Structure 4 cis Ionisation potentials

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Name | Image | Abs. energy | Rel. energy among neutrals | Geometry | Ionization energy | Name | Image | Abs. energy | Rel. energy among ions | Geometry |
| Conformer 1 (neutral) |  | -287.290001 | 16.87 | 15-6-4-11 = -67°  5-4-1-2 = 130° | 8.57 | Conformer 1 (ion) |  | -286.975132 | 0.45 | 15-6-4-11 = 19°  5-4-1-2 = 94° |
| Conformer 2 (neutral) |  | -287.291471 | 13.01 | 15-6-4-11 = 51°  5-4-1-2 = 102° | 8.61 |
| Conformer 3 (neutral) |  | -287.294833 | 4.19 | 15-6-4-11 = 179°  5-4-1-2 = -169° | 8.69 | Conformer 2 (ion) |  | -286.975303 | 0.0 | 15-6-4-11 = -152°  5-4-1-2 = 159° |
| Conformer 4 (neutral) |  | -287.290397 | 15.83 | 15-6-4-11 = -56°  5-4-1-2 = -95° | 8.57 |
| Conformer 5 (neutral) |  | -287.296426 | 0.0 | 15-6-4-11 = 156°  5-4-1-2 = -97° | 8.74 |