Structure 4 Ionisation potentials

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| Name | Image | Abs. energy, hartree | Rel. energy among neutrals, kJ/mol | Geometry | Ionization energy, eV | Name | Image | Abs. energy, hartree | Rel. energy among ions, kJ/mol | Geometry |
| Conformer 1 b(neutral) |  | -287.300967 | 1.26 | 15-6-4-11 = 46°  5-4-1-2 = 115° | 8.86 | Conformer 1 b(ion) |  | -286.975289 | 0.0 | 15-6-4-11 = 18°  5-4-1-2 = 100° |
| Conformer 2 f(neutral) |  | -287.298798 | 6.95 | 15-6-4-11 = 83°  5-4-1-2 = -26° | 8.8 |
| Conformer 3 a(neutral) |  | -287.301446 | 0.0 | 15-6-4-11 = 167°  5-4-1-2 = -116° | 8.88 | Conformer 2 d(ion) |  | -286.975127 | 0.43 | 15-6-4-11 = -154°  5-4-1-2 = 148° |
| Conformer 4 c(neutral) |  | -287.300607 | 2.21 | 15-6-4-11 = -165°  5-4-1-2 = 130° | 8.86 |
| Conformer 5 e(neutral) |  | -287.299753 | 4.45 | 15-6-4-11 = -64°  5-4-1-2 = 124° | 8.83 |
| Conformer 6 g(neutral) |  | -287.296805 | 12.19 | 15-6-4-11 = -73°  5-4-1-2 = -124° | 8.75 |
| Conformer 7 d(neutral) |  | -287.300268 | 3.1 | 15-6-4-11 = 74°  5-4-1-2 = -113° | 8.91 | Conformer 3 e(ion) |  | -286.972781 | 6.59 | 15-6-4-11 = 40°  5-4-1-2 = -136° |