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Cytosine-guanine base pairing in a hydrogen-bonded complex of stable open-shell molecules with $S = 1$ spins

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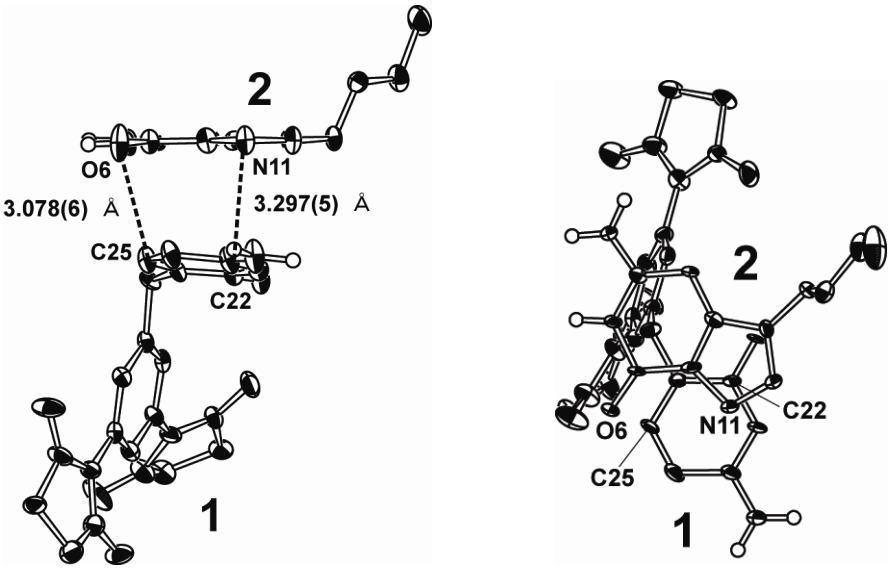

(a) Side view. **(b) Top view.**

Figure 1S. ORTEP drawings for the stacking of the nucleobase moieties of **1** and **2** in the complex. The thermal ellipsoids are given at the 50% probability level.

Table 1S. Atomic spin densities ρ of the biradical **1** calculated at UB3LYP/6-31+G(d,p) level.[a,b]

atom	ρ	atom	ρ
O1	0.352294	C2	-0.109897
N1	0.273734	C3	0.037390
C7	-0.175236	C4	-0.073281
N2	0.285690	C5	0.038672
O2	0.345182	C6	-0.076855
C8	-0.013145	H1	0.003451
C9	-0.013647	H2	0.002815
H4	0.013762	H3	0.002957
H5	0.004760	C13	-0.003585
H6	0.003800	H12	0.000137
H7	0.012561	H13	0.000574
O3	0.355549	N5	0.000328
N3	0.275721	N6	0.000020
C10	-0.221801	N7	0.000013
N4	0.288158	O5	-0.000255
O4	0.334104	C14	0.000700
C11	-0.016632	C15	0.000253
C12	-0.014678	C16	0.000721
H8	0.013859	C17	-0.000889
H9	0.004709	H14	-0.000001
H10	0.004710	H15	0.000000
H11	0.013806	H16	0.000003
C1	0.049451	H17	0.000018

[a] The convergence criteria was 1×10^{-8} hartree. The expectation values $<S^2>$ before and after the spin-projection, *i.e.*, the annihilation of higher spin multiplicity components, are 2.1247 and 2.0070, respectively.

[a] The atom numbering scheme is given in Scheme 1S.

Scheme 1S. Atom numbering scheme of the biradical **1**, corresponding to the DFT-calculated spin density distribution in Table 1S.