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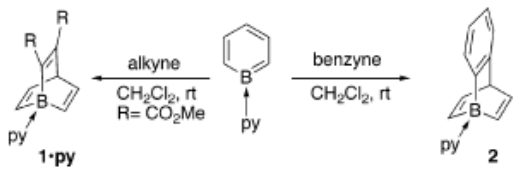
Citation:

1-Borabarrelene Derivatives via Diels-Alder Additions to Borabenzenes
Thomas K. Wood, Warren E. Piers, Brian A. Keay, and Masood Parvez
pp 2875 - 2878

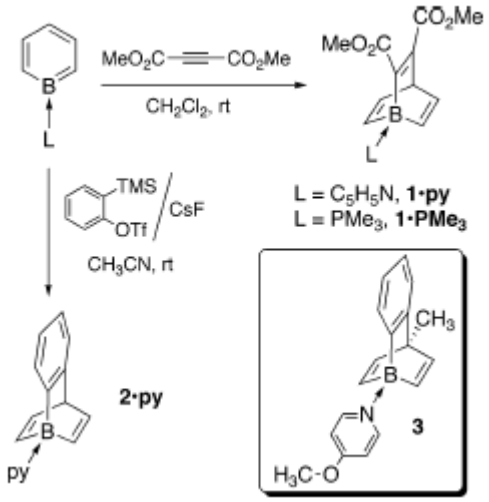
Abstract:



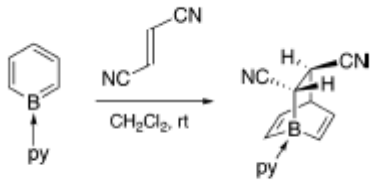
Borabenzene reacts with strong dienophiles such as dimethylacetylenedicarboxylate or benzyne to afford substituted borabarrelenes and borabenzobarrelene, respectively. The resultant Diels–Alder adducts display high stability due to increased Lewis acidity at boron.

Schemes:

Scheme 1



Scheme 2



4·py

Figures:

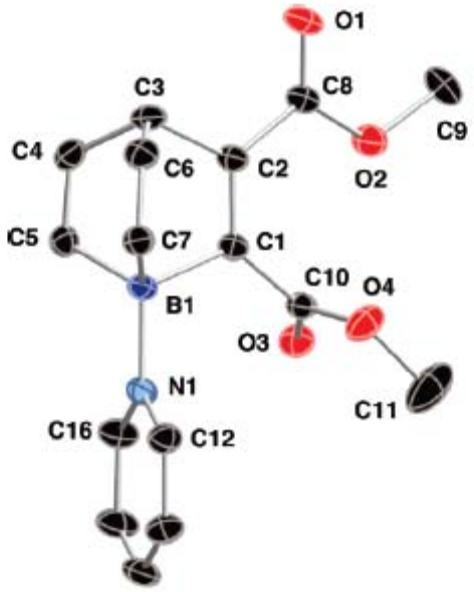


Figure 1. Thermal ellipsoid diagram of **1**·py (50%), with hydrogens omitted. Selected bond distances (Å): B(1)−N(1), 1.584-(3); B(1)−C(1), 1.646(3); B(1)−C(5), 1.624(3); B(1)−C(7), 1.616-(3); C(1)−C(2), 1.348(3); C(4)−C(5), 1.322(3); C(6)−C(7), 1.326-(3). Selected bond angles (deg): C(1)−B(1)−C(5), 103.01(15); C(1)−B(1)−C(7), 103.35(17); C(5)−B(1)−C(7), 105.66(17).

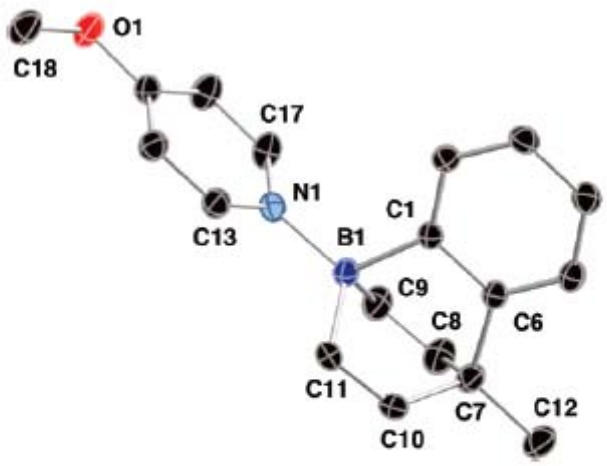


Figure 2. Thermal ellipsoid diagram of **3** (50%), with hydrogens omitted. Selected bond distances (Å): B(1)−N(1), 1.589(2); B(1)−C(1), 1.630(2); B(1)−C(9), 1.619(2); B(1)−C(11), 1.617(2); C(1)−C(6), 1.412(2); C(8)−C(9), 1.325(2); C(10)−C(11), 1.328(2). Selected bond angles (deg): C(1)−B(1)−C(9), 103.27(12); C(1)−B(1)−C(11), 103.56(12); C(9)−B(1)−C(11), 105.00(14).

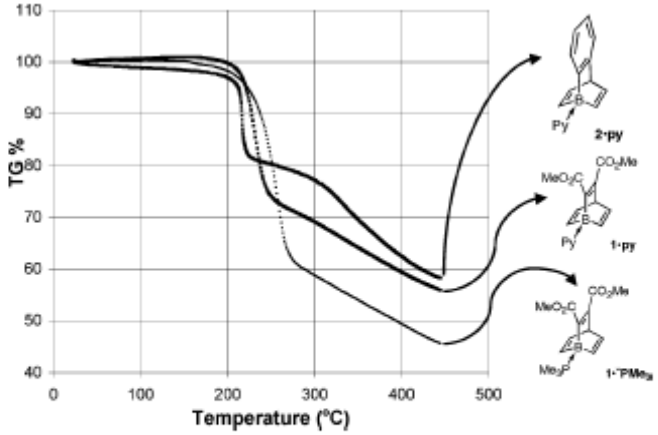


Figure 3. Thermal gravimetric analysis of compounds **1**·py, **1**·PMe_3, and **2**·py. Melting points for the three compounds as measured by differential scanning calorimetry are 222 °C (**1**·py), 162 °C (**1**·PMe_3), and 216 °C (**2**·py).

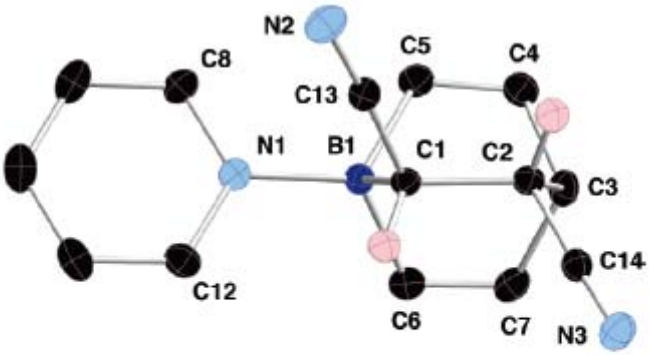


Figure 4. Thermal ellipsoid diagram of 4·py (50%), with hydrogens omitted. Selected bond distances (Å): B(1)−N(1), 1.586-(2); B(1)−C(1), 1.699(2); B(1)−C(5), 1.603(2); B(1)−C(6), 1.595-(2); C(1)−C(2), 1.560(2); C(4)−C(5), 1.333(2); C(6)−C(7), 1.334-(2). Selected bond angles (deg): C(1)−B(1)−C(5), 104.8(1); C(1)−B(1)−C(6), 102.6(1); C(5)−B(1)−C(6), 108.7(1). Selected torsion angle: C(13)−C(1)−C(2)−C(14), 110.7(1).

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