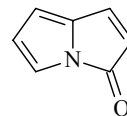
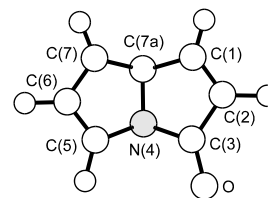


784 **C₇H₅NO**ED, *ab initio* and DFT
calculations**3H-Pyrrolizin-3-one**possibly C_s (see comment)

| $r_{\text{hl}}^{\text{a})}$ | $\text{\AA}^{\text{b})}$ | $\theta_{\text{hl}}^{\text{a})}$ | deg ^{b)} |
|-----------------------------|--------------------------|----------------------------------|-------------------|
| C(7)=C(7a) | 1.395(5) | O=C(3)–N(4) | 124.4(9) |
| C(6)–C(7) | 1.439(4) | C(5)–N(4)–C(7a) | 108.7(7) |
| C(5)=C(6) | 1.394(7) | C(3)–N(4)–C(5) | 137.5(6) |
| C(1)–C(7a) | 1.461(3) | C(3)–N(4)–C(7a) | 111.17(10) |
| C(1)=C(2) | 1.363(10) | C(7)=C(7a)–N(4) | 107.7(4) |
| C(2)–C(3) | 1.498(3) | C(1)–C(7a)–N(4) | 107.6(4) |
| N(4)–C(5) | 1.389(7) | C(1)–C(7a)=C(7) | 141.8(6) |
| N(4)–C(7a) | 1.380(7) | H–C(5)–N(4) | 121.5(5) |
| N(4)–C(3) | 1.437(4) | H–C(7)=C(7a) | 126.73(10) |
| C(3)=O | 1.215(4) | H–C(1)–C(7a) | 124.9(5) |
| C–H (average) | 1.090(4) | H–C(6)=C(5) | 125.4(5) |
| | | H–C(2)=C(1) | 128.5(5) |

The butterfly angle between the planes of the two rings was determined in the ED analysis to be between *ca.* 6 and 19°. It was difficult to assess whether the nonplanarity is an artifact of the refinement procedure (*i.e.*, as a result of the harmonicity of the force field used) or a structural fact. Differences between the C–C and C–N bond lengths were restrained to the values from B3LYP/6-311+G* or MP2/6-311+G* calculations. According to the results of the force field calculations by the B3LYP/6-311+G* method, the molecule is planar. The nozzle temperature was 78...100 °C.



^{a)} Curvilinear motions of the atoms were taken into account.

^{b)} Estimated standard errors.

Blockhuys, F., Hinchley, S.L., Robertson, H.E., Blake, A.J., McNab, H., Despinoy, X.L.M., Harris, S.G., Rankin, D.W.H.: J. Chem. Soc., Perkin Trans. 2 (2001) 2195.