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

SUPPLEMENTARY INFORMATION
Highly-Excited States of Cumulenenone Chlorides in the Vacuum-Ultraviolet

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1 Ground State Equilibrium Geometries

The ground state neutral geometry of formyl chloride, chloroketene, propadienone chloride, and butatrienone chloride are optimized with CCSD(T), MP2, and DFT/B3LYP levels of theory with the d-aug-cc-pV(T+d)Z basis set. The calculated geometries are shown in the following tables:

- Formyl Chloride: Tables 1, 2, 3.
- Chloroketene: Tables 4, 5, 6.
- Propadienone Chloride: Tables 7, 8, 9.
- Butatrienone Chloride: Tables 10, 11, 12

1.1 Formyl chloride

Table 1: Ground state equilibrium geometry of formyl chloride optimized at CCSD(T)

C	-0.0058154	0.8304188	0.0000000
O	1.1271554	1.1916396	0.0000000
H	-0.8900374	1.4757852	0.0000000
Cl	-0.4879190	-0.8725632	0.0000000

Table 2: Ground state equilibrium geometry of formyl chloride optimized at MP2

C	-0.00572620	0.82164784	0.00000000
O	1.12411717	1.18373052	0.00000000
H	-0.88683898	1.46114947	0.00000000
Cl	-0.48665209	-0.86551383	0.00000000

Table 3: Ground state equilibrium geometry of formyl chloride optimized at B3LYP

C	0.00265751	0.83881366	0.00000000
O	1.12585276	1.19613080	0.00000000
H	-0.88668608	1.47666344	0.00000000
Cl	-0.49032734	-0.87752357	0.00000000

1.2 Chloroketene

Table 4: Ground state equilibrium geometry of chloroketene optimized at CCSD(T)

C	-0.34147545	-0.67509679	0.00000000
C	0.98099146	-0.69629719	0.00000000
O	2.14797749	-0.71878511	0.00000000
Cl	-1.17575162	0.84522090	0.00000000
H	-0.90910965	-1.59032642	0.00000000

Table 5: Ground state equilibrium geometry of chloroketene optimized at MP2

C	-0.34329602	-0.66826238	0.00000000
C	0.97240523	-0.69038170	0.00000000
O	2.13524642	-0.71389700	0.00000000
Cl	-1.16651643	0.83833759	0.00000000
H	-0.90358301	-1.58088255	0.00000000

Table 6: Ground state equilibrium geometry of chloroketene optimized at B3LYP

C	-0.33024201	-0.67376907	0.00000000
C	0.98157003	-0.69571950	0.00000000
O	2.14090429	-0.71978335	0.00000000
Cl	-1.17673811	0.84486083	0.00000000
H	-0.90326777	-1.58467760	0.00000000

1.3 Propadienone chloride

Table 7: Ground state equilibrium geometry of propadienone chloride optimized at CCSD(T)

C	0.712348	-0.924082	0.000000
C	-0.616365	-0.952100	0.000000
C	-1.619551	-0.101810	0.000000
Cl	1.690642	0.516824	0.000000
H	1.327075	-1.815779	0.000000
O	-2.636740	0.468470	0.000000

Table 8: Ground state equilibrium geometry of propadienone chloride optimized at MP2

C	0.708632	-0.909143	0.000000
C	-0.611057	-0.921243	0.000000
C	-1.625311	-0.106416	0.000000
Cl	1.694985	0.504828	0.000000
H	1.311592	-1.802917	0.000000
O	-2.642133	0.462984	0.000000

Table 9: Ground state equilibrium geometry of propadienone chloride optimized at B3LYP

C	0.69008272	-0.88326582	0.00000000
C	-0.61870469	-0.81194743	0.00000000
C	-1.69644026	-0.10422902	0.00000000
Cl	1.77795717	0.48895120	0.00000000
H	1.25343918	-1.80660422	0.00000000
O	-2.74684948	0.39487461	0.00000000

1.4 Butatrienone chloride

Table 10: Ground state equilibrium geometry of butatrienone chloride optimized at CCSD(T)

C	-1.44265713	-0.45765886	0.00000000
C	-0.12315926	-0.50139359	0.00000000
O	3.61242298	-0.64598586	0.00000000
Cl	-2.28974316	1.05534629	0.00000000
H	-2.05462612	-1.34794362	0.00000000
C	1.15434828	-0.54420293	0.00000000
C	2.44146791	-0.59785037	0.00000000

Table 11: Ground state equilibrium geometry of butatrienone chloride optimized at MP2

C	-1.43471630	-0.44925163	0.00000000
C	-0.12171567	-0.49013832	0.00000000
O	3.59378652	-0.64448295	0.00000000
Cl	-2.27703490	1.04604731	0.00000000
H	-2.03465027	-1.34296191	0.00000000
C	1.14554305	-0.54127788	0.00000000
C	2.42701899	-0.59576166	0.00000000

Table 12: Ground state equilibrium geometry of butatrienonechloride optimized at B3LYP

C	-1.42257854	-0.45529812	0.00000000
C	-0.11508666	-0.49802775	0.00000000
O	3.59364944	-0.64393528	0.00000000
Cl	-2.28647464	1.05353630	0.00000000
H	-2.03546290	-1.34315424	0.00000000
C	1.15175256	-0.54779601	0.00000000
C	2.42980176	-0.59784488	0.00000000

2 Excited state properties

2.1 Electronic Excitation Characters

2.1.1 Chloroketene

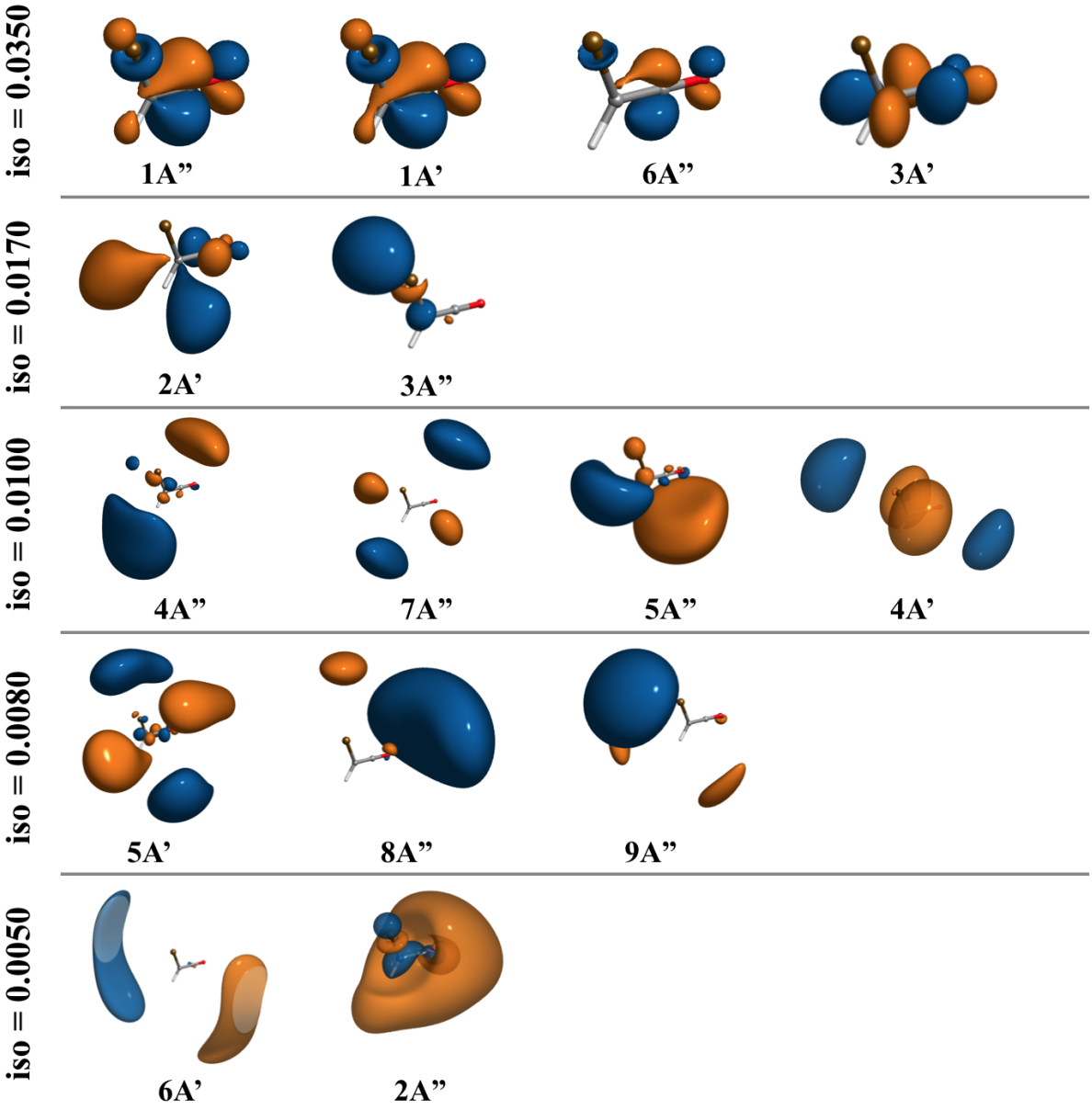

Figure 1: Linear combinations of virtual transition orbitals for each excited state of chloroketene. The lower panel shows a group of states with the same character. The upper panel shows the excited state character with the corresponding energy in red and the oscillator strength in parentheses. The iso value indicates the isosurface value used for the plotting the excited state wavefunctions in $e^2/Bohr$.

2.1.2 Propadienone chloride

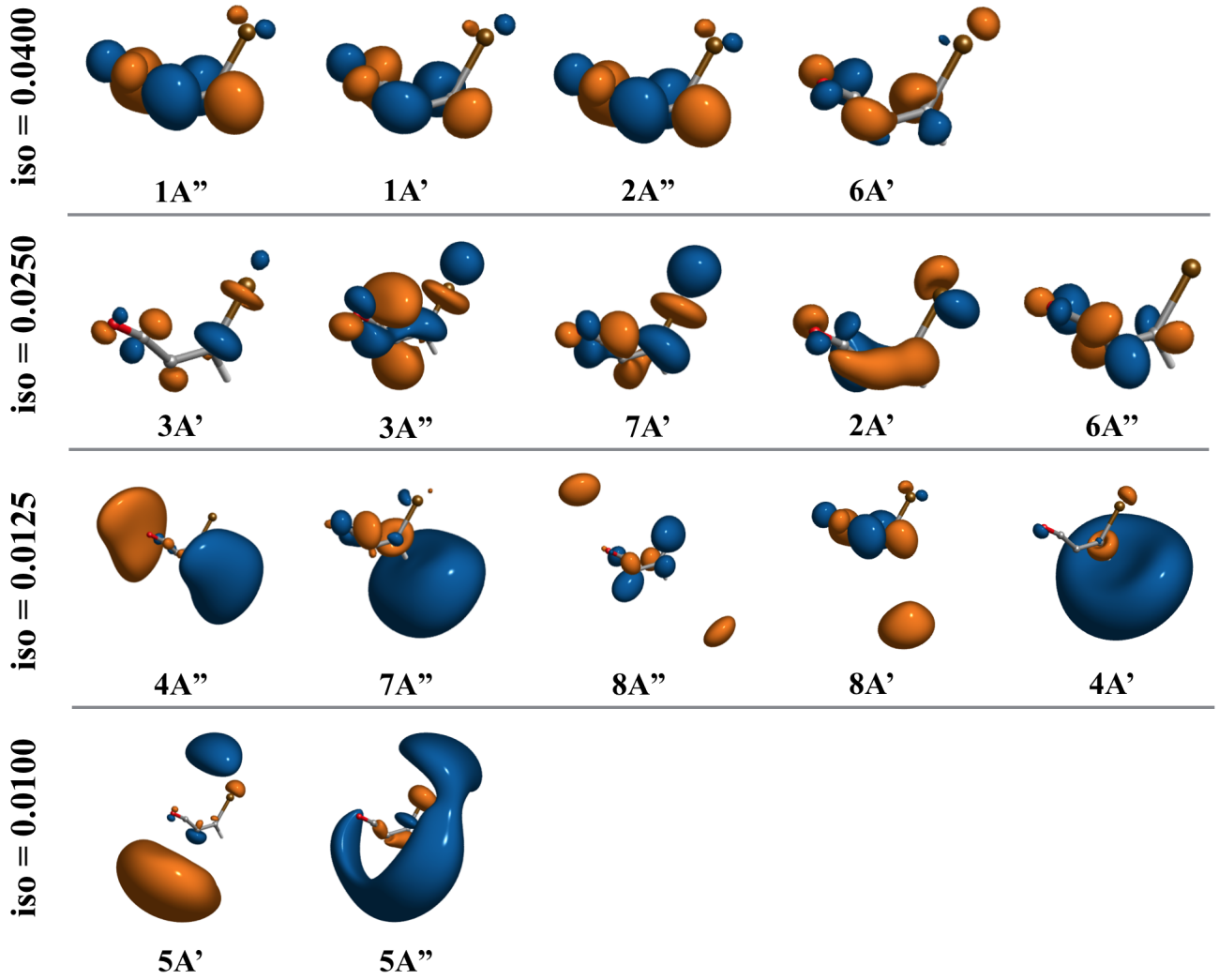

Figure 2: Excited state transition orbitals of chloro-propadienone. Lowest two panel shows the first and second sets of orbitals. Top panel shows the first Rydberd-valence transitions of two symmetries. The iso value indicates the isosurface value used for the plotting the excited state wavefunctions in $e^2/Bohr$.

2.1.3 Butatrienone chloride

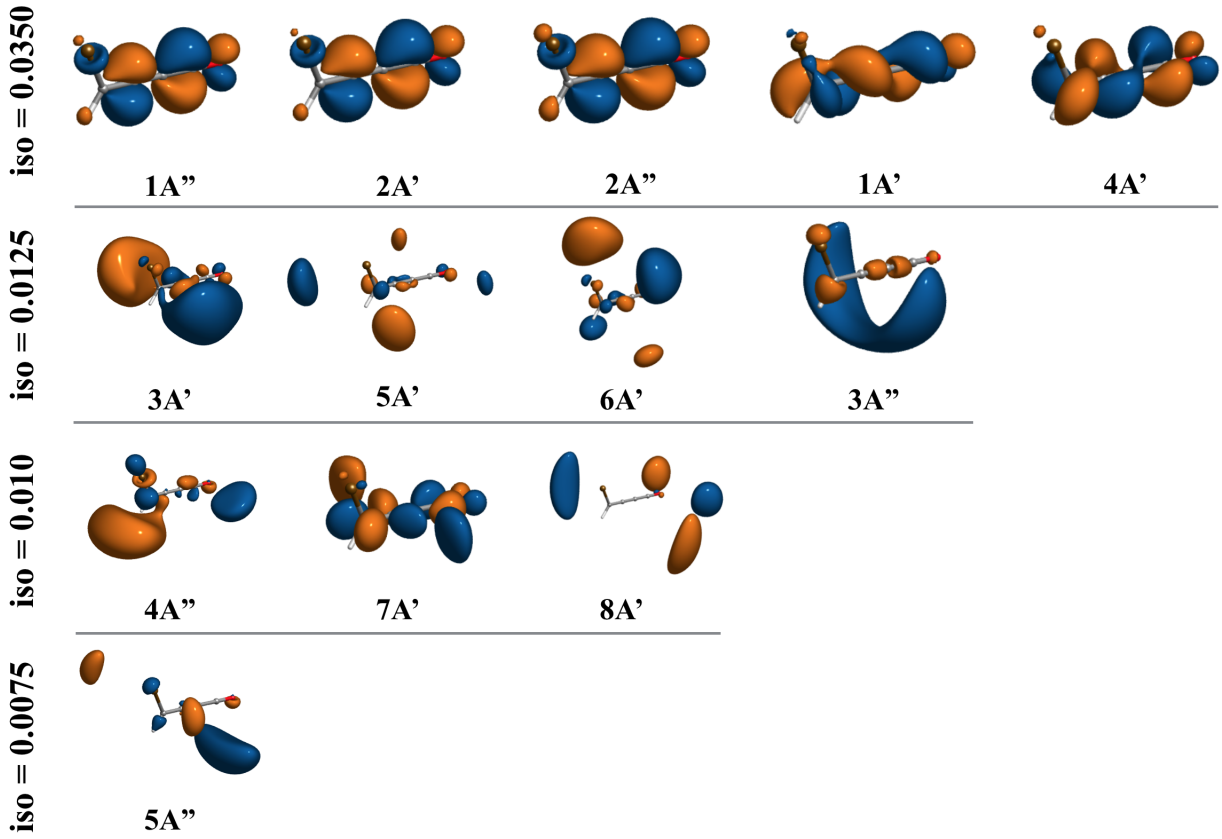

Figure 3: Excited state transition orbitals of chloro-butatrienone. The iso value indicates the isosurface value used for the plotting the excited state wavefunctions in $e^2/Bohr$.

3 Method Comparison

The excited state energies of chloromethane (Table 13) and formaldehyde (Table 14) computed with EOM-CCSD with three different basis sets: aug-cc-pV(T+d)Z, d-aug-cc-pV(T+d)Z, and t-aug-cc-pV(T+d)Z. The predicted energies are in excellent agreement with experimental values, validating the accuracy of our theoretical method for organics consisting of both chloride and carbonyl functional groups.
The ground state equilibrium geometry of each species are optimized with d-aug-cc-pV(T+d)Z at three different levels of theory: DFT/B3LYP, MP2, and CCSD(T). The vertical excitation energies are computed for each geometry at the EOM-CCSD level with different basis sets and reported in the following tables and figures:

- Formyl chloride: Tables 15, 17, 18 and Figure 5.
- Chloroketene: Tables 19, 20, 21 and Figure 6.
- Propadienone chloride: Tables 22, 23, 24 and Figure 7.
- Butatrienone chloride: Tables 25, 26, 27 and Figure 8.

As shown in these figures and tables, the vertical excitation energies computed with the same basis set for the geometries optimized at different levels of theory agree well quantitatively with discrepancies of less than 0.1 eV for formyl chloride, chloroketene, propadienone chloride, and butatrienone chloride. The center-of-mass technique provides comparable results calculated with the d-aug-cc-pV(T+d)Z basis for the geometries propadione chloride (Table 22) and butatrienone chloride (Table 25) optimized at all three levels .

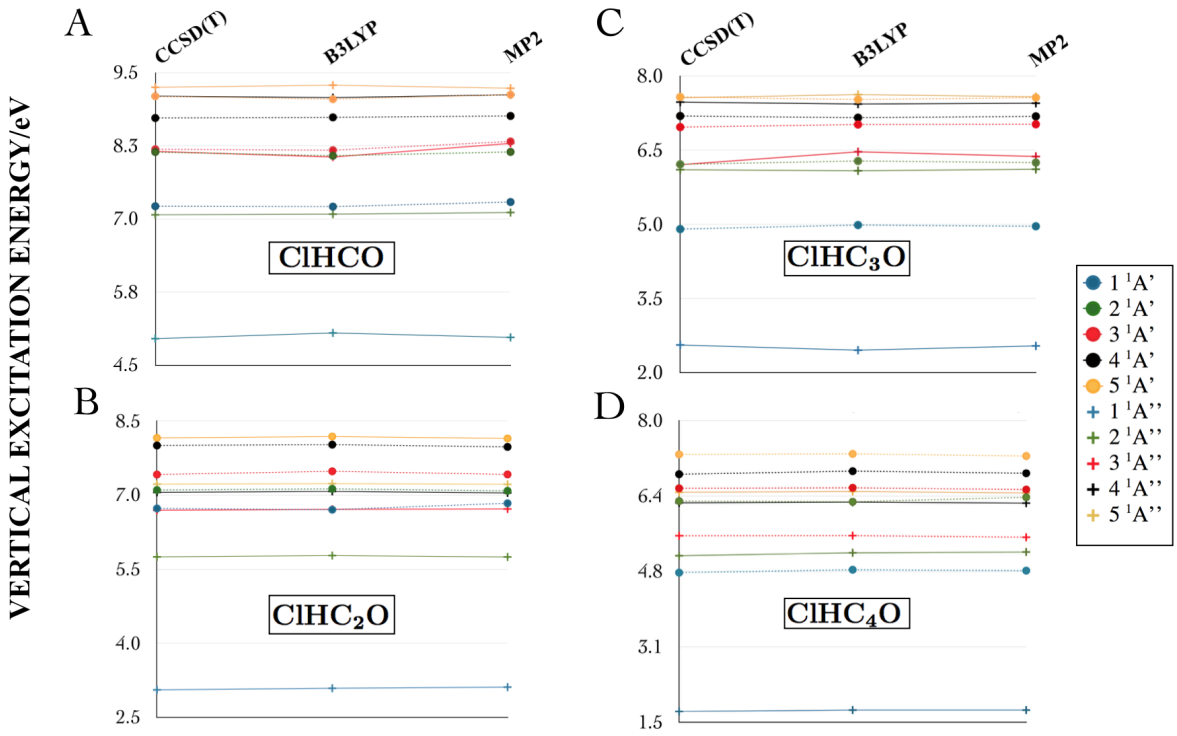

Figure 4: **Method comparison for vertical excitation energies:** Excited state energies are roughly dependent on the ground state geometries. The ground state geometries for (A) formyl chloride, (B) chloroketene, (C) propadienone chloride, (D) butatrienone chloride are optimized at CCSD(T), B3LYP, and MP2/d-aug-cc-pV(T+d)Z. Vertical excitation energies of the ten lowest states for each geometry calculated at EOM-CCSD/d-aug-cc-pV(T+d)Z are displayed.

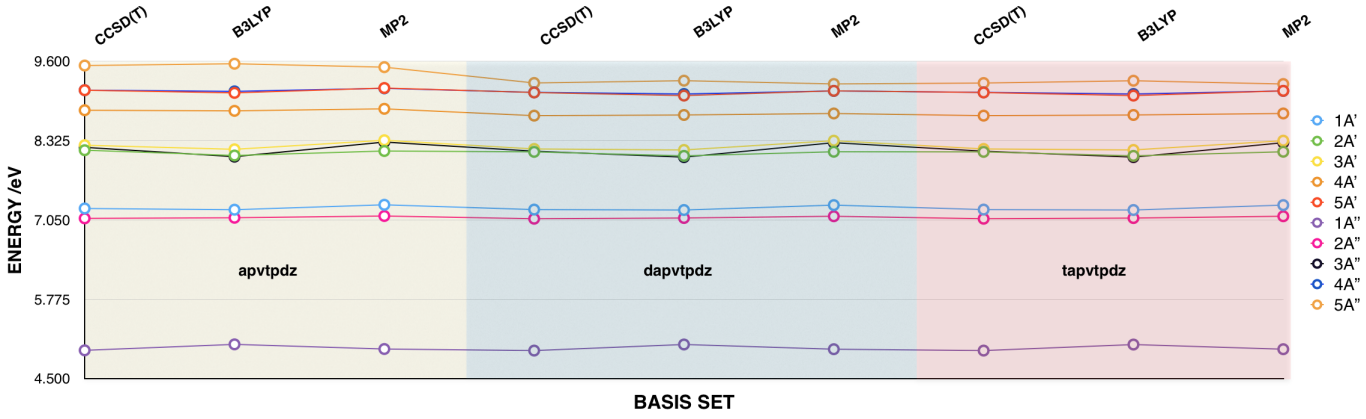

Figure 5: EOM-CCSD vertical excitation energies of formyl chloride equilibrium energies optimized at CCSD(T), B3LYP, MP2/d-aug-cc-pVTPDZ

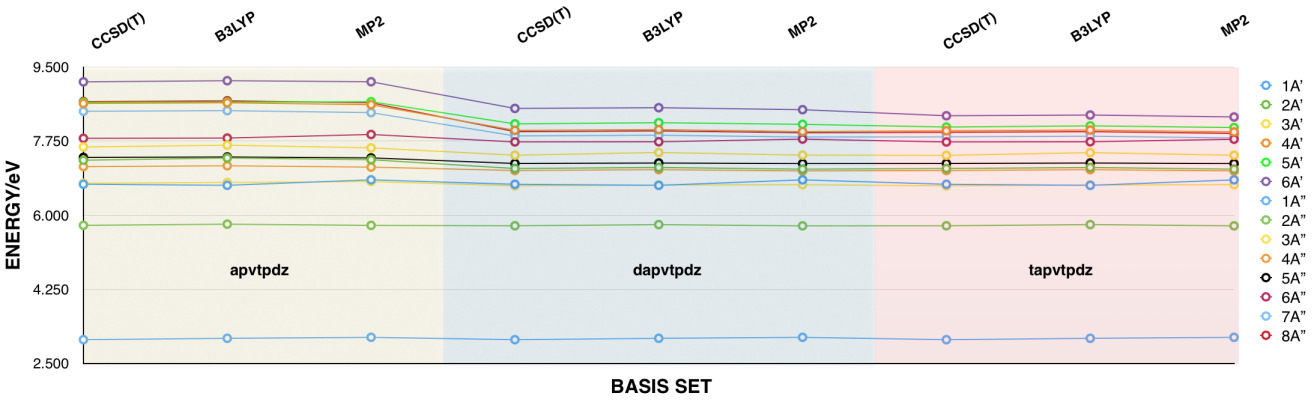

Figure 6: EOM-CCSD vertical excitation energies of chloroketene equilibrium energies optimized at CCSD(T), B3LYP, MP2/d-aug-cc-pVTPDZ

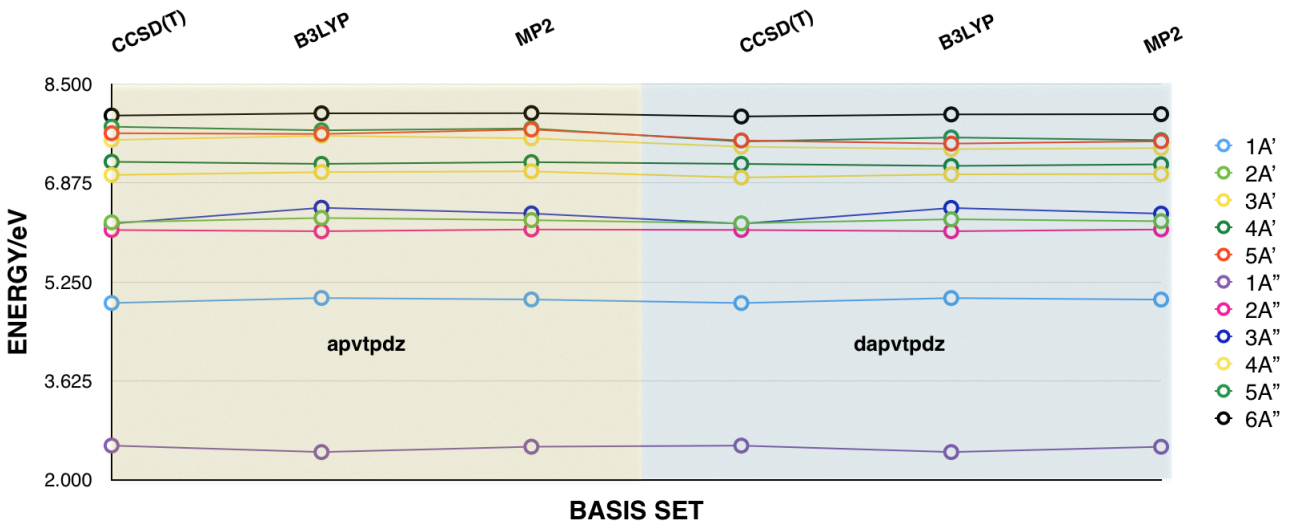

Figure 7: EOM-CCSD vertical excitation energies of propadienone chloride equilibrium energies optimized at CCSD(T), B3LYP, MP2/d-aug-cc-pVTPDZ

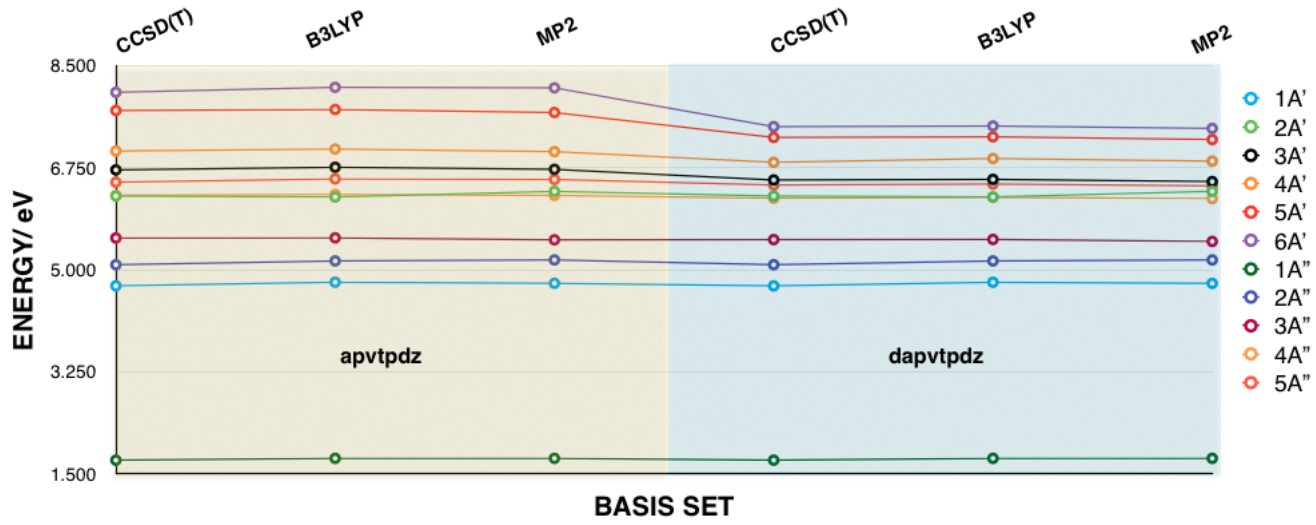

Figure 8: EOM-CCSD vertical excitation energies of butatrienone chloride equilibrium energies optimized at CCSD(T), B3LYP, MP2/d-aug-cc-pVTPDZ

3.1 Electronic Vertical Excitation Energies

3.1.1 Chloromethane and formaldehyde

Table 13: Excited state properties of **chloromethane** at EOM-CCSD where SA is the state assignment, E is the vertical excitation energy, and f is the oscillator strength

SA	Excitation Character		EOM-CCSD					
			aug-cc-pVTZ		d-aug-cc-pV(T+d)Z		aug-cc-pVDZ	
			E	f	E	f	E	f
1a	13a → 42a	0.3039	7.381	0.0031	7.353	0.0032	7.382	0.0035
	13a → 26a	0.2385						
	13a → 49a	0.2230						
	13a → 45a	0.2107						
2a	12a → 42a	0.3090	7.381	0.0031	7.353	0.0032	7.382	0.0035
	12a → 26a	0.2386						
	12a → 49a	0.2230						
	12a → 45a	0.2107						
3a	13a → 18a	0.3490	7.964	0.0246	7.939	0.0262	7.872	0.0240
	13a → 14a	0.2693						
	13a → 26a	0.2619						
	13a → 42a	0.2155						
	13a → 29a	0.2131						
4a	12a → 18a	0.3490	7.964	0.0246	7.939	0.0262	7.872	0.0240
	12a → 14a	0.2693						
	12a → 26a	0.2619						
	12a → 42a	0.2155						
	12a → 29a	0.2131						
5a	13a → 16a	0.2199	9.056	0.0022	8.952	0.0022	8.994	0.0771
	12a → 15a	0.2178						
	13a → 20a	0.1981						
	12a → 19a	0.1964						
	13a → 23a	0.1830						
	13a → 19a	0.1824						
	12a → 22a	0.1814						
	12a → 20a	0.1805						
6a	13a → 15a	0.2193	9.056	0.0022	8.952	0.0022	9.000	0.0028
	12a → 16a	0.2185						
	13a → 19a	0.1976						
	12a → 20a	0.1966						
7a	12a → 15a	0.2263	9.061	0.0732	8.964	0.0600	9.000	0.0028
	13a → 16a	0.2243						
	12a → 20a	0.2069						
	13a → 19a	0.2048						
8a	12a → 16a	0.2269	9.118	0.0000	9.009	0.0000	9.069	0.0000
	13a → 15a	0.2262						
	12a → 19a	0.2051						
	13a → 20a	0.2044						
9a	13a → 17a	0.4357	9.568	0.0443	9.321	0.0268	9.658	0.0467
	13a → 14a	0.2535						
	13a → 26a	0.2395						
	13a → 49a	0.2324						
10a	12a → 17a	0.4357	9.568	0.0443	9.321	0.0268	9.658	0.0467
	12a → 14a	0.2535						
	12a → 26a	0.2395						
	12a → 49a	0.2324						
11a	13a → 21a	0.3795	10.088	0.002	9.568	0.0012	10.250	0.0047
	13a → 14a	0.2837						
	13a → 34a	0.2345						
12a	12a → 21a	0.3795	10.088	0.002	9.569	0.0012	10.251	0.0047
	12a → 14a	0.2837						
	12a → 34a	0.2345						
13a	13a → 25a	0.3380	10.404	0.000	9.634	0.0000	10.629	0.0759
	12a → 24a	0.3378						
	13a → 41a	0.2322						
	12a → 40a	0.2321						
14a	13a → 24a	0.3404	10.438	0.0086	9.671	0.0027	10.662	0.0000
	12a → 25a	0.3392						
	13a → 40a	0.2280						
	12a → 41a	0.2273						
15a	12a → 25a	0.3222	10.572	0.0051	9.744	0.0093	10.733	0.0008
	13a → 24a	0.3211						
	12a → 41a	0.2006						
	13a → 40a	0.1999						

Table 14: Excited state properties of **formaldehyde** at EOM-CCSD where SA is the state assignment, E is the vertical excitation energy, and f is the oscillator strength

SA	Excitation Character		EOM-CCSD					
			aug-cc-pVTZ		d-aug-cc-pV(T+d)Z		aug-cc-pVDZ	
			E	f	E	f	E	f
1b2	2b2 → 8a1	0.4281	7.228	0.0184	7.221	0.0175	7.041	0.0184
	12b2 → 6a1	0.3320						
	2b2 → 12a1	0.3138						
2b2	2b2 → 11a1	0.4368	8.117	0.0404	8.023	0.0356	7.991	0.0441
	2b2 → 7a1	0.3589						
	2b2 → 16a1	0.2368						
1a1	2b2 → 4b2	0.4343	8.208	0.0545	8.167	0.0502	8.050	0.0587
	2b2 → 6b2	0.3405						
	2b2 → 3b2	0.2659						
3b2	2b2 → 10a1	0.3936	9.934	0.0495	9.088	0.022	10.326	0.0254
	2b2 → 6a1	0.3190						
	2b2 → 15a1	0.2624						
	2b2 → 9a1	0.2177						
1b1	5a1 → 5b1	0.5028	9.242	0.0006	9.238	0.0008	9.335	0.0008
	5a1 → 4b1	0.3005						
	5a1 → 7b1	0.2473						
4b2	2b2 → 10a1	0.3532	10.405	0.0100	9.316	0.0021	10.686	0.0494
	2b2 → 9a1	0.3267						
	2b2 → 14a1	0.2162						
	2b2 → 6a1	0.2115						
	2b2 → 7a1	0.2040						
2a1	2b2 → 5b2	0.5173	9.631	0.1445	9.328	0.0204	9.714	0.1628
	2b2 → 9b2	0.2523						
	1b1 → 5b1	0.2328						
5b2	2b2 → 6a1	0.4171	10.734	0.0183	9.392	0.0001	11.132	0.0335
	2b2 → 9a1	0.3295						
	2b2 → 12a1	0.2250						
2b1	2b2 → 1a2	0.5907	10.934	0.0439	9.394	0.0018	10.845	0.0435
	2b2 → 2a2	0.2567						
	2b2 → 3a2	0.1788						
3a1	2b2 → 3b2	0.5888	10.349	0.0000	9.593	0.0096	10.445	0.0009
	2b2 → 6b2	0.2524						
	2b2 → 10b2	0.1669						
6b2	2b2 → 7a1	0.5024	12.045	0.0079	9.645	0.0095	12.889	0.0053
	2b2 → 9a1	0.2646						
4a1	2b2 → 5b2	0.3898	11.607	0.1309	9.832	0.1273	12.39	0.0893
	1b1 → 5b1	0.3895						
	1b1 → 4b1	0.2643						
7b2	2b2 → 8a1	0.4449	13.47	0.0931	10.279	0.0056	13.39	0.1056
	2b2 → 12a1	0.2914						
5a1	2b2 → 4b2	0.5054	12.376	0.0068	10.368	0.0301	12.451	0.0007
	2b2 → 6b2	0.3149						
	2b2 → 10b2	0.2304						
	2b2 → 3b2	0.2012						
6a1	2b2 → 7b2	0.6093	12.665	0.0009	10.554	0.0282	12.734	0.0699
	2b2 → 6b2	0.2157						
7a1	2b2 → 8b2	0.6619	13.209	0.3143	10.792	0.0002	13.315	0.1745
3b1	1b1 → 8a1	0.4047	11.574	0.0093	10.927	0.0457	11.855	0.0373
	1b1 → 6a1	0.3118						
	1b1 → 12a1	0.2997						
4b1	2b2 → 2a2	0.5447	11.899	0.0478	10.945	0.0007	13.077	0.0341
	2b2 → 1a2	0.2988						
8a1	2b2 → 9b2	0.5959	13.356	0.1446	11.386	0.0324	14.163	0.3245
	2b2 → 5b2	0.2183						
5b1	1b1 → 11a1	0.4325	13.518	0.0026	11.786	0.0271	13.965	0.0185
	1b1 → 7a1	0.3601						
	1b1 → 16a1	0.2478						
9a1	2b2 → 10b2	0.4803	14.626	0.0172	12.015	0.0776	14.448	0.0199
	2b2 → 6b2	0.3466						
6b1	2b2 → 3a2	0.6049	13.918	0.0242	12.068	0.026	14.041	0.0074
	2b2 → 2a2	0.2094						
7b1	1b1 → 10a1	0.4256	14.071	0.0621	12.756	0.0088	14.283	0.0617
	1b1 → 6a1	0.3012						
	1b1 → 15a1	0.2654						

3.1.2 Formyl chloride

Table 15: Excited state properties of formyl chloride (optimized at CCSD(T)/d-aug-cc-pV(T+d)Z) at EOM-CCSD with Dunning's basis sets where SA is the state assignment, E is the vertical excitation energy and f is the oscillator strength.

SA	Excitation Character		EOM-CCSD								MRD-CI+Q*		Expt**
			aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		t-aug-cc-pV(T+d)Z		aug-cc-pVDZ		DZ+*spd*		
			E	f	E	f	E	f	E	f	E	f	E
$1\ ^1A''$	$13a' \rightarrow 14a''$	0.4299	4.963	0.1824	4.951	0.0001	4.951	0.0001	5.005	0.0001	5.04	0.00001	4.86
	$13a' \rightarrow 16a''$	0.3414											
	$13a' \rightarrow 13a''$	0.2395											
$2\ ^1A''$	$12a' \rightarrow 14a''$	0.4481	7.091	0.2606	7.069	0.0003	7.069	0.0003	7.123	0.0002	6.70	<0.0001	
	$12a' \rightarrow 16a''$	0.3378											
	$12a' \rightarrow 13a''$	0.2517											
$1\ ^1A'$	$3a'' \rightarrow 14a''$	0.3851	7.245	0.2663	7.216	0.0191	7.216	0.0191	7.274	0.0219	6.89	0.03	
	$3a'' \rightarrow 16a''$	0.2881											
	$3a'' \rightarrow 13a''$	0.2133											
$2\ ^1A'$	$13a' \rightarrow 32a'$	0.2713	8.166	0.3001	8.143	0.0617	8.143	0.0618	8.05	0.0476	8.06	0.03	
	$13a' \rightarrow 17a'$	0.2335											
	$13a' \rightarrow 41a'$	0.1979											
	$13a' \rightarrow 22a'$	0.1908											
	$13a' \rightarrow 23a'$	0.1804											
$3\ ^1A''$	$3a'' \rightarrow 47a'$	0.3398	8.230	0.3024	8.154	0.0002	8.154	0.0002	8.325	0.0002	9.07	0.006	
	$3a'' \rightarrow 38a'$	0.2310											
	$3a'' \rightarrow 58a'$	0.1754											
	$3a'' \rightarrow 44a'$	0.1640											
$3\ ^1A'$	$12a' \rightarrow 47a'$	0.3290	8.266	0.3038	8.190	0.0000	8.190	0.0001	8.345	0.0003	8.51	0.03	
	$12a' \rightarrow 38a'$	0.2187											
$4\ ^1A'$	$13a' \rightarrow 38a'$	0.2232	8.810	0.3238	8.725	0.3411	8.725	0.3407	8.77	0.3868	8.80	0.28	
	$13a' \rightarrow 47a'$	0.2128											
	$13a' \rightarrow 23a'$	0.1838											
	$13a' \rightarrow 32a'$	0.1608											
$5\ ^1A'$	$12a' \rightarrow 23a'$	0.2615	9.143	0.3360	9.097	0.0485	9.097	0.0485	9.045	0.0651	9.21	0.16	
	$12a' \rightarrow 17a'$	0.2540											
	$12a' \rightarrow 32a'$	0.2438											
$4\ ^1A''$	$3a'' \rightarrow 32a'$	0.2750	9.142	0.3360	9.099	0.0531	9.099	0.0532	9.041	0.0474	9.21	0.015	
	$3a'' \rightarrow 17a'$	0.2708											
	$3a'' \rightarrow 23a'$	0.2650											
	$3a'' \rightarrow 22a'$	0.1672											
$6\ ^1A'$	$13a' \rightarrow 16a'$	0.3691	9.419	0.3462	9.247	0.0897			9.383	0.0653			
	$13a' \rightarrow 23a'$	0.2249											
	$13a' \rightarrow 22a'$	0.1940											
	$13a' \rightarrow 25a'$	0.1916											
$5\ ^1A''$	$13a' \rightarrow 6a''$	0.3075	9.530	0.0032	9.250	0.0024	9.249	0.0024	9.540	0.0032	9.38	0.009	
	$13a' \rightarrow 8a''$	0.3055											
	$13a' \rightarrow 9a''$	0.2389											
	$13a' \rightarrow 13a''$	0.1853											
	$13a' \rightarrow 15a''$	0.1816											
$6\ ^1A''$	$11a' \rightarrow 8a''$	0.4512	10.030	0.0043	10.014	0.0070			10.148	0.0083	9.97	0.001	
	$10a' \rightarrow 8a''$	0.2296											
	$11a' \rightarrow 7a''$	0.1760											
	$11a' \rightarrow 11a''$	0.1297											
	$3a'' \rightarrow 22a'$	0.1229											
	$3a'' \rightarrow 15a'$	0.1054											
$7\ ^1A''$	$3a'' \rightarrow 16a'$	0.2802	10.253	0.0148	10.054	0.0011			10.277	0.0115			
	$3a'' \rightarrow 22a'$	0.2569											
	$12a' \rightarrow 4a''$	0.1869											
	$11a' \rightarrow 8a''$	0.1715											
	$3a'' \rightarrow 15a'$	0.1654											
	$3a'' \rightarrow 19a'$	0.1528											

* Reference [**?**]

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Table 16: Excited state properties of formyl chloride (optimized at CCSD(T)/d-aug-cc-pV(T+d)Z)) at EOM-CCSD where SA is the state assignment, E is the vertical excitation energy, and f is the oscillator strength

SA	Excitation Character		def2-TZVP-RI		def2-TZVPPD-RI		def2-TZVP-JFIT	
			E	f	E	f	E	f
$1\ ^1A''$	$13a' \rightarrow 14a''$	0.4299	4.978	0.0001	4.971	0.0001	5.023	0.0000
	$13a' \rightarrow 16a''$	0.3414						
	$13a' \rightarrow 13a''$	0.2395						
$2\ ^1A''$	$12a' \rightarrow 14a''$	0.4481	7.178	0.0002	7.129	0.0002	5.477	0.0000
	$12a' \rightarrow 16a''$	0.3378						
	$12a' \rightarrow 13a''$	0.2517						
$1\ ^1A'$	$3a'' \rightarrow 14a''$	0.3851	7.327	0.0214	7.285	0.0207	6.252	0.1046
	$3a'' \rightarrow 16a''$	0.2881						
	$3a'' \rightarrow 13a''$	0.2133						
$2\ ^1A'$	$13a' \rightarrow 32a'$	0.2713	8.397	0.0011	8.321	0.0007	7.475	0.0005
	$13a' \rightarrow 17a'$	0.2335						
	$13a' \rightarrow 41a'$	0.1979						
	$13a' \rightarrow 22a'$	0.1908						
	$13a' \rightarrow 23a'$	0.1804						
$3\ ^1A'$	$12a' \rightarrow 47a'$	0.3290	8.774	0.3069	8.746	0.3084	10.218	0.2671
	$12a' \rightarrow 38a'$	0.2187						
$3\ ^1A''$	$3a'' \rightarrow 47a'$	0.3398	8.342	0.0008	8.274	0.0004	7.731	0.0007
	$3a'' \rightarrow 38a'$	0.2310						
	$3a'' \rightarrow 58a'$	0.1754						
	$3a'' \rightarrow 44a'$	0.1640						
$4\ ^1A'$	$13a' \rightarrow 38a'$	0.2232	9.458	0.1817	9.389	0.1830	10.931	0.1343
	$13a' \rightarrow 47a'$	0.2128						
	$13a' \rightarrow 23a'$	0.1838						
	$13a' \rightarrow 32a'$	0.1608						
$4\ ^1A''$	$3a'' \rightarrow 32a'$	0.2750	9.935	0.093	9.836	0.0905	9.641	0.0080
	$3a'' \rightarrow 17a'$	0.2708						
	$3a'' \rightarrow 23a'$	0.2650						
	$3a'' \rightarrow 22a'$	0.1672						
$5\ ^1A'$	$12a' \rightarrow 23a'$	0.2615	9.927	0.0749	9.814	0.0737	11.962	0.0456
	$12a' \rightarrow 17a'$	0.2540						
	$12a' \rightarrow 32a'$	0.2438						
$6\ ^1A'$	$13a' \rightarrow 16a'$	0.3691	10.425	0.0259	10.396	0.0221	12.677	0.1973
	$13a' \rightarrow 23a'$	0.2249						
	$13a' \rightarrow 22a'$	0.1940						
	$13a' \rightarrow 25a'$	0.1916						
$5\ ^1A''$	$13a' \rightarrow 6a''$	0.3075	10.049	0.0047	10.044	0.0032	11.007	0.0039
	$13a' \rightarrow 8a''$	0.3055						
	$13a' \rightarrow 9a''$	0.2389						
	$13a' \rightarrow 13a''$	0.1853						
	$13a' \rightarrow 15a''$	0.1816						
$6\ ^1A''$	$11a' \rightarrow 5a''$	0.4139	11.015	0.0001	11.009	0.0000	12.049	0.0003
	$11a' \rightarrow 4a''$	0.3402						
	$10a' \rightarrow 5a''$	0.2288						
$7\ ^1A''$	$3a'' \rightarrow 16a'$	0.3331	11.744	0.0233	11.661	0.0182	12.79	0.0077
	$3a'' \rightarrow 15a'$	0.3323						
	$3a'' \rightarrow 14a'$	0.2646						
	$3a'' \rightarrow 17a'$	0.2552						

Table 17: Excited state properties of formyl chloride (optimized at B3LYP/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength. States are characterized with d-aug-cc-pV(T+d)Z basis.

SA	Excitation Character		aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		t-aug-cc-pV(D+d)Z		aug-cc-pVDZ		aug-cc-pV(D+d)Z	
			E	f	E	f	E	f	E	f	E	f
$1\ ^1A''$	$13a' \rightarrow 14a''$	0.4514	5.051	0.0001	5.049	0.0001	5.048	0.0001	5.102	0.0001	5.088	0.0001
	$13a' \rightarrow 16a''$	0.3449										
$2\ ^1A''$	$12a' \rightarrow 14a''$	0.4723	7.085	0.0002	7.081	0.0003	7.080	0.0003	7.132	0.0002	7.117	0.0002
	$12a' \rightarrow 16a''$	0.3420										
$1\ ^1A'$	$3a'' \rightarrow 14a''$	0.4042	7.214	0.0135	7.209	0.0133	7.209	0.0132	7.265	0.0156	7.233	0.0133
	$3a'' \rightarrow 16a''$	0.2909										
$3\ ^1A''$	$3a'' \rightarrow 47a'$	0.3476	8.066	0.0002	8.058	0.0001	8.058	0.0001	8.222	0.0002	8.135	0.0003
	$3a'' \rightarrow 38a'$	0.2316										
	$3a'' \rightarrow 44a'$	0.1713										
	$3a'' \rightarrow 58a'$	0.1635										
$2\ ^1A'$	$12a' \rightarrow 47a'$	0.3335	8.085	0.0015	8.079	0.0016	8.079	0.0016	8.082	0.0578	8.067	0.063
	$12a' \rightarrow 38a'$	0.2192										
	$12a' \rightarrow 44a'$	0.1751										
$3\ ^1A'$	$13a' \rightarrow 32a'$	0.2630	8.184	0.0776	8.174	0.0738	8.174	0.0739	8.228	0.0001	8.141	0.0003
	$13a' \rightarrow 17a'$	0.2266										
	$13a' \rightarrow 41a'$	0.1928										
$4\ ^1A'$	$13a' \rightarrow 47a'$	0.2186	8.802	0.3919	8.736	0.3560	8.736	0.3556	8.776	0.4008	8.758	0.4109
	$13a' \rightarrow 38a'$	0.2184										
	$13a' \rightarrow 23a'$	0.1850										
	$13a' \rightarrow 32a'$	0.1649										
	$13a' \rightarrow 17a'$	0.1616										
	$3a'' \rightarrow 14a''$	0.1547										
	$13a' \rightarrow 27a'$	0.1505										
$5\ ^1A'$	$12a' \rightarrow 23a'$	0.2592	9.091	0.052	9.047	0.0513	9.047	0.0513	8.995	0.0728	9.000	0.0632
	$12a' \rightarrow 17a'$	0.2543										
	$12a' \rightarrow 32a'$	0.2471										
$6\ ^1A'$			9.438	0.1011					9.416	0.0713		
$4\ ^1A''$	$3a'' \rightarrow 32a'$	0.2756	9.115	0.0552	9.073	0.0575	9.073	0.0576	9.014	0.0516	9.020	0.0521
	$3a'' \rightarrow 17a'$	0.2706										
	$3a'' \rightarrow 23a'$	0.2633										
	$3a'' \rightarrow 22a'$	0.1726										
$5\ ^1A''$	$13a' \rightarrow 8a''$	0.3061	9.559	0.0033	9.287	0.0026	9.286	0.0026	9.578	0.0032	9.575	0.0032
	$13a' \rightarrow 6a''$	0.3057										
	$13a' \rightarrow 9a''$	0.2365										
$6\ ^1A''$			10.128	0.0071					10.220	0.0228	10.204	0.0257
$7\ ^1A''$			10.22	0.0141					10.272	0.0005	10.259	0.0005

Table 18: Excited state properties of formyl chloride (optimized at MP2/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength. States are characterized with d-aug-cc-pV(T+d)Z basis.

SA	Excitation Character		aug-cc-pVTZ		aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		t-aug-cc-pV(T+d)Z		t-aug-cc-pVDZ		aug-cc-pV(D+d)Z	
			E	f	E	f	E	f	E	f	E	f	E	f
$1\ ^1A''$	$13a' \rightarrow 14a''$	0.4585	4.986	0.0001	4.976	0.0001	3.414	0.0001	4.973	0.0001	5.028	0.0001	5.012	0.0001
	$13a' \rightarrow 16a''$	0.3485												
	$13a' \rightarrow 13a''$	0.1588												
	$13a' \rightarrow 17a''$	0.1428												
	$13a' \rightarrow 24a''$	0.1272												
$2\ ^1A''$	$12a' \rightarrow 14a''$	0.4781	7.132	0.0003	7.113	0.0003	3.705	0.0003	7.109	0.0003	7.169	0.0002	7.151	0.0002
	$12a' \rightarrow 16a''$	0.3457												
	$12a' \rightarrow 13a''$	0.1675												
	$12a' \rightarrow 17a''$	0.1354												
	$12a' \rightarrow 9a''$	0.1132												
$1\ ^1A'$	$3a'' \rightarrow 14a''$	0.4137	7.319	0.0260	7.293	0.024	7.288	0.0237	7.288	0.0237	7.351	0.0270	7.316	0.0234
	$3a'' \rightarrow 16a''$	0.2970												
	$13a' \rightarrow 47a'$	0.1531												
	$3a'' \rightarrow 13a''$	0.1418												
	$3a'' \rightarrow 17a''$	0.1172												
	$13a' \rightarrow 58a'$	0.1064												
	$13a' \rightarrow 38a'$	0.1062												
$2\ ^1A'$	$13a' \rightarrow 32a'$	0.2770	8.169	0.0461	8.157	0.0503	8.145	0.0467	8.145	0.0468	8.049	0.0372	8.034	0.0415
	$13a' \rightarrow 17a'$	0.2397												
	$13a' \rightarrow 41a'$	0.1988												
	$13a' \rightarrow 22a'$	0.1925												
	$13a' \rightarrow 23a'$	0.1882												
	$13a' \rightarrow 24a'$	0.1446												
$3\ ^1A''$	$3a'' \rightarrow 47a'$	0.3199	8.372	0.0003	8.301	0.0005	3.736	0.0002	8.291	0.0003	8.468	0.0004	8.371	0.0006
	$3a'' \rightarrow 47a'$	0.3199												
	$3a'' \rightarrow 38a'$	0.2267												
	$3a'' \rightarrow 58a'$	0.1892												
	$3a'' \rightarrow 51a'$	0.1653												
	$3a'' \rightarrow 41a'$	0.1536												
	$3a'' \rightarrow 44a'$	0.1535												
$3\ ^1A'$	$12a' \rightarrow 47a'$	0.3096	8.403	0.0000	8.330	0.0001	8.323	0.0001	8.323	0.0001	8.483	0.0001	8.386	0.0000
	$12a' \rightarrow 38a'$	0.2123												
	$12a' \rightarrow 58a'$	0.1689												
	$12a' \rightarrow 41a'$	0.1646												
	$12a' \rightarrow 44a'$	0.1594												
	$12a' \rightarrow 55a'$	0.1521												
$4\ ^1A'$	$13a' \rightarrow 38a'$	0.2264	8.852	0.3663	8.835	0.3706	8.760	0.3277	8.760	0.3273	8.811	0.3667	8.791	0.3805
	$13a' \rightarrow 47a'$	0.1933												
	$13a' \rightarrow 23a'$	0.1759												
	$13a' \rightarrow 27a'$	0.1720												
	$3a'' \rightarrow 14a''$	0.1518												
	$13a' \rightarrow 32a'$	0.1508												
$4\ ^1A''$	$3a'' \rightarrow 32a'$	0.2734	9.165	0.0489	9.164	0.0493	3.808	0.0000	9.122	0.0519	9.066	0.0460	9.071	0.0464
	$3a'' \rightarrow 17a'$	0.2698												
	$3a'' \rightarrow 23a'$	0.2654												
	$3a'' \rightarrow 22a'$	0.1638												
	$3a'' \rightarrow 28a'$	0.1563												
	$3a'' \rightarrow 14a'$	0.1531												
$5\ ^1A'$	$12a' \rightarrow 23a'$	0.2612	9.171	0.0534	9.169	0.0498	9.124	0.0492	9.124	0.0492	9.075	0.0677	9.078	0.0602
	$12a' \rightarrow 17a'$	0.2520												
	$12a' \rightarrow 32a'$	0.2397												
	$12a' \rightarrow 28a'$	0.1745												
	$12a' \rightarrow 38a'$	0.1566												
$6\ ^1A'$	$13a' \rightarrow 16a'$	0.3758	9.427	0.0838	9.415	0.1144	9.250	0.0835			9.386	0.0513	9.375	0.0743
	$13a' \rightarrow 23a'$	0.2417												
$5\ ^1A''$	$13a' \rightarrow 6a''$	0.3069	9.507	0.0033	9.504	0.0033	3.912	0.0005	9.233	0.0023	9.520	0.0033	9.515	0.0034
	$13a' \rightarrow 8a''$	0.3038												
	$13a' \rightarrow 9a''$	0.2397												
	$13a' \rightarrow 15a''$	0.1831												
	$13a' \rightarrow 13a''$	0.1825												
	$13a' \rightarrow 4a''$	0.1598												
$6\ ^1A''$	$13a' \rightarrow 8a''$	0.1608	10.093	0.0050	10.083	0.005	3.923	0.0000			10.202	0 .0099	10.188	0.0107
	$12a' \rightarrow 8a''$	0.0782												
	$13a' \rightarrow 7a''$	0.0666												
	$13a' \rightarrow 12a''$	0.0445												
	$13a' \rightarrow 11a''$	0.0420												

3.1.3 Chloroketene

Table 19: Excited state properties of chloroketene (optimized at CCSD(T)/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation	Character	aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		COM/aug-cc-pV(T+d)Z		t-aug-cc-pV(T+d)Z	
			E	f	E	f	E	f	E	f
$1\ ^1A''$	$4a'' \rightarrow 45a'$	0.3926	3.057	0.0000	3.057	0.0000	3.057	0.000	3.057	0.0000
	$4a'' \rightarrow 46a'$	0.2457								
	$4a'' \rightarrow 41a'$	0.2350								
	$4a'' \rightarrow 48a'$	0.1943								
$2\ ^1A''$	$4a'' \rightarrow 40a'$	0.1905	5.759	0.0043	5.749	0.0040	5.751	0.0041	5.749	0.0040
	$4a'' \rightarrow 28a'$	0.1878								
	$4a'' \rightarrow 51a'$	0.1800								
	$4a'' \rightarrow 26a'$	0.1786								
	$4a'' \rightarrow 41a'$	0.1646								
	$4a'' \rightarrow 21a'$	0.1638								
	$4a'' \rightarrow 47a'$	0.1513								
$3\ ^1A''$	$4a'' \rightarrow 32a'$	0.1870	6.753	0.0015	6.692	0.0020	6.701	0.0020	6.692	0.0020
	$4a'' \rightarrow 28a'$	0.1867								
	$4a'' \rightarrow 52a'$	0.1574								
	$4a'' \rightarrow 46a'$	0.1564								
	$4a'' \rightarrow 23a'$	0.1537								
	$4a'' \rightarrow 70a'$	0.1537								
$1\ ^1A'$	$15a' \rightarrow 45a'$	0.3840	6.730	0.0019	6.729	0.0018	6.729	0.0018	6.729	0.0018
	$15a' \rightarrow 41a'$	0.2623								
	$15a' \rightarrow 46a'$	0.2079								
	$15a' \rightarrow 48a'$	0.1862								
$4\ ^1A''$	$4a'' \rightarrow 32a'$	0.2451	7.1460	0.0013	7.055	0.0008	7.073	0.0010	7.055	0.0008
	$4a'' \rightarrow 23a'$	0.1904								
	$4a'' \rightarrow 26a'$	0.1707								
	$4a'' \rightarrow 35a'$	0.1506								
$2\ ^1A'$	$4a'' \rightarrow 12a''$	0.2767	7.298	0.1385	7.102	0.0543	7.184	0.0773	7.102	0.0544
	$4a'' \rightarrow 7a''$	0.2763								
	$4a'' \rightarrow 18a''$	0.2272								
	$4a'' \rightarrow 28a''$	0.1968								
$5\ ^1A''$	$4a'' \rightarrow 30a'$	0.2445	7.3640	0.0065	7.221	0.0048	7.247	0.0051	7.221	0.0049
	$4a'' \rightarrow 22a'$	0.2259								
	$4a'' \rightarrow 60a'$	0.1589								
	$4a'' \rightarrow 23a'$	0.1562								
	$4a'' \rightarrow 47a'$	0.1506								
$3\ ^1A'$	$4a'' \rightarrow 28a''$	0.3200	7.611	0.0525	7.416	0.1153	7.444	0.0914	7.413	0.1136
	$4a'' \rightarrow 21a''$	0.2054								
	$4a'' \rightarrow 7a''$	0.1807								
$6\ ^1A''$	$3a'' \rightarrow 45a'$	0.2909	7.8150	0.0013	7.730	0.0001	7.733	0.0002	7.729	0.0002
	$4a'' \rightarrow 21a'$	0.2021								
	$3a'' \rightarrow 41a'$	0.1828								
	$3a'' \rightarrow 46a'$	0.1690								
	$4a'' \rightarrow 16a'$	0.1632								
$7\ ^1A''$	$4a'' \rightarrow 24a'$	0.2718	8.4540	0.0094	7.872	0.0089	7.876	0.0080	7.850	0.0079
	$4a'' \rightarrow 33a'$	0.2003								
	$4a'' \rightarrow 44a'$	0.1695								
	$4a'' \rightarrow 39a'$	0.1621								
$4\ ^1A'$	$4a'' \rightarrow 9a''$	0.4107	8.640	0.0365	8.004	0.0298	8.037	0.0297	7.994	0.0263
	$4a'' \rightarrow 16a''$	0.2380								
	$4a'' \rightarrow 6a''$	0.2227								
$8\ ^1A''$	$4a'' \rightarrow 30a'$	0.2214	8.6830	0.0101	7.973	0.0001	7.989	0.0007	7.957	0.0006
	$4a'' \rightarrow 26a'$	0.2028								
	$4a'' \rightarrow 19a'$	0.1906								
	$4a'' \rightarrow 22a'$	0.1902								
$9\ ^1A''$	$4a'' \rightarrow 29a'$	0.2471							8.031	0.0026
	$4a'' \rightarrow 20a''$	0.2078								
	$4a'' \rightarrow 38a''$	0.2029								
	$4a'' \rightarrow 28a''$	0.1847								
$5\ ^1A'$	$4a'' \rightarrow 8a''$	0.3962	8.6640	0.0388	8.157	0.0114	8.147	0.0143	8.082	0.0161
	$4a'' \rightarrow 13a''$	0.2287								
	$4a'' \rightarrow 16a''$	0.2031								
$6\ ^1A'$	$4a'' \rightarrow 5a''$	0.5010	9.1500	0.0656	8.522	0.0056	8.433	0.0062	8.349	0.0038
	$4a'' \rightarrow 7a''$	0.2917								
$7\ ^1A'$	$15a' \rightarrow 21a'$	0.3304	9.4960	0.0514	8.644	0.0171	8.646	0.0179		
	$15a' \rightarrow 16a'$	0.2530								
	$15a' \rightarrow 28a'$	0.1950								
	$15a' \rightarrow 30a'$	0.1684								
	$15a' \rightarrow 31a'$	0.1657								
$8\ ^1A'$	$4a'' \rightarrow 6a''$	0.3574	9.8220	0.5451	8.914	0.0193	8.838	0.0007		
	$4a'' \rightarrow 9a''$	0.3558								
	$4a'' \rightarrow 11a''$	0.3269								
$9\ ^1A'$	$4a'' \rightarrow 11a''$	0.4229	10.1100	0.1129	9.146	0.0140	9.183	0.0000		
	$4a'' \rightarrow 9a''$	0.3306								
	$4a'' \rightarrow 8a''$	0.2366								

Table 20: Excited state properties of chloroketene (optimized at B3LYP/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation	Character	aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		t-aug-cc-pV(T+d)Z	
			E	f	E	f	E	f
$1\ ^1A''$	$4a'' \rightarrow 45a'$	0.3392	3.090	0.0000	3.090	0.0000	3.090	0.0000
	$4a'' \rightarrow 46a'$	0.3133						
	$4a'' \rightarrow 41a'$	0.2324						
	$4a'' \rightarrow 48a'$	0.2025						
$2\ ^1A''$	$4a'' \rightarrow 28a'$	0.1889	5.787	0.0042	5.776	0.0039	5.777	0.0039
	$4a'' \rightarrow 40a'$	0.1836						
	$4a'' \rightarrow 26a'$	0.1804						
	$4a'' \rightarrow 51a'$	0.1801						
$1\ ^1A'$	$15a' \rightarrow 45a'$	0.3389	6.705	0.0022	6.704	0.0021	6.704	0.0021
	$15a' \rightarrow 46a'$	0.2755						
	$15a' \rightarrow 41a'$	0.2597						
	$15a' \rightarrow 48a'$	0.1947						
$3\ ^1A''$	$4a'' \rightarrow 32a'$	0.1857	6.773	0.0015	6.712	0.0021	6.713	0.0021
	$4a'' \rightarrow 28a'$	0.1849						
	$4a'' \rightarrow 52a'$	0.1576						
	$4a'' \rightarrow 70a'$	0.1546						
	$4a'' \rightarrow 23a'$	0.1532						
$4\ ^1A''$	$4a'' \rightarrow 32a'$	0.2468	7.167	0.0013	7.075	0.0008	7.075	0.0008
	$4a'' \rightarrow 23a'$	0.1921						
	$4a'' \rightarrow 26a'$	0.1683						
	$4a'' \rightarrow 35a'$	0.1525						
$2\ ^1A'$	$4a'' \rightarrow 7a''$	0.2866	7.351	0.1143	7.127	0.0429	7.126	0.0430
	$4a'' \rightarrow 12a''$	0.2842						
	$4a'' \rightarrow 18a''$	0.2363						
	$4a'' \rightarrow 13a''$	0.1798						
$5\ ^1A''$	$4a'' \rightarrow 30a'$	0.2485	7.375	0.0066	7.232	0.0048	7.232	0.0049
	$4a'' \rightarrow 22a'$	0.2279						
	$4a'' \rightarrow 23a'$	0.1545						
	$4a'' \rightarrow 60a'$	0.1542						
$3\ ^1A'$	$4a'' \rightarrow 28a''$	0.3078	7.654	0.0636	7.481	0.1115	7.477	0.1095
	$4a'' \rightarrow 21a''$	0.2140						
	$4a'' \rightarrow 29a''$	0.1908						
	$4a'' \rightarrow 7a''$	0.1642						
$6\ ^1A''$	$3a'' \rightarrow 45a'$	0.2526	7.822	0.0013	7.734	0.0002	7.734	0.0002
	$3a'' \rightarrow 46a'$	0.2182						
	$4a'' \rightarrow 21a'$	0.2024						
	$3a'' \rightarrow 41a'$	0.1797						
	$4a'' \rightarrow 16a'$	0.1624						
$7\ ^1A''$	$4a'' \rightarrow 24a'$	0.2707	8.469	0.0095	7.889	0.0088	7.866	0.0078
	$4a'' \rightarrow 33a'$	0.1981						
	$4a'' \rightarrow 44a'$	0.1718						
	$4a'' \rightarrow 39a'$	0.1591						
	$4a'' \rightarrow 38a'$	0.1540						
	$4a'' \rightarrow 53a'$	0.1504						
$8\ ^1A''$	$4a'' \rightarrow 30a'$	0.2224	8.702	0.0105	7.990	0.0001	7.973	0.0005
	$4a'' \rightarrow 26a'$	0.2031						
	$4a'' \rightarrow 19a'$	0.1901						
	$4a'' \rightarrow 22a'$	0.1896						
	$4a'' \rightarrow 16a'$	0.1777						
	$4a'' \rightarrow 35a'$	0.1579						
$9\ ^1A''$	$4a'' \rightarrow 29a'$	0.2462					8.050	0.0026
	$4a'' \rightarrow 20a'$	0.2090						
	$4a'' \rightarrow 38a'$	0.2041						
	$4a'' \rightarrow 28a'$	0.1850						
$4\ ^1A'$	$4a'' \rightarrow 9a''$	0.4182	8.656	0.0093	8.021	0.0301	8.011	0.0257
	$4a'' \rightarrow 16a''$	0.2452						
	$4a'' \rightarrow 6a''$	0.2235						
	$4a'' \rightarrow 15a''$	0.1971						
	$4a'' \rightarrow 18a''$	0.1795						
$5\ ^1A'$	$4a'' \rightarrow 8a''$	0.3990	8.671	0.0686	8.185	0.0137	8.110	0.0195
	$4a'' \rightarrow 13a''$	0.2256						
	$4a'' \rightarrow 16a''$	0.1906						
	$4a'' \rightarrow 11a''$	0.1803						
	$4a'' \rightarrow 9a''$	0.1762						
	$4a'' \rightarrow 14a''$	0.1545						
$6\ ^1A'$	$4a'' \rightarrow 5a''$	0.4999	9.177	0.0621	8.539	0.0056	8.366	0.0041
	$4a'' \rightarrow 7a''$	0.2918						
	$4a'' \rightarrow 18a''$	0.1869						
$7\ ^1A'$	$15a' \rightarrow 21a'$	0.3345	9.508	0.0514	8.645	0.0178		
	$15a' \rightarrow 16a'$	0.2562						
	$15a' \rightarrow 28a'$	0.1932						
	$15a' \rightarrow 30a'$	0.1731						
$8\ ^1A'$	$4a'' \rightarrow 9a''$	0.3563	9.857	0.5038	8.931	0.0192		
	$4a'' \rightarrow 6a''$	0.3550						
	$4a'' \rightarrow 11a''$	0.3302						
$9\ ^1A'$	$4a'' \rightarrow 11a''$	0.4238	10.145	0.2035	9.164	0.0139		
	$4a'' \rightarrow 9a''$	0.3309						
	$4a'' \rightarrow 8a''$	0.2348						

Table 21: Excited state properties of chloroketene (optimized at MP2/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation Character		aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		t-aug-cc-pV(T+d)Z	
			E	f	E	f	E	f
$1\ ^1A''$	$4a'' \rightarrow 46a'$	0.4513	3.113	0.000	3.113	0.000	3.113	0.0000
	$4a'' \rightarrow 48a'$	0.2313						
	$4a'' \rightarrow 41a'$	0.2070						
	$4a'' \rightarrow 50a'$	0.1556						
$2\ ^1A''$	$4a'' \rightarrow 28a'$	0.1930	5.758	0.0041	5.747	0.0039	5.747	0.0039
	$4a'' \rightarrow 51a'$	0.1856						
	$4a'' \rightarrow 26a'$	0.1814						
	$4a'' \rightarrow 40a'$	0.1814						
	$4a'' \rightarrow 21a'$	0.1682						
	$4a'' \rightarrow 41a'$	0.1624						
$3\ ^1A''$	$4a'' \rightarrow 32a'$	0.2172	6.794	0.0027	6.719	0.0034	6.720	0.0034
	$4a'' \rightarrow 23a'$	0.1821						
	$4a'' \rightarrow 28a'$	0.1799						
	$4a'' \rightarrow 45a'$	0.1627						
$1\ ^1A'$	$15a' \rightarrow 46a'$	0.4244	6.835	0.0019	6.834	0.0017	6.834	0.0017
	$15a' \rightarrow 41a'$	0.2369						
	$15a' \rightarrow 48a'$	0.2233						
$4\ ^1A''$	$4a'' \rightarrow 32a'$	0.2143	7.135	0.0007	7.044	0.0002	7.044	0.0002
	$4a'' \rightarrow 26a'$	0.1790						
	$4a'' \rightarrow 30a'$	0.1757						
	$4a'' \rightarrow 22a'$	0.1750						
$2\ ^1A'$	$4a'' \rightarrow 7a''$	0.2882	7.310	0.1263	7.086	0.0438	7.086	0.0439
	$4a'' \rightarrow 12a''$	0.2861						
	$4a'' \rightarrow 18a''$	0.2351						
	$4a'' \rightarrow 13a''$	0.1788						
$5\ ^1A''$	$4a'' \rightarrow 30a'$	0.2184	7.353	0.0064	7.218	0.0044	7.218	0.0045
	$4a'' \rightarrow 22a'$	0.2066						
	$4a'' \rightarrow 60a'$	0.1770						
	$4a'' \rightarrow 23a'$	0.1607						
	$4a'' \rightarrow 47a'$	0.1506						
$3\ ^1A'$	$4a'' \rightarrow 21a''$	0.2160	7.590	0.0682	7.418	0.1248	7.415	0.1226
	$4a'' \rightarrow 29a''$	0.1738						
	$4a'' \rightarrow 7a''$	0.1593						
	$4a'' \rightarrow 16a''$	0.1518						
$6\ ^1A''$	$3a'' \rightarrow 46a'$	0.2986	7.906	0.0008	7.797	0.0003	7.794	0.0007
	$4a'' \rightarrow 21a'$	0.2366						
	$4a'' \rightarrow 16a'$	0.2085						
	$3a'' \rightarrow 48a'$	0.1522						
$7\ ^1A''$	$4a'' \rightarrow 24a'$	0.2645	8.423	0.0094	7.846	0.0078	7.824	0.0064
	$4a'' \rightarrow 33a'$	0.2154						
	$4a'' \rightarrow 44a'$	0.1819						
	$4a'' \rightarrow 45a'$	0.1588						
	$4a'' \rightarrow 31a'$	0.1505						
$8\ ^1A''$	$4a'' \rightarrow 30a'$	0.2240	8.655	0.0096	7.947	0.0002	7.931	0.0006
	$4a'' \rightarrow 26a'$	0.2039						
	$4a'' \rightarrow 22a'$	0.1896						
	$4a'' \rightarrow 19a'$	0.1866						
	$4a'' \rightarrow 35a'$	0.1669						
	$4a'' \rightarrow 16a'$	0.1665						
$4\ ^1A'$	$4a'' \rightarrow 9a''$	0.4154	8.610	0.0555	7.975	0.0304	7.966	0.0262
	$4a'' \rightarrow 16a''$	0.2438						
	$4a'' \rightarrow 6a''$	0.2222						
	$4a'' \rightarrow 15a''$	0.1973						
	$4a'' \rightarrow 18a''$	0.1811						
$5\ ^1A'$	$4a'' \rightarrow 8a''$	0.4017	8.681	0.0271	8.146	0.0175	8.070	0.0232
	$4a'' \rightarrow 13a''$	0.2246						
	$4a'' \rightarrow 16a''$	0.1909						
	$4a'' \rightarrow 9a''$	0.1807						
	$4a'' \rightarrow 11a''$	0.1798						
$6\ ^1A'$	$4a'' \rightarrow 5a''$	0.5006	9.152	0.0374	8.492	0.0058	8.320	0.0041
	$4a'' \rightarrow 7a''$	0.2926						
	$4a'' \rightarrow 18a''$	0.1864						
	$4a'' \rightarrow 20a''$	0.1200						
$7\ ^1A'$	$15a' \rightarrow 21a'$	0.3343	9.517	0.0496	8.663	0.0192		
	$15a' \rightarrow 16a'$	0.2568						
	$15a' \rightarrow 28a'$	0.1940						
	$15a' \rightarrow 30a'$	0.1880						
$7\ ^1A'$	$4a'' \rightarrow 9a''$	0.3608	9.869	0.4879	8.889	0.0245		
	$4a'' \rightarrow 6a''$	0.3591						
	$4a'' \rightarrow 11a''$	0.3204						
$9\ ^1A''$	$4a'' \rightarrow 29a'$	0.2465	10.13	0.1621	9.123	0.0074	8.005	0.0025
	$4a'' \rightarrow 38a'$	0.2113						
	$4a'' \rightarrow 20a'$	0.2078						
	$4a'' \rightarrow 28a'$	0.1883						
	$4a'' \rightarrow 25a'$	0.1718						
	$4a'' \rightarrow 27a'$	0.1709						

3.1.4 Propadienone chloride

Table 22: Excited state properties of propadienone chloride (optimized at CCSD(T)/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation	Character	aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		COM/aug-cc-pV(T+d)Z	
			E	f	E	f	E	f
$1\ ^1A''$	$18a' \rightarrow 6a''$	0.6198	2.560	0.0002	2.559	0.0002	2.559	0.0002
	$18a' \rightarrow 7a''$	0.2039						
$1\ ^1A'$	$4a'' \rightarrow 6a''$	0.5040	4.903	0.0813	4.902	0.0809	4.902	0.0812
	$18a' \rightarrow 39a'$	0.1833						
	$4a'' \rightarrow 7a''$	0.1646						
$2\ ^1A''$	$17a' \rightarrow 6a''$	0.6197	6.103	0.0000	6.103	0.0000	6.103	0.0000
	$17a' \rightarrow 7a''$	0.2002						
$3\ ^1A''$	$4a'' \rightarrow 39a'$	0.3180	6.208	0.0023	6.205	0.0023	6.207	0.0023
	$4a'' \rightarrow 43a'$	0.2363						
	$4a'' \rightarrow 33a'$	0.2321						
	$4a'' \rightarrow 36a'$	0.2132						
$2\ ^1A'$	$4a'' \rightarrow 6a''$	0.2587	6.228	0.2265	6.212	0.2167	6.216	0.2172
	$18a' \rightarrow 25a'$	0.2327						
	$18a' \rightarrow 33a'$	0.2308						
	$18a' \rightarrow 24a'$	0.2184						
	$18a' \rightarrow 19a'$	0.1989						
	$18a' \rightarrow 35a'$	0.1842						
$3\ ^1A'$	$18a' \rightarrow 39a'$	0.2235	7.007	0.4432	6.965	0.4237	6.970	0.4284
	$18a' \rightarrow 43a'$	0.2071						
	$4a'' \rightarrow 6a''$	0.1968						
	$18a' \rightarrow 19a'$	0.1803						
$4\ ^1A'$	$18a' \rightarrow 28a'$	0.3304	7.224	0.0312	7.189	0.0429	7.198	0.0384
	$18a' \rightarrow 20a'$	0.2574						
	$18a' \rightarrow 19a'$	0.2468						
	$18a' \rightarrow 24a'$	0.2389						
	$18a' \rightarrow 37a'$	0.2131						
$4\ ^1A''$	$18a' \rightarrow 5a''$	0.4460	7.583	0.0004	7.471	0.0027	7.538	0.0014
	$18a' \rightarrow 10a''$	0.3245						
	$18a' \rightarrow 9a''$	0.1909						
$5\ ^1A''$	$4a'' \rightarrow 19a'$	0.2779	7.800	0.0033	7.557	0.0000	7.589	0.0014
	$4a'' \rightarrow 24a'$	0.2682						
	$4a'' \rightarrow 25a'$	0.2407						
$5\ ^1A'$	$18a' \rightarrow 21a'$	0.3995	7.693	0.0022	7.574	0.0145	7.604	0.0151
	$18a' \rightarrow 30a'$	0.3452						
	$18a' \rightarrow 40a'$	0.1366						
	$18a' \rightarrow 31a'$	0.1121						
$6\ ^1A'$	$3a'' \rightarrow 6a''$	0.3458	7.790	0.0508	7.697	0.006	7.703	0.0075
	$17a' \rightarrow 39a'$	0.1772						
	$17a' \rightarrow 43a'$	0.1758						
	$17a' \rightarrow 33a'$	0.1317						
$7\ ^1A'$	$3a'' \rightarrow 6a''$	0.2440	7.916	0.1847	7.876	0.1548	7.882	0.1598
	$17a' \rightarrow 43a'$	0.2059						
	$17a' \rightarrow 39a'$	0.1992						
	$17a' \rightarrow 33a'$	0.1417						
	$18a' \rightarrow 32a'$	0.1413						
$6\ ^1A''$	$15a' \rightarrow 6a''$	0.2878	7.983	0.0044	7.968	0.0054	7.973	0.0052
	$16a' \rightarrow 6a''$	0.2803						
	$18a' \rightarrow 27a''$	0.2395						
$7\ ^1A''$	$4a'' \rightarrow 28a'$	0.2840	8.077	0.0017	8.051	0.0018	8.058	0.0019
	$4a'' \rightarrow 20a'$	0.2121						
	$4a'' \rightarrow 37a'$	0.1758						
	$4a'' \rightarrow 24a'$	0.1610						
$8\ ^1A'$	$18a' \rightarrow 19a'$	0.2252	8.308	0.2169	8.098	0.0675	8.118	0.0753
	$3a'' \rightarrow 6a''$	0.2164						
	$18a' \rightarrow 25a'$	0.1903						
	$18a' \rightarrow 24a'$	0.1894						
	$18a' \rightarrow 32a'$	0.1835						
	$18a' \rightarrow 20a'$	0.1831						
$8\ ^1A''$	$18a' \rightarrow 7a''$	0.4380			8.216	0.0008	8.245	0.0009
	$18a' \rightarrow 11a''$	0.3054						
	$18a' \rightarrow 6a''$	0.1979						
	$18a' \rightarrow 8a''$	0.1797						
	$18a' \rightarrow 13a''$	0.1768						
$9\ ^1A'$	$18a' \rightarrow 37a'$	0.4126					8.261	0.0954
	$3a'' \rightarrow 10a''$	0.2533						
	$18a' \rightarrow 33a'$	0.2324						
	$18a' \rightarrow 45a'$	0.1835						

Table 23: Excited state properties of propadienone chloride (optimized at B3LYP/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation	Character	aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		COM/aug-cc-pV(T+d)Z	
			E	f	E	f	E	f
$1\ ^1A''$	$18a' \rightarrow 6a''$	0.6307	2.453	0.0001	2.453	0.0001	2.453	0.0001
	$18a' \rightarrow 7a''$	0.1735						
$1\ ^1A'$	$4a'' \rightarrow 6a''$	0.5235	4.985	0.0826	4.984	0.0821	4.985	0.0824
	$18a' \rightarrow 39a'$	0.1802						
$2\ ^1A''$	$17a' \rightarrow 6a''$	0.6298	6.082	0.0000	6.082	0.0000	6.082	0.0000
	$17a' \rightarrow 7a''$	0.1694						
$2\ ^1A'$	$18a' \rightarrow 24a'$	0.2742	6.301	0.1148	6.279	0.1078	6.283	0.1078
	$18a' \rightarrow 33a'$	0.2459						
	$18a' \rightarrow 19a'$	0.2388						
	$18a' \rightarrow 25a'$	0.2340						
$3\ ^1A''$	$4a'' \rightarrow 39a'$	0.3361	6.468	0.0019	6.465	0.0019	6.467	0.0019
	$4a'' \rightarrow 43a'$	0.2785						
	$4a'' \rightarrow 36a'$	0.1972						
	$4a'' \rightarrow 33a'$	0.1647						
$3\ ^1A'$	$18a' \rightarrow 39a'$	0.2267	7.054	0.5606	7.017	0.5100	7.023	0.5239
	$4a'' \rightarrow 6a''$	0.2254						
	$18a' \rightarrow 43a'$	0.2229						
$4\ ^1A'$	$18a' \rightarrow 28a'$	0.3161	7.189	0.0832	7.155	0.1200	7.163	0.1067
	$18a' \rightarrow 19a'$	0.2496						
	$18a' \rightarrow 20a'$	0.2425						
	$18a' \rightarrow 24a'$	0.2403						
$4\ ^1A''$	$18a' \rightarrow 5a''$	0.4622	7.651	0.0004	7.431	0.0011	7.520	0.0012
	$18a' \rightarrow 10a''$	0.3439						
	$18a' \rightarrow 9a''$	0.1992						
$5\ ^1A'$	$18a' \rightarrow 21a'$	0.3924	7.680	0.0024	7.522	0.0105	7.552	0.0104
	$18a' \rightarrow 30a'$	0.3258						
$5\ ^1A''$	$4a'' \rightarrow 24a'$	0.3272	7.740	0.0009	7.623	0.0000	7.627	0.0000
	$4a'' \rightarrow 19a'$	0.3084						
	$4a'' \rightarrow 25a'$	0.2372						
$6\ ^1A'$	$3a'' \rightarrow 6a''$	0.3163	7.760	0.0299	7.704	0.0039	7.709	0.0048
	$17a' \rightarrow 43a'$	0.2407						
	$17a' \rightarrow 39a'$	0.2380						
$7\ ^1A'$	$3a'' \rightarrow 6a''$	0.3018	7.866	0.2124	7.827	0.1538	7.832	0.1604
	$17a' \rightarrow 43a'$	0.1965						
	$17a' \rightarrow 39a'$	0.1851						
	$18a' \rightarrow 32a'$	0.1627						
$6\ ^1A''$	$15a' \rightarrow 6a''$	0.3416	8.020	0.0024	8.002	0.0026	8.008	0.0025
	$16a' \rightarrow 6a''$	0.3164						
	$18a' \rightarrow 27a''$	0.2401						
$8\ ^1A'$	$18a' \rightarrow 19a'$	0.2373	8.317	0.2095	8.068	0.0636	8.089	0.0685
	$18a' \rightarrow 25a'$	0.2240						
	$3a'' \rightarrow 6a''$	0.1901						
$7\ ^1A''$	$18a' \rightarrow 7a''$	0.2697			8.158	0.0001	8.171	0.0002
	$4a'' \rightarrow 28a'$	0.2599						
	$4a'' \rightarrow 20a'$	0.2047						
	$18a' \rightarrow 11a''$	0.1904						
$8\ ^1A''$	$18a' \rightarrow 7a''$	0.3502			8.189	0.0011	8.207	0.0013
	$18a' \rightarrow 11a''$	0.2366						
	$4a'' \rightarrow 28a'$	0.1791						
	$15a' \rightarrow 6a''$	0.1658						
$9\ ^1A'$	$18a' \rightarrow 22a'$	0.3116			8.228	0.0411	8.259	0.0592
	$18a' \rightarrow 25a'$	0.3048						
	$18a' \rightarrow 31a'$	0.2236						

Table 24: Excited state properties of propadienone chloride (optimized at MP2/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation Character		aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		COM/aug-cc-pV(T+d)Z	
			E	f	E	f	E	f
$1\ ^1A''$	$18a' \rightarrow 10a''$	0.6510	2.541	0.0002	2.540	0.0002	2.541	0.0002
	$18a' \rightarrow 12a''$	0.0778						
	$18a' \rightarrow 14a''$	0.0704						
	$18a' \rightarrow 11a''$	0.0670						
	$18a' \rightarrow 17a''$	0.0544						
$1\ ^1A'$	$4a'' \rightarrow 10a''$	0.5399	4.961	0.0969	4.959	0.0964	4.960	0.0967
	$18a' \rightarrow 42a'$	0.2318						
	$18a' \rightarrow 39a'$	0.1590						
	$18a' \rightarrow 48a'$	0.1436						
$2\ ^1A''$	$17a' \rightarrow 10a''$	0.6505	6.112	0.0000	6.112	0.0000	6.112	0.0000
	$17a' \rightarrow 12a''$	0.0749						
	$17a' \rightarrow 11a''$	0.0613						
	$17a' \rightarrow 14a''$	0.0545						
	$17a' \rightarrow 18a''$	0.0525						
$2\ ^1A'$	$18a' \rightarrow 34a'$	0.3439	6.265	0.1730	6.247	0.1646	6.250	0.1648
	$18a' \rightarrow 39a'$	0.2587						
	$18a' \rightarrow 40a'$	0.2448						
	$4a'' \rightarrow 10a''$	0.2395						
$3\ ^1A''$	$4a'' \rightarrow 42a'$	0.44564	6.374	0.0025	6.371	0.0025	6.373	0.0026
	$4a'' \rightarrow 39a'$	0.2609						
	$4a'' \rightarrow 48a'$	0.2451						
	$4a'' \rightarrow 38a'$	0.1586						
$3\ ^1A'$	$18a' \rightarrow 42a'$	0.3302	7.067	0.4731	7.022	0.4358	7.028	0.4459
	$18a' \rightarrow 34a'$	0.2766						
	$18a' \rightarrow 40a'$	0.2193						
	$4a'' \rightarrow 10a''$	0.2141						
$4\ ^1A'$	$18a' \rightarrow 38a'$	0.3512	7.218	0.0616	7.182	0.0835	7.190	0.0747
	$18a' \rightarrow 32a'$	0.3263						
	$18a' \rightarrow 39a'$	0.2530						
$4\ ^1A''$	$18a' \rightarrow 9a''$	0.4183	7.608	0.0003	7.448	0.0022	7.536	0.0020
	$18a' \rightarrow 13a''$	0.3820						
	$4a'' \rightarrow 34a'$	0.1979						
	$4a'' \rightarrow 40a'$	0.1473						
$5\ ^1A''$	$4a'' \rightarrow 34a'$	0.3689	7.771	0.0027	7.578	0.0000	7.589	0.0003
	$4a'' \rightarrow 40a'$	0.2856						
	$18a' \rightarrow 9a''$	0.2197						
	$18a' \rightarrow 13a''$	0.1934						
$5\ ^1A'$	$18a' \rightarrow 33a'$	0.3781	7.754	0.0188	7.561	0.0171	7.594	0.0174
	$18a' \rightarrow 39a'$	0.2548						
	$18a' \rightarrow 42a'$	0.2425						
	$18a' \rightarrow 40a'$	0.2279						
$6\ ^1A'$	$3a'' \rightarrow 10a''$	0.3852	7.827	0.0288			7.798	0.0220
	$17a' \rightarrow 42a'$	0.2314						
	$18a' \rightarrow 35a'$	0.1952						
	$18a' \rightarrow 41a'$	0.1656						
$7\ ^1A'$	$17a' \rightarrow 42a'$	0.3866	8.011	0.1534			7.978	0.0970
	$18a' \rightarrow 35a'$	0.2145						
	$17a' \rightarrow 39a'$	0.1724						
	$17a' \rightarrow 48a'$	0.1536						
$6\ ^1A''$	$16a' \rightarrow 10a''$	0.3476	8.023	0.0042	8.006	0.0051	8.012	0.0049
	$15a' \rightarrow 10a''$	0.3157						
	$18a' \rightarrow 19a''$	0.2232						
	$18a' \rightarrow 18a''$	0.1793						
$7\ ^1A''$	$4a'' \rightarrow 38a'$	0.3003	8.136	0.0006	8.100	0.0006	8.109	0.0006
	$4a'' \rightarrow 32a'$	0.2666						
	$4a'' \rightarrow 39a'$	0.2131						
	$4a'' \rightarrow 35a'$	0.1789						
$8\ ^1A'$	$18a' \rightarrow 37a'$	0.3896	8.340	0.2171			8.114	0.0488
	$18a' \rightarrow 35a'$	0.2394						
	$18a' \rightarrow 31a'$	0.2127						
	$3a'' \rightarrow 10a''$	0.2111						
$8\ ^1A''$	$18a' \rightarrow 11a''$	0.4949	8.600	0.0056	8.197	0.0009	8.223	0.0010
	$18a' \rightarrow 12a''$	0.2907						
	$18a' \rightarrow 14a''$	0.2340						
	$18a' \rightarrow 15a''$	0.1171						
$9\ ^1A'$	$18a' \rightarrow 37a'$	0.3585					8.276	0.0908
	$3a'' \rightarrow 10a''$	0.2639						
	$18a' \rightarrow 33a'$	0.2533						

3.1.5 Butatrienone chloride

Table 25: Excited state properties of butatrienone chloride (optimized at CCSD(T)/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation	Character	aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z		COM/aug-cc-pV(T+d)Z	
			E	f	E	f	E	f
$1\ ^1A''$	$5a'' \rightarrow 24a'$	0.4217	1.731	0.000	1.731	0.0000	1.731	0.000
	$5a'' \rightarrow 23a'$	0.3593						
	$5a'' \rightarrow 22a'$	0.2860						
	$5a'' \rightarrow 27a'$	0.1194						
	$5a'' \rightarrow 21a'$	0.1080						
$1\ ^1A'$	$5a'' \rightarrow 13a''$	0.4110	4.723	0.0431	4.722	0.0446	4.722	0.0431
	$20a' \rightarrow 24a'$	0.2718						
	$5a'' \rightarrow 12a''$	0.2521						
	$20a' \rightarrow 23a'$	0.2324						
	$20a' \rightarrow 22a'$	0.1844						
$2\ ^1A''$	$4a'' \rightarrow 24a'$	0.3728	5.085	0.0001	5.085	0.0002	5.085	0.0001
	$4a'' \rightarrow 23a'$	0.3231						
	$4a'' \rightarrow 22a'$	0.2562						
	$3a'' \rightarrow 24a'$	0.1403						
	$3a'' \rightarrow 23a'$	0.1160						
	$4a'' \rightarrow 27a'$	0.1042						
$3\ ^1A''$	$5a'' \rightarrow 27a'$	0.3675	5.544	0.0016	5.516	36.1168	5.520	0.0016
	$5a'' \rightarrow 21a'$	0.2919						
	$5a'' \rightarrow 40a'$	0.1956						
	$5a'' \rightarrow 38a'$	0.1898						
	$5a'' \rightarrow 36a'$	0.1595						
	$5a'' \rightarrow 29a'$	0.1569						
	$5a'' \rightarrow 25a'$	0.1556						
$2\ ^1A'$	$19a' \rightarrow 24a'$	0.3960	6.264	0.0133	6.264	0.0138	6.264	0.0136
	$19a' \rightarrow 23a'$	0.3588						
	$19a' \rightarrow 22a'$	0.2862						
	$19a' \rightarrow 21a'$	0.1115						
	$19a' \rightarrow 27a'$	0.1074						
$4\ ^1A''$	$5a'' \rightarrow 31a'$	0.2717	6.276	0.0081	6.226	0.0071	6.236	0.0073
	$5a'' \rightarrow 23a'$	0.2446						
	$5a'' \rightarrow 43a'$	0.1850						
	$5a'' \rightarrow 37a'$	0.1814						
	$5a'' \rightarrow 22a'$	0.1746						
$5\ ^1A''$	$5a'' \rightarrow 22a'$	0.2394	6.501	0.000	6.453	0.0006	6.468	0.0002
	$5a'' \rightarrow 31a'$	0.2313						
	$5a'' \rightarrow 24a'$	0.1815						
	$5a'' \rightarrow 21a'$	0.1755						
	$5a'' \rightarrow 39a'$	0.1536						
	$5a'' \rightarrow 35a'$	0.1414						
	$5a'' \rightarrow 28a'$	0.1411						
$6\ ^1A''$*	$20a' \rightarrow 13a''$	0.6143	6.536	0.0001			6.501	0.0000
	$20a' \rightarrow 14a''$	0.1760						
	$20a' \rightarrow 16a''$	0.1469						
$3\ ^1A'$	$5a'' \rightarrow 6a''$	0.4302	6.712	1.2530	6.539	0.2640	6.601	0.4516
	$5a'' \rightarrow 11a''$	0.3200						
	$5a'' \rightarrow 12a''$	0.2046						
	$5a'' \rightarrow 8a''$	0.1980						
$7\ ^1A''$*	$5a'' \rightarrow 34a'$	0.2394			6.816	0.0019	6.667	0.0005
	$5a'' \rightarrow 35a'$	0.2023						
	$5a'' \rightarrow 46a'$	0.2020						
	$5a'' \rightarrow 41a'$	0.1998						
	$5a'' \rightarrow 43a'$	0.1975						
$4\ ^1A'$	$5a'' \rightarrow 13a''$	0.3022	7.037	0.6768	6.842	1.3503		
	$5a'' \rightarrow 12a''$	0.2358						
	$20a' \rightarrow 24a'$	0.2330						
	$5a'' \rightarrow 6a''$	0.2055						
	$20a' \rightarrow 23a'$	0.1941						
	$4a'' \rightarrow 13a''$	0.1872						
$8\ ^1A''$**	$5a'' \rightarrow 25a'$	0.5802	7.254	0.0012				
	$5a'' \rightarrow 35a'$	0.1644						
	$5a'' \rightarrow 22a'$	0.1106						
	$5a'' \rightarrow 36a'$	0.1096						
	$5a'' \rightarrow 27a'$	0.1084						
$9\ ^1A''$**	$3a'' \rightarrow 21a'$	0.5092	7.501	0.0001				
	$4a'' \rightarrow 21a'$	0.2278						
	$3a'' \rightarrow 22a'$	0.1396						
	$5a'' \rightarrow 25a'$	0.1332						
	$4a'' \rightarrow 36a'$	0.1055						
$10\ ^{1''}$**	$5a'' \rightarrow 26a'$	0.5221	7.679	0.0018				
	$5a'' \rightarrow 28a'$	0.1918						
	$5a'' \rightarrow 41a'$	0.1483						
	$5a'' \rightarrow 30a'$	0.1264						
	$5a'' \rightarrow 35a'$	0.1215						
	$5a'' \rightarrow 36a'$	0.1163						
$5\ ^1A'$	$5a'' \rightarrow 7a''$	0.5090	7.732	0.0270	7.269	0.0678	7.312	0.0731
	$5a'' \rightarrow 10a''$	0.2233						
	$5a'' \rightarrow 13a''$	0.1794						
	$5a'' \rightarrow 12a''$	0.1754						
	$5a'' \rightarrow 11a''$	0.1545						
	$5a'' \rightarrow 15a''$	0.1483						
$6\ ^1A'$	$5a'' \rightarrow 9a''$	0.5251	8.044	0.5262	7.455	0.1007	7.408	0.1007
	$5a'' \rightarrow 14a''$	0.2508						
	$5a'' \rightarrow 13a''$	0.1854						
	$5a'' \rightarrow 16a''$	0.1458						
	$5a'' \rightarrow 18a''$	0.1186						
$7\ ^1A'$	$5a'' \rightarrow 6a''$	0.4166	8.264	0.0373	7.762	0.0014	7.762	0.0052
	$5a'' \rightarrow 8a''$	0.3810						
	$5a'' \rightarrow 15a''$	0.1712						
	$5a'' \rightarrow 16a''$	0.1672						
$8\ ^1A'$	$5a'' \rightarrow 8a''$	0.4198	8.565	0.0003	7.960		8.028	0.4527
	$5a'' \rightarrow 11a''$	0.4049						
	$5a'' \rightarrow 6a''$	0.2015						
	$5a'' \rightarrow 19a''$	0.1329						
	$5a'' \rightarrow 9a''$	0.1052						
$9\ ^1A'$*	$5a'' \rightarrow 9a''$	0.4722	8.640	0.2262			8.123	0.0692
	$5a'' \rightarrow 10a''$	0.3093						
	$5a'' \rightarrow 14a''$	0.2354						
	$5a'' \rightarrow 8a''$	0.1860						
	$4a'' \rightarrow 13a''$	0.1387						

*Excitation coefficients computed with COM/aug-cc-pV(T+d)Z

[b]Held constant to the values calculated with COM/aug-cc-pV(T+d)Z and aug-cc-pV(T+d)Z

Table 26: Excited state properties of butatrienone chloride (optimized at B3LYP/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation Character		aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z	
			E	f	E	f
E	f					
$1\ ^1A''$	$5a'' \rightarrow 24a'$	0.5002	1.762	0.0000	1.762	0.0000
	$5a'' \rightarrow 23a'$	0.2909				
	$5a'' \rightarrow 22a'$	0.2157				
$1\ ^1A'$	$5a'' \rightarrow 13a''$	0.4300	4.785	0.0406	4.784	0.0410
	$20a' \rightarrow 24a'$	0.3238				
	$5a'' \rightarrow 12a''$	0.2095				
	$20a' \rightarrow 23a'$	0.1890				
$2\ ^1A''$	$4a'' \rightarrow 24a'$	0.4399	5.150	0.0001	5.150	0.0001
	$4a'' \rightarrow 23a'$	0.2611				
	$4a'' \rightarrow 22a'$	0.1919				
	$3a'' \rightarrow 24a'$	0.1692				
$3\ ^1A''$	$5a'' \rightarrow 27a'$	0.3681	5.546	0.0017	5.519	0.0017
	$5a'' \rightarrow 21a'$	0.2942				
	$5a'' \rightarrow 40a'$	0.1948				
	$5a'' \rightarrow 38a'$	0.1896				
$4\ ^1A''$	$5a'' \rightarrow 31a'$	0.2785	6.291	0.0078	6.241	0.0078
	$5a'' \rightarrow 23a'$	0.2398				
	$5a'' \rightarrow 22a'$	0.2002				
	$5a'' \rightarrow 43a'$	0.1893				
	$5a'' \rightarrow 37a'$	0.1755				
$2\ ^1A'$	$19a' \rightarrow 24a'$	0.4763	6.247	0.0085	6.248	0.0088
	$19a' \rightarrow 23a'$	0.2963				
	$19a' \rightarrow 22a'$	0.2178				
	$19a' \rightarrow 27a'$	0.1248				
$5\ ^1A''$	$5a'' \rightarrow 22a'$	0.2390	6.558	0.0002	6.470	0.9354
	$5a'' \rightarrow 31a'$	0.2265				
	$5a'' \rightarrow 23a'$	0.1866				
	$5a'' \rightarrow 21a'$	0.1639				
	$5a'' \rightarrow 39a'$	0.1513				
$6\ ^1A''$	$20a' \rightarrow 7a''$	0.4562	6.610	0.0000		
	$20a' \rightarrow 8a''$	0.3218				
	$20a' \rightarrow 6a''$	0.3191				
$3\ ^1A'$	$5a'' \rightarrow 6a''$	0.4425	6.758	1.0212	6.550	
	$5a'' \rightarrow 11a''$	0.3257				
	$5a'' \rightarrow 8a''$	0.2050				
	$5a'' \rightarrow 12a''$	0.1896				
$7\ ^1A''$	$5a'' \rightarrow 24a'$	0.4204	6.820	0.0018		
	$5a'' \rightarrow 26a'$	0.2973				
	$5a'' \rightarrow 29a'$	0.1780				
	$5a'' \rightarrow 36a'$	0.1723				
$4\ ^1A'$	$5a'' \rightarrow 13a''$	0.3099	7.070	0.9373	6.908	0.0000
	$20a' \rightarrow 24a'$	0.2825				
	$5a'' \rightarrow 12a''$	0.2289				
	$4a'' \rightarrow 13a''$	0.1888				
	$5a'' \rightarrow 9a''$	0.1773				
	$5a'' \rightarrow 6a''$	0.1769				
$8\ ^1A''$	$5a'' \rightarrow 25a'$	0.5810	7.275	0.0013		
	$5a'' \rightarrow 35a'$	0.1776				
	$5a'' \rightarrow 22a'$	0.1178				
	$5a'' \rightarrow 27a'$	0.1075				
$5\ ^1A'$	$5a'' \rightarrow 7a''$	0.5057	7.749	0.0542	7.280	0.0961
	$5a'' \rightarrow 10a''$	0.2172				
	$5a'' \rightarrow 12a''$	0.1831				
	$5a'' \rightarrow 13a''$	0.1709				
$6\ ^1A'$	$5a'' \rightarrow 9a''$	0.5143	8.130	0.4993	7.466	0.1423
	$5a'' \rightarrow 14a''$	0.2400				
	$5a'' \rightarrow 13a''$	0.2038				
	$5a'' \rightarrow 16a''$	0.1492				
$7\ ^1A'$	$20a' \rightarrow 22a'$	0.4759	8.297	0.0440		
	$20a' \rightarrow 23a'$	0.2320				
	$20a' \rightarrow 28a'$	0.1920				
	$20a' \rightarrow 21a'$	0.1698				
	$20a' \rightarrow 25a'$	0.1628				
$8\ ^1A'$	$19a' \rightarrow 28a'$	0.2841	8.567	0.0025		
	$19a' \rightarrow 22a'$	0.2837				
	$19a' \rightarrow 36a'$	0.2067				
	$19a' \rightarrow 21a'$	0.2048				
	$5a'' \rightarrow 10a''$	0.1972				
$9\ ^1A'$	$5a'' \rightarrow 10a''$	0.3957	8.650	0.2304		
	$5a'' \rightarrow 9a''$	0.3866				
	$19a' \rightarrow 22a'$	0.1651				

Table 27: Excited state properties of butatrienone chloride (optimized at MP2/d-aug-cc-pV(T+d)Z) at EOM-CCSD where E is the vertical excitation energy and f is the oscillator strength

SA	Excitation Character		aug-cc-pV(T+d)Z		d-aug-cc-pV(T+d)Z	
			E	f	E	f
$1\ ^1A''$	$5a'' \rightarrow 24a'$	0.5495	1.762	0.0000	1.762	0.2755
	$5a'' \rightarrow 23a'$	0.1943				
	$5a'' \rightarrow 27a'$	0.1603				
	$5a'' \rightarrow 22a'$	0.1590				
$1\ ^1A'$	$5a'' \rightarrow 13a''$	0.4309	4.766	0.0510	4.765	0.0514
	$20a' \rightarrow 24a'$	0.3504				
	$5aa'' \rightarrow 12a''$	0.2235				
	$20a' \rightarrow 23a'$	0.1245				
$2\ ^1A''$	$4a'' \rightarrow 24a'$	0.4906	5.167	0.0001	5.167	0.0002
	$3a'' \rightarrow 24a'$	0.1805				
	$4a'' \rightarrow 23a'$	0.1777				
	$4a'' \rightarrow 22a'$	0.1434				
	$4a'' \rightarrow 27a'$	0.1407				
$3\ ^1A''$	$5a'' \rightarrow 27a'$	0.3666	5.512	0.0016	5.484	0.0018
	$5a'' \rightarrow 21a'$	0.2952				
	$5a'' \rightarrow 40a'$	0.1955				
	$5a'' \rightarrow 38a'$	0.1892				
	$5a'' \rightarrow 25a'$	0.1626				
$4\ ^1A''$	$5a'' \rightarrow 31a'$	0.2923	6.274	0.0080	6.220	0.0068
	$5a'' \rightarrow 23a'$	0.2372				
	$5a'' \rightarrow 22a'$	0.2287				
	$5a'' \rightarrow 43a'$	0.1978				
	$5a'' \rightarrow 37a'$	0.1625				
$2\ ^1A'$	$19a' \rightarrow 24a'$	0.5304	6.344	0.0145	6.345	0.0158
	$19a' \rightarrow 23a'$	0.2047				
	$19a' \rightarrow 22a'$	0.1634				
$5\ ^1A''$	$5a'' \rightarrow 23a'$	0.2781	6.548	0.0009	6.438	0.0009
	$5a'' \rightarrow 22a'$	0.2193				
	$5a'' \rightarrow 31a'$	0.2010				
	$5a'' \rightarrow 35a'$	0.1687				
	$5a'' \rightarrow 34a'$	0.1613				
$3\ ^1A'$	$5\ a'' \rightarrow 6a''$	0.4450	6.722	0.9961	6.512	0.164
	$5a'' \rightarrow 11a''$	0.3261				
	$5a'' \rightarrow 8a''$	0.2066				
	$5a'' \rightarrow 12a''$	0.1875				
$6\ ^1A''$	$20a' \rightarrow 13a''$	0.5743	6.576	0.0000	6.574	0.0012
	$20a' \rightarrow 12a''$	0.2842				
$7\ ^1A''$	$5a'' \rightarrow 24a'$	0.3455	6.804	0.0011		
	$5a'' \rightarrow 26a'$	0.3289				
	$5a'' \rightarrow 36a'$	0.2121				
	$5a'' \rightarrow 29a'$	0.1804				
	$5a'' \rightarrow 28a'$	0.1803				
	$5a'' \rightarrow 22a'$	0.1698				
$4\ ^1A'$	$20a' \rightarrow 24a'$	0.3113	7.026	0.8861	6.863	1.5502
	$5\ a'' \rightarrow 13a''$	0.3034				
	$5a'' \rightarrow 12a''$	0.2329				
	$4a'' \rightarrow 13a''$	0.1979				
	$5a'' \rightarrow 9a''$	0.1728				
	$5a'' \rightarrow 6a''$	0.1717				
$8\ ^1A''$	$5a'' \rightarrow 25a'$	0.5923	7.237	0.0011		
	$5a'' \rightarrow 35a'$	0.1945				
	$5a'' \rightarrow 27a'$	0.1110				
	$5a'' \rightarrow 22a'$	0.1085				
$5\ ^1A'$	$5a'' \rightarrow 7a''$	0.5058	7.697	0.0460	7.234	0.083
	$5a'' \rightarrow 10a''$	0.2179				
	$5a'' \rightarrow 12a''$	0.1836				
	$5a'' \rightarrow 13a''$	0.1718				
	$5a'' \rightarrow 15a''$	0.1539				
	$5a'' \rightarrow 11a''$	0.1504				
$6\ ^1A'$	$5a'' \rightarrow 9a''$	0.5042	8.121	0.5106	7.424	0.141
	$5a'' \rightarrow 14a''$	0.2425				
	$5a'' \rightarrow 13a''$	0.1982				
$7\ ^1A'$	$5a'' \rightarrow 6a''$	0.4197	8.288	0.0314	7.729	0.0032
	$5a'' \rightarrow 8a''$	0.3690				
	$5a'' \rightarrow 16a''$	0.1757				
	$5a'' \rightarrow 15a''$	0.1604				
	$5a'' \rightarrow 11a''$	0.1428				
$8\ ^1A'$	$5a'' \rightarrow 11a''$	0.4082	8.574	0.0905	7.923	0.0125
	$5a'' \rightarrow 8a''$	0.3915				
	$5a'' \rightarrow 6a''$	0.2076				
	$5a'' \rightarrow 9a''$	0.1786				
$9\ ^1A'$	$19a' \rightarrow 22a'$	0.3050	8.640	0.1667		
	$19a' \rightarrow 28a'$	0.2768				
	$5a'' \rightarrow 9a''$	0.2439				
	$19a' \rightarrow 21a'$	0.2099				
	$19a' \rightarrow 36a'$	0.1871				