Supplementary Data for "THE PHOTOELECTRON SPECTROSCOPY OF THE DICHLOROETHYLENES: THE GEMINAL ISOMER 1,1- $Cl_2C_2H_2$. AN EXPERIMENTAL AND QUANTUM CHEMICAL STUDY."

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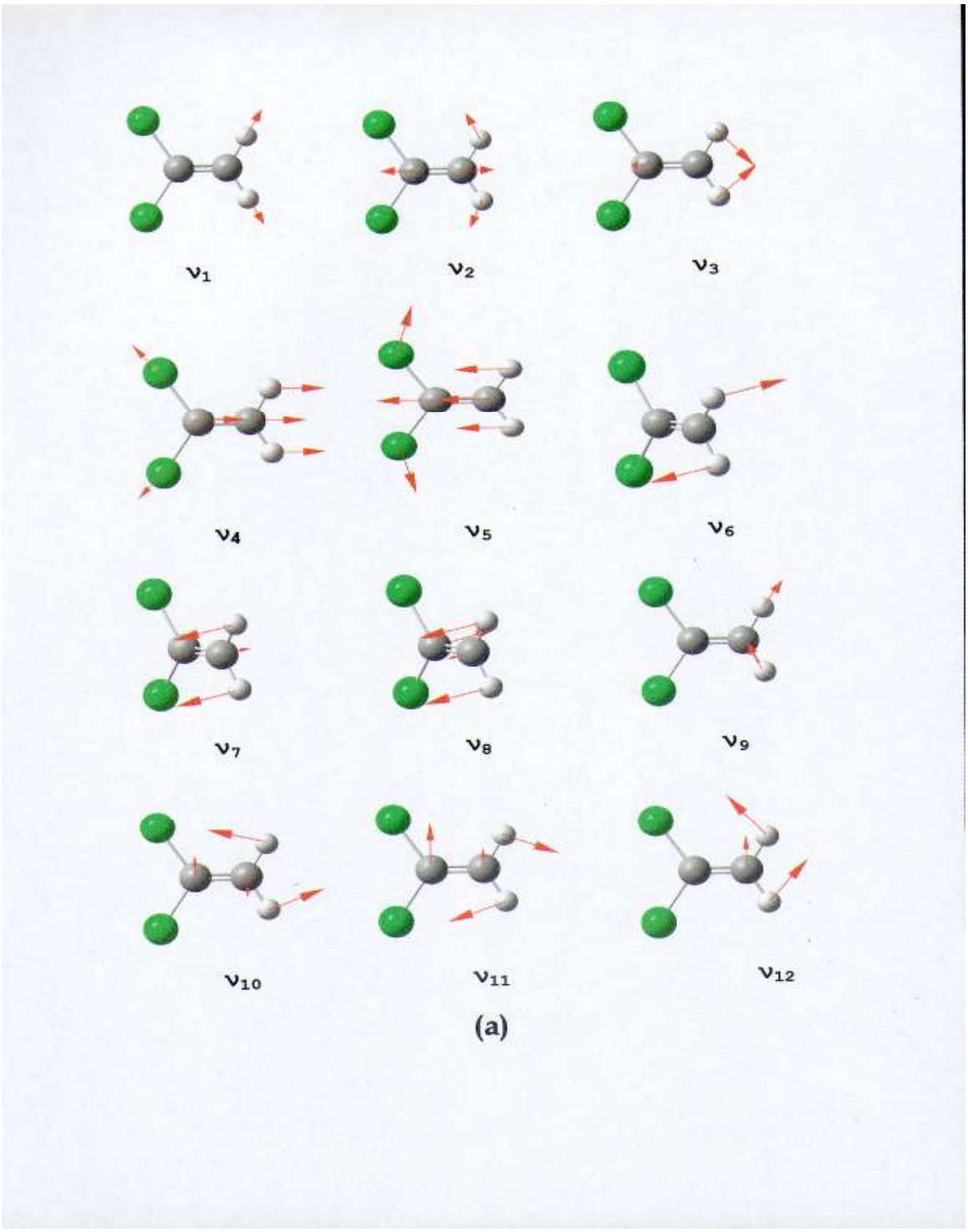
FIG.S1: Graphical representation and description of (a) the twelve nuclear normal modes of 1,1-$C_2H_2Cl_2^+$ in the C_{2v} point group for which the associated wavenumbers have been calculated, the two modified coordinates in (b) the $\widetilde{C}\,^2A_1$ and (c) the $\widetilde{D}\,^2B_2$ states and the modified coordinate in (d) the $\widetilde{F}\,^2A_1$ and (e) $\widetilde{H}\,^2A_1$ states.

FIG.S2: Isocontour lines of the ionized molecular orbitals (MO) calculated at RHF level for the neutral molecule optimized at the CCSF(FC) level. Contours correspond to 0.02 a.u. density. The positive and negative parts are colored in green and yellow respectively.

TABLE S1: Optimized geometry of the neutral and ionic ground and excited states of 1,1-$C_2H_2Cl_2$ in the C_{2v} point group at different calculation levels. Internuclear distances in Å and angles in degrees.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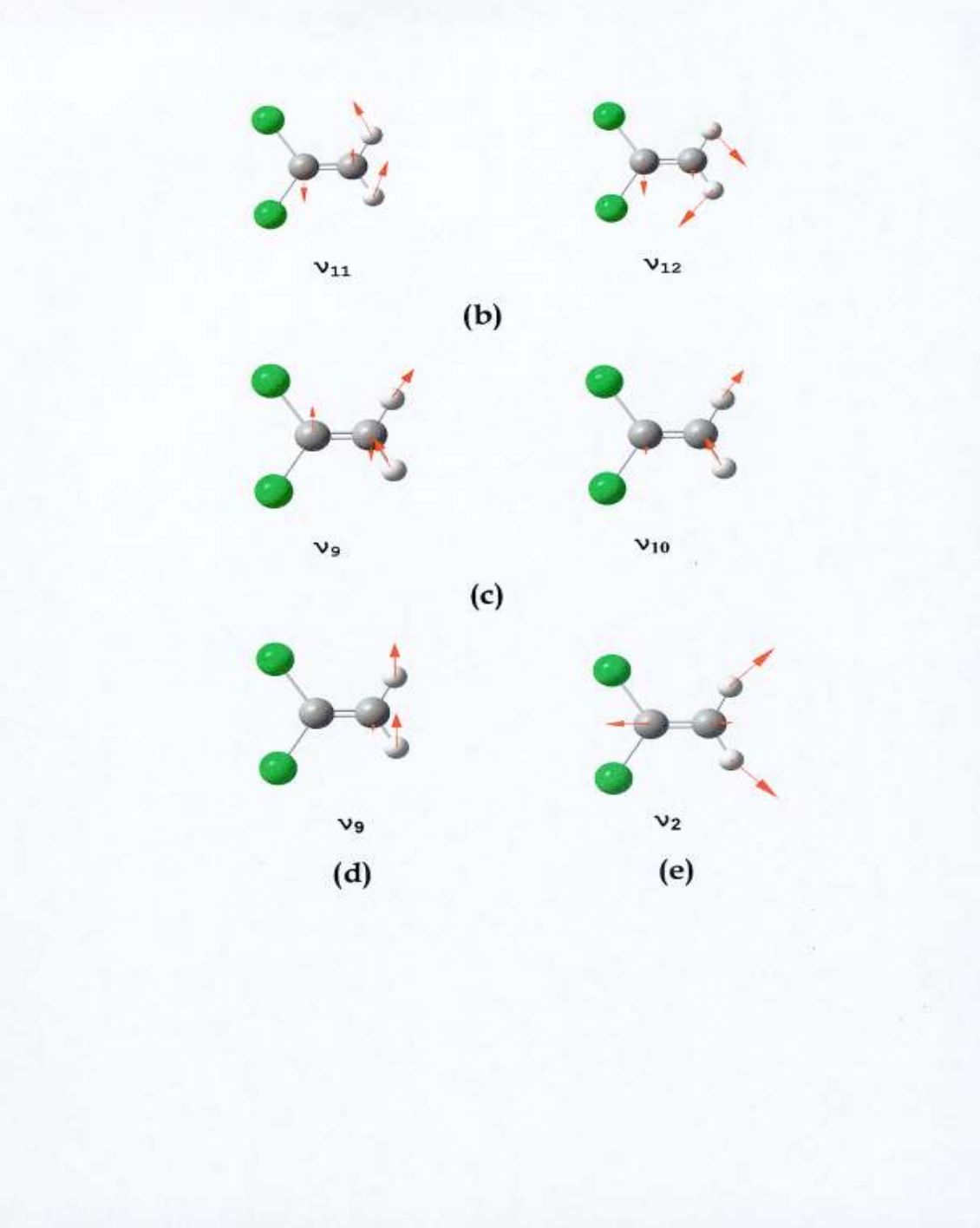

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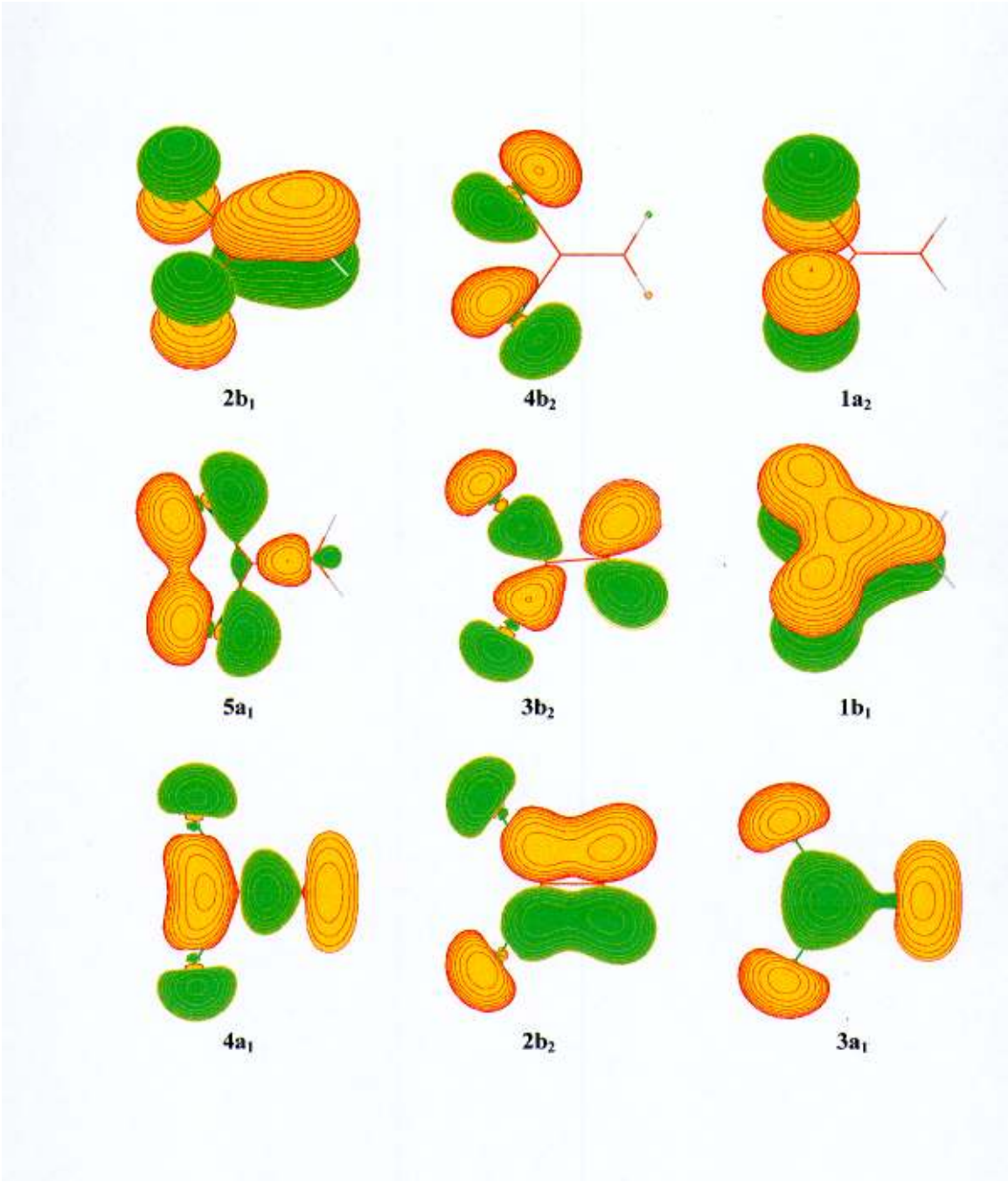

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TABLE S1: Optimized geometry of the neutral and ionic ground and excited states of 1,1-$C_2H_2Cl_2$ in the C_{2v} point group at different calculation levels. Internuclear distances in Å and angles in degrees.

Level	C1-C2	C-H	C-Cl	H-C-C	Cl-C-C
	Neutral $\widetilde{X}\,^1A_1$ state				
CCSD(FC)	1.3416	1.0917	1.7457	120.174	122.734
M06-2X	1.3271	1.0866	1.7325	120.054	122.914
B3LYP	1.3312	1.0877	1.7469	120.360	122.944
	Cation $\widetilde{X}\,^2B_1$ state				
CCSD(FC)	1.4213	1.0949	1.6783	119.577	120.132
M06-2X	1.4080	1.0904	1.6682	119.759	120.26
B3LYP	1.4067	1.0916	1.6832	120.062	120.3
	Cation $\widetilde{A}\,^2B_2$ state				
CCSD(FC)	1.3251	1.0941	1.7540	120.137	132.225
M06-2X	1.3115	1.0904	1.7419	120.143	132.67
B3LYP	1.3155	1.0913	1.7564	120.535	131.506
TD-DFT	1.3048	1.0894	1.7386	120.406	131.698
	Cation $\widetilde{B}\,^2A_2$ state				
CCSD(FC)	1.3319	1.0936	1.7688	120.209	126.074
M06-2X	1.3183	1.0897	1.7557	120.228	126.116
B3LYP	1.3216	1.0905	1.7761	120.570	125.625
TD-DFT	1.3186	1.0892	1.7584	120.380	125.504
	Cation $\widetilde{C}\,^2A_1$ state				
CCSD(FC)	1.3490	1.0923	1.7558	120.251	119.407
M06-2X	1.3412	1.0881	1.7343	120.043	119.323
B3LYP	1.3408	1.0889	1.7586	120.453	119.639
TD-DFT	1.3384	1.0876	1.7341	120.326	119.257
	Cation $\widetilde{D}\,^2B_2$ state				
TD-DFT	1.3005	1.1543	1.7308	135.696	123.442
	Cation $\widetilde{E}\,^2B_1$ state				
TD-DFT	1.3475	1.0920	1.8437	119.953	123.312
	Cation $\widetilde{F}\,^2A_1$ state				
TD-DFT	1.3699	1.1205	1.7634	106.516	119.704
	Cation $\widetilde{G}\,^2B_2$ state				

TD-DFT	1.3713	1.1230	1.7846	126.713	124.779
	Cation $\tilde{H}\,^2A_2$ state				
TD-DFT	1.3591	1.1312	1.7434	116.377	120.800