Crystal structure of (4*SR*,4*aSR*)-1-acetyl-4-hydroxy-4,8-dimethyl-1,2,3,4,4*a*,7-hexahydroquinoline, C₁₃H₁₉NO₂

S. Gross^I, I. Brüdgam^{II}, H. Hartl^{*II} and H.-U. Reißig^I^I Freie Universität Berlin, Institut für Chemie - Organische Chemie, Takustr. 3, D-14195 Berlin, Germany^{II} Freie Universität Berlin, Institut für Chemie - Anorganische Chemie, Fabeckstr. 34–36, D-14195 Berlin, Germany

Received December 18, 2003, accepted and available on-line February 5, 2004; CCDC no. 1267/1193

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
N(1)	4e	0.6136(2)	0.31472(7)	0.2931(2)	0.0214(5)	0.0225(5)	0.0246(6)	0.0039(4)	0.0044(4)	−0.0021(4)
O(1)	4e	0.0931(2)	0.32409(7)	0.2052(2)	0.0238(5)	0.0426(7)	0.0334(6)	−0.0090(5)	0.0129(4)	−0.0046(5)
O(2)	4e	0.8003(2)	0.22098(7)	0.4327(2)	0.0326(6)	0.0330(6)	0.0397(7)	0.0129(5)	0.0023(5)	0.0015(5)
C(2)	4e	0.5052(2)	0.26004(9)	0.1697(2)	0.0266(7)	0.0255(7)	0.0275(7)	0.0035(5)	0.0049(6)	−0.0060(5)
C(3)	4e	0.3257(2)	0.25439(8)	0.1739(2)	0.0279(7)	0.0222(6)	0.0263(7)	−0.0026(5)	0.0057(6)	−0.0023(5)
C(4)	4e	0.2365(2)	0.33274(8)	0.1599(2)	0.0197(6)	0.0257(6)	0.0220(6)	−0.0018(5)	0.0072(5)	−0.0004(5)
C(4A)	4e	0.3638(2)	0.38959(8)	0.2861(2)	0.0205(6)	0.0227(6)	0.0229(6)	−0.0003(5)	0.0083(5)	−0.0020(5)
C(5)	4e	0.2869(2)	0.46879(9)	0.2689(2)	0.0248(7)	0.0277(7)	0.0433(9)	0.0029(5)	0.0163(6)	−0.0047(6)
C(6)	4e	0.3614(2)	0.53145(9)	0.2418(2)	0.0333(8)	0.0240(7)	0.053(1)	0.0050(6)	0.0189(8)	−0.0024(7)
C(7)	4e	0.5333(2)	0.5305(1)	0.2298(3)	0.0357(9)	0.0230(7)	0.062(1)	−0.0001(6)	0.0238(8)	0.0031(7)
C(8)	4e	0.6151(2)	0.45212(9)	0.2463(2)	0.0238(6)	0.0265(7)	0.0349(8)	0.0012(5)	0.0127(6)	0.0009(6)
C(8A)	4e	0.5388(2)	0.39032(8)	0.2763(2)	0.0192(6)	0.0217(6)	0.0221(6)	0.0022(5)	0.0061(5)	−0.0018(5)
C(9)	4e	0.7540(2)	0.28908(9)	0.4228(2)	0.0214(6)	0.0316(7)	0.0257(7)	0.0046(5)	0.0063(5)	0.0004(5)
C(41)	4e	0.1745(2)	0.3641(1)	−0.0118(2)	0.0265(7)	0.0376(8)	0.0228(7)	0.0013(6)	0.0051(5)	0.0036(6)
C(91)	4e	0.8519(2)	0.3450(1)	0.5553(2)	0.0279(7)	0.0434(9)	0.0311(8)	0.0052(7)	−0.0003(6)	−0.0082(7)
C(81)	4e	0.7860(2)	0.4505(1)	0.2301(3)	0.0321(8)	0.0410(9)	0.064(1)	0.0004(7)	0.0285(9)	0.0069(9)

Acknowledgments. Support of this work by the Schering Research Foundation, the Volkswagen-Stiftung and the Fonds der Chemischen Industrie is gratefully acknowledged.

References

1. Gross, S.; Reissig, H.-U.: Samarium Diiodide-Induced Diastereoselective Synthesis of Hexahydroquinoline Derivatives. *Synlett* (2002) 2027-2030.
2. Gross, S.: Samariumdiiodid-induzierte Cyclisierungen zu *N*-Heterocyclen - Neue Möglichkeiten für die Alkaloidsynthese. Dissertation, Freie Universität Berlin (2003).
3. Sheldrick, G. M.: Phase Annealing in SHELX-90: Direct Methods for Larger Structures. *Acta Crystallogr. A* **46** (1990) 467-473.
4. Sheldrick, G. M.: SHELXL-97. A Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
5. Spek, A. L.: PLATON - A Multipurpose Crystallographic Tool. Utrecht University, The Netherlands 1998.