

Table S2: Frequencies of Transition states

TS1

| Mode # | Freq | Infrared |
|--------|---------|-----------|
| 1 | -842.67 | 1046.7297 |

TS2

| Mode # | Freq | Infrared |
|--------|----------|-----------|
| 1 | -2197.37 | 2162.0733 |

TS3

| Mode # | Freq | Infrared |
|--------|---------|----------|
| 1 | -433.46 | 995.5108 |

TS4

| Mode # | Freq | Infrared |
|--------|----------|-----------|
| 1 | -1151.23 | 1221.3764 |