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Quantum-chemical calculation of 1-bis(dimethylamino)-4-bis(trimethylsilyl)-2,3-diphospha-1,3-butadiene

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Abstract

According to the results of ab initio quantum-chemical calculation 1-bis(dimethylamino)-4-bis(trimethylsilyl)-2,3-diphosphabuta-1,3-diene exists as an E-isomer where electronic delocalization occurs involving donor dimethylamino and acceptor trimethylsilyl groups and also the multiple P=C bonds.

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