Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Chemical bonding analysis of excited states using the Adaptive Natural Density Partitioning method

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Supporting Information

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1. Cartesian coordinates and total electron energies of investigated molecules

H_2O ground state	CASSCF(8,10)/aug-cc-pvtz, E_{total}= -76.1910703			
	8	0.000000000	-0.065482000	0.000000000
	1	0.762915000	0.528725000	0.000000000
	1	-0.762915000	0.528725000	0.000000000
H_2O the first excited state	CASSCF(8,10)/aug-cc-pvtz, E_{total}= -75.9177191			
	8	0.000000000	-0.111490000	0.000000000
	1	0.834248000	0.551729000	0.000000000
	1	-0.834248000	0.551729000	0.000000000
B_5^+ ground state	CASSCF(14,10)/6-311G**, E_{total}= -122.9150924			
	5	0.000000000	0.000000000	1.117711000
	5	-1.388960000	0.000000000	0.430132000
	5	1.388960000	0.000000000	0.430132000
	5	-0.776338000	0.000000000	-0.988987000
	5	0.776338000	0.000000000	-0.988987000
B_5^+ the first excited state	CASSCF(14,10)/6-311G**, E_{total}= -122.8079403			
	5	0.000003000	1.124107000	0.000013000
	5	-1.427010000	0.423093000	-0.000010000
	5	1.427011000	0.423090000	-0.000010000
	5	-0.810368000	-0.985144000	0.000003000
	5	0.810365000	-0.985146000	0.000003000
$C_2H_4^+$ ground state (twisted geometry)	CCSD(T)/cc-pvqz, E_{total}=-78.0754243, ZPE correction = 0.049023			
	6	0.000000000	0.000000000	0.701246000
	6	0.000000000	0.000000000	-0.701246000
	1	-0.167502000	0.919959000	1.253913000
	1	0.167502000	-0.919959000	1.253913000

	1	0.167502000	0.919959000	-1.253913000
	1	-0.167502000	-0.919959000	-1.253913000
TS $C_2H_4^+$ ground state (planar geometry)	CCSD(T)/cc-pvqz, E_{total}= -78.0750645, ZPE correction= 0.048640 (1 imaginary frequency -316.5528 cm^{-1})			
	6	0.000000000	0.000000000	0.706737000
	6	0.000000000	0.000000000	-0.706737000
	1	0.000000000	0.932947000	1.258142000
	1	0.000000000	-0.932947000	1.258142000
	1	0.000000000	0.932947000	-1.258142000
	1	0.000000000	-0.932947000	-1.258142000
$C_2H_4^+$ ground state	CSSSCF(7,9)/aug-cc-pvdz, E_{total}= -77.7960898			
	6	0.000000000	0.716990000	0.000000000
	6	0.000000000	-0.716990000	0.000000000
	1	-0.935944000	1.260888000	0.000000000
	1	0.950805000	1.277414000	0.000000000
	1	-0.950805000	-1.277414000	0.000000000
	1	0.935944000	-1.260888000	0.000000000
$C_2H_4^+$ the first excited state	CSSSCF(7,9)/aug-cc-pvdz, E_{total}= -77.7066715			
	6	0.000000000	0.654218000	0.000000000
	6	0.000000000	-0.654218000	0.000000000
	1	1.179890000	0.898439000	0.000000000
	1	-0.631000000	1.529705000	0.000000000
	1	0.631000000	-1.529705000	0.000000000
	1	-1.179890000	-0.898439000	0.000000000