|  |  |  |  |
| --- | --- | --- | --- |
|  | **S1** | **S4** | **S3** |
| **HOMO** | -5.515 | -5.485 | -5.213 |
| **LUMO** | -1.204 | -1.217 | -1.288 |
| **Dipole moment** | 4.9558 | 5.3427 | 9.7960 |