

Relative Population

gpBTTT

pBTTT

pgT2_TT

0.0075
0.0050
0.0025
0.0000

-100

0

100

$\phi [^\circ]$

-100

0

100

-100

0

100

Method

- B3lyp/6-311+g(d,p)
- HF/aug-cc-pvdz
- MP2/aug-cc-pvdz
- wb97xd/6-311+g(d,p)

