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§ The data (without structure factors) should be sent by email to deposit@ccdc.cam.ac.uk as an ASCII file, preferably in CIF format. The CIF file must be validated before deposition using *Checkcif*, available at the IUCR website (www.iucr.org). Hard copy data should be sent to CCDC, 12 Union Road, Cambridge, CB2 1EZ, England. A checklist of data items for deposition can be obtained from the CCDC Home Page on the World Wide Web (<http://www.ccdc.cam.ac.uk/>) or by e-mail (to fileserv@ccdc.cam.ac.uk with the one-line message: send me checklist).

\*\* Ab initio electronic structure calculations: J. E. Boggs, *Pure Appl. Chem.* **1998**, *70*, 1015; <http://www.iupac.org/reports/1998/7004boggs/index.html>. Force-field calculations: D. J. Raber, W. C. Guida, *Pure Appl. Chem.* **1998**, *70*, 2047; <http://www.iupac.org/reports/1998/7010raber/index.html>.