Electronic supplementary information(ESI)

Coexistence of antiferromagnetically coupled dimer and isolated paramagnetic spin in 4-azaindol-2-yl nitronyl nitroxide crystal

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Table S1 Atomic spin population of **2**[a,b]

O(1)	0.368320	H(21)	-0.001492
O(2)	0.306082	H(22)	0.000223
N(3)	0.271512	H(23)	-0.000788
N(4)	0.284650	H(24)	-0.000630
N(5)	-0.002866	H(25)	-0.000467
N(6)	-0.015021	H(26)	0.000193
C(7)	-0.182771	H(27)	-0.000798
C(8)	-0.012303	H(28)	-0.000451
C(9)	-0.010888	H(29)	-0.000683
C(10)	0.018924	H(30)	0.000144
C(11)	0.001210	H(31)	-0.000784
C(12)	0.001538	H(32)	-0.000674
C(13)	0.019350	H(33)	0.000300
C(14)	0.041947	H(34)	0.003038
C(15)	-0.071726	H(35)	-0.000119
C(16)	-0.017701	H(36)	0.001394
C(17)	0.014302	H(37)	-0.000289
C(18)	0.004165		
C(19)	-0.024350		
C(20)	0.007507		

[a] UB3LYP/EPR-II//UB3LYP/cc-pVDZ
[b] see Fig. S1 for atomic numbering

Table S2 Final position parameters of **2**

atom	*x*	*y*	*z*	U_{iso}
O1	0.98722(9)	-0.1229(1)	0.1606(1)	0.0673(5)
O2	0.77211(8)	0.0332(1)	0.13737(9)	0.0604(4)
N3	0.92065(9)	-0.1058(1)	0.15604(9)	0.0454(4)
N4	0.81801(9)	-0.0317(1)	0.14415(8)	0.0424(3)
N5	0.89189(9)	0.1411(1)	0.15262(8)	0.0408(3)
N6	1.0735(1)	0.2214(1)	0.17528(9)	0.0516(4)
C7	0.8905(1)	-0.0233(1)	0.15193(9)	0.0389(4)
C8	0.8622(1)	-0.1788(1)	0.1445(1)	0.0470(4)
C9	0.7994(1)	-0.1260(1)	0.1551(1)	0.0454(4)
C10	0.8997(2)	-0.2548(2)	0.1951(2)	0.0665(7)
C11	0.8360(2)	-0.2118(2)	0.0712(2)	0.0715(7)
C12	0.8090(2)	-0.1287(2)	0.2282(1)	0.0666(6)
C13	0.7166(1)	-0.1474(2)	0.1041(2)	0.0649(6)
C14	0.9286(1)	0.0607(1)	0.15518(9)	0.0389(4)
C15	1.0019(1)	0.0767(1)	0.1628(1)	0.0437(4)
C16	0.9417(1)	0.2097(1)	0.15966(9)	0.0401(4)
C17	1.0110(1)	0.1717(1)	0.16622(9)	0.0409(4)
C18	1.0638(1)	0.3101(2)	0.1763(1)	0.0561(5)
C19	0.9960(1)	0.3524(2)	0.1681(1)	0.0538(5)
C20	0.9326(1)	0.3027(1)	0.1598(1)	0.0478(4)
O21	0.5531(1)	0.0552(2)	0.1333(1)	0.0970(7)
O22	0.77027(7)	0.22556(9)	0.18392(7)	0.0491(3)
N23	0.5993(1)	0.1113(1)	0.1276(1)	0.0577(5)
N24	0.70168(8)	0.1931(1)	0.15187(8)	0.0394(3)
N25	0.7792(1)	0.1207(1)	0.29220(8)	0.0466(4)
N26	0.7277(2)	-0.0178(1)	0.3974(1)	0.0731(6)
C27	0.6702(1)	0.1320(1)	0.1768(1)	0.0427(4)
C28	0.5833(1)	0.1514(2)	0.0593(1)	0.0535(5)
C29	0.6454(1)	0.2270(1)	0.0823(1)	0.0443(4)
C30	0.5002(2)	0.1845(3)	0.0229(2)	0.0820(9)
C31	0.5969(2)	0.0769(2)	0.0180(2)	0.0715(7)
C32	0.6169(2)	0.3176(2)	0.0946(1)	0.0573(5)
C33	0.6867(2)	0.2385(2)	0.0381(1)	0.0590(6)
C34	0.7059(1)	0.0953(1)	0.2453(1)	0.0444(4)
C35	0.6752(2)	0.0379(1)	0.2759(1)	0.0535(5)
C36	0.7960(1)	0.0799(1)	0.3537(1)	0.0504(5)
C37	0.7315(2)	0.0286(1)	0.3451(1)	0.0549(5)
C38	0.7909(2)	-0.0117(2)	0.4574(2)	0.0800(9)
C39	0.8571(2)	0.0362(2)	0.4690(1)	0.0749(8)
C40	0.8612(2)	0.0839(2)	0.4169(1)	0.0637(6)

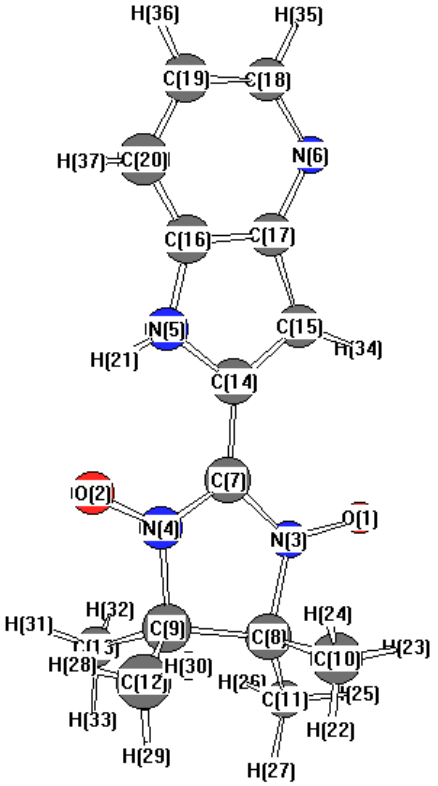
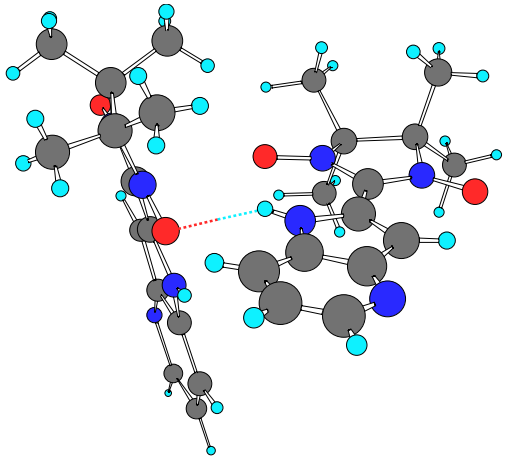
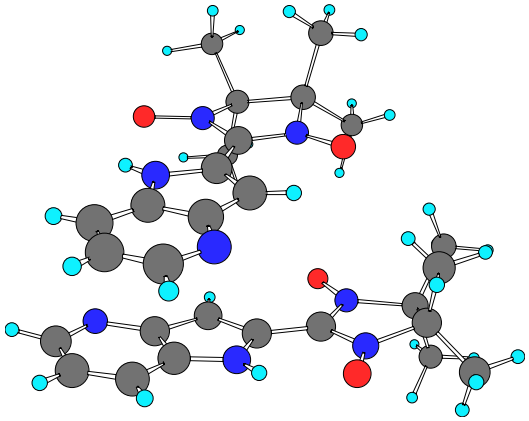


Fig. S1 UB3LYP/cc-pVDZ optimized structure of **2** and its atomic numbering.

A-B



A-A*



A-B*
(A*-B)

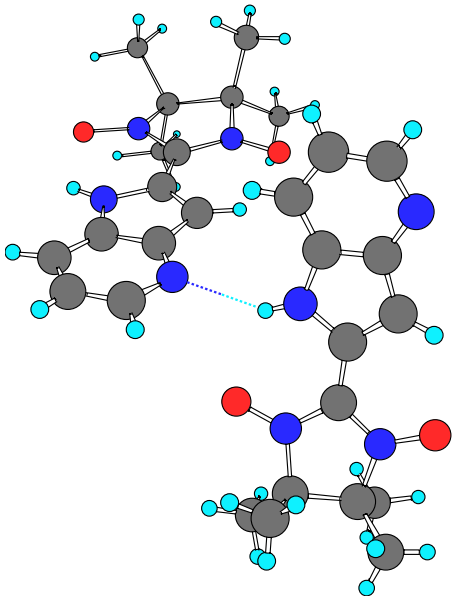


Fig. S2 Selected dimeric structures to calculate *J* values.