Table S2. Selected NBOs for 3FA (*trans* conformer) obtained from the B3LYP/6-311++G(d,p) calculations.

Bond orbital [a]	Occupancy [b] (*e*)	Coefficients (%) [c]		Description [d]
T(*A*-*B*)		*A*	*B*	
σ (O1-C2)	1.99122	69.07	30.93	0.8311 $sp^{2.11}$ + 0.5561 $sp^{3.13}$
σ (O1-C5)	1.99018	69.77	30.23	0.8353 $sp^{2.23}$ + 0.5561 $sp^{3.29}$
σ (C2-C3)	1.98425	48.80	51.20	0.6985 $sp^{1.43}$ + 0.7156 $sp^{2.03}$
π (C2-C3)	1.79569	46.05	53.95	0.6786 p + 0.7345 p
σ (C2-H9)	1.98472	60.37	39.63	0.7770 $sp^{1.89}$ + 0.6295 s
σ (C3-C4)	1.96342	51.24	48.76	0.7158 $sp^{2.07}$ + 0.6983 $sp^{2.10}$
σ (C3-C6)	1.98484	53.25	46.75	0.7297 $sp^{1.91}$ + 0.6837 $sp^{1.66}$
σ (C4-C5)	1.98600	50.45	49.55	0.7103 $sp^{1.91}$ + 0.7039 $sp^{1.39}$
π (C4-C5)	1.88181	49.91	50.09	0.7065 p + 0.7077 p
σ (C4-H10)	1.98030	62.06	37.94	0.7878 $sp^{2.00}$ + 0.6159 s
σ (C5-H11)	1.98613	60.35	39.65	0.7769 $sp^{1.87}$ + 0.6297 s
σ (C6-O7)	1.99652	35.16	64.84	0.5930 $sp^{2.05}$ + 0.8052 $sp^{1.44}$
π (C6-O7)	1.97886	33.32	66.68	0.5772 p + 0.8166 p
σ (C6-H8)	1.98603	57.20	42.80	0.7563 $sp^{2.32}$ + 0.6542 s
Cr (O1)	1.99974			s
Cr (C2)	1.99898			s
Cr (C3)	1.99902			s
Cr (C4)	1.99908			s
Cr (C5)	1.99906			s
Cr (C6)	1.99935			s
Cr (O7)	1.99977			s
LP1 (O1)	1.97293			$sp^{1.69}$
LP2 (O1)	1.69231			p
LP1 (O7)	1.98516			$sp^{0.69}$
LP2 (O7)	1.88351			p
Ry* (C6)	0.01156			$sp^{4.22}d^{0.02}$
σ* (O1-C2)	0.01476	30.93	69.07	0.5561 $sp^{2.11}$ – 0.8311 $sp^{3.13}$
σ* (O1-C5)	0.02099	30.23	69.77	0.5498 $sp^{2.23}$ – 0.8353 $sp^{3.29}$
σ* (C2-C3)	0.01842	51.20	48.80	0.7156 $sp^{1.43}$ – 0.6985 $sp^{2.03}$
π* (C2-C3)	0.29732	53.95	46.05	0.7345 p – 0.6786 p
σ* (C2-H9)	0.01548	39.63	60.37	0.6295 $sp^{1.89}$ – 0.7770 s
σ* (C3-C4)	0.02162	48.76	51.24	0.6983 $sp^{2.07}$ – 0.7158 $sp^{2.10}$
σ* (C3-C6)	0.05529	46.75	53.25	0.6837 $sp^{1.91}$ – 0.7297 $sp^{1.66}$
σ* (C4-C5)	0.01188	49.55	50.45	0.7039 $sp^{1.91}$ – 0.7103 $sp^{1.39}$
π* (C4-C5)	0.21420	50.09	49.91	0.7077 p – 0.7065 p
σ* (C4-H10)	0.01100	37.94	62.06	0.6159 $sp^{2.00}$ – 0.7878 s
σ* (C5-H11)	0.01484	39.65	60.35	0.6297 $sp^{1.87}$ – 0.7769 s
σ* (C6-O7)	0.00363	64.84	35.16	0.8052 $sp^{2.05}$ – 0.5930 $sp^{1.44}$
π* (C6-O7)	0.12316	66.68	33.32	0.8166 p – 0.5772 p
σ* (C6-H8)	0.06647	42.80	57.20	0.6542 $sp^{2.32}$ – 0.7563 s

[a] See atom numbering in Figure 1. Cr, core orbital; LP, lone electron pair orbital; Ry*, Rydberg orbital. [b] Occupancy is given with an exaggerated accuracy, as in the Gaussian output file. [c] The *A* and *B* values correspond to the contributions of the atomic orbitals of the two atoms forming a bond (by order of appearance in the corresponding entry in the first column) for the NBO orbitals, extracted from the polarization coefficients given in the description of the NBO orbitals. [d] The presented description is made in the space of the input atomic orbitals, as given by 6-311++G(d,p) basis set used in the calculations.