

Table: values of the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) energy levels (hartree)

Cd-CDCA1

| Species | HOMO | LUMO |
|---------|----------|---------|
| ES | -0.10254 | 0.05104 |
| TS1 | -0.07873 | 0.02946 |
| INT1 | -0.07928 | 0.03049 |
| TS4 | -0.08455 | 0.03609 |
| PROD | -0.08759 | 0.04438 |
| TS2 | -0.08142 | 0.03747 |
| INT2 | -0.09140 | 0.04477 |
| TS3 | -0.08696 | 0.04500 |

Zn-CDCA1

| Species | HOMO | LUMO |
|---------|----------|---------|
| ES | -0.09797 | 0.04991 |
| TS1 | -0.07168 | 0.03079 |
| INT1 | -0.07243 | 0.02837 |
| TS4 | -0.07667 | 0.03329 |
| PROD | -0.07336 | 0.03004 |
| TS2 | -0.08472 | 0.04602 |
| INT2 | -0.08268 | 0.04498 |
| TS3 | -0.07827 | 0.04374 |