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Molecular Mechanics: The Cross-conjugated Carbonyl group in Heterocyclic Compounds

1. Parameterisation (MM2) of the $>\text{C}=\text{O}$ bond

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An uncorrected version of Table 5 was printed in the above-titled paper. In accordance with the plain text, it should be read that, for the C(44)=O(7) bond, the respective values of the parameters TSLOPE and SSLOPE are 0.662 Å and 25.35 mdyn·Å⁻¹.

The online version of the original article can be found at <http://link.springer.de/link/service/journals/00894/papers/8004012/80040405.pdf>

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