

```
%chk=test.chk
%mem=100MB
%nproc=1
# b3lyp/6-31g scf
```

Title Card Required

0 1

| | | | | | |
|----|---|----|---|----|---|
| C | | | | | |
| H | 1 | B1 | | | |
| H | 1 | B2 | 2 | A1 | |
| C | 1 | B3 | 3 | A2 | 2 |
| D1 | | | | | |
| H | 4 | B4 | 1 | A3 | 3 |
| D2 | | | | | |
| H | 4 | B5 | 1 | A4 | 3 |
| D3 | | | | | |

| | |
|----|--------------|
| B1 | 1.07000000 |
| B2 | 1.07000000 |
| B3 | 1.35520000 |
| B4 | 1.07000000 |
| B5 | 1.07000000 |
| A1 | 119.88652694 |
| A2 | 119.88652694 |
| A3 | 120.00000000 |
| A4 | 120.00000000 |
| D1 | 180.00000000 |
| D2 | -90.00000000 |
| D3 | 90.00000000 |