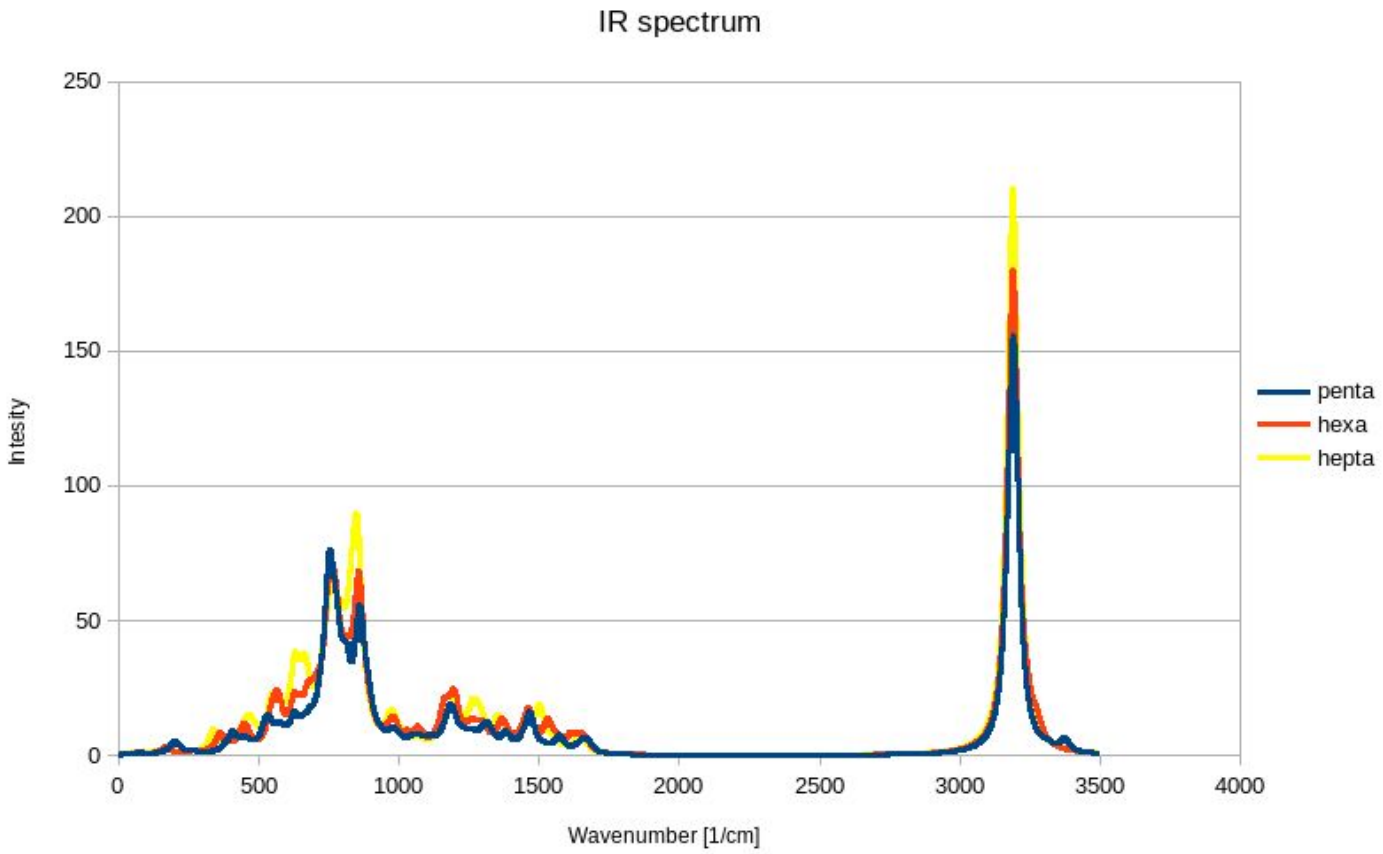
heptahelicene (TS)
G=-1153.800177 Ha



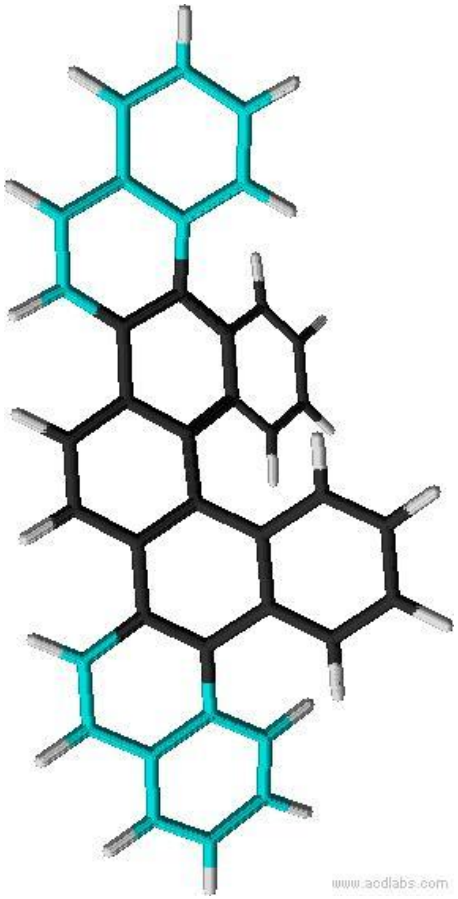
P-heptahelicene
G=-1153.869094 Ha

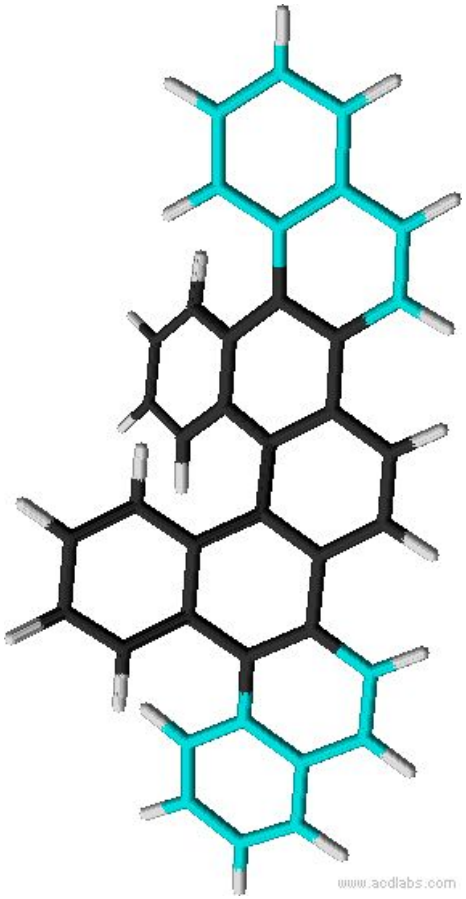
B3LYP/cc-pVDZ
EmpiricalDispersion=GD3

IR spectrum


IR spectrum
250
200
150
100
50
0
Intesity
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber [1/cm]
penta
hexa
hepta

Dinaphtho[5]helicene 3



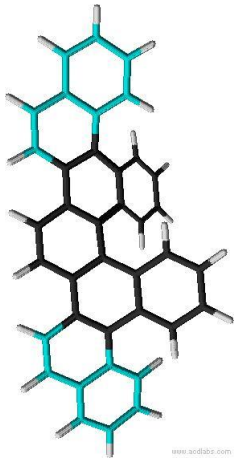


P-M-P-dinaphtho[5]helicene

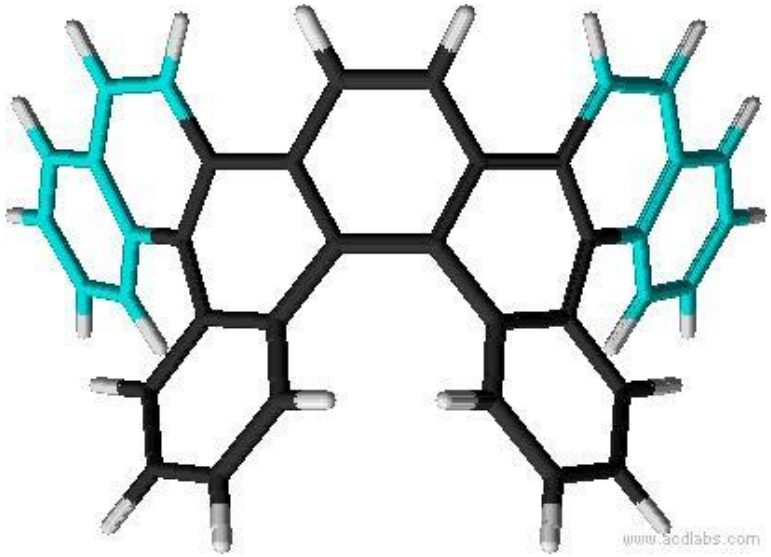
M-P-M-dinaphtho[5]helicene

B3LYP/cc-pVDZ
EmpiricalDispersion=GD3

Dinaphtho[5]helicene



P-M-P-dinaphtho[5]helicene
G=-1461.094760 Ha

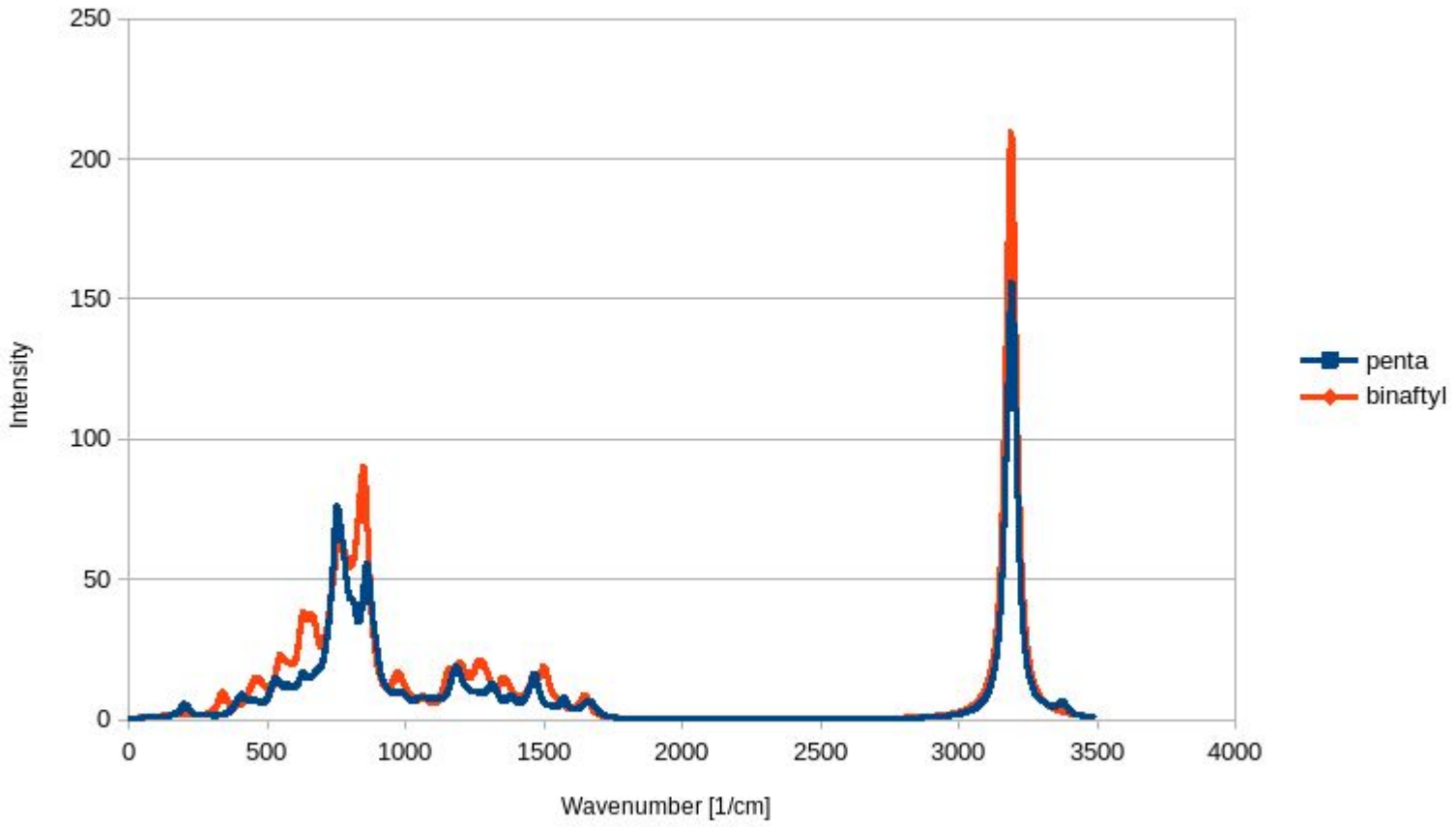


dinaphtho[5]helicene (TS
)G=-1461.053973 Ha

M-P-M-dinaphtho[5]helicene
G=-1461.094761 Ha

B3LYP/cc-pVDZ
EmpiricalDispersion=GD3

IR spectrum


250
200
150
100
50
0
Intensity
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber [1/cm]
penta
binaftyl

Plans

- calculate ECD spectrums
- calculate reaction path of racemization

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