|  |  |  |
| --- | --- | --- |
|  | My Full-CI | PySCF |
| H2 STO-3G | -1.079192944969 | -1.079192944969 |
| H2 6-31G | -1.111269880064 | -1.111269880064 |
| He2 STO-3G | -5.497612660169 | -5.497612660169 |
| He2 6-31G | -5.672662691270 | -5.633464683353 |
| HF STO-3G | -98.620456095434 | -98.595121449138 |

R = 1.1 au

After correcting the problem of sign

|  |  |  |
| --- | --- | --- |
|  | My Full-CI | PySCF |
| H2 STO-3G | -1.079192944969 | -1.079192944969 |
| H2 6-31G | -1.111269880064 | -1.111269880064 |
| He2 STO-3G | -5.497612660169 | -5.497612660169 |
| He2 6-31G | -5.633464683353 | -5.633464683353 |
| HF STO-3G | -98.595121449139 | -98.595121449138 |

R = 1.1 au