Synthesis and Structure of 2,6-Diazidotrichloropyridine *N*-Oxide

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Abstract—Pentachloropyridine *N*-oxide readily reacted with sodium azide in aqueous acetone at room temperature to produce 2,6-diazidotrichloropyridine *N*-oxide in high yield. The molecular and crystalline structures of the product were studied in detail by X-ray analysis and quantum-chemical calculations. Unusual geometric parameters of the azido groups and reactivity of the diazide were rationalized by the presence of strong intramolecular contacts N⋯O with an energy of ~6.1 kcal/mol.

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