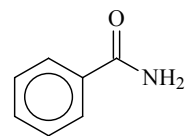


796 **C₇H₇NO****Benzamide****C₁**ED, *ab initio*
calculations

| r_g | Å ^{a)} | θ_α | deg ^{a)} |
|--------------------------|---------------------|------------------------|---------------------|
| C(1)–C(7) | 1.511(5) | C–C=O | 121.2(17) |
| C–C (ring) ^{b)} | 1.401(2) | C–C–N | 117.8(16) |
| C=O | 1.225(3) | N–C=O | 121.0 ^{c)} |
| C–N | 1.380(11) | C(2)–C(1)–C(7) | 118.2(17) |
| C–H ^{b)} | 1.112(7) | C–C–C (ring) | 120.0 ^{d)} |
| N–H ^{b)} | 1.022 ^{c)} | C–C–H (ring) | 120.0 ^{d)} |
| | | C(7)–N–H(10) | 114.7 ^{f)} |
| | | C(7)–N–H(11) | 118.9 ^{f)} |
| | | τ_1 ^{g)} | 19(5) |
| | | τ_2 ^{h)} | 171.1 ^{f)} |



The skeleton of the amide group was assumed to be planar.
The nozzle temperature was 445 K.

^{a)} Three times the estimated standard errors.

^{b)} Average value.

^{c)} Dependent parameter.

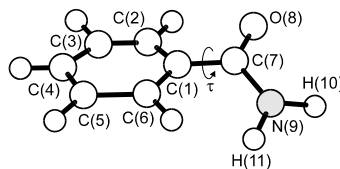
^{d)} Assumed.

^{e)} Assumed at the value for acetamide.

^{f)} Assumed at the value from MP2/6-31G* calculations.

^{g)} C(2)–C(1)–C(7)=O torsional angle from the *syn* position.

^{h)} C(1)–C(7)–N–H(10) torsional angle from the *syn* position.



Takeuchi, H., Sato, M., Tsuji, T., Takashima, H., Egawa, T., Konaka, S.: J. Mol. Struct. **485-486** (1999) 175.