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环双(对-蒽基-对草快)的分子识别与谱学性质

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Binding Affinities and Spectroscopic Properties of Cyclobis(paraquat-*p*-anthracene)

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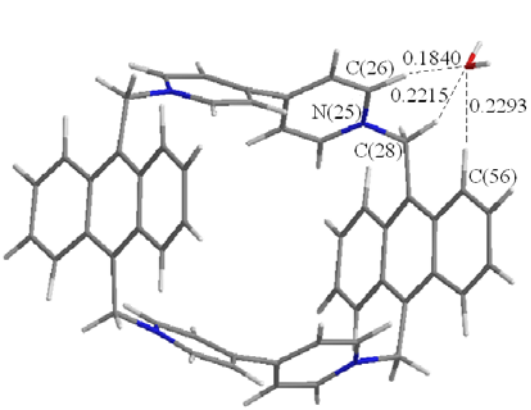
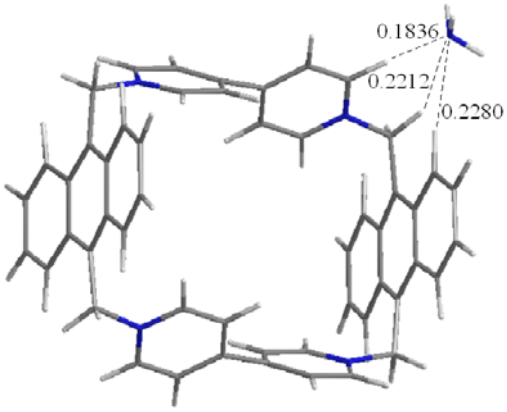


(a) complex **5**



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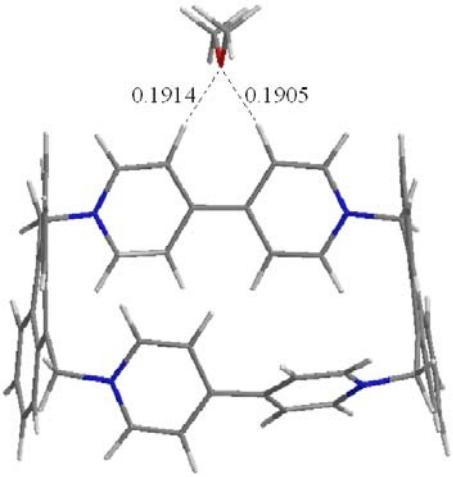
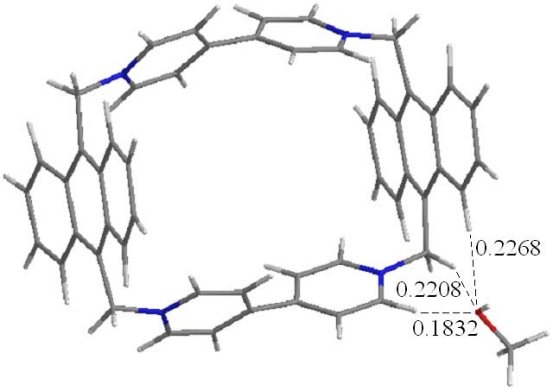


(c) complex **7**



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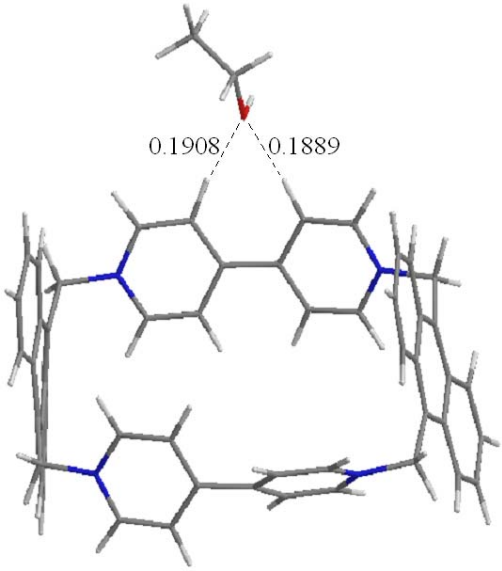
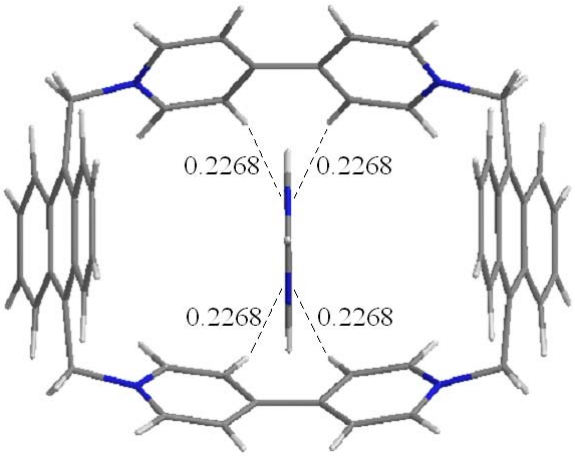


(e) complex **9**



(f) complex **10**

图 S1　复合物 5-10 的 B3LYP/3-21G 优化构型

Fig.S1　The optimized geometries of the complexes 5-10 at B3LYP/3-21G level

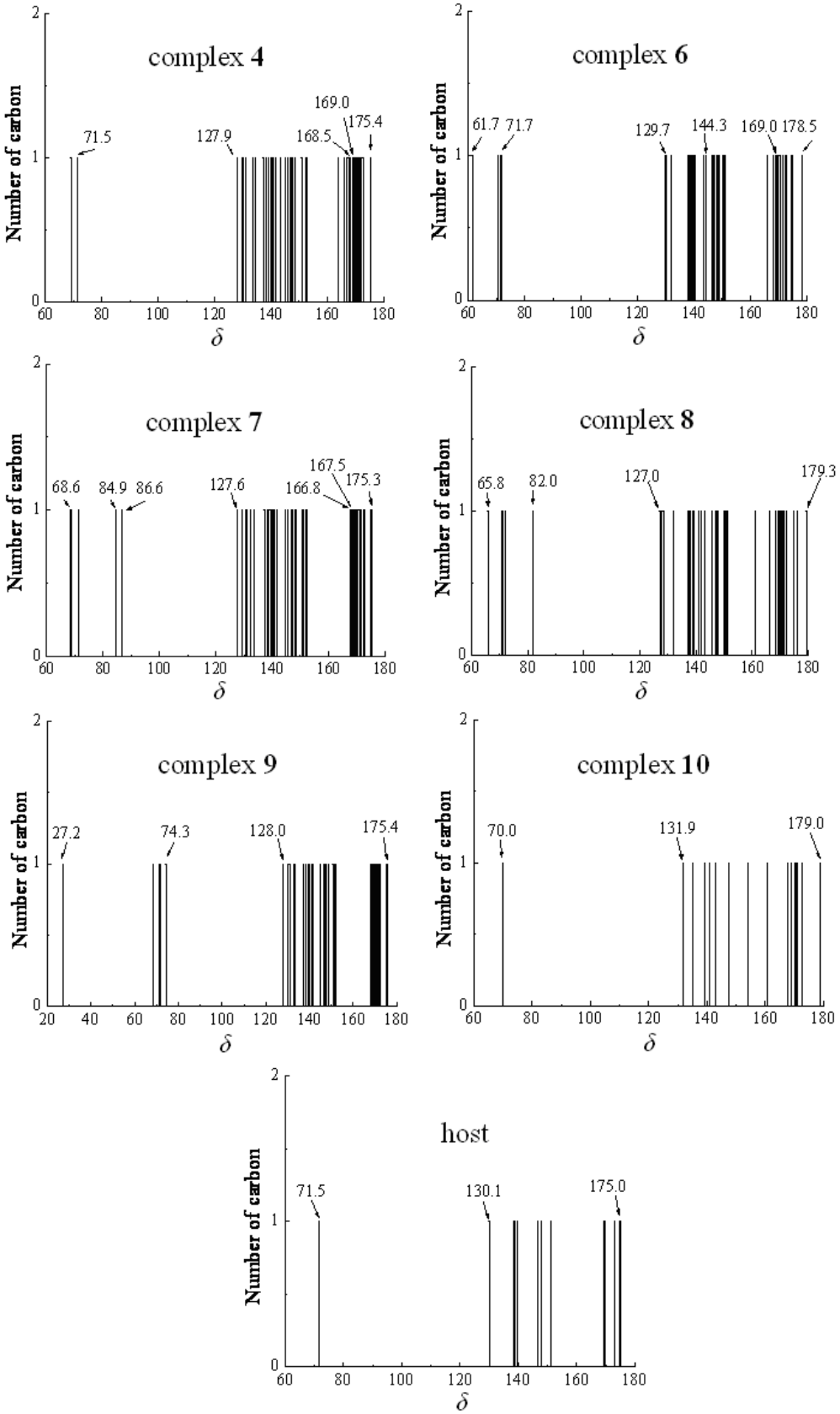


图 S2　B3LYP/3-21G 方法计算的复合物 4,6-10 和主体的核磁共振谱

Fig.S2　^{13}C-NMR spectra of the complexes 4, 6-10 and host at B3LYP/3-21G level