SUPPORTING INFORMATION for:

Beyond the molecular orbital conception of electronically excited states through the quantum theory of atoms in molecules

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Keywords: Formaldehyde, electronic excited states, QTAIM, IQA scheme, nπ^* states, ELF, electronic structure theory.

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Table S1: Change in the diatomic terms (in kJ mol^{-1}) arising from the IQA scheme for the vertical electronic excitation process (Figure 4a). In the core attraction matrix, $\Delta V_{ne}(\alpha, \Omega)$, columns represent the nuclei (α) and rows the basins (Ω). The data correspond to the CASSCF(4,3)/cc-pVTZ level of calculation.

	$\Delta V_{coul}(\Omega, \Omega')$				$\Delta V_{xc}(\Omega, \Omega')$			
	C	O	H1	H2	C	O	H1	H2
C	3449.7				-496.1			
O	1818.0	-3450.5			132.5	175.0		
H1	-75.9	-737.2	-169.5		1.7	-3.3	91.0	
H2	-75.9	-737.2	-117.1	-169.5	1.7	-3.3	5.1	91.0

	$\Delta V_{ne}(\alpha, \Omega)$				$\Delta V_{nn}(\alpha, \alpha')$			
	C	O	H1	H2	C	O	H1	H2
C	-4252.7	-3230.4	-502.2	-502.2				
O	2411.3	2733.9	251.3	251.3	0.0			
H1	613.1	445.5	255.7	64.0	0.0	0.0		
H2	613.1	445.5	64.0	255.7	0.0	0.0	0.0	

Table S2: Change in the diatomic terms (in kJ mol^{-1}) arising from the IQA scheme for the C−O elongation process (Figure 4b). In the core attraction matrix, $\Delta V_{ne}(\alpha, \Omega)$, columns represent the nuclei (α) and rows the basins (Ω). The data correspond to the CASSCF(4,3)/cc-pVTZ level of calculation.

	$\Delta V_{coul}(\Omega, \Omega')$				$\Delta V_{xc}(\Omega, \Omega')$			
	C	O	H1	H2	C	O	H1	H2
C	1080.1				-158.6			
O	-3697.9	-2853.3			133.4	219.9		
H1	148.6	-251.1	9.3		-28.3	14.5	-6.4	
H2	148.6	-251.1	-17.5	9.3	-28.3	14.5	0.4	-6.4

	$\Delta V_{ne}(\alpha, \Omega)$				$\Delta V_{nn}(\alpha, \alpha')$			
	C	O	H1	H2	C	O	H1	H2
C1	-1298.3	2725.2	-197.1	-197.1				
O2	7571.4	3274.5	288.0	288.0	-6077.7			
H3	-80.4	157.6	-36.5	19.3	125.3	-180.8		
H4	-80.4	157.6	19.3	-36.5	125.3	-180.8	-21.5	

Table S3: Change in the diatomic terms (in kJ mol^{-1}) arising from the IQA scheme for the C pyramidalization process (Figure 4c). In the core attraction matrix, $\Delta V_{ne}(\alpha, \Omega)$, columns represent the nuclei (α) and rows the basins (Ω). The data correspond to the CASSCF(4,3)/cc-pVTZ level of calculation.

	$\Delta V_{coul}(\Omega, \Omega')$				$\Delta V_{xc}(\Omega, \Omega')$			
	C	O	H1	H2	C	O	H1	H2
C	-613.1				41.1			
O	-388.7	158.4			8.8	-12.9		
H1	99.4	296.8	61.5		8.7	-5.2	-30.8	
H2	99.4	296.8	62.7	61.5	8.7	-5.2	-1.2	-30.8

	$\Delta V_{ne}(\alpha, \Omega)$				$\Delta V_{nn}(\alpha, \alpha')$			
	C	O	H1	H2	C	O	H1	H2
C	716.9	404.9	153.9	153.9				
O	-205.0	-175.9	-99.5	-99.5	117.8			
H1	-213.1	-264.4	-82.3	-44.1	-54.9	83.9		
H2	-213.1	-264.4	-44.1	-82.3	-54.9	83.9	20.1	

Table S4: Changes in the intra-atomic net energies and the inter-atomic interaction energies (kJ mol^{-1}) for the processes (a to c) considered in Figure 4. However, instead of the singlet S_1 state, the triplet T_1 is considered (*planar*T_1 and *min*T_1 in place of *planar*S_1 and *min*S_1). The data correspond to the CASSCF(4,3)/cc-pVTZ level of calculation.

	(a)	(b)	(c)
$\Delta E_{net}(C)$	-629.3	-264.1	81.9
$\Delta E_{net}(O)$	-201.9	-374.8	37.4
$\Delta E_{net}(H)$	40.2	-11.3	-11.1
$\Delta V_{int}(C, O)$	1110.5	621.7	-116.9
$\Delta V_{int}(C, H)$	44.6	-36.7	-1.0
$\Delta V_{int}(O, H)$	-50.7	31.2	10.6
$\Delta V_{int}(H, H')$	18.0	-1.5	-7.2

Table S5: Difference in the intra-atomic net energies and the inter-atomic interaction energies (kJ mol^{-1}) between T_1 and S_1 (both in *planar*S_1 geometry). The data correspond to the CASSCF(4,3)/cc-pVTZ level of calculation.

	$T_1 - S_1$
$\Delta E_{net}(C)$	-18.1
$\Delta E_{net}(O)$	-2.8
$\Delta E_{net}(H1)$	1.2
$\Delta V_{int}(C, O)$	-5.0
$\Delta V_{int}(C, H1)$	1.7
$\Delta V_{int}(O, H1)$	-2.3
$\Delta V_{int}(H1, H2)$	0.9

Table S6: Change in the atomic kinetic energies (kJ mol^{-1}) for the processes (a to c) considered in Figure 4. The data correspond to the CASSCF(4,3)/cc-pVTZ level of calculation.

	(a)	(b)	(c)
$\Delta T(C)$	693.1	86.6	-87.1
$\Delta T(O)$	338.5	-1039.5	40.9
$\Delta T(H)$	-139.5	23.9	41.5