Quantum Mechanical Studies of 2,5-didehydropyrrole

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This study focuses on the diradical structure of pyrrole with radicals at the 2, 5 positions. These species are likely formed via the high temperature pyrolysis of asphaltenes contained in oil shale. Also, a better understanding of diradical behavior may advance the development of anti-cancer drugs and allow the design of more selective Bergman cyclization and subsequent formation of the active diradical species. The structure of 2,5-didehydropyrrole was optimized using single-(CCSD(T)/DZ and TZ) and multi-reference (CAS(8,8), MCSCF, MR-CI, MR-AQCC) methods. Optimized structures and energies of the singlet and triplet spin states were examined in order to determine adiabatic singlet-triplet energy splittings. Single point calculations were also performed to calculate vertical excitations between the singlet and triplet state. All multi-reference calculations were done using COLUMBUS software.