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Table A. Supplemental Material for Table 1.

4 (C_{2v}, $^1A_1$)	Curvature[2]	C2–C3	C1–C2	C3–H4	C2–H6	C1–C3–C2	C1–C2–C3	α	β
HF	min	1.498	1.278	1.083	1.068	50.5	64.8	56.6	
MP2	min	1.510	1.305	1.087	1.075	51.2	64.4	57.0	
B-LYP	min	1.526	1.308	1.100	1.086	50.7	64.6	56.8	
5 (C_s, $^1A'$)									
HF	min	1.556	1.288	1.107	1.075	48.9	65.6	69.6	11.4
MP2	min	1.564	1.315	1.108	1.083	49.7	65.2	69.8	17.9
B-LYP	271i cm^{-1}	1.593	1.316	1.129	1.096	48.8	65.6	70.5	13.9
6 (C_2, ^1A)									
HF	794i cm^{-1}	1.365	1.615	1.081	1.084	72.5	53.7		52.6
MP2	min	1.376	1.698	1.090	1.089	76.2	51.9		52.2
B-LYP	min	1.386	1.737	1.109	1.104	77.6	51.2		53.8
7 (C_s,$^2A'$)									
HF	min	1.453	1.296	1.081	1.068	53.0	63.5	45.0	0.5
MP2	min	1.463	1.324	1.087	1.075	53.8	63.0	45.4	0.8
B-LYP	min	1.476	1.329	1.100	1.087	53.5	63.3	45.0	0.5
8 (C_2, ^2A)									
HF	min	1.350	1.469	1.071	1.069	65.9	57.0		26.5
MP2	1061i cm^{-1}	1.357	1.491	1.078	1.076	66.7	56.7		28.0
B-LYP	663i cm^{-1}	1.376	1.518	1.091	1.090	67.0	56.5		28.7
9 (C_s, $^3A''$)									
HF	min	1.443	1.445	1.082	1.085	60.1	60.0	39.0	42.1
MP2	min	1.452	1.458	1.088	1.092	60.3	59.8	39.2	42.4
B-LYP	min	1.466	1.469	1.104	1.108	60.2	59.9	39.0	42.1
10 (C_2,^3B)									
HF	729i cm^{-1}	1.423	1.460	1.066	1.087	61.8	59.0		41.6
MP2	759i cm^{-1}	1.432	1.472	1.074	1.094	61.9	59.0		42.0
B-LYP	689i cm^{-1}	1.447	1.484	1.086	1.100	61.7	59.0		42.5
11 (C_{3v}, $^3A_2$)									
HF	min	1.443		1.087				43.9	
MP2	min	1.456		1.094				44.4	
B-LYP	min	1.470		1.100				43.8	

[1]α and β correspond to the H4 and H5(H6) out of plane angles, respectively. [2]Curvature associated with the potential energy surface in the vicinity of the stationary point: min ≡ minimum energy structure; xi cm^{-1} ≡ transition structure. [3]Ref 26.

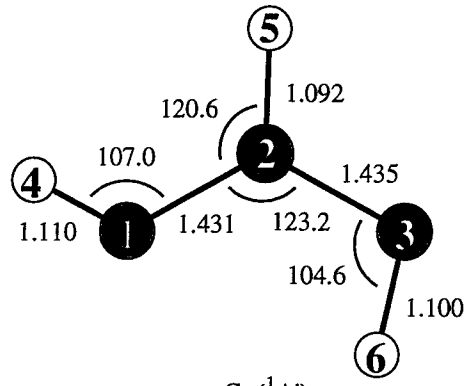
Table B. Mulliken Atomic Charges (in units of e^-) for Cyclopropene and Cyclopropenyl Species.[1]

4 (C_{2v}, $^1A_1$)	C1/C2	ΔC1/ΔC2	C3	ΔC3
MP2//HF	-0.02		0.04	
MP2	-0.03		0.06	
CCSD(T)//MCSCF	-0.03		0.06	
B-VWN5	0.00		0.00	
B-LYP	0.00		0.00	
B3-LYP	0.00		0.00	
5 (C_s, $^1A'$)				
MP2//HF	-0.16	-0.14	-0.68	-0.72
MP2	-0.25	-0.22	-0.50	-0.56
CCSD(T)//MCSCF	-0.24	-0.21	-0.52	-0.58
B-VWN5	-0.24	-0.24	-0.52	-0.52
B-LYP	-0.25	-0.24	-0.50	-0.50
B3-LYP	-0.25	-0.25	-0.50	-0.50
6 (C_2, ^1A)				
MP2//HF	-0.51	-0.35	0.02	0.66
MP2	-0.45	-0.20	-0.10	0.40
CCSD(T)//MCSCF	-0.50	-0.26	0.00	0.52
B-VWN5	-0.45	-0.21	-0.10	0.42
B-LYP	-0.44	-0.20	-0.12	0.38
B3-LYP	-0.41	-0.16	-0.18	0.32
7 (C_s, $^2A'$)				
MP2//HF	0.04	0.20	-0.08	0.59
MP2	-0.01	0.24	0.02	0.52
CCSD(T)//MCSCF	-0.01	0.23	0.02	0.54
B-VWN5	0.04	0.28	-0.08	0.44
B-LYP	0.04	0.28	-0.08	0.42
B3-LYP	0.03	0.28	-0.06	0.44
8 (C_2, ^2A)				
MP2//HF	-0.11	0.05	0.22	0.89
MP2	-0.03	0.22	0.06	0.56
CCSD(T)//MCSCF	-0.02	0.22	0.04	0.56
B-VWN5	-0.04	0.20	0.08	0.60
B-LYP	-0.05	0.19	0.10	0.62
B3-LYP	-0.04	0.21	0.08	0.58
9 (C_s, $^3A''$)				
MP2//HF	-0.28	-0.12	-0.44	0.24
MP2	-0.28	-0.03	-0.44	0.06
CCSD(T)//MCSCF	-0.28	-0.04	-0.44	0.08
B-VWN5	-0.29	-0.05	-0.42	0.10
B-LYP	-0.29	-0.05	-0.42	0.08
B3-LYP	-0.29	-0.04	-0.42	0.08

10 (C_2, ^3B)	C1/C2	ΔC1/ΔC2	C3	ΔC3
MP2//HF	-0.32	-0.16	-0.36	0.32
MP2	-0.28	-0.03	-0.44	0.06
CCSD(T)//MCSCF	-0.28	-0.04	-0.44	0.08
B-VWN5	-0.31	-0.07	-0.38	0.14
B-LYP	-0.31	-0.08	-0.38	0.16
B3-LYP	-0.31	-0.05	-0.38	0.12
11 (C_{3v}, $^3A_2$)				
MP2//HF	-0.33	-0.17		
MP2	-0.33	-0.08		
CCSD(T)//MCSCF	-0.33	-0.09		
B-VWN5	-0.33	-0.09		
B-LYP	-0.33	-0.10		
B3-LYP	-0.33	-0.09		

[1]Hydrogen atom contributions have been summed into the carbons. The charge differences (e.g., ΔC1) for **5** are relative to **4** while for all of the others species they are given in comparison to **5**. See Figure 1 for the labeling scheme.

Table C. Structural Parameters and the Relative Energy of an Acyclic $C_3H_3^-$ Anion.[1]



C_s ($^1A'$)

Level	C1–C2	C2–C3	H4–C1	H5–C2	H6–C3	C1–C2–C3	H4–C1–C2	H5–C2–C1	H6–C3–C2
HF	1.400	1.408	1.107	1.093	1.097	122.8	108.2	120.6	105.7
MP2	1.409	1.413	1.116	1.100	1.107	122.4	107.4	121.0	103.8
MCSCF	1.431	1.435	1.110	1.092	1.100	123.2	107.0	120.6	104.6
B-VWN5[2]	1.417	1.415	1.130	1.112	1.116	118.9	107.7	123.2	107.0
B-LYP[2]	1.413	1.410	1.132	1.114	1.117	115.4	108.2	125.0	108.3
B3-LYP	1.408	1.414	1.124	1.108	1.114	123.2	107.6	120.8	104.4

[1]Distances are in angstroms, angles in degrees, and ΔE (C_s ($^1A'$) open ion - C_s ($^1A'$) cyclopropenyl anion) in kcal/mol. The values in the figure are from the MCSCF optimization. [2]The acyclic structure has C_1 (^1A) symmetry. Dihedral angles are as follows: B-VWN5: H4–C1–C2–H5 = 18.5°; H6–C3–C2–H5 = 171.8°. B-LYP: H4–C1–C2–H5 = 24.3°; H6–C3–C2–H5 = 169.8°.

Table D. Supplemental Material for Table 7.

12(C_s, $^1A'$)	curv[2]	C2–C3	C1–C2	C3–C4	C4–N	H3–C3	H1–C1	C1–C3–C2	C2–C1–C3	N–C4–C3	α	β
HF	min	1.497	1.274	1.465	1.137	1.079	1.067	50.4	64.8	180.0	56.1	0.3
B-LYP	min	1.532	1.303	1.460	1.176	1.100	1.085	50.4	64.8	179.4	56.0	0.6
B3-LYP	min	1.516	1.292	1.456	1.163	1.092	1.078	50.4	64.8	179.6	56.1	0.6
expt[3]		1.511	1.292	1.453	1.162	1.092	1.071	50.6	64.7		57.1	
13(C_s, $^1A'$)												
HF	min	1.540	1.280	1.456	1.151		1.071	49.0	65.5	173.9	64.2	7.9
B-LYP	min	1.573	1.308	1.431	1.198		1.091	49.2	65.4	169.3	59.9	7.9
B3-LYP	min	1.555	1.298	1.426	1.183		1.083	49.4	65.3	170.9	60.6	8.6
14(C_2, ^1A)												
HF	1004i cm^{-1}	1.362	1.616	1.435	1.140		1.083	72.8	53.6			53.8
B-LYP	155i cm^{-1}	1.395	1.716	1.424	1.184		1.103	76.0	52.0			56.3
B3-LYP	413i cm^{-1}	1.381	1.672	1.420	1.170		1.095	74.4	52.8			55.4
15(C_s, $^2A'$)												
HF	min	1.446	1.295	1.431	1.139		1.068	53.2	63.4	176.2	40.5	0.3
B-LYP	min	1.463	1.331	1.377	1.194		1.087	54.0	63.0	173.9	21.2	0.3
B3-LYP	min	1.450	1.320	1.376	1.179		1.079	54.0	63.0	173.9	23.0	0.0
16(C_2, ^2A)												
HF	min	1.348	1.474	1.426	1.135		1.069	66.4	56.8			27.2
B-LYP	1080i cm^{-1}	1.384	1.516	1.415	1.177		1.090	66.4	56.8			30.8
B3-LYP	1136i cm^{-1}	1.371	1.500	1.412	1.164		1.083	66.4	56.8			30.1

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17(C_s, $^3A''$)	curv[2]	C2–C3	C1–C2	C3–C4	C4–N	H3–C3	H1–C1	C1–C3–C2	C2–C1–C3	N–C4–C3	α	β
HF	min	1.431	1.455	1.402	1.152		1.083	61.0	59.5	176.8	33.7	
B-LYP	min	1.458	1.468	1.373	1.207		1.107	60.4	59.8	175.9	17.8	44.0
B3-LYP	min	1.443	1.459	1.367	1.192		1.097	60.8	59.6	176.6	16.2	43.6
18(C_2, ^3B)												
HF	116i cm^{-1}	1.419	1.460	1.374	1.158		1.082	62.0	59.0			41.9
B-LYP	min	1.439	1.461	1.362	1.193		1.095	61.0	59.5			42.8
B3-LYP	min	1.453	1.472	1.367	1.207		1.104	60.8	59.6			42.2

[1]α and β correspond to the C4 and hydrogen out of plane angles, respectively. [2]Curvature of the potential surface in the vicinity of the stationary point. [3]See: Staley, S. W.; Norden, T. D.; Su, C.-F.; Rall, M.; Harmony, M. D. *J. Am. Chem. Soc.* **1987**, *109*, 2880.

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Table E. Mulliken Atomic Charges (in units of electrons) for Cyanocyclopropene and Cyanocyclopropenyl Species.[1]

12 (C_s, $^1A'$)	C1/C2	ΔC1/ΔC2	C3	ΔC3	C4	ΔC4	N	ΔN
MP2//HF	0.05		0.37		-0.02		-0.45	
MP2	0.04		0.19		0.11		-0.38	
B-VWN5	0.05		0.12		0.08		-0.30	
B-LYP	0.05		0.11		0.08		-0.29	
B3-LYP	0.05		0.12		0.09		-0.31	
13 (C_s, $^1A'$)								
MP2//HF	-0.02	-0.07	-0.76	-1.13	0.49	0.94	-0.70	-0.25
MP2	-0.07	-0.11	-0.58	-0.77	0.34	0.23	-0.62	-0.24
B-VWN5	-0.04	-0.09	-0.59	-0.71	0.18	0.10	-0.51	-0.21
B-LYP	-0.03	-0.08	-0.60	-0.71	0.16	0.08	-0.50	-0.21
B3-LYP	-0.04	-0.09	-0.60	-0.72	0.23	0.14	-0.53	-0.22
14 (C_2, ^1A)								
MP2//HF	-0.85	-0.83	0.78	1.54	0.44	-0.05	-0.54	0.16
MP2	-0.71	-0.64	1.21	1.79	-0.34	-0.68	-0.44	0.18
B-VWN5	-0.55	-0.51	0.70	1.29	-0.23	-0.41	-0.37	0.14
B-LYP	-0.55	-0.52	0.61	1.21	-0.15	-0.31	-0.36	0.14
B3-LYP	-0.59	-0.55	0.74	1.34	-0.17	-0.40	-0.38	0.15
15 (C_s, $^2A'$)	C1/C2	ΔC1/ΔC2	C3	ΔC3	C4	ΔC4	N	ΔN
MP2//HF	0.09	0.11	0.31	1.07	-0.06	-0.55	-0.44	0.26
MP2	0.02	0.09	0.36	0.94	-0.02	-0.36	-0.37	0.25
B-VWN5	0.05	0.09	0.41	1.00	-0.20	-0.38	-0.31	0.20
B-LYP	0.07	0.10	0.34	0.94	-0.19	-0.35	-0.30	0.20
B3-LYP	0.05	0.09	0.45	1.05	-0.22	-0.45	-0.32	0.21
16 (C_2, ^2A)								
MP2//HF	0.06	0.08	0.62	1.38	-0.37	-0.86	-0.39	0.31
MP2	0.02	0.09	0.98	1.56	-0.72	-1.06	-0.29	0.33
B-VWN5	-0.02	0.02	0.67	1.26	-0.42	-0.60	-0.22	0.29
B-LYP	-0.02	0.01	0.61	1.21	-0.35	-0.51	-0.21	0.29
B3-LYP	-0.02	0.02	0.71	1.31	-0.44	-0.67	-0.23	0.30

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17 (C_s, $^3A''$)	C1/C2	ΔC1/ΔC2	C3	ΔC3	C4	ΔC4	N	ΔN
MP2//HF	-0.38	-0.36	0.37	1.13	0.05	-0.44	-0.65	0.05
MP2	-0.28	-0.21	0.29	0.87	-0.16	-0.50	-0.57	0.05
B-VWN5	-0.21	-0.17	0.33	0.92	-0.43	-0.61	-0.48	0.03
B-LYP	-0.22	-0.19	0.28	0.88	-0.39	-0.55	-0.47	0.03
B3-LYP	-0.21	-0.17	0.37	0.97	-0.44	-0.67	-0.50	0.03
18 (C_2, ^3B)								
MP2//HF	-0.09	-0.07	0.16	0.92	-0.28	-0.77	-0.69	0.01
MP2	-0.17	-0.10	0.75	1.33	-0.85	-1.19	-0.56	0.06
B-VWN5	-0.23	-0.19	0.43	1.02	-0.50	-0.68	-0.48	0.03
B-LYP	-0.23	-0.20	0.35	0.95	-0.42	-0.58	-0.46	0.04
B3-LYP	-0.23	-0.19	0.47	1.07	-0.51	-0.74	-0.49	0.04

[1]Hydrogen atom contributions have been summed into the carbons. The charge differences (e.g., ΔC1) for **13** are relative to **12** while for all of the others species they are given in comparison to **13**. See Figure 3 for the labeling scheme.

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Table F. Supplemental Material for Table 8.

19(C_{2v}, $^1A_1$)	Curvature[2]	C1–C2	C1–C3[3]	C1–C4[4]	C4–N1[5]	C3–H[6]	C1–C3–C2	C2–C1–C3[7]	C1–C4–N1[8]	α[9]	β[10]
HF	min	1.280	1.496	1.414	1.136	1.079	50.7	64.7	178.7	57.5	
B-LYP	min	1.327	1.527	1.398	1.180	1.097	51.5	64.2	178.2	57.7	
B3-LYP	min	1.311	1.512	1.398	1.166	1.090	51.4	64.3	178.3	57.6	
20(C_1, ^1A)											
HF	min	1.276	1.493 (1.496)	1.415 (1.465)	1.136 (1.136)	1.078 (1.068)	50.5	64.9 (64.6)	179.1 (179.4)	56.4 (56.2)	0.2 (0.4)
B-LYP[11]	min	1.312	1.521 (1.547)	1.401 (1.459)	1.179 (1.175)	1.098 (1.086)	50.6	63.7 (65.7)	178.0 (179.5)	57.5 (56.0)	0.9 (0.0)
B3-LYP	min	1.299	1.524 (1.509)	1.400 (1.455)	1.165 (1.162)	1.091 (1.079)	50.7	64.0 (65.2)	178.4 (179.6)	57.3 (56.0)	0.6 (0.1)
21(C_s, $^1A'$)											
HF	min	1.288	1.569	1.411	1.143	1.100	48.5	65.8	178.0	72.5	10.1
B-LYP	449i cm^{-1}	1.335	1.596	1.389	1.192	1.128	49.5	65.3	176.4	72.7	2.0
B3-LYP	299i cm^{-1}	1.319	1.580	1.389	1.176	1.118	49.3	65.3	177.0	73.0	4.4
22(C_2, ^1A)											
HF	293i cm^{-1}	1.589	1.359	1.411	1.148	1.076	71.6	54.2	176.3		45.7
B-LYP	min	1.764	1.374	1.381	1.197	1.100	79.8	50.0	173.9		37.1
B3-LYP	60i cm^{-1}	1.670	1.366	1.385	1.181	1.089	75.4	52.3	174.4		38.3
23(C_1, ^1A)[11]											
HF	min	1.572	1.285 (1.500)	1.404 (1.457)	1.144 (1.148)	1.072	68.2	62.4 (49.4)	179.0 (173.9)	6.6	11.0 (64.2)

[1]α and β correspond to the hydrogen and C4 out-of-plane angles, respectively; see Figure 4. [2]Curvature associated with the potential energy surface in the vicinity of the stationary point: min ≡ minimum energy structure; xi cm^{-1} ≡ transition structure. [3]Parenthetical values correspond to C2–C3 bond distances. [4]Parenthetical values correspond to C2–C5 or C3–C5 bond lengths. [5]Parenthetical values correspond to the C5–N2 bond distances. [6]Parenthetical values correspond to the C2–H bond lengths. [7]Parenthetical values correspond to the C1–C2–C3 bond angles. [8]Parenthetical values correspond to the C2–C5–N2 or C3–C5–N2 bond angles. [9]Parenthetical values correspond to the H–C3 out-of-plane angles. [10]Parenthetical values correspond to the C5 out-of-plane angle. [11]Attempts to locate C_1 structures with B-VWN5 and B-LYP led to C_2 structures.

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Table G. Additional Supplemental Material for Table 8.

24(C_s, $^1A'$)	Curv[2]	C1–C2	C1–C3[3]	C1–C4[4]	C3–C6	C4–N1[5]	C6–N3	C3–H	C2–C1–C3[6]	C1–C3–C2	C1–C4–N1[7]	C3–C6–N3	α	β	δ
HF	min	1.278	1.494	1.414	1.463	1.135	1.135	1.078	64.7	50.6	179.0	179.6	56.9	0.4	56.2
B-LYP	min	1.323	1.536	1.398	1.457	1.180	1.175	1.098	64.5	51.0	178.2	179.3	58.3	0.1	56.0
B3-LYP	min	1.307	1.518	1.398	1.453	1.165	1.162	1.090	64.5	51.0	178.4	179.5	58.0	0.1	56.1
25(C_s, $^1A'$)															
HF	min	1.283	1.542	1.412	1.462	1.140	1.146		65.4	49.2	178.8	173.8		8.9	65.6
B-LYP	315i cm^{-1}	1.330	1.572	1.391	1.438	1.188	1.191		65.0	50.0	177.0	168.3		2.3	61.2
B3-LYP	90i cm^{-1}	1.314	1.555	1.391	1.435	1.172	1.176		65.0	50.0	177.9	170.2		4.2	62.3
26(C_2, ^1A)															
HF	422i cm^{-1}	1.592	1.356	1.414	1.431	1.145	1.137		54.0	72.0	176.0			46.2	
B-LYP	46i cm^{-1}	1.748	1.382	1.385	1.425	1.194	1.179		50.8	78.4	173.4			39.7	
B3-LYP	90i cm^{-1}	1.669	1.371	1.388	1.420	1.178	1.166		52.5	75.0	174.0			40.8	
27(C_1, ^1A)[8]															
B-LYP	min	1.338	1.462 (1.700)	1.415 (1.367)	1.420	1.181 (1.196)	1.192		74.6 (56.0)	49.4	178.3 (177.6)	169.6	5.6	0.0	56.2
B3-LYP	min	1.316	1.510 (1.600)	1.400 (1.382)	1.423	1.170 (1.175)	1.176		68.6 (61.4)	49.9	179.7 (179.4)	170.4	5.6	2.9	62.1

[1]α, β, and δ correspond to the hydrogen (or C5 in **27**), C4, and C6 out of plane angles, respectively; see Figure 5. [2]Curvature associated with the potential energy surface in the vicinity of the stationary point: min ≡ minimum energy structure; xi cm^{-1} ≡ transition structure. [3]Parenthetical values correspond to C2–C3 bond distances. [4]Parenthetical values correspond to C2–C5 bond lengths. [5]Parenthetical values correspond to the C5–N2 bond distance. [6]Parenthetical values correspond to the C1–C2–C3 bond angle. [7]Parenthetical values correspond to the C2–C5–N2 bond angle. [8]Attempts to locate HF and MP2 C_1 structures led back to the C_2 species.

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Table H. Mulliken Atomic Charges (in units of electrons) for Dicyanocyclopropene and Dicyanocyclopropenyl Species.[1]

19 (C_{2v}, $^1A_1$)	C1	ΔC1	C3	ΔC3	C4	ΔC4	N1	ΔN1
MP2//HF	0.82		0.36		-0.61		-0.38	
MP2	1.39		0.06		-1.14		-0.29	
B-VWN5	1.02		0.00		-0.80		-0.22	
B-LYP	0.95		0.00		-0.74		-0.21	
B3-LYP	1.06		0.01		-0.83		-0.23	
20 (C_1, ^1A)[2]								
MP2//HF	0.56 (-0.11)		0.43		0.04 (-0.10)		-0.40 (-0.41)	
MP2	1.12 (-0.42)		0.42		-0.39 (-0.09)		-0.30 (-0.34)	
B-VWN5	0.22 (0.70)		-0.20		-0.22 (-0.01)		-0.23 (-0.27)	
B-LYP	0.62 (-0.16)		0.20		-0.19 (0.01)		-0.22 (-0.26)	
B3-LYP	0.75 (-0.22)		0.24		-0.24 (-0.01)		-0.24 (-0.28)	
21 (C_s, $^1A'$)								
MP2//HF	0.90	0.08	-0.72	-1.08	-0.60	0.01	-0.44	-0.06
MP2	0.86	-0.53	-0.74	-0.80	-0.54	0.60	-0.45	-0.16
B-VWN5	0.65	-0.37	-0.62	-0.62	-0.47	0.33	-0.38	-0.16
B-LYP	0.54	-0.41	-0.65	-0.65	-0.35	0.39	-0.37	-0.16
B3-LYP	0.68	-0.38	-0.72	-0.73	-0.43	0.40	-0.39	-0.16
22 (C_2, ^1A)								
MP2//HF	-0.55	-1.45	0.41	1.13	0.45	1.05	-0.60	-0.16
MP2	-0.07	-0.93	0.27	1.01	-0.04	0.50	-0.53	-0.08
B-VWN5	-0.06	-0.71	0.04	0.66	-0.01	0.46	-0.45	-0.07
B-LYP	-0.12	-0.66	0.04	0.69	0.04	0.39	-0.43	-0.06
B3-LYP	-0.12	-0.80	0.00	0.72	0.09	0.52	-0.47	-0.08
23 (C_1, ^1A)[3]								
MP2//HF	0.36 (-0.84)	-0.54 (-0.12)	0.24	0.84	0.05 (0.39)	0.49 (0.99)	-0.56 (-0.64)	-0.12 (-0.20)
MP2	0.83 (-0.51)	-0.03 (0.23)	-0.06	0.48	-0.35 (0.14)	0.10 (0.68)	-0.49 (-0.55)	-0.04 (-0.10)
B3-LYP	0.42 (-0.47)	-0.26 (0.25)	-0.08	0.35	-0.04 (0.08)	0.35 (0.51)	-0.45 (-0.47)	-0.06 (-0.08)

[1]Hydrogen atom contributions have been summed into the carbons. The charge differences (e.g., ΔC1) for **21** are relative to **19** while for all of the others species they are given in comparison to **21**. See Figure 3 for the labeling scheme. [2]Parenthetical values in the C1, C4, and N1 columns correspond to C2, C5, and N2, respectively. [3]Parenthetical values in the C1 and ΔC1, C4 and ΔC4, and N1 and ΔN1 columns correspond to C2 and ΔC2, C5 and ΔC5, and N2 and ΔN2, respectively.

Table I. Mulliken Atomic Charges (in units of electrons) for Tricyanocyclopropene and Tricyanocyclopropenyl Species.[1]

24 (C_s, $^1A'$)	C1	ΔC1	C3	ΔC3	C4	ΔC4	C6	ΔC6	N1	ΔN1	N3	ΔN3
MP2//HF	0.45		0.54		-0.11		-0.12		-0.37		-0.38	
MP2	0.85		0.51		-0.58		-0.21		-0.27		-0.31	
B-VWN5	0.59		0.26		-0.36		-0.08		-0.20		-0.24	
B-LYP	0.55		0.22		-0.33		-0.05		-0.19		-0.23	
B3-LYP	0.69		0.29		-0.45		-0.08		-0.21		-0.25	
25 (C_s, $^1A'$)												
MP2//HF	0.76	0.31	-0.85	-1.39	-0.22	-0.11	0.35	0.47	-0.49	-0.12	-0.59	-0.21
MP2	1.08	0.23	-0.54	-1.05	-0.67	-0.09	0.04	0.25	-0.41	-0.14	-0.52	-0.21
B-VWN5	0.61	0.02	-0.54	-0.80	-0.31	0.05	0.03	0.11	-0.34	-0.14	-0.41	-0.17
B-LYP	0.54	-0.01	-0.59	-0.81	-0.24	0.09	0.06	0.11	-0.32	-0.13	-0.41	-0.18
B3-LYP	0.70	0.01	-0.62	-0.91	-0.35	0.10	0.07	0.15	-0.35	-0.14	-0.44	-0.19
26 (C_2, ^1A)												
MP2//HF	-0.80	-1.56	1.29	2.14	0.30	0.52	0.28	-0.07	-0.56	-0.07	-0.45	0.14
MP2	-0.39	-1.47	1.59	2.13	-0.24	0.43	0.01	-0.03	-0.49	-0.08	-0.37	0.15
B-VWN5	-0.24	-0.85	0.89	1.43	-0.10	0.21	-0.08	-0.11	-0.41	-0.07	-0.30	0.11
B-LYP	-0.30	-0.84	0.81	1.40	-0.03	0.21	-0.05	-0.11	-0.40	-0.08	-0.29	0.12
B3-LYP	-0.35	-1.05	0.99	1.61	-0.06	0.29	-0.02	-0.09	-0.43	-0.08	-0.31	0.13
27 (C_1, ^1A)[2]												
B-VWN5	0.97 (0.18)	0.36 (-0.43)	-0.44	0.10	-0.20 (-0.41)	0.11 (-0.10)	0.00	-0.03	-0.31 (-0.38)	0.03 (-0.04)	-0.42	-0.01
B-LYP	0.92 (0.09)	0.38 (-0.45)	-0.50	0.09	-0.14 (-0.34)	0.10 (-0.10)	0.03	-0.03	-0.30 (-0.36)	0.02 (-0.04)	-0.41	0.00
B3-LYP	0.93 (0.45)	0.23 (-0.25)	-0.61	0.01	-0.27 (-0.42)	0.08 (-0.07)	0.06	-0.01	-0.34 (-0.36)	0.01 (-0.01)	-0.44	0.00

[1]Hydrogen atom contributions have been summed into the carbons. The charge differences (e.g., ΔC1) for **25** are relative to **24** while for all the other species they are given in comparison to **25**. See Figure 5 for the labeling scheme. [2]Parenthetical values in the C1 and ΔC1, C4 and ΔC4, and N1 and ΔN1 columns correspond to C2 and ΔC2, C5 and ΔC5, and N2 and ΔN2, respectively.

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