

Chemistry–A European Journal

Supporting Information

Twisting versus Delocalization in CAAC- and NHC-Stabilized Boron-Based Biradicals: The Roles of Sterics and Electronics

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I. Further information on CAAC-stabilized compounds

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$$y_i = 1 - \frac{2T_i}{1+T_i^2} \quad (1)$$

$$T_i = \frac{n_{HOMO-i} - n_{LUMO+i}}{2} \quad (2)$$

Table S1: Selected bond distances within the characterized compounds (S_0). Distances are given in Å. The enumeration of the centers is given in Scheme 1.

Comp.	$R_{N^1C^1}$	$R_{C^1B^1}$	$R_{B^1C^2}$	$R_{C^2C^3}$	$R_{C^3B^2}$	$R_{B^2C^4}$	$R_{C^4N^2}$
Full system with bulky substituents							
CAAC_Full_C ₂ H ₅ _Cl (crystal data)	1.37	1.50	1.59	1.34	1.59	1.50	1.37
CAAC_Full_C ₂ H ₅ _Cl (full opt.)	1.36	1.52	1.57	1.35	1.57	1.52	1.36
CAAC_Full_C ₂ H ₅ _Cl (twisted)	1.36	1.52	1.57	1.35	1.57	1.52	1.36
CAAC_Full_C ₂ H ₅ _Cl (planar)	1.36	1.54	1.57	1.38	1.57	1.54	1.36
CAAC_Full_CH ₃ _Cl (crystal data)	1.37	1.51	1.60	1.35	1.60	1.51	1.37
CAAC_Full_CH ₃ _Cl (full opt.)	1.36	1.52	1.57	1.35	1.57	1.52	1.36
CAAC_Full_CH ₃ _Cl (twisted)	1.36	1.52	1.57	1.35	1.57	1.52	1.36
CAAC_Full_CH ₃ _Cl (planar)	1.37	1.55	1.55	1.39	1.55	1.55	1.37
CAAC_Full_H_Cl (full opt.)	1.34	1.54	1.49	1.40	1.49	1.54	1.34
CAAC_Full_H_Cl (twisted)	1.36	1.51	1.56	1.34	1.56	1.51	1.36
CAAC_Full_H_Cl (planar)	1.34	1.54	1.49	1.40	1.49	1.54	1.34
CAAC_Full_C ₂ H ₅ _H (full opt.)	1.36	1.52	1.57	1.36	1.57	1.52	1.35
CAAC_Full_C ₂ H ₅ _H (twisted)	1.36	1.52	1.58	1.35	1.58	1.52	1.36
CAAC_Full_C ₂ H ₅ _H (planar)	1.36	1.55	1.52	1.44	1.52	1.55	1.36
CAAC_Full_CH ₃ _H (full opt.)	1.36	1.52	1.57	1.35	1.57	1.52	1.36
CAAC_Full_CH ₃ _H (twisted)	1.35	1.52	1.57	1.35	1.57	1.52	1.35
CAAC_Full_CH ₃ _H (planar)	1.35	1.55	1.51	1.44	1.51	1.55	1.35
CAAC_Full_H_H (full opt.)	1.34	1.53	1.49	1.41	1.49	1.53	1.34
CAAC_Full_H_H (twisted)	1.36	1.52	1.56	1.35	1.56	1.52	1.36
CAAC_Full_H_H (planar)	1.34	1.53	1.49	1.41	1.49	1.53	1.34
Model compound without bulky substituents							
CAAC_Mod_C ₂ H ₅ _Cl (twisted)	1.35	1.50	1.56	1.35	1.56	1.50	1.35
CAAC_Mod_C ₂ H ₅ _Cl (planar)	1.34	1.56	1.51	1.43	1.51	1.56	1.34
CAAC_Mod_CH ₃ _Cl (twisted)	1.35	1.50	1.56	1.35	1.56	1.50	1.35
CAAC_Mod_CH ₃ _Cl (planar)	1.34	1.54	1.51	1.43	1.51	1.54	1.34
CAAC_Mod_H_Cl (twisted)	1.35	1.50	1.56	1.34	1.56	1.50	1.35
CAAC_Mod_H_Cl (planar)	1.33	1.52	1.48	1.40	1.48	1.52	1.33
CAAC_Mod_C ₂ H ₅ _H (twisted)	1.35	1.51	1.57	1.35	1.57	1.51	1.35
CAAC_Mod_C ₂ H ₅ _H (planar)	1.34	1.53	1.50	1.43	1.50	1.53	1.34
CAAC_Mod_CH ₃ _H (twisted)	1.35	1.51	1.57	1.35	1.57	1.51	1.35
CAAC_Mod_CH ₃ _H (planar)	1.34	1.53	1.50	1.43	1.50	1.53	1.34
CAAC_Mod_H_H (twisted)	1.35	1.51	1.56	1.35	1.56	1.51	1.35
CAAC_Mod_H_H (planar)	1.34	1.52	1.49	1.40	1.49	1.52	1.34

Table S2: Selected bond angles within the characterized compounds (S_0). The enumeration of the centers is given in Scheme 1.

Comp.	$\sphericalangle N^1 C^1 B^1$	$\sphericalangle C^1 B^1 C^2$	$\sphericalangle B^1 C^2 C^3$	$\sphericalangle C^2 C^3 B^2$	$\sphericalangle C^3 B^2 C^4$	$\sphericalangle B^2 C^4 N^2$
Full system with bulky substituents						
CAAC_Full_C ₂ H ₅ _Cl (crystal data)	129.2	126.6	121.1	121.1	126.6	129.2
CAAC_Full_C ₂ H ₅ _Cl (full opt.)	129.0	124.8	120.0	120.0	124.8	129.0
CAAC_Full_C ₂ H ₅ _Cl (twisted)	128.9	125.0	120.1	120.1	125.0	128.9
CAAC_Full_C ₂ H ₅ _Cl (planar)	126.7	124.9	125.3	125.3	124.9	126.7
CAAC_Full_CH ₃ _Cl (crystal data)	128.9	126.3	121.9	121.9	126.3	128.9
CAAC_Full_CH ₃ _Cl (full opt.)	128.5	124.6	124.2	124.2	124.6	128.5
CAAC_Full_CH ₃ _Cl (twisted)	128.2	126.6	124.1	124.1	126.6	128.2
CAAC_Full_CH ₃ _Cl (planar)	124.9	124.6	126.0	126.0	124.6	124.9
CAAC_Full_H_Cl (full opt.)	127.5	121.2	126.3	126.3	121.2	127.5
CAAC_Full_H_Cl (twisted)	127.7	125.3	126.5	126.5	125.3	127.7
CAAC_Full_H_Cl (planar)	127.8	121.0	126.7	126.7	121.0	127.8
CAAC_Full_C ₂ H ₅ _H (full opt.)	123.9	126.0	120.1	124.2	124.2	124.0
CAAC_Full_C ₂ H ₅ _H (twisted)	124.3	124.1	122.2	122.2	124.1	124.3
CAAC_Full_C ₂ H ₅ _H (planar)	118.1	134.1	120.7	120.7	134.1	118.1
CAAC_Full_CH ₃ _H (full opt.)	123.3	126.5	126.5	126.5	126.5	123.3
CAAC_Full_CH ₃ _H (twisted)	123.4	126.5	125.7	125.7	126.5	123.4
CAAC_Full_CH ₃ _H (planar)	118.7	133.3	120.5	120.5	133.3	118.7
CAAC_Full_H_H (full opt.)	123.2	123.5	124.1	124.1	123.5	123.2
CAAC_Full_H_H (twisted)	123.9	124.8	127.1	127.0	124.7	123.9
CAAC_Full_H_H (planar)	123.0	123.9	124.0	124.0	123.9	123.0
Model compound without bulky substituents						
CAAC_Mod_C ₂ H ₅ _Cl (twisted)	126.4	121.6	122.3	122.3	121.6	126.4
CAAC_Mod_C ₂ H ₅ _Cl (planar)	120.1	126.8	129.9	129.9	126.8	120.1
CAAC_Mod_CH ₃ _Cl (twisted)	126.3	123.5	123.4	123.4	123.5	126.3
CAAC_Mod_CH ₃ _Cl (planar)	121.7	125.2	127.9	127.9	125.2	121.7
CAAC_Mod_H_Cl (twisted)	125.7	123.9	125.3	125.3	123.9	125.7
CAAC_Mod_H_Cl (planar)	124.9	121.7	127.4	127.4	121.7	124.9
CAAC_Mod_C ₂ H ₅ _H (twisted)	126.3	117.7	123.6	123.6	117.7	126.3
CAAC_Mod_C ₂ H ₅ _H (planar)	118.5	126.9	123.5	123.5	126.9	118.5
CAAC_Mod_CH ₃ _H (twisted)	126.3	119.3	125.2	125.2	119.3	126.3
CAAC_Mod_CH ₃ _H (planar)	118.9	127.2	122.3	122.3	127.2	118.9
CAAC_Mod_H_H (twisted)	125.3	120.8	127.0	127.0	120.8	125.3
CAAC_Mod_H_H (planar)	124.7	119.0	126.6	126.6	119.0	124.7

Table S3: Sum of bonding angles around C² and C³. The unexpected <S²> value for **CAAC_Full_C₂H₅Cl** (planar) and **CAAC_Full_CH₃Cl** (planar) result from pyramidalization of the C² and the C³ centers. *S* always gives the first atom center of the substituent R³.

Comp.	$\angle B^1C^2S$	$\angle SC^2C^3$	$\angle B^1C^2C^3$	$\angle SC^3B^2$	$\angle C^2C^3S$	$\angle C^2C^3B^2$
Full system with bulky substituents						
CAAC_Full_C₂H₅Cl (crystal data)	119.2	119.6	121.1	119.2	119.6	121.1
CAAC_Full_C₂H₅Cl (full opt.)	119.4	120.4	120.0	119.4	120.4	120.0
CAAC_Full_C₂H₅Cl (twisted)	119.5	120.4	120.1	119.5	120.4	120.1
CAAC_Full_C₂H₅Cl (planar)	108.9	112.4	125.3	108.9	112.4	125.3
CAAC_Full_CH₃Cl (crystal data)	117.0	120.7	121.9	117.0	120.7	121.9
CAAC_Full_CH₃Cl (full opt.)	114.0	121.1	124.2	114.0	121.1	124.2
CAAC_Full_CH₃Cl (twisted)	114.0	121.0	124.1	114.0	121.0	124.1
CAAC_Full_CH₃Cl (planar)	110.3	114.9	126.0	110.3	114.9	126.0
CAAC_Full_HCl (full opt.)	119.6	114.0	126.3	119.6	114.0	126.3
CAAC_Full_HCl (twisted)	116.4	116.3	126.5	116.4	116.3	126.5
CAAC_Full_HCl (planar)	119.2	113.9	126.7	119.2	113.9	126.7
CAAC_Full_C₂H₅H (full opt.)	120.3	119.5	120.1	117.6	118.1	124.2
CAAC_Full_C₂H₅H (twisted)	118.5	119.3	122.2	118.5	119.3	122.2
CAAC_Full_C₂H₅H (planar)	120.7	118.2	120.7	120.7	118.2	120.7
CAAC_Full_CH₃H (full opt.)	113.0	120.2	126.5	113.0	120.2	126.5
CAAC_Full_CH₃H (twisted)	113.4	120.0	125.7	113.4	120.0	125.7
CAAC_Full_CH₃H (planar)	122.4	116.6	120.5	122.4	116.6	120.5
CAAC_Full_HH (full opt.)	122.7	113.2	124.1	122.7	113.2	124.1
CAAC_Full_HH (twisted)	117.1	115.2	127.1	117.1	115.3	127.0
CAAC_Full_HH (planar)	122.8	113.1	124.0	122.8	113.1	124.0

Table S4: Selected dihedral angles for the ground state of the fully optimized CAAC structures. The enumeration is given in Scheme 1.

Comp.	$\angle N^1C^1B^1C^2$	$\angle C^1B^1C^2C^3$	$\angle B^1C^2C^3B^2$	$\angle C^2C^3B^2C^4$	$\angle C^3B^2C^4N^2$
Full systems with bulky substituents					
CAAC_Full_C₂H₅Cl (cry. data)	178.1	-96.8	180.0	96.8	-178.1
CAAC_Full_C₂H₅Cl (full opt.)	174.5	-97.0	180.0	97.0	-174.5
CAAC_Full_CH₃Cl (cry. data)	-169.6	-97.7	180.0	97.7	169.6
CAAC_Full_CH₃Cl (full opt.)	-163.6	-99.4	180.0	99.4	163.6
CAAC_Full_HCl (full opt.)	-161.0	170.3	180.0	-170.3	161.0
CAAC_Full_C₂H₅H (full opt.)	178.4	-112.3	-179.0	83.9	-179.4
CAAC_Full_CH₃H (full opt.)	-173.0	-86.8	180.0	86.8	173.0
CAAC_Full_HH (full opt.)	-167.7	174.8	180.0	-174.7	167.7

Table S5: Selected calculated interatomic distances $R_{\text{calc.}}$ [Å] and the dihedral angle $\angle C^1B^1C^2S$ [°] of the characterized compounds (S_0). S gives the first atom center of the substituent R^3 . The difference between the calculated atomic distance $R_{\text{calc.}}$ and the sum of the van der Waals radii $R_{\text{v.d.W.-r.}}$ is defined as $R_{\text{diff.}}$ [Å]. The abbreviations of H_{bridge} , H_{CAAC} , H_{Dip} and H_{Nitrogen} are H_b , H_c , H_D and H_N . The interatomic distances for the full and model system (twisted/planar) are shown by colored lines in Figure S1.

Comp.	$R_{\text{calc.}}$			$R_{\text{diff.}} = R_{\text{calc.}} - R_{\text{v.d.W.-r.}}$			Dihedral
	Cl- H_b	H_c - H_b	Cl- H_D	Cl- H_b	H_c - H_b	Cl- H_D	$\angle C^1B^1C^2S$
	purple	yellow	red	purple	yellow	red	-
Full system with bulky substituents							
CAAC_Full_C₂H₅_Cl (crystal data)	3.15	2.27	2.77	0.30	0.07	-0.08	87.5
CAAC_Full_C₂H₅_Cl (full opt.)	3.06	2.17	2.67	0.21	-0.03	-0.18	87.7
CAAC_Full_C₂H₅_Cl (twisted)	3.04	2.13	2.68	0.19	-0.07	-0.17	90.3
CAAC_Full_C₂H₅_Cl (planar)	2.44	2.04	2.68	-0.41	-0.16	-0.17	42.6
CAAC_Full_CH₃_Cl (crystal data)	3.21	2.25	2.85	0.36	0.05	0.00	89.3
CAAC_Full_CH₃_Cl (full opt.)	3.21	2.19	2.75	0.36	-0.01	-0.10	90.1
CAAC_Full_CH₃_Cl (twisted)	3.04	2.15	2.74	0.19	-0.05	-0.11	100.6
CAAC_Full_CH₃_Cl (planar)	2.68	2.18	2.63	-0.17	-0.02	-0.22	34.6
CAAC_Full_H_Cl (full opt.)	2.66	1.98	2.67	-0.19	-0.22	-0.18	-6.2
CAAC_Full_H_Cl (twisted)	3.23	2.56	2.82	0.38	0.36	-0.03	101.2
CAAC_Full_H_Cl (planar)	2.65	1.90	2.70	-0.20	-0.30	-0.15	5.0
Comp.	$R_{\text{calc.}}$			$R_{\text{diff.}} = R_{\text{calc.}} - R_{\text{v.d.W.-r.}}$			Dihedral
	Cl- H_b	H_c - H_b	Cl- H_N	Cl- H_b	H_c - H_b	Cl- H_N	$\angle C^1B^1C^2S$
	purple	yellow	green	purple	yellow	green	-
Model compound without bulky substituents							
CAAC_Mod_C₂H₅_Cl (twisted)	3.03	2.31	2.78	0.18	0.11	-0.07	85.7
CAAC_Mod_C₂H₅_Cl (planar)	2.38	1.79	2.28	-0.47	-0.41	-0.57	-5.4
CAAC_Mod_CH₃_Cl (twisted)	3.37	3.06	2.77	0.52	0.86	-0.08	92.0
CAAC_Mod_CH₃_Cl (planar)	2.54	2.09	2.38	-0.31	-0.11	-0.47	14.2
CAAC_Mod_H_Cl (twisted)	3.44	3.35	2.73	0.59	1.15	-0.12	93.6
CAAC_Mod_H_Cl (planar)	2.88	2.38	2.66	0.03	0.18	-0.19	-0.4

Figure S1: Sketch of the color-coded atomic distances summarized in Table S5 using the full system **CAAC_Full_CH₃_Cl** (left) and the model system **CAAC_Mod_CH₃_Cl** (right) as examples. The two upper pictures show the twisted structures while the lower pictures give the planar structures.

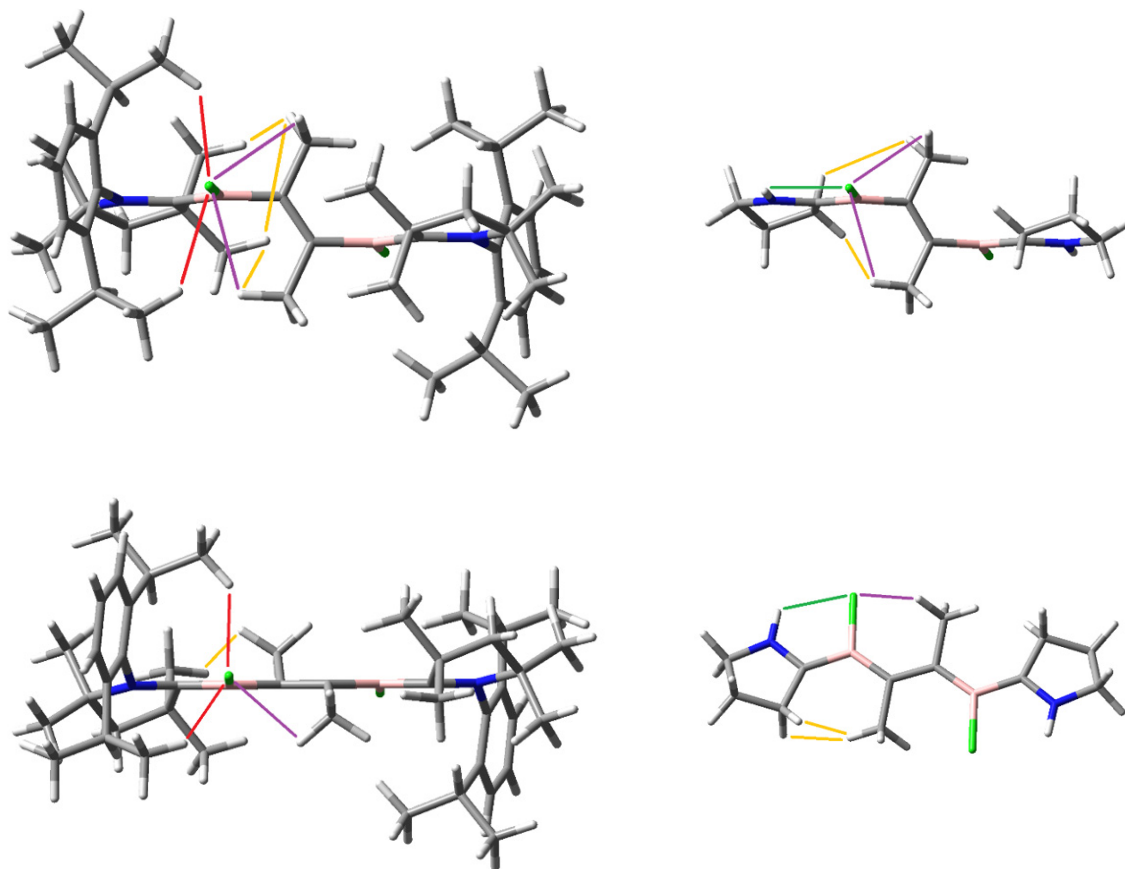


Figure S2: SOMO orbitals of the twisted structure of the systems **CAAC_Mod_R³_X** with R³ = C₂H₅, CH₃, H and X = Cl, H and of the diborane obtained from UMN12L/6-311G(d,p) computations for the lowest triplet state. S-T gaps are obtained from NEVPT2/cc-pVDZ computations. A positive value means a singlet ground state.

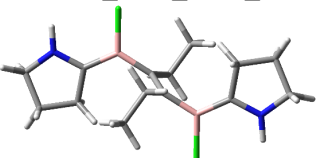
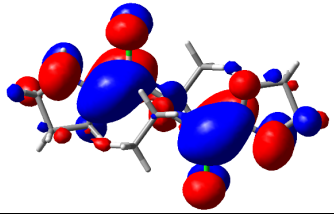
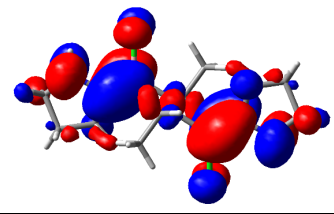

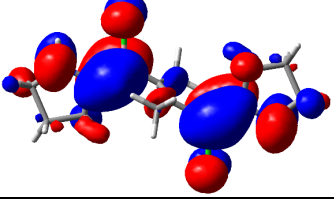
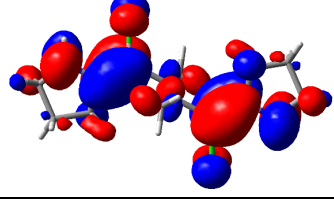
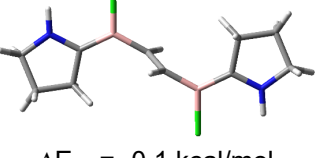
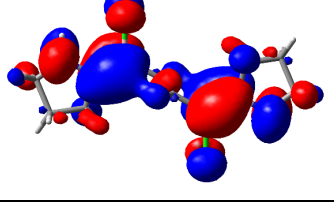
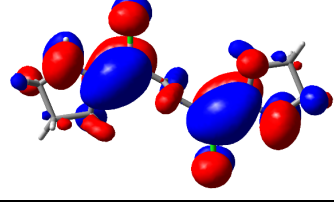
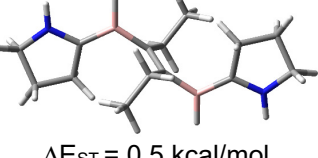
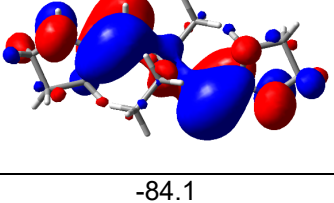
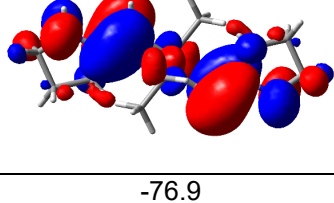
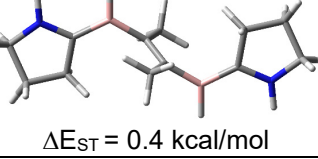
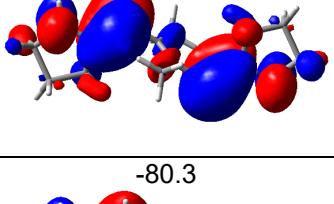
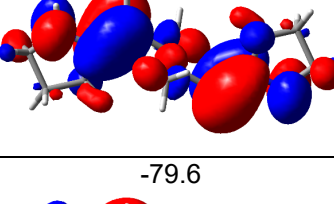
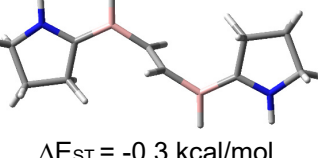
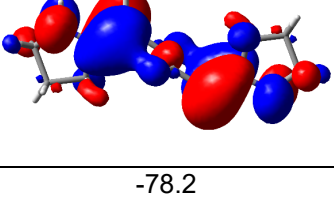
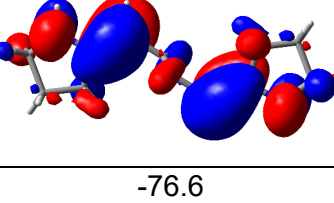
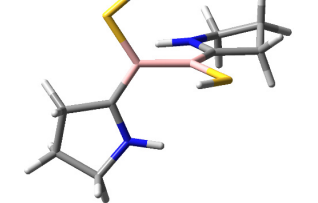
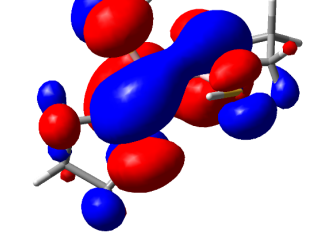
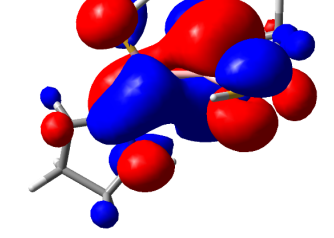
Comp. S-T gap	SOMO1	SOMO2
CAAC_Mod_C₂H₅_Cl  $\Delta E_{ST} = 0.4$ kcal/mol	-88.8 	-84.0 
CAAC_Mod_CH₃_Cl  $\Delta E_{ST} = 0.4$ kcal/mol	-88.6 	-82.8 
CAAC_Mod_H_Cl  $\Delta E_{ST} = -0.1$ kcal/mol	-86.6 	-85.8 
CAAC_Mod_C₂H₅_H  $\Delta E_{ST} = 0.5$ kcal/mol	-84.3 	-78.4 
CAAC_Mod_CH₃_H  $\Delta E_{ST} = 0.4$ kcal/mol	-84.1 	-76.9 
CAAC_Mod_H_H  $\Delta E_{ST} = -0.3$ kcal/mol	-80.3 	-79.6 
CAAC-Diborene  $\Delta E_{ST} = -0.4$ kcal/mol	-78.2 	-76.6 

Figure S3: SOMO orbitals of the twisted structure of the systems **CAAC_Mod_R³_X** with R³ = C₂H₅, CH₃, H and X = Cl, H and of the diborane obtained from CASSCF(4,6)/cc-pVDZ computations for the lowest triplet state. S-T gaps are obtained from NEVPT2/cc-pVDZ computations. A positive value means a singlet ground state.

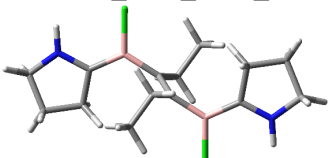
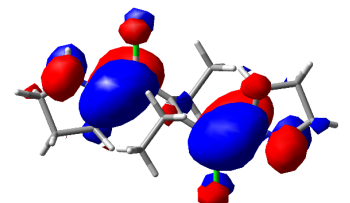
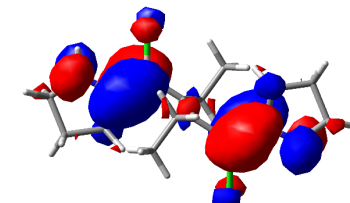
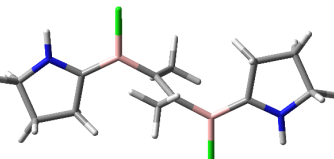
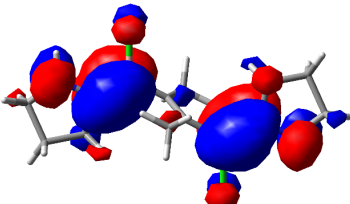
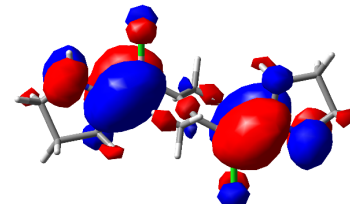
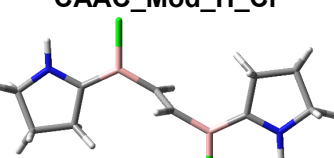
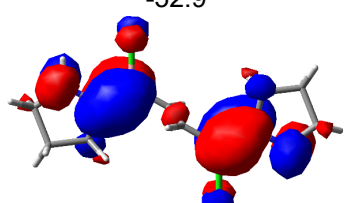
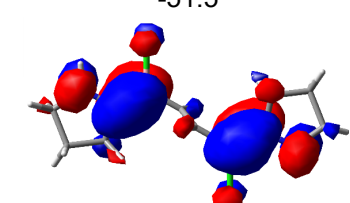
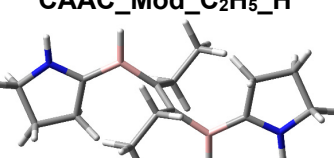
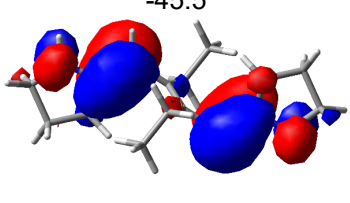
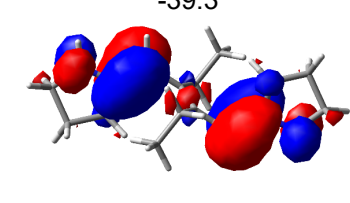
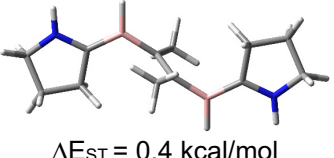
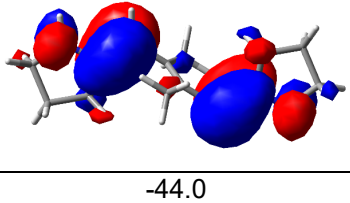
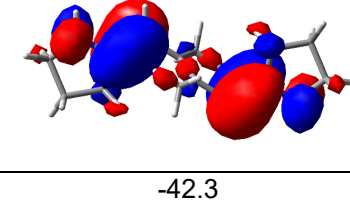
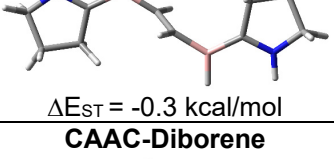
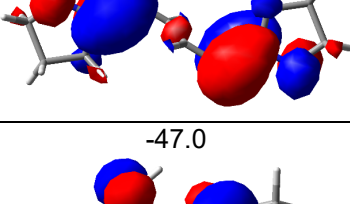
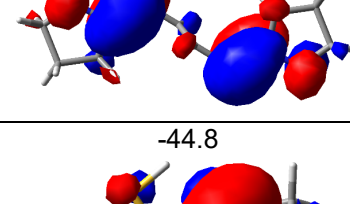
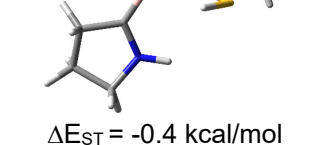
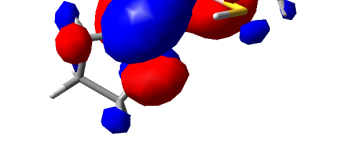
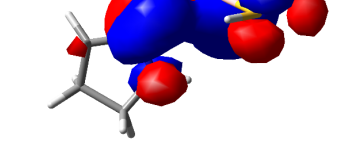
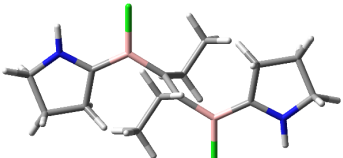
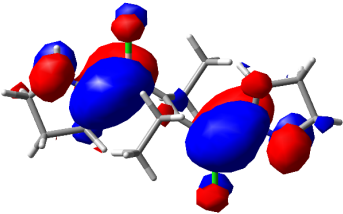
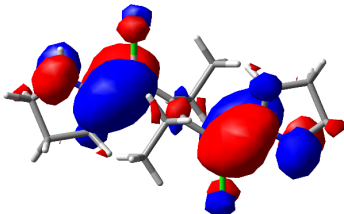
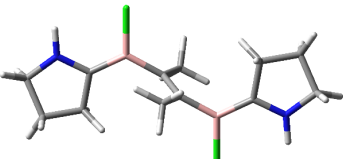
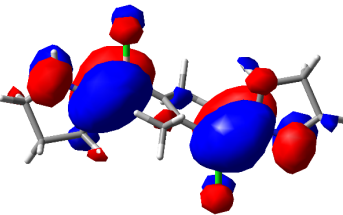
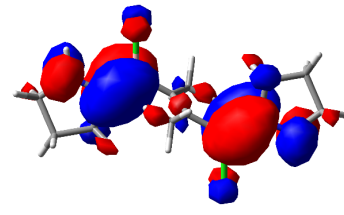
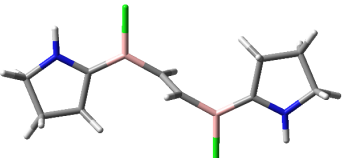
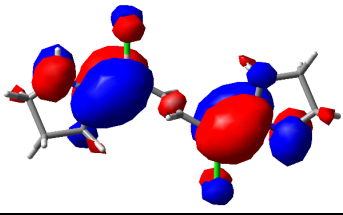
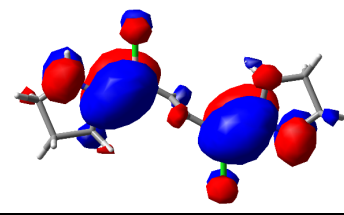
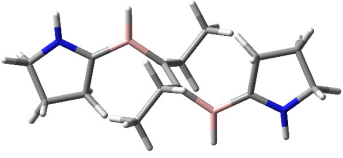
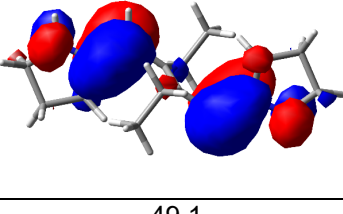
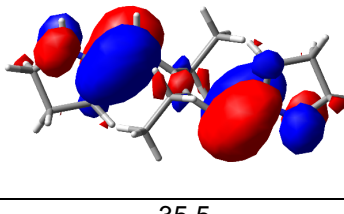
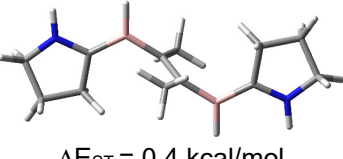
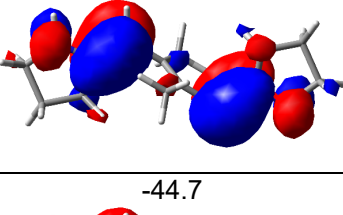
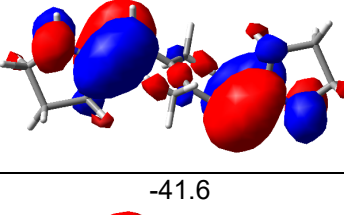
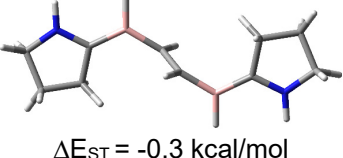
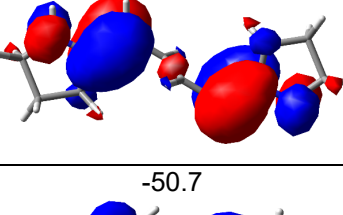
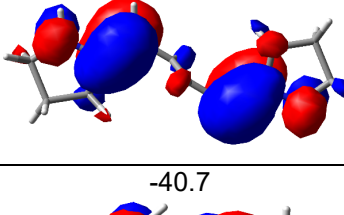
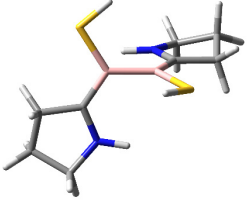
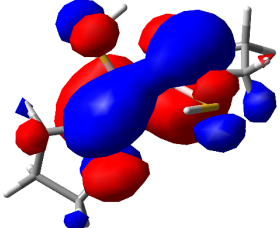
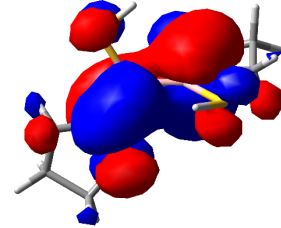
Comp. S-T gap	SOMO1	SOMO2
CAAC_Mod_C₂H₅_Cl  $\Delta E_{ST} = 0.4$ kcal/mol	-53.7 	-48.4 
CAAC_Mod_CH₃_Cl  $\Delta E_{ST} = 0.4$ kcal/mol	-54.1 	-47.8 
CAAC_Mod_H_Cl  $\Delta E_{ST} = -0.1$ kcal/mol	-52.9 	-51.5 
CAAC_Mod_C₂H₅_H  $\Delta E_{ST} = 0.5$ kcal/mol	-45.5 	-39.3 
CAAC_Mod_CH₃_H  $\Delta E_{ST} = 0.4$ kcal/mol	-46.1 	-38.8 
CAAC_Mod_H_H  $\Delta E_{ST} = -0.3$ kcal/mol	-44.0 	-42.3 
CAAC-Diborene  $\Delta E_{ST} = -0.4$ kcal/mol	-47.0 	-44.8 

Figure S4: SOMO orbitals of the twisted structure of the systems **CAAC_Mod_R³_X** with R³ = C₂H₅, CH₃, H and X = Cl, H and of the diborane obtained from CASSCF(4,6)/cc-pVDZ computations for the lowest singlet state. S-T gaps obtained from NEVPT2/cc-pVDZ computations. A positive value means a singlet ground state.

Comp. S-T gap	SOMO1	SOMO2
CAAC_Mod_C₂H₅_Cl  $\Delta E_{ST} = 0.4$ kcal/mol	-55.9 	-46.0 
CAAC_Mod_CH₃_Cl  $\Delta E_{ST} = 0.4$ kcal/mol	-56.7 	-45.0 
CAAC_Mod_H_Cl  $\Delta E_{ST} = -0.1$ kcal/mol	-53.5 	-50.9 
CAAC_Mod_C₂H₅_H  $\Delta E_{ST} = 0.5$ kcal/mol	-48.2 	-36.4 
CAAC_Mod_CH₃_H  $\Delta E_{ST} = 0.4$ kcal/mol	-49.1 	-35.5 
CAAC_Mod_H_H  $\Delta E_{ST} = -0.3$ kcal/mol	-44.7 	-41.6 
CAAC-Diborene  $\Delta E_{ST} = -0.4$ kcal/mol	-50.7 	-40.7 

II. Further information on the saturated hydrocarbon-bridged model compounds

Figure S5: CASCI(2,2) triplet MOs of the planar and twisted structure of the saturated hydrocarbon-bridged diborenes together with the orbital energies. The S-T gaps [kcal/mol] are computed with the CASCI(2,2)/cc-pVDZ and the NEVPT2/cc-pVDZ approach. A negative sign indicates a triplet ground state.

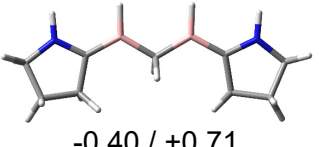
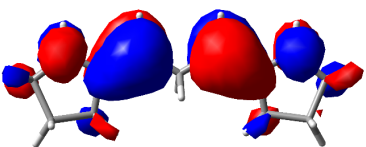
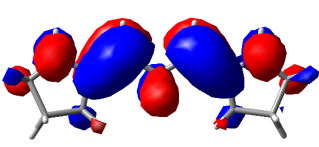
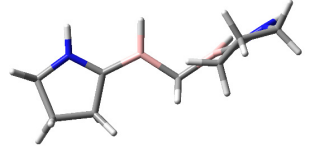
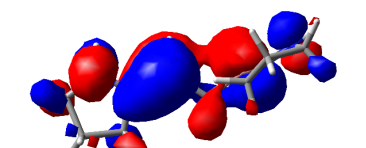
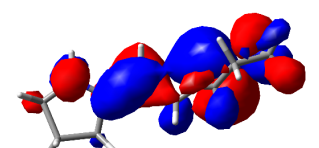
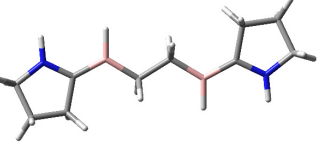
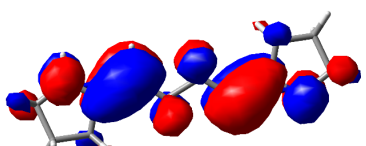
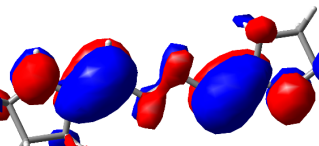
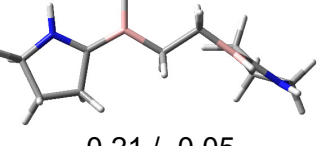
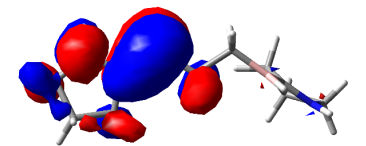
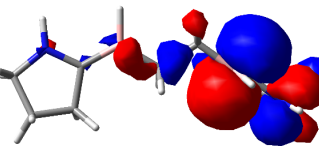
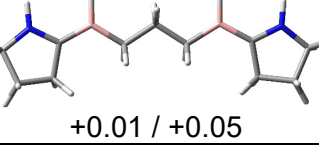
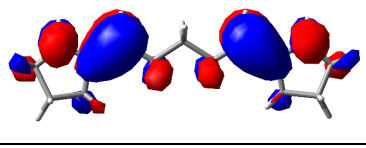
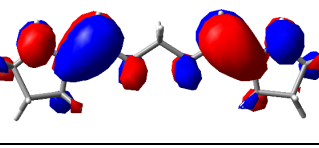
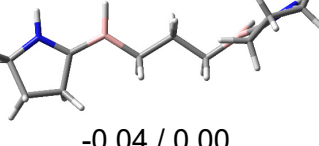
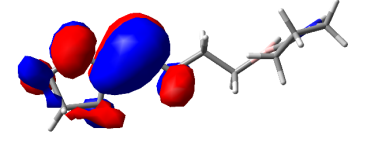
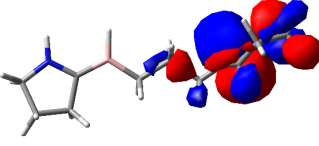
conformer S-T gap in [kcal/mol]: CASCI(2,2) / NEVPT2(2,2)	SOMO1	SOMO2
CH₂		
 -0.40 / +0.71 planar	 57.4	 64.1
 -0.85 / -0.21 twisted	 61.9	 65.3
C₂H₄		
 -0.13 / +0.22 planar	 51.7	 56.2
 -0.21 / -0.05 twisted	 53.1	 57.5
C₃H₆		
 +0.01 / +0.05 planar	 49.7	 52.5
 -0.04 / 0.00 twisted	 50.2	 54.7

Table S6: CASCI(2,2) wavefunction for the lowest singlet state of the planar and the twisted structure of the saturated hydrocarbon-bridged diborenes. The structures and the orbital shapes are depicted in Figure S5. The occupation pattern gives the occupation of SOMO1 and SOMO2 within the given determinants. The column 2 0 contains the coefficients c_i and its square c_i^2 of the determinant in which the SOMO1 is doubly occupied while SOMO2 is empty. For 1 1 both orbitals are singly occupied, etc.

coeff.	occupation pattern		
	2 0	0 2	1 1
CH₂: planar structure			
c_i	0.7388896	-0.6737217	-0.01188106
c_i^2	0.54596	0.45390	0.00014
CH₂: twisted structure			
c_i	0.6241019	-0.6000098	-0.5004848
c_i^2	0.38950	0.36001	0.25049
C₂H₄: planar structure			
c_i	0.7269007	-0.6867425	-0.0001753747
c_i^2	0.52838	0.47162	0.00000
C₂H₄: twisted structure			
c_i	0.1572038	-0.1454666	0.9767940
c_i^2	0.02471	0.02116	0.95413
C₃H₆: planar structure			
c_i	0.7178663	-0.6949993	-0.04054588
c_i^2	0.51533	0.48302	0.00164
C₃H₆: twisted structure			
c_i	-0.04016355	0.03941161	0.9984156
c_i^2	0.00161	0.00155	0.99683

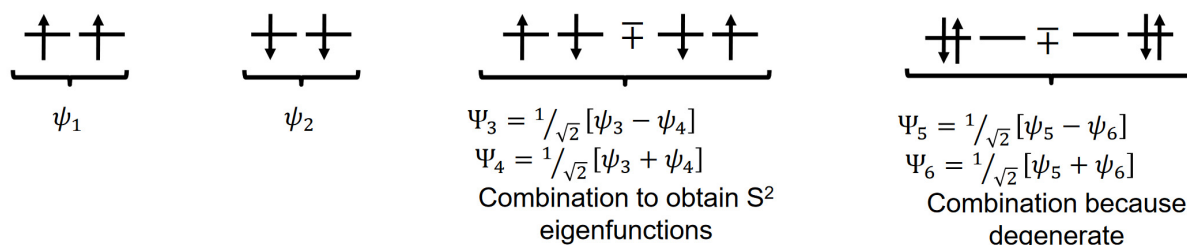
Description of the orbital shapes and the related wavefunctions of the saturated hydrocarbon-bridged compounds

The electronic structures of the singlet states of the saturated hydrocarbon-bridged compounds are characterized by means of the occupation numbers of the SOMOs (Figure S5) and the wavefunctions (Table S6). Obviously, the forms of SOMOs and wavefunctions depend on the conformers. The differences are best seen for the (CH₂)₃-bridged compound. For the planar structure, the CASCI(2,2)/cc-pVDZ computation provides orbitals which are delocalized over the whole molecule while orbitals located either on the left or the right B-CAAC unit are calculated for the twisted conformer. Coincidentally, the form of the wavefunction changes. For localized orbitals (twisted form) the lowest-lying singlet state is dominated by one determinant in which both SOMOs are singly occupied. For the planar structure, the orbitals are delocalized and the wavefunction is dominated by two determinants in which either SOMO1 or SOMO2 are doubly occupied. Both determinants have similar coefficients and according to the sign of the coefficients both determinants form a negative linear combination. For the compounds with a (CH₂)₂ bridge we find the same pattern. The planar structure of the CH₂-bridged system resembles the other systems. For the twisted conformer the wavefunction is more complicated, however, the MOs are also a mixture of localized and delocalized orbitals. For the interpretation of these data, one has to know how the electronic wavefunctions and the energy order of the various states are related to the shape of the underlying MOs (localized vs. delocalized MOs).

III. Discussion of the 4*4 CI model to describe biradicaloid systems

These relationships are explained in the excellent reviews of Bonačić-Koutecký, Koutecký and Michl^[2] about biradicaloid compounds. As such, we provide only a brief summary and refer the reader to the original papers for more information. If two electrons are distributed in two spatial orbitals, six different determinants can be generated as shown in Scheme S1. The determinants ψ_3 and ψ_4 have to be combined to obtain correct eigenfunctions of the S^2 operator. The determinants ψ_5 and ψ_6 should be combined because they have the same energy if both orbitals are energetically degenerate. With this we obtain six electronic states whose wavefunctions will be abbreviated as $\Psi_1 - \Psi_6$. For each of these wavefunctions, the spin and space portions can be separated as shown in Scheme S2. Scheme S2 also gives the S_z and S^2 quantum numbers M_S and $\langle S^2 \rangle$ together with the energies. The data reveal that the three states Ψ_1, Ψ_2, Ψ_4 form the triplet manifold with the M_S quantum numbers 1, -1 and 0. These states are energetically degenerate. They do not interact with each other because they show different M_S quantum numbers. They also do not interact with the singlet states if the spin-orbit interaction is neglected. Because the various triplet states do not interact with any other state their energies can simply be obtained by applying the Slater-Condon rules. The Slater-Condon rules reduce matrix elements between determinants to the connected integrals.^[3] Because we neglect spin-orbit effects we only include the triplet state with $M_S=0$. According to its open-shell spatial wavefunction structure we abbreviate it as $^3|\phi_1\phi_2\rangle$, in which ϕ_1 and ϕ_2 give the two degenerate or near-degenerate spatial orbitals. This state also does not interact with the remaining singlet state, but it is of interest to explain why biradical boron species show singlet or triplet ground states. The remaining states, Ψ_3, Ψ_5 and Ψ_6 form three singlet states which interact with each other. According to their spatial forms (Scheme S2) they will be abbreviated as $^1|\phi_1\phi_2\rangle, ^1|\phi_1^2 - \phi_2^2\rangle$ and $^1|\phi_1^2 + \phi_2^2\rangle$.

Scheme S1: Principle determinants and states arising if two electrons are distributed in two spatial orbitals ϕ_1 and ϕ_2 . In the following we always assume that both orbitals are orthogonal to each other.



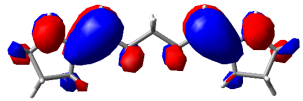
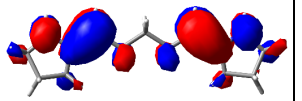
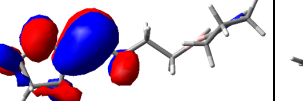
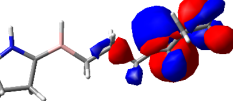
Scheme S2: Electronic wavefunctions and energies of the states obtained from the six determinants depicted in Scheme S1.

$$\begin{aligned}
 \psi_1 &= \frac{1}{\sqrt{2}} \underbrace{\alpha(1)\alpha(2)}_{\text{symmetric}} \underbrace{[\phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1)]}_{\text{antisymmetric}} \quad M_S = 1, \langle S^2 \rangle = 2 \\
 \psi_2 &= \frac{1}{\sqrt{2}} \underbrace{\beta(1)\beta(2)}_{\text{symmetric}} \underbrace{[\phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1)]}_{\text{antisymmetric}} \quad M_S = -1, \langle S^2 \rangle = 2 \\
 \Psi_4 &= \frac{1}{2} \left(\underbrace{[\phi_1(r_1)\phi_2(r_2) - \phi_1(r_2)\phi_2(r_1)]}_{\text{antisymmetric}} \cdot \underbrace{[\alpha(1)\beta(2) + \alpha(2)\beta(1)]}_{\text{symmetric}} \right) \quad M_S = 0, \langle S^2 \rangle = 2
 \end{aligned}$$

$$\begin{aligned}
 E(\text{triplets}) &= \\
 &h_{11} + h_{22} \\
 &+ J_{12} - K_{12}
 \end{aligned}$$

$$\begin{aligned}
 \Psi_3 &= \frac{1}{2} \left(\underbrace{[\phi_1(r_1)\phi_2(r_2) + \phi_1(r_2)\phi_2(r_1)]}_{\text{symmetric}} \cdot \underbrace{[\alpha(1)\beta(2) - \alpha(2)\beta(1)]}_{\text{antisymmetric}} \right) \quad h_{11} + h_{22} + J_{12} + K_{12} \\
 \Psi_5 &= \frac{1}{2} \left(\underbrace{[\phi_1(r_1)\phi_1(r_2) - \phi_2(r_1)\phi_2(r_2)]}_{\text{symmetric}} \cdot \underbrace{[\alpha(1)\beta(2) - \alpha(2)\beta(1)]}_{\text{antisymmetric}} \right) \quad h_{11} + h_{22} + \frac{1}{2}(J_{11} + J_{22}) - K_{12} \\
 \Psi_6 &= \frac{1}{2} \left(\underbrace{[\phi_1(r_1)\phi_1(r_2) + \phi_2(r_1)\phi_2(r_2)]}_{\text{symmetric}} \cdot \underbrace{[\alpha(1)\beta(2) - \alpha(2)\beta(1)]}_{\text{antisymmetric}} \right) \quad h_{11} + h_{22} + \frac{1}{2}(J_{11} + J_{22}) + K_{12}
 \end{aligned}$$

Scheme S3: Relationship between localized MOs A, B and delocalized MOs a, b. The left-hand side shows how localized orbitals A and B could be obtained from the delocalized orbitals a, b given by the CASCI(2,2)/cc-pVDZ computations of the planar form. The orbital A would be located at the left part of the molecule, B would be located at the right side. The right-hand side indicates how delocalized orbitals a, b could be obtained from the localized orbitals A and B given by the CASCI(2,2) computations of the twisted form. Orbital a gives the bonding linear combination of the two localized π systems, while b gives the antibonding form.

delocalized orbitals a, b for planar form		localized orbitals A, B for twisted form	
			
$A = \frac{1}{\sqrt{2}}(a + b)$		$a = \frac{1}{\sqrt{2}}(A - B)$	
$B = \frac{1}{\sqrt{2}}(a - b)$		$b = \frac{1}{\sqrt{2}}(A + B)$	

Depending on the CASCI computations, the involved orbitals ϕ_1 and ϕ_2 can be localized or delocalized. However, both orbital sets can be transformed into each other as indicated in Scheme S3. As in the reviews of Bonačić-Koutecký, Koutecký and Michl^[2] we will abbreviate delocalized MOs (Scheme S3 left-hand side) as a and b, while A and B are used for the localized ones (Scheme S3 right-hand side). The corresponding energy expressions as well as the 4*4 CI matrix indicating the various interactions are given in Scheme S4 for localized MOs and in Scheme S5 for delocalized MOs.

Scheme S4: The quantities characterizing the interactions in the 4×4 CI model description of two electrons contained in two orthogonal localized orbitals A and B, i.e. their overlap $S_{AB} = \int A(1)B(1)d\tau_1$ vanishes.

	$^1 A^2 + B^2\rangle$	$^1 A^2 - B^2\rangle$	$^1 AB\rangle$	$^3 AB\rangle$
$^1 A^2 + B^2\rangle$	$E(T) + 2(K'_{AB} + K_{AB})$	δ_{AB}	γ_{AB}	0
$^1 A^2 - B^2\rangle$	δ_{AB}	$E(T) + 2K'_{AB}$	γ_{AB}^-	0
$^1 AB\rangle$	γ_{AB}	γ_{AB}^-	$E(T) + 2K_{AB}$	0
$^3 AB\rangle$	0	0	0	$E(T)$

With

$$E(T) = E_0 - (K'_{AB} + K_{AB})$$

$$E_0 = h_{AA} + h_{BB} + (J_{AA} + J_{BB})/4 + J_{AA}/2$$

$$2K'_{AB} = [(J_{AA} + J_{BB})/2 - J_{AB}]/2$$

$$\delta_{AB} = h_{AA} - h_{BB} + (J_{AA} - J_{BB})/2$$

$$\gamma_{AB}^- = (AA|AB) - (BB|BA)$$

$$\gamma_{AB} = 2h_{AB} + (AA|AB) + (BB|BA)$$

$$J_{AB} = \int \int A(1) \cdot A(1) \frac{1}{r_{12}} B(2) \cdot B(2) d\tau_1 d\tau_2$$

$$K_{AB} = \int \int A(1) \cdot B(1) \frac{1}{r_{12}} A(2) \cdot B(2) d\tau_1 d\tau_2$$

$$(AA|AB) = \int \int A(1) \cdot A(1) \frac{1}{r_{12}} A(2) \cdot B(2) d\tau_1 d\tau_2$$

$$h_{AB} = \int A(1) h(1) B(1) d\tau_1$$

Scheme S5: The quantities characterizing the interactions in the 4×4 CI model description of two electrons contained in two orthogonal delocalized orbitals a and b, i.e. their overlap $S_{ab} = \int a(1)b(1)d\tau_1$ vanishes.

	$^1 a^2 + b^2\rangle$	$^1 ab\rangle$	$^1 a^2 - b^2\rangle$	$^3 ab\rangle$
$^1 a^2 + b^2\rangle$	$E(T) + 2(K_{ab} + K'_{ab})$	γ_{ab}	δ_{ab}	0
$^1 ab\rangle$	γ_{ab}	$E(T) + 2K_{ab}$	γ_{ab}^-	0
$^1 a^2 - b^2\rangle$	δ_{ab}	γ_{ab}^-	$E(T) + 2K'_{ab}$	0
$^3 ab\rangle$	0	0	0	$E(T)$

The expressions for the matrix elements can be taken from Scheme S4 by changing A, B by a, b. However, while the expressions remain, the actual number changes (see text).

As depicted in Scheme S3 delocalized and localized MOs can be transformed into each other. As nicely explained in the aforementioned reviews,^[2] some expressions in Scheme S4 and S5 remain invariant while others interchange. Going from the localized to the delocalized orbitals,

E_0 , $E(T)$, $K'_{xy} \pm K_{xy}$, $(K'_{xy} - K_{xy})^2 - \gamma_{xy}^-$, and $\delta_{xy}^2 + \gamma_{xy}^2$ ($xy \equiv A, B$ or a, b) stay invariant. The same holds for $^1|A^2 + B^2\rangle$, which transform into $^1|a^2 + b^2\rangle$. In contrast, $^1|A^2 - B^2\rangle$ transforms into $^1|ab\rangle$ and $^1|AB\rangle$ into $^1|a^2 - b^2\rangle$. Finally, K'_{AB} and K_{ab} are connected through $K'_{AB} = K_{ab}$ and $K'_{ab} = K_{AB}$. Similarly, $\delta_{AB} = \gamma_{ab}$ and $\delta_{ab} = \gamma_{AB}$ holds. Using these relationships, the matrix describing the interactions between the states in the localized basis (Scheme S4) transforms into the matrix describing the interactions between the states in delocalized basis (Scheme S5).

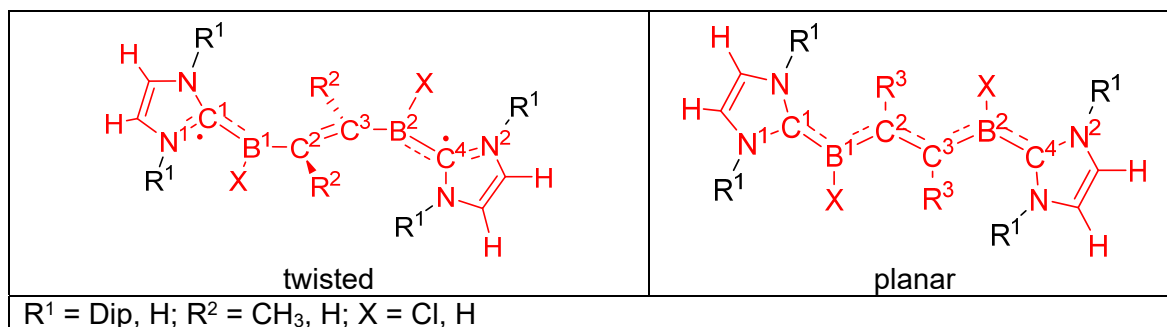
The question arises when we expect a triplet ground state and what is the energy sequence of the singlet states. If the interactions between the singlet states are zero or neglected, the triplet state is the lowest state because all quantities are positive. For both types of orbitals, $^1|\phi_1^2 + \phi_2^2\rangle$ represents the highest lying state but the states $^1|\phi_1\phi_2\rangle$ and $^1|\phi_1^2 - \phi_2^2\rangle$ change their energy position. For localized orbitals, $^1|AB\rangle$ is lower in energy than $^1|A^2 - B^2\rangle$. This order comes about because K_{AB} is smaller than K'_{AB} . The exchange integral K_{AB} depend on the so-called differential overlap $A(1) \cdot B(1) d\tau$. However, this product is always small because the localized orbitals are far apart, so K_{AB} is also quite small. On the other hand, K'_{AB} is large. J_{AA} (J_{BB}) represents the coulomb repulsion between two electrons occupying the localized orbital

A (B). Because the orbitals are localized this interaction will be quite large. J_{AB} on the other side represents the coulomb repulsion between two electrons whereby one occupies A but the other B. Since A and B are far apart, J_{AB} will be much smaller than J_{AA} or J_{BB} . Going from localized to delocalized orbitals (Scheme S3) both states interchange their form and their energy position. Now, ${}^1|ab\rangle$ lies above ${}^1|a^2 - b^2\rangle$. This results, because K_{ab} and K'_{ab} interchange. For delocalized orbitals K_{ab} is large because the delocalized orbitals cover the whole space so that their differential overlap $a(1) \cdot b(1) d\tau$ becomes large. On the other hand, K'_{ab} is small because J_{aa} , J_{bb} and J_{ab} are similar in size. The latter also arise from the delocalized forms of a and b. J_{aa} (J_{bb}) are smaller than J_{AA} (J_{BB}) because the electrons can avoid each other in the delocalized orbitals. J_{ab} on the other hand is larger than J_{AB} because the both orbitals spread in the same space. The switching of the states as a function of the shape of the orbitals explains the qualitative behavior for the lowest-lying singlet states of the saturated hydrocarbon-bridged compounds.

Whether the saturated hydrocarbon- or C_2R_2 -bridged compounds possess a singlet or triplet ground state can be explained on the basis of possible interactions between the spin centers. Due to the interaction the degeneracy of the orbitals is lifted and the singlet state in which the lower lying orbital is doubly occupied becomes lower in energy than the triplet state in which both orbitals are occupied. This picture can be transferred into the picture of the interacting states discussed above. If the orbital ϕ_1 becomes considerably more stable than orbital ϕ_2 , the states ${}^1|\phi_1^2 - \phi_2^2\rangle$ and ${}^1|\phi_1^2 + \phi_2^2\rangle$ start to mix, leading to the lower lying state ${}^1|\phi_1^2\rangle$ and the higher lying ${}^1|\phi_2^2\rangle$. This mixing is introduced either by the explicit expressions for the diagonal elements of the matrices or by an increase of the outer-diagonal matrix element δ_{ab} , which is a measure of the energy difference of both orbitals. For more information, refer to the original articles.²

We explain above that the interaction between the spin centers is responsible for the twisted structures of the saturated hydrocarbon-bridged systems possessing triplet ground states while singlet ground states are found for the planar conformers. Additionally, Figure S5 shows that the size of the S-T gap nicely correlates with the distance of the spin centers. For the parallel orientation, the S-T gap computed with NEVPT2 becomes increasingly positive with decreasing bridge size, i.e. as expected, the interaction between the spin centers increases with decreasing distance. For the twisted conformer we always find a triplet ground state, but the S-T gap decreases with increasing size of the bridge. This can easily be explained by the decreasing size of the exchange integral K_{AB} as a function of the distance between the localized orbitals A and B. Besides NEVPT2 results, Figure S5 also gives the CASCI(2,2) energies. This less sophisticated level of theory always predicts a triplet ground state. This indicates that dynamic correlation effects are essential for an accurate description of the S-T gap.

IV. Further information on the NHC-stabilized systems



Scheme S6: Sketch of the characterized NHC compounds. In the naming of the compounds $R^1 = \text{Dip}$ are denoted *Full* while $R^1 = \text{H}$ is denoted *Mod*. The substituents R^2 and X are explicitly given. For examples the compound with $R^1 = \text{Dip}$, $R^2 = \text{CH}_3$ and $X = \text{Cl}$ is abbreviated as **NHC_Full_CH₃_Cl** while the one with $R^1 = \text{H}$, $R^2 = \text{H}$ and $X = \text{H}$ is called **NHC_Mod_H_H**. In the planar geometry the dihedral angles $\angle N^1C^1B^1C^2$, $\angle C^1B^1C^2C^3$, $\angle B^1C^2C^3B^2$, $\angle C^2C^3B^2C^4$, and $\angle C^3B^2C^4N^2$ are equal to 180° . For the twisted geometry, the dihedral angles $\angle N^1C^1B^1C^2$, $\angle B^1C^2C^3B^2$, and $\angle C^3B^2C^4N^2$ are equal to 180° while $\angle C^1B^1C^2C^3 = -90^\circ$ and $\angle C^2C^3B^2C^4 = 90^\circ$. Geometries obtained by optimization without constraints are denoted “full opt.”. The corresponding dihedral angles for the fully optimized structures are given in Table S9. For more information see main text and below.

Table S7: Selected bond distances within the characterized NHC stabilized compounds (S_0). Distances are given in Å. The enumeration of the centers is given in Scheme S6.

Comp.	$R_{N^1C^1}$	$R_{C^1B^1}$	$R_{B^1C^2}$	$R_{C^2C^3}$	$R_{C^3B^2}$	$R_{B^2C^4}$	$R_{C^4N^2}$
Full system with bulky substituents							
NHC_Full_C₂H₅_Cl (full opt.)	1.36	1.56	1.46	1.45	1.47	1.55	1.36
NHC_Full_C₂H₅_Cl (twisted)	1.39	1.51	1.56	1.36	1.57	1.51	1.39
NHC_Full_C₂H₅_Cl (planar)	1.39	1.55	1.50	1.44	1.50	1.58	1.38
NHC_Full_CH₃_Cl (full opt.)	1.37	1.55	1.48	1.44	1.47	1.57	1.36
NHC_Full_CH₃_Cl (twisted)	1.39	1.52	1.58	1.36	1.58	1.52	1.39
NHC_Full_CH₃_Cl (planar)	1.39	1.55	1.51	1.43	1.51	1.55	1.39
NHC_Full_H_Cl (full opt.)	1.37	1.55	1.48	1.41	1.48	1.55	1.38
NHC_Full_H_Cl (twisted)	1.39	1.51	1.56	1.35	1.55	1.51	1.39
NHC_Full_H_Cl (planar)	1.37	1.55	1.48	1.41	1.48	1.54	1.38
NHC_Full_C₂H₅_H (full opt.)	1.38	1.54	1.50	1.44	1.49	1.54	1.38
NHC_Full_C₂H₅_H (twisted)	1.39	1.51	1.57	1.36	1.58	1.51	1.38
NHC_Full_C₂H₅_H (planar)	1.39	1.55	1.50	1.44	1.50	1.55	1.39
NHC_Full_CH₃_H (full opt.)	1.38	1.54	1.49	1.43	1.49	1.54	1.38
NHC_Full_CH₃_H (twisted)	1.39	1.52	1.57	1.36	1.57	1.52	1.39
NHC_Full_CH₃_H (planar)	1.38	1.54	1.49	1.44	1.49	1.54	1.38
NHC_Full_H_H (full opt.)	1.38	1.54	1.48	1.41	1.48	1.53	1.38
NHC_Full_H_H (twisted)	1.37	1.52	1.56	1.34	1.56	1.52	1.38
NHC_Full_H_H (planar)	1.37	1.54	1.48	1.41	1.48	1.54	1.38
Model compound without bulky substituents							
NHC_Mod_C₂H₅_Cl (twisted)	1.37	1.50	1.56	1.36	1.56	1.50	1.37
NHC_Mod_C₂H₅_Cl (planar)	1.36	1.56	1.49	1.44	1.49	1.56	1.36
NHC_Mod_CH₃_Cl (twisted)	1.37	1.50	1.56	1.36	1.56	1.50	1.37
NHC_Mod_CH₃_Cl (planar)	1.36	1.55	1.49	1.44	1.49	1.55	1.36
NHC_Mod_H_Cl (twisted)	1.37	1.50	1.56	1.35	1.56	1.50	1.37
NHC_Mod_H_Cl (planar)	1.36	1.53	1.46	1.41	1.46	1.53	1.36
NHC_Mod_C₂H₅_H (twisted)	1.37	1.51	1.58	1.36	1.58	1.51	1.37
NHC_Mod_C₂H₅_H (planar)	1.37	1.54	1.49	1.44	1.49	1.54	1.37
NHC_Mod_CH₃_H (twisted)	1.37	1.51	1.58	1.36	1.58	1.51	1.37
NHC_Mod_CH₃_H (planar)	1.37	1.53	1.49	1.43	1.49	1.53	1.37
NHC_Mod_H_H (twisted)	1.37	1.51	1.57	1.35	1.57	1.51	1.37
NHC_Mod_H_H (planar)	1.36	1.53	1.48	1.41	1.48	1.53	1.36

Table S8: Selected bond angles of the characterized NHC-stabilized compounds (S_0). The enumeration of the centers is given in Scheme S6.

Comp.	$\angle N^1 C^1 B^1$	$\angle C^1 B^1 C^2$	$\angle B^1 C^2 C^3$	$\angle C^2 C^3 B^2$	$\angle C^3 B^2 C^4$	$\angle B^2 C^4 N^2$
Full system with bulky substituents						
NHC_Full_C₂H₅_Cl (full opt.)	126.2	126.0	124.3	124.8	123.3	128.1
NHC_Full_C₂H₅_Cl (twisted)	128.2	131.9	122.6	118.1	126.7	129.3
NHC_Full_C₂H₅_Cl (planar)	128.5	125.5	125.7	128.7	124.2	125.4
NHC_Full_CH₃_Cl (full opt.)	127.4	123.2	126.8	128.2	122.9	124.7
NHC_Full_CH₃_Cl (twisted)	129.1	132.3	122.1	121.7	130.8	128.3
NHC_Full_CH₃_Cl (planar)	128.0	124.9	124.5	124.5	124.9	128.1
NHC_Full_H_Cl (full opt.)	128.8	125.0	124.3	126.7	122.9	129.1
NHC_Full_H_Cl (twisted)	129.3	123.6	125.2	126.7	126.8	129.1
NHC_Full_H_Cl (planar)	128.8	123.4	125.6	125.9	123.1	129.0
NHC_Full_C₂H₅_H (full opt.)	124.9	131.5	116.8	122.7	127.6	123.7
NHC_Full_C₂H₅_H (twisted)	123.7	130.5	125.3	119.4	123.9	126.5
NHC_Full_C₂H₅_H (planar)	120.3	133.7	122.1	122.1	133.7	120.3
NHC_Full_CH₃_H (full opt.)	124.9	124.5	122.5	122.6	124.4	125.0
NHC_Full_CH₃_H (twisted)	125.6	127.1	123.2	123.2	127.1	125.6
NHC_Full_CH₃_H (planar)	122.6	127.0	122.0	122.0	127.0	122.6
NHC_Full_H_H (full opt.)	125.8	121.7	128.2	119.3	127.3	123.1
NHC_Full_H_H (twisted)	126.0	122.8	126.9	125.4	120.5	126.6
NHC_Full_H_H (planar)	125.4	124.1	125.4	122.5	124.8	125.0
Model compound without bulky substituents						
NHC_Mod_C₂H₅_Cl (twisted)	130.1	122.6	123.2	123.2	122.6	130.1
NHC_Mod_C₂H₅_Cl (planar)	123.6	125.4	130.4	130.4	125.4	123.6
NHC_Mod_CH₃_Cl (twisted)	130.4	121.0	123.7	123.7	121.0	130.4
NHC_Mod_CH₃_Cl (planar)	124.6	124.5	128.8	128.8	124.5	124.6
NHC_Mod_H_Cl (twisted)	129.6	121.6	125.4	125.4	121.6	129.6
NHC_Mod_H_Cl (planar)	127.6	122.6	128.0	128.0	122.6	127.6
NHC_Mod_C₂H₅_H (twisted)	131.5	117.5	125.2	125.2	117.5	131.5
NHC_Mod_C₂H₅_H (planar)	122.6	125.0	125.0	125.0	125.0	122.6
NHC_Mod_CH₃_H (twisted)	131.9	115.4	125.7	125.7	115.4	131.9
NHC_Mod_CH₃_H (planar)	123.1	123.7	125.9	126.0	123.7	123.1
NHC_Mod_H_H (twisted)	131.2	116.8	127.0	127.0	116.8	131.2
NHC_Mod_H_H (planar)	127.9	119.3	127.7	127.7	119.3	127.9

Table S9: Selected dihedral angles for the ground state of the fully optimized NHC structures. The enumeration is given in Scheme S6.

Comp.	$\angle N^1C^1B^1C^2$	$\angle C^1B^1C^2C^3$	$\angle B^1C^2C^3B^2$	$\angle C^2C^3B^2C^4$	$\angle C^3B^2C^4N^2$
Full systems with bulky substituents					
NHC_Full_C₂H₅_Cl (full opt.)	141.4	162.4	140.2	173.8	125.3
NHC_Full_CH₃_Cl (full opt.)	156.3	148.7	165.6	-177.9	119.3
NHC_Full_H_Cl (full opt.)	174.8	-166.1	163.6	-170.3	178.6
NHC_Full_C₂H₅_H (full opt.)	-160.9	-167.0	-144.7	144.9	172.6
NHC_Full_CH₃_H (full opt.)	167.3	157.0	179.8	-156.3	-167.4
NHC_Full_H_H (full opt.)	171.1	-166.5	163.4	-165.9	157.4

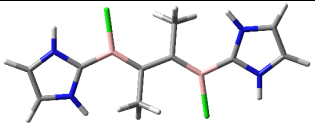
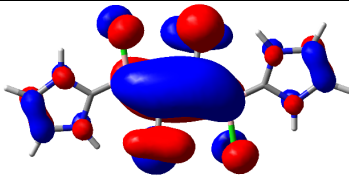
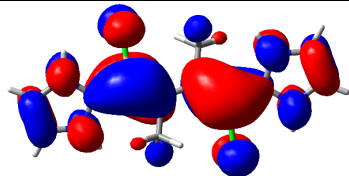
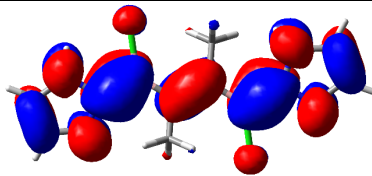
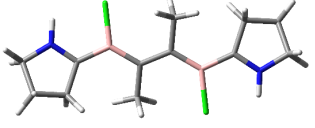
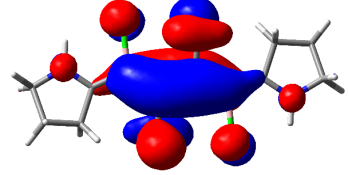
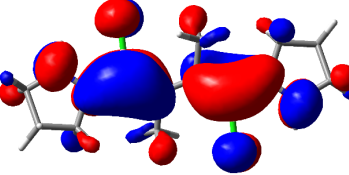
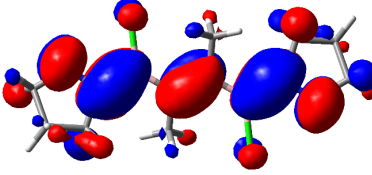
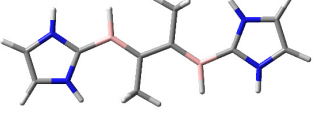
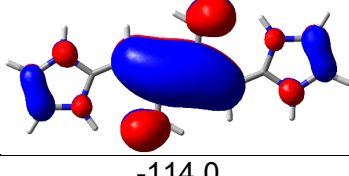
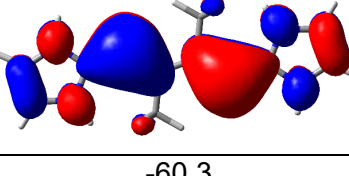
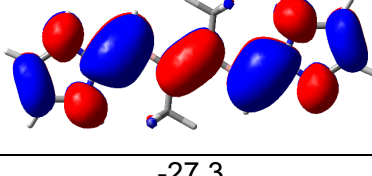
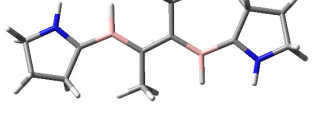
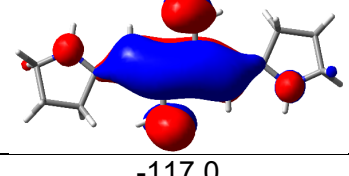
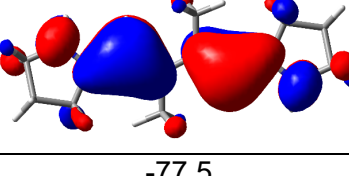
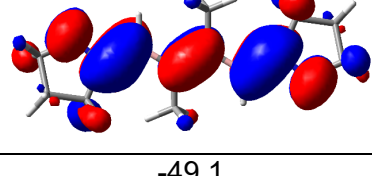
Table S10: Computed NHC-stabilized compounds. Relative energies [kcal/mol] with respect to the S₀ state of the planar structure of the characterized compounds ($\Delta E_{p \rightarrow t}$). $\Delta E_{p \rightarrow t}$ is positive if the planar structure is more stable.

Comp.	NEVPT2(4,6)/cc-pVDZ				UMN12L/6-311G(d,p)			
	S ₀	T ₀	S-T gap	Y (S ₀)	S ₀	T ₀	S-T gap	S ² (S ₀)
Full systems with bulky substituents								
NHC_Full_C₂H₅_Cl (full opt.)	-	-	-	-	-28.8	-22.2	6.6	0.00
NHC_Full_C₂H₅_Cl (twisted)	-	-	-	-	-18.6	-18.4	0.2	1.00
NHC_Full_C₂H₅_Cl (planar)	-	-	-	-	0.0	10.7	10.7	0.00
NHC_Full_CH₃_Cl (full opt.)	-	-	-	-	-27.3	-19.0	8.3	0.00
NHC_Full_CH₃_Cl (twisted)	-	-	-	-	-9.8	-10.6	-0.8	0.95
NHC_Full_CH₃_Cl (planar)	-	-	-	-	0.0	5.5	5.5	0.00
NHC_Full_H_Cl (full opt.)	-	-	-	-	-2.0	12.6	14.6	0.00
NHC_Full_H_Cl (twisted)	-	-	-	-	28.0	28.0	0.0	1.01
NHC_Full_H_Cl (planar)	-	-	-	-	0.0	16.3	16.3	0.00
NHC_Full_C₂H₅_H (full opt.)	-	-	-	-	-13.4	-7.7	5.7	0.00
NHC_Full_C₂H₅_H (twisted)	-	-	-	-	-1.1	-0.9	0.2	1.01
NHC_Full_C₂H₅_H (planar)	-	-	-	-	0.0	12.1	12.1	0.00
NHC_Full_CH₃_H (full opt.)	-	-	-	-	-10.4	-4.5	5.9	0.00
NHC_Full_CH₃_H (twisted)	-	-	-	-	-2.7	-0.1	2.6	0.94
NHC_Full_CH₃_H (planar)	-	-	-	-	0.0	14.9	14.9	0.00
NHC_Full_H_H (full opt.)	-	-	-	-	-0.7	11.6	12.3	0.00
NHC_Full_H_H (twisted)	-	-	-	-	20.5	20.5	0.0	1.01
NHC_Full_H_H (planar)	-	-	-	-	0.0	14.0	14.0	0.00
Model system without the bulky substituents								
NHC_Mod_C₂H₅_Cl (twisted)	15.9	16.4	0.5	0.77	14.5	15.2	0.7	0.96
NHC_Mod_C₂H₅_Cl (planar)	0.0	27.2	27.2	0.01	0.0	20.5	20.5	0.00
NHC_Mod_CH₃_Cl (twisted)	11.3	11.8	0.5	0.77	14.4	15.2	0.8	0.95
NHC_Mod_CH₃_Cl (planar)	0.0	21.7	21.7	0.01	0.0	19.1	19.1	0.00
NHC_Mod_H_Cl (twisted)	33.8	33.5	-0.3	0.91	35.4	35.5	0.1	1.01
NHC_Mod_H_Cl (planar)	0.0	25.7	25.7	0.01	0.0	21.5	21.5	0.00
NHC_Mod_C₂H₅_H (twisted)	24.8	25.5	0.7	0.76	22.0	22.8	0.8	0.96
NHC_Mod_C₂H₅_H (planar)	0.0	26.4	26.4	0.01	0.0	19.6	19.6	0.00
NHC_Mod_CH₃_H (twisted)	24.5	25.2	0.7	0.73	22.4	23.4	1.0	0.95
NHC_Mod_CH₃_H (planar)	0.0	25.3	25.3	0.02	0.0	19.1	19.1	0.00

NHC_Mod_H_H (twisted)	31.9	31.6	-0.3	0.91	30.5	30.6	0.1	1.01
NHC_Mod_H_H (planar)	0.0	25.7	25.7	0.01	0.0	20.7	20.7	0.00

V. Comparison of planar structures of CAAC- and NHC-stabilized compounds

Table S11: Influence of cyclic carbenes CAAC and NHC, respectively, for selected model systems of C_2R_2 -bridged and non-bridged diborenes. $\Delta E_{p \rightarrow t}$ gives the relative energy between the planar and the twisted structure. A negative sign would indicate a twisted structure as a ground state. In the twisted structure of the C_2R_2 -bridged diborenes, the C_2R_2 -bridge is rotated by 90° with respect to the boron / cyclic carbene planes. For the twisted diborenes both boron / carbene moieties are rotated by 90° with respect to each other. ΔE_{ST} gives the S-T gap for the planar structure. A positive sign indicates a singlet ground state. For the bridged systems we employed NEVPT2(4,6)/cc-pVDZ while NEVPT2(2,4)/cc-pVDZ were used for the diborenes. The singlet orbital energies are taken from UMN12L computations, which show nearly identical trends and orbitals.

Comp.	$\Delta E_{p \rightarrow t}$	S-T gap	HOMO-1	HOMO	LUMO
	11.3	21.7			
NHC Mod CH₃ Cl			-121.6	-69.7	-37.1
	3.5	10.6			
CAAC Mod CH₃ Cl			-128.9	-84.5	-59.7
	24.5	25.3			
NHC Mod CH₃ H			-114.0	-60.3	-27.3
	13.1	14.7			
CAAC Mod CH₃ H			-117.0	-77.5	-49.1

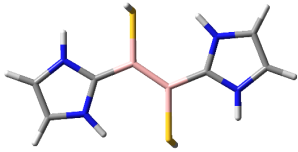
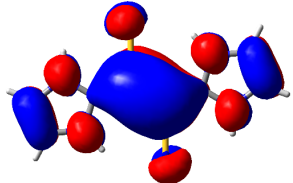
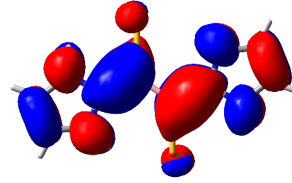
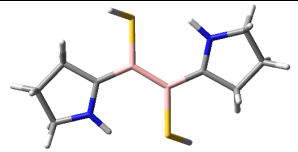
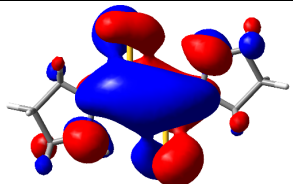
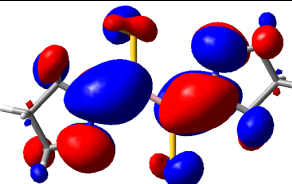
Comp.	$\Delta E_{p \rightarrow t}$	ΔE_{ST}	HOMO	LUMO
	26.1	25.1		
NHC-Diborene			-73.3	-28.7
	5.2	9.6		
CAAC-Diborene			-83.1	-53.3

Table S12: Reaction energies $\Delta E_{\text{Reac.}}$ of the exchange reaction replacing CAAC ligands by NHC ligands. (see Scheme 2 of main text)

Substituents	$\Delta E_{\text{Reac.}}$ [kcal/mol]
	UMN12L/6-311G(d,p)
XX Full C₂H₅ Cl	10.1
XX Full CH₃ Cl	4.3
XX Full H Cl	2.6
XX Full C₂H₅ H	8.1
XX Full CH₃ H	4.4
XX Full H H	11.2

VI. References

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- [S2] a) V. Bonačić-Koutecký, J. Koutecký, J. Michl, *Angew. Chem. Int. Ed.* **1987**, *26*, 170–189; b) J. Michl, V. Bonačić-Koutecký, *Tetrahedron* **1988**, *44*, 7559–7585.
- [S3] Szabo, A.; Ostlund, N. S. *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*; Dover Publications: New York, 1996.

VII. XYZ-coordinates of all *full* systems optimized with UMN12L/6-311G(d,p)

1. CAAC_Full_C₂H₅_Cl (fully optimized)-singlet:

C	-6.03386000	3.92112300	-2.00974700
N	-7.79107100	3.88786600	-0.47364600
C	-5.87620500	2.70970900	-1.07590400
C	-7.20725100	2.52248100	-0.34951500
H	-5.09546000	2.93666000	-0.33600600
H	-5.56783400	1.80730700	-1.61708100
C	-7.14401900	4.72105700	-1.32741400
C	-6.54464000	7.08866700	-2.56246700
C	-5.62990400	7.91550800	-2.00900000
C	-6.79548100	7.11180300	-4.05976900
H	-6.52745600	8.10117500	-4.47144400
H	-6.10195900	6.40940200	-4.56059300
C	-5.37905200	7.89237200	-0.51170200
H	-5.64714100	6.90302300	-0.10001600
H	-6.07251400	8.59483000	-0.01087400
C	-6.50975000	3.49485800	-3.40730100
H	-6.62369700	4.37002600	-4.05392300
H	-7.47311000	2.97539900	-3.38049200
H	-5.77185700	2.82601100	-3.87012300
C	-4.68869800	4.63732600	-2.15158700
H	-3.90989000	3.89138600	-2.35762000
H	-4.41590800	5.16746900	-1.22965800
H	-4.67846000	5.36215900	-2.96916500
C	-7.00077600	2.12454300	1.10853900
H	-6.29346400	2.78469100	1.61575400
H	-6.59448600	1.10814700	1.14137200
H	-7.94945200	2.12272400	1.65779400
C	-8.12008100	1.46563300	-0.97338400
H	-8.31781300	1.62970300	-2.03448000
H	-9.07580900	1.44416000	-0.43850300
H	-7.65508500	0.48033300	-0.86309800
C	-6.14068400	11.08305100	-2.56163800

N	-4.38361300	11.11630300	-4.09789800
C	-6.29845900	12.29442900	-3.49550600
C	-4.96748500	12.48166700	-4.22202700
H	-6.60680000	13.19684200	-2.95432900
H	-7.07926800	12.06743400	-4.23532100
C	-5.66466100	11.50937500	-1.16414700
H	-4.70134200	12.02890300	-1.19107700
H	-5.55057600	10.63422600	-0.51752300
H	-6.40254800	12.17817800	-0.70125300
C	-7.48581500	10.36682200	-2.41962900
H	-7.49596400	9.64206400	-1.60198300
H	-7.75866700	9.83657900	-3.34148200
H	-8.26462700	11.11275700	-2.21359800
C	-4.05462900	13.53857200	-3.59829300
H	-3.85680600	13.37457200	-2.53720300
H	-4.51965900	14.52385400	-3.70859800
H	-3.09894400	13.56003800	-4.13325200
C	-5.17411200	12.87953100	-5.68007800
H	-5.88143400	12.21931900	-6.18719700
H	-4.22548600	12.88137700	-6.22941900
H	-5.58046200	13.89590300	-5.71292000
B	-4.74009700	8.82735300	-2.92684000
B	-7.43446600	6.17683000	-1.64463800
Cl	-8.82445900	7.11526800	-0.91269000
C	-5.03057500	10.28312000	-3.24405500
Cl	-3.35012000	7.88893000	-3.65883400
C	-8.98687100	4.23977100	0.22985200
C	-10.23125100	4.09101400	-0.40854600
C	-8.88640200	4.78796300	1.52126400
C	-11.37979800	4.41795100	0.31160100
C	-10.06588500	5.09811100	2.19580700
C	-11.30419400	4.90020500	1.60739400
H	-12.35034000	4.31167900	-0.16777600
H	-12.21168100	5.14963000	2.14993000

H	-10.00581300	5.52654400	3.19371100
C	-7.56578900	5.15963200	2.17752600
C	-7.38634100	4.47491500	3.53650000
H	-7.51796300	3.39084600	3.49426100
H	-8.11693200	4.86604800	4.25509200
H	-6.39134100	4.68601900	3.94424100
C	-7.46760300	6.67563700	2.38703900
H	-6.74807900	4.86760700	1.50398500
H	-6.49518000	6.93048600	2.82482500
H	-8.24262600	7.01890800	3.08373400
H	-7.58540500	7.23061500	1.45464900
C	-10.39010300	3.70079100	-1.87023300
C	-11.26590200	2.45792400	-2.05241600
H	-11.31830200	2.18120600	-3.11142600
H	-12.29172000	2.66398600	-1.72325800
H	-10.90953100	1.59087600	-1.49109500
C	-11.01291900	4.85040800	-2.67215700
H	-9.39434500	3.50968800	-2.28953100
H	-11.07051500	4.57985500	-3.73309600
H	-10.44152000	5.77623500	-2.57980800
H	-12.03527600	5.05059400	-2.32783200
C	-3.18785100	10.76441500	-4.80147000
C	-1.94343600	10.91323200	-4.16315500
C	-2.10892900	9.90606400	-6.76747000
C	-0.87059000	10.10402900	-6.17914100
C	-0.79492100	10.58631600	-4.88336300
H	0.03687100	9.85462300	-6.72172700
H	0.17564600	10.69263200	-4.40404900
C	-1.78450900	11.30351100	-2.70149100
C	-1.16164400	10.15392900	-1.89955400
H	-1.73306100	9.22810400	-1.99180900
H	-1.10396300	10.42453900	-0.83863400
H	-0.13931700	9.95371200	-2.24394800
C	-0.90871400	12.54639400	-2.51940400

H	-2.78024400	11.49462200	-2.28214800
H	-0.85627400	12.82316500	-1.46041000
H	-1.26512200	13.41341100	-3.08075200
H	0.11709300	12.34033200	-2.84859500
C	-3.28838200	10.21618300	-6.09286000
C	-4.60902000	9.84443000	-6.74902300
C	-4.70712500	8.32841700	-6.95852000
H	-5.67958700	8.07349800	-7.39618000
H	-4.58916300	7.77345000	-6.02614400
H	-3.93216900	7.98520100	-7.65531500
C	-4.78861300	10.52912000	-8.10799200
H	-5.42669800	10.13640900	-6.07542100
H	-4.65707400	11.61319900	-8.06577900
H	-5.78362300	10.31793100	-8.51566500
H	-4.05803800	10.13803400	-8.82662700
H	-2.16904800	9.47760500	-7.76536000
C	-8.23347900	6.77183700	-4.43548500
H	-8.50564000	5.76172600	-4.09422000
H	-8.93508900	7.46654200	-3.95502000
H	-8.39667800	6.81281900	-5.51690500
C	-3.94102100	8.23223600	-0.13601800
H	-3.23947200	7.53748600	-0.61650700
H	-3.66880000	9.24233000	-0.47728300
H	-3.77779700	8.19123600	0.94539800

2. CAAC_Full_C₂H₅_Cl (fully optimized)-triplet:

C	-6.03329000	3.92024300	-2.00857400
N	-7.79057700	3.88746400	-0.47222300
C	-5.87635500	2.70869900	-1.07472600
C	-7.20772600	2.52163200	-0.34902000

H	-5.09602200	2.93551100	-0.33434500
H	-5.56778100	1.80628400	-1.61576000
C	-7.14388100	4.72020100	-1.32693600
C	-6.54389300	7.08806500	-2.56238300
C	-5.63075300	7.91613300	-2.00913200
C	-6.79486700	7.10893300	-4.06008200
H	-6.53144700	8.09845600	-4.47391100
H	-6.09879200	6.40868500	-4.56028700
C	-5.37977000	7.89526000	-0.51143400
H	-5.64318600	6.90573400	-0.09760700
H	-6.07583900	8.59550600	-0.01122100
C	-6.50722300	3.49431000	-3.40684300
H	-6.61839200	4.36938600	-4.05402600
H	-7.47147000	2.97638500	-3.38177700
H	-5.76944900	2.82428000	-3.86813300
C	-4.68798400	4.63664100	-2.14849500
H	-3.90882300	3.89096400	-2.35415000
H	-4.41632600	5.16612000	-1.22583500
H	-4.67689800	5.36207800	-2.96553000
C	-7.00221300	2.12176900	1.10862700
H	-6.29432200	2.78042800	1.61696700
H	-6.59715500	1.10484700	1.14038800
H	-7.95110100	2.12036500	1.65751500
C	-8.12109300	1.46623600	-0.97457600
H	-8.31871100	1.63225200	-2.03539300
H	-9.07685300	1.44450100	-0.43976200
H	-7.65669900	0.48047100	-0.86589500
C	-6.14137300	11.08394300	-2.56298300
N	-4.38408700	11.11671300	-4.09933500
C	-6.29830500	12.29548700	-3.49683100
C	-4.96694100	12.48254200	-4.22255200
H	-6.60686400	13.19790600	-2.95579400
H	-7.07865000	12.06868500	-4.23720200
C	-5.66744600	11.50987600	-1.16471200

H	-4.70321000	12.02782200	-1.18977900
H	-5.55625600	10.63479500	-0.51753700
H	-6.40523300	12.17988500	-0.70341300
C	-7.48668100	10.36754600	-2.42307400
H	-7.49777700	9.64210800	-1.60604000
H	-7.75833100	9.83807100	-3.34573700
H	-8.26584300	11.11322500	-2.21742500
C	-4.05357000	13.53794700	-3.59702100
H	-3.85594700	13.37194800	-2.53620100
H	-4.51796400	14.52371100	-3.70571600
H	-3.09781300	13.55967400	-4.13184100
C	-5.17246900	12.88237700	-5.68020400
H	-5.88036100	12.22370300	-6.18852400
H	-4.22358600	12.88377600	-6.22910100
H	-5.57753500	13.89929600	-5.71198100
B	-4.74146000	8.82780700	-2.92851100
B	-7.43318800	6.17638500	-1.64301100
Cl	-8.82095800	7.11584200	-0.90860600
C	-5.03077800	10.28398400	-3.24461000
Cl	-3.35368400	7.88834700	-3.66290000
C	-8.98637400	4.23952500	0.23111100
C	-10.23070400	4.09251700	-0.40781600
C	-8.88587700	4.78609800	1.52321300
C	-11.37918900	4.41941300	0.31246700
C	-10.06528200	5.09637100	2.19782600
C	-11.30358200	4.90006500	1.60885500
H	-12.34969500	4.31437700	-0.16725700
H	-12.21103500	5.14948300	2.15145000
H	-10.00515600	5.52357400	3.19625400
C	-7.56510600	5.15578900	2.18026700
C	-7.38694200	4.46976600	3.53874800
H	-7.52031200	3.38594200	3.49563700
H	-8.11698600	4.86152100	4.25756000
H	-6.39165500	4.67894000	3.94678600

C	-7.46521100	6.67149200	2.39097100
H	-6.74750600	4.86330300	1.50680800
H	-6.49322400	6.92471900	2.83065300
H	-8.24099600	7.01537800	3.08650800
H	-7.58060900	7.22726900	1.45875400
C	-10.38959600	3.70432000	-1.87006000
C	-11.26542900	2.46173600	-2.05405000
H	-11.31848000	2.18706400	-3.11356200
H	-12.29104100	2.66716900	-1.72385200
H	-10.90871000	1.59361500	-1.49463900
C	-11.01267900	4.85508500	-2.67018000
H	-9.39381600	3.51393900	-2.28975300
H	-11.06906500	4.58672100	-3.73174000
H	-10.44215300	5.78119500	-2.57537800
H	-12.03552800	5.05363000	-2.32637500
C	-3.18829200	10.76464600	-4.80266700
C	-1.94395900	10.91167000	-4.16374900
C	-2.10939000	9.90777100	-6.76937400
C	-0.87108800	10.10409600	-6.18041300
C	-0.79547600	10.58476900	-4.88403300
H	0.03636300	9.85467500	-6.72301000
H	0.17503200	10.68981700	-4.40431600
C	-1.78506300	11.29988800	-2.70151100
C	-1.16197000	10.14913600	-1.90137800
H	-1.73249800	9.22302500	-1.99615800
H	-1.10557100	10.41751900	-0.83982300
H	-0.13912600	9.95058300	-2.24519300
C	-0.90923500	12.54247800	-2.51754000
H	-2.78084200	11.49026800	-2.28181600
H	-0.85618200	12.81716400	-1.45803200
H	-1.26595900	13.41059000	-3.07696100
H	0.11637700	12.33704400	-2.84773800
C	-3.28879300	10.21804800	-6.09475900
C	-4.60956600	9.84833000	-6.75179500

C	-4.70943900	8.33262300	-6.96248100
H	-5.68144200	8.07937000	-7.40211100
H	-4.59398300	7.77685600	-6.03026500
H	-3.93368100	7.98874800	-7.65805400
C	-4.78775500	10.53433400	-8.11028300
H	-5.42716300	10.14081200	-6.07832900
H	-4.65441600	11.61816200	-8.06718500
H	-5.78303800	10.32512600	-8.51831400
H	-4.05770300	10.14259100	-8.82909300
H	-2.16951900	9.48055000	-7.76779400
C	-8.23181000	6.76243000	-4.43288400
H	-8.50002400	5.75319000	-4.08542600
H	-8.93524800	7.45712400	-3.95502400
H	-8.39673700	6.79700300	-5.51425500
C	-3.94282300	8.24176200	-0.13864300
H	-3.23938800	7.54706800	-0.61650600
H	-3.67461200	9.25100200	-0.48610500
H	-3.77788900	8.20719200	0.94272700

3. CAAC_Full_C₂H₅_Cl (twisted)-singlet:

C	-5.99986300	3.96342800	-1.95251700
N	-7.79806500	3.89490800	-0.47204000
C	-5.86017800	2.73503700	-1.03960400
C	-7.20705900	2.53222200	-0.34728700
H	-5.09605500	2.94875300	-0.27854700
H	-5.53790500	1.84424000	-1.59176800
C	-7.11270000	4.75842900	-1.26487500
C	-6.57999300	7.12029700	-2.54765400

C	-5.59443700	7.88390700	-2.02377700
C	-6.86431900	7.15113400	-4.03913800
H	-6.62345400	8.14622300	-4.45202200
H	-6.16001100	6.46789700	-4.55176700
C	-5.31001800	7.85285900	-0.53232500
H	-5.55124400	6.85781400	-0.11956600
H	-6.01400300	8.53632600	-0.01955400
C	-6.47767300	3.56330800	-3.35767000
H	-6.56334800	4.44740400	-3.99593000
H	-7.45549200	3.07139400	-3.34142400
H	-5.75518900	2.87919500	-3.82273700
C	-4.64611500	4.66218100	-2.08481400
H	-3.88358800	3.91052300	-2.32768200
H	-4.34943900	5.15102200	-1.14837000
H	-4.63518500	5.41425400	-2.87741500
C	-7.03221200	2.11355700	1.11021800
H	-6.32852100	2.75844600	1.64115800
H	-6.63570400	1.09306300	1.13596500
H	-7.99092100	2.11235900	1.64184500
C	-8.10091500	1.47920300	-1.00400600
H	-8.28718400	1.66233800	-2.06401300
H	-9.06264800	1.43912200	-0.48130000
H	-7.62867000	0.49606800	-0.90634200
C	-6.17467400	11.04067000	-2.61882500
N	-4.37657500	11.10935400	-4.09941100
C	-6.31458200	12.26899100	-3.53178800
C	-4.96775000	12.47196700	-4.22417400
H	-6.63696300	13.15976800	-2.97965300
H	-7.07869700	12.05512500	-4.29281200
C	-5.69672700	11.44095500	-1.21376800
H	-4.71916700	11.93336700	-1.23022300
H	-5.61046100	10.55685500	-0.57557700
H	-6.41944500	12.12468700	-0.74850600
C	-7.52829800	10.34172100	-2.48625200

H	-7.53903400	9.58993000	-1.69338000
H	-7.82494900	9.85246500	-3.42248800
H	-8.29094900	11.09332000	-2.24359400
C	-4.07395000	13.52511000	-3.56757800
H	-3.88738800	13.34194400	-2.50763200
H	-4.54638200	14.50817100	-3.66508000
H	-3.11233900	13.56538800	-4.09049500
C	-5.14276800	12.89055900	-5.68168200
H	-5.84648500	12.24561000	-6.21251300
H	-4.18412000	12.89178600	-6.21342000
H	-5.53933700	13.91103000	-5.70743000
B	-4.73044100	8.80476900	-2.95718800
B	-7.44401200	6.19942500	-1.61428300
Cl	-8.85219000	7.11951100	-0.89131400
C	-5.06183900	10.24576100	-3.30656600
Cl	-3.32196200	7.88493600	-3.67988100
C	-8.99503500	4.23971900	0.23250700
C	-10.23918400	4.09165100	-0.40548800
C	-8.89398400	4.78186600	1.52644000
C	-11.38788100	4.41363300	0.31689900
C	-10.07309800	5.09170700	2.20149900
C	-11.31167900	4.89413200	1.61321800
H	-12.35871400	4.30698300	-0.16181800
H	-12.21897800	5.14186900	2.15684500
H	-10.01288800	5.51742400	3.20055900
C	-7.57247600	5.13976300	2.18868700
C	-7.41388400	4.45952100	3.55234300
H	-7.57350500	3.37871900	3.51364200
H	-8.13509000	4.87216200	4.26825200
H	-6.41436400	4.64645900	3.96080900
C	-7.45080300	6.65524900	2.38445100
H	-6.75347500	4.83011900	1.52549400
H	-6.48853600	6.89617600	2.85153300
H	-8.24236500	7.02326900	3.04925100

H	-7.52533900	7.19965700	1.44122300
C	-10.39666300	3.71382700	-1.87042900
C	-11.25649600	2.46161500	-2.06464800
H	-11.31552700	2.20151100	-3.12751200
H	-12.28161500	2.64973400	-1.72250600
H	-10.88456400	1.59010000	-1.52108600
C	-11.04023700	4.86212100	-2.65826400
H	-9.39805100	3.54243400	-2.29280500
H	-11.08304500	4.60843100	-3.72404800
H	-10.49234600	5.79961800	-2.54558100
H	-12.06995800	5.03134700	-2.31949300
C	-3.17971600	10.76457200	-4.80414400
C	-1.93548000	10.91280500	-4.16640000
C	-2.10194400	9.91244000	-6.77324000
C	-0.86327200	10.11016400	-6.18519000
C	-0.78688400	10.59081400	-4.88893900
H	0.04395100	9.86241600	-6.72893800
H	0.18402100	10.69757900	-4.41039400
C	-1.77783200	11.29082700	-2.70152500
C	-1.13384300	10.14285200	-1.91358000
H	-1.68174700	9.20527600	-2.02558600
H	-1.09053400	10.39699100	-0.84792300
H	-0.10426500	9.97355500	-2.25273800
C	-0.91819900	12.54325200	-2.50767700
H	-2.77641200	11.46210800	-2.27900000
H	-0.85920400	12.80369700	-1.44489500
H	-1.29023900	13.41453900	-3.05152500
H	0.10694800	12.35516800	-2.84976100
C	-3.28096000	10.22228400	-6.09801200
C	-4.60255400	9.86419400	-6.75998200
C	-4.72411200	8.34866900	-6.95552700
H	-5.68656100	8.10755300	-7.42214000
H	-4.64906600	7.80438100	-6.01227100
H	-3.93280100	7.98068900	-7.62065100

C	-4.76145300	10.54424900	-8.12369500
H	-5.42147600	10.17383300	-6.09668500
H	-4.60193600	11.62507200	-8.08516000
H	-5.76102400	10.35715500	-8.53196600
H	-4.04032800	10.13159300	-8.83967700
H	-2.16229500	9.48660900	-7.77224300
C	-8.29708700	6.77471800	-4.39536500
H	-8.53845400	5.75886400	-4.04701100
H	-9.01058300	7.45312100	-3.90940700
H	-8.47414100	6.80687100	-5.47477900
C	-3.87706600	8.22857400	-0.17617000
H	-3.16403400	7.55002300	-0.66259600
H	-3.63531200	9.24442500	-0.52418800
H	-3.69978400	8.19587900	0.90318600

4. CAAC_Full_C₂H₅_Cl (twisted)-triplet:

C	-5.99965900	3.96355700	-1.95205400
N	-7.79795300	3.89479900	-0.47143000
C	-5.86041800	2.73477500	-1.03956400
C	-7.20737400	2.53193100	-0.34746800
H	-5.09638600	2.94806200	-0.27829000
H	-5.53820200	1.84411600	-1.59198400
C	-7.11279200	4.75836800	-1.26465600
C	-6.58010100	7.12072600	-2.54775400
C	-5.59466400	7.88350200	-2.02380400
C	-6.86523500	7.15115300	-4.03948700
H	-6.62887900	8.14656300	-4.45372700
H	-6.15867800	6.47039200	-4.55226200

C	-5.30951300	7.85289500	-0.53207700
H	-5.54626600	6.85754800	-0.11789300
H	-6.01579100	8.53390500	-0.01925000
C	-6.47629300	3.56432400	-3.35781600
H	-6.56068200	4.44875900	-3.99580500
H	-7.45444100	3.07298800	-3.34280000
H	-5.75368900	2.88012400	-3.82257100
C	-4.64572500	4.66224300	-2.08306600
H	-3.88324600	3.91070600	-2.32645400
H	-4.34923100	5.14992600	-1.14597000
H	-4.63432100	5.41513100	-2.87488700
C	-7.03288600	2.11191500	1.10970200
H	-6.32867600	2.75571900	1.64127400
H	-6.63728300	1.09104800	1.13462300
H	-7.99162500	2.11108000	1.64128300
C	-8.10150700	1.47982000	-1.00526100
H	-8.28807200	1.66453000	-2.06495200
H	-9.06309100	1.43917000	-0.48232500
H	-7.62936000	0.49648700	-0.90909500
C	-6.17511300	11.04071700	-2.61962300
N	-4.37664800	11.10946400	-4.10004800
C	-6.31429800	12.26943800	-3.53220300
C	-4.96725000	12.47231000	-4.22412100
H	-6.63662600	13.16011400	-2.97987600
H	-7.07821500	12.05607400	-4.29357000
C	-5.69868900	11.44007700	-1.21383000
H	-4.72054600	11.93142100	-1.22873500
H	-5.61441500	10.55568000	-0.57575400
H	-6.42137400	12.12431000	-0.74925100
C	-7.52901600	10.34196700	-2.48869400
H	-7.54038300	9.58899600	-1.69694500
H	-7.82548800	9.85437600	-3.42584300
H	-8.29152500	11.09345100	-2.24523600
C	-4.07322400	13.52444900	-3.56622700

H	-3.88661400	13.33966000	-2.50656000
H	-4.54544900	14.50775300	-3.66230900
H	-3.11165000	13.56522400	-4.08916900
C	-5.14157100	12.89228000	-5.68132100
H	-5.84576700	12.24848100	-6.21291800
H	-4.18278900	12.89304500	-6.21282500
H	-5.53713200	13.91316100	-5.70632000
B	-4.73071200	8.80485300	-2.95790000
B	-7.44401700	6.19940000	-1.61360800
Cl	-8.85140600	7.11982600	-0.89007100
C	-5.06187600	10.24591200	-3.30685600
Cl	-3.32293400	7.88464200	-3.68097500
C	-8.99484500	4.23959300	0.23313000
C	-10.23906600	4.09258500	-0.40499600
C	-8.89356900	4.78073400	1.52746200
C	-11.38760300	4.41442100	0.31772500
C	-10.07250600	5.09064000	2.20279500
C	-11.31117800	4.89393600	1.61440100
H	-12.35850800	4.30846500	-0.16100400
H	-12.21837300	5.14159600	2.15823600
H	-10.01209700	5.51562700	3.20215600
C	-7.57179800	5.13745800	2.18977700
C	-7.41367400	4.45687600	3.55329100
H	-7.57425400	3.37621500	3.51433800
H	-8.13441000	4.86999200	4.26939900
H	-6.41393200	4.64281800	3.96167000
C	-7.44891900	6.65282100	2.38548500
H	-6.75308000	4.82719400	1.52654700
H	-6.48670500	6.89304600	2.85303900
H	-8.24057200	7.02162900	3.04974200
H	-7.52248800	7.19711600	1.44210500
C	-10.39681400	3.71614600	-1.87029300
C	-11.25618600	2.46375700	-2.06553600
H	-11.31605700	2.20518100	-3.12872700

H	-12.28107700	2.65096500	-1.72219600
H	-10.88341700	1.59161600	-1.52359100
C	-11.04140400	4.86483000	-2.65678500
H	-9.39820600	3.54577100	-2.29320300
H	-11.08343900	4.61256700	-3.72293600
H	-10.49470200	5.80282200	-2.54258000
H	-12.07148900	5.03230400	-2.31825300
C	-3.17978000	10.76459300	-4.80460300
C	-1.93552700	10.91177400	-4.16663100
C	-2.10225100	9.91319200	-6.77420100
C	-0.86353900	10.10998600	-6.18592000
C	-0.78703800	10.58975500	-4.88934600
H	0.04362300	9.86219600	-6.72975300
H	0.18389500	10.69578600	-4.41068700
C	-1.77770800	11.28851500	-2.70141200
C	-1.13288400	10.14018400	-1.91461200
H	-1.67969100	9.20216000	-2.02802400
H	-1.09041800	10.39304700	-0.84861700
H	-0.10293100	9.97248000	-2.25341400
C	-0.91840400	12.54103500	-2.50658800
H	-2.77629800	11.45893600	-2.27845400
H	-0.85868800	12.80008600	-1.44350400
H	-1.29108800	13.41292800	-3.04898600
H	0.10653900	12.35368300	-2.84969500
C	-3.28114000	10.22322300	-6.09884600
C	-4.60294000	9.86640100	-6.76106100
C	-4.72579100	8.35101200	-6.95661300
H	-5.68819800	8.11067500	-7.42371400
H	-4.65173700	7.80677500	-6.01324100
H	-3.93441100	7.98223900	-7.62121500
C	-4.76111400	10.54681300	-8.12465800
H	-5.42165000	10.17672500	-6.09784200
H	-4.60053000	11.62747700	-8.08585700
H	-5.76086600	10.36081200	-8.53298400

H	-4.04039700	10.13360400	-8.84073000
H	-2.16272700	9.48803300	-7.77348500
C	-8.29676500	6.76854100	-4.39280000
H	-8.53411200	5.75365200	-4.03826100
H	-9.01212600	7.44685300	-3.90942200
H	-8.47539000	6.79418500	-5.47211300
C	-3.87782800	8.23478100	-0.17872800
H	-3.16290500	7.55637300	-0.66263000
H	-3.64007300	9.24971500	-0.53276300
H	-3.69902700	8.20842500	0.90053300

5. CAAC_Full_C₂H₅_Cl (planar)-singlet:

C	-6.16912200	4.03383100	-1.12523100
N	-8.38602600	3.40970200	-1.51837300
C	-6.70038300	3.13545500	0.00607500
C	-7.85974300	2.36246300	-0.59545600
H	-7.09928200	3.77318400	0.80967600
H	-5.92393500	2.49301200	0.43544400
C	-7.46336300	4.32411700	-1.93356100
C	-6.65391600	6.70997800	-3.06235600
C	-6.90214700	7.93038200	-3.65859400
C	-5.50531600	5.93556100	-3.75726300
H	-4.90394900	5.34325300	-3.06867000
H	-4.80853200	6.63549100	-4.22249900
C	-8.05073600	8.70477300	-2.96359000
H	-8.74729800	8.00478400	-2.49810100
H	-8.65236300	9.29686100	-3.65215300
C	-5.09048300	3.25877900	-1.94098600

H	-4.88458200	2.28179100	-1.49190900
H	-4.14290800	3.80660500	-1.95873300
H	-5.38964800	3.08653900	-2.98098800
C	-5.56885600	5.28579800	-0.46952600
H	-4.80202900	4.97264000	0.25191900
H	-6.34600900	5.83347900	0.07732500
H	-5.10261700	5.98220500	-1.16958800
C	-8.87155000	1.93119500	0.45978300
H	-9.09682000	2.72925000	1.16908000
H	-8.44095300	1.09765300	1.02424700
H	-9.80587000	1.57849800	0.00847600
C	-7.44946800	1.10945600	-1.37341100
H	-6.78848600	1.32478400	-2.21466500
H	-8.34513800	0.61151700	-1.75769000
H	-6.94047700	0.40964800	-0.70122100
C	-7.38730900	10.60638800	-5.59570900
N	-5.17046900	11.23082800	-5.20266700
C	-6.85620700	11.50478900	-6.72706900
C	-5.69693400	12.27796300	-6.12559700
H	-7.63275400	12.14711000	-7.15644400
H	-6.45724600	10.86708400	-7.53065700
C	-8.46604200	11.38133000	-4.77997700
H	-8.67192900	12.35835400	-5.22898000
H	-8.16700000	11.55348400	-3.73993300
H	-9.41359900	10.83346400	-4.76238600
C	-7.98741200	9.35430200	-6.25134400
H	-8.45358000	8.65787700	-5.55124900
H	-7.21018100	8.80668400	-6.79815000
H	-8.75426800	9.66732300	-6.97281900
C	-6.10737100	13.53094500	-5.34767600
H	-6.76811100	13.31552700	-4.50625400
H	-6.61670200	14.23054400	-6.01982800
H	-5.21175600	14.02918100	-4.96365000
C	-4.68522000	12.70934400	-7.18087400

H	-4.45976500	11.91126500	-7.89008600
H	-3.75098500	13.06229400	-6.72959400
H	-5.11600300	13.54273400	-7.74542400
B	-5.80495900	8.95387800	-4.12148100
B	-7.75120800	5.68656600	-2.59951400
C	-6.09299400	10.31629700	-4.78742500
C	-9.73744200	3.33059600	-1.98154100
C	-10.03953600	2.68424200	-3.19101300
C	-10.73161900	3.95732000	-1.21170900
C	-11.37704600	2.63244000	-3.58447100
C	-12.04928500	3.88653100	-1.65595500
C	-12.37547500	3.22014300	-2.82649400
H	-11.63120700	2.14257300	-4.52175600
H	-13.40882900	3.17603000	-3.15861400
H	-12.82902900	4.38182400	-1.08183100
C	-10.42927700	4.77489000	0.03426400
C	-11.28816300	4.31957800	1.21919100
H	-11.27823100	3.23333900	1.35309800
H	-12.33240400	4.62179700	1.07533800
H	-10.94500000	4.78839100	2.14814900
C	-10.66710900	6.26972100	-0.20402200
H	-9.36751000	4.64900200	0.28705100
H	-10.54540500	6.82277700	0.73454400
H	-11.68796600	6.44452800	-0.56633500
H	-9.97558100	6.68648300	-0.94040300
C	-8.99199700	2.13984800	-4.14844600
C	-9.19828400	0.64900700	-4.43385600
H	-8.38588900	0.26081300	-5.05809500
H	-10.13248800	0.49656300	-4.98834700
H	-9.25647000	0.03924000	-3.52838000
C	-9.02309800	2.89443900	-5.48355900
H	-7.99891600	2.29202100	-3.70473500
H	-8.22524300	2.52697200	-6.13970300
H	-8.89740500	3.97109000	-5.35360400

H	-9.97686400	2.72433900	-5.99822200
C	-3.81899100	11.31000900	-4.73970300
C	-3.51677000	11.95645100	-3.53031300
C	-1.50717400	10.75413800	-5.06554500
C	-1.18085700	11.42063400	-3.89510200
C	-2.17921200	12.00834600	-3.13703400
H	-0.14746000	11.46481500	-3.56312100
H	-1.92495100	12.49828300	-2.19981300
C	-4.56423200	12.50080400	-2.57277100
C	-4.53292000	11.74625800	-1.23763600
H	-4.65870200	10.66960600	-1.36753400
H	-5.33064200	12.11378900	-0.58136600
H	-3.57905700	11.91632400	-0.72314500
C	-4.35804200	13.99167200	-2.28746300
H	-5.55735400	12.34852600	-3.01634600
H	-5.17034700	14.37980400	-1.66306700
H	-4.30012500	14.60139900	-3.19298300
H	-3.42373500	14.14424600	-1.73317900
C	-2.82489300	10.68325300	-5.50961800
C	-3.12734500	9.86560000	-6.75551200
C	-2.88934700	8.37079500	-6.51722300
H	-3.01111600	7.81771300	-7.45576600
H	-3.58073800	7.95396800	-5.78075000
H	-1.86842500	8.19609400	-6.15504300
C	-2.26865400	10.32092400	-7.94058000
H	-4.18915600	9.99140200	-7.00816400
H	-2.27866200	11.40715800	-8.07452400
H	-2.61192600	9.85206100	-8.86947200
H	-1.22437500	10.01876700	-7.79686700
H	-0.72748100	10.25883200	-5.63973100
C	-7.51744700	9.60643500	-1.84415700
H	-6.87616100	9.02529900	-1.16758700
H	-6.90937000	10.43849900	-2.22148800
H	-8.33915400	10.03309500	-1.25631800

C	-6.03856400	5.03410500	-4.87687900
H	-5.21683800	4.60739200	-5.46465300
H	-6.64679100	4.20208300	-4.49969700
H	-6.67968800	5.61539500	-5.55347200
Cl	-9.34865800	5.86368800	-3.50493800
Cl	-4.20746600	8.77696500	-3.21613300

6. CAAC_Full_C₂H₅_Cl (planar)-triplet:

C	-6.17253600	4.03464700	-1.13323000
N	-8.38996600	3.40378400	-1.52081300
C	-6.70046900	3.13978600	0.00224300
C	-7.86017500	2.36236800	-0.59457500
H	-7.09916300	3.78031200	0.80377100
H	-5.92281700	2.49972200	0.43315900
C	-7.46788800	4.31980300	-1.93904800
C	-6.65396400	6.71243300	-3.06669600
C	-6.90222600	7.92804200	-3.65421700
C	-5.51994900	5.93513300	-3.78115300
H	-4.90455000	5.34557400	-3.10167200
H	-4.83527900	6.63981400	-4.25935000
C	-8.03625800	8.70532500	-2.93974300
H	-8.72080100	8.00060700	-2.46140800
H	-8.65178200	9.29474000	-3.61924000
C	-5.09443200	3.26007800	-1.94993400
H	-4.88508100	2.28440200	-1.49957700
H	-4.14785300	3.80946800	-1.97183100
H	-5.39692100	3.08513000	-2.98869000
C	-5.57321800	5.29115000	-0.48601000

H	-4.80426200	4.98462300	0.23584400
H	-6.35032300	5.84115800	0.05892600
H	-5.10821500	5.98369600	-1.19111600
C	-8.86997300	1.93488700	0.46401900
H	-9.09395700	2.73606400	1.17026300
H	-8.43918600	1.10330000	1.03121500
H	-9.80514100	1.58098600	0.01528100
C	-7.44813100	1.10640700	-1.36683000
H	-6.79013600	1.31960900	-2.21102700
H	-8.34336300	0.60395400	-1.74622300
H	-6.93520600	0.41134700	-0.69265000
C	-7.38389900	10.60574200	-5.58771300
N	-5.16651900	11.23681200	-5.20016000
C	-6.85605700	11.50069200	-6.72316600
C	-5.69646900	12.27824000	-6.12628900
H	-7.63377900	12.14066200	-7.15409200
H	-6.45725700	10.86023700	-7.52469800
C	-8.46214400	11.38016600	-4.77105200
H	-8.67152500	12.35585800	-5.22135800
H	-8.15976800	11.55506300	-3.73225400
H	-9.40868600	10.83070900	-4.74929000
C	-7.98301800	9.34915200	-6.23495600
H	-8.44793400	8.65653300	-5.52986000
H	-7.20581300	8.79926300	-6.77987300
H	-8.75200300	9.65556500	-6.95682700
C	-6.10875100	13.53405400	-5.35390700
H	-6.76659500	13.32060900	-4.50965300
H	-6.62194700	14.22901500	-6.02798400
H	-5.21362700	14.03674100	-4.97456900
C	-4.68672900	12.70598100	-7.18482400
H	-4.46248300	11.90485400	-7.89104500
H	-3.75168500	13.06013800	-6.73603200
H	-5.11771300	13.53744500	-7.75205200
B	-5.79972100	8.95792200	-4.12299100

B	-7.75654700	5.68261600	-2.59795500
C	-6.08850500	10.32071700	-4.78189200
C	-9.74033300	3.32296200	-1.98579400
C	-10.04079500	2.67395400	-3.19449900
C	-10.73680200	3.95121500	-1.21974000
C	-11.37772800	2.61967400	-3.58964800
C	-12.05395000	3.87762100	-1.66534800
C	-12.37801300	3.20764000	-2.83433700
H	-11.63010000	2.12680700	-4.52584600
H	-13.41094300	3.16099100	-3.16743800
H	-12.83500300	4.37313000	-1.09315500
C	-10.43764800	4.77268000	0.02432000
C	-11.29302200	4.31609600	1.21129200
H	-11.27600800	3.23055400	1.34948500
H	-12.33926700	4.61086100	1.06640300
H	-10.95277800	4.79070900	2.13839700
C	-10.68484500	6.26524500	-0.21812000
H	-9.37473500	4.65324100	0.27582300
H	-10.55415800	6.82387800	0.71589600
H	-11.71094300	6.43371000	-0.56848700
H	-10.00459000	6.68091000	-0.96550100
C	-8.99196600	2.12675600	-4.14886000
C	-9.19408300	0.63370200	-4.42563600
H	-8.38210200	0.24480400	-5.05000700
H	-10.12933900	0.47545000	-4.97674500
H	-9.24782000	0.02855900	-3.51687500
C	-9.02624700	2.87300500	-5.48863900
H	-7.99930000	2.28455500	-3.70604400
H	-8.22385500	2.50854500	-6.14091400
H	-8.91016500	3.95146400	-5.36498400
H	-9.97724800	2.69162800	-6.00452200
C	-3.81604400	11.31754800	-4.73548000
C	-3.51527200	11.96656200	-3.52685900
C	-1.50255500	10.76263000	-5.05637400

C	-1.17818600	11.43261400	-3.88747300
C	-2.17825400	12.02072100	-3.13198200
H	-0.14518500	11.47915800	-3.55457800
H	-1.92563900	12.51358800	-2.19584900
C	-4.56386600	12.51390700	-2.57233100
C	-4.52947500	11.76771000	-1.23252700
H	-4.64598100	10.68927900	-1.35610300
H	-5.33156100	12.13248800	-0.58005400
H	-3.57827100	11.94877100	-0.71690800
C	-4.36150300	14.00695200	-2.29569300
H	-5.55662400	12.35621300	-3.01496900
H	-5.17338800	14.39604800	-1.67132000
H	-4.30771600	14.61198300	-3.20453100
H	-3.42618800	14.16511500	-1.74465900
C	-2.81979800	10.68916300	-5.50172000
C	-3.11928600	9.86770300	-6.74570600
C	-2.87232100	8.37510700	-6.50324900
H	-3.00317000	7.81647700	-7.43724300
H	-3.55260400	7.95957400	-5.75581700
H	-1.84623100	8.20647200	-6.15294100
C	-2.26402700	10.32411300	-7.93282700
H	-4.18221300	9.98731500	-6.99706400
H	-2.28084500	11.40966400	-8.07099400
H	-2.60453900	9.84958800	-8.85987700
H	-1.21781500	10.02913300	-7.78813700
H	-0.72166600	10.26702300	-5.62870600
C	-7.48832100	9.60889900	-1.82916700
H	-6.84200000	9.02761400	-1.15763400
H	-6.88295800	10.43910600	-2.21431600
H	-8.30321600	10.03943800	-1.23515000
C	-6.06791200	5.03173300	-4.89185800
H	-5.25303300	4.60114500	-5.48586200
H	-6.67340500	4.20157600	-4.50682700
H	-6.71411900	5.61316100	-5.56337900

Cl	-9.34017000	5.85796900	-3.52386200
Cl	-4.21606600	8.78266300	-3.19713000

7. CAAC_Full_CH₃_Cl (fully optimized)-singlet:

C	-5.74013100	3.95074500	-1.56385100
N	-7.63708900	3.85956900	-0.20517900
C	-5.72791900	2.65709400	-0.72479800
C	-7.13996100	2.45534000	-0.18651400
H	-5.04319000	2.79978500	0.12385600
H	-5.37241900	1.79260400	-1.29721900
C	-6.91298300	4.72476500	-0.95712300
C	-6.52650500	7.01156400	-2.40495400
C	-5.48504100	7.85209400	-2.23128100
C	-7.28111000	6.96560600	-3.71230500
H	-7.46870100	5.93556100	-4.04558500
H	-6.76045900	7.50681100	-4.51861300
H	-8.27646600	7.42406800	-3.59757100
C	-4.73044500	7.89806100	-0.92392400
H	-4.54279200	8.92810900	-0.59068600
H	-3.73511700	7.43953500	-1.03862400
H	-5.25113800	7.35692000	-0.11759800
C	-5.98643900	3.69416800	-3.05954700
H	-5.77436300	4.60499200	-3.62990100
H	-7.02016800	3.39696700	-3.27318000
H	-5.31482800	2.90783800	-3.42762200
C	-4.38407800	4.64347100	-1.41671900
H	-3.58745500	3.92708000	-1.65679800
H	-4.22961000	4.98943500	-0.38728600

H	-4.28379300	5.49326000	-2.09711800
C	-7.15924400	1.85618400	1.21683200
H	-6.45830400	2.35274900	1.89125800
H	-6.87166200	0.80190100	1.15490700
H	-8.16462200	1.90164400	1.65269500
C	-7.99545800	1.55281000	-1.07889400
H	-7.98261900	1.85839600	-2.12744500
H	-9.03162400	1.54439900	-0.72515200
H	-7.61372400	0.52805100	-1.02167100
C	-6.27140100	10.91291900	-3.07235600
N	-4.37444900	11.00410400	-4.43103800
C	-6.28362300	12.20657100	-3.91140500
C	-4.87158200	12.40833300	-4.44968500
H	-6.63912700	13.07105700	-3.33898200
H	-6.96835100	12.06387700	-4.76005900
C	-6.02506400	11.16949100	-1.57666400
H	-4.99132200	11.46666300	-1.36304600
H	-6.23715900	10.25867400	-1.00630600
H	-6.69664600	11.95584200	-1.20857900
C	-7.62746000	10.22020100	-3.21946800
H	-7.72774000	9.37040600	-2.53907600
H	-7.78195200	9.87424900	-4.24890000
H	-8.42407300	10.93659600	-2.97936600
C	-4.01609100	13.31084900	-3.55728600
H	-4.02893000	13.00523800	-2.50874200
H	-4.39783200	14.33560700	-3.61448600
H	-2.97992500	13.31927500	-3.91102900
C	-4.85229900	13.00751200	-5.85301900
H	-5.55323900	12.51095700	-6.52745200
H	-3.84692100	12.96206200	-6.28888200
H	-5.13988300	14.06179400	-5.79107700
B	-4.81412600	8.67342700	-3.38350500
B	-7.19743300	6.19023100	-1.25273900
Cl	-8.46473100	7.20229600	-0.40531400

C	-5.09855700	10.13890000	-3.67910300
Cl	-3.54687400	7.66135600	-4.23099000
C	-8.84576800	4.24321000	0.45260700
C	-10.05432800	4.26643000	-0.26256500
C	-8.76380800	4.69609000	1.77971900
C	-11.19965800	4.69345500	0.40920400
C	-9.93653000	5.11469500	2.40365100
C	-11.14789300	5.10494400	1.73041100
H	-12.14467900	4.72648600	-0.12835900
H	-12.05135700	5.44160300	2.23094100
H	-9.89065100	5.48048400	3.42700200
C	-7.44858300	4.83457900	2.52867900
C	-7.48388000	4.08341400	3.86211400
H	-7.80322800	3.04281500	3.74729500
H	-8.17937100	4.56596800	4.55933000
H	-6.49593700	4.09169100	4.33608400
C	-7.10408500	6.30570800	2.77997000
H	-6.64750600	4.42040800	1.90430100
H	-6.19912400	6.37890000	3.39415200
H	-7.91558700	6.81095200	3.31844400
H	-6.93385600	6.84918800	1.84674500
C	-10.16554900	3.94300700	-1.74369300
C	-11.18544900	2.83121100	-2.00597600
H	-11.17543700	2.54133200	-3.06245900
H	-12.19959700	3.18077900	-1.77703700
H	-11.00655000	1.93635100	-1.40286900
C	-10.56565800	5.18084500	-2.55264200
H	-9.18129800	3.62420500	-2.10537300
H	-10.66154200	4.92099800	-3.61326200
H	-9.83328800	5.98598900	-2.45949800
H	-11.53507100	5.56961500	-2.21691100
C	-3.16573600	10.62049600	-5.08878600
C	-1.95720200	10.59726900	-4.37356500
C	-2.07486800	9.74911900	-7.03982400

C	-0.86353500	9.75886000	-6.36653200
C	-0.81183600	10.17029300	-5.04530500
H	0.03995800	9.42224000	-6.86703700
H	0.13316400	10.13726200	-4.50770500
C	-1.84603900	10.92063100	-2.89241700
C	-1.44593200	9.68276100	-2.08352100
H	-2.17820600	8.87755100	-2.17684700
H	-1.35023000	9.94252400	-1.02286400
H	-0.47642700	9.29412100	-2.41914100
C	-0.82616500	12.03242600	-2.63003500
H	-2.83030800	11.23939800	-2.53075200
H	-0.83616700	12.32218900	-1.57352000
H	-1.00509700	12.92734900	-3.23303700
H	0.18798900	11.68290900	-2.85902600
C	-3.24762400	10.16767500	-6.41592400
C	-4.56280400	10.02921100	-7.16496900
C	-4.90723300	8.55809500	-7.41642600
H	-5.81218200	8.48493100	-8.03062900
H	-5.07744600	8.01449800	-6.48326800
H	-4.09570200	8.05295200	-7.95495200
C	-4.52745900	10.78049400	-8.49833700
H	-5.36392700	10.44329800	-6.54059600
H	-4.20814700	11.82109200	-8.38341800
H	-5.51537600	10.77222700	-8.97236100
H	-3.83191600	10.29801600	-9.19555600
H	-2.12069500	9.38338200	-8.06319600

8. CAAC_Full_CH₃_Cl (fully optimized)-triplet:

C	-5.79284600	3.92365600	-1.64384100
N	-7.67465100	3.83972000	-0.26411800
C	-5.75416800	2.65055700	-0.77476800
C	-7.15803100	2.44323800	-0.21664000
H	-5.06246400	2.82219400	0.06277200
H	-5.39347200	1.77736200	-1.33051800
C	-6.96783400	4.69721900	-1.04187400
C	-6.60000800	6.98237100	-2.51350500
C	-5.58030200	7.84510900	-2.32671100
C	-7.34737200	6.92918600	-3.82568500
H	-7.50017000	5.89803400	-4.17178100
H	-6.84177200	7.49423100	-4.62335900
H	-8.35792000	7.35289800	-3.71042100
C	-4.83188400	7.90078000	-1.01407800
H	-4.61540900	8.93499700	-0.70978500
H	-3.84956800	7.41238500	-1.11072000
H	-5.36929100	7.39754200	-0.19502900
C	-6.05713500	3.62827100	-3.12894900
H	-5.87046000	4.52915800	-3.72277600
H	-7.08878200	3.30926200	-3.31904400
H	-5.37814900	2.84520500	-3.49049800
C	-4.44517200	4.63840300	-1.52999500
H	-3.64066100	3.92979200	-1.76665300
H	-4.28299700	5.00680400	-0.50951900
H	-4.36748200	5.47751100	-2.22705200
C	-7.15416700	1.87902600	1.20124300
H	-6.45446200	2.40289700	1.85595200
H	-6.85089200	0.82804100	1.16262300

H	-8.15583000	1.92007500	1.64598200
C	-8.01049200	1.50681300	-1.07669500
H	-8.00915000	1.78288800	-2.13342400
H	-9.04389600	1.49699700	-0.71462600
H	-7.61691100	0.48831100	-0.99404000
C	-6.46841100	10.89782800	-3.03580300
N	-4.52789100	11.13537800	-4.32034800
C	-6.48289600	12.25154500	-3.77334600
C	-5.05876200	12.52555100	-4.24231200
H	-6.87859400	13.06135400	-3.14967300
H	-7.13362100	12.16168000	-4.65515600
C	-6.30651900	11.04974300	-1.51431500
H	-5.30244600	11.38091700	-1.22394000
H	-6.50245900	10.09105600	-1.02095200
H	-7.03443500	11.77524700	-1.12883900
C	-7.79310300	10.17745200	-3.29668600
H	-7.89949000	9.28879500	-2.66960600
H	-7.88340600	9.88545700	-4.35020500
H	-8.62413500	10.85443300	-3.05891200
C	-4.24861800	13.36580100	-3.25316600
H	-4.26447800	12.96354200	-2.23785400
H	-4.65951400	14.38037300	-3.22203200
H	-3.20904200	13.43603600	-3.58951500
C	-5.00841200	13.24209900	-5.58793700
H	-5.66589700	12.78403400	-6.33018400
H	-3.98591100	13.26611000	-5.98353000
H	-5.33374700	14.27790200	-5.44784500
B	-4.93739100	8.72813000	-3.45002900
B	-7.26656400	6.15415800	-1.36086400
Cl	-8.54888300	7.16370500	-0.53138900
C	-5.25029300	10.20279200	-3.64968200
Cl	-3.66044000	7.80160400	-4.37179000
C	-8.88380500	4.22190500	0.39345000
C	-10.09642400	4.21457400	-0.31509400

C	-8.80018300	4.70560000	1.70967300
C	-11.24307400	4.64355600	0.35303700
C	-9.97480200	5.12273300	2.33106500
C	-11.18938000	5.08421000	1.66476600
H	-12.19108800	4.65422100	-0.18013000
H	-12.09416400	5.42112000	2.16273300
H	-9.92795500	5.51142900	3.34589300
C	-7.48267600	4.88058500	2.44700000
C	-7.49720600	4.15833300	3.79664600
H	-7.79874000	3.11003600	3.70686800
H	-8.19717300	4.64397600	4.48720500
H	-6.50691600	4.19447400	4.26435500
C	-7.16054300	6.36215000	2.66432100
H	-6.67885000	4.46649200	1.82612100
H	-6.25130600	6.46340000	3.26809800
H	-7.97531900	6.86549100	3.19957600
H	-7.00832300	6.88815000	1.71815300
C	-10.21157500	3.85397300	-1.78732400
C	-11.22579800	2.72981200	-2.01656400
H	-11.21668900	2.41139300	-3.06478800
H	-12.24165300	3.07859700	-1.79431300
H	-11.03886400	1.85288800	-1.38977100
C	-10.61976300	5.06883600	-2.62635300
H	-9.22764200	3.53039500	-2.14477300
H	-10.73471600	4.77756800	-3.67683100
H	-9.88146500	5.87228600	-2.57040600
H	-11.58108200	5.47344400	-2.28615700
C	-3.26019500	10.85098000	-4.91664300
C	-2.10627500	10.78983800	-4.11549100
C	-1.98648400	10.24995400	-6.86104700
C	-0.82943100	10.23212500	-6.09913500
C	-0.89579300	10.48870700	-4.73991000
H	0.12403100	9.99347800	-6.56181500
H	0.00781300	10.43232600	-4.13710200

C	-2.11339900	10.93423600	-2.60125800
C	-1.67035500	9.62915800	-1.93049700
H	-2.27177400	8.77705400	-2.25308700
H	-1.74892500	9.71872200	-0.84062200
H	-0.62264400	9.40777300	-2.16977200
C	-1.19469200	12.06146300	-2.12172200
H	-3.14043300	11.13745300	-2.27395400
H	-1.26487100	12.17410800	-1.03405500
H	-1.42083700	13.02765700	-2.57981300
H	-0.14911800	11.82536600	-2.35439400
C	-3.22076900	10.54825400	-6.28838900
C	-4.46766300	10.44019800	-7.15095400
C	-4.71374700	8.99314800	-7.58834500
H	-5.57390600	8.94793500	-8.26630500
H	-4.90921100	8.33870000	-6.73566700
H	-3.84424900	8.59469300	-8.12585300
C	-4.37497200	11.33421600	-8.39023700
H	-5.33215400	10.74500100	-6.54944000
H	-4.12112300	12.36984300	-8.14467500
H	-5.32401600	11.33229100	-8.93803000
H	-3.60650700	10.96141600	-9.07813100
H	-1.94004500	10.00222500	-7.91915900

9. CAAC_Full_CH₃_Cl (twisted)-singlet:

C	-5.94281900	3.92722000	-1.85196500
N	-7.75360700	3.86321400	-0.38139900
C	-5.86189500	2.65542500	-0.98458900
C	-7.21901500	2.47440500	-0.31121900
H	-5.09521200	2.80515200	-0.21185900
H	-5.57211100	1.77496700	-1.57007100
C	-7.09088400	4.70963300	-1.20927600
C	-6.60752200	7.11720100	-2.47597500
C	-5.56677200	7.88709800	-2.09519600
C	-7.25332000	7.29631400	-3.82894100
H	-7.32566600	6.35091000	-4.38341800
H	-6.71822200	8.02299800	-4.46026100
H	-8.28937800	7.65426800	-3.71115000
C	-4.92090100	7.70800200	-0.74226700
H	-4.84844600	8.65344000	-0.18785900
H	-3.88486200	7.34999400	-0.86013200
H	-5.45598200	6.98136500	-0.11086100
C	-6.31025800	3.61786500	-3.31032300
H	-6.28396400	4.53863600	-3.90181700
H	-7.31317200	3.18642500	-3.40561700
H	-5.58685800	2.91647500	-3.74639900
C	-4.57879100	4.61679800	-1.82891400
H	-3.81764600	3.90133800	-2.16696600
H	-4.31651300	4.92584400	-0.81098800
H	-4.53336600	5.48995200	-2.48484600
C	-7.09477400	1.99660600	1.13258400
H	-6.38601900	2.59890300	1.70563500
H	-6.73461800	0.96288600	1.13447800
H	-8.06766200	2.01243200	1.63833400
C	-8.12098100	1.47698600	-1.04282600
H	-8.17942300	1.66259200	-2.11780200
H	-9.13214200	1.49729300	-0.62246300

H	-7.71958800	0.46822500	-0.90001200
C	-6.23165800	11.07701900	-2.71937600
N	-4.42090600	11.14102000	-4.18995800
C	-6.31275200	12.34862000	-3.58701700
C	-4.95559700	12.52979800	-4.26027500
H	-6.60282300	13.22916300	-3.00180200
H	-7.07929700	12.19849100	-4.35981200
C	-5.86409900	11.38652000	-1.26108000
H	-4.86102200	11.81761100	-1.16587700
H	-5.89065300	10.46581600	-0.66948400
H	-6.58726400	12.08818400	-0.82505300
C	-7.59566400	10.38738000	-2.74227100
H	-7.64102900	9.51423700	-2.08631800
H	-7.85801100	10.07831700	-3.76017100
H	-8.35680300	11.10283200	-2.40418700
C	-4.05385500	13.52734500	-3.52853900
H	-3.99641000	13.34239900	-2.45339700
H	-4.45474000	14.53617500	-3.67230900
H	-3.04235600	13.50641100	-3.94802000
C	-5.07986300	13.00758500	-5.70408700
H	-5.78794900	12.40469600	-6.27735600
H	-4.10686000	12.99267800	-6.20965600
H	-5.44096700	14.04097400	-5.70595500
B	-4.77233600	8.83316800	-3.06237800
B	-7.40203000	6.17109800	-1.50888100
Cl	-8.79419400	7.10322300	-0.76461700
C	-5.08356700	10.29461100	-3.36199800
Cl	-3.38000200	7.90117400	-3.80647600
C	-8.96961200	4.22542800	0.27773500
C	-10.18443300	4.15882000	-0.42567800
C	-8.89867100	4.74870300	1.57932300
C	-11.34295300	4.56369900	0.23562300
C	-10.08699100	5.13347200	2.19674800
C	-11.30148000	5.03434700	1.53757600

H	-12.29160400	4.53184000	-0.29554600
H	-12.21637100	5.34908500	2.03160800
H	-10.05085200	5.54813600	3.20166500
C	-7.58713700	5.01800000	2.29901800
C	-7.53073800	4.31339600	3.65680200
H	-7.73520200	3.24115400	3.58580900
H	-8.27044000	4.74440200	4.34242300
H	-6.54659000	4.44689900	4.11980200
C	-7.37454800	6.52136200	2.50442000
H	-6.76409100	4.65972700	1.66774300
H	-6.43446500	6.69771500	3.03973500
H	-8.18510300	6.95093300	3.10620800
H	-7.34106900	7.06191900	1.55548900
C	-10.29348100	3.75287400	-1.88730500
C	-11.30422600	2.61794600	-2.07984500
H	-11.27172300	2.24636500	-3.10996800
H	-12.32535100	2.97489900	-1.89929900
H	-11.12914100	1.77488600	-1.40465600
C	-10.69625500	4.93300000	-2.77927000
H	-9.31036400	3.41520000	-2.22848700
H	-10.90903900	4.57496000	-3.79332300
H	-9.90968300	5.68986900	-2.84360600
H	-11.60209800	5.42162800	-2.39969200
C	-3.20508700	10.77876300	-4.84941600
C	-1.99006900	10.84550300	-4.14639100
C	-2.08819100	9.87099600	-6.76881000
C	-0.87349200	9.97033300	-6.11004200
C	-0.83167600	10.44088500	-4.80807200
H	0.04129700	9.65582600	-6.60441200
H	0.11712000	10.47283000	-4.27717100
C	-1.88076500	11.25131800	-2.68475600
C	-1.47855400	10.07096300	-1.79281900
H	-2.26648200	9.31567600	-1.72643200
H	-1.26320300	10.42927200	-0.77939700

H	-0.57437200	9.58034000	-2.17378900
C	-0.86949600	12.38579100	-2.49226100
H	-2.86369500	11.58951500	-2.34358200
H	-0.90257000	12.75815400	-1.46244400
H	-1.04361700	13.22844600	-3.16823000
H	0.15158100	12.02816200	-2.67177700
C	-3.27639300	10.25548700	-6.15097800
C	-4.58810000	9.98588300	-6.87018500
C	-4.80026600	8.48246900	-7.07561600
H	-5.74082900	8.30584100	-7.61001200
H	-4.83253000	7.94174700	-6.12672400
H	-3.99014800	8.05335400	-7.67831300
C	-4.64538700	10.69054200	-8.22788000
H	-5.41104900	10.34376900	-6.23854200
H	-4.44198700	11.76297900	-8.15678700
H	-5.62951100	10.55609100	-8.69067700
H	-3.90540700	10.26032200	-8.91368700
H	-2.12455800	9.45641300	-7.77374700

10. CAAC_Full_CH₃_Cl (twisted)-triplet:

C	-5.94497500	3.92570600	-1.85303600
N	-7.75366000	3.86141000	-0.37953600

C	-5.86271200	2.65391600	-0.98566400
C	-7.21882600	2.47283400	-0.31012100
H	-5.09480500	2.80368400	-0.21415900
H	-5.57381500	1.77340500	-1.57153500
C	-7.09181800	4.70829800	-1.20869000
C	-6.60831300	7.11807000	-2.47429300
C	-5.56596000	7.88623100	-2.09681400
C	-7.26256900	7.29719400	-3.82451700
H	-7.34686700	6.34870800	-4.37195300
H	-6.72943000	8.01490700	-4.46587900
H	-8.29506400	7.66278300	-3.69988800
C	-4.91164500	7.70712700	-0.74661900
H	-4.82727900	8.65564000	-0.19924000
H	-3.87915500	7.34151800	-0.87131100
H	-5.44475500	6.98943300	-0.10519300
C	-6.31452700	3.61663700	-3.31082900
H	-6.29161200	4.53803000	-3.90165800
H	-7.31659200	3.18286400	-3.40451100
H	-5.59040200	2.91743400	-3.74926700
C	-4.58097800	4.61536400	-1.83188900
H	-3.81985100	3.89967500	-2.16949000
H	-4.31803600	4.92568100	-0.81452700
H	-4.53613500	5.48767000	-2.48903500
C	-7.09252800	1.99537800	1.13370200
H	-6.38318200	2.59792900	1.70578300
H	-6.73233400	0.96167400	1.13558600
H	-8.06483600	2.01132200	1.64059500
C	-8.12143700	1.47461500	-1.04007000
H	-8.18007700	1.65858900	-2.11531600
H	-9.13253700	1.49574500	-0.61950600
H	-7.72026900	0.46594300	-0.89598300
C	-6.22946900	11.07855100	-2.71825300
N	-4.42084100	11.14281200	-4.19179300
C	-6.31192800	12.35011300	-3.58593700

C	-4.95578500	12.53135400	-4.26138500
H	-6.60112700	13.23072800	-3.00036800
H	-7.07969800	12.19989400	-4.35749600
C	-5.85974100	11.38780900	-1.26054700
H	-4.85749500	11.82120400	-1.16700200
H	-5.88291700	10.46649900	-0.66958800
H	-6.58359800	12.08731800	-0.82215300
C	-7.59344600	10.38883300	-2.73917200
H	-7.63820200	9.51655200	-2.08198500
H	-7.85650000	10.07848100	-3.75649000
H	-8.35455200	11.10452300	-2.40152100
C	-4.05340700	13.52973300	-3.53133600
H	-3.99583500	13.34650500	-2.45590700
H	-4.45402700	14.53847300	-3.67648400
H	-3.04194400	13.50791400	-3.95095400
C	-5.08214100	13.00876100	-5.70522500
H	-5.79074700	12.40553500	-6.27752800
H	-4.10971200	12.99383500	-6.21193100
H	-5.44339300	14.04209500	-5.70709700
B	-4.77290700	8.83407000	-3.06586300
B	-7.40144600	6.17019600	-1.50534500
Cl	-8.79575200	7.10097800	-0.76462900
C	-5.08262200	10.29594600	-3.36254300
Cl	-3.37839400	7.90343700	-3.80637100
C	-8.96990800	4.22356000	0.27880500
C	-10.18408900	4.15769100	-0.42580700
C	-8.89995700	4.74731100	1.58024200
C	-11.34294000	4.56405500	0.23394800
C	-10.08857900	5.13342300	2.19627500
C	-11.30241300	5.03530400	1.53574500
H	-12.29104100	4.53291400	-0.29825400
H	-12.21753500	5.35122800	2.02859600
H	-10.05316600	5.54846700	3.20107000
C	-7.58880300	5.01592200	2.30078100

C	-7.53402900	4.31239500	3.65911500
H	-7.73834300	3.24008500	3.58841500
H	-8.27452100	4.74374700	4.34366500
H	-6.55039500	4.44612800	4.12314200
C	-7.37462500	6.51925800	2.50441800
H	-6.76582200	4.65606400	1.67048100
H	-6.43544100	6.69529200	3.04141800
H	-8.18591300	6.95105600	3.10361000
H	-7.33838800	7.05819700	1.55461900
C	-10.29166000	3.75045400	-1.88715800
C	-11.30455600	2.61750300	-2.07981800
H	-11.27089600	2.24415900	-3.10926800
H	-12.32530900	2.97672000	-1.90170600
H	-11.13224900	1.77522800	-1.40288800
C	-10.68949500	4.93038300	-2.78158800
H	-9.30886300	3.40988200	-2.22604500
H	-10.90526800	4.57099900	-3.79453700
H	-9.89891900	5.68293200	-2.84884900
H	-11.59214600	5.42501400	-2.40215700
C	-3.20480100	10.78061300	-4.85049400
C	-1.99039700	10.84664700	-4.14632000
C	-2.08665500	9.87106300	-6.76838700
C	-0.87258600	9.96943500	-6.10831100
C	-0.83168300	10.44058500	-4.80649700
H	0.04242500	9.65377700	-6.60153900
H	0.11658100	10.47184100	-4.27459600
C	-1.88254300	11.25375800	-2.68496500
C	-1.48533000	10.07358900	-1.79055800
H	-2.27738300	9.32279200	-1.72105100
H	-1.26675400	10.43326000	-0.77830300
H	-0.58450900	9.57677600	-2.17149000
C	-0.86908100	12.38621800	-2.49236100
H	-2.86513200	11.59490500	-2.34608800
H	-0.90335700	12.76041100	-1.46324700

H	-1.04035700	13.22804800	-3.17013500
H	0.15161800	12.02627800	-2.66936100
C	-3.27515200	10.25685500	-6.15190200
C	-4.58649100	9.98790300	-6.87191300
C	-4.80017700	8.48451100	-7.07561500
H	-5.73993900	8.30816300	-7.61151400
H	-4.83495600	7.94534700	-6.12587400
H	-3.98941300	8.05326700	-7.67591200
C	-4.64223700	10.69151400	-8.23014000
H	-5.40937200	10.34731400	-6.24120200
H	-4.43901600	11.76402400	-8.15932000
H	-5.62586400	10.55681300	-8.69392300
H	-3.90148300	10.26098600	-8.91491800
H	-2.12232000	9.45611100	-7.77320500

11. CAAC_Full_CH₃_Cl (planar)-singlet:

C	-6.72440800	3.67824800	-2.04388200
N	-8.12023700	4.02880100	-0.18327500
C	-6.54957600	2.57160400	-0.98494300
C	-7.83083700	2.55940300	-0.18117100
H	-5.72781200	2.85051300	-0.30957900
H	-6.30985900	1.59871800	-1.42671900

C	-7.66153800	4.67565100	-1.30467000
C	-7.04198200	6.93452700	-2.73580300
C	-6.93999900	8.31425000	-2.91056500
C	-7.44547800	6.14830400	-4.00009500
H	-6.62190200	5.65276500	-4.52310300
H	-7.90587600	6.81894900	-4.72935600
H	-8.19981100	5.39251000	-3.76329200
C	-6.53647100	9.10045600	-1.64626900
H	-7.36001100	9.59609000	-1.12329800
H	-5.78205600	9.85617200	-1.88306700
H	-6.07615200	8.42978600	-0.91698200
C	-7.30776200	3.07108800	-3.35342700
H	-6.83116900	3.50566200	-4.23509200
H	-8.38460400	3.22747200	-3.46660200
H	-7.12895100	1.99037100	-3.38131500
C	-5.32971700	4.25352300	-2.32650000
H	-4.67488700	3.44070500	-2.66922300
H	-4.89787400	4.67386200	-1.41145200
H	-5.32238600	5.03198400	-3.08925700
C	-7.63188100	1.99290700	1.21428400
H	-6.79896700	2.46134300	1.74277300
H	-7.41153000	0.92447400	1.12074900
H	-8.54390800	2.08982900	1.81251800
C	-8.96589300	1.76026800	-0.83001600
H	-9.15657200	2.03641600	-1.86748300
H	-9.89062300	1.89624100	-0.25739500
H	-8.71213900	0.69508800	-0.80575300
C	-7.25761300	11.57052400	-3.60239200
N	-5.86177700	11.22004600	-5.46301200
C	-7.43245600	12.67719600	-4.66129800
C	-6.15118000	12.68944300	-5.46504800
H	-7.67220000	13.65006300	-4.21949700
H	-8.25420100	12.39829000	-5.33668700
C	-6.67427500	12.17766500	-2.29282700

H	-5.59746100	12.02115300	-2.17956900
H	-7.15098900	11.74318300	-1.41118000
H	-6.85295200	13.25840400	-2.26498800
C	-8.65229700	10.99521500	-3.31980100
H	-8.65962500	10.21673800	-2.55705900
H	-9.08412100	10.57488500	-4.23486300
H	-9.30714600	11.80801400	-2.97707200
C	-5.01613100	13.48853800	-4.81614100
H	-4.82543400	13.21229400	-3.77870200
H	-5.26989800	14.55371700	-4.84030300
H	-4.09140500	13.35262800	-5.38878500
C	-6.35011400	13.25601900	-6.86047300
H	-7.18302700	12.78762300	-7.38899800
H	-5.43808100	13.15912100	-7.45870200
H	-6.57045300	14.32445000	-6.76688000
B	-6.41952800	9.03846300	-4.18359300
B	-7.56246200	6.21033900	-1.46275900
Cl	-8.33658800	7.21427600	-0.15295500
C	-6.32046700	10.57315800	-4.34163500
Cl	-5.64547100	8.03458600	-5.49347700
C	-9.25617200	4.48609300	0.57168400
C	-10.49835500	4.64615600	-0.07562600
C	-9.10539300	4.79613700	1.93791800
C	-11.58620100	5.07280800	0.68603400
C	-10.23245500	5.19537300	2.65270000
C	-11.46713400	5.32931500	2.04058200
H	-12.54591400	5.21498600	0.19489500
H	-12.33029600	5.65552300	2.61357700
H	-10.12538900	5.44126500	3.70666700
C	-7.76433000	4.84610000	2.65642000
C	-7.73687000	3.95379300	3.90351800
H	-8.05399300	2.92574000	3.71738600
H	-8.39970600	4.36581700	4.67430800
H	-6.72854100	3.92956200	4.33224000

C	-7.42735500	6.27320500	3.10863100
H	-6.98638400	4.53012200	1.95034100
H	-6.46529800	6.27589300	3.63406700
H	-8.18375400	6.64189600	3.81206600
H	-7.36898100	6.97287900	2.27544500
C	-10.73120500	4.44702100	-1.56713300
C	-11.88765400	3.48313800	-1.84501700
H	-11.96360500	3.28307000	-2.91969800
H	-12.84616100	3.91214900	-1.53091100
H	-11.76803500	2.52658200	-1.32700000
C	-11.00253400	5.78407100	-2.26480500
H	-9.82678400	4.02823200	-2.01821800
H	-11.19114600	5.62077000	-3.33252000
H	-10.16402900	6.48049700	-2.16729300
H	-11.89059800	6.26808500	-1.83918900
C	-4.72583100	10.76279600	-6.21797800
C	-3.48365600	10.60269500	-5.57066100
C	-3.74951700	10.05364500	-8.29902500
C	-2.51484500	9.91967100	-7.68689900
C	-2.39579800	10.17609400	-6.33233400
H	-1.65167400	9.59350100	-8.25990200
H	-1.43609100	10.03388900	-5.84119000
C	-3.25081900	10.80173600	-4.07913900
C	-2.97947100	9.46464300	-3.38155700
H	-3.81795800	8.76820300	-3.47913400
H	-2.79088300	9.62787100	-2.31382700
H	-2.09138800	8.98068000	-3.80719100
C	-2.09438900	11.76562100	-3.80118300
H	-4.15525000	11.22048000	-3.62802800
H	-2.01844000	11.96560800	-2.72648700
H	-2.21402900	12.72221300	-4.31912600
H	-1.13587400	11.33665300	-4.11532400
C	-4.87658900	10.45283400	-7.58423300
C	-6.21764200	10.40291000	-8.30275700

C	-6.55460800	8.97582900	-8.75505000
H	-7.51665900	8.97316600	-9.28049700
H	-6.61299100	8.27611000	-7.92190200
H	-5.79820000	8.60717800	-9.45849500
C	-6.24508800	11.29528400	-9.54980700
H	-6.99559800	10.71884800	-7.59667100
H	-5.92796600	12.32332600	-9.36361700
H	-7.25341200	11.31953900	-9.97853900
H	-5.58224500	10.88330000	-10.32061200
H	-3.85656800	9.80781700	-9.35300900

12. CAAC_Full_CH₃_Cl (planar)-triplet:

C	-6.73559400	3.68817200	-2.05252300
N	-8.14231900	4.01691100	-0.19478500
C	-6.55313200	2.57994200	-0.99613500
C	-7.83746600	2.55300200	-0.19490900
H	-5.73608400	2.86540400	-0.31765100
H	-6.30252700	1.61057800	-1.43998600
C	-7.68104500	4.67419800	-1.31346700
C	-7.04379800	6.94189500	-2.74587300
C	-6.93835500	8.30722200	-2.90053900
C	-7.49053600	6.17581500	-4.00553700

H	-6.69287800	5.62289100	-4.51029400
H	-7.90630900	6.86257900	-4.74694800
H	-8.28513300	5.46045100	-3.76194900
C	-6.49152300	9.07330800	-1.64088500
H	-7.28902100	9.62650000	-1.13618600
H	-5.69672900	9.78848300	-1.88446500
H	-6.07593600	8.38650200	-0.89941200
C	-7.31962600	3.08342100	-3.36283100
H	-6.83647200	3.50992700	-4.24482000
H	-8.39439500	3.25313500	-3.47773000
H	-7.15311800	2.00067800	-3.39046600
C	-5.34626100	4.27673600	-2.33372500
H	-4.68321500	3.47308300	-2.68161900
H	-4.91743000	4.69600000	-1.41641500
H	-5.34380700	5.05975200	-3.09285800
C	-7.63673000	1.99025200	1.20253700
H	-6.80472700	2.46247500	1.72919900
H	-7.41489700	0.92175300	1.11423200
H	-8.54865400	2.08901100	1.80111600
C	-8.96059500	1.73930000	-0.84685000
H	-9.14834600	2.00950800	-1.88648800
H	-9.88955000	1.86859600	-0.27941500
H	-8.69690700	0.67661800	-0.81706800
C	-7.24641700	11.56092900	-3.59372400
N	-5.83982500	11.23203900	-5.45167000
C	-7.42912400	12.66896900	-4.65037400
C	-6.14480500	12.69591700	-5.45164400
H	-7.67973900	13.63848400	-4.20686000
H	-8.24612600	12.38322000	-5.32877100
C	-6.66207400	12.16573800	-2.28357900
H	-5.58752500	11.99506300	-2.16826800
H	-7.14599100	11.74007700	-1.40156800
H	-6.82752800	13.24865700	-2.25645400
C	-8.63566800	10.97227100	-3.31215600

H	-8.63785700	10.18918300	-2.55310400
H	-9.06476900	10.55306400	-4.22936400
H	-9.29866600	11.77582800	-2.96396300
C	-5.02175500	13.50973500	-4.79971100
H	-4.83406600	13.23964800	-3.76003000
H	-5.28547800	14.57240700	-4.82964300
H	-4.09274200	13.38039600	-5.36705100
C	-6.34548600	13.25850200	-6.84915100
H	-7.17725400	12.78598000	-7.37593100
H	-5.43340900	13.15986100	-7.44751300
H	-6.56756200	14.32696600	-6.76106200
B	-6.40869900	9.04453200	-4.18652900
B	-7.57346500	6.20455600	-1.45986300
Cl	-8.41344200	7.22812500	-0.21090500
C	-6.30110900	10.57485100	-4.33294600
Cl	-5.56933200	8.02112700	-5.43600300
C	-9.27431200	4.47453500	0.56208700
C	-10.52191500	4.62674900	-0.07625800
C	-9.11087400	4.80690700	1.92141100
C	-11.60205200	5.06849800	0.68738600
C	-10.23021600	5.22124300	2.64001600
C	-11.46982200	5.34801100	2.03646000
H	-12.56616800	5.20406700	0.20289000
H	-12.32713600	5.68592300	2.61150700
H	-10.11324900	5.48411800	3.68886700
C	-7.76256800	4.86162100	2.62496600
C	-7.72699700	3.98564900	3.88286500
H	-8.04594900	2.95572200	3.70923500
H	-8.38509000	4.40647800	4.65297600
H	-6.71590500	3.96535900	4.30526400
C	-7.41480300	6.29424700	3.04968200
H	-6.99358700	4.53089200	1.91599600
H	-6.44596100	6.30319700	3.56241700
H	-8.16115100	6.67810300	3.75581900

H	-7.36557000	6.97961900	2.20366100
C	-10.76482300	4.40228100	-1.56225600
C	-11.92217400	3.43259200	-1.81476900
H	-12.00616300	3.21331100	-2.88510200
H	-12.87865200	3.86630100	-1.50071500
H	-11.79782100	2.48551600	-1.28072000
C	-11.04352100	5.72632200	-2.28145700
H	-9.86209200	3.97785800	-2.01077500
H	-11.24412400	5.54358700	-3.34387800
H	-10.20373500	6.42389600	-2.20625200
H	-11.92614600	6.21973600	-1.85531900
C	-4.70767100	10.77428500	-6.20827600
C	-3.46016400	10.62201300	-5.56973000
C	-3.75143500	10.02738000	-8.28601200
C	-2.51192500	9.90063300	-7.68226300
C	-2.37992100	10.18018200	-6.33318300
H	-1.65452800	9.56268200	-8.25716100
H	-1.41588900	10.04459900	-5.84852600
C	-3.21741800	10.84654700	-4.08373000
C	-2.93910200	9.52247500	-3.36444400
H	-3.77886800	8.82490900	-3.44010500
H	-2.73902400	9.70514800	-2.30191100
H	-2.05627000	9.02908100	-3.79017700
C	-2.05994000	11.81604700	-3.83109300
H	-4.12013500	11.27116900	-3.63540400
H	-1.97612400	12.03544000	-2.76076900
H	-2.18403700	12.76307900	-4.36528100
H	-1.10347400	11.38214200	-4.14491000
C	-4.87088900	10.44175700	-7.56761100
C	-6.21905600	10.38699300	-8.27144100
C	-6.56665300	8.95440900	-8.69648600
H	-7.53532800	8.94554200	-9.20954000
H	-6.61620800	8.26890000	-7.85059700
H	-5.82008800	8.57065500	-9.40244400

C	-6.25446500	11.26308800	-9.52927200
H	-6.98819900	10.71755700	-7.56256500
H	-5.93559400	12.29301500	-9.35554400
H	-7.26549000	11.28335300	-9.95183500
H	-5.59622700	10.84232700	-10.29930000
H	-3.86824100	9.76445700	-9.33487100

13. CAAC_Full_H_CI (fully optimized)-singlet:

C	-5.66662400	4.07027700	-1.62632100
N	-7.52692600	4.05490700	-0.21701200
C	-5.69574800	2.75923700	-0.81491800
C	-7.10012100	2.62077600	-0.24026000
H	-4.97910600	2.83553300	0.01471100
H	-5.40999700	1.89240000	-1.42140200
C	-6.79632900	4.88258800	-0.98303400
C	-6.42435800	7.07395500	-2.40288600
C	-6.71447800	8.36861500	-2.84358300
C	-5.94521700	3.78852100	-3.11456900
H	-5.86405200	4.68965600	-3.72467500
H	-6.94372900	3.37298000	-3.27785900
H	-5.21291200	3.05892500	-3.48392100
C	-4.28524300	4.71505900	-1.47569800

H	-3.51724200	3.98683700	-1.76744300
H	-4.10278700	5.00054100	-0.43384300
H	-4.16198400	5.60374500	-2.09652500
C	-7.09539700	1.98951700	1.14602500
H	-6.38915800	2.47281900	1.82471600
H	-6.79957400	0.94011300	1.04619900
H	-8.09661900	2.01087500	1.59029400
C	-8.05089100	1.78506300	-1.10092000
H	-8.10470500	2.11500800	-2.13938200
H	-9.05913000	1.81298500	-0.67298100
H	-7.71355300	0.74351700	-1.09354100
C	-7.47246800	11.37217800	-3.62021700
N	-5.61216600	11.38771600	-5.02952700
C	-7.44350100	12.68321100	-4.43164500
C	-6.03917000	12.82178600	-5.00638800
H	-7.72927000	13.55002700	-3.82513900
H	-8.16020200	12.60686900	-5.26121700
C	-7.19389300	11.65402100	-2.13198300
H	-6.19546200	12.06977700	-1.96873600
H	-7.27485500	10.75288800	-1.52184900
H	-7.92633900	12.38347700	-1.76263300
C	-8.85378000	10.72723400	-3.77081400
H	-8.97695800	9.83857200	-3.14993200
H	-9.03618900	10.44166200	-4.81265300
H	-9.62186400	11.45539400	-3.47913100
C	-5.08847900	13.65770100	-4.14583600
H	-5.03473000	13.32793300	-3.10731400
H	-5.42586600	14.69922900	-4.15340800
H	-4.08020600	13.62974800	-4.57370200
C	-6.04403400	13.45289400	-6.39274200
H	-6.75029100	12.96947900	-7.07133400
H	-5.04283900	13.43154200	-6.83706700
H	-6.33991000	14.50229300	-6.29301600
B	-6.10226800	9.06115200	-4.01072000

B	-7.03659000	6.38144300	-1.23574500
Cl	-8.16561200	7.36582800	-0.17265100
C	-6.34267400	10.55997600	-4.26348500
Cl	-4.97314600	8.07684100	-5.07375900
C	-8.78915800	4.41499700	0.36802700
C	-9.92015600	4.52791900	-0.46153300
C	-8.85324000	4.70160600	1.74312400
C	-11.13423200	4.86357900	0.13717000
C	-10.09401700	5.02638000	2.28729200
C	-11.22979500	5.09583700	1.49819700
H	-12.01783900	4.96225700	-0.48883300
H	-12.18667000	5.35755300	1.94073700
H	-10.15902100	5.25938100	3.34751900
C	-7.63254700	4.79415300	2.64530500
C	-7.75024800	3.88313000	3.87160300
H	-7.98173300	2.84505300	3.62004000
H	-8.54339400	4.24383800	4.53763400
H	-6.81866400	3.89723200	4.44848000
C	-7.41743800	6.23178900	3.13268200
H	-6.74874400	4.51140100	2.06126500
H	-6.54454700	6.27256700	3.79442000
H	-8.28433000	6.57569200	3.71012700
H	-7.26435000	6.92832000	2.30748200
C	-9.89629900	4.38372300	-1.97658600
C	-10.87449500	3.30941800	-2.46257000
H	-10.77933900	3.17195300	-3.54543900
H	-11.90989700	3.61314900	-2.26741100
H	-10.72020400	2.34022400	-1.98022800
C	-10.24310000	5.71043400	-2.66306000
H	-8.88403100	4.10985200	-2.29329000
H	-10.24215700	5.57648400	-3.75057000
H	-9.53488000	6.50508000	-2.41678700
H	-11.24641100	6.04414900	-2.37067900
C	-4.34986900	11.02778200	-5.61452500

C	-3.21888500	10.91506000	-4.78492400
C	-3.04487500	10.41642900	-7.53370700
C	-1.90911500	10.34715600	-6.74457100
C	-2.00474800	10.57950800	-5.38356400
H	-0.95219600	10.08551200	-7.18706000
H	-1.12114900	10.48098500	-4.75752700
C	-3.24282000	11.05936100	-3.26988300
C	-2.89589300	9.73274300	-2.58329600
H	-3.60395200	8.93797500	-2.82962600
H	-2.89700700	9.86674600	-1.49579300
H	-1.89248700	9.39917600	-2.87552200
C	-2.26479500	12.13383500	-2.78393900
H	-4.25513900	11.33312700	-2.95324700
H	-2.35993000	12.27127600	-1.70106500
H	-2.41929800	13.10300300	-3.26626800
H	-1.22934700	11.83029700	-2.97914700
C	-4.28571100	10.74109800	-6.98960400
C	-5.50634400	10.64840100	-7.89185700
C	-5.72121500	9.21074000	-8.37926000
H	-6.59408400	9.16982300	-9.04101800
H	-5.87421000	8.51418500	-7.55406600
H	-4.85425400	8.86697600	-8.95668300
C	-5.38867100	11.55944900	-9.11814200
H	-6.39021700	10.93102500	-7.30786500
H	-5.15728200	12.59754500	-8.86657300
H	-6.32023100	11.54527900	-9.69505600
H	-4.59547100	11.19880600	-9.78414400
H	-2.97981200	10.18336400	-8.59391600
H	-5.71580600	6.53941300	-3.03342800
H	-7.42303600	8.90314400	-2.21303900

14. CAAC_Full_H_CI (fully optimized)-triplet:

C	-5.76776300	4.00280900	-1.70307600
N	-7.58094900	3.98782800	-0.21884700
C	-5.75245200	2.70701900	-0.86795600
C	-7.13391800	2.56379000	-0.23610500
H	-5.00519300	2.80510500	-0.06828600
H	-5.48180300	1.83105600	-1.46897500
C	-6.88169700	4.81374200	-1.03963400
C	-6.49035600	7.05970100	-2.48344300
C	-6.64844600	8.38304800	-2.76281600
C	-6.09117800	3.69658500	-3.17552800
H	-6.11600100	4.60247800	-3.78516500
H	-7.05781600	3.19795400	-3.29049100
H	-5.32008500	3.03332100	-3.58892300
C	-4.39268600	4.67212700	-1.61132500
H	-3.62021900	3.95963800	-1.92871500
H	-4.17669800	4.96870100	-0.57882900
H	-4.30762000	5.55835900	-2.24386100
C	-7.06486700	1.96110700	1.16160800

H	-6.35252600	2.48103200	1.80636800
H	-6.74254200	0.91812300	1.07690900
H	-8.05211700	1.96536200	1.63674700
C	-8.09966000	1.68910400	-1.04154500
H	-8.18570800	1.98104600	-2.08916100
H	-9.09664500	1.72240500	-0.58769700
H	-7.75224100	0.65118400	-1.00838500
C	-7.37120800	11.43986500	-3.54328900
N	-5.55809200	11.45487500	-5.02761000
C	-7.38662500	12.73560000	-4.37848600
C	-6.00517900	12.87889800	-5.01035900
H	-7.65735600	13.61158300	-3.77753500
H	-8.13387100	12.63737900	-5.17815400
C	-7.04776100	11.74616600	-2.07086100
H	-6.08110200	12.24476700	-1.95594100
H	-7.02295900	10.84030500	-1.46117600
H	-7.81882600	12.40947500	-1.65748700
C	-8.74625300	10.77047200	-3.63497800
H	-8.83127000	9.88426400	-3.00240200
H	-8.96224400	10.47384600	-4.66745900
H	-9.51874800	11.48294000	-3.31760700
C	-5.03946100	13.75362300	-4.20493800
H	-4.95336800	13.46165800	-3.15733200
H	-5.38693900	14.79152400	-4.23806400
H	-4.04248700	13.72038800	-4.65881400
C	-6.07430100	13.48155300	-6.40807700
H	-6.78665900	12.96157700	-7.05277200
H	-5.08707800	13.47731400	-6.88327700
H	-6.39666000	14.52452800	-6.32339200
B	-6.01545300	9.14099700	-3.94535300
B	-7.12339000	6.30174100	-1.30093100
Cl	-8.21681000	7.29092700	-0.23398900
C	-6.25725400	10.62896300	-4.20673400
Cl	-4.92201600	8.15182200	-5.01228700

C	-8.83640700	4.34320600	0.37549700
C	-9.98128400	4.43118000	-0.43939400
C	-8.88825200	4.66037000	1.74522000
C	-11.18994600	4.77474900	0.16506800
C	-10.12508000	4.98696600	2.29838300
C	-11.27082100	5.03471400	1.52248700
H	-12.08217900	4.85324800	-0.45174200
H	-12.22393300	5.29933500	1.97144400
H	-10.17912800	5.23901200	3.35500500
C	-7.65778300	4.78145700	2.63065400
C	-7.74409000	3.88118800	3.86734600
H	-7.95270000	2.83543200	3.62900700
H	-8.54067600	4.23051900	4.53556300
H	-6.80861600	3.92327100	4.43664400
C	-7.46026300	6.22636400	3.10405300
H	-6.77858200	4.50844200	2.03540600
H	-6.57489200	6.28896300	3.74722100
H	-8.32083200	6.55927900	3.69714400
H	-7.33562100	6.91998200	2.27174800
C	-9.97476900	4.24229000	-1.94946500
C	-10.96294600	3.15893300	-2.39219800
H	-10.87472500	2.98145500	-3.46990100
H	-11.99577900	3.47441100	-2.20223700
H	-10.80964800	2.20735900	-1.87531300
C	-10.31805500	5.55021200	-2.67182700
H	-8.96759900	3.95188000	-2.26622100
H	-10.34630700	5.38233600	-3.75438400
H	-9.59267000	6.34245600	-2.46924600
H	-11.30735800	5.91253900	-2.36614700
C	-4.30268500	11.09950400	-5.62207100
C	-3.15769500	11.01163400	-4.80733400
C	-3.01423500	10.45579000	-7.54511700
C	-1.86838400	10.40814700	-6.76937700
C	-1.94909100	10.66813200	-5.41195200

H	-0.91531300	10.14359600	-7.21846200
H	-1.05676700	10.58971600	-4.79526500
C	-3.16402100	11.20056100	-3.29727000
C	-2.82051400	9.89268300	-2.57493800
H	-3.54578200	9.10033200	-2.77751400
H	-2.79225600	10.06054700	-1.49237900
H	-1.83116100	9.53051700	-2.88065000
C	-2.17585900	12.28399900	-2.85470900
H	-4.17117100	11.49089100	-2.98036800
H	-2.26390000	12.46146800	-1.77699000
H	-2.32932200	13.23556300	-3.37156400
H	-1.14303400	11.96860200	-3.04485700
C	-4.25101200	10.78231000	-6.99179400
C	-5.48160100	10.66110400	-7.87705200
C	-5.67911200	9.21614800	-8.35031300
H	-6.56460300	9.15343700	-8.99330300
H	-5.80353500	8.52257700	-7.51793600
H	-4.81863300	8.88326000	-8.94355000
C	-5.39549100	11.56127100	-9.11383200
H	-6.36073700	10.93413500	-7.28170500
H	-5.18710100	12.60709900	-8.87561600
H	-6.33096700	11.51893200	-9.68310700
H	-4.59885200	11.21202900	-9.78203000
H	-2.96030500	10.20373100	-8.60174100
H	-5.87971600	6.50770000	-3.19793700
H	-7.25908100	8.93504900	-2.04831900

15. CAAC_Full_H_CI (twisted)-singlet:

C	-5.94244100	4.01662900	-1.73507200
N	-8.21069800	3.76377600	-1.14118500
C	-6.15255000	2.69139800	-0.97239300
C	-7.65124500	2.38681200	-1.01680000
H	-5.84819400	2.82818300	0.07584400
H	-5.55037700	1.87405400	-1.38597500
C	-7.33180200	4.65607300	-1.67870600
C	-6.56304000	7.04102500	-2.75937600
C	-5.80151700	7.91612200	-2.08326200
C	-5.45648100	3.81353300	-3.17554800
H	-5.37183500	4.78290600	-3.68043600
H	-6.12550900	3.17996800	-3.76472300
H	-4.46142500	3.35104600	-3.17321100
C	-4.87906300	4.85011800	-0.99806400
H	-4.02215500	4.20427800	-0.76353300
H	-5.26875200	5.25349200	-0.05359200
H	-4.51442200	5.68376000	-1.60166700
C	-8.15509800	1.69659100	0.24026200
H	-7.91520400	2.27545200	1.13830300
H	-7.68191900	0.71327300	0.32715500
H	-9.24127900	1.54953200	0.20454100
C	-7.99539800	1.53221400	-2.24266200

H	-7.81275400	2.07847600	-3.17255300
H	-9.03839300	1.20856700	-2.23470000
H	-7.36929500	0.63310200	-2.24305300
C	-6.42211400	10.94052100	-3.10756700
N	-4.15385900	11.19336900	-3.70146100
C	-6.21200500	12.26575000	-3.87024800
C	-4.71330900	12.57033400	-3.82584700
H	-6.81417400	13.08309600	-3.45666500
H	-6.51636500	12.12896600	-4.91848400
C	-6.90806700	11.14362000	-1.66708900
H	-6.99271300	10.17424700	-1.16220000
H	-7.90312200	11.60610900	-1.66942200
H	-6.23903500	11.77718400	-1.07791800
C	-7.48549700	10.10703400	-3.84457000
H	-7.85013500	9.27339100	-3.24096600
H	-7.09581300	9.70366000	-4.78904400
H	-8.34240600	10.75287300	-4.07909600
C	-4.36915000	13.42493300	-2.59998700
H	-4.55179600	12.87867600	-1.67009500
H	-4.99524800	14.32404900	-2.59960000
H	-3.32615400	13.74857400	-2.60795200
C	-4.20946000	13.26055200	-5.08291100
H	-4.44935600	12.68168900	-5.98095100
H	-3.12327800	13.40761000	-5.04719400
H	-4.68263800	14.24387000	-5.16980500
B	-4.74845500	8.89161600	-2.69168300
B	-7.61610300	6.06553100	-2.15095800
Cl	-9.29028400	6.77555600	-2.15972500
C	-5.03275500	10.30107400	-3.16393800
Cl	-3.07427500	8.18158800	-2.68292800
C	-9.40670400	4.17316300	-0.46839700
C	-10.66761000	3.97403000	-1.04730100
C	-9.27041000	4.82042500	0.77363600
C	-11.79224300	4.42292800	-0.35722300

C	-10.42196900	5.28096600	1.40851400
C	-11.67610600	5.08184800	0.85486700
H	-12.77524600	4.27349500	-0.79782100
H	-12.56271100	5.44469700	1.36683400
H	-10.32831000	5.80585800	2.35641800
C	-7.92895100	5.06824400	1.43999500
C	-7.91596700	4.59083000	2.89400400
H	-8.23571300	3.54748000	2.98836800
H	-8.58195700	5.19659400	3.51891700
H	-6.90882300	4.68099300	3.31531400
C	-7.56092300	6.55306800	1.37991900
H	-7.16213700	4.50203900	0.89691800
H	-6.56331700	6.72595500	1.80213400
H	-8.27922200	7.14502200	1.96223600
H	-7.57467200	6.93612000	0.35349400
C	-10.85721900	3.33015700	-2.40447600
C	-11.55286600	1.97432300	-2.24666300
H	-11.59364500	1.43262700	-3.19885700
H	-12.58529500	2.12253600	-1.90460700
H	-11.05924400	1.33617900	-1.50473100
C	-11.66874500	4.21119700	-3.35683000
H	-9.86564400	3.18899600	-2.85030300
H	-11.73212400	3.73866700	-4.34342700
H	-11.21892400	5.19967900	-3.47443000
H	-12.69538800	4.34428800	-2.99612800
C	-2.95785500	10.78397900	-4.37425200
C	-1.69694700	10.98311000	-3.79535100
C	-1.94259600	9.67617400	-6.25116600
C	-0.68845700	9.87528900	-5.69752200
C	-0.57231600	10.53420900	-4.48543200
H	0.19814600	9.51243800	-6.20949100
H	0.41068800	10.68364000	-4.04483600
C	-1.50733300	11.62698100	-2.43817600
C	-0.69580900	10.74593800	-1.48582400

H	-1.14563300	9.75745700	-1.36822400
H	-0.63242700	11.21846700	-0.49922700
H	0.33083300	10.61284400	-1.84652800
C	-0.81168300	12.98281300	-2.59599000
H	-2.49890800	11.76814600	-1.99234700
H	-0.77089900	13.52450800	-1.64379600
H	-1.30530400	13.62095900	-3.33792100
H	0.22074600	12.83459700	-2.93804800
C	-3.09415300	10.13671700	-5.61628400
C	-4.43561500	9.88889900	-6.28263900
C	-4.80364300	8.40407500	-6.22256100
H	-5.80125300	8.23118900	-6.64476600
H	-4.78988300	8.02102200	-5.19613600
H	-4.08535000	7.81212100	-6.80488500
C	-4.44860400	10.36631200	-7.73664900
H	-5.20242700	10.45510400	-5.73956000
H	-4.12886000	11.40966200	-7.83101400
H	-5.45574800	10.27614600	-8.15795500
H	-3.78261400	9.76054800	-8.36156300
H	-2.03625900	9.15128200	-7.19906900
H	-6.56764100	7.14385500	-3.85739200
H	-5.79691500	7.81329200	-0.98524600

16. CAAC_Full_H_CI (twisted)-triplet:

C	-5.94135800	4.01842000	-1.73378800
N	-8.20935900	3.76530200	-1.13946000
C	-6.15139200	2.69278200	-0.97169200
C	-7.65004200	2.38824700	-1.01618800
H	-5.84695600	2.82898800	0.07659300
H	-5.54924600	1.87567200	-1.38577100
C	-7.33091400	4.65760300	-1.67767700
C	-6.56207200	7.04124200	-2.76086900
C	-5.80263700	7.91607000	-2.08193900
C	-5.45452100	3.81602800	-3.17404200
H	-5.36961800	4.78559500	-3.67851400
H	-6.12307300	3.18254100	-3.76387500
H	-4.45938000	3.35373100	-3.17127800
C	-4.87865800	4.85190400	-0.99572100
H	-4.02196000	4.20606600	-0.76040100
H	-5.26928200	5.25519500	-0.05159700
H	-4.51351900	5.68561700	-1.59890600
C	-8.15397000	1.69685900	0.24019000
H	-7.91364200	2.27453800	1.13885800
H	-7.68123300	0.71322000	0.32586100
H	-9.24022500	1.55032600	0.20449200
C	-7.99434900	1.53489800	-2.24283600
H	-7.81192900	2.08223100	-3.17216300
H	-9.03734800	1.21124900	-2.23491800
H	-7.36821400	0.63580400	-2.24427100
C	-6.42338600	10.93879200	-3.10937000

N	-4.15527600	11.19200000	-3.70327900
C	-6.21328800	12.26442600	-3.87145400
C	-4.71465300	12.56903200	-3.82677100
H	-6.81552500	13.08152300	-3.45748400
H	-6.51757800	12.12817200	-4.91977300
C	-6.91064800	11.14109700	-1.66926200
H	-6.99581100	10.17148800	-1.16491200
H	-7.90573500	11.60350700	-1.67227200
H	-6.24218500	11.77441700	-1.07916900
C	-7.48577900	10.10522300	-3.84777200
H	-7.85089300	9.27136100	-3.24477700
H	-7.09486500	9.70217200	-4.79188200
H	-8.34254700	10.75093700	-4.08318200
C	-4.37072800	13.42265300	-2.60017100
H	-4.55401700	12.87573200	-1.67078400
H	-4.99656000	14.32195500	-2.59941800
H	-3.32762700	13.74596200	-2.60741500
C	-4.21050300	13.26020200	-5.08318100
H	-4.45027200	12.68214400	-5.98176900
H	-3.12430600	13.40710100	-5.04709100
H	-4.68353300	14.24365400	-5.16935000
B	-4.74899800	8.89094200	-2.69103300
B	-7.61571100	6.06637700	-2.15174400
Cl	-9.28862600	6.77945800	-2.15327700
C	-5.03375600	10.29971900	-3.16509100
Cl	-3.07597200	8.17808100	-2.68896000
C	-9.40560000	4.17417700	-0.46694700
C	-10.66619100	3.97608500	-1.04680900
C	-9.26973100	4.81990500	0.77588800
C	-11.79105300	4.42465600	-0.35687800
C	-10.42144600	5.28017600	1.41065500
C	-11.67533900	5.08219700	0.85600700
H	-12.77387200	4.27606700	-0.79817500
H	-12.56210200	5.44483000	1.36785600

H	-10.32814300	5.80398400	2.35919300
C	-7.92841200	5.06658000	1.44293500
C	-7.91638000	4.58851000	2.89672400
H	-8.23720300	3.54541900	2.99043400
H	-8.58199100	5.19461200	3.52171300
H	-6.90930200	4.67748800	3.31843400
C	-7.55943000	6.55115000	1.38339900
H	-7.16169500	4.50015400	0.89992300
H	-6.56250000	6.72350400	1.80741400
H	-8.27848700	7.14363400	1.96423300
H	-7.57107600	6.93387900	0.35682100
C	-10.85518300	3.33353500	-2.40470900
C	-11.55193500	1.97806300	-2.24869300
H	-11.59220800	1.43723800	-3.20140100
H	-12.58458000	2.12669100	-1.90748100
H	-11.05946900	1.33889500	-1.50688800
C	-11.66524900	4.21606800	-3.35690400
H	-9.86337400	3.19202600	-2.84991000
H	-11.72862900	3.74426400	-4.34384900
H	-11.21429200	5.20414200	-3.47358200
H	-12.69192500	4.35007300	-2.99663100
C	-2.95883800	10.78316200	-4.37553300
C	-1.69834200	10.98125300	-3.79542900
C	-1.94260600	9.67705100	-6.25287400
C	-0.68881700	9.87518100	-5.69805700
C	-0.57334200	10.53271200	-4.48514900
H	0.19805000	9.51259100	-6.20975600
H	0.40938700	10.68130900	-4.04365600
C	-1.50961700	11.62359700	-2.43741100
C	-0.69910200	10.74126400	-1.48539100
H	-1.14930800	9.75278000	-1.36928400
H	-0.63636100	11.21264900	-0.49820800
H	0.32778400	10.60826300	-1.84543700
C	-0.81343900	12.97938200	-2.59331200

H	-2.50149400	11.76458100	-1.99217600
H	-0.77340800	13.52022300	-1.64060300
H	-1.30617500	13.61830300	-3.33516900
H	0.21926800	12.83116400	-2.93452800
C	-3.09446400	10.13724300	-5.61830300
C	-4.43568700	9.89018200	-6.28540000
C	-4.80437300	8.40553100	-6.22557300
H	-5.80148500	8.23294900	-6.64907400
H	-4.79212000	8.02284800	-5.19898800
H	-4.08550000	7.81313800	-6.80673000
C	-4.44778700	10.36791500	-7.73928900
H	-5.20251700	10.45658100	-5.74252800
H	-4.12746200	11.41113400	-7.83321800
H	-5.45478700	10.27837500	-8.16106900
H	-3.78184000	9.76196800	-8.36407000
H	-2.03571200	9.15315200	-7.20137900
H	-6.56094000	7.14162600	-3.85894600
H	-5.80371200	7.81566500	-0.98386400

17. CAAC_Full_H_CI (planar)-singlet:

C	-5.87198400	4.00119000	-1.83453700
N	-7.67775600	3.97040400	-0.35834700
C	-5.82726600	2.71496900	-0.98239100
C	-7.18746400	2.55812100	-0.31812100
H	-5.06172500	2.83241900	-0.20332400
H	-5.55526100	1.83850900	-1.58195700
C	-7.03098600	4.78869100	-1.20591200
C	-6.49818000	7.04761000	-2.46126700
C	-6.65115200	8.39365900	-2.80203000
C	-6.19188400	3.68989000	-3.30528400
H	-6.23127800	4.60569600	-3.90100400
H	-7.15593600	3.18185200	-3.41665100
H	-5.41412900	3.03649800	-3.72120800
C	-4.48701700	4.65949000	-1.73421400
H	-3.72622300	3.87996500	-1.87287400
H	-4.33760600	5.10431300	-0.74450200
H	-4.30541200	5.42874200	-2.48461700
C	-7.07963100	2.03123500	1.10803200
H	-6.36179000	2.59600800	1.70720800
H	-6.73939100	0.99143800	1.06972000
H	-8.05485600	2.04423700	1.60782600
C	-8.13104300	1.61825900	-1.07140500
H	-8.22394200	1.85632000	-2.13292100
H	-9.12640800	1.63861100	-0.61556900
H	-7.74649500	0.59643000	-0.98897200
C	-7.27738900	11.44006300	-3.42881200
N	-5.47155300	11.47084700	-4.90496200
C	-7.32200400	12.72638600	-4.28080300
C	-5.96184000	12.88312300	-4.94519000
H	-7.59378500	13.60280900	-3.68108200

H	-8.08766300	12.60919800	-5.05978700
C	-6.95769700	11.75131100	-1.95800800
H	-5.99390700	12.25982200	-1.84653200
H	-6.91793500	10.83547400	-1.36236500
H	-7.73578000	12.40431600	-1.54208700
C	-8.66233600	10.78174100	-3.52928800
H	-8.84392200	10.01236200	-2.77901000
H	-8.81172600	10.33706500	-4.51906600
H	-9.42315300	11.56122400	-3.39051300
C	-5.01811200	13.82297100	-4.19205600
H	-4.92494800	13.58487500	-3.13056500
H	-5.40267000	14.84480400	-4.27437600
H	-4.02284700	13.80262000	-4.64811300
C	-6.06973900	13.40993200	-6.37137000
H	-6.78781000	12.84532200	-6.97042600
H	-5.09457300	13.39660600	-6.87125800
H	-6.40966100	14.44983500	-6.33311400
B	-5.83326600	9.16295600	-3.78051100
B	-7.31607200	6.27832000	-1.48278100
Cl	-8.60939800	7.21858600	-0.57008800
C	-6.11834200	10.65258300	-4.05739000
Cl	-4.54004100	8.22271800	-4.69334100
C	-8.92246600	4.30584100	0.27569200
C	-10.10927700	4.28051400	-0.47858600
C	-8.90987500	4.71594300	1.61913200
C	-11.29761400	4.61130600	0.17155100
C	-10.12683900	5.03362500	2.21826700
C	-11.31415700	4.97206600	1.50806800
H	-12.22513400	4.60741200	-0.39609400
H	-12.25243100	5.23048700	1.99064100
H	-10.13402400	5.36533900	3.25392900
C	-7.63529000	4.94623300	2.41487500
C	-7.62713900	4.15613900	3.72681100
H	-7.82172300	3.08935200	3.58603500

H	-8.39284300	4.54229500	4.41039600
H	-6.66170100	4.26563600	4.23345600
C	-7.45219600	6.43395900	2.73463400
H	-6.78178400	4.63793500	1.79982100
H	-6.54287000	6.57823900	3.32936600
H	-8.29722600	6.80715300	3.32634400
H	-7.38023200	7.04235900	1.83144400
C	-10.17235500	3.99745800	-1.97279800
C	-11.13638600	2.85069700	-2.29458300
H	-11.08424200	2.59814200	-3.35946700
H	-12.17104200	3.14858600	-2.08661600
H	-10.93465000	1.94395500	-1.71769400
C	-10.61112800	5.23830500	-2.75897700
H	-9.17049600	3.73026100	-2.32603200
H	-10.71811100	4.98437300	-3.81977800
H	-9.89689000	6.05923900	-2.67257200
H	-11.58502400	5.59684200	-2.40368700
C	-4.22656700	11.13562400	-5.53858800
C	-3.04009700	11.16088000	-4.78377000
C	-3.02127600	10.40820600	-7.48073000
C	-1.83428200	10.46971400	-6.76998700
C	-1.85144600	10.83027500	-5.43342200
H	-0.89577900	10.21141500	-7.25217800
H	-0.92418100	10.83416200	-4.86535900
C	-2.97770400	11.44376400	-3.28950100
C	-2.53882400	10.20295800	-2.50332200
H	-3.25266300	9.38173500	-2.59032400
H	-2.43257100	10.45670700	-1.44240500
H	-1.56456500	9.84491600	-2.85811400
C	-2.01427000	12.59088700	-2.96721000
H	-3.97979300	11.71053800	-2.93661000
H	-2.06684200	12.84321900	-1.90229300
H	-2.21626900	13.49764600	-3.54398600
H	-0.97941800	12.29350700	-3.17493700

C	-4.23852900	10.72573800	-6.88209800
C	-5.51274500	10.49555700	-7.67845100
C	-5.69575600	9.00787500	-7.99843400
H	-6.60467200	8.86376700	-8.59384500
H	-5.76847000	8.39941400	-7.09534800
H	-4.85033500	8.63462900	-8.58954500
C	-5.52028800	11.28565000	-8.99039300
H	-6.36649700	10.80387200	-7.06376700
H	-5.32574500	12.35244600	-8.84961600
H	-6.48552700	11.17614400	-9.49742300
H	-4.75432500	10.89943700	-9.67365400
H	-3.01362000	10.07663600	-8.51643600
H	-5.74316400	6.52819500	-3.04638400
H	-7.40616100	8.91307700	-2.21690500

18. CAAC_Full_H_CI (planar)-triplet:

C	-5.87797000	3.97299700	-1.80998100
N	-7.65821300	3.95549900	-0.28615900
C	-5.82955900	2.68671100	-0.95841300
C	-7.18195700	2.54105700	-0.27160300
H	-5.05044000	2.79615200	-0.19181200
H	-5.57698000	1.80616700	-1.56094100
C	-7.02428300	4.76548200	-1.17441100
C	-6.48790100	7.06156500	-2.48572500
C	-6.66152400	8.37982900	-2.77763900
C	-6.19589200	3.66442100	-3.28066800
H	-6.28061800	4.58352300	-3.86826200
H	-7.13824000	3.11659600	-3.38776600
H	-5.39640200	3.05154800	-3.71711300
C	-4.49967600	4.64323700	-1.70863500
H	-3.72816400	3.88813800	-1.90884300
H	-4.33363300	5.03333200	-0.69812200
H	-4.34874700	5.45722700	-2.41808900
C	-7.05479800	2.00040900	1.14758500
H	-6.33458200	2.56554200	1.74413400
H	-6.71064900	0.96223500	1.09912000
H	-8.02560400	2.00548600	1.65605100
C	-8.14207800	1.61071200	-1.01764700
H	-8.24399100	1.85216600	-2.07759800
H	-9.13317500	1.63933700	-0.55231000
H	-7.76708200	0.58455000	-0.94259200
C	-7.27163500	11.46830800	-3.45368300
N	-5.49114300	11.48585700	-4.97725800
C	-7.31988000	12.75462200	-4.30521900
C	-5.96729900	12.90034300	-4.99165200
H	-7.57266600	13.63514600	-3.70274900
H	-8.09877300	12.64515500	-5.07204500
C	-6.95425900	11.77688100	-1.98287400
H	-6.01213700	12.32501500	-1.87542800
H	-6.86943700	10.85778300	-1.39529000

H	-7.75408300	12.38947800	-1.54665700
C	-8.64981300	10.79790500	-3.55550500
H	-8.80070400	9.98361400	-2.84638600
H	-8.81561000	10.40815500	-4.56619200
H	-9.42148500	11.55280100	-3.35514900
C	-5.00728700	13.83048300	-4.24519900
H	-4.90558700	13.58881800	-3.18528100
H	-5.38221400	14.85668000	-4.32013000
H	-4.01609000	13.80189700	-4.71034000
C	-6.09400600	13.44123500	-6.41077300
H	-6.81412900	12.87627000	-7.00759300
H	-5.12305900	13.43607100	-6.91896800
H	-6.43800900	14.47945400	-6.36227100
B	-5.86697700	9.19044200	-3.81985200
B	-7.28243900	6.25094400	-1.44351700
Cl	-8.50461400	7.20861300	-0.49004600
C	-6.12511200	10.67590200	-4.08897800
Cl	-4.64479900	8.23276800	-4.77332200
C	-8.90949600	4.29174000	0.32849900
C	-10.08511300	4.29258500	-0.44646900
C	-8.92298300	4.68084400	1.67927700
C	-11.28226800	4.62712800	0.18507500
C	-10.14866500	4.99899500	2.26116700
C	-11.32249400	4.96372600	1.52768700
H	-12.19900800	4.64011000	-0.39988700
H	-12.26763500	5.22223800	1.99666500
H	-10.17282700	5.30983700	3.30315400
C	-7.66309300	4.88921000	2.50395800
C	-7.67537900	4.06641300	3.79549000
H	-7.85512900	3.00169400	3.62510100
H	-8.46012900	4.42809700	4.47103700
H	-6.72250800	4.17291900	4.32616000
C	-7.48904100	6.36770700	2.86921300
H	-6.80071600	4.59847300	1.89303400

H	-6.58152500	6.50032400	3.46938700
H	-8.33641400	6.71859400	3.47108300
H	-7.41844400	7.00398900	1.98551200
C	-10.12752800	4.02124800	-1.94387900
C	-11.10165500	2.89012200	-2.28941000
H	-11.03306100	2.64179500	-3.35444800
H	-12.13629200	3.19933000	-2.09868200
H	-10.92052800	1.97856300	-1.71325500
C	-10.53507400	5.27340000	-2.72879500
H	-9.12417500	3.74192300	-2.28207900
H	-10.63357300	5.02872200	-3.79257800
H	-9.80796400	6.08252200	-2.63100700
H	-11.50593600	5.64923900	-2.38320200
C	-4.23952000	11.14973200	-5.59132000
C	-3.06431700	11.14860900	-4.81571000
C	-2.99930100	10.44310100	-7.52355200
C	-1.82587900	10.47806300	-6.78941200
C	-1.86683800	10.81418800	-5.44670400
H	-0.88049000	10.21968500	-7.25796100
H	-0.95041800	10.80097800	-4.86124500
C	-3.02258300	11.41961300	-3.31821500
C	-2.61548100	10.16728500	-2.53334600
H	-3.34269100	9.35828400	-2.63145900
H	-2.51730700	10.41181000	-1.46949700
H	-1.64456200	9.79133700	-2.87865500
C	-2.04858800	12.55065800	-2.97203600
H	-4.02605600	11.69891900	-2.98036700
H	-2.11762700	12.79875100	-1.90697100
H	-2.22950600	13.46233700	-3.54806900
H	-1.01387000	12.24150900	-3.16240800
C	-4.22530100	10.76107000	-6.94222700
C	-5.48475000	10.55287900	-7.76765300
C	-5.65857100	9.07444500	-8.13330300
H	-6.56589600	8.94187100	-8.73377500

H	-5.72936200	8.43796800	-7.24977200
H	-4.81098700	8.72377700	-8.73500200
C	-5.47180600	11.37589500	-9.05903300
H	-6.34745300	10.84348800	-7.15711300
H	-5.29248400	12.44064700	-8.88839200
H	-6.42428900	11.26920000	-9.59036000
H	-4.68650600	11.01453200	-9.73411300
H	-2.97456800	10.13262500	-8.56563300
H	-5.77901300	6.54006000	-3.12719100
H	-7.37042800	8.90134300	-2.13619100

19. CAAC_Full_C₂H₅_H (fully optimized)-singlet:

C	-6.14984000	3.67000800	-2.19271200
N	-7.75223700	3.82401000	-0.50969800
C	-6.12202000	2.38848500	-1.33989800
C	-7.40733900	2.37781800	-0.50786600

H	-5.26029100	2.43196400	-0.65894400
H	-6.01797500	1.48194300	-1.94786900
C	-7.07135600	4.58679800	-1.40145000
C	-6.42348700	7.03290700	-2.49760100
C	-5.51225100	7.91753000	-2.01787500
C	-6.73153700	7.00814500	-3.98547800
H	-6.42957000	7.96683500	-4.44151000
H	-6.10290600	6.25464200	-4.49436100
C	-5.21969100	7.90786300	-0.52117800
H	-5.19655600	6.86935200	-0.14352100
H	-6.07831900	8.37158500	0.00033500
C	-6.74389900	3.39288000	-3.58223800
H	-6.73097300	4.29458400	-4.19876300
H	-7.78134400	3.04523200	-3.52769300
H	-6.15375900	2.62294400	-4.09670300
C	-4.74240800	4.24409300	-2.34964400
H	-4.06941800	3.48187700	-2.76326200
H	-4.34538100	4.56506000	-1.37811500
H	-4.72951400	5.11170700	-3.01510800
C	-7.15392400	1.85410800	0.90191300
H	-6.31232400	2.36712100	1.37416300
H	-6.90954100	0.78794700	0.84506200
H	-8.04098200	1.96116400	1.53745800
C	-8.53974100	1.54724400	-1.11529000
H	-8.77665800	1.83577500	-2.14214800
H	-9.44624700	1.65424600	-0.50782300
H	-8.25868400	0.48865700	-1.11391200
C	-6.46306300	10.98655500	-2.94836600
N	-4.48745700	11.11044700	-4.17144600
C	-6.53271300	12.20342400	-3.89048900
C	-5.12877000	12.41712600	-4.46692100
H	-6.90272200	13.10114500	-3.38075300
H	-7.22930700	11.98275600	-4.71072900
C	-6.27055200	11.40633900	-1.48365700

H	-5.34233600	11.97639000	-1.34604100
H	-6.21489200	10.51880400	-0.84266700
H	-7.11113400	12.02582200	-1.14337400
C	-7.74406700	10.16256000	-3.06899000
H	-7.74388500	9.30516800	-2.38906300
H	-7.87456900	9.79117700	-4.09321300
H	-8.60826000	10.79579600	-2.82890100
C	-4.37016800	13.56001300	-3.79576500
H	-4.30651300	13.43552300	-2.71031300
H	-4.87911900	14.50759700	-4.00287000
H	-3.35550700	13.62828100	-4.20304800
C	-5.17270800	12.69054800	-5.96840800
H	-5.76227600	11.93345800	-6.49304300
H	-4.16616400	12.72085500	-6.40271100
H	-5.64389300	13.66400300	-6.14171000
B	-4.68686400	8.91066400	-2.91560100
B	-7.21295900	6.09864000	-1.50847200
C	-5.19879300	10.26323500	-3.38909700
C	-8.81445400	4.30827300	0.31495900
C	-10.11720100	4.38268500	-0.20716200
C	-8.53946700	4.69478200	1.63774500
C	-11.15624000	4.71878800	0.66152200
C	-9.61152900	5.02557800	2.46591900
C	-10.91420100	5.00786100	1.99430200
H	-12.17072700	4.77512200	0.27346700
H	-11.73804700	5.25838800	2.65657900
H	-9.41305800	5.32434900	3.49274100
C	-7.12810300	4.90115400	2.15827200
C	-6.85704800	4.15709900	3.46709200
H	-7.07640600	3.08768800	3.40351900
H	-7.46897700	4.57069900	4.27774700
H	-5.80967200	4.27609300	3.76578200
C	-6.89777200	6.40140400	2.37424900
H	-6.42076100	4.56448800	1.38704900

H	-5.85180600	6.60040100	2.63618100
H	-7.52565000	6.76827400	3.19660400
H	-7.14662700	6.97330100	1.47678800
C	-10.42629000	4.25719300	-1.68933100
C	-11.52279100	3.23823000	-1.99841600
H	-11.69117700	3.17794100	-3.07932900
H	-12.47418500	3.53641600	-1.54210600
H	-11.28218000	2.23477800	-1.63597900
C	-10.84508700	5.63707600	-2.21121200
H	-9.50790700	3.96787500	-2.21809000
H	-10.99091000	5.61567700	-3.29762800
H	-10.08778500	6.39335400	-1.97782500
H	-11.79086900	5.94827200	-1.74971400
C	-3.20604500	10.79762200	-4.71921100
C	-2.03866100	11.14122300	-4.01713400
C	-1.89283200	9.96617700	-6.55129800
C	-0.73659900	10.40078500	-5.92239000
C	-0.81128900	10.95410700	-4.65469000
H	0.22840700	10.26927800	-6.40367800
H	0.10248800	11.22293900	-4.12928800
C	-2.04089300	11.54144600	-2.55048400
C	-1.35621500	10.42920000	-1.74482400
H	-1.78162900	9.44981700	-1.97766200
H	-1.46316300	10.60841700	-0.66857700
H	-0.28343400	10.39847600	-1.97413600
C	-1.32305100	12.86179500	-2.26766400
H	-3.08465600	11.60618900	-2.20934800
H	-1.34275600	13.07995900	-1.19410200
H	-1.75871700	13.71442700	-2.79361700
H	-0.26835200	12.79498400	-2.56122600
C	-3.14332600	10.14229800	-5.96026900
C	-4.35975600	9.51244400	-6.61574600
C	-4.24757600	7.98790100	-6.50049200
H	-5.14812000	7.50066800	-6.89324400

H	-4.11386700	7.67754000	-5.45820100
H	-3.38634000	7.62448600	-7.07627000
C	-4.51741100	9.91385300	-8.08247100
H	-5.25710100	9.81929300	-6.06024400
H	-4.52333000	10.99989200	-8.21892900
H	-5.44919000	9.51018400	-8.49352100
H	-3.69845300	9.50979000	-8.68930600
H	-1.82779900	9.46242700	-7.51305600
C	-8.19789100	6.72993600	-4.29923900
H	-8.50945100	5.74805000	-3.91430700
H	-8.84541200	7.47511800	-3.81823700
H	-8.40183500	6.74809000	-5.37570900
C	-3.93971000	8.62437000	-0.11312400
H	-3.06094100	8.14039000	-0.55380100
H	-3.93568500	9.66898300	-0.46182900
H	-3.80916400	8.63451100	0.97412300
H	-7.94881400	6.61878500	-0.70471200
H	-3.55474000	8.62872000	-3.21479300

20. CAAC_Full_C₂H₅_H (fully optimized)-triplet:

C	-5.76256400	4.00587400	-1.78016100
N	-7.65569200	3.88030800	-0.43293800
C	-5.62786000	2.79973400	-0.83152800
C	-7.00069300	2.56965800	-0.19009200
H	-4.90084200	3.04431500	-0.04470000
H	-5.26306500	1.90351700	-1.34772800
C	-6.99008600	4.73289900	-1.25007400
C	-6.67580200	7.12402100	-2.52256700

C	-5.76656000	7.99634300	-2.02837400
C	-6.94158800	7.12219600	-4.02305700
H	-6.89481600	8.15223000	-4.42167800
H	-6.10902700	6.59411700	-4.52681900
C	-5.46047100	8.00639500	-0.53940600
H	-5.73426400	7.03447700	-0.09322900
H	-6.10617100	8.73906300	-0.02055900
C	-6.05513500	3.56554200	-3.22218700
H	-6.15208800	4.44241900	-3.87160300
H	-6.98815300	2.99314800	-3.29349300
H	-5.23743600	2.94215000	-3.60814100
C	-4.47502100	4.82959000	-1.76535200
H	-3.62446800	4.17873000	-2.00734600
H	-4.29791400	5.26068100	-0.77204500
H	-4.50027100	5.64755900	-2.49234900
C	-6.88140700	2.27352400	1.30261200
H	-6.26904200	3.02423900	1.80967200
H	-6.40020200	1.29887200	1.43724200
H	-7.86563700	2.23284900	1.78470200
C	-7.79275700	1.43343300	-0.83577800
H	-7.90526200	1.56112100	-1.91625400
H	-8.78935300	1.36760300	-0.38482500
H	-7.27995900	0.48248800	-0.65547000
C	-6.14375600	11.30883600	-2.46650000
N	-4.46412700	11.17973200	-4.07344400
C	-6.19340900	12.56406000	-3.35585600
C	-4.88240500	12.60471400	-4.14719800
H	-6.35235400	13.48174800	-2.77701000
H	-7.03090200	12.46818600	-4.06109400
C	-5.60653200	11.63915200	-1.06615600
H	-4.59470200	12.05812700	-1.10023000
H	-5.57119700	10.73961700	-0.44560500
H	-6.26122900	12.36854900	-0.57088100
C	-7.53211900	10.68328400	-2.33835600

H	-7.53895300	9.85307800	-1.62666300
H	-7.87447300	10.29527700	-3.30640200
H	-8.25159300	11.43797200	-1.99514400
C	-3.81631700	13.51849100	-3.54058500
H	-3.60070700	13.28449700	-2.49506200
H	-4.15268400	14.55938800	-3.59550800
H	-2.88531000	13.43643700	-4.11367100
C	-5.11421100	13.05209200	-5.58691700
H	-5.91086400	12.47318400	-6.06132400
H	-4.20143100	12.96436600	-6.18813700
H	-5.41643500	14.10486300	-5.58757300
B	-4.93561900	8.91943200	-3.00009800
B	-7.49144400	6.11938200	-1.62509700
C	-5.15152700	10.41276500	-3.19145600
C	-8.91477400	4.18174100	0.171104200
C	-10.10591800	3.86136600	-0.50169300
C	-8.93548500	4.80438500	1.43009700
C	-11.31206000	4.03938100	0.17734600
C	-10.16613600	4.97013300	2.06446900
C	-11.34415400	4.55971900	1.46069800
H	-12.24315200	3.78913800	-0.32634200
H	-12.29291600	4.68443800	1.97494600
H	-10.19790400	5.44849900	3.04078800
C	-7.69799900	5.41453300	2.06416800
C	-7.48421400	4.95743800	3.50752900
H	-7.46588800	3.86750400	3.60346900
H	-8.28434300	5.33208300	4.15699700
H	-6.54142600	5.35347000	3.90062600
C	-7.82081200	6.94204000	2.01793300
H	-6.82209600	5.13569200	1.46159100
H	-6.90513700	7.41675900	2.39052100
H	-8.65583200	7.27672900	2.64710700
H	-8.00209400	7.29508100	0.99728800
C	-10.15016200	3.49017400	-1.97474800

C	-10.90010300	2.18858800	-2.25905300
H	-10.90179700	1.97952600	-3.33458600
H	-11.94837700	2.27121800	-1.94741300
H	-10.47045800	1.32391500	-1.74695700
C	-10.82658700	4.63399000	-2.74144600
H	-9.11836600	3.40740800	-2.34426000
H	-10.76741700	4.46439800	-3.82299700
H	-10.35734700	5.59539100	-2.51455900
H	-11.88786100	4.69973500	-2.46965400
C	-3.34971700	10.71957200	-4.84088200
C	-2.06275400	10.74317800	-4.27685500
C	-2.44372800	9.95993000	-6.93330300
C	-1.16020500	10.07582100	-6.42441100
C	-0.97837200	10.43351500	-5.09860800
H	-0.30213600	9.84788900	-7.05042500
H	0.02458900	10.45312800	-4.67824700
C	-1.81187200	10.94372600	-2.79189400
C	-1.32363400	9.61438900	-2.20290700
H	-2.01637900	8.79990000	-2.43833800
H	-1.22586100	9.68349400	-1.11310600
H	-0.33974700	9.35408500	-2.61350100
C	-0.79107000	12.04005800	-2.48774000
H	-2.76479300	11.19210800	-2.30467500
H	-0.66127600	12.14776900	-1.40517800
H	-1.07973600	13.01365000	-2.89332500
H	0.19073400	11.78511000	-2.90423000
C	-3.55923200	10.26091400	-6.15249800
C	-4.93914900	9.94542400	-6.70178400
C	-5.07036500	8.42461200	-6.84469000
H	-6.09522800	8.14503900	-7.11688800
H	-4.80807500	7.91707500	-5.91254200
H	-4.39994400	8.05722300	-7.63252200
C	-5.21382100	10.60708200	-8.05298700
H	-5.68943400	10.27554400	-5.96905500

H	-5.06382000	11.69022800	-8.03478900
H	-6.24170300	10.40779100	-8.37550300
H	-4.55178900	10.19614100	-8.82462500
H	-2.59120100	9.60654500	-7.95133100
C	-8.26137000	6.47889600	-4.42698400
H	-8.31880000	5.43536600	-4.08070300
H	-9.10900600	7.00796200	-3.97523800
H	-8.40257200	6.47900600	-5.51301500
C	-4.00062000	8.32001400	-0.23197700
H	-3.33752400	7.60431400	-0.73670600
H	-3.72374000	9.31891400	-0.60123800
H	-3.78368000	8.28702900	0.84128100
H	-8.57800100	6.43520200	-1.21224500
H	-4.09535000	8.40022600	-3.69611100

21. CAAC_Full_C₂H₅_H (twisted)-singlet:

C	-5.91982500	3.88518700	-1.93680700
N	-7.74752100	3.87351800	-0.50024400
C	-5.85049000	2.63107700	-1.04743100
C	-7.20899600	2.49636100	-0.34998900
H	-5.07040900	2.77542300	-0.28685400
H	-5.59149900	1.73031800	-1.61691300
C	-7.03158700	4.70425100	-1.29734500
C	-6.57992800	7.10616800	-2.52764300
C	-5.59454400	7.89800700	-2.04376800
C	-6.91341300	7.15550700	-4.01145800
H	-6.71646200	8.16498700	-4.41396600
H	-6.21283400	6.50069700	-4.56275300

C	-5.26123900	7.84897000	-0.55989700
H	-5.45773300	6.83944900	-0.15726800
H	-5.96224500	8.50348200	-0.00880300
C	-6.35208900	3.53363700	-3.36874700
H	-6.41953800	4.44057700	-3.97788600
H	-7.33364500	3.04581500	-3.39111400
H	-5.62186400	2.85939300	-3.83623700
C	-4.56188300	4.58367100	-1.98475900
H	-3.79386800	3.86928600	-2.30885500
H	-4.27668600	4.96037800	-0.99444000
H	-4.56238000	5.42761600	-2.68092100
C	-7.04692200	2.10988400	1.11806900
H	-6.33698800	2.76621400	1.62826700
H	-6.66014300	1.08674600	1.17599000
H	-8.00490200	2.13797500	1.65104700
C	-8.14065800	1.47513800	-1.00219700
H	-8.30321500	1.67003200	-2.06567800
H	-9.11180700	1.47980800	-0.49416700
H	-7.71368200	0.47180900	-0.89909000
C	-6.25511600	11.11885200	-2.63520000
N	-4.42716300	11.13055400	-4.07146300
C	-6.32429300	12.37290800	-3.52467100
C	-4.96561100	12.50772800	-4.22170000
H	-6.58354500	13.27368600	-2.95533600
H	-7.10413200	12.22842800	-4.28547000
C	-5.82342200	11.47041600	-1.20309300
H	-4.84168300	11.95786100	-1.18029700
H	-5.75659300	10.56352900	-0.59381900
H	-6.55361900	12.14497400	-0.73601500
C	-7.61305100	10.42028500	-2.58783000
H	-7.61257200	9.57575200	-1.89237600
H	-7.89822800	10.04442900	-3.57847000
H	-8.38108800	11.13440500	-2.26320300
C	-4.03408900	13.52879200	-3.56906000

H	-3.87189800	13.33376100	-2.50554900
H	-4.46091400	14.53218200	-3.67220200
H	-3.06278600	13.52405300	-4.07678700
C	-5.12723500	12.89439300	-5.68975600
H	-5.83704700	12.23815000	-6.20023300
H	-4.16910300	12.86631800	-6.22246500
H	-5.51395300	13.91755400	-5.74767500
B	-4.75885200	8.85956700	-2.97125200
B	-7.41569400	6.14457200	-1.60029500
C	-5.14302900	10.29987300	-3.27425600
C	-8.93380200	4.26153800	0.19522900
C	-10.18669500	4.09709100	-0.41843700
C	-8.82230900	4.80285000	1.48705800
C	-11.32951800	4.34567200	0.34320900
C	-9.99308100	5.04470500	2.20470900
C	-11.23793900	4.78600100	1.65323000
H	-12.30760100	4.21533900	-0.11457500
H	-12.13930300	4.96723700	2.23187700
H	-9.92254300	5.46190400	3.20667300
C	-7.49790100	5.25373300	2.07707700
C	-7.25086700	4.69831000	3.48009900
H	-7.33785800	3.60836900	3.52209700
H	-7.97060700	5.11397600	4.19525800
H	-6.25217700	4.97766100	3.83332200
C	-7.47452300	6.78583200	2.11600000
H	-6.68795900	4.92902200	1.40896600
H	-6.49435200	7.15244200	2.44393900
H	-8.22936800	7.16065500	2.81952400
H	-7.68993800	7.20916400	1.12979700
C	-10.35032800	3.82063300	-1.90363600
C	-11.23509200	2.61196100	-2.20970600
H	-11.31872800	2.46791400	-3.29262700
H	-12.25104600	2.77061500	-1.82825600
H	-10.85932300	1.68330300	-1.77273500

C	-10.95904700	5.06562300	-2.56207200
H	-9.35381700	3.66537500	-2.34126200
H	-10.98516900	4.95474300	-3.65244900
H	-10.38566200	5.96469500	-2.31791000
H	-11.98973300	5.21405800	-2.21574900
C	-3.24073900	10.74256700	-4.76669100
C	-1.98794700	10.90708500	-4.15287900
C	-2.18120500	9.95956400	-6.77610300
C	-0.93642400	10.21828900	-6.22445000
C	-0.84502200	10.65856100	-4.91439800
H	-0.03497900	10.03710100	-6.80298600
H	0.13300100	10.78888000	-4.45648400
C	-1.82451300	11.18334100	-2.66762100
C	-1.21582000	9.93825500	-2.00932600
H	-1.78892100	9.03914600	-2.25400700
H	-1.19024900	10.04878300	-0.91890000
H	-0.18492900	9.79018200	-2.35518900
C	-0.93981700	12.39198400	-2.36121700
H	-2.82106400	11.33853200	-2.23003500
H	-0.85608600	12.53563000	-1.27825000
H	-1.31569300	13.32078000	-2.79779200
H	0.07611300	12.23355600	-2.74281800
C	-3.35206200	10.20133900	-6.05857000
C	-4.67640800	9.75045000	-6.64872700
C	-4.69982400	8.21834700	-6.68753000
H	-5.67994700	7.85173600	-7.01561300
H	-4.48459100	7.79508700	-5.70125800
H	-3.94486200	7.84345000	-7.39089100
C	-4.92324100	10.30577700	-8.05182100
H	-5.48643500	10.07524100	-5.98075500
H	-4.83618200	11.39571100	-8.09388400
H	-5.92190300	10.02645500	-8.40514700
H	-4.20343800	9.89002500	-8.76686600
H	-2.25160600	9.54241300	-7.77809600

C	-8.34182200	6.73661000	-4.33239400
H	-8.53044800	5.70160700	-4.00802000
H	-9.06283300	7.37130600	-3.80053400
H	-8.56061400	6.79675100	-5.40369300
C	-3.83307800	8.26860700	-0.23882000
H	-3.11172400	7.63411100	-0.77048700
H	-3.64489100	9.30363400	-0.56341000
H	-3.61437200	8.20877600	0.83251400
H	-8.42945500	6.55659100	-1.09241300
H	-3.74507800	8.44757800	-3.47911200

22. CAAC_Full_C₂H₅_H (twisted)-triplet:

C	-5.91992400	3.88475500	-1.93826200
N	-7.74907700	3.87185800	-0.50339900
C	-5.85185100	2.62947600	-1.05043500
C	-7.21078500	2.49456900	-0.35388200
H	-5.07204800	2.77233100	-0.28930100
H	-5.59312000	1.72928000	-1.62093400
C	-7.03239900	4.70327000	-1.29935300
C	-6.57945500	7.10639200	-2.52861900
C	-5.59540200	7.89790200	-2.04285800
C	-6.91357100	7.15745700	-4.01266600
H	-6.72000800	8.16739000	-4.41522500
H	-6.21187300	6.50485200	-4.56496300
C	-5.26145700	7.84715600	-0.55872500
H	-5.45404700	6.83703900	-0.15613700
H	-5.96394000	8.49901200	-0.00658300
C	-6.35030600	3.53558100	-3.37130900

H	-6.41644200	4.44356600	-3.97910400
H	-7.33215900	3.04838600	-3.39568100
H	-5.61981700	2.86177000	-3.83901100
C	-4.56177200	4.58304400	-1.98317600
H	-3.79367500	3.86942200	-2.30875100
H	-4.27718100	4.95658200	-0.99149500
H	-4.56151500	5.42905200	-2.67681600
C	-7.04973000	2.10686500	1.11399200
H	-6.33981400	2.76248600	1.62513700
H	-6.66344100	1.08351300	1.17139000
H	-8.00800900	2.13498700	1.64644500
C	-8.14202600	1.47404600	-1.00766500
H	-8.30314000	1.66968600	-2.07124600
H	-9.11375100	1.47879400	-0.50076900
H	-7.71552600	0.47050400	-0.90463500
C	-6.25547100	11.11951600	-2.63450100
N	-4.42536400	11.13227000	-4.06822100
C	-6.32268900	12.37490900	-3.52227300
C	-4.96326900	12.50968600	-4.21783900
H	-6.58168300	13.27509500	-2.95188600
H	-7.10196600	12.23225600	-4.28398200
C	-5.82695500	11.46855700	-1.20088800
H	-4.84480100	11.95512700	-1.17517400
H	-5.76230800	10.56060100	-0.59290400
H	-6.55769100	12.14286800	-0.73430300
C	-7.61365000	10.42112900	-2.59146300
H	-7.61439400	9.57424200	-1.89888500
H	-7.89750100	10.04889300	-3.58384900
H	-8.38200700	11.13434500	-2.26560800
C	-4.03231600	13.52983900	-3.56306900
H	-3.87175800	13.33356800	-2.49950900
H	-4.45872100	14.53345800	-3.66576400
H	-3.06033700	13.52532500	-4.06947700
C	-5.12314900	12.89772400	-5.68573900

H	-5.83268500	12.24222700	-6.19757200
H	-4.16445700	12.86966700	-6.21744700
H	-5.50936000	13.92110100	-5.74322000
B	-4.75855900	8.86078300	-2.96917400
B	-7.41627000	6.14354100	-1.60230500
C	-5.14225900	10.30107800	-3.27223100
C	-8.93567600	4.25955400	0.19162200
C	-10.18836600	4.09585900	-0.42257700
C	-8.82451700	4.80009200	1.48382400
C	-11.33138900	4.34456000	0.33876100
C	-9.99543600	5.04204100	2.20119200
C	-11.24018200	4.78420100	1.64903200
H	-12.30934000	4.21486200	-0.11948600
H	-12.14171800	4.96556000	2.22737400
H	-9.92512700	5.45864600	3.20341800
C	-7.50012400	5.25026500	2.07440200
C	-7.25387500	4.69471700	3.47747700
H	-7.34111500	3.60477500	3.51923600
H	-7.97383300	5.11042200	4.19239200
H	-6.25527600	4.97378800	3.83117600
C	-7.47609700	6.78232400	2.11301000
H	-6.69006500	4.92513100	1.40664700
H	-6.49610200	7.14867600	2.44174600
H	-8.23149700	7.15767800	2.81565400
H	-7.69051900	7.20537200	1.12643400
C	-10.35180800	3.81980700	-1.90782300
C	-11.23618800	2.61095500	-2.21449600
H	-11.32060500	2.46814300	-3.29752500
H	-12.25191100	2.76872900	-1.83207500
H	-10.85971500	1.68193900	-1.77895500
C	-10.96113000	5.06470900	-2.56593000
H	-9.35522000	3.66508200	-2.34552300
H	-10.98466000	4.95514200	-3.65650300
H	-10.38965500	5.96436400	-2.31956000

H	-11.99283700	5.21103700	-2.22175600
C	-3.23866600	10.74441900	-4.76292500
C	-1.98604400	10.90845900	-4.14862500
C	-2.17858000	9.96167600	-6.77220000
C	-0.93393200	10.21999600	-6.22003600
C	-0.84291300	10.65992000	-4.90984000
H	-0.03231900	10.03877800	-6.79830000
H	0.13497600	10.78992700	-4.45154500
C	-1.82299300	11.18424000	-2.66320800
C	-1.21363200	9.93939800	-2.00506700
H	-1.78527600	9.03977300	-2.25108100
H	-1.18968100	10.04920100	-0.91452800
H	-0.18208100	9.79286800	-2.34961900
C	-0.93877300	12.39309300	-2.35607300
H	-2.81974200	11.33878100	-2.22576600
H	-0.85483500	12.53582200	-1.27299700
H	-1.31504900	13.32214500	-2.79170600
H	0.07712600	12.23533600	-2.73804200
C	-3.34961400	10.20355400	-6.05499200
C	-4.67391200	9.75324200	-6.64567500
C	-4.69798300	8.22116900	-6.68378100
H	-5.67785000	7.85473700	-7.01280500
H	-4.48395300	7.79840400	-5.69699700
H	-3.94231200	7.84558700	-7.38601200
C	-4.91982500	10.30831300	-8.04900200
H	-5.48410100	10.07868500	-5.97820200
H	-4.83220400	11.39821200	-8.09117800
H	-5.91847600	10.02943500	-8.40270500
H	-4.19992700	9.89208500	-8.76367200
H	-2.24871800	9.54483300	-7.77433700
C	-8.34099800	6.73433700	-4.33118200
H	-8.52617000	5.69984100	-4.00248500
H	-9.06309700	7.36876100	-3.80050500
H	-8.56150200	6.78998900	-5.40234200

C	-3.83452300	8.27164200	-0.23995100
H	-3.11179100	7.63778900	-0.77043100
H	-3.65012800	9.30624800	-0.56873500
H	-3.61420200	8.21629500	0.83126400
H	-8.43242400	6.55445900	-1.09846400
H	-3.74211600	8.44995600	-3.47247900

23. CAAC_Full_C₂H₅_H (planar)-singlet:

C	-5.44943700	3.63711800	-1.44812500
N	-7.61380500	3.85525500	-0.63048300
C	-5.83201700	2.38399800	-0.61997700
C	-7.35248400	2.39798200	-0.49791300
H	-5.39197000	2.45192800	0.38521400
H	-5.46292100	1.45948700	-1.07916300
C	-6.68878500	4.53958700	-1.35313300
C	-6.27896900	7.06151900	-2.55160600
C	-6.87131400	8.35366100	-2.77382200
C	-4.97296800	6.74085600	-3.25701900
H	-4.53896700	5.85229300	-2.80489500
H	-4.22967400	7.53469800	-3.12203100
C	-8.17737700	8.67421600	-2.06846400
H	-8.92053500	7.88025200	-2.20348900
H	-8.61150600	9.56270200	-2.52065300
C	-5.07543300	3.23041000	-2.87955600
H	-5.82920600	2.56441900	-3.31031100
H	-4.12386300	2.68383700	-2.86769100
H	-4.97152600	4.08228300	-3.55244900
C	-4.26555000	4.31146900	-0.73064600

H	-3.43722000	3.59384600	-0.65524000
H	-4.55581500	4.59736000	0.28771000
H	-3.89536800	5.20677800	-1.22896400
C	-7.86348100	1.82810400	0.81774500
H	-7.41056900	2.31339300	1.68640900
H	-7.61696400	0.76209100	0.85878700
H	-8.95276100	1.92460600	0.89312700
C	-8.01458200	1.63031700	-1.64761800
H	-7.77089800	2.07335000	-2.61801500
H	-9.10274400	1.61786600	-1.53927000
H	-7.66471400	0.59192000	-1.64097500
C	-7.70020000	11.77831900	-3.87745300
N	-5.53590700	11.55962900	-4.69511200
C	-7.31730700	13.03141000	-4.70548100
C	-5.79685100	13.01694500	-4.82782900
H	-7.68597000	13.95598800	-4.24608100
H	-7.75758500	12.96379400	-5.71059300
C	-8.07398300	12.18491300	-2.44594600
H	-7.31952300	12.84992100	-2.01485300
H	-8.17896400	11.33289800	-1.77341500
H	-9.02495400	12.73253300	-2.45777200
C	-8.88425500	11.10423000	-4.59486600
H	-9.25429000	10.20878200	-4.09668100
H	-8.59422700	10.81859800	-5.61336200
H	-9.71260800	11.82186600	-4.66989400
C	-5.13433700	13.78461300	-3.67837000
H	-5.37810100	13.34190200	-2.70784400
H	-5.48382300	14.82313600	-3.68522100
H	-4.04618100	13.79663600	-3.78684000
C	-5.28594300	13.58652700	-6.14366000
H	-5.73937900	13.10148700	-7.01218500
H	-4.19673600	13.48946600	-6.21937400
H	-5.53191500	14.65266800	-6.18464300
B	-6.13216100	9.41951300	-3.55673400

B	-7.01802900	5.99558200	-1.76870800
C	-6.46110500	10.87554300	-3.97246800
C	-8.71256900	4.48435800	0.03865900
C	-9.96433500	4.61286200	-0.57514800
C	-8.45556600	5.02955600	1.30848100
C	-10.97559400	5.26921600	0.12666100
C	-9.49113600	5.69780700	1.95908600
C	-10.74573600	5.81112800	1.38020000
H	-11.95260700	5.38093100	-0.33876100
H	-11.54175600	6.33380300	1.90282300
H	-9.30488400	6.14481200	2.93257400
C	-7.08633000	4.97581800	1.96591500
C	-7.17000900	4.54679700	3.43176900
H	-7.75470500	3.62887700	3.55961200
H	-7.63564700	5.32311100	4.04955500
H	-6.16670100	4.37641700	3.83695300
C	-6.37269500	6.32448700	1.85081200
H	-6.47633000	4.23574000	1.43287900
H	-5.40448600	6.29266800	2.36566600
H	-6.97531700	7.11706000	2.31414600
H	-6.19852500	6.59916700	0.80391000
C	-10.24178000	4.14624800	-1.99025200
C	-11.34998200	3.08998800	-2.00530900
H	-11.47537100	2.66449700	-3.00726400
H	-12.30877800	3.53997200	-1.71822500
H	-11.15664700	2.27162500	-1.30273500
C	-10.62977100	5.31366800	-2.90039400
H	-9.31852500	3.71701000	-2.39465100
H	-10.83829200	4.94912700	-3.91273100
H	-9.82622500	6.05239100	-2.96181200
H	-11.53524400	5.81484900	-2.53730700
C	-4.43729600	10.93011900	-5.36411900
C	-3.18561800	10.80124100	-4.75020900
C	-3.65918300	9.71577700	-7.28416300

C	-2.40468500	9.60199800	-6.70514700
C	-2.17463300	10.14419900	-5.45176400
H	-1.60888900	9.07876200	-7.22755100
H	-1.19770100	10.03215900	-4.98625000
C	-2.90803000	11.26814700	-3.33522700
C	-2.52056500	10.10087100	-2.42467700
H	-3.32438800	9.36246800	-2.36307800
H	-2.31201100	10.46568200	-1.41244200
H	-1.61523700	9.59923700	-2.78750500
C	-1.79939200	12.32395200	-3.32044800
H	-3.83111400	11.69788900	-2.93099500
H	-1.67382700	12.74965200	-2.31860400
H	-1.99237900	13.14221200	-4.02323400
H	-0.84078300	11.87349000	-3.60741100
C	-4.69447300	10.38471400	-6.63381400
C	-6.06363400	10.43893800	-7.29136700
C	-6.77783700	9.09057400	-7.17629400
H	-7.74598700	9.12279100	-7.69123700
H	-6.95222900	8.81602300	-6.12939400
H	-6.17552100	8.29771500	-7.63953200
C	-5.97959800	10.86792400	-8.75721000
H	-6.67341000	11.17925600	-6.75841200
H	-5.39458000	11.78565500	-8.88494300
H	-6.98278400	11.03862900	-9.16256300
H	-5.51409800	10.09146500	-9.37491800
H	-3.84558700	9.26857800	-8.25753400
C	-8.01138300	8.94933500	-0.57290800
H	-7.76570600	8.03535800	-0.02349900
H	-7.19984900	9.66939000	-0.40203700
H	-8.93034300	9.36320800	-0.13838500
C	-5.13916900	6.46578700	-4.75258700
H	-4.22037500	6.05170900	-5.18726300
H	-5.95089000	5.74589800	-4.92336300
H	-5.38471700	7.37981700	-5.30195900

H	-8.09632300	6.28303100	-1.36000200
H	-5.05384900	9.13194000	-3.96525500

24. CAAC_Full_C₂H₅_H (planar)-triplet:

C	-5.69496700	3.41027800	-1.97858200
N	-7.57166500	3.78691300	-0.68742500
C	-5.84530000	2.26056600	-0.96639200
C	-7.23907100	2.37681200	-0.35410700
H	-5.09049200	2.38810200	-0.17698300
H	-5.67256700	1.28214900	-1.43201100
C	-6.64783000	4.48050600	-1.43266400
C	-6.26891400	7.08571500	-2.59535300
C	-6.88117400	8.32903900	-2.73035400
C	-4.78708400	6.93322100	-2.91201800
H	-4.36522300	6.21995800	-2.19748000
H	-4.24692900	7.86697200	-2.73107500
C	-8.36306300	8.48142800	-2.41387400
H	-8.90309300	7.54753600	-2.59434900
H	-8.78501000	9.19431100	-3.12877100
C	-6.22302400	2.99973000	-3.36397900
H	-7.27763000	2.70991700	-3.32838100
H	-5.64254800	2.15568000	-3.76144000
H	-6.14008300	3.83627900	-4.06481200
C	-4.20847700	3.73586800	-2.10530400
H	-3.65909400	2.79238500	-2.22270200
H	-3.82374200	4.23589800	-1.20965600
H	-3.98321500	4.34732600	-2.98038000
C	-7.21738600	2.13867200	1.15742600

H	-6.44767700	2.73265700	1.65508700
H	-6.99617900	1.08276400	1.34572200
H	-8.18967000	2.36452300	1.61152700
C	-8.25195700	1.38988900	-0.94315000
H	-8.26647100	1.38604500	-2.03512000
H	-9.25994100	1.61571900	-0.57639500
H	-7.99559600	0.37876600	-0.60993800
C	-7.45516800	12.00433800	-3.34735600
N	-5.57836400	11.62774500	-4.63828400
C	-7.30477600	13.15405400	-4.35953400
C	-5.91090100	13.03783900	-4.97163300
H	-7.47760800	14.13246900	-3.89395200
H	-8.05947100	13.02644900	-5.14903800
C	-6.92723000	12.41489100	-1.96194700
H	-5.87277800	12.70522600	-1.99768600
H	-7.00964700	11.57824100	-1.26119900
H	-7.50797900	13.25866600	-1.56432600
C	-8.94168700	11.67873500	-3.22095800
H	-9.16720500	11.06714600	-2.34605600
H	-9.32619600	11.17882800	-4.11677500
H	-9.49109300	12.62220300	-3.10357700
C	-4.89803700	14.02472000	-4.38246100
H	-4.88387200	14.02876300	-3.29048800
H	-5.15410100	15.03583100	-4.71592800
H	-3.88997100	13.79863600	-4.74883600
C	-5.93244700	13.27599300	-6.48317700
H	-6.70214100	12.68204400	-6.98091100
H	-4.96015000	13.05011200	-6.93722000
H	-6.15360200	14.33191100	-6.67148200
B	-6.17018500	9.46850700	-3.52756800
B	-6.97993900	5.94620000	-1.79810600
C	-6.50221900	10.93417200	-3.89303600
C	-8.69679900	4.42603900	-0.07701300
C	-9.93461900	4.40727100	-0.73708300

C	-8.51123500	5.16327700	1.10575300
C	-11.00841100	5.07634200	-0.14920800
C	-9.61520100	5.81349100	1.65512100
C	-10.85828800	5.76373900	1.04359800
H	-11.96990500	5.08173600	-0.65774600
H	-11.70406800	6.28359100	1.48458900
H	-9.48644100	6.39350400	2.56645900
C	-7.15452700	5.37110400	1.75907000
C	-7.17079900	4.96045400	3.23342600
H	-7.55194200	3.94438000	3.37762800
H	-7.80509500	5.63622800	3.81943800
H	-6.16295700	5.01511200	3.66007300
C	-6.70909400	6.83166700	1.63538700
H	-6.41237500	4.76443800	1.22709600
H	-5.75528100	6.98162300	2.15451900
H	-7.44701900	7.50452500	2.09155000
H	-6.57981000	7.13080000	0.58935200
C	-10.11674100	3.81405900	-2.12277500
C	-11.31370000	2.86591900	-2.19775000
H	-11.35649600	2.37855700	-3.17793200
H	-12.25681000	3.41042600	-2.06940600
H	-11.27755700	2.08654400	-1.42945700
C	-10.26545100	4.92778900	-3.16292100
H	-9.21017600	3.25871800	-2.37799400
H	-10.46246400	4.50172000	-4.15365000
H	-9.35602800	5.53378100	-3.22681200
H	-11.10182500	5.59158900	-2.90878400
C	-4.45292700	10.98871900	-5.24822300
C	-3.21534200	11.00751900	-4.58769300
C	-3.53379300	9.60151800	-6.98018300
C	-2.29093600	9.65131400	-6.36820800
C	-2.14130000	10.33858400	-5.17526000
H	-1.44494700	9.13159300	-6.80895100
H	-1.17997800	10.33322200	-4.66640000

C	-3.03373900	11.60065600	-3.20189400
C	-2.88529800	10.48686900	-2.16175600
H	-3.79467900	9.88078700	-2.09815500
H	-2.68860600	10.91290000	-1.17094900
H	-2.04878500	9.82315900	-2.41567800
C	-1.83679800	12.54878500	-3.12640400
H	-3.94040700	12.15597900	-2.94696000
H	-1.79442300	13.03613700	-2.14620000
H	-1.87256400	13.32816600	-3.89470200
H	-0.89365000	12.00424100	-3.25432200
C	-4.63800700	10.25157600	-6.43111800
C	-5.99450300	10.04362900	-7.08482700
C	-6.43976900	8.58300500	-6.96125900
H	-7.39345100	8.43291900	-7.48059400
H	-6.56922700	8.28386200	-5.91524700
H	-5.70165000	7.91024300	-7.41725300
C	-5.97790900	10.45432700	-8.55916100
H	-6.73686800	10.65018400	-6.55302600
H	-5.59696200	11.47049500	-8.70322300
H	-6.98561900	10.39945800	-8.98609000
H	-5.34329800	9.77871900	-9.14502300
H	-3.66218200	9.02158500	-7.89162400
C	-8.65473500	8.94363700	-0.98792600
H	-8.47051200	8.13429800	-0.27165000
H	-8.01472600	9.78590300	-0.69717900
H	-9.69878600	9.25937600	-0.86721700
C	-4.49545500	6.47164800	-4.33810200
H	-3.45191200	6.15415000	-4.45856700
H	-5.13676400	5.63065600	-4.62979800
H	-4.67790100	7.28179400	-5.05391300
H	-8.00909300	6.26698400	-1.30389600
H	-5.14092600	9.14771900	-4.02151300

25. CAAC_Full_CH₃_H (fully optimized)-singlet:

C	-5.83011800	3.85100900	-1.79189100
N	-7.69507800	3.82374000	-0.40465700
C	-5.81447300	2.56004500	-0.94947600
C	-7.19193800	2.43098300	-0.28977900
H	-5.04821900	2.65382400	-0.16761800
H	-5.56576100	1.67546100	-1.54807400
C	-6.95943200	4.66101600	-1.17571100
C	-6.63133900	7.10600800	-2.41530900
C	-5.55231300	7.87896600	-2.15249800
C	-7.38180700	7.26554800	-3.71926200
H	-7.50232700	6.30604500	-4.24439900
H	-6.88690200	7.97326100	-4.40510200
H	-8.40548200	7.63342900	-3.54327200
C	-4.80184600	7.71942500	-0.84854500
H	-4.68133800	8.67892400	-0.32340000
H	-3.77816700	7.35155600	-1.02453600
H	-5.29674600	7.01170200	-0.16271200
C	-6.18079500	3.58173100	-3.26217600
H	-6.18209900	4.52427600	-3.82088400
H	-7.17151700	3.12450800	-3.37037500
H	-5.43952300	2.91249000	-3.71893000
C	-4.46924700	4.53895800	-1.72978900
H	-3.69264400	3.85288100	-2.09211100
H	-4.21988300	4.82227700	-0.70041400
H	-4.45084100	5.43938200	-2.35024500
C	-7.09190700	1.99556300	1.17010200
H	-6.38276900	2.61322300	1.72756000
H	-6.74197900	0.95881700	1.21313200
H	-8.06896900	2.04184200	1.66646100

C	-8.11576400	1.44734300	-1.00965100
H	-8.18363500	1.64197100	-2.08352500
H	-9.12249900	1.49049000	-0.57896500
H	-7.73622300	0.42901200	-0.87393600
C	-6.35353800	11.13396400	-2.77593800
N	-4.48859100	11.16121800	-4.16318800
C	-6.36919700	12.42491300	-3.61837500
C	-4.99174000	12.55397000	-4.27808900
H	-6.61790600	13.30950600	-3.01978900
H	-7.13546100	12.33111700	-4.40022200
C	-6.00284200	11.40326900	-1.30566200
H	-5.01212100	11.86049800	-1.19748400
H	-6.00152600	10.46073300	-0.74693800
H	-6.74411100	12.07251400	-0.84890900
C	-7.71440800	10.44601000	-2.83801000
H	-7.73280300	9.54559500	-2.21754200
H	-7.96378600	10.16267800	-3.86737700
H	-8.49100700	11.13209100	-2.47568500
C	-4.06791500	13.53763300	-3.55824900
H	-4.00003700	13.34303400	-2.48437100
H	-4.44746100	14.55595800	-3.69398900
H	-3.06118200	13.49448000	-3.98893900
C	-5.09179200	12.98935600	-5.73798000
H	-5.80092700	12.37167300	-6.29541600
H	-4.11473400	12.94307900	-6.23434800
H	-5.44173500	14.02609600	-5.78103000
B	-4.84878800	8.86876800	-3.14641700
B	-7.33486400	6.11620400	-1.42139300
C	-5.22422700	10.32395100	-3.39211600
C	-8.90314900	4.23406900	0.23732300
C	-10.12210000	4.15035900	-0.45581000
C	-8.83307900	4.77719800	1.53019600
C	-11.28837500	4.50156100	0.22437900
C	-10.02625300	5.11546100	2.16765500

C	-11.24768500	4.95496500	1.53302800
H	-12.24163100	4.44194300	-0.29626400
H	-12.16771200	5.21916800	2.04679100
H	-9.98989200	5.53611700	3.17011700
C	-7.51761500	5.12285000	2.20608400
C	-7.40485700	4.51989400	3.60679600
H	-7.56549300	3.43725800	3.60934000
H	-8.14494100	4.96467100	4.28282600
H	-6.41685300	4.72226200	4.03493000
C	-7.36663800	6.64601400	2.28280000
H	-6.69556100	4.74603300	1.58341200
H	-6.40341500	6.91409700	2.73206200
H	-8.15963800	7.08094800	2.90480300
H	-7.42623700	7.10357600	1.28976600
C	-10.21003000	3.82451800	-1.93723300
C	-11.19575000	2.69589700	-2.24174500
H	-11.18480800	2.45822300	-3.31120700
H	-12.22049800	2.99506000	-1.99073100
H	-10.97539100	1.77900800	-1.68738600
C	-10.61773100	5.07933700	-2.71721300
H	-9.21258700	3.53481600	-2.28720400
H	-10.65222100	4.86672200	-3.79190200
H	-9.91529800	5.90169200	-2.54855600
H	-11.61623200	5.41663300	-2.41051600
C	-3.28052600	10.75088300	-4.80517500
C	-2.06156600	10.83461700	-4.11206000
C	-2.15744100	9.86945200	-6.73550000
C	-0.93600100	10.02997300	-6.10089300
C	-0.89529800	10.48340800	-4.79225500
H	-0.01597900	9.76576600	-6.61466300
H	0.05796500	10.54304500	-4.27162500
C	-1.97362000	11.16049400	-2.63064600
C	-1.56591300	9.90569500	-1.85063700
H	-2.26836000	9.08334200	-2.01925000

H	-1.53139400	10.11834300	-0.77595500
H	-0.56742400	9.56837800	-2.15734700
C	-0.98789400	12.28912100	-2.32617300
H	-2.97105800	11.45020800	-2.28067100
H	-0.99883200	12.52683100	-1.25672000
H	-1.20825200	13.20599300	-2.88056200
H	0.03685200	11.98994700	-2.57718200
C	-3.35060900	10.20772000	-6.09803300
C	-4.66607800	9.86203700	-6.77389300
C	-4.81703400	8.33886900	-6.85058000
H	-5.78026200	8.07076400	-7.29981900
H	-4.75740800	7.88132400	-5.85754000
H	-4.02404100	7.90393600	-7.47259300
C	-4.77886600	10.46496300	-8.17461700
H	-5.48812900	10.23885200	-6.15121700
H	-4.61824900	11.54760200	-8.17718500
H	-5.76687200	10.26256900	-8.60273200
H	-4.03878400	10.02018400	-8.85064800
H	-2.19381200	9.44877200	-7.73795200
H	-8.33281500	6.51454200	-0.87764700
H	-3.85083300	8.47043000	-3.69015300

26. CAAC_Full_CH₃_H (fully optimized)-triplet:

C	-5.84667400	3.84132400	-1.83445300
N	-7.70730000	3.81727700	-0.44244300
C	-5.82439400	2.55418000	-0.98645100
C	-7.19573800	2.42934600	-0.31204100
H	-5.04956400	2.64958200	-0.21339800
H	-5.58348900	1.66673400	-1.58410800
C	-6.97048100	4.65500400	-1.21305700
C	-6.63525000	7.11624000	-2.42869600
C	-5.54841900	7.86872000	-2.13914500
C	-7.38267600	7.31692000	-3.72985700
H	-7.48439300	6.37538900	-4.29028900
H	-6.89942400	8.05485800	-4.38941400
H	-8.41311300	7.65921700	-3.54212800
C	-4.80099400	7.66803900	-0.83798300
H	-4.69927700	8.60957000	-0.27755100
H	-3.77055600	7.32574300	-1.02571300
H	-5.28424500	6.93010100	-0.17842700
C	-6.21924900	3.56504500	-3.29831300
H	-6.23779700	4.50636100	-3.85954900
H	-7.20872800	3.10091800	-3.38752600
H	-5.48145400	2.89951700	-3.76612300
C	-4.48291600	4.52420500	-1.79484400
H	-3.71682800	3.83756500	-2.17780600
H	-4.21061000	4.79800300	-0.76895400
H	-4.47253700	5.42923300	-2.40889300
C	-7.07892500	2.02018100	1.15450100
H	-6.37051800	2.65472000	1.69382000
H	-6.71887900	0.98765800	1.21328500
H	-8.05177500	2.06708700	1.65909200
C	-8.11947200	1.42782200	-1.00667300
H	-8.19302200	1.60019100	-2.08405400
H	-9.12423800	1.47525100	-0.57195900
H	-7.73474400	0.41408500	-0.85240600

C	-6.33699400	11.14363600	-2.73339100
N	-4.47636900	11.16768000	-4.12540200
C	-6.35927400	12.43077800	-3.58139500
C	-4.98793100	12.55561000	-4.25580700
H	-6.60017900	13.31822600	-2.98374000
H	-7.13410600	12.33537500	-4.35444800
C	-5.96441700	11.41991700	-1.26953200
H	-4.97493800	11.88404500	-1.18032000
H	-5.94586900	10.47860300	-0.70829400
H	-6.70221200	12.08544700	-0.80172200
C	-7.70075200	10.46075500	-2.77299600
H	-7.71113000	9.55572800	-2.15894600
H	-7.97306000	10.18695600	-3.79888500
H	-8.46683900	11.14739600	-2.39003400
C	-4.06419700	13.55713600	-3.56117800
H	-3.99064600	13.38477000	-2.48379600
H	-4.44892500	14.57087300	-3.71544800
H	-3.05943000	13.50970600	-3.99589300
C	-5.10474600	12.96477200	-5.72235000
H	-5.81315200	12.33023100	-6.26166600
H	-4.13189600	12.91786500	-6.22694200
H	-5.46479200	13.99729400	-5.78113600
B	-4.82827600	8.87983900	-3.09917900
B	-7.35539300	6.10512000	-1.46866200
C	-5.21318700	10.32995400	-3.35478600
C	-8.90967200	4.23317100	0.20610600
C	-10.13579000	4.13032600	-0.47141100
C	-8.82731600	4.80523700	1.48579800
C	-11.29604600	4.49111700	0.21394000
C	-10.01490700	5.15121600	2.12954100
C	-11.24268800	4.97186500	1.51235300
H	-12.25471900	4.41722300	-0.29479200
H	-12.15802500	5.24297400	2.03088600
H	-9.96925000	5.59329600	3.12237400

C	-7.50618700	5.17377600	2.13831800
C	-7.37110600	4.59893000	3.54880600
H	-7.52042400	3.51491900	3.57342300
H	-8.10815000	5.04873600	4.22484300
H	-6.38042900	4.81941000	3.96150800
C	-7.36656000	6.69942700	2.18350000
H	-6.68861700	4.79144900	1.51278500
H	-6.39765800	6.98388200	2.61007300
H	-8.15216400	7.13990900	2.81095400
H	-7.44735900	7.13777800	1.18310700
C	-10.23750600	3.77292500	-1.94461000
C	-11.22810100	2.63961100	-2.21423700
H	-11.22132800	2.37125200	-3.27642700
H	-12.25112300	2.94921500	-1.96888800
H	-11.00914200	1.73831100	-1.63417200
C	-10.64876800	5.00992400	-2.75073800
H	-9.24395200	3.47272100	-2.29603100
H	-10.71065800	4.76629600	-3.81758400
H	-9.93315700	5.82842300	-2.62297300
H	-11.63599000	5.36801100	-2.43148400
C	-3.27399700	10.75178400	-4.77395100
C	-2.04787900	10.85463100	-4.09643600
C	-2.16876400	9.83373300	-6.69738500
C	-0.94098300	10.01308700	-6.08019800
C	-0.88762400	10.49383800	-4.78178700
H	-0.02564600	9.74197600	-6.59873100
H	0.07105000	10.56773300	-4.27305500
C	-1.94616100	11.21203600	-2.62323700
C	-1.53490000	9.97503900	-1.81710600
H	-2.25051200	9.15654100	-1.94486700
H	-1.47300800	10.21867100	-0.75026100
H	-0.54767900	9.61694900	-2.13636100
C	-0.95556600	12.34535000	-2.35361400
H	-2.93971500	11.51224200	-2.27181600

H	-0.96233800	12.61371300	-1.29142500
H	-1.17452400	13.24664800	-2.93368200
H	0.06745600	12.03574500	-2.59896300
C	-3.35635500	10.17971500	-6.05364200
C	-4.67748400	9.81117300	-6.70615900
C	-4.81711000	8.28552200	-6.75133800
H	-5.78601300	8.00106500	-7.17790800
H	-4.73630900	7.84717300	-5.75094400
H	-4.03150800	7.84503900	-7.37879100
C	-4.81256800	10.38601600	-8.11664800
H	-5.49505400	10.19350100	-6.08062500
H	-4.66325000	11.47002700	-8.14126700
H	-5.80324500	10.16553400	-8.52934900
H	-4.07552400	9.93620800	-8.79268400
H	-2.21442200	9.39165200	-7.69021700
H	-8.38103400	6.48755700	-0.96676700
H	-3.80263400	8.49740100	-3.60107300

27. CAAC_Full_CH₃_H (twisted)-singlet:

C	-5.87566000	3.81403500	-1.89289100
N	-7.70666500	3.81776400	-0.45764300
C	-5.84004700	2.54015500	-1.02392700

C	-7.19757200	2.42978800	-0.31969000
H	-5.04929500	2.64382500	-0.26854900
H	-5.61529600	1.64217300	-1.61199000
C	-7.00563300	4.62868600	-1.28542800
C	-6.60514900	7.09176200	-2.46640800
C	-5.57836100	7.89309100	-2.10122500
C	-7.29151000	7.30146900	-3.79807100
H	-7.34066300	6.37628600	-4.39111100
H	-6.79687700	8.07366400	-4.41046700
H	-8.33875700	7.61379300	-3.65141200
C	-4.89203900	7.68338600	-0.76954900
H	-4.84317700	8.60849700	-0.17637500
H	-3.84470500	7.37133700	-0.91616900
H	-5.38653200	6.91099700	-0.15729900
C	-6.23642100	3.50830400	-3.35304900
H	-6.27432100	4.43919900	-3.92986400
H	-7.21517600	3.02056700	-3.43755700
H	-5.48319100	2.85136500	-3.80785200
C	-4.52124000	4.51851100	-1.85004500
H	-3.74100700	3.84092100	-2.22053100
H	-4.26400500	4.80312400	-0.82291400
H	-4.51792400	5.42194600	-2.46689200
C	-7.05219200	2.04335900	1.14962000
H	-6.33594600	2.68957600	1.66444800
H	-6.68754700	1.01307500	1.21803600
H	-8.01550600	2.09542200	1.67167100
C	-8.13747400	1.42225800	-0.98309600
H	-8.23110300	1.58228800	-2.06101800
H	-9.13372600	1.47747400	-0.53004600
H	-7.75202900	0.40943800	-0.82435200
C	-6.30793500	11.17078700	-2.67475200
N	-4.47696900	11.16707500	-4.11004300
C	-6.34370000	12.44454200	-3.54387500
C	-4.98620500	12.55496200	-4.24816100

H	-6.56857000	13.34257700	-2.95594200
H	-7.13443700	12.34066200	-4.29924500
C	-5.94709700	11.47674900	-1.21465700
H	-4.96838700	11.96458200	-1.13025300
H	-5.90909700	10.54594400	-0.63770200
H	-6.70035400	12.13369500	-0.75990900
C	-7.66231100	10.46622500	-2.71739300
H	-7.66553700	9.56290600	-2.10038000
H	-7.91958600	10.18140700	-3.74445700
H	-8.44256300	11.14383600	-2.34698600
C	-4.04631200	13.56262100	-3.58495200
H	-3.95232500	13.40253700	-2.50706000
H	-4.43194100	14.57539400	-3.74354700
H	-3.05019300	13.50756000	-4.03829900
C	-5.13173400	12.94119500	-5.71751700
H	-5.84779000	12.29471600	-6.23229600
H	-4.16841200	12.88939500	-6.23957300
H	-5.49669100	13.97136600	-5.78600700
B	-4.82131900	8.89659800	-3.04046400
B	-7.36221900	6.08824400	-1.52720600
C	-5.17795500	10.35614600	-3.28223400
C	-8.90701100	4.23852400	0.19229800
C	-10.13672000	4.12630800	-0.47795200
C	-8.82048500	4.81891100	1.46776300
C	-11.29469400	4.48301900	0.21338400
C	-10.00620600	5.15848600	2.11845000
C	-11.23659200	4.96757100	1.51024000
H	-12.25604200	4.40136100	-0.28901500
H	-12.15057200	5.23357600	2.03377400
H	-9.95690600	5.60566900	3.10882600
C	-7.49791000	5.20933900	2.10430700
C	-7.33428000	4.64002700	3.51407800
H	-7.45821100	3.55320000	3.54412000
H	-8.07467200	5.07509700	4.19619500

H	-6.34484800	4.88476000	3.91590700
C	-7.38830600	6.73784400	2.14924500
H	-6.68192400	4.84192100	1.46675300
H	-6.41307400	7.04163500	2.54724700
H	-8.16360600	7.15984800	2.80168200
H	-7.50803100	7.17662900	1.15332700
C	-10.24741400	3.76133800	-1.94890000
C	-11.23587300	2.62345100	-2.20698300
H	-11.23613500	2.35202900	-3.26842400
H	-12.25828100	2.92930000	-1.95471800
H	-11.00822200	1.72478800	-1.62619000
C	-10.66874000	4.99416100	-2.75634000
H	-9.25586600	3.46284700	-2.30761000
H	-10.73768000	4.74659200	-3.82180600
H	-9.95464000	5.81540900	-2.63671800
H	-11.65466300	5.35007900	-2.43080500
C	-3.27668400	10.74635000	-4.76010000
C	-2.04688300	10.85888600	-4.09010100
C	-2.17771000	9.82635600	-6.68634900
C	-0.94723800	10.01761200	-6.07841200
C	-0.88896800	10.50234300	-4.78163100
H	-0.03330900	9.75174600	-6.60210500
H	0.07246700	10.58427300	-4.27943600
C	-1.93603300	11.22393000	-2.61919100
C	-1.51405700	9.99123500	-1.81186700
H	-2.22771400	9.16962200	-1.93161200
H	-1.44524900	10.23868600	-0.74636800
H	-0.52795100	9.63588700	-2.13746000
C	-0.94794200	12.36215900	-2.36125700
H	-2.92763300	11.52203800	-2.26029500
H	-0.94719500	12.63317600	-1.29971200
H	-1.17631400	13.26095000	-2.94156400
H	0.07445200	12.05683300	-2.61422500
C	-3.36336500	10.16578700	-6.03547100

C	-4.68600100	9.77526800	-6.67181400
C	-4.79543100	8.24679500	-6.71719400
H	-5.77086400	7.94307800	-7.11476700
H	-4.67511900	7.80768700	-5.72148600
H	-4.02046300	7.82509700	-7.37022300
C	-4.84988000	10.34498500	-8.08140300
H	-5.50193100	10.14240900	-6.03400700
H	-4.72591600	11.43182500	-8.11111000
H	-5.83936700	10.10038500	-8.48318000
H	-4.10956100	9.91013100	-8.76373800
H	-2.22711700	9.37906800	-7.67667400
H	-8.36519500	6.49620800	-1.00000500
H	-3.81832700	8.48864400	-3.56764500

28. CAAC_Full_CH₃_H (twisted)-triplet:

C	-5.87780500	3.81045500	-1.89764800
N	-7.71000600	3.81338500	-0.46382700
C	-5.84196400	2.53676700	-1.02837200
C	-7.19946500	2.42640700	-0.32363700
H	-5.05099500	2.64063600	-0.27323700
H	-5.61730900	1.63861500	-1.61624700
C	-7.00690200	4.62554200	-1.28957800

C	-6.60417200	7.09151100	-2.46772400
C	-5.57927400	7.89337100	-2.09992600
C	-7.29925600	7.30660700	-3.79544500
H	-7.35010300	6.38269100	-4.39019300
H	-6.81399500	8.08038200	-4.41094100
H	-8.34645700	7.61425400	-3.63907100
C	-4.88423600	7.67827300	-0.77218700
H	-4.83361600	8.60213200	-0.17733300
H	-3.83697100	7.37082400	-0.92851000
H	-5.36941400	6.90435600	-0.15681700
C	-6.24094100	3.50471300	-3.35716900
H	-6.28162500	4.43595800	-3.93351200
H	-7.21929100	3.01573500	-3.43952300
H	-5.48793400	2.84912600	-3.81434400
C	-4.52338200	4.51479700	-1.85656100
H	-3.74357800	3.83778000	-2.22896100
H	-4.26418000	4.79854200	-0.82967500
H	-4.52118300	5.41876500	-2.47269600
C	-7.05328100	2.04345900	1.14666400
H	-6.33740400	2.69151900	1.65971800
H	-6.68784900	1.01362600	1.21765400
H	-8.01648500	2.09625500	1.66889400
C	-8.13806100	1.41597200	-0.98451100
H	-8.23071500	1.57225300	-2.06307400
H	-9.13478300	1.47200200	-0.53260100
H	-7.75209200	0.40394100	-0.82202700
C	-6.30577500	11.17438000	-2.67002200
N	-4.47359300	11.17149300	-4.10385500
C	-6.34178200	12.44793200	-3.53948000
C	-4.98429700	12.55837700	-4.24423100
H	-6.56659600	13.34614100	-2.95175400
H	-7.13271900	12.34381500	-4.29461900
C	-5.94259800	11.48035500	-1.21055700
H	-4.96430300	11.96945000	-1.12829200

H	-5.90179600	10.54919600	-0.63408400
H	-6.69565500	12.13592500	-0.75343900
C	-7.66014500	10.46993300	-2.71094000
H	-7.66226100	9.56607300	-2.09464900
H	-7.91936000	10.18599400	-3.73777000
H	-8.43998200	11.14696100	-2.33863200
C	-4.04578600	13.56898200	-3.58350300
H	-3.95287200	13.41265900	-2.50496200
H	-4.43197700	14.58094600	-3.74587500
H	-3.04914900	13.51315200	-4.03561700
C	-5.13057800	12.94110500	-5.71458500
H	-5.84627800	12.29277600	-6.22755700
H	-4.16736800	12.88851900	-6.23682100
H	-5.49630000	13.97082900	-5.78569000
B	-4.82097100	8.90024300	-3.03672500
B	-7.36250200	6.08462900	-1.53096200
C	-5.17664200	10.35932200	-3.27808600
C	-8.90873200	4.23636800	0.18708700
C	-10.13968600	4.12210000	-0.48044900
C	-8.81937700	4.82315500	1.45943200
C	-11.29614800	4.48348500	0.21094800
C	-10.00364000	5.16721300	2.11044700
C	-11.23526100	4.97458200	1.50523700
H	-12.25844500	4.40037500	-0.28940600
H	-12.14804300	5.24427900	2.02897800
H	-9.95226000	5.61919100	3.09854600
C	-7.49522000	5.21475500	2.09193700
C	-7.33044800	4.65182200	3.50409100
H	-7.45653200	3.56534300	3.53897400
H	-8.06892600	5.09133200	4.18543100
H	-6.33987700	4.89630600	3.90325400
C	-7.38277800	6.74323900	2.12866400
H	-6.68081400	4.84261600	1.45511300
H	-6.40700400	7.04752700	2.52499200

H	-8.15738800	7.17034700	2.77858300
H	-7.50181600	7.17689100	1.13027500
C	-10.25270600	3.74978400	-1.94933300
C	-11.24389100	2.61265000	-2.20011200
H	-11.24471900	2.33412800	-3.25970800
H	-12.26559600	2.92259700	-1.94997800
H	-11.01847600	1.71734700	-1.61323900
C	-10.67170500	4.97898900	-2.76340300
H	-9.26214100	3.44710700	-2.30710700
H	-10.74551200	4.72459400	-3.82694000
H	-9.95369500	5.79796100	-2.65179700
H	-11.65490400	5.34139600	-2.43680400
C	-3.27494700	10.74855200	-4.75491000
C	-2.04388000	10.86316800	-4.08766200
C	-2.18030000	9.81775900	-6.67841800
C	-0.94858000	10.01074900	-6.07351600
C	-0.88749300	10.50198700	-4.77929200
H	-0.03586100	9.74122400	-6.59745500
H	0.07490700	10.58536100	-4.27917600
C	-1.93071700	11.23552500	-2.61880500
C	-1.51097200	10.00642400	-1.80493600
H	-2.22846400	9.18702600	-1.91673500
H	-1.43732600	10.26062200	-0.74134400
H	-0.52755300	9.64470000	-2.13162600
C	-0.93990400	12.37301300	-2.36818200
H	-2.92132400	11.53777600	-2.26080600
H	-0.93871500	12.65126500	-1.30851600
H	-1.16594200	13.26837600	-2.95471900
H	0.08181200	12.06352700	-2.61885200
C	-3.36449000	10.16161000	-6.02716000
C	-4.68873100	9.76976100	-6.65933400
C	-4.80083800	8.24128100	-6.69624800
H	-5.77685900	7.93688600	-7.09188900
H	-4.68095900	7.80750100	-5.69800900

H	-4.02664000	7.81444500	-7.34683300
C	-4.85405200	10.33292200	-8.07133600
H	-5.50306300	10.14160700	-6.02222000
H	-4.72892700	11.41952400	-8.10591700
H	-5.84443900	10.08769900	-8.47050600
H	-4.11522800	9.89424600	-8.75283700
H	-2.23179200	9.36568200	-7.66646600
H	-8.37512600	6.48905800	-1.01980700
H	-3.80833700	8.49584000	-3.54789600

29. CAAC_Full_CH₃_H (planar)-singlet:

C	-5.60998500	3.52780000	-1.85468000
N	-7.49094800	3.84971900	-0.53650900
C	-5.77977000	2.32387600	-0.90113500
C	-7.18441000	2.41064800	-0.31244400
H	-5.04626900	2.39659700	-0.08719500
H	-5.60756900	1.36933500	-1.41238700
C	-6.70483600	4.50450900	-1.42309900
C	-6.33191800	7.02897000	-2.59411500
C	-6.82593800	8.38328100	-2.63549800
C	-5.84865600	3.06533300	-3.30159100
H	-5.86856300	3.88884700	-4.01644800

H	-6.80798800	2.54274600	-3.38608900
H	-5.05937500	2.36396000	-3.60129400
C	-4.19767900	4.08744300	-1.64915000
H	-3.46421700	3.29377500	-1.84419300
H	-4.07629500	4.40749900	-0.60785000
H	-3.95639800	4.93701700	-2.28484500
C	-7.20071300	2.03712600	1.16741000
H	-6.44044600	2.57957300	1.73476700
H	-6.98513900	0.96723700	1.25796100
H	-8.18271800	2.21985600	1.61889700
C	-8.20623700	1.51651500	-1.01922300
H	-8.25527900	1.69326700	-2.09634300
H	-9.20375700	1.67686500	-0.59504300
H	-7.93748900	0.46710700	-0.85785400
C	-7.54843600	11.88403100	-3.37460000
N	-5.66737200	11.56283200	-4.69281500
C	-7.37921100	13.08795900	-4.32823800
C	-5.97454800	13.00174100	-4.91699200
H	-7.55174400	14.04246800	-3.81704000
H	-8.11273400	13.01490100	-5.14213000
C	-7.30964000	12.34692700	-1.92784100
H	-7.29007500	11.52380100	-1.21255800
H	-8.09870900	13.04869600	-1.62849200
H	-6.35015000	12.86924300	-1.84353500
C	-8.96044700	11.32357400	-3.57979500
H	-9.20056100	10.47310100	-2.94485700
H	-9.08225300	11.00451000	-4.62134600
H	-9.69443400	12.11643300	-3.38342100
C	-4.95302700	13.89639800	-4.21041500
H	-4.90378800	13.71982900	-3.13327700
H	-5.22221200	14.94567400	-4.37190800
H	-3.95547900	13.73639400	-4.63466900
C	-5.95851600	13.37514200	-6.39688300
H	-6.71858500	12.83231700	-6.96414200

H	-4.97645900	13.19282400	-6.84842300
H	-6.17457100	14.44492900	-6.48749900
B	-6.17618800	9.40894400	-3.53252000
B	-6.98164500	6.00328600	-1.69710500
C	-6.45327200	10.90770800	-3.80629100
C	-8.69353200	4.38849200	0.02901100
C	-9.88171100	4.39125600	-0.72047700
C	-8.64623600	4.91862200	1.32750000
C	-11.04863000	4.82528700	-0.09071200
C	-9.83872700	5.34419100	1.91060400
C	-11.03767400	5.27436200	1.21979800
H	-11.97854200	4.83354100	-0.65476700
H	-11.95929700	5.60453000	1.69058800
H	-9.81697900	5.76184200	2.91455800
C	-7.34082600	5.17162200	2.06099100
C	-7.35103300	4.62285200	3.48848800
H	-7.63567500	3.56687800	3.53094900
H	-8.05715000	5.18010700	4.11547600
H	-6.36265300	4.73134100	3.94856200
C	-7.05472200	6.67657600	2.08846000
H	-6.52763900	4.69777800	1.49712500
H	-6.11392900	6.87824900	2.61345700
H	-7.85581500	7.20946300	2.61658500
H	-6.98072300	7.08334800	1.07559300
C	-9.93786100	4.07452200	-2.20638300
C	-10.98630100	3.01463700	-2.55011500
H	-10.95803400	2.78694200	-3.62146700
H	-11.99645600	3.37838600	-2.32743900
H	-10.84376200	2.08005400	-2.00008900
C	-10.24161100	5.35646600	-2.99191500
H	-8.95137300	3.71903700	-2.53018600
H	-10.25511300	5.14789700	-4.06770800
H	-9.49488800	6.13380200	-2.80160600
H	-11.22882700	5.74828000	-2.71553000

C	-4.46459600	11.02449600	-5.25833100
C	-3.27644600	11.02217600	-4.50880500
C	-3.31899500	10.06913800	-7.13984700
C	-2.12010100	10.13939300	-6.44899200
C	-2.10935100	10.58851400	-5.13849600
H	-1.19834700	9.80952400	-6.91973400
H	-1.17946100	10.58059600	-4.57440100
C	-3.22048900	11.33902900	-3.02292100
C	-2.91642500	10.05721500	-2.23730200
H	-3.66289400	9.27964600	-2.42767100
H	-2.90310100	10.26581800	-1.16151400
H	-1.92906500	9.66568800	-2.51357600
C	-2.17240600	12.39926900	-2.67920700
H	-4.20710100	11.69425100	-2.69921400
H	-2.20078600	12.62702100	-1.60787000
H	-2.31525300	13.33376900	-3.22929800
H	-1.16212100	12.03585100	-2.90183100
C	-4.51166200	10.49430200	-6.55680700
C	-5.81693900	10.24082100	-7.29036900
C	-6.10243700	8.73575600	-7.31797600
H	-7.04314400	8.53376000	-7.84300400
H	-6.17628400	8.32886800	-6.30514700
H	-5.30112900	8.20323400	-7.84614100
C	-5.80689000	10.78968000	-8.71783500
H	-6.63033900	10.71429200	-6.72649700
H	-5.52264800	11.84576300	-8.76024500
H	-6.79521100	10.68083500	-9.17795100
H	-5.10053700	10.23272000	-9.34482100
H	-3.34055600	9.65145400	-8.14379200
H	-7.89561600	6.36452500	-1.02307400
H	-5.26206000	9.04787100	-4.20642200
C	-5.27799900	6.66034300	-3.61461500
H	-5.55780400	6.98548500	-4.62175400
H	-4.30592900	7.13247800	-3.40939400

H	-5.11976300	5.58834500	-3.66444000
C	-7.87974900	8.75204400	-1.61489300
H	-8.85232200	8.28117700	-1.82078900
H	-7.60052900	8.42579000	-0.60797900
H	-8.03690100	9.82414300	-1.56416400

30. CAAC_Full_CH₃_H (planar)-triplet:

C	-5.64157700	3.48752300	-1.89760300
N	-7.67505200	3.73729900	-0.78767000
C	-6.22749300	2.09982300	-1.55512400
C	-7.33041500	2.31730400	-0.52332000
H	-5.45877800	1.40454100	-1.19720800
H	-6.67149300	1.66265500	-2.45993500
C	-6.74885000	4.45937100	-1.49061000
C	-6.29529900	7.07325900	-2.55705500
C	-6.86279000	8.33933400	-2.67226500
C	-5.34258400	3.51861300	-3.39986200
H	-4.89643800	4.45299800	-3.73802700
H	-6.26725700	3.36380000	-3.96767500
H	-4.65145400	2.70329200	-3.65206300
C	-4.36521000	3.71982100	-1.07187600
H	-3.60526500	2.97584400	-1.34506000

H	-4.56444800	3.61559900	-0.00025300
H	-3.93709500	4.71218500	-1.22286200
C	-6.87589400	2.11795700	0.92622200
H	-6.01266900	2.73068300	1.19453300
H	-6.60839200	1.06703100	1.08044200
H	-7.69696400	2.35908200	1.61134600
C	-8.51285700	1.37922900	-0.75452500
H	-8.85174500	1.39428400	-1.79335600
H	-9.35606900	1.62820300	-0.09958800
H	-8.19937500	0.35646400	-0.51988600
C	-7.51660700	11.92510200	-3.33154500
N	-5.48318500	11.67537500	-4.44160000
C	-6.93063000	13.31282000	-3.67381500
C	-5.82777600	13.09542200	-4.70571100
H	-6.48655000	13.74979800	-2.76895100
H	-7.69928900	14.00824100	-4.03157400
C	-7.81564300	11.89381400	-1.82930700
H	-6.89095800	12.04842200	-1.26146000
H	-8.26197100	10.95945900	-1.49129500
H	-8.50666000	12.70921400	-1.57701800
C	-8.79297100	11.69296200	-4.15731200
H	-9.22129600	10.70071700	-4.00619300
H	-8.59365300	11.79697800	-5.22894000
H	-9.55278100	12.43712500	-3.88426400
C	-4.64529400	14.03340100	-4.47436800
H	-4.30635800	14.01804500	-3.43555300
H	-4.95876700	15.05623900	-4.70871000
H	-3.80213100	13.78457600	-5.12942400
C	-6.28234600	13.29500900	-6.15520500
H	-7.14569600	12.68245700	-6.42352000
H	-5.46136100	13.05383000	-6.84041200
H	-6.54969500	14.34599500	-6.30928900
B	-6.10084300	9.47515900	-3.42366500
B	-7.05729700	5.93747800	-1.80564200

C	-6.40935800	10.95326200	-3.73866300
C	-8.79862100	4.31407400	-0.11565600
C	-10.06345100	4.22455900	-0.71733000
C	-8.61998500	4.97819700	1.11030400
C	-11.16744000	4.70576000	-0.01467800
C	-9.75539000	5.44089700	1.77564800
C	-11.02184700	5.28636800	1.23477700
H	-12.15288200	4.64579100	-0.47119200
H	-11.89252900	5.65113000	1.77233500
H	-9.63549100	5.95532400	2.72653300
C	-7.25481600	5.32681200	1.68053700
C	-7.08203700	4.86670900	3.12912200
H	-7.25414000	3.79370800	3.25485000
H	-7.77750700	5.39339500	3.79340800
H	-6.06966600	5.09305000	3.48181700
C	-7.03623500	6.84295600	1.60074400
H	-6.48320600	4.85212200	1.06203400
H	-6.04472700	7.10554000	1.98674100
H	-7.78189400	7.36907900	2.21045000
H	-7.11376500	7.21316400	0.57253600
C	-10.25107900	3.75510300	-2.14897900
C	-11.34708900	2.69798600	-2.28612500
H	-11.38674600	2.31646300	-3.31243300
H	-12.33265300	3.12553900	-2.06649000
H	-11.19784500	1.85005200	-1.61035500
C	-10.57625500	4.95786700	-3.03993700
H	-9.30010600	3.33874000	-2.50281200
H	-10.71386900	4.64096800	-4.08015100
H	-9.77329100	5.70079300	-3.00831600
H	-11.50377700	5.44271500	-2.70943300
C	-4.35970900	11.09864200	-5.11381600
C	-3.09477200	11.18807700	-4.51233900
C	-3.40322300	9.97212800	-7.00546100
C	-2.13667600	10.12663600	-6.46480200

C	-1.99089200	10.70703900	-5.21527300
H	-1.26607300	9.76200200	-7.00257400
H	-1.00537400	10.76696400	-4.75891800
C	-2.90687900	11.65722000	-3.08061900
C	-2.58120800	10.45429200	-2.19006000
H	-3.38389100	9.71107900	-2.22185100
H	-2.44360700	10.77091800	-1.14976100
H	-1.65353700	9.96988900	-2.52079700
C	-1.81100100	12.71448000	-2.94345700
H	-3.85784900	12.07331200	-2.72644400
H	-1.77116800	13.09574600	-1.91706000
H	-1.96049800	13.56256500	-3.61897500
H	-0.82543000	12.28711300	-3.16341800
C	-4.53852600	10.43468500	-6.33984300
C	-5.90377900	10.08607900	-6.90987100
C	-6.12225400	8.56991700	-6.83011800
H	-7.11385000	8.30728900	-7.21585900
H	-6.04440600	8.19964800	-5.80195200
H	-5.37672200	8.04388500	-7.44005800
C	-6.07684700	10.54627400	-8.35839000
H	-6.67529700	10.56070000	-6.29120400
H	-5.90481300	11.61929300	-8.48406900
H	-7.08927600	10.31991800	-8.71090800
H	-5.38148600	10.01966600	-9.02285100
H	-3.52327600	9.45783500	-7.95640000
H	-8.10848600	6.24235100	-1.33799100
H	-5.04954500	9.17043600	-3.89118100
C	-4.84810800	6.88156600	-2.96819700
H	-4.72430900	6.81490900	-4.05958300
H	-4.20576600	7.70134700	-2.63827800
H	-4.43547800	5.97147300	-2.54083800
C	-8.31000700	8.53094100	-2.26115500
H	-8.95228300	7.71109900	-2.59102600
H	-8.43384600	8.59764700	-1.16977300

H -8.72268500 9.44098700 -2.68857700

31. CAAC_Full_H_H (fully optimized)-singlet:

C -5.66987200 3.88555200 -1.76743700
N -7.56027700 3.93962100 -0.42291800
C -5.74621200 2.57919900 -0.94881400
C -7.14827700 2.51137300 -0.33783200
H -5.00300800 2.61571000 -0.14058700
H -5.52494900 1.69530000 -1.55868300
C -6.79013900 4.73371100 -1.18418300
C -6.40746600 7.04224900 -2.46165600
C -6.74561400 8.37318100 -2.75989900
C -5.95002200 3.62906400 -3.25656000
H -5.92850900 4.56276100 -3.82462500
H -6.93413300 3.17208200 -3.41011700
H -5.19222000 2.94905000 -3.66738800
C -4.28792400 4.51987800 -1.60252300
H -3.51568200 3.80172400 -1.90771000
H -4.10815100 4.78922800 -0.55573400
H -4.17384600 5.42204800 -2.20574800
C -7.12537200 2.01422200 1.10437900
H -6.39826700 2.55902300 1.71213900

H	-6.84323500	0.95617600	1.11045700
H	-8.11439600	2.09994100	1.57018900
C	-8.11470800	1.62146300	-1.12088800
H	-8.15788400	1.87525500	-2.18319100
H	-9.12359800	1.70111200	-0.70046400
H	-7.79603300	0.57745400	-1.03346200
C	-7.48320000	11.52992600	-3.45385000
N	-5.59276800	11.47595600	-4.79833000
C	-7.40693000	12.83624400	-4.27253500
C	-6.00484000	12.90417100	-4.88344600
H	-7.62833700	13.72016200	-3.66274500
H	-8.15008200	12.79958400	-5.08080700
C	-7.20290300	11.78643000	-1.96476000
H	-7.22447000	10.85274600	-1.39667300
H	-7.96059800	12.46653200	-1.55388100
H	-6.21872900	12.24329800	-1.81129900
C	-8.86517600	10.89562400	-3.61862900
H	-8.97925200	9.99350200	-3.01533500
H	-9.04503800	10.62621200	-4.66538200
H	-9.63737200	11.61382700	-3.31343800
C	-5.03847300	13.79412700	-4.10034600
H	-4.99547100	13.54046100	-3.03800900
H	-5.35704800	14.83815100	-4.18794800
H	-4.02952200	13.71434800	-4.52061800
C	-6.02770200	13.40135900	-6.32565900
H	-6.75483900	12.85666100	-6.93347200
H	-5.03867500	13.31559500	-6.79145200
H	-6.30974400	14.45943100	-6.33168900
B	-6.06259300	9.19614400	-3.80169000
B	-7.09048900	6.21932900	-1.41983400
C	-6.36295800	10.68177900	-4.03720300
C	-8.78463100	4.38340300	0.17414700
C	-9.96272000	4.40479000	-0.59141400
C	-8.76763800	4.82884300	1.50516400

C	-11.14965600	4.76211700	0.04903900
C	-9.98008200	5.17877400	2.09810000
C	-11.16755800	5.12063200	1.38695100
H	-12.07240300	4.78180900	-0.52630800
H	-12.10431200	5.39111800	1.86599300
H	-9.98355900	5.52769800	3.12821400
C	-7.48158600	5.06990300	2.27529600
C	-7.47969000	4.39056600	3.64525200
H	-7.69338600	3.31898400	3.58290300
H	-8.23269800	4.83939100	4.30391100
H	-6.50857800	4.51903300	4.13600200
C	-7.26539900	6.57762200	2.44339000
H	-6.64339900	4.68536300	1.68162600
H	-6.32731200	6.77275600	2.97543200
H	-8.08131500	7.01804600	3.03062200
H	-7.22938000	7.08447800	1.47497100
C	-9.99231700	4.17809100	-2.09408100
C	-10.99485000	3.10068900	-2.51165800
H	-10.94833600	2.93845000	-3.59420300
H	-12.02033600	3.41123600	-2.27845400
H	-10.82037000	2.14117500	-2.01632400
C	-10.33592300	5.49262200	-2.80466500
H	-8.98995200	3.88113800	-2.42511700
H	-10.32620500	5.34980100	-3.89103800
H	-9.62349600	6.28412900	-2.55501300
H	-11.34143900	5.82887700	-2.52109400
C	-4.36849000	11.03218800	-5.39554500
C	-3.19031000	11.01082000	-4.63015700
C	-3.17336800	10.23659600	-7.31960700
C	-1.98578900	10.29469900	-6.60861900
C	-2.00348400	10.65334500	-5.27073600
H	-1.04912100	10.02408700	-7.08775600
H	-1.08065900	10.63365100	-4.69551800
C	-3.16057500	11.23768400	-3.12752200

C	-2.81699300	9.92321100	-2.41682900
H	-3.52937900	9.13166700	-2.66648200
H	-2.82678900	10.06610000	-1.33046700
H	-1.81144500	9.58696600	-2.70030700
C	-2.15793400	12.31505900	-2.71014400
H	-4.16290000	11.53473900	-2.79645100
H	-2.20431900	12.47738500	-1.62760700
H	-2.33240200	13.27454800	-3.20553300
H	-1.13249800	12.00441900	-2.94343300
C	-4.38569800	10.58664900	-6.72651700
C	-5.67187400	10.34573800	-7.49646600
C	-5.88822400	8.83806900	-7.66474800
H	-6.82623400	8.64317100	-8.19703100
H	-5.92454100	8.33110700	-6.69639400
H	-5.07225800	8.39758100	-8.25185500
C	-5.67399300	11.02514700	-8.86636200
H	-6.50997400	10.73024100	-6.90265900
H	-5.45980800	12.09663500	-8.80406600
H	-6.64537600	10.89709200	-9.35669900
H	-4.92145300	10.57599300	-9.52533700
H	-3.17007600	9.88759000	-8.34969700
H	-7.98052200	6.71389200	-0.77759700
H	-5.17256300	8.70162600	-4.44397600
H	-5.61493700	6.64293800	-3.10762800
H	-7.53813400	8.77248800	-2.11391500

32. CAAC_Full_H_H (fully optimized)-triplet:

C	-5.70092700	3.84271200	-1.76918900
N	-7.57715600	3.91285000	-0.39071400
C	-5.76992700	2.54690000	-0.93354400
C	-7.16636300	2.48781800	-0.30418100
H	-5.01772100	2.59295000	-0.13417300
H	-5.55728500	1.65375900	-1.53329000
C	-6.80621200	4.70053200	-1.17932600
C	-6.41550900	7.05221000	-2.50439100
C	-6.73802500	8.36317900	-2.71785500
C	-5.99729400	3.57785500	-3.25273300
H	-6.01018100	4.51463300	-3.81879200
H	-6.97148000	3.09559500	-3.39050300
H	-5.22938200	2.92232100	-3.68459900
C	-4.31963500	4.48425700	-1.62907800
H	-3.54473900	3.78233800	-1.96349300
H	-4.11812900	4.74238800	-0.58323200
H	-4.22934900	5.39577900	-2.22437000
C	-7.12758600	1.99941000	1.14114100
H	-6.39439900	2.54896600	1.73750500
H	-6.84790900	0.94073900	1.15475500
H	-8.11227900	2.09174200	1.61526700
C	-8.14038700	1.58940900	-1.06996200
H	-8.18715000	1.82704400	-2.13582400

H	-9.14756700	1.68022700	-0.64697400
H	-7.82688700	0.54489200	-0.96892200
C	-7.45265700	11.57261200	-3.45296200
N	-5.57602700	11.50283900	-4.83091400
C	-7.38348100	12.86854200	-4.28840300
C	-5.98676000	12.92791400	-4.91706500
H	-7.59664700	13.76158800	-3.68870500
H	-8.13524200	12.82236600	-5.08818900
C	-7.15679600	11.83723100	-1.96926700
H	-7.14437400	10.90038900	-1.40331100
H	-7.92472000	12.49289800	-1.53762600
H	-6.18254500	12.31921500	-1.83101900
C	-8.83386900	10.93101400	-3.59362300
H	-8.92429600	10.01939400	-2.99849700
H	-9.03499700	10.67302700	-4.63957800
H	-9.60892000	11.63283600	-3.25936200
C	-5.01311400	13.82604800	-4.15047500
H	-4.96670300	13.58787400	-3.08472400
H	-5.32674300	14.87056600	-4.25109100
H	-4.00576000	13.73561700	-4.57315000
C	-6.02481700	13.41689400	-6.36221500
H	-6.75820000	12.86801800	-6.95895900
H	-5.04006900	13.32415700	-6.83616900
H	-6.30389600	14.47572400	-6.37553800
B	-6.05565700	9.23815700	-3.79020000
B	-7.09777600	6.17728400	-1.43194500
C	-6.34715800	10.71495200	-4.04268000
C	-8.79828300	4.36939000	0.19517500
C	-9.97230300	4.40053600	-0.57753400
C	-8.78618300	4.82979100	1.52156700
C	-11.15839900	4.78311100	0.04937100
C	-9.99762300	5.20239700	2.10316200
C	-11.18060100	5.15544100	1.38382500
H	-12.07709600	4.80908600	-0.53236100

H	-12.11673000	5.44436200	1.85327900
H	-10.00349600	5.56058700	3.13023300
C	-7.50088500	5.06303800	2.29484400
C	-7.50847100	4.39222700	3.66866700
H	-7.72316400	3.32066000	3.61044700
H	-8.26515400	4.84565000	4.32008600
H	-6.54016500	4.52151300	4.16483000
C	-7.27130200	6.56960600	2.45381000
H	-6.66608200	4.66727500	1.70414700
H	-6.33156000	6.76108000	2.98427800
H	-8.08338000	7.02265500	3.03673700
H	-7.23102800	7.07014800	1.48197700
C	-9.99352800	4.14808600	-2.07590700
C	-11.01420500	3.08374900	-2.48202100
H	-10.95817600	2.89482200	-3.55981800
H	-12.03589500	3.41987800	-2.26842100
H	-10.86417000	2.13320300	-1.96172600
C	-10.29980000	5.45545900	-2.81554400
H	-8.99497300	3.82245200	-2.38972000
H	-10.29572200	5.28959400	-3.89874300
H	-9.56603200	6.23401800	-2.58432800
H	-11.29371900	5.82945400	-2.53846800
C	-4.35471700	11.04639000	-5.41650700
C	-3.18100500	11.01497800	-4.64332500
C	-3.15464100	10.21395600	-7.32423400
C	-1.97194900	10.26068700	-6.60441500
C	-1.99466200	10.63256100	-5.26985000
H	-1.03564600	9.97191800	-7.07361600
H	-1.07620300	10.60634300	-4.68775500
C	-3.16043100	11.26692100	-3.14485900
C	-2.85455600	9.95929000	-2.40551200
H	-3.58836100	9.18090200	-2.63718600
H	-2.85894100	10.12484100	-1.32226600
H	-1.86060400	9.58524400	-2.68240100

C	-2.13989000	12.33109100	-2.73793300
H	-4.15909600	11.59248900	-2.83134300
H	-2.19648100	12.51978300	-1.66012600
H	-2.28956100	13.28176400	-3.25811000
H	-1.11811200	11.99493800	-2.95105200
C	-4.36634300	10.58635200	-6.74302900
C	-5.65138000	10.35316000	-7.51682800
C	-5.88102300	8.84659600	-7.67554800
H	-6.82094000	8.65502800	-8.20565100
H	-5.92097200	8.34622600	-6.70361000
H	-5.06914700	8.39343800	-8.25866800
C	-5.64306200	11.02395800	-8.89064800
H	-6.48633500	10.74910900	-6.92644800
H	-5.42856000	12.09553500	-8.83228800
H	-6.61104700	10.89463800	-9.38740500
H	-4.88596000	10.57064600	-9.54165500
H	-3.14827600	9.85608200	-8.35140100
H	-7.96477600	6.69375600	-0.77947100
H	-5.18862000	8.72169600	-4.44262100
H	-5.65075600	6.65707300	-3.18612000
H	-7.50276900	8.75831200	-2.03611800

33. CAAC_Full_H_H (twisted)-singlet:

C	-5.94134400	3.83266000	-1.84238900
N	-7.88958100	3.79851600	-0.56874800
C	-5.94254900	2.57568400	-0.94862900
C	-7.35322400	2.42788200	-0.36824700
H	-5.22913300	2.72354500	-0.12619200
H	-5.63093300	1.67706000	-1.49471700
C	-7.14322000	4.61885000	-1.34767000
C	-6.68262700	7.01621400	-2.57443500
C	-5.71412400	7.85942400	-2.17031100
C	-6.16669300	3.49801600	-3.32331800
H	-6.21587500	4.42369100	-3.90938400
H	-7.10501000	2.95193700	-3.47900800
H	-5.34274100	2.88534400	-3.71244900
C	-4.61368200	4.57649200	-1.69342900
H	-3.78253400	3.88254200	-1.87621900
H	-4.50588800	4.97972700	-0.67875200
H	-4.53208200	5.40743100	-2.39681600
C	-7.33141000	2.04902800	1.11085200
H	-6.67068700	2.70244300	1.68670900
H	-6.96251100	1.02316200	1.21361400
H	-8.33729900	2.08952200	1.54655200
C	-8.20132600	1.38921500	-1.10357900
H	-8.21870900	1.54956200	-2.18512200
H	-9.23033600	1.40765400	-0.72762100
H	-7.79362800	0.39017200	-0.91585300
C	-6.45618300	11.04241400	-2.90328300
N	-4.51080600	11.07518300	-4.18117100

C	-6.45703500	12.29844200	-3.79835800
C	-5.04781200	12.44543100	-4.38251400
H	-6.76715200	13.19768300	-3.25242800
H	-7.17256700	12.14979800	-4.61882200
C	-6.22646400	11.37860100	-1.42337900
H	-6.17648000	10.45358400	-0.83635100
H	-7.04870200	11.99255000	-1.03263400
H	-5.28711300	11.92389000	-1.27105600
C	-7.78442600	10.29879700	-3.04790500
H	-7.86442100	9.46860300	-2.34345400
H	-7.89493000	9.89447600	-4.06187400
H	-8.61492200	10.99315700	-2.86372300
C	-4.19792400	13.48524800	-3.65092300
H	-4.17793900	13.32654200	-2.56918300
H	-4.60603400	14.48401700	-3.83920900
H	-3.16983900	13.46614900	-4.02933500
C	-5.07350700	12.82196900	-5.86216100
H	-5.73593300	12.16777800	-6.43515300
H	-4.06884400	12.78060400	-6.30059400
H	-5.44254900	13.84772300	-5.96552200
B	-4.87142800	8.82191700	-3.06745600
B	-7.52666100	6.05286000	-1.67950300
C	-5.25581600	10.25543300	-3.40038300
C	-9.14167400	4.19924700	-0.01043500
C	-10.32193800	4.04402700	-0.75684900
C	-9.15347200	4.80099100	1.25805400
C	-11.53052400	4.38798000	-0.15045500
C	-10.38595900	5.13395700	1.81869700
C	-11.56890500	4.90523800	1.13408700
H	-12.45467000	4.27142500	-0.71227800
H	-12.52085500	5.16450000	1.58881400
H	-10.41200200	5.60151100	2.80047000
C	-7.88340000	5.20318600	1.98674600
C	-7.84311100	4.67419300	3.42075600

H	-7.99782400	3.59148900	3.46852000
H	-8.61969600	5.14591100	4.03453400
H	-6.87999400	4.90503300	3.88929600
C	-7.75309500	6.72972200	1.98796800
H	-7.02376100	4.80515800	1.43342600
H	-6.83478500	7.03585500	2.50194400
H	-8.60076100	7.18897100	2.51266000
H	-7.72929400	7.12807700	0.96792800
C	-10.33139200	3.64918200	-2.22395200
C	-11.25715300	2.46786000	-2.51788100
H	-11.19263300	2.18682300	-3.57488100
H	-12.30239500	2.73492300	-2.32086500
H	-11.02462100	1.58445300	-1.91657300
C	-10.76078800	4.84989400	-3.07449100
H	-9.30824200	3.38844200	-2.51952500
H	-10.73707300	4.59174800	-4.13931000
H	-10.10770800	5.71160000	-2.91006200
H	-11.78707500	5.14922600	-2.82651900
C	-3.26161000	10.67251400	-4.74447500
C	-2.07773000	10.82902700	-4.00419500
C	-2.02679600	9.73199500	-6.57699800
C	-0.84042000	9.96183100	-5.89869700
C	-0.87225400	10.48267700	-4.61543900
H	0.10916600	9.70069700	-6.35728100
H	0.05465600	10.60015300	-4.05837900
C	-2.06127500	11.22746100	-2.53814500
C	-1.62918300	10.02837900	-1.68668300
H	-2.28383300	9.16693600	-1.84613700
H	-1.64782300	10.28906800	-0.62238200
H	-0.60432400	9.72746700	-1.93861500
C	-1.13307900	12.40861100	-2.25131600
H	-3.08286700	11.48989000	-2.23865100
H	-1.19281300	12.69262300	-1.19483400
H	-1.36720700	13.29061800	-2.85407300

H	-0.08895500	12.13991700	-2.45202400
C	-3.25636500	10.06729600	-6.01139200
C	-4.53014100	9.66434600	-6.73321300
C	-4.66197300	8.13793900	-6.73021000
H	-5.58270500	7.83155700	-7.23968800
H	-4.68204500	7.74200400	-5.70912800
H	-3.81693900	7.67655200	-7.25726700
C	-4.57635700	10.18990100	-8.16833100
H	-5.38696700	10.06450600	-6.17702500
H	-4.42039700	11.27228200	-8.21943400
H	-5.54191300	9.95919900	-8.63188900
H	-3.80320800	9.71567300	-8.78450700
H	-2.00574800	9.26175800	-7.55760800
H	-8.58389500	6.44814500	-1.26312300
H	-3.81477800	8.42631200	-3.48498800
H	-7.00327300	7.13620000	-3.62594600
H	-5.39306200	7.73994400	-1.11898400

34. CAAC_Full_H_H (twisted)-triplet:

C	-5.93896200	3.83482600	-1.83950300
N	-7.88674700	3.80117600	-0.56474300
C	-5.94064800	2.57767000	-0.94594200
C	-7.35154100	2.42985600	-0.36624800
H	-5.22766900	2.72537400	-0.12309000
H	-5.62876400	1.67912400	-1.49200200
C	-7.14134900	4.62088000	-1.34561600
C	-6.68296800	7.01551300	-2.57825000
C	-5.71586200	7.85886700	-2.16966700
C	-6.16242500	3.50074500	-3.32080200
H	-6.21127600	4.42669800	-3.90645300
H	-7.10029800	2.95435800	-3.47797400
H	-5.33769800	2.88870300	-3.70931200
C	-4.61144100	4.57871800	-1.68877800
H	-3.78004000	3.88472000	-1.87027900
H	-4.50496700	4.98196500	-0.67396100
H	-4.52881000	5.40959100	-2.39211600
C	-7.33074700	2.04810300	1.11210800
H	-6.66926400	2.69929400	1.68959900
H	-6.96349100	1.02146400	1.21294800
H	-8.33674300	2.08921700	1.54750500
C	-8.20016600	1.39318500	-1.10387700
H	-8.21740400	1.55586700	-2.18506500
H	-9.22920500	1.41148200	-0.72796600
H	-7.79309900	0.39348300	-0.91826500
C	-6.46029800	11.03923100	-2.90889800
N	-4.51423000	11.07205500	-4.18621300
C	-6.45978700	12.29588900	-3.80315400
C	-5.04978000	12.44316900	-4.38516900
H	-6.77068300	13.19478600	-3.25710800
H	-7.17408400	12.14783100	-4.62480300

C	-6.23425100	11.37413100	-1.42818000
H	-6.18490500	10.44853500	-0.84201300
H	-7.05797600	11.98688900	-1.03867500
H	-5.29577500	11.92006800	-1.27297400
C	-7.78818200	10.29550400	-3.05712500
H	-7.86989200	9.46502700	-2.35321200
H	-7.89624800	9.89168400	-4.07155500
H	-8.61918900	10.98974800	-2.87476800
C	-4.20000000	13.48048100	-3.64979300
H	-4.18103500	13.31865400	-2.56850600
H	-4.60737500	14.48002700	-3.83557200
H	-3.17156500	13.46187100	-4.02731300
C	-5.07295100	12.82358300	-5.86384600
H	-5.73550700	12.17197000	-6.43961900
H	-4.06770900	12.78193300	-6.30092600
H	-5.44026000	13.85017400	-5.96499200
B	-4.87273900	8.82049200	-3.06861900
B	-7.52688100	6.05337500	-1.68059900
C	-5.25883000	10.25269600	-3.40424300
C	-9.13905300	4.20165400	-0.00683400
C	-10.31887600	4.04919100	-0.75450400
C	-9.15134100	4.80039800	1.26307400
C	-11.52760800	4.39289900	-0.14822900
C	-10.38390500	5.13326200	1.82356000
C	-11.56652300	4.90725300	1.13745900
H	-12.45144400	4.27840400	-0.71098800
H	-12.51859600	5.16635700	1.59202100
H	-10.41028900	5.59861100	2.80637100
C	-7.88131600	5.19996900	1.99325200
C	-7.84255200	4.66900400	3.42654400
H	-7.99849100	3.58640000	3.47267100
H	-8.61897400	5.14073100	4.04052000
H	-6.87946800	4.89809200	3.89601300
C	-7.74913000	6.72632200	1.99639300

H	-7.02187400	4.80153200	1.43997400
H	-6.83089400	7.03080600	2.51148700
H	-8.59669900	7.18598100	2.52088100
H	-7.72416200	7.12573000	0.97681200
C	-10.32773400	3.65713400	-2.22237000
C	-11.25391900	2.47680700	-2.51896800
H	-11.18917400	2.19788000	-3.57651500
H	-12.29911000	2.74389900	-2.32172300
H	-11.02191500	1.59209900	-1.91937700
C	-10.75614300	4.85964000	-3.07086900
H	-9.30454900	3.39646700	-2.51794300
H	-10.73176400	4.60358600	-4.13617600
H	-10.10287600	5.72084400	-2.90432200
H	-11.78248700	5.15888600	-2.82302500
C	-3.26366700	10.67042300	-4.74714500
C	-2.08166300	10.82362000	-4.00314600
C	-2.02452300	9.73543400	-6.57965700
C	-0.83983400	9.96207500	-5.89733300
C	-0.87480300	10.47850400	-4.61237000
H	0.11081800	9.70187500	-6.35423600
H	0.05070500	10.59352100	-4.05246900
C	-2.06857700	11.21776800	-2.53588000
C	-1.63849800	10.01621000	-1.68688900
H	-2.29268000	9.15514200	-1.85048400
H	-1.65982200	10.27373700	-0.62187200
H	-0.61299900	9.71607100	-1.93714100
C	-1.14093700	12.39800600	-2.24352100
H	-3.09083100	11.47940500	-2.23790100
H	-1.20276500	12.67865900	-1.18625800
H	-1.37394600	13.28190300	-2.84392700
H	-0.09641900	12.12997300	-2.44304800
C	-3.25533200	10.06966200	-6.01615200
C	-4.52760000	9.66964900	-6.74219500
C	-4.66070600	8.14337000	-6.74277000

H	-5.58041300	7.83871800	-7.25513600
H	-4.68340300	7.74543700	-5.72254800
H	-3.81472500	7.68242400	-7.26869400
C	-4.56994300	10.19855100	-8.17615900
H	-5.38534300	10.06937000	-6.18718200
H	-4.41325900	11.28096500	-8.22428500
H	-5.53450400	9.96954100	-8.64262300
H	-3.79559300	9.72532700	-8.79159500
H	-2.00115200	9.26852600	-7.56180500
H	-8.57742300	6.45310200	-1.25184600
H	-3.82255400	8.42056200	-3.49804100
H	-6.99241800	7.12648500	-3.63336600
H	-5.40616100	7.74818500	-1.11466000

35. CAAC_Full_H_H (planar)-singlet:

C	-5.74416200	3.84245300	-1.85670600
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N	-7.61433700	3.90584500	-0.48309800
C	-5.79360800	2.55298900	-1.00777800
C	-7.17762000	2.48811800	-0.35891100
H	-5.02870100	2.60957700	-0.22153700
H	-5.58291800	1.65801500	-1.60523100
C	-6.88750800	4.68127500	-1.30445800
C	-6.42744600	7.03202300	-2.48778400
C	-6.73069400	8.38065500	-2.74154400
C	-6.01137300	3.55948000	-3.34205000
H	-6.01723500	4.49191700	-3.91494200
H	-6.98293100	3.07294400	-3.49087700
H	-5.23369900	2.89914500	-3.74752500
C	-4.36832600	4.49365300	-1.69153700
H	-3.59009100	3.75598900	-1.92779800
H	-4.21881700	4.82619500	-0.65823500
H	-4.22855900	5.35374100	-2.34662000
C	-7.11474200	2.04452000	1.09944700
H	-6.38262900	2.62231100	1.66973200
H	-6.81653800	0.99168600	1.13833600
H	-8.09402900	2.13402500	1.58479100
C	-8.14220400	1.55521400	-1.09179000
H	-8.20477800	1.77233700	-2.16178200
H	-9.14527200	1.63011100	-0.65763200
H	-7.80155200	0.52100700	-0.97464900
C	-7.41399800	11.57025500	-3.37271300
N	-5.54377700	11.50679100	-4.74623500
C	-7.36476600	12.85940000	-4.22211300
C	-5.98068900	12.92441700	-4.87080100
H	-7.57588600	13.75455800	-3.62508400
H	-8.12950300	12.80220100	-5.00848400
C	-7.14658100	11.85367900	-1.88749900
H	-7.14058800	10.92138500	-1.31436800
H	-7.92423600	12.51407200	-1.48208100
H	-6.17502800	12.34029500	-1.73893800

C	-8.78982500	10.91894400	-3.53750000
H	-8.92963000	10.05927800	-2.88187200
H	-8.93930400	10.58575800	-4.57059800
H	-9.56806200	11.65675900	-3.30171900
C	-5.01622500	13.85756600	-4.13805800
H	-4.95382000	13.64082500	-3.06798300
H	-5.35677000	14.89175700	-4.25563400
H	-4.01308800	13.78242800	-4.57204200
C	-6.04356000	13.36776400	-6.32925400
H	-6.77558700	12.78981800	-6.89949200
H	-5.06424300	13.27833300	-6.81455000
H	-6.34188200	14.42056000	-6.36828800
B	-5.93616500	9.25894400	-3.65033900
B	-7.22196600	6.15372100	-1.57899100
C	-6.27062800	10.73138500	-3.92486800
C	-8.83330100	4.34779500	0.12641100
C	-10.03382900	4.31109300	-0.60298100
C	-8.78544200	4.85384900	1.43442500
C	-11.20776500	4.67614300	0.05684600
C	-9.98601400	5.20955100	2.04768300
C	-11.19263300	5.09715900	1.37649600
H	-12.14757700	4.65248100	-0.49006600
H	-12.11979300	5.37322000	1.87078000
H	-9.96565400	5.60581000	3.06028300
C	-7.48106000	5.14958300	2.15302500
C	-7.43092400	4.53845700	3.55355300
H	-7.63105400	3.46225500	3.54772800
H	-8.17123200	5.00833500	4.21186500
H	-6.44817000	4.70258800	4.00921800
C	-7.28123800	6.66647400	2.23619500
H	-6.65490000	4.74497800	1.55578300
H	-6.33194000	6.90139400	2.73094000
H	-8.08750100	7.12713800	2.82136800
H	-7.27787800	7.12156900	1.24122300

C	-10.10480700	4.01490000	-2.09236000
C	-11.09854100	2.90133600	-2.42894600
H	-11.07856500	2.68706500	-3.50322300
H	-12.12248900	3.20705200	-2.18286600
H	-10.89531200	1.97004800	-1.89277300
C	-10.49789900	5.28635800	-2.85379900
H	-9.10692600	3.72228300	-2.44055100
H	-10.52361100	5.08882500	-3.93138300
H	-9.79352800	6.10175100	-2.66847900
H	-11.49935700	5.61866700	-2.55206200
C	-4.32480200	11.06485700	-5.35569600
C	-3.12432500	11.10169000	-4.62629000
C	-3.17208400	10.20299900	-7.27690400
C	-1.96547000	10.31549100	-6.60569800
C	-1.95036600	10.73660000	-5.28607000
H	-1.03828700	10.03942300	-7.09993700
H	-1.01055100	10.76035700	-4.73917100
C	-3.05355000	11.39811800	-3.13695200
C	-2.66029800	10.12684000	-2.37530900
H	-3.36443700	9.31126300	-2.56071300
H	-2.63486800	10.32447500	-1.29773900
H	-1.65869200	9.79473900	-2.67679600
C	-2.06010100	12.51194300	-2.80039500
H	-4.05154200	11.69057100	-2.78891800
H	-2.07986000	12.72594200	-1.72605900
H	-2.26380300	13.44330400	-3.33626500
H	-1.03612100	12.20663200	-3.04684100
C	-4.37265800	10.55866400	-6.66364000
C	-5.67708700	10.26274900	-7.38206800
C	-5.87669500	8.74581700	-7.46535900
H	-6.82580700	8.51081300	-7.96043000
H	-5.88034900	8.29068600	-6.47040700
H	-5.07018600	8.28526900	-8.05027400
C	-5.72757800	10.87380600	-8.78258200

H	-6.50329200	10.66710800	-6.78473100
H	-5.52715000	11.94995500	-8.77693800
H	-6.71057400	10.70986800	-9.23781100
H	-4.98766300	10.40362800	-9.44113200
H	-3.19244700	9.80665900	-8.28947400
H	-8.16884700	6.62110700	-1.00138400
H	-4.98931800	8.79152000	-4.22798600
H	-5.57297700	6.66579500	-3.07011500
H	-7.58514100	8.74690100	-2.15919600

36. CAAC_Full_H_H (planar)-triplet:

C	-5.74394600	3.80796700	-1.84380000
N	-7.61006300	3.87876100	-0.44995000
C	-5.79575400	2.52117300	-0.99111300
C	-7.17996600	2.46142000	-0.33776100
H	-5.02935500	2.57809600	-0.20629800

H	-5.58945300	1.62249500	-1.58481900
C	-6.87916600	4.65167900	-1.29033300
C	-6.41055800	7.05220400	-2.51069300
C	-6.74768600	8.36047400	-2.71867600
C	-6.00796900	3.52912800	-3.32962100
H	-6.03235000	4.46722000	-3.89537200
H	-6.97140000	3.02714600	-3.47926100
H	-5.22022300	2.88962400	-3.74942900
C	-4.37200300	4.46683200	-1.67875300
H	-3.58460000	3.75098900	-1.94888400
H	-4.21279000	4.77025100	-0.63762000
H	-4.25380500	5.34896100	-2.31005200
C	-7.11569600	2.00980000	1.11853800
H	-6.37961400	2.58191700	1.68975200
H	-6.82494300	0.95477400	1.15524600
H	-8.09397400	2.10514700	1.60531400
C	-8.14711400	1.53179600	-1.07330800
H	-8.20330800	1.74702600	-2.14404100
H	-9.15207700	1.61435000	-0.64437600
H	-7.81445500	0.49514500	-0.95332300
C	-7.41430000	11.60471000	-3.38557700
N	-5.54817700	11.53391500	-4.77942000
C	-7.36248800	12.89150500	-4.23826400
C	-5.97827300	12.95125600	-4.89161000
H	-7.56879000	13.79018200	-3.64455800
H	-8.12888400	12.83458300	-5.02308200
C	-7.15028800	11.88354900	-1.89975500
H	-7.12591000	10.94545700	-1.33400200
H	-7.93803600	12.52305200	-1.47995200
H	-6.18685700	12.38553100	-1.75010800
C	-8.78624100	10.94584200	-3.55063400
H	-8.90443800	10.06370700	-2.91934600
H	-8.94545000	10.64243500	-4.59177100
H	-9.57364600	11.66168100	-3.28049800

C	-5.01112700	13.88087900	-4.15605800
H	-4.95493900	13.66564800	-3.08532500
H	-5.34378600	14.91753100	-4.27604300
H	-4.00616200	13.79832500	-4.58498600
C	-6.04253700	13.40287800	-6.34790900
H	-6.77861700	12.83076300	-6.91912700
H	-5.06425700	13.30753100	-6.83468100
H	-6.33328900	14.45790400	-6.38461600
B	-5.95938700	9.29396900	-3.66079800
B	-7.19885600	6.11870900	-1.56857100
C	-6.27907600	10.76099800	-3.93903800
C	-8.82784400	4.33030100	0.14688100
C	-10.02225800	4.31348500	-0.59440500
C	-8.78791100	4.83857700	1.45467900
C	-11.19716700	4.69996500	0.05118100
C	-9.98884600	5.21408200	2.05562100
C	-11.18961400	5.12193900	1.37093400
H	-12.13164000	4.69011300	-0.50540600
H	-12.11753600	5.41376200	1.85468000
H	-9.97321100	5.61000100	3.06858300
C	-7.48497000	5.11617900	2.18250400
C	-7.45103800	4.50410500	3.58269900
H	-7.65713100	3.42906500	3.57262700
H	-8.19479800	4.97698900	4.23507800
H	-6.47142200	4.66124200	4.04758900
C	-7.26547200	6.63013200	2.26566100
H	-6.66204500	4.70044000	1.58872800
H	-6.31551200	6.85461100	2.76398100
H	-8.06857300	7.10374700	2.84478700
H	-7.25216700	7.08430600	1.26993500
C	-10.08111400	4.00712600	-2.08207800
C	-11.09332000	2.91111100	-2.42065100
H	-11.06102800	2.68144500	-3.49147900
H	-12.11457000	3.24044300	-2.19456200

H	-10.91669600	1.98367800	-1.86839100
C	-10.43587100	5.27891000	-2.86111200
H	-9.08534200	3.68981200	-2.41333800
H	-10.46387500	5.06952000	-3.93643200
H	-9.71055900	6.07855900	-2.68422200
H	-11.42749900	5.64558700	-2.56685800
C	-4.33039400	11.08237600	-5.37624600
C	-3.13598400	11.09918900	-4.63495400
C	-3.16938300	10.19859600	-7.28498200
C	-1.96861900	10.29073700	-6.60028900
C	-1.96107200	10.71270800	-5.28053600
H	-1.04069500	9.99891400	-7.08403200
H	-1.02660100	10.72255900	-4.72394400
C	-3.07713400	11.40554600	-3.14728100
C	-2.72238100	10.13376200	-2.36824700
H	-3.44769400	9.33411300	-2.54513900
H	-2.69438000	10.34315200	-1.29292600
H	-1.73075200	9.76708300	-2.66249700
C	-2.06492900	12.50156000	-2.80870300
H	-4.07290700	11.72286100	-2.81602500
H	-2.09722600	12.73122600	-1.73787500
H	-2.24154900	13.42899400	-3.36096300
H	-1.04367800	12.17222700	-3.03478700
C	-4.37032100	10.57410100	-6.68404500
C	-5.67325900	10.29650000	-7.41187700
C	-5.89275600	8.78254800	-7.49503600
H	-6.84271400	8.55806900	-7.99336000
H	-5.90606500	8.32837200	-6.49931100
H	-5.08965300	8.30893300	-8.07415900
C	-5.70718400	10.90857500	-8.81207100
H	-6.49618700	10.71223900	-6.81810500
H	-5.50109200	11.98361500	-8.80199700
H	-6.68679800	10.75143800	-9.27696600
H	-4.96342100	10.43569300	-9.46444700

H	-3.18501400	9.80267800	-8.29794500
H	-8.13087100	6.60251800	-0.98473700
H	-5.02737300	8.81015800	-4.24463000
H	-5.56487000	6.70198900	-3.11623900
H	-7.59337300	8.71068900	-2.11312900

37. NHC_Full_C₂H₅_Cl (fully optimized)-singlet:

N	-10.24743300	5.14764000	-1.96066900
C	-10.28829000	5.99024400	0.05854200
C	-11.07134400	5.46023200	-0.90225200
C	-8.95260400	5.46416800	-1.68334300
C	-6.55467900	5.97862400	-2.79169000
C	-5.27400300	5.51109200	-3.29409000
C	-6.71547300	7.46418800	-2.51783500
H	-7.66177500	7.61778200	-1.98208700
H	-6.84350300	8.02774700	-3.45312400
C	-4.80575500	4.17526000	-2.72144400

H	-5.57844200	3.79358800	-2.04304300
H	-3.95403700	4.37600600	-2.05993300
N	-1.98646100	5.44576900	-3.83459600
N	-2.53768900	5.51879700	-5.92731700
C	-0.91724500	4.94679600	-4.55906900
C	-1.25950100	5.00744000	-5.86325300
B	-4.44236500	6.22912000	-4.26651300
B	-7.71414200	5.11494600	-2.55742600
Cl	-7.87310800	3.41152200	-3.26525600
C	-3.01572200	5.76546800	-4.67565300
Cl	-5.02459800	7.67999100	-5.25733100
C	-10.73314600	4.71562500	-3.23626200
C	-11.25503700	3.42033700	-3.33993600
C	-10.67703400	5.60191800	-4.31879600
C	-11.78765200	3.03380500	-4.56645700
C	-11.19966800	5.15161600	-5.53245600
C	-11.76053200	3.89140600	-5.65551800
H	-12.20906500	2.03735600	-4.67177400
H	-12.16983700	3.57112500	-6.60940000
H	-11.17193400	5.81543700	-6.39297200
C	-10.12288600	7.01526000	-4.24845100
C	-11.23409700	8.03405700	-4.51598300
H	-12.06553200	7.92558600	-3.81107000
H	-11.63884100	7.91520500	-5.52840700
H	-10.84517600	9.05487400	-4.43505300
C	-8.97318300	7.20230800	-5.24247000
H	-9.72799500	7.20374200	-3.24030100
H	-8.55570300	8.21228300	-5.16069600
H	-9.32463300	7.07481800	-6.27372000
H	-8.16128600	6.48748600	-5.06120400
C	-11.22405000	2.43605400	-2.18618600
C	-12.62372400	2.25050100	-1.59491900
H	-12.60742800	1.53854200	-0.76228500
H	-13.30490100	1.85587700	-2.35995200

H	-13.05263000	3.18999300	-1.23034700
C	-10.66194400	1.08036300	-2.61699300
H	-10.55613500	2.83747100	-1.41212900
H	-10.53585900	0.43155200	-1.74360400
H	-9.69248200	1.19007500	-3.10948500
H	-11.34406700	0.56618100	-3.30417500
C	-3.13773100	5.99178000	-7.14539600
C	-4.20607600	5.30785800	-7.72756000
C	-3.17828100	7.66496900	-8.85187800
C	-4.22231500	6.99309300	-9.47038100
C	-4.73725200	5.83931700	-8.90371200
H	-4.64839200	7.38289700	-10.39054500
H	-5.57596700	5.33181300	-9.37448500
C	-4.81384300	4.05660700	-7.13291400
C	-6.27271500	4.29024600	-6.72631200
H	-6.36788600	5.10009700	-5.99350300
H	-6.69286700	3.38492200	-6.27215500
H	-6.88437900	4.53834600	-7.60384000
C	-4.71598300	2.88254800	-8.10928500
H	-4.24921500	3.80169900	-6.23184900
H	-5.10849200	1.97015500	-7.64756700
H	-3.68340600	2.69281600	-8.42121300
H	-5.30750700	3.07270500	-9.01345700
C	-2.63186300	7.19248500	-7.66236300
C	-1.57249600	8.00941100	-6.94621300
C	-2.04576000	9.44449200	-6.70414700
H	-1.28963600	10.00278700	-6.13808800
H	-2.98631900	9.46267000	-6.14352800
H	-2.20050800	9.98093200	-7.64769100
C	-0.25069300	7.99811000	-7.71352100
H	-1.39169700	7.55964600	-5.96325300
H	0.12592100	6.97889900	-7.85745800
H	0.51399200	8.57254700	-7.17698400
H	-0.37540900	8.44897300	-8.70636900

H	-2.79627500	8.58811900	-9.28164200
N	-8.99250300	5.99388100	-0.42152100
C	-7.92373500	6.59963800	0.32458300
C	-6.90648700	5.80047600	0.86472600
C	-7.99324200	7.98445800	0.54381600
C	-5.94910300	6.43111700	1.65866100
C	-6.01097600	7.79338000	1.91750200
C	-7.02286600	8.55892200	1.36591300
H	-5.14546100	5.84203800	2.08911100
H	-5.26108000	8.25913200	2.55061600
H	-7.06314200	9.62741300	1.56341400
C	-9.07584100	8.87417900	-0.05111500
C	-8.50314300	10.09317400	-0.77829400
H	-7.92860400	10.73250200	-0.09832700
H	-9.32157100	10.70171400	-1.17835000
H	-7.85379300	9.81005400	-1.60987800
C	-10.03043000	9.35078500	1.04836600
H	-9.64633300	8.29286600	-0.79023400
H	-9.48600200	9.96613100	1.77586700
H	-10.48475800	8.52221400	1.60067900
H	-10.83488300	9.96438100	0.62859900
C	-6.88565900	4.29736100	0.67684200
C	-5.48114100	3.71494800	0.80405500
H	-4.75292900	4.30160800	0.22698400
H	-5.46632600	2.68614300	0.42804000
H	-5.14710400	3.68381900	1.84925200
C	-7.84016500	3.63737700	1.67661100
H	-7.24062600	4.07453500	-0.33754100
H	-7.52532900	3.85274500	2.70571400
H	-7.84875900	2.54978800	1.54532500
H	-8.86782300	4.00000800	1.55657900
H	-0.72113800	4.74027100	-6.75838300
H	-0.01008600	4.62481600	-4.07559800
H	-12.13385300	5.28737400	-0.94916400

H	-10.51214500	6.35727000	1.04643300
C	-1.93933600	5.82857800	-2.44827400
C	-1.80528900	4.84301800	-1.45990600
C	-2.02433700	7.20112000	-2.13433600
C	-1.87791100	5.24923800	-0.12466000
C	-2.12435400	7.54501600	-0.78961900
C	-2.08335600	6.57635800	0.20666500
H	-1.79308500	4.50133600	0.65941200
H	-2.23070900	8.58916500	-0.51479000
H	-2.17271100	6.86929100	1.24918000
C	-1.84420200	8.27892100	-3.19464400
C	-2.22575700	9.68719500	-2.75029500
H	-3.24372400	9.74589800	-2.35594900
H	-2.16098100	10.36033200	-3.61251300
H	-1.53473600	10.06930300	-1.98795900
C	-0.36630300	8.28580100	-3.61833100
H	-2.46712600	8.04414700	-4.06781700
H	0.26485100	8.53267900	-2.75521400
H	-0.18718200	9.04227500	-4.39239700
H	-0.03352400	7.31904700	-4.01010200
C	-1.53739700	3.38286300	-1.78089600
C	-0.04126500	3.09511900	-1.60152900
H	0.19592700	2.05927800	-1.86830700
H	0.23893600	3.24482700	-0.55080500
H	0.59372400	3.75942000	-2.19703000
C	-2.33010000	2.40642300	-0.90950900
H	-1.81746800	3.19918700	-2.82635700
H	-2.19162800	1.38438200	-1.27866400
H	-3.40118900	2.62591100	-0.90971300
H	-1.97784000	2.42003000	0.12884000
C	-4.43832400	3.05345300	-3.69055900
H	-4.21899200	2.12211900	-3.14964100
H	-5.27141000	2.85274500	-4.37418400
H	-3.55280700	3.28246800	-4.29850300

C	-5.54648200	8.05865300	-1.73558600
H	-5.27426500	7.40922200	-0.89058100
H	-4.66504600	8.12407500	-2.38002600
H	-5.76021000	9.06288700	-1.34604900

38. NHC_Full_C₂H₅_Cl (fully optimized)-triplet:

N	-9.31002300	4.72159000	-0.40653200
C	-10.48171400	6.58095600	-0.39812400
C	-10.43587100	5.33381800	0.10392600
C	-8.59959800	5.59908900	-1.22058900
C	-6.30706600	6.35461100	-2.63303800
C	-6.51386300	6.64542300	-3.94450400
C	-4.97670600	6.73668800	-1.97811100
H	-4.66552900	7.73277000	-2.32651600
H	-4.21087600	6.05597800	-2.38158300
C	-7.71234900	6.03913700	-4.65908200
H	-8.53601200	5.87999400	-3.94634700
H	-7.41416600	5.01815100	-4.96093900
N	-3.45612700	5.95344800	-5.06351500
N	-3.08528900	8.05134200	-5.56459000
C	-2.13600700	6.07331700	-5.46000700

C	-1.91330100	7.35992400	-5.77973300
B	-5.51564100	7.54561000	-4.74667000
B	-7.22171100	5.38369700	-1.81940200
Cl	-6.38037600	3.77687600	-1.53382100
C	-4.08507000	7.19783600	-5.11893000
Cl	-6.14119600	9.22485100	-5.15473100
C	-9.10419700	3.31273300	-0.29493300
C	-8.69209400	2.78914900	0.93905600
C	-9.32637100	2.51312800	-1.42163200
C	-8.49546700	1.41264600	1.01746900
C	-9.11525200	1.14219200	-1.29079500
C	-8.69970400	0.59675800	-0.08775700
H	-8.16990000	0.96757300	1.95178000
H	-8.53596000	-0.47401000	-0.00475400
H	-9.28463700	0.49678700	-2.14946100
C	-9.80999200	3.07044200	-2.74740500
C	-11.29547700	2.75160700	-2.92535200
H	-11.89811300	3.21971200	-2.13570700
H	-11.46955400	1.66871100	-2.87966100
H	-11.65826000	3.11008900	-3.89516100
C	-8.98271100	2.56904000	-3.93171700
H	-9.69789100	4.15938000	-2.73669300
H	-9.28063100	3.10061200	-4.84675400
H	-9.13341100	1.49753300	-4.11431300
H	-7.91319200	2.74843400	-3.76818800
C	-8.39491100	3.70609400	2.11383200
C	-8.30617300	2.96918300	3.44566200
H	-8.22259300	3.69021000	4.26449800
H	-7.41524200	2.33121500	3.48839400
H	-9.18275900	2.33998000	3.63366400
C	-7.10019600	4.49116000	1.87049200
H	-9.21413300	4.43618900	2.19516400
H	-6.84976100	5.09132000	2.75289400
H	-7.17628900	5.16476500	1.01101500

H	-6.26905500	3.80178500	1.67459000
C	-3.27740000	9.34278300	-6.15157900
C	-3.56896900	9.39670100	-7.51507800
C	-3.35817300	11.71567500	-5.95706900
C	-3.59964600	11.80493100	-7.32323900
C	-3.72139400	10.65834400	-8.09102400
H	-3.72215000	12.78065200	-7.78520500
H	-3.96058400	10.73452000	-9.14984200
C	-3.83711200	8.14636500	-8.32898100
C	-5.31770500	8.09580300	-8.71670200
H	-5.95852900	8.18963900	-7.83235500
H	-5.55472000	7.15097500	-9.22403700
H	-5.57137400	8.91533100	-9.40139100
C	-2.94260100	8.05045200	-9.56204900
H	-3.63354000	7.27058900	-7.70150100
H	-3.14497700	7.12208100	-10.10945900
H	-1.88109500	8.06203400	-9.29207700
H	-3.12281600	8.88467400	-10.25114200
C	-3.20490200	10.47800100	-5.34074500
C	-3.04648200	10.32871900	-3.84112400
C	-3.71433500	11.45999900	-3.06726000
H	-3.72832100	11.22717400	-1.99692600
H	-4.75017600	11.60358300	-3.39835000
H	-3.17733400	12.40921700	-3.18522500
C	-1.57059400	10.20003700	-3.46074300
H	-3.56062800	9.39530100	-3.55837100
H	-1.09593000	9.35169500	-3.96593900
H	-1.45363700	10.05940700	-2.38049800
H	-1.02473800	11.10861600	-3.74463900
H	-3.31772000	12.62232100	-5.36098800
N	-9.39613900	6.74752000	-1.23821400
C	-9.46472700	7.77084800	-2.24682100
C	-8.61165100	8.87661400	-2.16900000
C	-10.47676700	7.67242800	-3.21444500

C	-8.77880000	9.89973600	-3.09761700
C	-9.78670000	9.84004100	-4.04868600
C	-10.62868700	8.74193700	-4.09892300
H	-8.10661900	10.75236900	-3.07798800
H	-9.90874200	10.65132200	-4.76060700
H	-11.41175600	8.69646300	-4.85292700
C	-11.43383600	6.49386000	-3.32498600
C	-11.40402000	5.84358600	-4.71123000
H	-11.46656000	6.58778300	-5.51342200
H	-12.25623800	5.16411800	-4.82554800
H	-10.48690700	5.26339600	-4.86561900
C	-12.85829700	6.94644700	-2.99027900
H	-11.14753300	5.72445100	-2.59727300
H	-13.21545900	7.67845100	-3.72508600
H	-12.91265500	7.41895600	-2.00353400
H	-13.54883900	6.09588000	-3.00268100
C	-7.60882200	8.98168300	-1.04438000
C	-6.37779800	9.80118800	-1.41613100
H	-5.98460900	9.51109500	-2.39739000
H	-5.58736800	9.66386100	-0.66811000
H	-6.60392000	10.87532900	-1.44976800
C	-8.28856600	9.56049100	0.19988300
H	-7.28803300	7.96097900	-0.80750900
H	-8.65358500	10.57543500	-0.00264800
H	-7.58483100	9.61483100	1.03871300
H	-9.14303800	8.95024600	0.51395200
H	-1.03694700	7.86358300	-6.15559100
H	-1.49326100	5.21054000	-5.49654800
H	-11.09722000	4.80602900	0.77225200
H	-11.20166200	7.37467000	-0.27484600
C	-4.02766200	4.66139500	-4.81437900
C	-5.00233400	4.15776900	-5.70081500
C	-3.49387300	3.86709900	-3.78354300
C	-5.53672000	2.90045800	-5.43420500

C	-4.02389600	2.58869900	-3.60420000
C	-5.06090300	2.12198300	-4.38788600
H	-6.31895800	2.50815200	-6.07796200
H	-3.63338200	1.96806900	-2.80191500
H	-5.49243300	1.14321300	-4.19819100
C	-2.33588300	4.28515100	-2.88905400
C	-2.61763600	4.02490000	-1.40513800
H	-3.60041000	4.38779700	-1.09782000
H	-1.85296700	4.50749100	-0.78658500
H	-2.57869400	2.95225300	-1.18146700
C	-1.06711900	3.51562100	-3.27732000
H	-2.15573900	5.36047400	-3.01866200
H	-1.22624900	2.44089100	-3.12316100
H	-0.22098200	3.81995600	-2.65108500
H	-0.78151800	3.64869100	-4.32534700
C	-5.33329600	4.86747900	-7.00204800
C	-4.16563500	4.65449000	-7.97914900
H	-4.35092400	5.17937400	-8.92578900
H	-4.06157000	3.58508000	-8.20288400
H	-3.20930100	5.00756000	-7.57950400
C	-6.61603200	4.39265900	-7.68002100
H	-5.43344100	5.94539600	-6.80854200
H	-6.86318100	5.07214400	-8.50436300
H	-7.47497000	4.36569400	-7.00165800
H	-6.49184500	3.39111100	-8.11094700
C	-8.22806600	6.79332100	-5.87770600
H	-7.43271500	6.96261300	-6.61549400
H	-9.02200300	6.23352300	-6.38543300
H	-8.62212000	7.77581900	-5.60005800
C	-4.88561800	6.68525700	-0.45472100
H	-3.86704400	6.92828500	-0.12986400
H	-5.55835200	7.39448200	0.03919000
H	-5.12113000	5.69113900	-0.05956800

39. NHC_Full_C₂H₅_Cl (twisted)-singlet:

N	-9.41618100	4.70740300	-0.45451800
C	-10.55028300	6.59184500	-0.39424600
C	-10.55390800	5.31659200	0.03526300
C	-8.63500800	5.62544600	-1.15083700
C	-6.33326300	6.36471900	-2.58102000
C	-6.39734100	6.50417800	-3.93087300
C	-5.06032100	6.84760900	-1.86747100
H	-4.87516400	7.90500100	-2.12219300
H	-4.21015100	6.30856400	-2.31897300
C	-7.56496400	5.89411200	-4.68032200
H	-8.39547200	5.73877900	-3.97224700
H	-7.27304200	4.87558500	-4.99095700
N	-3.37785400	5.92263500	-5.12933300
N	-3.08565800	7.99240800	-5.76283500
C	-2.10013700	6.03308700	-5.64285000
C	-1.92344300	7.30645800	-6.03943000
B	-5.39427200	7.49518200	-4.61928600
B	-7.28048900	5.40781400	-1.78610000
Cl	-6.47535800	3.76374800	-1.59456500
C	-4.01367400	7.16435600	-5.14788200

Cl	-6.03750600	9.19433200	-4.83769600
C	-9.19213000	3.30211200	-0.31771500
C	-8.82218100	2.79487700	0.93559400
C	-9.35378000	2.48762400	-1.44439300
C	-8.62088500	1.41971800	1.03778500
C	-9.14068600	1.12037200	-1.29165600
C	-8.77657700	0.59052900	-0.06436100
H	-8.32892100	0.98845600	1.98963200
H	-8.61078500	-0.47833900	0.03759800
H	-9.26187400	0.46517400	-2.15027400
C	-9.78168200	3.04564900	-2.78698000
C	-11.29415400	2.86686800	-2.93926600
H	-11.83723700	3.41091200	-2.15395700
H	-11.56554400	1.80628200	-2.85749900
H	-11.63934500	3.22986000	-3.91342300
C	-9.02148100	2.43816000	-3.96522800
H	-9.55935700	4.11815800	-2.80394400
H	-9.26677300	2.98833100	-4.88458800
H	-9.28800400	1.38787800	-4.13696600
H	-7.93709400	2.50600600	-3.81001400
C	-8.55322900	3.72406000	2.10613900
C	-8.55526200	3.01380200	3.45544200
H	-8.49589200	3.74949900	4.26332700
H	-7.68533000	2.35443200	3.55963600
H	-9.45706700	2.41121800	3.60818900
C	-7.21621000	4.44698900	1.90226700
H	-9.34476400	4.48735000	2.13174000
H	-6.97726800	5.06288300	2.77702900
H	-7.22593000	5.09509300	1.02025500
H	-6.40926800	3.71598300	1.76382300
C	-3.29913800	9.30890600	-6.27357200
C	-3.66464000	9.42806200	-7.61536900
C	-3.31454600	11.67325100	-5.97712600
C	-3.64869000	11.82521300	-7.31805000

C	-3.83529000	10.71532400	-8.12616000
H	-3.78555600	12.82180600	-7.72864800
H	-4.13858700	10.84170200	-9.16321100
C	-4.00364700	8.21206800	-8.45319300
C	-5.52416500	8.13607900	-8.61122500
H	-6.01729700	8.23817600	-7.63834100
H	-5.82695100	7.18112400	-9.06374700
H	-5.88817500	8.94770000	-9.25511800
C	-3.30852500	8.20263500	-9.81079600
H	-3.68545100	7.31519000	-7.90767800
H	-3.55653600	7.28449000	-10.35641200
H	-2.21938100	8.25534200	-9.71169800
H	-3.63083500	9.04653600	-10.43252600
C	-3.14165400	10.40833500	-5.42450300
C	-2.83939900	10.20182200	-3.95378300
C	-3.44476900	11.28921300	-3.07185800
H	-3.36227800	11.00703300	-2.01662800
H	-4.50557400	11.43991800	-3.30343100
H	-2.92522700	12.24819000	-3.19059900
C	-1.32967900	10.09452700	-3.72969000
H	-3.30207700	9.24782600	-3.65611600
H	-0.89268800	9.27420600	-4.30986300
H	-1.10090500	9.92083000	-2.67231800
H	-0.83314500	11.02432700	-4.03503600
H	-3.20939100	12.55262800	-5.34859900
N	-9.41332300	6.78506200	-1.15838800
C	-9.43030600	7.80323200	-2.17706100
C	-8.61648700	8.93243900	-2.03307400
C	-10.35464000	7.67479800	-3.22469900
C	-8.74358000	9.95611800	-2.96582400
C	-9.66624900	9.86631300	-3.99780500
C	-10.46400500	8.74154300	-4.11970500
H	-8.10177000	10.82884500	-2.89037200
H	-9.75719800	10.67650700	-4.71556400

H	-11.18431000	8.67734900	-4.93254700
C	-11.28697200	6.48262500	-3.38460700
C	-11.22826100	5.85585000	-4.78134100
H	-11.22834300	6.61272800	-5.57324000
H	-12.10412100	5.21716500	-4.94139100
H	-10.33354500	5.23733600	-4.91200000
C	-12.72573300	6.91066500	-3.07568400
H	-11.00260600	5.70656700	-2.66348500
H	-13.07750000	7.63692200	-3.81939400
H	-12.81026400	7.38178000	-2.09093300
H	-13.40052800	6.04735200	-3.10392700
C	-7.68505300	9.04057900	-0.84934000
C	-6.48349100	9.94517300	-1.10478300
H	-6.03396000	9.75745600	-2.08586700
H	-5.71929300	9.78444700	-0.33482600
H	-6.76716100	11.00507400	-1.06197300
C	-8.45552200	9.52187500	0.38413400
H	-7.32292300	8.02607800	-0.64647000
H	-8.86697000	10.52333000	0.20496700
H	-7.79476700	9.58031700	1.25679700
H	-9.28654700	8.85374800	0.63376000
H	-1.08919500	7.80216800	-6.50976400
H	-1.45875000	5.17059100	-5.71185800
H	-11.25475500	4.76689900	0.64349200
H	-11.26433100	7.38970900	-0.26530000
C	-3.94051000	4.63710500	-4.83788100
C	-4.88748400	4.08848300	-5.72713900
C	-3.42395000	3.90061500	-3.76146900
C	-5.39106300	2.82354100	-5.43569400
C	-3.92851500	2.61761900	-3.54570200
C	-4.92234000	2.09411200	-4.35068400
H	-6.15001100	2.39061900	-6.08148200
H	-3.55244000	2.03964200	-2.70526200
H	-5.33110300	1.10926400	-4.14236300

C	-2.31714300	4.40588800	-2.85245400
C	-2.64450300	4.17158200	-1.37374400
H	-3.68348300	4.41541900	-1.14118300
H	-1.98690100	4.77139000	-0.73515900
H	-2.48486100	3.12120000	-1.10104100
C	-0.99454600	3.70295800	-3.17803100
H	-2.19449600	5.48497000	-3.01640000
H	-1.10571000	2.62054600	-3.03425500
H	-0.19769500	4.04823200	-2.50966600
H	-0.66439100	3.86226200	-4.20888800
C	-5.26493900	4.79257900	-7.01962700
C	-4.13270200	4.63741800	-8.04653000
H	-4.38366800	5.17373800	-8.97248400
H	-4.00037500	3.57760800	-8.29872100
H	-3.17374300	5.02096000	-7.68694200
C	-6.55147300	4.28306900	-7.66665200
H	-5.38867800	5.86501800	-6.80602800
H	-6.84425000	4.96130700	-8.47687200
H	-7.39135300	4.21568200	-6.96852800
H	-6.40241300	3.29168200	-8.11311800
C	-8.06902600	6.68547500	-5.88057900
H	-7.26612900	6.89312900	-6.59569200
H	-8.84888600	6.14096300	-6.42473300
H	-8.47883000	7.65190400	-5.56588200
C	-4.97694500	6.67452100	-0.35322700
H	-3.98240300	6.96316900	0.00639100
H	-5.70543800	7.28626800	0.18992400
H	-5.14393700	5.63597700	-0.04711400

40. NHC_Full_C₂H₅_Cl (twisted)-triplet:

N	-9.41494300	4.70704500	-0.45499700
C	-10.54780800	6.59225100	-0.39339500
C	-10.55207000	5.31676300	0.03546800
C	-8.63346200	5.62502800	-1.15116600
C	-6.33252300	6.36531700	-2.58251700
C	-6.39895800	6.50517800	-3.93155100
C	-5.05767300	6.84501500	-1.86881100
H	-4.86949700	7.90221200	-2.12112300
H	-4.20827100	6.30449000	-2.31987000
C	-7.56952200	5.89764200	-4.67956700
H	-8.40147100	5.74663000	-3.97281900
H	-7.28067700	4.87732000	-4.98734300
N	-3.37904000	5.92442500	-5.12577300
N	-3.08689100	7.99391600	-5.76199700
C	-2.10036300	6.03530300	-5.63718600
C	-1.92401000	7.30813400	-6.03564100
B	-5.39567700	7.49769300	-4.61896400
B	-7.27951300	5.40692900	-1.78743600
Cl	-6.47412900	3.76349100	-1.59702900
C	-4.01579000	7.16593500	-5.14787500
Cl	-6.04083200	9.19531700	-4.84191200
C	-9.19176500	3.30151700	-0.31917900
C	-8.82307500	2.79305100	0.93405000
C	-9.35333900	2.48786100	-1.44651800
C	-8.62298600	1.41765200	1.03542000

C	-9.14148000	1.12034100	-1.29453700
C	-8.77862800	0.58933400	-0.06736700
H	-8.33208100	0.98550200	1.98718300
H	-8.61384100	-0.47974600	0.03397200
H	-9.26283300	0.46579900	-2.15362500
C	-9.78033800	3.04677300	-2.78904300
C	-11.29289800	2.86901400	-2.94178300
H	-11.83591700	3.41322500	-2.15655200
H	-11.56483700	1.80855300	-2.86017500
H	-11.63763000	3.23225500	-3.91600200
C	-9.02025100	2.43888600	-3.96716500
H	-9.55707900	4.11910900	-2.80569300
H	-9.26435900	2.98971300	-4.88646600
H	-9.28793600	1.38899700	-4.13948200
H	-7.93590800	2.50534800	-3.81119500
C	-8.55404200	3.72112300	2.10544200
C	-8.55714200	3.00988300	3.45421800
H	-8.49741500	3.74494000	4.26265800
H	-7.68782700	2.34968100	3.55824800
H	-9.45952300	2.40797200	3.60621900
C	-7.21648300	4.44324000	1.90250400
H	-9.34496700	4.48502000	2.13133200
H	-6.97767300	5.05896200	2.77742300
H	-7.22541700	5.09138400	1.02052700
H	-6.40989400	3.71177000	1.76449900
C	-3.30086200	9.30959400	-6.27451000
C	-3.66634600	9.42706700	-7.61641600
C	-3.31838000	11.67430000	-5.98062000
C	-3.65218100	11.82454700	-7.32183200
C	-3.83783000	10.71362600	-8.12871100
H	-3.78963700	12.82059200	-7.73356500
H	-4.14098700	10.83855500	-9.16599600
C	-4.00399300	8.20998500	-8.45309900
C	-5.52408700	8.13449300	-8.61503400

H	-6.01967400	8.23847400	-7.64360700
H	-5.82610900	7.17888200	-9.06664100
H	-5.88611100	8.94507200	-9.26135600
C	-3.30512100	8.19812300	-9.80877500
H	-3.68771800	7.31388600	-7.90525900
H	-3.55267200	7.27967700	-10.35409200
H	-2.21619400	8.24964800	-9.70663400
H	-3.62463300	9.04180100	-10.43226900
C	-3.14476800	10.41012700	-5.42653000
C	-2.84375800	10.20551800	-3.95525700
C	-3.44981400	11.29407500	-3.07523800
H	-3.36801900	11.01334300	-2.01956500
H	-4.51047900	11.44440900	-3.30771600
H	-2.93022600	12.25290300	-3.19494300
C	-1.33427100	10.09840600	-3.72951600
H	-3.30682000	9.25190300	-3.65686900
H	-0.89671500	9.27735900	-4.30820200
H	-1.10656500	9.92605600	-2.67169400
H	-0.83742300	11.02781700	-4.03552900
H	-3.21422000	12.55446300	-5.35303400
N	-9.41125600	6.78512400	-1.15820000
C	-9.42882200	7.80371100	-2.17661800
C	-8.61502300	8.93293400	-2.03270800
C	-10.35339200	7.67564100	-3.22410500
C	-8.74263200	9.95707400	-2.96485700
C	-9.66582900	9.86774800	-3.99635600
C	-10.46329600	8.74280100	-4.11853600
H	-8.10059400	10.82964400	-2.88946000
H	-9.75726700	10.67828500	-4.71366400
H	-11.18397200	8.67891100	-4.93106200
C	-11.28556600	6.48338700	-3.38428100
C	-11.22807900	5.85782000	-4.78169900
H	-11.22758700	6.61546000	-5.57286300
H	-12.10476700	5.22034700	-4.94203100

H	-10.33423600	5.23829400	-4.91353100
C	-12.72418000	6.91088300	-3.07384800
H	-11.00037700	5.70689400	-2.66393600
H	-13.07679100	7.63732300	-3.81698300
H	-12.80800600	7.38158200	-2.08885300
H	-13.39872500	6.04736100	-3.10187000
C	-7.68180000	9.03987800	-0.85030200
C	-6.47901500	9.94218800	-1.10820100
H	-6.03129400	9.75271600	-2.08985400
H	-5.71397000	9.78075100	-0.33922100
H	-6.76058900	11.00266900	-1.06594500
C	-8.44965000	9.52245700	0.38423300
H	-7.32100600	8.02484500	-0.64793900
H	-8.85958500	10.52466600	0.20582000
H	-7.78771900	9.57948500	1.25609400
H	-9.28158400	8.85571500	0.63469200
H	-1.08928800	7.80339600	-6.50563000
H	-1.45829900	5.17318800	-5.70447900
H	-11.25313900	4.76721800	0.64357200
H	-11.26141500	7.39040700	-0.26379600
C	-3.94117400	4.63878100	-4.83427600
C	-4.89010100	4.09054200	-5.72195800
C	-3.42240600	3.90101200	-3.75959700
C	-5.39363300	2.82574200	-5.43010000
C	-3.92682400	2.61802600	-3.54376000
C	-4.92289000	2.09537600	-4.34655700
H	-6.15366600	2.39333300	-6.07497700
H	-3.54884900	2.03935400	-2.70463200
H	-5.33147200	1.11051000	-4.13797800
C	-2.31443700	4.40518300	-2.85133900
C	-2.64122900	4.17080500	-1.37242100
H	-3.68015900	4.41453100	-1.13945700
H	-1.98345900	4.77061000	-0.73399300
H	-2.48142500	3.12041700	-1.09985000

C	-0.99261100	3.70115300	-3.17763800
H	-2.19095400	5.48420500	-3.01496200
H	-1.10462700	2.61883300	-3.03387400
H	-0.19507700	4.04566000	-2.50968500
H	-0.66282800	3.86014700	-4.20867000
C	-5.26726100	4.79373700	-7.01489600
C	-4.13429500	4.63754900	-8.04089500
H	-4.38482700	5.17231800	-8.96785800
H	-4.00140900	3.57739000	-8.29131400
H	-3.17571200	5.02198300	-7.68119600
C	-6.55332900	4.28351700	-7.66225400
H	-5.39102600	5.86639200	-6.80248200
H	-6.84692300	4.96210800	-8.47191500
H	-7.39307000	4.21467700	-6.96405400
H	-6.40335800	3.29255400	-8.10937500
C	-8.06930000	6.68767700	-5.88214500
H	-7.26332000	6.89475000	-6.59408000
H	-8.84712300	6.14271800	-6.42883500
H	-8.48020300	7.65454700	-5.57021400
C	-4.97684700	6.67030900	-0.35469000
H	-3.98233500	6.95616400	0.00718200
H	-5.70490300	7.28348100	0.18746800
H	-5.14708300	5.63201500	-0.04966200

41. NHC_Full_C₂H₅_Cl (planar)-singlet:

N	-8.57596100	3.48546500	-0.98783300
C	-6.99970000	2.08893300	-1.58869000
C	-8.11942500	2.18980900	-0.85645800
C	-7.85533800	4.18638500	-1.94187100
C	-7.07022000	6.40143900	-3.30711300
C	-7.09494500	7.81152400	-3.59630800
C	-6.72049500	5.48964400	-4.48782700
H	-6.86024800	4.44714000	-4.20527600
H	-5.67129000	5.58875800	-4.79597900
C	-7.15261900	8.69377200	-2.30243900
H	-8.15445900	8.84518000	-1.88456000
H	-6.76452200	9.69362200	-2.53748200
N	-7.52063000	10.93700300	-4.59684200
N	-5.72081400	10.85208200	-5.79804500
C	-7.44157100	12.11604100	-5.30168600
C	-6.31904700	12.06854500	-6.04280000
B	-6.31539700	8.57037200	-4.62850200
B	-7.88482500	5.70844300	-2.25094400
Cl	-9.21730600	6.62111200	-1.34597200
C	-6.42621400	10.12680900	-4.85537500
Cl	-5.25215800	7.84180500	-5.93439200
C	-9.82356600	3.85639600	-0.39458300
C	-10.99178200	3.81011700	-1.15876400
C	-9.80303200	4.25449700	0.94535900
C	-12.16165700	4.27610300	-0.56145800
C	-10.99829300	4.70298000	1.50069200
C	-12.16277400	4.73553600	0.74720600
H	-13.08349200	4.28742000	-1.13843400
H	-13.08280000	5.10857700	1.18840200
H	-11.00866700	5.05120500	2.53111300

C	-8.52565600	4.25919000	1.76261600
C	-8.70484600	3.53314200	3.09575900
H	-9.08856100	2.51667100	2.95912900
H	-9.40229400	4.06757800	3.75177100
H	-7.74665200	3.46968300	3.62435500
C	-8.02130500	5.68379300	2.00036000
H	-7.75455800	3.72426000	1.19602700
H	-7.09072800	5.66316900	2.58314800
H	-8.75998500	6.26438700	2.56864800
H	-7.83793900	6.21550800	1.06024800
C	-11.01234500	3.31278700	-2.59162200
C	-12.10070100	2.25719100	-2.79471800
H	-12.04312300	1.84161200	-3.80640400
H	-13.10114200	2.69044900	-2.67987400
H	-12.00974900	1.43348400	-2.07918100
C	-11.20612300	4.47289500	-3.57046600
H	-10.04401600	2.84207500	-2.81032500
H	-11.25545000	4.10423300	-4.60184100
H	-10.38815100	5.19569100	-3.49850600
H	-12.14431600	5.00112600	-3.35449800
C	-4.30955800	10.72275600	-6.06274700
C	-3.41914800	11.03274800	-5.02665300
C	-2.51320300	10.33774200	-7.58348200
C	-1.60526100	10.58713200	-6.56454600
C	-2.05518700	10.93156900	-5.29990900
H	-0.53893100	10.52104700	-6.76089700
H	-1.33930400	11.14101700	-4.50941100
C	-3.89631200	11.46722100	-3.65465600
C	-3.85511500	10.30378500	-2.66103100
H	-4.32578500	9.40339500	-3.07004400
H	-4.37655600	10.56719500	-1.72921700
H	-2.81440300	10.05674500	-2.41230600
C	-3.11015100	12.65811700	-3.10862100
H	-4.93871400	11.79603000	-3.75364200

H	-3.56745300	13.00951200	-2.17671400
H	-3.08673500	13.49362000	-3.81568400
H	-2.07533000	12.38551600	-2.87249900
C	-3.88523200	10.39073800	-7.35214700
C	-4.86552800	10.09926600	-8.47004000
C	-4.47711900	8.85558700	-9.26884400
H	-5.27307900	8.59904700	-9.97567700
H	-4.30840500	7.99570200	-8.61522100
H	-3.56801900	9.02645600	-9.85768100
C	-4.97092300	11.30525000	-9.40743700
H	-5.84588900	9.91211100	-8.01297100
H	-5.30206000	12.20973600	-8.88589900
H	-5.67606800	11.10748400	-10.22232400
H	-3.99223300	11.52298100	-9.85456200
H	-2.15273300	10.08064200	-8.57602300
N	-6.77396100	3.32018400	-2.17508000
C	-5.40504600	3.67066100	-2.46763700
C	-4.81023800	3.13924000	-3.61897700
C	-4.66973000	4.42124800	-1.52687000
C	-3.47276200	3.44481700	-3.87107100
C	-2.75461000	4.25389400	-3.01074200
C	-3.34717900	4.72358600	-1.84647400
H	-2.99926000	3.04666600	-4.76486700
H	-1.72099200	4.50394400	-3.23130100
H	-2.75764600	5.31346300	-1.15211100
C	-5.20167000	4.76723100	-0.14414200
C	-4.46453800	5.92188100	0.53669500
H	-3.49647700	5.58634700	0.93066000
H	-5.05298400	6.27711200	1.38991200
H	-4.28538300	6.77021500	-0.12448500
C	-5.07710100	3.54809600	0.78389000
H	-6.26417800	5.03640600	-0.22864600
H	-4.02244400	3.25725000	0.87313600
H	-5.64133900	2.67950300	0.43659200

H	-5.43759800	3.80705700	1.78947500
C	-5.54918300	2.22640200	-4.58044000
C	-5.37930500	2.66000900	-6.03825300
H	-5.60059700	3.72092900	-6.17787300
H	-6.04219400	2.07791400	-6.68726300
H	-4.35430600	2.48175800	-6.38420400
C	-5.04921400	0.78628200	-4.42513500
H	-6.61897400	2.25639700	-4.33468500
H	-3.97972400	0.73322900	-4.66592100
H	-5.57963800	0.11296000	-5.10765000
H	-5.17180400	0.40375100	-3.40654200
H	-5.85574200	12.79004200	-6.69552800
H	-8.21610900	12.86089800	-5.20998100
H	-8.65458000	1.48096200	-0.24535900
H	-6.28963700	1.28632000	-1.70565100
C	-8.63832100	10.73073500	-3.71624600
C	-8.66136800	11.46157400	-2.52109100
C	-9.65917400	9.84797000	-4.08025000
C	-9.75668300	11.29378300	-1.67681500
C	-10.71093000	9.68249800	-3.17961800
C	-10.76469900	10.39868000	-1.99342900
H	-9.79660700	11.85151500	-0.74417700
H	-11.50325400	8.97927500	-3.41279500
H	-11.59662400	10.25196200	-1.31097400
C	-9.68216100	9.14842700	-5.42310700
C	-10.34418100	7.77750700	-5.33546600
H	-9.92035800	7.20426000	-4.50013500
H	-10.18137100	7.21355700	-6.25938900
H	-11.42850300	7.85931400	-5.19221700
C	-10.38767400	10.04378000	-6.44541300
H	-8.64596600	8.99468100	-5.75129000
H	-11.42345800	10.23436600	-6.13641100
H	-10.40983200	9.56868400	-7.43251700
H	-9.88515400	11.01370200	-6.54637000

C	-7.52319500	12.36517600	-2.08522400
C	-7.93899300	13.83556700	-2.15093400
H	-7.12313000	14.49019900	-1.82512600
H	-8.79702500	14.01499400	-1.49058700
H	-8.23380600	14.13569200	-3.16222400
C	-7.03700900	12.01757400	-0.67642400
H	-6.67759700	12.21063300	-2.76691900
H	-6.12002100	12.57162900	-0.44383400
H	-6.83045600	10.94732700	-0.57689400
H	-7.78083100	12.28785200	0.08230700
C	-6.21698400	8.15970800	-1.21774300
H	-6.64404300	7.31335600	-0.67056200
H	-5.28302500	7.80971500	-1.67735800
H	-5.96775200	8.93252200	-0.47665400
C	-7.66767400	5.68654500	-5.67515700
H	-7.34880500	5.09978200	-6.54616400
H	-8.67268700	5.34593000	-5.38982100
H	-7.75110500	6.73039400	-5.98927900

42. NHC_Full_C₂H₅_Cl (planar)-triplet:

N	-8.59574200	3.40699500	-1.02080600
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C	-6.99369500	2.06049400	-1.67267700
C	-8.12014400	2.11736100	-0.94185500
C	-7.87606300	4.15702100	-1.94347700
C	-7.08751300	6.43525300	-3.27886300
C	-7.14912300	7.80186700	-3.51857500
C	-6.79969200	5.53744800	-4.50283500
H	-7.06324200	4.50039800	-4.27228900
H	-5.72970400	5.53050300	-4.74291800
C	-7.21571400	8.68489900	-2.23101400
H	-8.22519500	8.82388500	-1.82591000
H	-6.84698400	9.68746100	-2.47387100
N	-7.52656600	10.93177100	-4.59234000
N	-5.67096400	10.85125800	-5.74976300
C	-7.41905500	12.10944400	-5.29987500
C	-6.27580100	12.06374100	-6.00684800
B	-6.31391300	8.59639900	-4.57246600
B	-7.93714800	5.67574300	-2.21762900
Cl	-9.34524000	6.55880200	-1.44442700
C	-6.40555600	10.11561700	-4.81464100
Cl	-4.83315600	7.82681800	-5.32522600
C	-9.82617200	3.77857200	-0.40096100
C	-11.01199200	3.72214900	-1.13802100
C	-9.76877300	4.22048800	0.92354500
C	-12.16461000	4.20810400	-0.52405400
C	-10.94859000	4.68611400	1.49832400
C	-12.13094400	4.70000900	0.77324300
H	-13.10111800	4.21123100	-1.07612000
H	-13.03929100	5.08642400	1.22703000
H	-10.93202300	5.06213200	2.51905100
C	-8.46679900	4.25349600	1.69865500
C	-8.58557800	3.52028200	3.03423100
H	-8.92974900	2.48902100	2.90434900
H	-9.29157400	4.02580700	3.70413800
H	-7.61473600	3.49588000	3.54257400

C	-7.99323000	5.69074600	1.92124800
H	-7.70228000	3.74052000	1.10301200
H	-7.01993400	5.69540700	2.42985400
H	-8.70417100	6.24011300	2.55237900
H	-7.89920700	6.23816700	0.97719300
C	-11.05945100	3.19484600	-2.56048200
C	-12.23819400	2.23993800	-2.76001400
H	-12.17468200	1.76101400	-3.74265500
H	-13.19479500	2.77402800	-2.72576000
H	-12.26482300	1.45636400	-1.99583700
C	-11.13357000	4.33567400	-3.58154100
H	-10.13499900	2.63051600	-2.74815000
H	-11.31345100	3.93563600	-4.58624800
H	-10.20901400	4.92199400	-3.60667200
H	-11.95678500	5.01879500	-3.33346800
C	-4.25506900	10.73082100	-5.97154000
C	-3.38417700	11.16001700	-4.96289500
C	-2.43287300	10.16861400	-7.40511900
C	-1.54434100	10.57604600	-6.41965700
C	-2.01526500	11.05898000	-5.20828000
H	-0.47434600	10.51063600	-6.59637000
H	-1.31176100	11.36840300	-4.43979400
C	-3.90585000	11.67025600	-3.63477400
C	-3.92612300	10.54649400	-2.59086300
H	-4.35174600	9.62201300	-2.99421300
H	-4.51775200	10.83856000	-1.71023300
H	-2.90380100	10.32556700	-2.25604900
C	-3.12456500	12.86929400	-3.10293100
H	-4.93728600	12.00695000	-3.79739800
H	-3.61466600	13.26589300	-2.20635500
H	-3.05676500	13.67531000	-3.84076100
H	-2.10550300	12.59088900	-2.81079400
C	-3.80801700	10.22517700	-7.19431000
C	-4.79034700	9.72048100	-8.23150100

C	-4.28615700	8.47082700	-8.94829400
H	-5.08088700	8.04838500	-9.57171200
H	-3.96725200	7.70578600	-8.23342200
H	-3.44409300	8.69723300	-9.61338500
C	-5.11433200	10.82062900	-9.24426500
H	-5.71228300	9.44916500	-7.69734600
H	-5.54977200	11.70325800	-8.76393100
H	-5.82348100	10.46331100	-9.99934500
H	-4.20073300	11.13928700	-9.76270300
H	-2.05138900	9.77702400	-8.34388700
N	-6.77746800	3.31637300	-2.20728500
C	-5.44076200	3.71311100	-2.55642100
C	-4.87950000	3.20392300	-3.73430100
C	-4.70815000	4.54174100	-1.67835900
C	-3.59696900	3.62209200	-4.08747000
C	-2.90966300	4.53602100	-3.30965000
C	-3.45619100	4.97614500	-2.11140500
H	-3.15102000	3.24593100	-5.00457800
H	-1.93154500	4.89098300	-3.62005100
H	-2.87882200	5.64512400	-1.48230900
C	-5.16637400	4.83050000	-0.25611000
C	-4.37599500	5.93177200	0.44912600
H	-3.37377400	5.57471900	0.71984400
H	-4.88424700	6.20100200	1.38167300
H	-4.26263700	6.83968600	-0.14344700
C	-5.02902200	3.56623700	0.60730800
H	-6.22812400	5.11727200	-0.27377600
H	-3.97913500	3.24829500	0.63939800
H	-5.62807000	2.72702600	0.24800500
H	-5.34230000	3.78625700	1.63773300
C	-5.61218500	2.23023500	-4.63865100
C	-5.55442400	2.64684000	-6.10987900
H	-5.84726800	3.69023100	-6.24982500
H	-6.21940000	2.01604300	-6.70930500

H	-4.54368000	2.52409000	-6.51592800
C	-5.01395700	0.82721500	-4.49185000
H	-6.66693200	2.20093000	-4.33453700
H	-3.95972800	0.83794900	-4.79717400
H	-5.53981500	0.10805000	-5.12970300
H	-5.04774100	0.45856400	-3.46138300
H	-5.80189500	12.78976100	-6.64737800
H	-8.19706800	12.85418200	-5.24223900
H	-8.64224100	1.37432000	-0.36071100
H	-6.27399200	1.27067400	-1.81464600
C	-8.64245300	10.74631800	-3.71035600
C	-8.66829600	11.49345200	-2.52352600
C	-9.66660200	9.85581600	-4.05413900
C	-9.76587200	11.34392100	-1.67918800
C	-10.71977600	9.70459900	-3.15185000
C	-10.77655800	10.44574500	-1.98133900
H	-9.80450200	11.91406000	-0.75394300
H	-11.51063600	8.99510200	-3.37008800
H	-11.61057200	10.31446300	-1.29809500
C	-9.67927800	9.14176800	-5.38887800
C	-10.46704800	7.83784200	-5.34227400
H	-10.15133100	7.22073700	-4.48952400
H	-10.30896300	7.26754700	-6.26298200
H	-11.54540600	8.02220400	-5.25850600
C	-10.24585100	10.07909000	-6.45992500
H	-8.64194600	8.90054000	-5.65853300
H	-11.27730700	10.36066700	-6.21212700
H	-10.25445500	9.59025100	-7.44067800
H	-9.65696600	10.99940100	-6.54588300
C	-7.51432300	12.37743200	-2.08950200
C	-7.87770700	13.85811900	-2.20804500
H	-7.04810100	14.49404200	-1.87949700
H	-8.74495500	14.08393900	-1.57404400
H	-8.13614500	14.13919000	-3.23410800

C	-7.07090600	12.06167900	-0.65888800
H	-6.66034800	12.16830000	-2.74630200
H	-6.13711200	12.58777200	-0.42730600
H	-6.90676900	10.98816700	-0.51748500
H	-7.81693100	12.38754300	0.07545700
C	-6.26982100	8.16255200	-1.15539000
H	-6.65417700	7.26758500	-0.65543800
H	-5.31363200	7.88943400	-1.62392700
H	-6.07340100	8.91306800	-0.37696100
C	-7.62461400	5.89443000	-5.73680700
H	-7.35939500	5.26100400	-6.59229200
H	-8.68797400	5.73393200	-5.52484500
H	-7.50031800	6.93633700	-6.05187400

43. NHC_Full_CH₃_Cl (fully optimized)-singlet:

N	-10.18146800	5.00708400	-1.79420100
C	-9.98829400	6.17514700	0.04986400
C	-10.84626400	5.41375500	-0.65729100
C	-8.90839300	5.51071200	-1.82519900
C	-6.63520400	6.04177400	-3.11999500
C	-5.29603000	5.65249900	-3.46599500
C	-6.96193300	7.51802300	-3.09205500

H	-7.98983100	7.68305100	-2.74329600
H	-6.92483100	7.94572800	-4.10244400
H	-6.27197200	8.11355200	-2.46747400
C	-4.95527400	4.18675900	-3.26637700
H	-5.32755300	3.54795700	-4.07710200
H	-5.40293300	3.78580300	-2.34784100
H	-3.87710100	4.02370100	-3.20479200
N	-1.82939100	5.38343500	-3.64231800
N	-2.28123000	5.91498000	-5.67809000
C	-0.72479900	5.05096800	-4.40374300
C	-1.00973600	5.38527600	-5.67863800
B	-4.22672600	6.48345200	-4.05017000
B	-7.77115500	5.14101200	-2.81599600
Cl	-7.96515500	3.39686200	-3.40153600
C	-2.80841900	5.91329200	-4.42636700
Cl	-4.32883200	8.22400600	-4.66327000
C	-10.87454500	4.47855800	-2.93154800
C	-11.23841200	3.12766600	-2.93676100
C	-11.18862200	5.35321100	-3.97799000
C	-11.95800100	2.65746100	-4.03176500
C	-11.88268100	4.82420800	-5.06706700
C	-12.27069700	3.49488600	-5.09269900
H	-12.25893500	1.61359500	-4.06111400
H	-12.81783200	3.10633300	-5.94698300
H	-12.12722500	5.47602200	-5.90264400
C	-10.82882200	6.82777700	-3.97840800
C	-12.07739800	7.69917600	-4.12700500
H	-12.81514800	7.48964600	-3.34529300
H	-12.56258900	7.53630800	-5.09656600
H	-11.80937700	8.75995800	-4.07102200
C	-9.81963800	7.13698000	-5.08584300
H	-10.36180800	7.08169900	-3.01691400
H	-9.51247700	8.18876900	-5.04415100
H	-10.26582300	6.95526400	-6.07218300

H	-8.92262400	6.51335300	-4.99262300
C	-10.86205700	2.19167400	-1.80598800
C	-12.06611800	1.94806000	-0.89254100
H	-11.80583000	1.27064800	-0.07158400
H	-12.88356500	1.48746600	-1.46257600
H	-12.45236800	2.87566400	-0.45679400
C	-10.32409900	0.85707400	-2.32117700
H	-10.06193500	2.67185400	-1.22719800
H	-9.93126000	0.26377700	-1.48874400
H	-9.52113800	1.00504900	-3.04816100
H	-11.11479800	0.26222200	-2.79371300
C	-2.95045100	6.36491500	-6.86418000
C	-3.97105900	5.58236400	-7.41251000
C	-3.12946800	7.97543000	-8.61860000
C	-4.12559600	7.20846600	-9.20432000
C	-4.54693300	6.03561400	-8.60092400
H	-4.58443400	7.53463900	-10.13342000
H	-5.33401100	5.44401300	-9.06117500
C	-4.43194300	4.26135500	-6.82612700
C	-5.94669700	4.23688600	-6.60876400
H	-6.27050000	5.03027900	-5.92469000
H	-6.25540600	3.27850500	-6.17597600
H	-6.48460300	4.35194100	-7.55726300
C	-4.00272800	3.11217800	-7.74305200
H	-3.95212800	4.11943400	-5.84907300
H	-4.30207900	2.14768800	-7.31884000
H	-2.91806400	3.09796100	-7.89874100
H	-4.47796000	3.20499000	-8.72775500
C	-2.53278200	7.57923500	-7.42488200
C	-1.48536300	8.46004800	-6.76910300
C	-1.90919600	9.92921400	-6.74813900
H	-1.20784300	10.51292500	-6.14257700
H	-2.91185100	10.05068300	-6.33066200
H	-1.89851800	10.36155200	-7.75555700

C	-0.13960200	8.32594600	-7.48653100
H	-1.37149700	8.13540300	-5.72407100
H	0.23762600	7.29829100	-7.48223400
H	0.61779600	8.96767500	-7.02283300
H	-0.24396000	8.63342200	-8.53513100
H	-2.81956000	8.90713400	-9.08416600
N	-8.80341900	6.23004700	-0.65746700
C	-7.71100700	7.04776900	-0.21257700
C	-6.50345600	6.45455500	0.18703300
C	-7.91860000	8.43409200	-0.16864300
C	-5.48815600	7.30339100	0.62279200
C	-5.68547600	8.67538700	0.72039900
C	-6.89153600	9.23107700	0.33905000
H	-4.52270500	6.88556700	0.89867400
H	-4.88455400	9.31240000	1.08586200
H	-7.03808000	10.30652000	0.40154000
C	-9.17413900	9.11501600	-0.68847000
C	-8.83766000	10.24596800	-1.66637700
H	-8.37236300	11.09194000	-1.14735700
H	-9.75357200	10.62202500	-2.13533400
H	-8.15320600	9.91806600	-2.45386800
C	-10.00990600	9.67805200	0.46382300
H	-9.77749900	8.37547200	-1.23267500
H	-9.42363200	10.41646600	1.02552200
H	-10.32561600	8.90498600	1.17144100
H	-10.90688300	10.18171600	0.08694000
C	-6.33384700	4.95033800	0.24689300
C	-4.87108900	4.52858700	0.18017600
H	-4.34486400	5.04126100	-0.63844200
H	-4.78923300	3.44720200	0.01682100
H	-4.34451100	4.75094600	1.11741500
C	-6.99441800	4.41712800	1.52245300
H	-6.84685500	4.51116100	-0.61832700
H	-6.51244700	4.84543500	2.41071000

H	-6.90328200	3.32668400	1.58013200
H	-8.06060500	4.66929300	1.56409800
H	-0.44811400	5.27932400	-6.59195500
H	0.15601500	4.62689500	-3.95101500
H	-11.87072200	5.13207400	-0.47711300
H	-10.08281300	6.66763100	1.00378100
C	-1.82327400	5.29758600	-2.21116100
C	-1.70318100	4.02993200	-1.61791700
C	-1.81796400	6.48214300	-1.45898100
C	-1.56501200	3.97333600	-0.23077800
C	-1.70772600	6.36172900	-0.07282300
C	-1.56927800	5.12511500	0.53768900
H	-1.45703000	3.00353600	0.24869900
H	-1.69652000	7.26679700	0.53042400
H	-1.46495500	5.05935600	1.61721800
C	-1.85431600	7.87456600	-2.05999100
C	-3.06236100	8.65056400	-1.53630600
H	-3.99082000	8.08620000	-1.68789600
H	-3.15718500	9.61223600	-2.05151900
H	-2.95445800	8.84974100	-0.46129400
C	-0.55499200	8.62377700	-1.75291100
H	-1.94751900	7.80282500	-3.15014300
H	-0.42693500	8.76453200	-0.67279500
H	-0.57166800	9.61644000	-2.21532900
H	0.32414900	8.08708300	-2.12525000
C	-1.68976000	2.72920000	-2.40395400
C	-0.29917200	2.08932400	-2.35981200
H	-0.28052300	1.15817600	-2.93629600
H	-0.02606700	1.84698300	-1.32523700
H	0.48010700	2.74987400	-2.75443500
C	-2.72508300	1.73881500	-1.86435600
H	-1.94402600	2.94378700	-3.45056200
H	-2.76880500	0.85003500	-2.50273200
H	-3.72449200	2.18088100	-1.82153500

H -2.45851700 1.40082000 -0.85610300

44. NHC_Full_CH₃_Cl (fully optimized)-triplet:

N -9.83959600 4.52111800 -1.20208200
C -10.60159800 6.58343800 -1.09123100
C -10.84882200 5.31973700 -0.70248500
C -8.91883900 5.28779000 -1.91240900
C -6.67833000 5.74156300 -3.46136200
C -5.33482800 5.84253400 -3.23741200
C -7.28176000 6.41442900 -4.68246900
H -8.27684200 6.00357000 -4.90532100
H -6.65003600 6.26874000 -5.57249500
H -7.38727600 7.50009700 -4.56190000
C -4.71553900 5.16893600 -2.02531700
H -4.77344900 4.07167000 -2.06415300

H	-5.21939900	5.48085200	-1.10049900
H	-3.65793000	5.44785200	-1.92192900
N	-2.59740300	5.01358800	-4.88354100
N	-2.08129100	7.08884400	-5.31344700
C	-1.40703900	5.01289100	-5.57828100
C	-1.08827900	6.29400300	-5.84484700
B	-4.38304000	6.73966600	-4.08994500
B	-7.63567200	4.84595100	-2.60129000
Cl	-7.26652400	3.05001100	-2.53808400
C	-3.05096200	6.31092600	-4.69349800
Cl	-4.81719300	8.51131400	-4.25662000
C	-9.58637700	3.25859100	-0.57041300
C	-8.89284200	3.26670500	0.64053500
C	-10.04893000	2.08782900	-1.17568000
C	-8.69210100	2.04074300	1.27628900
C	-9.83663500	0.88926000	-0.50182500
C	-9.16985100	0.86689300	0.71749800
H	-8.14162100	2.01302900	2.21448800
H	-9.00629700	-0.07977700	1.22495300
H	-10.17431300	-0.04314300	-0.94434600
C	-10.70883700	2.14601700	-2.53742400
C	-12.21418100	2.37960700	-2.39461800
H	-12.43059500	3.30729400	-1.85389400
H	-12.67626400	1.55256900	-1.84075800
H	-12.69769100	2.44024900	-3.37612800
C	-10.43293900	0.90216400	-3.37462100
H	-10.27088500	3.00546500	-3.06622700
H	-10.79159400	1.04934600	-4.39831800
H	-10.95099600	0.02096100	-2.97722800
H	-9.36046600	0.68377600	-3.41451200
C	-8.28206700	4.52962400	1.21484100
C	-8.76507100	4.81201100	2.63506000
H	-8.31568500	5.73688200	3.01542400
H	-8.48414400	4.00310600	3.32052300

H	-9.85436100	4.92222000	2.67415700
C	-6.75640500	4.42192600	1.15394200
H	-8.57685800	5.38177400	0.59060000
H	-6.28340500	5.38608200	1.38979200
H	-6.42991500	4.10874900	0.15557600
H	-6.38827500	3.68117200	1.87593600
C	-1.87042200	8.49402900	-5.12777200
C	-2.35566400	9.38154400	-6.09228700
C	-0.98072200	10.28355100	-3.82232000
C	-1.43728000	11.18493900	-4.77082800
C	-2.11528400	10.73817100	-5.89736200
H	-1.27150000	12.24918100	-4.62795200
H	-2.48452800	11.45799400	-6.62173800
C	-3.14521900	8.87048700	-7.28014100
C	-4.23668900	9.84073600	-7.72018400
H	-4.86434200	10.13955900	-6.87445400
H	-4.87690100	9.36909500	-8.47251100
H	-3.81624100	10.74387500	-8.17886600
C	-2.20752600	8.55424600	-8.44761000
H	-3.63834600	7.93939600	-6.96418600
H	-2.76839800	8.17568800	-9.30943700
H	-1.45813100	7.80293400	-8.17691100
H	-1.67476100	9.46056500	-8.76264700
C	-1.17981800	8.91238900	-3.98609700
C	-0.72253000	7.92864400	-2.92684900
C	-1.73931800	7.87234400	-1.78142500
H	-1.49656700	7.06014800	-1.08212900
H	-2.75813200	7.71251000	-2.15217400
H	-1.73184800	8.81726400	-1.22195000
C	0.66905000	8.24732200	-2.38407300
H	-0.67359600	6.93348100	-3.38900200
H	1.40761700	8.34944300	-3.18572400
H	1.00261400	7.45032900	-1.71096400
H	0.67169500	9.17645800	-1.80278400

H	-0.46448800	10.64613900	-2.93738100
N	-9.42475100	6.57703600	-1.81050900
C	-8.90052100	7.78874900	-2.35509100
C	-7.75098700	8.35435000	-1.78023000
C	-9.59924900	8.40070500	-3.40331900
C	-7.30782400	9.56824000	-2.29626900
C	-7.99816900	10.21037200	-3.31544700
C	-9.13588200	9.63629200	-3.85656000
H	-6.39932000	10.01447700	-1.90526500
H	-7.63486800	11.16034600	-3.69676800
H	-9.66224600	10.13609900	-4.66601500
C	-10.78690000	7.75038100	-4.08954500
C	-10.65157400	7.79629300	-5.61481800
H	-10.79600500	8.81514800	-5.99279600
H	-11.41921200	7.16988600	-6.08141700
H	-9.67020900	7.45072000	-5.95087100
C	-12.09823200	8.43278600	-3.68978900
H	-10.82348600	6.69486800	-3.78475000
H	-12.06349000	9.49423800	-3.96763100
H	-12.29201900	8.37951200	-2.61460800
H	-12.94907800	7.97892600	-4.21005000
C	-7.06451800	7.70514800	-0.59385900
C	-5.60107600	8.10828300	-0.44499000
H	-5.05082700	7.98699500	-1.38625400
H	-5.12176500	7.48155300	0.31735700
H	-5.49857300	9.15010800	-0.11653200
C	-7.82828600	8.03159100	0.69528400
H	-7.09090200	6.61494800	-0.74159400
H	-7.80213200	9.11133000	0.89012000
H	-7.36828900	7.52401500	1.55392600
H	-8.87969600	7.72403500	0.64716700
H	-0.24156400	6.73093000	-6.34922200
H	-0.92943900	4.08480800	-5.84719300
H	-11.62822700	4.89926500	-0.08731700

H	-11.12810000	7.50603500	-0.90956900
C	-3.12957800	3.80143400	-4.33904400
C	-4.25749400	3.22111500	-4.93401300
C	-2.45971600	3.21610200	-3.25571600
C	-4.69948500	2.00479800	-4.42142400
C	-2.92175000	1.98084100	-2.80179800
C	-4.03116000	1.38257800	-3.37638200
H	-5.59142000	1.54472200	-4.83420900
H	-2.42068000	1.50053000	-1.96520200
H	-4.39309200	0.43214200	-2.99485800
C	-1.31424000	3.90429000	-2.53394200
C	-1.45229900	3.80513400	-1.01139200
H	-2.45715900	4.06762500	-0.66798900
H	-0.73314400	4.47454600	-0.52582200
H	-1.23059900	2.79101600	-0.65828500
C	0.04067800	3.32000200	-2.94243800
H	-1.34324600	4.97173200	-2.80157100
H	0.06539400	2.24760900	-2.70872900
H	0.85511000	3.80126700	-2.38911100
H	0.24513100	3.43310100	-4.01028800
C	-4.92513800	3.86721400	-6.13113900
C	-4.15696200	3.50762200	-7.40712800
H	-4.61533200	3.98088600	-8.28290100
H	-4.17215900	2.42156700	-7.56422600
H	-3.11009100	3.82665100	-7.36075000
C	-6.39495500	3.48777500	-6.27647900
H	-4.87316000	4.95730700	-5.99326400
H	-6.86676500	4.11284000	-7.04232300
H	-6.94213800	3.62257200	-5.33669400
H	-6.51139900	2.44463500	-6.59653700

45. NHC_Full_CH₃_Cl (twisted)-singlet:

N	-9.58836700	4.66891800	-0.63369100
C	-10.67282400	6.58382900	-0.63121700
C	-10.73538800	5.30895300	-0.20641000
C	-8.78876400	5.53745400	-1.36860100
C	-6.43307800	6.22645900	-2.78434100
C	-6.46189600	6.25662800	-4.14367600
C	-5.46858300	7.10774900	-2.02946700
H	-5.97751100	8.00372900	-1.64120200
H	-4.64279100	7.46259200	-2.66472300
H	-5.03366400	6.58716400	-1.16390700
C	-7.40896700	5.34208200	-4.88428200
H	-7.79479400	5.79806600	-5.80669000
H	-8.26686400	5.04420700	-4.26321500
H	-6.90108500	4.40910700	-5.17135500
N	-3.46607600	5.68573400	-5.67164600
N	-3.28518700	7.76977700	-6.26030000
C	-2.35217200	5.79368400	-6.47354200

C	-2.23055800	7.08785200	-6.82542800
B	-5.48936400	7.18041900	-4.97378900
B	-7.40168900	5.30594400	-1.94683800
Cl	-6.70270200	3.63084000	-1.65409600
C	-4.09938300	6.91318600	-5.53243400
Cl	-5.99710400	8.95029300	-5.00899800
C	-9.43789700	3.25961100	-0.44877200
C	-9.09890100	2.80166300	0.83204800
C	-9.66411300	2.40136700	-1.52764100
C	-8.97646800	1.42524100	1.00862600
C	-9.52926000	1.03302000	-1.30002000
C	-9.18549500	0.54941300	-0.04854800
H	-8.70879800	1.02885500	1.98271500
H	-9.08260800	-0.52047100	0.10980200
H	-9.70112600	0.33983600	-2.11992700
C	-10.06431400	2.90116400	-2.90237000
C	-11.54471900	2.59746100	-3.14598400
H	-12.18051000	3.06396400	-2.38501500
H	-11.72369300	1.51492800	-3.11215000
H	-11.86318900	2.96070100	-4.12941000
C	-9.19977100	2.29769300	-4.01172900
H	-9.93021400	3.99059200	-2.93563800
H	-9.45133300	2.75587200	-4.97527400
H	-9.37386400	1.21913900	-4.11022500
H	-8.13133900	2.45994900	-3.82609200
C	-8.79632000	3.77845600	1.95651900
C	-8.89994900	3.15011400	3.34236900
H	-8.81880700	3.92508100	4.11078700
H	-8.08417500	2.43912300	3.51954400
H	-9.84762200	2.62098700	3.48924200
C	-7.40340800	4.39188300	1.76999000
H	-9.52830700	4.59916400	1.90846100
H	-7.16982900	5.06508800	2.60423000
H	-7.31789000	4.95971800	0.83726000

H	-6.64256300	3.60190700	1.74252900
C	-3.34059200	9.19377800	-6.34971900
C	-3.86727600	9.75625200	-7.51350800
C	-2.82534600	11.34373800	-5.45945700
C	-3.29246100	11.92978800	-6.62707500
C	-3.81935700	11.14275500	-7.64070700
H	-3.26197000	13.00987400	-6.74009800
H	-4.21412900	11.60995200	-8.53998100
C	-4.52476000	8.90236800	-8.57933600
C	-5.91963400	9.42678200	-8.92008100
H	-6.53293600	9.52219600	-8.01830000
H	-6.42439800	8.74479200	-9.61277400
H	-5.87123000	10.40789800	-9.40734000
C	-3.64896600	8.82863900	-9.83023200
H	-4.64641300	7.88721000	-8.17340600
H	-4.12187900	8.22093100	-10.60961300
H	-2.66613100	8.39641600	-9.61033700
H	-3.48593100	9.83385300	-10.24032100
C	-2.84393500	9.96033700	-5.29335900
C	-2.36697600	9.34296100	-3.99332300
C	-3.09260800	9.95823900	-2.79423700
H	-2.82063100	9.43031300	-1.87321100
H	-4.18071600	9.90239800	-2.91436900
H	-2.81573700	11.01150700	-2.66218400
C	-0.85207600	9.49809300	-3.85289600
H	-2.60382800	8.26907800	-4.00590900
H	-0.32053700	9.01966900	-4.68304900
H	-0.49671000	9.05369000	-2.91678600
H	-0.57438400	10.56002000	-3.84658800
H	-2.43892200	11.96904500	-4.65765700
N	-9.50770500	6.72187700	-1.35447600
C	-8.93762200	8.00478200	-1.61198600
C	-8.31230300	8.65943200	-0.54738300
C	-9.07217000	8.55942400	-2.88948900

C	-7.79929400	9.93401300	-0.79791100
C	-7.89815600	10.50190200	-2.05841700
C	-8.53342700	9.82528200	-3.09359200
H	-7.30932300	10.47922200	0.00628000
H	-7.47738300	11.48674200	-2.24101600
H	-8.58736400	10.27908200	-4.07817600
C	-9.85125000	7.81263000	-3.95524600
C	-9.48488300	8.19567100	-5.38281200
H	-9.79350400	9.22391100	-5.61108300
H	-10.01272500	7.54140000	-6.08524600
H	-8.41271400	8.11405800	-5.56994200
C	-11.35392300	8.03776500	-3.74852300
H	-9.63827200	6.74135000	-3.82104800
H	-11.58690300	9.10595400	-3.84298600
H	-11.69808800	7.70403900	-2.76599300
H	-11.93268100	7.49971700	-4.50786100
C	-8.21170400	8.05468900	0.84357300
C	-6.76487700	7.96720300	1.32607200
H	-6.18516500	7.28169100	0.69932000
H	-6.72990100	7.59667400	2.35707700
H	-6.27127400	8.94629600	1.30844600
C	-9.06665800	8.86353700	1.82147600
H	-8.60335100	7.02715000	0.82095000
H	-8.70576100	9.89728600	1.89093600
H	-9.03059900	8.42770800	2.82594700
H	-10.11411400	8.90000900	1.50050700
H	-1.48003600	7.61090500	-7.39632500
H	-1.74333600	4.93170600	-6.69247000
H	-11.48834600	4.77157400	0.34759300
H	-11.33403400	7.42256800	-0.48272100
C	-4.00938900	4.41585400	-5.31039600
C	-4.68996400	3.68638400	-6.29166200
C	-3.78320900	3.93420000	-4.01378700
C	-5.16085800	2.42062700	-5.93697800

C	-4.29337200	2.67840700	-3.70187000
C	-4.97831800	1.93152300	-4.65314900
H	-5.69025800	1.82159800	-6.67377400
H	-4.17211700	2.28479200	-2.69784000
H	-5.37140800	0.95435400	-4.38619700
C	-2.94630600	4.74069100	-3.03772200
C	-3.15927600	4.36320800	-1.57730800
H	-4.21378800	4.36313100	-1.29703400
H	-2.62699000	5.07148900	-0.93349600
H	-2.74881900	3.36762500	-1.36401800
C	-1.45656200	4.58256700	-3.36924700
H	-3.22274200	5.79882700	-3.16582000
H	-1.16833300	3.52681800	-3.28793000
H	-0.84529000	5.15049700	-2.65871700
H	-1.20393400	4.92540000	-4.37540000
C	-4.90089100	4.21818800	-7.69872400
C	-3.91000700	3.55640600	-8.66166300
H	-4.04611100	3.93010900	-9.68264100
H	-4.07409100	2.47098500	-8.67521500
H	-2.86935000	3.72971300	-8.37132600
C	-6.32401800	3.99003800	-8.20816400
H	-4.71992000	5.30403900	-7.69092600
H	-6.45373300	4.47215400	-9.18289800
H	-7.07313800	4.39487300	-7.52365500
H	-6.53192500	2.92296300	-8.34927200

46. NHC_Full_CH₃_Cl (twisted)-triplet:

N	-9.59568500	4.60159100	-0.84190600
C	-10.54122400	6.55414800	-0.49217600
C	-10.68484000	5.23134400	-0.27915300
C	-8.74406900	5.52242100	-1.43381200
C	-6.34516700	6.28148000	-2.68119000
C	-6.36991400	6.47130200	-4.02551200
C	-5.41732700	7.10199600	-1.81342700
H	-5.83069400	8.11138800	-1.66143500
H	-4.42496900	7.23963300	-2.26959400
H	-5.28005100	6.64892000	-0.82436600
C	-7.32371700	5.64863200	-4.86946600
H	-7.43126300	6.04036300	-5.89087200
H	-8.32757900	5.57591500	-4.43021300
H	-6.95970100	4.61591200	-4.94493000
N	-3.40982400	5.82977200	-5.34703200
N	-3.06306100	7.91848100	-5.88620200
C	-2.16064200	5.91462800	-5.92677700
C	-1.95204500	7.19857900	-6.27397900
B	-5.36066400	7.45096800	-4.72156400
B	-7.36162600	5.29811600	-2.00119500
Cl	-6.72127200	3.57185900	-1.98958500
C	-3.99115800	7.08997300	-5.26336300

Cl	-5.73040300	9.23826700	-4.54709200
C	-9.52085900	3.17778500	-0.89605700
C	-9.11547700	2.50336500	0.25785100
C	-9.86510100	2.51375500	-2.07744200
C	-9.13144500	1.11013100	0.23571300
C	-9.85355900	1.12073200	-2.05680200
C	-9.50616000	0.42326100	-0.90888900
H	-8.82808300	0.56001800	1.12374900
H	-9.51178100	-0.66309800	-0.91251500
H	-10.12296400	0.57626600	-2.95903300
C	-10.22245800	3.24515300	-3.35663400
C	-11.71054300	3.07685300	-3.66826500
H	-12.33742200	3.46399700	-2.85749300
H	-11.95626000	2.01557900	-3.80282600
H	-11.97998200	3.60252600	-4.59100300
C	-9.36516000	2.75852700	-4.52989500
H	-10.01880300	4.31585500	-3.21836900
H	-9.52652800	3.39534400	-5.40863900
H	-9.63277500	1.73332700	-4.81492900
H	-8.29653400	2.77726700	-4.28221900
C	-8.60760300	3.24316800	1.47964400
C	-9.58425000	3.10295900	2.64710700
H	-9.21733000	3.62935300	3.53510100
H	-9.71283900	2.04589300	2.91349900
H	-10.57311900	3.50390900	2.39720900
C	-7.21408300	2.74944000	1.87035000
H	-8.51896600	4.30817500	1.22235800
H	-6.81237200	3.35007600	2.69367900
H	-6.52433600	2.81459300	1.02284900
H	-7.24104600	1.70704100	2.20955400
C	-3.35687700	9.19034500	-6.47231700
C	-4.01985600	9.20456500	-7.70144200
C	-3.29618100	11.57300500	-6.38999700
C	-3.94819100	11.61950200	-7.61614700

C	-4.31576300	10.44903300	-8.25902200
H	-4.18487600	12.58032600	-8.06475200
H	-4.84797100	10.49397200	-9.20684700
C	-4.45747400	7.93380800	-8.40309700
C	-5.98307400	7.80558600	-8.38558100
H	-6.37827300	7.85844400	-7.36123400
H	-6.29108500	6.84737800	-8.82822000
H	-6.44872000	8.61045000	-8.96903100
C	-3.92855500	7.87288000	-9.83586100
H	-4.04374300	7.07452900	-7.86042800
H	-4.21890700	6.92989200	-10.31302700
H	-2.83648900	7.94815300	-9.86549300
H	-4.33694500	8.68637200	-10.44714100
C	-3.00231700	10.35502400	-5.78534900
C	-2.38048600	10.26897200	-4.40655100
C	-2.79217100	11.42892000	-3.50631000
H	-2.45390700	11.24752300	-2.48115500
H	-3.88039100	11.55016600	-3.49235300
H	-2.34102900	12.37473600	-3.83004900
C	-0.85626600	10.18032200	-4.50551000
H	-2.75652200	9.34301200	-3.94538400
H	-0.53585200	9.30972600	-5.08732700
H	-0.40207500	10.10661700	-3.51103400
H	-0.45470600	11.07682500	-4.99475400
H	-3.04304000	12.49946600	-5.88325800
N	-9.37389500	6.73804500	-1.19936200
C	-8.78458300	8.02908000	-1.36524100
C	-8.13360700	8.60990900	-0.27046800
C	-8.93366900	8.67878700	-2.59582000
C	-7.64236800	9.90632700	-0.43199600
C	-7.77011400	10.56906800	-1.64271000
C	-8.40650800	9.96041400	-2.71632500
H	-7.13787300	10.39280300	0.39883800
H	-7.36333400	11.57003200	-1.75569900

H	-8.47668800	10.48046900	-3.66699300
C	-9.72893000	8.02918900	-3.70949200
C	-9.26751900	8.42145700	-5.10849300
H	-9.51347400	9.46681900	-5.33306300
H	-9.77931400	7.80381300	-5.85485300
H	-8.18851800	8.29559300	-5.23573100
C	-11.21270500	8.37030500	-3.53342900
H	-9.61615900	6.94178400	-3.60305800
H	-11.35791300	9.45644500	-3.59377300
H	-11.59800300	8.03382600	-2.56504800
H	-11.81726200	7.90401000	-4.31962500
C	-7.97447500	7.88844300	1.05543100
C	-6.58923400	8.09867500	1.66848100
H	-5.78894800	7.91066400	0.94834400
H	-6.44966100	7.42973700	2.52385500
H	-6.47335600	9.12281300	2.04262500
C	-9.03632200	8.36368100	2.05255500
H	-8.10725700	6.80952900	0.87772400
H	-8.93003200	9.44375200	2.21816000
H	-8.91664500	7.86201000	3.01943800
H	-10.05445100	8.17914100	1.69838500
H	-1.13285500	7.67625900	-6.78677200
H	-1.55527800	5.03154300	-6.05479100
H	-11.47036900	4.65962400	0.18868900
H	-11.16223800	7.39302400	-0.22270500
C	-3.92425900	4.55235500	-4.94388200
C	-4.74338100	3.83590500	-5.83206600
C	-3.46332400	4.00444900	-3.74245400
C	-5.08920500	2.53203100	-5.47950300
C	-3.80306800	2.68382800	-3.45439400
C	-4.60707300	1.95403100	-4.31276800
H	-5.73861000	1.95692800	-6.13332400
H	-3.46024900	2.23909400	-2.52362800
H	-4.88172800	0.93324700	-4.06295600

C	-2.62187800	4.80398700	-2.76871900
C	-3.09950800	4.60674800	-1.32851700
H	-4.18986100	4.65016700	-1.25678200
H	-2.67148500	5.37559900	-0.67593400
H	-2.77722200	3.63375300	-0.93716900
C	-1.14420700	4.41938500	-2.87835200
H	-2.72992500	5.86739700	-3.02502300
H	-1.02275500	3.34684800	-2.67766100
H	-0.54372000	4.96816300	-2.14407400
H	-0.73201300	4.62365300	-3.87145500
C	-5.23462600	4.46007200	-7.12618000
C	-4.17832100	4.38040100	-8.23439100
H	-4.55530800	4.86876200	-9.14347700
H	-3.96731500	3.33233900	-8.48145500
H	-3.23466500	4.86236500	-7.96368100
C	-6.52387700	3.83344800	-7.65648200
H	-5.43199100	5.52296200	-6.91560000
H	-6.93181600	4.45653800	-8.46084800
H	-7.29497800	3.72295900	-6.88713100
H	-6.33232900	2.84250400	-8.08704100

47. NHC_Full_CH₃_Cl (planar)-singlet:

N	-9.88160600	4.44133300	-1.30462400
C	-10.79856700	6.42664200	-1.15199100
C	-11.00149200	5.12365100	-0.88959700
C	-8.96153700	5.29206500	-1.89664900
C	-6.53648600	5.98307000	-2.89965000
C	-5.17642000	5.70668400	-3.22358600
C	-7.23653600	6.93777900	-3.88754100
H	-8.29554900	6.68334300	-4.00491300
H	-6.77850200	6.80054700	-4.87992200
H	-7.16517900	8.00613700	-3.66541900
C	-4.47627800	4.75181200	-2.23599200
H	-4.54791500	3.68348300	-2.45820400
H	-4.93400600	4.88906800	-1.24346900
H	-3.41719200	5.00604600	-2.11889300
N	-2.16244100	5.14697800	-4.39624400
N	-1.83145300	7.24878900	-4.81869500
C	-0.91475200	5.26340900	-4.97207300
C	-0.71176200	6.56643300	-5.23420600
B	-4.23491400	6.69047500	-3.87010400
B	-7.47813400	4.99941900	-2.25313500
C	-2.75150300	6.39800400	-4.22665500
C	-9.69028700	3.10195200	-0.82296000
C	-9.22352800	2.95330600	0.48367900
C	-9.99551800	2.02265200	-1.65486500
C	-9.08865000	1.65225700	0.97037800
C	-9.85661500	0.74523700	-1.12317000
C	-9.41217200	0.56173100	0.18084900

H	-8.70754900	1.49930900	1.97760300
H	-9.30041800	-0.44420200	0.57567600
H	-10.07347700	-0.12042600	-1.74173300
C	-10.39973900	2.26088700	-3.09463000
C	-11.91343500	2.45801100	-3.20259200
H	-12.25898300	3.29718700	-2.58897900
H	-12.43873000	1.55623600	-2.86338400
H	-12.21152100	2.65245500	-4.23893000
C	-9.93210600	1.14710500	-4.02464700
H	-9.90169500	3.18684300	-3.41713800
H	-10.10433700	1.43087300	-5.06769500
H	-10.48182600	0.21412000	-3.85103400
H	-8.86289700	0.94921100	-3.89433100
C	-8.77438700	4.12930700	1.33082300
C	-9.43312900	4.13277100	2.70943700
H	-9.13845000	5.03049200	3.26561200
H	-9.12621500	3.26405100	3.30393300
H	-10.52579900	4.11987000	2.63616800
C	-7.24778600	4.12194300	1.46435600
H	-9.06730600	5.06160300	0.82995500
H	-6.91153300	4.96135000	2.08576100
H	-6.75286300	4.19230000	0.48755900
H	-6.90930500	3.19438300	1.94340900
C	-2.02281100	8.58828100	-5.30007700
C	-2.48926800	8.73725900	-6.60679100
C	-1.85669600	10.94493100	-4.99918800
C	-2.30070500	11.12875000	-6.30331900
C	-2.62395500	10.03842700	-7.09323200
H	-2.41237600	12.13478300	-6.69791500
H	-3.00480700	10.19162800	-8.10051200
C	-2.93864300	7.56148300	-7.45412600
C	-4.46530300	7.56896400	-7.58711800
H	-4.95990800	7.49811700	-6.61019800
H	-4.80180400	6.72991700	-8.20888100

H	-4.80388700	8.49681700	-8.06553300
C	-2.28043200	7.55835000	-8.83299000
H	-2.64560600	6.62904600	-6.95358800
H	-2.57498600	6.66054900	-9.38909700
H	-1.18773900	7.57167600	-8.76016700
H	-2.58793600	8.42696700	-9.42733400
C	-1.71782100	9.66738500	-4.46781300
C	-1.31380400	9.42865000	-3.02807100
C	-1.78011200	10.54285100	-2.09792000
H	-1.60834700	10.25869300	-1.05490500
H	-2.84905900	10.74213600	-2.22830400
H	-1.22918800	11.47517000	-2.27131800
C	0.19968300	9.22982000	-2.92020000
H	-1.81285200	8.50320800	-2.70562900
H	0.54428400	8.39036500	-3.53395700
H	0.49757100	9.03485800	-1.88390100
H	0.72597400	10.13107100	-3.25924800
H	-1.64014900	11.81045300	-4.38032600
N	-9.55076100	6.54305000	-1.72757500
C	-8.99128200	7.85895300	-1.85312500
C	-7.95651300	8.25710200	-0.99560800
C	-9.55416300	8.72765900	-2.79736300
C	-7.46223300	9.55155400	-1.14150300
C	-8.00790600	10.43503600	-2.06130000
C	-9.05687600	10.02783800	-2.86809300
H	-6.64539200	9.87614400	-0.50343300
H	-7.61165700	11.44233000	-2.14846400
H	-9.48133800	10.71710100	-3.59411200
C	-10.61572900	8.29071800	-3.78998400
C	-10.19353300	8.60967100	-5.22780100
H	-10.19756300	9.69086600	-5.40816900
H	-10.89540500	8.16032700	-5.93863400
H	-9.18899800	8.23679300	-5.44830200
C	-11.95783300	8.96259800	-3.49079900

H	-10.73834200	7.20234100	-3.70978400
H	-11.85521000	10.05346100	-3.55329700
H	-12.33059600	8.72632600	-2.48869700
H	-12.71933000	8.65726600	-4.21691100
C	-7.42222300	7.37555300	0.11316800
C	-5.90704200	7.48378200	0.27037600
H	-5.40803100	7.39925100	-0.70434400
H	-5.53999400	6.67719100	0.91682200
H	-5.60596400	8.43153200	0.73371200
C	-8.16247000	7.69735400	1.41414600
H	-7.63180600	6.33535200	-0.14327700
H	-8.00092400	8.74199700	1.71030500
H	-7.81400800	7.05578600	2.23410400
H	-9.24492100	7.54429200	1.30087400
H	0.10768400	7.08969000	-5.70025800
H	-0.30951000	4.38940300	-5.14969500
H	-11.82101000	4.60041700	-0.42364200
H	-11.40394100	7.30063000	-0.97473200
C	-2.72190700	3.83105500	-4.27081400
C	-3.75673400	3.43303700	-5.12832300
C	-2.15886200	2.96215700	-3.32685200
C	-4.25095700	2.13853900	-4.98264600
C	-2.65611400	1.66195300	-3.25632100
C	-3.70517300	1.25489600	-4.06307000
H	-5.06782100	1.81402600	-5.62072400
H	-2.23152400	0.97254500	-2.53051300
H	-4.10138500	0.24757400	-3.97606300
C	-1.09709000	3.39888500	-2.33436200
C	-1.51904400	3.07974900	-0.89651300
H	-2.52350100	3.45269500	-0.67576600
H	-0.81699500	3.52891400	-0.18574300
H	-1.51509000	1.99852500	-0.71631200
C	0.24491000	2.72695000	-2.63389000
H	-0.97442500	4.48726700	-2.41442800

H	0.14221000	1.63608500	-2.57153000
H	1.00656100	3.03211600	-1.90787000
H	0.61751100	2.96333800	-3.63602400
C	-4.29108900	4.31481500	-6.23688400
C	-3.55092300	3.99332900	-7.53798300
H	-3.89938700	4.63516500	-8.35773100
H	-3.71254800	2.94878100	-7.83443700
H	-2.46845800	4.14629500	-7.42471900
C	-5.80626600	4.20660300	-6.39403000
H	-4.08146700	5.35495700	-5.98020500
H	-6.17333200	5.01314200	-7.04052800
H	-6.30522300	4.29120000	-5.41929200
H	-6.10737400	3.25882400	-6.85728400
Cl	-4.65082200	8.48617200	-3.94576900
Cl	-7.06243900	3.20372200	-2.17672000

48. NHC_Full_CH₃_Cl (planar)-triplet:

N	-9.91978400	4.41706800	-1.37099200
C	-10.77863400	6.42223800	-1.11232000
C	-11.00817200	5.11424600	-0.89746700
C	-8.98694700	5.27304300	-1.94825400
C	-6.51387600	6.00260300	-2.92730200
C	-5.19915800	5.68727500	-3.19597900
C	-7.17897900	6.89301400	-3.99621700
H	-8.21931600	6.58761900	-4.17576600
H	-6.64345500	6.77746800	-4.95156000
H	-7.18130300	7.96263300	-3.76802600
C	-4.53388000	4.79684500	-2.12715900
H	-4.53201900	3.72715600	-2.35516400
H	-5.06900700	4.91277600	-1.17164100
H	-3.49336500	5.10189900	-1.94802300
N	-2.17009800	5.15526100	-4.40849000
N	-1.79344700	7.27298900	-4.75229400
C	-0.93466900	5.26779600	-5.01100400
C	-0.70507100	6.57578200	-5.22581100
B	-4.20040200	6.70102100	-3.84887000
B	-7.51280900	4.98902100	-2.27441600
Cl	-7.13603400	3.19929600	-2.48728900
C	-2.72628600	6.41702300	-4.17503500
Cl	-4.57730900	8.49068500	-3.63600200
C	-9.70018000	3.07679300	-0.91270000
C	-9.15434300	2.91409000	0.36110500
C	-10.04052700	2.00344000	-1.73968100
C	-8.98595100	1.60912700	0.82647300
C	-9.86348000	0.72080600	-1.23181700
C	-9.34748400	0.52549400	0.04394900
H	-8.55213700	1.44869200	1.81130900
H	-9.20957800	-0.48419300	0.42065300
H	-10.10828400	-0.13952300	-1.84742300

C	-10.52876400	2.25535600	-3.15080600
C	-12.04628700	2.45098300	-3.16801200
H	-12.35510500	3.28521600	-2.52889900
H	-12.54996300	1.54603700	-2.80531200
H	-12.40511500	2.65292600	-4.18351100
C	-10.11599000	1.15203500	-4.11844200
H	-10.05224400	3.18639600	-3.49078200
H	-10.34864000	1.44634300	-5.14676200
H	-10.65425500	0.21668400	-3.92302900
H	-9.04105600	0.95264900	-4.05297700
C	-8.67721000	4.08521600	1.19802500
C	-9.35847100	4.12425100	2.56468000
H	-9.02124200	4.99866600	3.13385100
H	-9.11949600	3.23217400	3.15637400
H	-10.44831400	4.18028200	2.46792900
C	-7.15413600	4.03387500	1.34633700
H	-8.93231800	5.01793900	0.67939900
H	-6.79014300	4.90562500	1.90497800
H	-6.65870700	4.01566800	0.36706200
H	-6.84582100	3.13442800	1.89432900
C	-2.01294900	8.61329000	-5.21056300
C	-2.55868800	8.77601700	-6.48441400
C	-1.84937200	10.96928300	-4.89154100
C	-2.36528900	11.16460700	-6.16733300
C	-2.72690500	10.08098200	-6.94983100
H	-2.50306300	12.17429500	-6.54408300
H	-3.16064400	10.24144000	-7.93469200
C	-3.03586100	7.60490700	-7.32135200
C	-4.55892100	7.65638700	-7.46976400
H	-5.05440200	7.67451400	-6.49051900
H	-4.92299300	6.78476000	-8.02853200
H	-4.86712000	8.55593800	-8.01764800
C	-2.35453400	7.56578000	-8.68797200
H	-2.78083500	6.67216000	-6.80270100

H	-2.69182200	6.69138300	-9.25713400
H	-1.26470100	7.50964000	-8.59116100
H	-2.59338300	8.45786100	-9.27970800
C	-1.67251100	9.68664700	-4.38360900
C	-1.18423300	9.43481400	-2.97248300
C	-1.59678500	10.53822600	-2.00485300
H	-1.36409700	10.24390100	-0.97654700
H	-2.67167900	10.73780800	-2.07022500
H	-1.05836300	11.47347600	-2.20031800
C	0.33328800	9.23911100	-2.95542200
H	-1.66075800	8.50381800	-2.63240700
H	0.64198900	8.40476300	-3.59444100
H	0.69223600	9.03731900	-1.93993500
H	0.83694500	10.14398900	-3.31833100
H	-1.60446900	11.82960500	-4.27596700
N	-9.54322600	6.53478500	-1.71483800
C	-8.96481400	7.82934600	-1.90123800
C	-7.86560900	8.21875300	-1.11833200
C	-9.54680000	8.68115700	-2.84983800
C	-7.32812600	9.48327900	-1.34913300
C	-7.89463800	10.34982100	-2.27278900
C	-9.00626000	9.95698200	-3.00029900
H	-6.45391100	9.79708100	-0.78723200
H	-7.46249400	11.33405600	-2.42778100
H	-9.44287900	10.63477200	-3.72994700
C	-10.67437400	8.24370500	-3.76651800
C	-10.33241600	8.51124700	-5.23551100
H	-10.32505200	9.58614400	-5.45003300
H	-11.08398000	8.05617000	-5.88956100
H	-9.35064800	8.10976800	-5.50357400
C	-11.98007200	8.95743300	-3.40872000
H	-10.81712600	7.16142800	-3.64797300
H	-11.85403200	10.04319000	-3.50819600
H	-12.29743400	8.75800900	-2.38001900

H	-12.79074800	8.65257900	-4.07970500
C	-7.32317500	7.35405300	0.00189900
C	-5.82489200	7.53324300	0.22903500
H	-5.27465800	7.47886000	-0.71994300
H	-5.45336600	6.73964800	0.88870300
H	-5.59014600	8.48991400	0.71222000
C	-8.12501900	7.62298300	1.27904800
H	-7.47023100	6.30306800	-0.26780400
H	-8.01859100	8.66944600	1.59274000
H	-7.77508300	6.98595000	2.10222600
H	-9.19495600	7.42341500	1.12911100
H	0.11723800	7.09343800	-5.69341900
H	-0.35147400	4.38927200	-5.23515900
H	-11.83044700	4.59656500	-0.42982800
H	-11.36186000	7.30075100	-0.88821200
C	-2.74855400	3.86071700	-4.22229500
C	-3.84768800	3.47139100	-5.00527300
C	-2.16651400	3.00870700	-3.27389100
C	-4.38501900	2.20673300	-4.77486800
C	-2.70692800	1.73279200	-3.12375400
C	-3.81846800	1.33999900	-3.85141000
H	-5.25912100	1.89297000	-5.33696600
H	-2.27020100	1.05484900	-2.39430600
H	-4.25048700	0.35566200	-3.69671700
C	-1.03879500	3.44588400	-2.35727700
C	-1.38049500	3.17802300	-0.88829400
H	-2.36193700	3.58001500	-0.61981000
H	-0.62846400	3.63242400	-0.23430600
H	-1.38846000	2.10306700	-0.67411300
C	0.26676500	2.73213700	-2.71554800
H	-0.89598600	4.52817300	-2.47558700
H	0.14070700	1.64637800	-2.61606800
H	1.07770800	3.03694000	-2.04486200
H	0.58373200	2.93156100	-3.74438000

C	-4.39011800	4.33627700	-6.12533900
C	-3.58851600	4.06716700	-7.40259500
H	-3.93837600	4.70424300	-8.22576000
H	-3.69517500	3.02071200	-7.71623700
H	-2.51852000	4.26653500	-7.25273500
C	-5.88850600	4.15745300	-6.35211000
H	-4.24278100	5.38721900	-5.85561600
H	-6.26009600	4.95129600	-7.01145200
H	-6.43840300	4.21168200	-5.40292800
H	-6.12361000	3.20095600	-6.83545400

49. NHC_Full_H_CI (fully optimized)-singlet:

N	-8.66435100	3.59956800	-0.90844400
C	-6.82988100	2.40244400	-0.98573800
C	-8.02446000	2.50332100	-0.37024000

C	-7.89266900	4.19898500	-1.87519200
C	-7.21609600	6.14209700	-3.60518300
C	-7.33816400	7.45972200	-4.09021700
N	-7.53236600	10.56645900	-4.77978500
N	-5.54692400	10.62995800	-5.64214800
C	-7.30147500	11.86449500	-5.18638600
C	-6.06783000	11.90549900	-5.72172600
B	-6.28859600	8.25634100	-4.75443400
B	-8.15858100	5.51284800	-2.65415200
Cl	-9.69649000	6.43818600	-2.22581400
C	-6.44456200	9.76533700	-5.05813400
Cl	-4.67281600	7.46373200	-5.14678800
C	-10.04101800	3.87333600	-0.63930800
C	-10.98702700	3.46121600	-1.57881400
C	-10.36868500	4.54562300	0.54500700
C	-12.31958000	3.78587400	-1.32396500
C	-11.71234700	4.84135500	0.75378600
C	-12.67595300	4.47661600	-0.17903400
H	-13.08326600	3.49589300	-2.04198300
H	-13.71779000	4.72849200	-0.00167600
H	-12.01532500	5.37092500	1.65110100
C	-9.28876700	4.98148800	1.52218900
C	-9.83354300	5.26854100	2.91792200
H	-10.45427300	4.45052700	3.29883900
H	-10.43638500	6.18446800	2.92821500
H	-9.00583600	5.42397300	3.61658300
C	-8.52702600	6.21091400	1.00798000
H	-8.56563900	4.15619600	1.61214500
H	-7.82177500	6.56062500	1.77127700
H	-9.22505100	7.02723700	0.78068000
H	-7.96379200	6.00985200	0.09010200
C	-10.63124200	2.70358800	-2.84635300
C	-11.33123200	1.34303300	-2.87099900
H	-11.03662800	0.77727300	-3.76188700

H	-12.42092800	1.46289200	-2.90290500
H	-11.08779500	0.74392300	-1.98732500
C	-10.99731300	3.51486000	-4.09140600
H	-9.54570400	2.52221500	-2.86870900
H	-10.77201000	2.94339300	-4.99874300
H	-10.45012400	4.46211600	-4.13276300
H	-12.07020500	3.74373800	-4.10124100
C	-4.13161800	10.43459400	-5.77601900
C	-3.33025700	10.78093700	-4.68623300
C	-2.24263800	9.78811500	-7.07358700
C	-1.41438200	10.14133400	-6.01530400
C	-1.95150600	10.62047500	-4.83180100
H	-0.33864200	10.02221000	-6.11059900
H	-1.29701800	10.85819700	-3.99657000
C	-3.91204200	11.19040300	-3.34483800
C	-3.81340100	10.00166400	-2.38466000
H	-4.32444400	9.12474900	-2.79651500
H	-4.26121300	10.24260100	-1.41085100
H	-2.76251500	9.73033300	-2.21696600
C	-3.23579600	12.42527700	-2.75502100
H	-4.97787300	11.42958300	-3.47136100
H	-3.73806500	12.71909000	-1.82601100
H	-3.26677400	13.27633000	-3.44319000
H	-2.18574800	12.23078200	-2.50739300
C	-3.62352600	9.91921300	-6.97028100
C	-4.56505900	9.48351800	-8.07382300
C	-4.00821700	8.32844000	-8.89759100
H	-4.77669400	7.94759400	-9.57748600
H	-3.68398300	7.50590700	-8.25133400
H	-3.15891300	8.64238600	-9.51656900
C	-4.91982700	10.67082500	-8.97184500
H	-5.48492400	9.12504700	-7.58851600
H	-5.37968100	11.48691500	-8.40366500
H	-5.62006700	10.37153400	-9.75961700

H	-4.01659300	11.06532600	-9.45420300
H	-1.80787500	9.38086000	-7.98118800
N	-6.75892600	3.42517500	-1.90281000
C	-5.62532900	3.60046000	-2.75352100
C	-5.57981600	2.87333000	-3.94796400
C	-4.62802800	4.49861600	-2.36482600
C	-4.48595000	3.08908700	-4.78478000
C	-3.48021200	3.97454500	-4.42682900
C	-3.54442000	4.66129100	-3.22488400
H	-4.42585300	2.56112100	-5.73216300
H	-2.64131900	4.13788600	-5.09705800
H	-2.75681300	5.36287700	-2.96180300
C	-4.70365600	5.29690000	-1.07849400
C	-4.53581600	6.79243400	-1.34669000
H	-3.55149100	7.01418200	-1.77893100
H	-4.61802400	7.35834300	-0.41031000
H	-5.29945000	7.15864900	-2.04422000
C	-3.64783200	4.79575500	-0.09109100
H	-5.69673400	5.14967100	-0.63181800
H	-2.64117900	4.92455300	-0.50895900
H	-3.77876400	3.73142600	0.13577600
H	-3.69389100	5.35546300	0.84959200
C	-6.70609700	1.94489100	-4.36104800
C	-7.69542100	2.69572200	-5.25640800
H	-8.09418900	3.58930200	-4.76173200
H	-8.53189100	2.04364600	-5.53841100
H	-7.19430600	3.02397900	-6.17627600
C	-6.20400000	0.68582700	-5.06487200
H	-7.24369000	1.62858700	-3.45488700
H	-5.79662800	0.91655000	-6.05581500
H	-7.03060500	-0.01563800	-5.21775200
H	-5.42331100	0.17621900	-4.49055300
H	-5.48521600	12.71390700	-6.13281200
H	-8.05673900	12.62226600	-5.05131800

H	-8.49859100	1.90368300	0.38955200
H	-6.01741400	1.70242500	-0.87625400
C	-8.72809300	10.25770600	-4.04631800
C	-8.64657000	10.13466400	-2.65341300
C	-9.93382500	10.15254000	-4.74922300
C	-9.83241000	9.92010900	-1.95725800
C	-11.09272900	9.93156700	-4.00450500
C	-11.04371100	9.82428800	-2.62386000
H	-9.80084000	9.79983400	-0.87810500
H	-12.04584000	9.83632500	-4.51459300
H	-11.95633200	9.64280900	-2.06368200
C	-9.96374100	10.17463500	-6.26550400
C	-9.56521100	8.79246300	-6.79346500
H	-8.57115500	8.49057300	-6.44776500
H	-9.57669100	8.77684100	-7.88951300
H	-10.27653500	8.03904000	-6.43214300
C	-11.31538200	10.58633500	-6.84004900
H	-9.21661500	10.90089400	-6.61631500
H	-12.07095900	9.80852200	-6.67934600
H	-11.23342200	10.72946500	-7.92199400
H	-11.68892200	11.51698200	-6.39927900
C	-7.32124900	10.21070600	-1.92348900
C	-7.05241600	11.63917200	-1.44621700
H	-6.06932000	11.71060700	-0.96116200
H	-7.81141900	11.96122700	-0.72143300
H	-7.06685800	12.34870000	-2.28456700
C	-7.22887100	9.19874700	-0.78387800
H	-6.53376500	9.93624000	-2.63239600
H	-6.20820500	9.18848500	-0.38265600
H	-7.46879900	8.18732200	-1.14337800
H	-7.90142200	9.44146100	0.04857400
H	-8.29499600	7.92650200	-3.86055900
H	-6.29661900	5.63826700	-3.90591800

50. NHC_Full_H_CI (fully optimized)-triplet:

N	-8.54450200	3.50495900	-0.79932900
C	-6.70184100	2.36340500	-1.16356800
C	-7.87083600	2.34044400	-0.49371300
C	-7.81750200	4.27760800	-1.68554200
C	-7.34718400	6.33929000	-3.39144400
C	-7.67057300	7.50943200	-4.01409500
N	-7.48139200	10.67906700	-4.83045000
N	-5.64326900	10.38137000	-5.97735000

C	-7.06384300	11.91505300	-5.27463400
C	-5.91729900	11.73696500	-5.96041900
B	-6.74383600	8.19028200	-5.04008700
B	-8.16560200	5.63668400	-2.30059600
Cl	-9.68576700	6.48853300	-1.74946900
C	-6.63108800	9.68546900	-5.28883200
Cl	-5.56758800	7.10678800	-5.92364000
C	-9.92797600	3.69224500	-0.50594900
C	-10.85790200	3.38459700	-1.50087100
C	-10.28044900	4.20903700	0.74605900
C	-12.19697500	3.66442700	-1.22964200
C	-11.63052000	4.46016100	0.97325500
C	-12.57647600	4.20643600	-0.01293000
H	-12.94777500	3.45673000	-1.98885700
H	-13.62346900	4.42482300	0.17811000
H	-11.95069700	4.86864800	1.92661200
C	-9.21430500	4.53423700	1.77816000
C	-9.75597500	4.55134300	3.20428200
H	-10.33030400	3.64912000	3.44012800
H	-10.40502200	5.41898100	3.37245600
H	-8.93043300	4.62872300	3.91855800
C	-8.53546800	5.87543500	1.46943800
H	-8.44320400	3.75040800	1.72116700
H	-7.79953400	6.11329600	2.24768800
H	-9.28094100	6.68041000	1.44323000
H	-8.02525200	5.87735400	0.50006400
C	-10.46701600	2.77575000	-2.83598400
C	-11.17792000	1.43564800	-3.04009300
H	-10.85580000	0.96986900	-3.97768900
H	-12.26465100	1.57120300	-3.09722900
H	-10.97214900	0.73829500	-2.22133700
C	-10.77954800	3.72394600	-3.99598700
H	-9.38404000	2.58211500	-2.83885200
H	-10.50237900	3.26051200	-4.95005800

H	-10.24139200	4.67381200	-3.90762600
H	-11.85332900	3.94768200	-4.03243800
C	-4.30422500	9.89203300	-6.12580300
C	-3.49915400	9.83411700	-4.98532600
C	-2.59003400	8.93014700	-7.47834700
C	-1.76366500	8.86470500	-6.36348200
C	-2.21730100	9.30128100	-5.12904600
H	-0.76108800	8.45665800	-6.45839100
H	-1.57057500	9.23114700	-4.25669800
C	-3.97928600	10.28178500	-3.61808200
C	-4.10127200	9.08652800	-2.66929800
H	-4.75071600	8.29260300	-3.07070000
H	-4.51262300	9.41041000	-1.70218000
H	-3.11234700	8.64532700	-2.47878700
C	-3.05453600	11.34345900	-3.02116300
H	-4.97399900	10.73547700	-3.71762200
H	-3.44159800	11.68600300	-2.05437200
H	-2.96170200	12.21351600	-3.67943800
H	-2.04765500	10.94458800	-2.84861600
C	-3.88538300	9.42767700	-7.37603700
C	-4.85105100	9.40635200	-8.54259500
C	-4.59293500	8.24485100	-9.49608800
H	-5.40379400	8.17144100	-10.22775900
H	-4.53303400	7.29520300	-8.95392100
H	-3.66295200	8.38126000	-10.06133000
C	-4.82178400	10.73742200	-9.29639700
H	-5.85560100	9.26828600	-8.11612900
H	-5.08039100	11.57928000	-8.64563100
H	-5.52826000	10.72995300	-10.13402000
H	-3.81918900	10.92335700	-9.70190000
H	-2.23271700	8.55336400	-8.43193300
N	-6.66947400	3.52874000	-1.89963100
C	-5.47204900	4.03916800	-2.48613700
C	-5.14301400	3.66258900	-3.79490900

C	-4.71816400	4.95090900	-1.74467000
C	-4.04975700	4.29138600	-4.38508100
C	-3.31686800	5.24824800	-3.69365800
C	-3.63156500	5.55328200	-2.37998700
H	-3.78583200	4.05915000	-5.41200400
H	-2.49541000	5.75978300	-4.18875400
H	-3.03689000	6.28243700	-1.83348400
C	-5.05225000	5.32836600	-0.31487200
C	-5.32453900	6.83000500	-0.22051600
H	-4.39459300	7.39972600	-0.35347900
H	-5.74197200	7.09705200	0.75814700
H	-6.02774400	7.14923700	-1.00100600
C	-3.92453200	4.91759000	0.63257500
H	-5.96359500	4.79712800	-0.00559200
H	-2.98820500	5.42290700	0.36536200
H	-3.74161300	3.83830300	0.60042200
H	-4.16708100	5.19372700	1.66469400
C	-6.01420600	2.68935600	-4.56733800
C	-7.22921900	3.42032000	-5.15128900
H	-7.88656800	3.81804800	-4.37117600
H	-7.81543500	2.74329500	-5.78477300
H	-6.90089300	4.27259800	-5.76209700
C	-5.25696800	1.97251000	-5.68090800
H	-6.38065200	1.92866200	-3.86055800
H	-5.02884000	2.65560300	-6.50737000
H	-5.87264900	1.16785000	-6.09472000
H	-4.31471500	1.53828500	-5.32974300
H	-5.24309300	12.44477400	-6.41500500
H	-7.63499800	12.80282600	-5.05391200
H	-8.31048600	1.60322400	0.15866300
H	-5.87287900	1.67425600	-1.18380600
C	-8.72072800	10.46770900	-4.15228700
C	-8.70842700	10.31366500	-2.75603300
C	-9.88218900	10.34942900	-4.91771700

C	-9.92842700	10.08726700	-2.12713300
C	-11.08038300	10.11260500	-4.24030300
C	-11.10435000	9.99562700	-2.86178300
H	-9.95940300	9.92932800	-1.05419100
H	-11.99837800	9.99192000	-4.81046100
H	-12.04236000	9.79686200	-2.35146200
C	-9.85652800	10.34175200	-6.43340200
C	-10.05657400	8.90410500	-6.92243100
H	-9.30014700	8.23307600	-6.49813500
H	-9.99824700	8.84987900	-8.01530700
H	-11.04312600	8.53292000	-6.61624300
C	-10.90668000	11.27142300	-7.03881800
H	-8.86858100	10.67938100	-6.77243200
H	-11.92261700	10.93639600	-6.79968200
H	-10.82080400	11.28438400	-8.13051300
H	-10.80002900	12.29888400	-6.67591000
C	-7.39312800	10.27303800	-2.00070200
C	-6.78650600	11.66302000	-1.79324500
H	-5.79899600	11.57336300	-1.31963200
H	-7.42016500	12.26596300	-1.13073600
H	-6.65639900	12.21349700	-2.73056800
C	-7.49555400	9.55281300	-0.66095000
H	-6.70350400	9.68559000	-2.62619600
H	-6.49450400	9.44680200	-0.22548300
H	-7.93158000	8.55073100	-0.77082500
H	-8.09978800	10.11930900	0.05918800
H	-8.61430600	7.97126500	-3.71351800
H	-6.40428300	5.89740000	-3.71836600

51. NHC_Full_H_Cl (twisted)-singlet:

N	-9.50183700	4.75543600	-0.35734900
C	-10.61674000	6.63026300	-0.64615300
C	-10.68463100	5.41107500	-0.07861500
C	-8.69719600	5.53379200	-1.17441600
C	-6.49074200	6.26336300	-2.56785300
C	-6.48157400	6.21519200	-3.91202600
N	-3.45454100	5.93406900	-5.11302100
N	-3.58113100	7.79541600	-6.24997200
C	-2.27023000	6.08247100	-5.80357900
C	-2.33816000	7.24032500	-6.49058600
B	-5.71209700	7.16657400	-4.87148500
B	-7.27826800	5.28729900	-1.63895900
Cl	-6.41966100	3.80090100	-1.03618900

C	-4.31120600	6.98051000	-5.39558300
Cl	-6.75250000	8.42799800	-5.69403400
C	-9.38625100	3.33493900	-0.23020500
C	-8.83683100	2.81482000	0.94567500
C	-9.79254400	2.53255500	-1.29945900
C	-8.75519900	1.43086100	1.06306000
C	-9.67052600	1.15073000	-1.14537900
C	-9.17366600	0.60560000	0.02711300
H	-8.33131500	0.99138200	1.96117800
H	-9.09067700	-0.47289600	0.12914000
H	-9.96188400	0.49770300	-1.96489000
C	-10.27032800	3.10559800	-2.62070900
C	-11.59800800	2.49600700	-3.06946300
H	-12.37789200	2.61724700	-2.31074900
H	-11.49775900	1.42475300	-3.27988400
H	-11.94069900	2.97701600	-3.99245400
C	-9.19477700	2.88778300	-3.69156600
H	-10.42754200	4.18788500	-2.50534100
H	-9.50313100	3.32660400	-4.64877300
H	-9.02863900	1.81389800	-3.84906200
H	-8.23514100	3.33472200	-3.39779700
C	-8.29748200	3.74359200	2.01471800
C	-9.38485800	4.08757000	3.03439400
H	-9.00061600	4.76390200	3.80615000
H	-9.74024600	3.17560000	3.53084900
H	-10.24778500	4.56948300	2.56308200
C	-7.06911600	3.17181000	2.71565000
H	-7.98737500	4.66964300	1.50626600
H	-6.61594100	3.93155900	3.36056800
H	-6.31749600	2.84317500	1.99032100
H	-7.32701100	2.32054100	3.35710000
C	-3.82311400	9.19854300	-6.40523500
C	-4.42870800	9.66040600	-7.57755500
C	-3.74813100	11.40387800	-5.49319400

C	-4.32336600	11.89259400	-6.65474600
C	-4.65709100	11.02843500	-7.68969900
H	-4.52529800	12.95563300	-6.75297100
H	-5.13108000	11.42175100	-8.58399700
C	-4.85663100	8.68623100	-8.65525800
C	-6.12571400	9.12961500	-9.37546000
H	-6.91936400	9.37514700	-8.66217700
H	-6.48681900	8.32896400	-10.02887300
H	-5.94732200	10.00517200	-10.01133200
C	-3.72137600	8.46193000	-9.65630800
H	-5.07459700	7.73247600	-8.15377700
H	-4.01840900	7.75030300	-10.43482900
H	-2.82093700	8.07265600	-9.16943300
H	-3.45450900	9.40704900	-10.14612200
C	-3.47655100	10.04296300	-5.34667300
C	-2.84739300	9.53338300	-4.06401500
C	-3.81119600	9.68316900	-2.88360200
H	-3.36276800	9.25676700	-1.97375600
H	-4.76774800	9.17231200	-3.07300700
H	-4.02625100	10.74224500	-2.68529000
C	-1.52645200	10.24623300	-3.77188400
H	-2.62424400	8.46473400	-4.17950600
H	-0.82037200	10.14067000	-4.60216700
H	-1.05909600	9.83240800	-2.87099600
H	-1.68058500	11.31770500	-3.59760700
H	-3.50343100	12.08434000	-4.68026600
N	-9.40304500	6.72266300	-1.29831200
C	-8.96017200	7.93624000	-1.91488600
C	-7.93483800	8.68069100	-1.31347800
C	-9.60901400	8.35119000	-3.08819900
C	-7.53672100	9.85579500	-1.95166100
C	-8.16973400	10.29309700	-3.10436700
C	-9.20471200	9.55594300	-3.65716700
H	-6.72670300	10.44521800	-1.53240500

H	-7.84151000	11.20865100	-3.58762500
H	-9.67209300	9.90121800	-4.57315900
C	-10.63984000	7.46563400	-3.76754100
C	-9.92554100	6.30815000	-4.47218500
H	-9.26302200	6.69908300	-5.25577300
H	-10.65270700	5.62654200	-4.93416000
H	-9.30288500	5.73394600	-3.77897300
C	-11.52258200	8.21090300	-4.76219200
H	-11.29700500	7.03337400	-2.99905900
H	-10.94922200	8.52421700	-5.64265700
H	-11.98502500	9.10154300	-4.32316200
H	-12.32113200	7.55245500	-5.11812600
C	-7.31840400	8.26025100	0.00867300
C	-5.93887900	8.86349700	0.25150600
H	-5.27600300	8.71889700	-0.61006900
H	-5.47162100	8.39088800	1.12171800
H	-5.99605500	9.93955900	0.45892200
C	-8.25774300	8.62082900	1.16406600
H	-7.19733500	7.16626900	0.00099000
H	-8.41846600	9.70582700	1.19692800
H	-7.82602100	8.31503000	2.12393800
H	-9.23523100	8.13770400	1.06559200
H	-1.61476000	7.74505500	-7.11012900
H	-1.49165200	5.34000200	-5.72604900
H	-11.46464400	4.92908200	0.48818400
H	-11.29800600	7.46610000	-0.62973300
C	-3.69111500	4.79539500	-4.27682700
C	-4.22289300	3.64234400	-4.85266900
C	-3.31166000	4.86476800	-2.92862600
C	-4.24331700	2.48318900	-4.07441000
C	-3.33065000	3.68132000	-2.19927200
C	-3.76250700	2.49407500	-2.77661000
H	-4.63709600	1.56305300	-4.49864400
H	-3.05421500	3.69465300	-1.14914500

H	-3.77765400	1.58244900	-2.18624300
C	-2.98047200	6.20126700	-2.29041600
C	-3.35926700	6.25613600	-0.81121600
H	-4.38585800	5.91225300	-0.63307200
H	-3.26937300	7.28728000	-0.44699900
H	-2.68554300	5.64358800	-0.19902300
C	-1.51110000	6.59656200	-2.45211800
H	-3.59850500	6.94932600	-2.81177800
H	-0.86190300	5.88553400	-1.92552800
H	-1.33985200	7.59101500	-2.01702500
H	-1.19554000	6.63191200	-3.50005500
C	-4.75458800	3.63519900	-6.27112200
C	-3.74583000	2.98252100	-7.21786900
H	-4.11975500	2.96912500	-8.24773700
H	-3.55779200	1.94493800	-6.91240100
H	-2.78611400	3.51153400	-7.21129400
C	-6.10846900	2.93099500	-6.35610700
H	-4.90488400	4.67837400	-6.58183700
H	-6.54310400	3.05912700	-7.35300400
H	-6.81321300	3.33090100	-5.61792800
H	-6.01347500	1.85304100	-6.18022900
H	-5.86133900	7.04846600	-2.11407800
H	-7.11775200	5.44119400	-4.37611900

52. NHC_Full_H_Cl (twisted)-triplet:

N	-9.50184800	4.75611400	-0.36500600
C	-10.61326600	6.63430700	-0.64271100
C	-10.68238700	5.41284100	-0.08032600
C	-8.69715700	5.53571400	-1.18111500
C	-6.48906400	6.27167800	-2.56990100
C	-6.48264200	6.21248800	-3.91420100
N	-3.45632900	5.93156900	-5.10554600
N	-3.57845800	7.79209700	-6.24523900
C	-2.26997600	6.07901600	-5.79307400
C	-2.33524200	7.23599000	-6.48170300
B	-5.71422900	7.16493400	-4.87373000
B	-7.27583500	5.29377700	-1.64123100
Cl	-6.43145600	3.77752100	-1.09577900
C	-4.31153200	6.97909500	-5.39117100
Cl	-6.74708200	8.44542400	-5.67429800
C	-9.38902000	3.33502500	-0.24255500
C	-8.82436700	2.81077700	0.92410900
C	-9.81173700	2.53691200	-1.30841000

C	-8.74495000	1.42636200	1.03700800
C	-9.69234000	1.15430300	-1.15912900
C	-9.18104000	0.60499700	0.00517100
H	-8.30911200	0.98327600	1.92756200
H	-9.09990300	-0.47399600	0.10342400
H	-9.99600300	0.50395900	-1.97626700
C	-10.29995200	3.11526500	-2.62367200
C	-11.63166000	2.50863200	-3.06422000
H	-12.40530000	2.62691800	-2.29867800
H	-11.53381500	1.43826600	-3.28017400
H	-11.98159100	2.99372500	-3.98228600
C	-9.23224200	2.89938500	-3.70267200
H	-10.45429100	4.19773100	-2.50410800
H	-9.55000000	3.33384700	-4.65860100
H	-9.06173900	1.82592200	-3.85800100
H	-8.27296200	3.35188200	-3.41699900
C	-8.26670300	3.73677700	1.98618500
C	-9.34120100	4.09207000	3.01556400
H	-8.94409500	4.76767900	3.78142100
H	-9.69872200	3.18439200	3.51826800
H	-10.20490700	4.57938800	2.55123300
C	-7.03605600	3.15642100	2.67573300
H	-7.95396700	4.65938200	1.47283500
H	-6.57072800	3.91343200	3.31516800
H	-6.29423000	2.82122200	1.94329000
H	-7.29411300	2.30788200	3.32075200
C	-3.81991800	9.19480100	-6.40429000
C	-4.42712000	9.65303700	-7.57721900
C	-3.74624800	11.40248400	-5.49798100
C	-4.32167600	11.88780200	-6.66083400
C	-4.65603200	11.02063300	-7.69311600
H	-4.52408400	12.95048700	-6.76190200
H	-5.13146800	11.41133400	-8.58776100
C	-4.85871300	8.67444200	-8.64951300

C	-6.12459200	9.11969600	-9.37404500
H	-6.91796400	9.37345800	-8.66330000
H	-6.48878600	8.31685000	-10.02302400
H	-5.94110300	9.99050600	-10.01498500
C	-3.72372100	8.43695200	-9.64779400
H	-5.08252400	7.72512800	-8.14194300
H	-4.02404700	7.72167800	-10.42169800
H	-2.82606200	8.04583600	-9.15736100
H	-3.45110900	9.37714000	-10.14385600
C	-3.47426400	10.04205400	-5.34780400
C	-2.84935500	9.53511100	-4.06207100
C	-3.81935400	9.68383400	-2.88643700
H	-3.37427400	9.25923400	-1.97411200
H	-4.77424400	9.17121300	-3.07965000
H	-4.03753600	10.74268500	-2.69026200
C	-1.53162700	10.25124200	-3.76375300
H	-2.62334600	8.46682200	-4.17562000
H	-0.82129800	10.14735200	-4.59058500
H	-1.06758500	9.83870800	-2.86057200
H	-1.68918700	11.32233300	-3.59024200
H	-3.50255600	12.08519000	-4.68664600
N	-9.40139000	6.72684100	-1.29797700
C	-8.96195100	7.94254900	-1.91319200
C	-7.93952100	8.68959100	-1.31032100
C	-9.61368700	8.35839400	-3.08447000
C	-7.54663400	9.86830400	-1.94515500
C	-8.18282100	10.30658500	-3.09565000
C	-9.21498900	9.56669600	-3.65002800
H	-6.73838100	10.45953100	-1.52502200
H	-7.85891500	11.22506600	-3.57627500
H	-9.68490400	9.91299100	-4.56434900
C	-10.64164700	7.47074100	-3.76528000
C	-9.92343000	6.31858700	-4.47457900
H	-9.25951000	6.71465200	-5.25441300

H	-10.64859000	5.63875300	-4.94211700
H	-9.30198800	5.74110400	-3.78293400
C	-11.52888200	8.21560700	-4.75622200
H	-11.29580600	7.03320600	-2.99711000
H	-10.95821700	8.53384600	-5.63666300
H	-11.99407700	9.10309700	-4.31373200
H	-12.32544500	7.55514900	-5.11286300
C	-7.32045000	8.26679500	0.00966100
C	-5.94215000	8.87287500	0.25186600
H	-5.28110800	8.73363900	-0.61191200
H	-5.47142400	8.39822200	1.11910300
H	-6.00194800	9.94796600	0.46352700
C	-8.25853100	8.62178300	1.16777300
H	-7.19682300	7.17298400	-0.00173900
H	-8.42138600	9.70635100	1.20430400
H	-7.82435600	8.31392400	2.12588800
H	-9.23516200	8.13692900	1.06979600
H	-1.60989000	7.73932700	-7.10010100
H	-1.49192900	5.33631400	-5.71227100
H	-11.46156700	4.92998400	0.48692100
H	-11.29291800	7.47136800	-0.62170800
C	-3.68857300	4.79362200	-4.26652700
C	-4.20860300	3.63458400	-4.84116200
C	-3.30709800	4.86639900	-2.91925000
C	-4.21167600	2.47455200	-4.06411100
C	-3.30898500	3.68221800	-2.19060400
C	-3.72614600	2.48985100	-2.76804800
H	-4.59566500	1.55012500	-4.48806300
H	-3.02829500	3.69831000	-1.14159400
H	-3.72610800	1.57706000	-2.17927000
C	-2.98777500	6.20569000	-2.28150700
C	-3.37802200	6.26011400	-0.80524100
H	-4.40461700	5.91154500	-0.63520100
H	-3.29577400	7.29188800	-0.44107700

H	-2.70644800	5.65110500	-0.18725600
C	-1.51901700	6.60664000	-2.43428700
H	-3.60538300	6.95009700	-2.80840400
H	-0.87040100	5.89892200	-1.90248700
H	-1.35393700	7.60261100	-2.00031000
H	-1.19755300	6.64064100	-3.48062700
C	-4.74744600	3.62312400	-6.25680000
C	-3.73926500	2.97872800	-7.20968600
H	-4.11944400	2.96198200	-8.23721300
H	-3.54077300	1.94277200	-6.90528100
H	-2.78397900	3.51572200	-7.20920000
C	-6.09605500	2.90775000	-6.33306100
H	-4.90814400	4.66522600	-6.56612500
H	-6.53869200	3.03262800	-7.32685000
H	-6.79889600	3.30124700	-5.58959500
H	-5.99075000	1.83059500	-6.15812200
H	-5.87206500	7.06941800	-2.12281900
H	-7.10790900	5.42619900	-4.37149600

53. NHC_Full_H_CI (planar)-singlet:

N	-8.74363500	3.47600900	-0.95959200
C	-6.89792400	2.30068400	-1.07689800
C	-8.14204700	2.30096800	-0.56032600
C	-7.90323200	4.21701900	-1.75466700
C	-7.10680800	6.33907900	-3.14930800
C	-7.23334800	7.63921700	-3.66710000
N	-7.51263500	10.60767400	-4.79110500
N	-5.62353500	10.51900900	-5.84956900
C	-7.32589500	11.82984400	-5.40358900
C	-6.15124900	11.77747800	-6.05893600
B	-6.24747700	8.33091200	-4.51960700
B	-8.09661000	5.65276500	-2.29708000
Cl	-9.61108600	6.57196300	-1.79231100
C	-6.45408500	9.76428400	-5.05369500
Cl	-4.70171700	7.44400900	-4.98531700
C	-10.14317300	3.71247400	-0.78953800
C	-10.98276900	3.52993500	-1.89052200
C	-10.60210700	4.12209200	0.46951900
C	-12.33445100	3.82862300	-1.71640500
C	-11.96044000	4.39779500	0.59192500
C	-12.81545900	4.26767000	-0.49578000
H	-13.01406400	3.71592600	-2.55794100
H	-13.87008100	4.50227400	-0.38199500

H	-12.35971100	4.72853000	1.54505000
C	-9.63773500	4.31431600	1.62812700
C	-10.33174200	4.31554100	2.98647800
H	-10.98919900	3.44965800	3.11893000
H	-10.93300400	5.22201800	3.12470500
H	-9.58511100	4.30342600	3.78637200
C	-8.82667800	5.60561200	1.46661000
H	-8.92934400	3.47235300	1.62092700
H	-8.18401000	5.75620400	2.34171000
H	-9.49984500	6.46657100	1.37930000
H	-8.19453700	5.60186100	0.57279100
C	-10.50019600	3.03332900	-3.24244400
C	-11.22093800	1.74013800	-3.63047600
H	-10.82211200	1.35336200	-4.57539300
H	-12.29423500	1.91369700	-3.77387300
H	-11.10731600	0.96435200	-2.86621500
C	-10.70321900	4.09672900	-4.32478500
H	-9.42523500	2.80718600	-3.18274300
H	-10.40717600	3.70510600	-5.30447700
H	-10.11961900	5.00125800	-4.12422200
H	-11.76054400	4.38294500	-4.38724000
C	-4.22172700	10.28479700	-6.05008500
C	-3.34766100	10.71184300	-5.04869100
C	-2.43120800	9.44571800	-7.37738400
C	-1.53162300	9.88225800	-6.41259400
C	-1.98469400	10.49578000	-5.25660900
H	-0.46691600	9.72087500	-6.55681200
H	-1.27577800	10.79827900	-4.48916800
C	-3.82935500	11.29319800	-3.73168700
C	-3.61453300	10.27214100	-2.60874700
H	-4.13956500	9.32962300	-2.81078500
H	-3.97317200	10.67273600	-1.65158500
H	-2.54641100	10.04494100	-2.49807100
C	-3.13956300	12.61412900	-3.39500300

H	-4.90682100	11.49878600	-3.80104000
H	-3.55768100	13.03260700	-2.47198400
H	-3.26625900	13.35321300	-4.19294600
H	-2.06409400	12.47574300	-3.23281800
C	-3.79965600	9.62801300	-7.20792000
C	-4.81797800	9.08914300	-8.19102500
C	-4.33214500	7.83574400	-8.90946000
H	-5.14973600	7.39334400	-9.48718400
H	-3.97234800	7.08770900	-8.19510700
H	-3.52413000	8.05983500	-9.61650900
C	-5.21913600	10.16969500	-9.19752100
H	-5.70666400	8.80805500	-7.60646700
H	-5.63404500	11.05388400	-8.70166200
H	-5.97139600	9.79263800	-9.89927800
H	-4.34526100	10.49026400	-9.77858500
H	-2.06251500	8.92998700	-8.25864300
N	-6.75473700	3.46117100	-1.80408800
C	-5.55834400	3.71837300	-2.54881300
C	-5.40970900	3.07080600	-3.78141300
C	-4.59742400	4.58977200	-2.02711600
C	-4.23470200	3.30754100	-4.49388700
C	-3.25321000	4.14610000	-3.98882500
C	-3.43389300	4.77899100	-2.76958000
H	-4.09271000	2.83558700	-5.46149100
H	-2.34742200	4.32404900	-4.56111300
H	-2.67113200	5.45634100	-2.39488700
C	-4.79736700	5.34320400	-0.72765200
C	-4.48450400	6.83369800	-0.89030500
H	-3.41256600	7.00415200	-1.05143600
H	-4.76682600	7.37620100	0.01939400
H	-5.03355900	7.26923600	-1.73569600
C	-3.93765800	4.72191800	0.37471400
H	-5.85330500	5.26010700	-0.43878000
H	-2.87502700	4.77163600	0.10363500

H	-4.19031000	3.66756000	0.53709800
H	-4.06803200	5.25522300	1.32290800
C	-6.52425300	2.23466600	-4.38177200
C	-7.41689000	3.13548900	-5.24143600
H	-7.80461300	3.98807100	-4.67035500
H	-8.26431100	2.56659800	-5.64664600
H	-6.84025900	3.53906000	-6.08377000
C	-6.01401100	1.05326400	-5.20296300
H	-7.13998900	1.83056800	-3.56514700
H	-5.53694100	1.38626700	-6.13171800
H	-6.84916000	0.40673500	-5.49097000
H	-5.28809000	0.44870800	-4.64909000
H	-5.61587900	12.51135600	-6.63918500
H	-8.06727300	12.60747200	-5.31077900
H	-8.67279400	1.58244700	0.04252400
H	-6.09260400	1.58638200	-1.01768300
C	-8.64109700	10.40114200	-3.92735900
C	-8.44594100	10.45198100	-2.54141900
C	-9.89628100	10.18832000	-4.50842600
C	-9.56666400	10.31184300	-1.72806300
C	-10.98682300	10.04880800	-3.64942400
C	-10.82550200	10.11854500	-2.27511400
H	-9.44484700	10.33142100	-0.64913500
H	-11.97423800	9.87298000	-4.06397400
H	-11.68615100	9.99860400	-1.62360500
C	-10.04738500	9.99240900	-6.00448400
C	-9.69283700	8.54115700	-6.34693300
H	-8.67233400	8.28570700	-6.04282100
H	-9.79793400	8.35714900	-7.42255200
H	-10.36938900	7.86091300	-5.81346000
C	-11.44110700	10.33112400	-6.52397800
H	-9.33038400	10.64934800	-6.51698800
H	-12.18071900	9.59218400	-6.19449900
H	-11.44593300	10.31731200	-7.61836100

H	-11.77931200	11.31899400	-6.19287400
C	-7.06613200	10.60391000	-1.93575700
C	-6.75703400	12.07408100	-1.65063500
H	-5.74130100	12.18894700	-1.24859400
H	-7.45961500	12.49134200	-0.91771800
H	-6.82746400	12.67825700	-2.56564300
C	-6.88108900	9.72181700	-0.70283400
H	-6.34149500	10.24337700	-2.67044100
H	-5.82257400	9.70564200	-0.41498400
H	-7.19370700	8.68845900	-0.91427900
H	-7.44798600	10.08761400	0.16204600
H	-8.16778500	8.12999700	-3.39977000
H	-6.20736300	5.82056400	-3.47800200

54. NHC_Full_H_CI (planar)-triplet:

N	-9.00483400	3.29564700	-1.43855000
C	-7.16455100	2.09711700	-1.57634000
C	-8.42478200	2.09009300	-1.10122600
C	-8.10528300	4.09276900	-2.12995800
C	-7.18922400	6.29234100	-3.40031600
C	-7.31578300	7.56665200	-3.86874800
N	-7.49796900	10.59637800	-4.95136100
N	-5.49899200	10.56283400	-5.83078600
C	-7.26517900	11.83592000	-5.51170800
C	-6.02963800	11.81785100	-6.04757200
B	-6.23069800	8.33904800	-4.62558900
B	-8.27411600	5.51982100	-2.64350400
Cl	-9.87312200	6.36376900	-2.40072500
C	-6.39861700	9.76596400	-5.13944900
Cl	-4.67020200	7.45621500	-4.96111300
C	-10.14576600	3.78183100	-0.72118700
C	-11.40686100	3.69441400	-1.31671400
C	-9.93341500	4.35538600	0.53398500
C	-12.49688600	4.15281600	-0.58407000
C	-11.05484300	4.81216400	1.22811700
C	-12.32243100	4.69948100	0.68145100
H	-13.49210300	4.10940900	-1.01577800
H	-13.18422300	5.06095300	1.23566800
H	-10.92366000	5.27631300	2.20324000
C	-8.54652100	4.57937500	1.10735800
C	-8.39968800	3.99804600	2.51245100
H	-8.62971200	2.92769700	2.53363000
H	-9.06535500	4.49884400	3.22554400

H	-7.37283700	4.13377200	2.87202900
C	-8.22935200	6.07846400	1.10710000
H	-7.80851000	4.07719700	0.46706800
H	-7.21845900	6.26128900	1.49367100
H	-8.93600100	6.62140000	1.74767500
H	-8.29876700	6.50238300	0.09702600
C	-11.54211200	3.17248900	-2.73227400
C	-11.65275200	1.64635500	-2.73669200
H	-11.72980700	1.26137900	-3.75967100
H	-12.54845400	1.32901700	-2.18792500
H	-10.78494600	1.17470500	-2.26344600
C	-12.71386400	3.79942400	-3.47887500
H	-10.62172200	3.45691700	-3.26449400
H	-12.68102600	3.51640600	-4.53568300
H	-12.68325000	4.89235800	-3.41507900
H	-13.67794600	3.45562300	-3.08466100
C	-4.08229900	10.35321000	-5.87105100
C	-3.33122400	10.74847400	-4.76222600
C	-2.14021900	9.57049700	-7.01084700
C	-1.36097800	9.98355800	-5.93698200
C	-1.95060300	10.55251800	-4.82028500
H	-0.28462500	9.83804800	-5.96492900
H	-1.33706000	10.83735200	-3.96828600
C	-3.96722300	11.27994500	-3.49117400
C	-3.83048700	10.23818500	-2.37577300
H	-4.29163400	9.28321100	-2.65929800
H	-4.30553900	10.59421400	-1.45253500
H	-2.77245600	10.04708900	-2.15542200
C	-3.36505600	12.61531200	-3.05736000
H	-5.03837800	11.44700900	-3.66931600
H	-3.88314700	12.99239500	-2.16771200
H	-3.44702800	13.37101800	-3.84556500
H	-2.30414900	12.51236800	-2.79981300
C	-3.52127400	9.73594000	-6.99196700

C	-4.41568600	9.22289200	-8.10159400
C	-3.83880100	7.99750000	-8.80102200
H	-4.58056200	7.57013600	-9.48308400
H	-3.55465400	7.22668600	-8.07666500
H	-2.95750600	8.25012300	-9.40311300
C	-4.71160300	10.33325100	-9.11197700
H	-5.36281700	8.91838900	-7.63095800
H	-5.18826500	11.19757400	-8.63725300
H	-5.37653800	9.97491100	-9.90575200
H	-3.78118700	10.67810700	-9.58051000
H	-1.66744000	9.08774000	-7.86070300
N	-6.95683900	3.31170900	-2.19799000
C	-5.66927600	3.65372600	-2.72574000
C	-5.26749500	3.06522900	-3.93188600
C	-4.85846800	4.55293200	-2.01945100
C	-3.99247300	3.37092000	-4.40729000
C	-3.16242400	4.23782300	-3.71385900
C	-3.59679600	4.83094400	-2.53864100
H	-3.65158700	2.93741300	-5.34201000
H	-2.17755300	4.47330900	-4.10657500
H	-2.95384400	5.53875800	-2.02426200
C	-5.34524800	5.23350600	-0.75680100
C	-4.86271200	6.67815900	-0.64637900
H	-3.78823700	6.74795200	-0.43736900
H	-5.38744300	7.18139000	0.17526000
H	-5.07570800	7.22995400	-1.57473200
C	-4.97253900	4.40504300	0.47421700
H	-6.43788200	5.28447300	-0.80825400
H	-3.88290100	4.31625300	0.57175800
H	-5.38828100	3.39036400	0.40913400
H	-5.35763100	4.86913500	1.39196300
C	-6.23836100	2.24636300	-4.76035700
C	-7.15707600	3.21059300	-5.52082200
H	-7.72359800	3.85829300	-4.84311200

H	-7.86643800	2.66054300	-6.15004800
H	-6.55556600	3.86224600	-6.16772900
C	-5.55661900	1.29331600	-5.73636300
H	-6.86010600	1.64499400	-4.08216300
H	-5.06829700	1.83890200	-6.55223300
H	-6.29964600	0.63424700	-6.19598400
H	-4.80146700	0.66830600	-5.24764400
H	-5.45481100	12.58119700	-6.54696200
H	-8.02008800	12.60529200	-5.47360000
H	-8.97101000	1.35494800	-0.53226300
H	-6.38182100	1.35569100	-1.54634600
C	-8.70131900	10.33767600	-4.21782400
C	-8.65317100	10.30039300	-2.81741200
C	-9.88721200	10.13611800	-4.93584000
C	-9.84772300	10.08636200	-2.13489600
C	-11.05789600	9.93044300	-4.20635100
C	-11.04022000	9.91418500	-2.82043200
H	-9.83869700	10.03267100	-1.05045900
H	-11.99312900	9.76359700	-4.73105500
H	-11.96017600	9.73999500	-2.27000800
C	-9.87003300	10.00002500	-6.44603000
C	-9.40211100	8.58262100	-6.79830800
H	-8.39814900	8.37410000	-6.41332900
H	-9.39635000	8.43124000	-7.88401400
H	-10.08225200	7.84623800	-6.35090800
C	-11.21781700	10.28408100	-7.10056800
H	-9.14034800	10.71273200	-6.85561900
H	-11.94487700	9.49480700	-6.87648200
H	-11.10641400	10.31265000	-8.18890600
H	-11.64435000	11.23922200	-6.77570700
C	-7.34596800	10.44591700	-2.06614500
C	-7.08308500	11.91534500	-1.73084600
H	-6.11707900	12.03576100	-1.22261700
H	-7.86446300	12.31302100	-1.07055200

H	-7.06508600	12.53151900	-2.64006000
C	-7.27768100	9.55211100	-0.82977100
H	-6.54321200	10.10547100	-2.72851800
H	-6.25555900	9.54950800	-0.43119800
H	-7.54555100	8.51549400	-1.08542100
H	-7.93961100	9.89555800	-0.02543100
H	-8.28662800	8.02700600	-3.69054100
H	-6.23621500	5.81380600	-3.62204200

55. NHC_Full_C₂H₅_H (fully optimized)-singlet:

N	-8.87277700	3.69372600	-1.93261700
C	-7.43557300	2.05903500	-1.66256200
C	-8.74011800	2.37635100	-1.54831200
C	-7.64828400	4.24200600	-2.26796100
C	-6.27421600	6.47731500	-3.14156300
C	-6.16272700	7.88735100	-2.87428600
C	-5.50389400	5.87857900	-4.30616800
H	-4.77211400	5.14178200	-3.93499500
H	-4.90326000	6.64801400	-4.79818500
C	-6.52113800	8.30853200	-1.45125000
H	-6.37948200	7.43849500	-0.79510700
H	-7.57998000	8.56660400	-1.32249200
N	-7.40123500	10.95041200	-3.69314100
N	-5.68184300	11.22072900	-4.98622500
C	-7.53487300	12.17940000	-4.31288500
C	-6.47518500	12.33848700	-5.12857200
B	-5.73921700	8.87498000	-3.91285300
B	-7.37649800	5.74347200	-2.44331000
C	-6.23391200	10.32771000	-4.08936700
C	-10.06628300	4.45406000	-1.73521600
C	-11.08852900	4.39335200	-2.69074100
C	-10.17259900	5.19824800	-0.55454600
C	-12.21801900	5.18386300	-2.46898200
C	-11.32984300	5.94973500	-0.36404200
C	-12.33297100	5.96086300	-1.32266900
H	-13.03215200	5.16971100	-3.18692900
H	-13.22593300	6.56064800	-1.16708300
H	-11.44213900	6.52535900	0.55279300
C	-9.10487000	5.13845300	0.51792500
C	-9.55104800	4.20417400	1.64456500
H	-9.74027400	3.18990900	1.27221900
H	-10.47515100	4.56998100	2.11122800
H	-8.78013300	4.14215000	2.42220200

C	-8.73682300	6.51839200	1.05965200
H	-8.20063500	4.70896400	0.07588000
H	-7.80331200	6.45747900	1.63670700
H	-9.51087200	6.90733200	1.73500600
H	-8.58962700	7.24051400	0.24923500
C	-10.97999000	3.45364500	-3.88009900
C	-12.33778500	3.05495600	-4.44951600
H	-12.21131600	2.26636000	-5.19787300
H	-12.82071700	3.89918100	-4.95591200
H	-13.02148300	2.68747500	-3.67691300
C	-10.10279600	4.03219700	-4.99094500
H	-10.49110000	2.53743100	-3.51645400
H	-9.94366500	3.28814700	-5.77971500
H	-9.12633700	4.36094600	-4.61913400
H	-10.59847600	4.89970400	-5.44243500
C	-4.67312800	10.89322300	-5.94726300
C	-3.35551600	11.30781500	-5.73611900
C	-4.10666600	9.89463000	-8.04186200
C	-2.78904300	10.28462700	-7.85607100
C	-2.41807500	10.98728800	-6.71788200
H	-2.04214700	10.04430200	-8.60760000
H	-1.38398000	11.29280400	-6.59156100
C	-2.96853200	12.03379500	-4.46295300
C	-2.72327900	11.01934200	-3.34150700
H	-3.59697000	10.38094400	-3.16636400
H	-2.47137600	11.52992900	-2.40481500
H	-1.88362400	10.36539300	-3.60879600
C	-1.74985900	12.93558300	-4.63135300
H	-3.82041200	12.66441200	-4.16882600
H	-1.60681500	13.54504200	-3.73360100
H	-1.84710100	13.60841400	-5.49015100
H	-0.83396700	12.34767600	-4.76456300
C	-5.07829600	10.19331600	-7.08923400
C	-6.51946400	9.77913200	-7.31091200

C	-6.65395600	8.27069400	-7.52054500
H	-7.71522400	7.98657900	-7.55470300
H	-6.18046000	7.71419400	-6.70434200
H	-6.19857900	7.95449500	-8.46778800
C	-7.12584000	10.55363400	-8.48158800
H	-7.09500000	10.03490800	-6.41501600
H	-7.08454000	11.63555800	-8.30910200
H	-8.17520000	10.27138300	-8.62881100
H	-6.58726700	10.34193400	-9.41415100
H	-4.39387800	9.35063500	-8.93944400
N	-6.77199800	3.19546600	-2.08849300
C	-5.34773000	3.26297400	-2.17488200
C	-4.71090000	2.52730700	-3.18259000
C	-4.63187800	4.02641500	-1.23143000
C	-3.31608700	2.56444200	-3.23824100
C	-2.59077200	3.33321200	-2.34764600
C	-3.24598300	4.06035400	-1.36161500
H	-2.80157700	1.99395600	-4.00731900
H	-1.50723300	3.36929700	-2.41561500
H	-2.66232300	4.65606800	-0.66801200
C	-5.31882200	4.74883100	-0.08602400
C	-4.49298400	5.89468500	0.48675600
H	-3.61599600	5.54438100	1.04554400
H	-5.11020000	6.47636700	1.18225900
H	-4.15603400	6.57239100	-0.30805700
C	-5.73984300	3.77603000	1.01850500
H	-6.22801500	5.21150300	-0.48895200
H	-4.87005200	3.28141900	1.46927200
H	-6.41867400	2.99789400	0.64679000
H	-6.26743500	4.32115400	1.81395800
C	-5.46309700	1.70394600	-4.21164300
C	-4.94383800	1.96624500	-5.62810600
H	-4.82911800	3.03538400	-5.82446300
H	-5.63084400	1.54795100	-6.37120200

H	-3.96999300	1.48757900	-5.78542500
C	-5.34032500	0.20884000	-3.90252500
H	-6.52365400	1.98788600	-4.17800000
H	-4.28350000	-0.08775300	-3.91471100
H	-5.86447400	-0.39028900	-4.65548700
H	-5.74225200	-0.05438700	-2.91929000
H	-6.20345700	13.13537800	-5.80223100
H	-8.39233300	12.80447700	-4.12886700
H	-9.59321300	1.79397500	-1.23805200
H	-6.89988600	1.14765100	-1.45451500
C	-8.41819900	10.39280700	-2.85199900
C	-8.66762200	10.99970600	-1.61024700
C	-9.14332900	9.26711500	-3.29791600
C	-9.62454500	10.41402800	-0.77924900
C	-10.04517400	8.69168900	-2.40276300
C	-10.28161100	9.25551600	-1.15532900
H	-9.84065900	10.87140300	0.18273500
H	-10.57535300	7.78353600	-2.67862600
H	-10.99574200	8.78793200	-0.48212800
C	-9.02878800	8.74242000	-4.71887600
C	-9.66614100	7.37275500	-4.91047900
H	-9.29157000	6.65179000	-4.17550700
H	-9.42265900	6.99368700	-5.91157000
H	-10.76356500	7.41362900	-4.83564500
C	-9.66604600	9.73360900	-5.70134500
H	-7.96195200	8.62776900	-4.96185200
H	-10.74049200	9.83161100	-5.49923400
H	-9.55199900	9.36882400	-6.73142100
H	-9.22111500	10.73328200	-5.65247100
C	-8.00209800	12.29133600	-1.16535600
C	-8.97715700	13.46097800	-1.35222800
H	-8.51004000	14.41125000	-1.07013700
H	-9.85351100	13.31328900	-0.70788300
H	-9.34687600	13.55105600	-2.37808800

C	-7.55436200	12.26927600	0.29715800
H	-7.11319800	12.46197700	-1.78735600
H	-6.96911300	13.16736300	0.52181000
H	-6.94421100	11.39451100	0.52776600
H	-8.41476000	12.27340600	0.97612500
C	-5.64619200	9.43973000	-0.92588700
H	-4.58365800	9.20619100	-1.07585600
H	-5.83544200	10.39145600	-1.44232200
H	-5.80704600	9.60053600	0.14732800
C	-6.40993800	5.20587800	-5.33888300
H	-5.88812900	4.99244900	-6.28134200
H	-6.81676900	4.25826400	-4.95851600
H	-7.26952000	5.85414900	-5.56661000
H	-8.22163400	6.38142500	-1.87462600
H	-5.08817700	8.57545800	-4.87068900

56. NHC_Full_C₂H₅_H (fully optimized)-triplet:

N	-8.86340100	3.67122300	-1.41583300
C	-7.29681700	2.13461200	-1.40952400
C	-8.54599500	2.40522900	-0.98046800
C	-7.81869400	4.22369300	-2.13850400

C	-6.79295400	6.47230700	-3.46386600
C	-6.47841900	7.73304100	-3.01991800
C	-6.24594400	5.98181200	-4.79695200
H	-5.17757300	5.72333600	-4.67074200
H	-6.25489500	6.81125100	-5.52010100
C	-6.92774500	8.11307700	-1.61159300
H	-6.82984100	7.23450800	-0.95817000
H	-8.00718600	8.33066900	-1.58386600
N	-7.36894100	10.83679700	-3.85286400
N	-5.40663400	11.20580300	-4.73021000
C	-7.35461400	12.13643200	-4.32727200
C	-6.14796100	12.35821200	-4.88054500
B	-5.67826700	8.77854800	-3.86466000
B	-7.84896700	5.64698900	-2.66932900
C	-6.14760000	10.21631900	-4.10048500
C	-10.05166800	4.37802300	-1.05307300
C	-11.21806000	4.16851900	-1.79523000
C	-9.98277100	5.29607900	0.00400200
C	-12.35525100	4.89240500	-1.43185400
C	-11.14278000	5.99346000	0.33173600
C	-12.31955000	5.79001500	-0.37617000
H	-13.27868200	4.75245300	-1.98567600
H	-13.21609700	6.34182600	-0.10580600
H	-11.12069500	6.71252900	1.14594900
C	-8.69562300	5.52136300	0.77104800
C	-8.58352700	4.53104400	1.93339600
H	-8.58553500	3.49287200	1.58091400
H	-9.42482400	4.65551600	2.62741900
H	-7.65510900	4.69371500	2.49354100
C	-8.55080400	6.95872400	1.26926400
H	-7.86113500	5.32897800	0.08372000
H	-7.51121000	7.14665000	1.56778600
H	-9.18088300	7.15037900	2.14724700
H	-8.81624000	7.68380200	0.48812000

C	-11.22562100	3.26258000	-3.01112600
C	-12.58415900	2.61816600	-3.27321500
H	-12.49383000	1.85622900	-4.05373000
H	-13.31372800	3.35338700	-3.63249000
H	-12.99694700	2.14310300	-2.37689200
C	-10.77453700	4.06201600	-4.23937800
H	-10.49519800	2.45845700	-2.84343900
H	-10.80780300	3.44262300	-5.14344700
H	-9.75563000	4.44773000	-4.11744200
H	-11.44146800	4.92275800	-4.39102200
C	-4.23584600	10.97376000	-5.51725500
C	-2.98438200	11.36079100	-5.02498400
C	-3.27741800	10.23748700	-7.57991100
C	-2.02233300	10.58850400	-7.10882200
C	-1.87840000	11.15149200	-5.84745000
H	-1.14632900	10.43463500	-7.73282600
H	-0.89022200	11.43777700	-5.50094500
C	-2.85175300	11.95621900	-3.63691900
C	-2.84843700	10.84021200	-2.58890300
H	-3.74701000	10.21760700	-2.65834100
H	-2.78871400	11.25655100	-1.57670600
H	-1.97916800	10.18810100	-2.74118800
C	-1.61621400	12.83510000	-3.47337200
H	-3.73941600	12.58157000	-3.45992000
H	-1.65031900	13.35445000	-2.51059100
H	-1.53407600	13.58739400	-4.26523400
H	-0.69737200	12.23668500	-3.47893100
C	-4.41181900	10.42831700	-6.79237400
C	-5.78226500	10.07842900	-7.33335500
C	-5.83720200	8.62237800	-7.79140300
H	-6.87565300	8.31179800	-7.97071100
H	-5.40682500	7.96305000	-7.03121800
H	-5.28161100	8.47373400	-8.72643200
C	-6.18260900	11.03128500	-8.45926600

H	-6.51392200	10.19593400	-6.52776600
H	-6.20452100	12.07124900	-8.11276200
H	-7.17934500	10.77880200	-8.84096400
H	-5.47551800	10.96971400	-9.29662200
H	-3.38868100	9.81510900	-8.57661000
N	-6.84164000	3.24098800	-2.10518400
C	-5.51318300	3.34701900	-2.62571900
C	-5.11781100	2.48604600	-3.66319900
C	-4.63241400	4.29151500	-2.06342400
C	-3.82671900	2.62798900	-4.17129800
C	-2.96372300	3.58998000	-3.67398200
C	-3.36295000	4.40690700	-2.62633300
H	-3.50049100	1.97414900	-4.97572700
H	-1.96898100	3.69823800	-4.09671500
H	-2.67197400	5.14484500	-2.23345400
C	-5.03643700	5.12293100	-0.86476500
C	-4.15644900	6.34373100	-0.63978700
H	-3.14349900	6.07358900	-0.31458100
H	-4.59564600	6.96634000	0.14936900
H	-4.08677800	6.95499500	-1.54946200
C	-5.12986700	4.28545900	0.41484700
H	-6.04120000	5.49818100	-1.07213800
H	-4.16464100	3.82874500	0.66717000
H	-5.87793500	3.48674000	0.33882000
H	-5.42519600	4.93089600	1.25348700
C	-6.01001400	1.38621900	-4.21435400
C	-5.99518900	1.29869300	-5.74162300
H	-6.23099400	2.25397800	-6.21349800
H	-6.72990700	0.55911800	-6.07757300
H	-5.01888200	0.96673700	-6.11253600
C	-5.56290500	0.03169400	-3.65009200
H	-7.04364600	1.58436200	-3.89934900
H	-4.54517900	-0.19115900	-3.99569400
H	-6.21870600	-0.77449000	-3.99738600

H	-5.54066900	0.00976500	-2.55645900
H	-5.73767700	13.22405200	-5.37560700
H	-8.22216000	12.76821200	-4.23865300
H	-9.24159800	1.81995700	-0.40040500
H	-6.66851000	1.27279900	-1.26183400
C	-8.53389300	10.24293800	-3.27294700
C	-9.04044800	10.76241800	-2.06952100
C	-9.14890600	9.15628900	-3.93077000
C	-10.13057000	10.11339500	-1.48529400
C	-10.20081800	8.51704700	-3.27651100
C	-10.67907400	8.97738300	-2.05663400
H	-10.53418000	10.49737600	-0.55196300
H	-10.65756900	7.63655600	-3.71994400
H	-11.49609200	8.45435400	-1.56676000
C	-8.74620500	8.75729000	-5.33769200
C	-9.31222300	7.41060700	-5.76336200
H	-9.13106600	6.64785800	-4.99830700
H	-8.83261800	7.08526100	-6.69502400
H	-10.39365700	7.46419500	-5.94905200
C	-9.18042400	9.83424400	-6.34074500
H	-7.64981400	8.67102500	-5.37648400
H	-10.27347000	9.93223500	-6.34603100
H	-8.86514100	9.55527800	-7.35572700
H	-8.75400800	10.81938600	-6.12006400
C	-8.49054500	12.00251100	-1.38524600
C	-9.41149800	13.19914300	-1.65388100
H	-9.02341700	14.10741300	-1.17909000
H	-10.40487400	12.99834400	-1.23237900
H	-9.55159700	13.40252300	-2.71982900
C	-8.35672500	11.82974600	0.13082800
H	-7.49410100	12.21924300	-1.79251900
H	-7.76523800	12.64795000	0.55499200
H	-7.87949800	10.88341800	0.39556900
H	-9.33764700	11.86039200	0.61909600

C	-6.14700100	9.24865700	-0.95916700
H	-5.06582100	9.08597800	-1.05145100
H	-6.35742800	10.22784700	-1.40632100
H	-6.37966900	9.31258500	0.11219000
C	-6.95859100	4.78928000	-5.42718400
H	-6.41530100	4.44668000	-6.31559600
H	-7.03901500	3.94106700	-4.73879200
H	-7.97817700	5.03174600	-5.74235800
H	-8.85277200	6.21988900	-2.33449700
H	-4.64045500	8.51584500	-4.41225100

57. NHC_Full_C₂H₅_H (twisted)-singlet:

N	-9.31819900	4.82904100	-0.34001400
C	-10.58512200	6.62403400	-0.38642200
C	-10.49369500	5.38184100	0.12511100
C	-8.59434300	5.76219600	-1.07760600
C	-6.31201800	6.38524000	-2.57492300
C	-6.35521300	6.51436600	-3.92839300
C	-5.08664200	6.97374700	-1.84946400
H	-4.98739000	8.04074600	-2.11390800
H	-4.17319700	6.51697400	-2.26555600

C	-7.52614100	5.94530000	-4.69604300
H	-8.31528100	5.65581500	-3.98025400
H	-7.22728900	5.00842200	-5.19332100
N	-3.43500500	5.76957900	-5.25767000
N	-3.03986100	7.84144700	-5.78517500
C	-2.17887300	5.82455000	-5.83439400
C	-1.93643100	7.10905300	-6.16434700
B	-5.33702000	7.47757800	-4.64683200
B	-7.25685100	5.46826400	-1.71968200
C	-3.97497800	7.04435000	-5.14869800
C	-8.92872400	3.47717900	-0.10611400
C	-8.57789300	3.08417700	1.19695700
C	-8.93288200	2.57800100	-1.18151200
C	-8.25411900	1.74496500	1.40668900
C	-8.58615000	1.25289400	-0.92012100
C	-8.25667600	0.83590000	0.35837700
H	-7.98547500	1.40774700	2.40244600
H	-7.99783600	-0.20303200	0.54241400
H	-8.58904700	0.53744600	-1.73953400
C	-9.32611900	2.96492100	-2.59571900
C	-10.61879500	2.25566400	-3.00383800
H	-11.45508300	2.53623900	-2.35231700
H	-10.50742000	1.16549500	-2.95003500
H	-10.88526500	2.51019000	-4.03593200
C	-8.20586300	2.67288300	-3.59500000
H	-9.50544600	4.04403700	-2.62872300
H	-8.50976100	2.98287200	-4.60531300
H	-7.96963500	1.60128500	-3.63559900
H	-7.28677900	3.21921200	-3.34470600
C	-8.45647700	4.10556800	2.31373800
C	-8.48412600	3.49399500	3.71001400
H	-8.52551000	4.28723600	4.46279200
H	-7.57623200	2.91250700	3.90989900
H	-9.34717800	2.83644700	3.86023300

C	-7.16780500	4.91141400	2.11883600
H	-9.29966900	4.80622800	2.24279100
H	-7.06041300	5.67036500	2.90249400
H	-7.14422200	5.41055100	1.14504900
H	-6.29879700	4.24301800	2.17040900
C	-3.22718700	9.21747000	-6.10071200
C	-3.62366200	9.53753000	-7.40200900
C	-3.19926700	11.51919600	-5.46969100
C	-3.55381500	11.86787200	-6.76741700
C	-3.77380200	10.88751000	-7.72129100
H	-3.67692800	12.91514700	-7.02927600
H	-4.08965900	11.16544700	-8.72448400
C	-3.99904600	8.46326000	-8.40153600
C	-5.52293300	8.43217800	-8.53948100
H	-5.99648100	8.35563900	-7.55342400
H	-5.84345400	7.57936000	-9.15351000
H	-5.88791800	9.35048300	-9.01836300
C	-3.33032600	8.64498300	-9.76069500
H	-3.68537000	7.49236900	-7.99956800
H	-3.59816000	7.81682800	-10.42740800
H	-2.23898100	8.67557500	-9.67819500
H	-3.65608800	9.57163200	-10.24837500
C	-3.03410000	10.18461700	-5.10747000
C	-2.63529200	9.77587400	-3.70430500
C	-3.13347100	10.74867700	-2.64143000
H	-3.00931400	10.31310000	-1.64392800
H	-4.19448900	10.98144100	-2.78069300
H	-2.57232500	11.69163400	-2.65454300
C	-1.11576800	9.61132300	-3.61777600
H	-3.10292400	8.80198000	-3.50001200
H	-0.74799200	8.86631600	-4.33194800
H	-0.81261800	9.29533100	-2.61337600
H	-0.61736800	10.56411600	-3.83793600
H	-3.05661400	12.29745400	-4.72563400

N	-9.46498600	6.84906500	-1.17298000
C	-9.57918900	7.74125300	-2.29672400
C	-8.81375100	8.91156700	-2.32999300
C	-10.53971600	7.45239000	-3.28003300
C	-9.06195400	9.83246600	-3.34550800
C	-10.05687300	9.60288200	-4.28627100
C	-10.77621600	8.42060100	-4.25856100
H	-8.47845700	10.74706600	-3.39013200
H	-10.25311300	10.34041100	-5.05939600
H	-11.53247200	8.23014700	-5.01731400
C	-11.36193500	6.17173300	-3.30508200
C	-11.24557600	5.42103200	-4.63406900
H	-11.48875600	6.06468000	-5.48770600
H	-11.95116000	4.58226000	-4.64651500
H	-10.23811900	5.01811500	-4.79240700
C	-12.83353600	6.48577700	-3.01920100
H	-10.99986000	5.49883400	-2.51901600
H	-13.25123700	7.12371400	-3.80810100
H	-12.95943100	7.01345300	-2.06811000
H	-13.42858900	5.56660100	-2.98335800
C	-7.80397500	9.18177600	-1.24008800
C	-6.66165500	10.07389600	-1.70881500
H	-6.27841000	9.74226800	-2.68261500
H	-5.83722500	10.04554700	-0.98567000
H	-6.97676200	11.12170000	-1.80100200
C	-8.49907600	9.78425400	-0.01635800
H	-7.38257900	8.21146700	-0.95242200
H	-8.95675100	10.74751600	-0.27575700
H	-7.78100400	9.95887200	0.79306200
H	-9.28734000	9.12662900	0.36606100
H	-1.08795800	7.57961100	-6.63537000
H	-1.59833900	4.92768000	-5.98251000
H	-11.15529500	4.82675800	0.77092600
H	-11.35872500	7.37128700	-0.30507100

C	-4.12493700	4.52020400	-5.12493100
C	-5.00351200	4.10783500	-6.14621600
C	-3.80389200	3.69187300	-4.04545700
C	-5.55207700	2.83029800	-6.04744200
C	-4.37037600	2.41715100	-3.99855000
C	-5.23000600	1.98638300	-4.99333600
H	-6.23896700	2.48626200	-6.81517900
H	-4.12889400	1.76184000	-3.16506900
H	-5.66563500	0.99202400	-4.94432800
C	-2.85630700	4.12222100	-2.94682700
C	-3.48389500	3.88597300	-1.57179600
H	-4.53007400	4.20881700	-1.55565500
H	-2.93715600	4.43222200	-0.79454800
H	-3.45858500	2.82243400	-1.30393100
C	-1.52233600	3.38221000	-3.06316700
H	-2.66470500	5.19599900	-3.06274700
H	-1.68127200	2.29824800	-2.99482500
H	-0.84210200	3.67293300	-2.25492600
H	-1.02202800	3.58470600	-4.01671900
C	-5.32082200	4.98795900	-7.34410500
C	-4.22926500	4.86368700	-8.41551600
H	-4.45479000	5.52236100	-9.26617800
H	-4.19018200	3.83327100	-8.79183200
H	-3.23537600	5.12604400	-8.04167100
C	-6.66686700	4.67472100	-7.99762000
H	-5.35115100	6.03165800	-6.99240700
H	-6.92183200	5.46863400	-8.70911500
H	-7.48443600	4.59871900	-7.27355800
H	-6.62571500	3.73701000	-8.56597900
C	-8.08222000	6.91873400	-5.72949000
H	-7.38810200	7.04513700	-6.56923600
H	-9.04221500	6.58551700	-6.14402900
H	-8.22746000	7.90614200	-5.27850900
C	-5.04610300	6.83335800	-0.33106900

H	-4.13135100	7.27923800	0.07695600
H	-5.89630500	7.32737900	0.15695500
H	-5.07365500	5.78416600	-0.01564400
H	-6.80633700	4.42062300	-1.32668900
H	-5.59374400	8.64568200	-4.80236600

58. NHC_Full_C₂H₅_H (twisted)-triplet:

N	-9.31865500	4.83049200	-0.33783900
C	-10.58100300	6.62876800	-0.38534000
C	-10.49274600	5.38662300	0.12683300
C	-8.59266700	5.76138300	-1.07638100
C	-6.31090100	6.38323200	-2.57359400
C	-6.35544100	6.51151300	-3.92637700
C	-5.08502200	6.97046500	-1.84657700
H	-4.98633800	8.03854100	-2.10547200
H	-4.17062100	6.51616900	-2.26322500
C	-7.52880400	5.94499800	-4.69312600
H	-8.32005900	5.65884000	-3.97895500
H	-7.23197900	5.00666300	-5.18896800
N	-3.43345200	5.77087900	-5.25493100
N	-3.04088700	7.84367800	-5.78251700

C	-2.17739000	5.82756800	-5.83185300
C	-1.93685000	7.11234100	-6.16212300
B	-5.33740800	7.47608700	-4.64452900
B	-7.25535100	5.46499700	-1.71752500
C	-3.97523800	7.04502500	-5.14649100
C	-8.93260600	3.47771700	-0.10412700
C	-8.58481900	3.08315200	1.19938800
C	-8.93669600	2.57902200	-1.17999200
C	-8.26418100	1.74319300	1.40896900
C	-8.59291900	1.25310900	-0.91866100
C	-8.26655600	0.83471000	0.36014400
H	-7.99805900	1.40489400	2.40503000
H	-8.01005200	-0.20482400	0.54403300
H	-8.59589400	0.53808600	-1.73844000
C	-9.32769700	2.96671300	-2.59462300
C	-10.62123700	2.25974700	-3.00403500
H	-11.45777100	2.54217100	-2.35362200
H	-10.51201600	1.16939500	-2.94967200
H	-10.88597500	2.51439900	-4.03653900
C	-8.20695900	2.67273800	-3.59274900
H	-9.50512600	4.04612600	-2.62791100
H	-8.50973300	2.98233300	-4.60348900
H	-7.97184700	1.60088300	-3.63244700
H	-7.28746300	3.21824100	-3.34203500
C	-8.46271700	4.10366000	2.31688900
C	-8.49325300	3.49151000	3.71284200
H	-8.53420900	4.28448700	4.46592000
H	-7.58664400	2.90834000	3.91365300
H	-9.35765900	2.83541300	3.86164800
C	-7.17210600	4.90676900	2.12360300
H	-9.30422800	4.80623700	2.24539500
H	-7.06408900	5.66563100	2.90726600
H	-7.14632200	5.40562000	1.14972600
H	-6.30460000	4.23652700	2.17634700

C	-3.23150000	9.21825600	-6.10241000
C	-3.62429000	9.53321700	-7.40604200
C	-3.21240000	11.52219300	-5.47878800
C	-3.56296800	11.86578900	-6.77900300
C	-3.77676700	10.88177600	-7.73037700
H	-3.68789100	12.91188800	-7.04466300
H	-4.08960200	11.15544500	-8.73571900
C	-3.99279200	8.45517900	-8.40413900
C	-5.51530500	8.42538700	-8.55624000
H	-5.99828600	8.35172600	-7.57456400
H	-5.83075600	7.57132400	-9.17109700
H	-5.87512500	9.34262100	-9.04100400
C	-3.31109500	8.63048100	-9.75771700
H	-3.68407400	7.48561900	-7.99535300
H	-3.57562400	7.80131400	-10.42451900
H	-2.22043600	8.65746700	-9.66512100
H	-3.62894000	9.55702100	-10.25084700
C	-3.04468000	10.18932700	-5.11155900
C	-2.65006200	9.78602900	-3.70559700
C	-3.14089800	10.76878200	-2.64846400
H	-3.02079800	10.33759900	-1.64858700
H	-4.19969600	11.01047300	-2.78916900
H	-2.57132800	11.70662000	-2.66653800
C	-1.13180000	9.61096100	-3.61597600
H	-3.12495800	8.81653700	-3.49649800
H	-0.76782500	8.85945800	-4.32511900
H	-0.83262200	9.29856900	-2.60926100
H	-0.62649600	10.55910400	-3.84038700
H	-3.07483600	12.30334500	-4.73686100
N	-9.46048700	6.85072000	-1.17237800
C	-9.57402400	7.74232700	-2.29687900
C	-8.80743700	8.91196700	-2.33109900
C	-10.53592800	7.45458900	-3.27918500
C	-9.05572400	9.83297100	-3.34653800

C	-10.05182900	9.60441000	-4.28624000
C	-10.77236000	8.42288900	-4.25763800
H	-8.47131500	10.74693000	-3.39193800
H	-10.24807700	10.34207500	-5.05923200
H	-11.52961300	8.23318100	-5.01556400
C	-11.35952300	6.17480900	-3.30362100
C	-11.24533700	5.42456000	-4.63310100
H	-11.48867400	6.06896000	-5.48611900
H	-11.95190100	4.58661800	-4.64529200
H	-10.23857100	5.02054300	-4.79286000
C	-12.83056200	6.49023100	-3.01629900
H	-10.99734600	5.50138400	-2.51802300
H	-13.24843400	7.12846600	-3.80486700
H	-12.95510000	7.01804700	-2.06512700
H	-13.42639300	5.57158000	-2.97985800
C	-7.79673900	9.18223300	-1.24198900
C	-6.65417800	10.07380300	-1.71170800
H	-6.26924500	9.74025500	-2.68425000
H	-5.83083000	10.04799200	-0.98730000
H	-6.96978200	11.12121500	-1.80674700
C	-8.49096300	9.78637900	-0.01857200
H	-7.37590600	8.21193200	-0.95363900
H	-8.94793800	10.74977600	-0.27871400
H	-7.77255700	9.96109500	0.79052400
H	-9.27966600	9.12970000	0.36456100
H	-1.08921500	7.58385200	-6.63375000
H	-1.59553000	4.93160000	-5.98024000
H	-11.15598000	4.83359300	0.77273300
H	-11.35262900	7.37807800	-0.30406900
C	-4.12308100	4.52133400	-5.12282300
C	-5.00298100	4.11000500	-6.14345100
C	-3.80195700	3.69197700	-4.04408000
C	-5.55333400	2.83329600	-6.04437000
C	-4.36962500	2.41778900	-3.99723400

C	-5.23086900	1.98838800	-4.99120400
H	-6.24135300	2.49034500	-6.81159800
H	-4.12779500	1.76174500	-3.16442900
H	-5.66762600	0.99452800	-4.94213700
C	-2.85315200	4.12061500	-2.94588300
C	-3.48023600	3.88321900	-1.57081600
H	-4.52679600	4.20479000	-1.55475500
H	-2.93421800	4.42977300	-0.79329300
H	-3.45375400	2.81960300	-1.30338600
C	-1.51978100	3.37979500	-3.06384300
H	-2.66090500	5.19436300	-3.06088900
H	-1.67945600	2.29588500	-2.99633600
H	-0.83873900	3.66932100	-2.25584600
H	-1.02001800	3.58275100	-4.01758200
C	-5.31796900	4.98887000	-7.34269900
C	-4.22564900	4.85920900	-8.41278000
H	-4.44840200	5.51633200	-9.26536400
H	-4.18898100	3.82770300	-8.78635900
H	-3.23147400	5.11979200	-8.03842500
C	-6.66418800	4.67803700	-7.99694300
H	-5.34583700	6.03341300	-6.99323500
H	-6.91607000	5.47173000	-8.70972000
H	-7.48281600	4.60526900	-7.27385700
H	-6.62485400	3.73951500	-8.56407000
C	-8.07907600	6.91896100	-5.72859300
H	-7.37938300	7.04538600	-6.56387600
H	-9.03677100	6.58654000	-6.14902400
H	-8.22615900	7.90624200	-5.27804100
C	-5.04751900	6.82400100	-0.32882300
H	-4.13410400	7.26819500	0.08389400
H	-5.89935900	7.31609600	0.15846300
H	-5.07625500	5.77361400	-0.01756200
H	-6.80376700	4.41921200	-1.32128200
H	-5.60081100	8.64109100	-4.81089600

59. NHC_Full_C₂H₅_H (planar)-singlet:

N	-8.57839300	3.27971500	-1.51149200
C	-6.93607100	1.84691900	-1.69798200
C	-8.18225600	1.99860000	-1.21225000
C	-7.60192600	3.96857000	-2.21640300
C	-6.86724800	6.52135400	-3.12296700
C	-7.22632300	7.91982700	-3.16917000
C	-5.85813300	6.05251000	-4.16778700
H	-5.04245900	5.46578400	-3.73763800
H	-5.36783700	6.89643400	-4.65066000
C	-8.23498000	8.38859400	-2.12387100
H	-8.72689600	7.54480900	-1.64236800
H	-9.04939600	8.97747200	-2.55329100
N	-7.51446600	11.40229400	-3.99296000
N	-5.51490200	11.16137100	-4.78078800
C	-7.15706000	12.59444300	-4.59445900
C	-5.91088500	12.44252200	-5.08016600
B	-6.37043700	8.94368400	-3.86471200
B	-7.72320000	5.49758800	-2.42740200
C	-6.49151400	10.47269900	-4.07582600

C	-9.72564400	3.86150800	-0.88575900
C	-10.97013000	3.77514000	-1.51641300
C	-9.54356700	4.47130500	0.36009400
C	-12.06068800	4.35043000	-0.86518300
C	-10.66182100	5.03901200	0.96803800
C	-11.90645700	4.98387000	0.35999900
H	-13.04374000	4.30523800	-1.32404600
H	-12.76741700	5.43265500	0.84750600
H	-10.54860600	5.53316100	1.93070500
C	-8.19049900	4.54618300	1.04312600
C	-8.23365200	3.90595300	2.43143600
H	-8.58485300	2.86936300	2.38930600
H	-8.89987400	4.45839100	3.10509200
H	-7.23341600	3.91055200	2.88074900
C	-7.69913900	5.99345600	1.13861700
H	-7.46349000	3.97788300	0.44749500
H	-6.72737100	6.03097900	1.64827300
H	-8.40100800	6.60385800	1.72144000
H	-7.58650300	6.45044400	0.14725200
C	-11.10778100	3.13007100	-2.88172100
C	-12.48632400	2.51864900	-3.11624200
H	-12.48403300	1.93004200	-4.03903400
H	-13.25171700	3.29428100	-3.23772400
H	-12.79567000	1.86514000	-2.29347200
C	-10.79369600	4.15090600	-3.98094000
H	-10.36407600	2.32246600	-2.94539500
H	-10.89709800	3.69291800	-4.97149300
H	-9.78168700	4.56189900	-3.89089000
H	-11.49815100	4.99023500	-3.91988900
C	-4.36847000	10.57913500	-5.40764500
C	-3.12329000	10.66521200	-4.77832800
C	-3.43454400	9.40158100	-7.26253300
C	-2.18922200	9.45651600	-6.65587700
C	-2.03353200	10.08983700	-5.43081600

H	-1.32887200	9.00764400	-7.14437900
H	-1.04995700	10.13485400	-4.97305500
C	-2.98415900	11.31025400	-3.41316100
C	-3.29815500	10.28970400	-2.31365800
H	-4.31027000	9.87888600	-2.40332800
H	-3.19435600	10.74784700	-1.32321900
H	-2.59391100	9.45020800	-2.37475100
C	-1.60505000	11.92075400	-3.17967700
H	-3.72726800	12.11837200	-3.34901000
H	-1.60614000	12.50899600	-2.25664900
H	-1.29608800	12.57442400	-4.00246300
H	-0.84001400	11.14460400	-3.05924100
C	-4.55203700	9.96944300	-6.65333300
C	-5.90583200	9.89502300	-7.33498500
C	-6.39754400	8.44788200	-7.43066400
H	-7.36973100	8.41078200	-7.93954600
H	-6.50948700	7.99048500	-6.43940300
H	-5.69629400	7.83757500	-8.01432700
C	-5.86402600	10.53588900	-8.72304500
H	-6.63215600	10.46315900	-6.73837400
H	-5.51265100	11.57241500	-8.68078600
H	-6.86473900	10.53163400	-9.17131200
H	-5.19856600	9.98367700	-9.39764200
H	-3.54889000	8.90752600	-8.22511500
N	-6.57879800	3.03917700	-2.29946500
C	-5.22750400	3.24233900	-2.71746300
C	-4.76758400	2.57096000	-3.85989200
C	-4.38809100	4.04621300	-1.92873300
C	-3.42992600	2.74259200	-4.21682900
C	-2.58205500	3.53370400	-3.45850500
C	-3.05815800	4.17224500	-2.32328200
H	-3.04887700	2.23649200	-5.10012800
H	-1.54311900	3.65236800	-3.75276200
H	-2.38874000	4.79031500	-1.73179100

C	-4.87974500	4.76028000	-0.68479500
C	-4.33340200	6.18167000	-0.56608800
H	-3.25725900	6.20426300	-0.35470600
H	-4.83667000	6.70095200	0.25866400
H	-4.52575800	6.75393700	-1.48384300
C	-4.58382400	3.91942000	0.55807400
H	-5.96301700	4.86970000	-0.76291600
H	-3.50411700	3.77327400	0.69368700
H	-5.05154300	2.92807100	0.48346900
H	-4.97591000	4.40992500	1.45941600
C	-5.64024300	1.62862700	-4.67116600
C	-5.51944900	1.84753100	-6.17999900
H	-5.71226300	2.88341600	-6.46374500
H	-6.23538500	1.20761000	-6.70677200
H	-4.52176800	1.57336700	-6.54208200
C	-5.26226800	0.17501900	-4.36107500
H	-6.68791500	1.79492300	-4.38602800
H	-4.22151600	-0.00772100	-4.65841600
H	-5.89733400	-0.52116700	-4.92002500
H	-5.34317000	-0.06935000	-3.29791200
H	-5.26534800	13.11446500	-5.62229500
H	-7.84324400	13.42389400	-4.62850100
H	-8.82774300	1.32646300	-0.67030100
H	-6.24976100	1.01757400	-1.66398200
C	-8.86526500	11.19933500	-3.57325200
C	-9.32334800	11.86939200	-2.42932800
C	-9.70573600	10.39579900	-4.36121300
C	-10.66039800	11.69717900	-2.07038400
C	-11.03505200	10.26932500	-3.96476100
C	-11.50939000	10.90676700	-2.82818000
H	-11.04011400	12.20225400	-1.18593500
H	-11.70527800	9.65146700	-4.55554500
H	-12.54782600	10.78765500	-2.53233500
C	-9.21525400	9.68176600	-5.60563400

C	-9.76313200	8.26101500	-5.72479700
H	-9.57167600	7.68838400	-4.80707700
H	-9.26013100	7.74134600	-6.54945600
H	-10.83923200	8.23958200	-5.93654200
C	-9.51024500	10.52341200	-6.84819000
H	-8.13209100	9.57101700	-5.52762100
H	-10.58977400	10.67095400	-6.98366500
H	-9.11884000	10.03272600	-7.74973500
H	-9.04126500	11.51414900	-6.77332400
C	-8.44952000	12.81129600	-1.61885600
C	-8.82731600	14.26505600	-1.92846600
H	-8.19136600	14.96100100	-1.37022100
H	-9.86768000	14.44813700	-1.62996800
H	-8.74749400	14.50937500	-2.99171800
C	-8.56876800	12.59227800	-0.10993500
H	-7.40222000	12.64470300	-1.90520600
H	-7.85213400	13.23198300	0.41614900
H	-8.37591100	11.55628800	0.17348400
H	-9.56598300	12.86666000	0.25325700
C	-7.54223000	9.20113000	-1.03040500
H	-6.67298300	8.64362600	-0.64783900
H	-7.16180600	10.16310300	-1.40442500
H	-8.21821800	9.40143100	-0.18768900
C	-6.54971900	5.23744600	-5.26013600
H	-5.87310200	5.03636300	-6.10212700
H	-6.92951800	4.27575300	-4.88482000
H	-7.41916200	5.79364300	-5.64411400
H	-8.76441600	5.80153400	-1.93523000
H	-5.32947300	8.63963100	-4.35737500

60. NHC_Full_C₂H₅_H (planar)-triplet:

N	-8.47339800	3.41546300	-1.12448500
C	-6.87796200	1.96504000	-1.54452600
C	-8.03106900	2.13538700	-0.87066300
C	-7.63679900	4.06447400	-2.02195100
C	-6.90943300	6.53794800	-3.14961400
C	-7.18378400	7.90265900	-3.14232000
C	-6.36233600	5.95854200	-4.45963500
H	-5.36189900	5.51906800	-4.33862100
H	-6.23835300	6.76367100	-5.18971100
C	-7.73111500	8.48203400	-1.83235700
H	-7.85484500	7.67691700	-1.10224000
H	-8.73175400	8.92101900	-1.95348100
N	-7.46607600	11.30771700	-4.04742700
N	-5.61995800	11.02532600	-5.16735000
C	-7.21560600	12.47553700	-4.74736100
C	-6.06244500	12.30535400	-5.42117300
B	-6.38411900	8.86962900	-4.06323600
B	-7.70914500	5.57102200	-2.22866100
C	-6.45648200	10.37619800	-4.26993300
C	-9.69624000	3.93583400	-0.60910200
C	-10.76126800	4.23034500	-1.47231500
C	-9.77752400	4.14175700	0.77845800
C	-11.94629800	4.68751000	-0.89577700
C	-10.99099000	4.58081700	1.30403300

C	-12.07119600	4.84447800	0.47505100
H	-12.78839000	4.92034300	-1.54359200
H	-13.00943500	5.19021300	0.89955700
H	-11.08381200	4.74233400	2.37376700
C	-8.54013800	4.06159300	1.65625300
C	-8.83493700	3.68086700	3.10383600
H	-9.44065000	2.77126000	3.17614200
H	-9.36496600	4.48218200	3.63156600
H	-7.89928200	3.51143000	3.64606200
C	-7.82432600	5.41754500	1.59806800
H	-7.85277100	3.30939700	1.24830900
H	-6.86182800	5.37418500	2.12543000
H	-8.44321600	6.18778500	2.07638300
H	-7.64192600	5.73642700	0.56330800
C	-10.69649600	4.08630800	-2.98386000
C	-11.74458500	3.08637200	-3.47890100
H	-11.65934700	2.94717300	-4.56215800
H	-12.76102000	3.44335700	-3.27296700
H	-11.63231300	2.10921800	-2.99807300
C	-10.89410300	5.44208400	-3.67664400
H	-9.70539500	3.71173600	-3.26759600
H	-10.84856500	5.31628600	-4.76584400
H	-10.12736100	6.17356000	-3.38590500
H	-11.87932100	5.86198400	-3.43429800
C	-4.39677700	10.50533100	-5.68228900
C	-3.33187200	10.21150600	-4.81871000
C	-3.10117100	9.86074900	-7.59495600
C	-2.02110600	9.59766000	-6.76559700
C	-2.14646400	9.75477800	-5.39482800
H	-1.08258100	9.25230100	-7.18977800
H	-1.30443300	9.52246800	-4.74674900
C	-3.39718100	10.35591500	-3.30723200
C	-3.19942500	9.00033400	-2.61414100
H	-3.96580000	8.26859800	-2.90515600

H	-3.24548700	9.12623900	-1.52497600
H	-2.21396100	8.58074300	-2.85602500
C	-2.34956000	11.35623300	-2.81199600
H	-4.38849400	10.73023500	-3.02390800
H	-2.43555700	11.49594600	-1.72886600
H	-2.46161100	12.33313600	-3.29338600
H	-1.33293700	10.99926000	-3.01701200
C	-4.31499400	10.29931300	-7.06980400
C	-5.55215000	10.37911400	-7.94795700
C	-6.26804500	9.02322300	-7.88958400
H	-7.23044200	9.06655700	-8.41713400
H	-6.45067300	8.70458100	-6.85479200
H	-5.64914600	8.25281800	-8.36761500
C	-5.25694000	10.75941000	-9.39556900
H	-6.23963800	11.13145500	-7.54045300
H	-4.65128000	11.66904500	-9.46796500
H	-6.19244600	10.92861000	-9.93812800
H	-4.72668200	9.95797900	-9.92289400
H	-3.00791100	9.69921500	-8.66464900
N	-6.62731900	3.13284400	-2.24441600
C	-5.31994200	3.48514400	-2.69763100
C	-4.81502100	2.90604800	-3.87149500
C	-4.56948300	4.39257400	-1.92983000
C	-3.57012900	3.33928100	-4.32609000
C	-2.85902800	4.31471200	-3.64339100
C	-3.34666900	4.81866900	-2.44620600
H	-3.15952800	2.91163800	-5.23697800
H	-1.90529300	4.66185200	-4.03024400
H	-2.75278200	5.53283500	-1.88015600
C	-4.95206200	4.79203500	-0.51415000
C	-4.86588100	6.29790300	-0.27010900
H	-3.83715200	6.66308100	-0.38707000
H	-5.17597700	6.53538900	0.75407500
H	-5.50494200	6.85177900	-0.96680800

C	-4.05020400	4.03700600	0.46827700
H	-5.98269700	4.47245600	-0.31650700
H	-2.99912500	4.32422200	0.33651100
H	-4.12245600	2.95243900	0.32601600
H	-4.33630200	4.26793300	1.50194600
C	-5.53691100	1.79035900	-4.60305900
C	-5.51339600	1.95687100	-6.12238100
H	-5.84523000	2.95138100	-6.42886100
H	-6.16495500	1.21411700	-6.59454200
H	-4.50556900	1.79656300	-6.52284100
C	-4.89650500	0.44568200	-4.23880200
H	-6.58437800	1.78300200	-4.27219100
H	-3.84996100	0.43183700	-4.56978300
H	-5.41635000	-0.38390500	-4.73106700
H	-4.89601500	0.25880300	-3.16008000
H	-5.49640200	12.97583300	-6.04794300
H	-7.89098700	13.31362900	-4.69550100
H	-8.59715500	1.46498400	-0.24385000
H	-6.20270200	1.12685200	-1.59644500
C	-8.77348400	10.95512000	-3.59452000
C	-9.27861700	11.53387400	-2.42058100
C	-9.52363600	10.04762300	-4.36253200
C	-10.52342700	11.10025100	-1.96613700
C	-10.74638400	9.62113400	-3.84631000
C	-11.23422700	10.12475900	-2.64906400
H	-10.93418600	11.52761400	-1.05518700
H	-11.34006300	8.90690400	-4.41250300
H	-12.18789600	9.77729700	-2.26233700
C	-9.14079200	9.64848000	-5.77823400
C	-9.22662400	8.14264900	-6.02251800
H	-8.58740300	7.58884100	-5.32592700
H	-8.91654100	7.90538500	-7.04675300
H	-10.25525900	7.77721200	-5.90555600
C	-10.04267900	10.40348900	-6.76065300

H	-8.11020700	9.96833700	-5.97572900
H	-11.09371100	10.11598100	-6.62913600
H	-9.75632800	10.17286400	-7.79432300
H	-9.97072200	11.48804300	-6.61814200
C	-8.55711900	12.64971500	-1.68887700
C	-9.19769600	13.99426200	-2.05332700
H	-8.67823700	14.82394000	-1.56080600
H	-10.24437200	14.00783800	-1.72275200
H	-9.19780100	14.18121600	-3.13203300
C	-8.58101200	12.48322300	-0.16956000
H	-7.50957600	12.65727000	-2.01948300
H	-7.92918200	13.22564200	0.30274700
H	-8.24974600	11.48854300	0.13697700
H	-9.58885000	12.64403100	0.23068300
C	-6.78600600	9.50545700	-1.19007600
H	-5.74688500	9.14908100	-1.23878000
H	-6.80383000	10.48680600	-1.67670500
H	-7.03271300	9.65526800	-0.13210300
C	-7.30792400	4.93542000	-5.10170400
H	-7.06174800	4.78579200	-6.15982700
H	-7.28994900	3.95394900	-4.61532700
H	-8.34698900	5.29186100	-5.05238800
H	-8.64141100	5.98955000	-1.61354700
H	-5.45153000	8.45129800	-4.67805400

61. NHC_Full_CH₃_H (fully optimized)-singlet:

N	-9.81201900	4.51298000	-1.32092700
C	-10.72288500	6.49015900	-1.06421300
C	-10.91059000	5.17774700	-0.81929700
C	-8.90442200	5.39140600	-1.86642400
C	-6.56395700	5.89943200	-3.08072500
C	-5.14079300	5.80739600	-3.03104000
C	-7.15655900	6.82063900	-4.12572200
H	-8.24442400	6.69888000	-4.18769600
H	-6.75188500	6.58389700	-5.12286300
H	-6.93277700	7.88614100	-3.94932200
C	-4.54796200	4.88640300	-1.98614300
H	-4.77824900	3.82167900	-2.15822800
H	-4.94703300	5.12839200	-0.98789400
H	-3.45915900	5.00286900	-1.92948600
N	-2.22709500	5.06329600	-4.44019800
N	-1.89192700	7.16945100	-4.80699900
C	-1.00308300	5.18348900	-5.07276200
C	-0.80361100	6.49430300	-5.31707300
B	-4.25098600	6.66703600	-3.86287900
B	-7.45290500	5.03589800	-2.25192000
C	-2.80475800	6.29952300	-4.25695300
C	-9.48541100	3.17159200	-0.94704100
C	-8.93886500	2.97726000	0.32476800
C	-9.68965000	2.13020300	-1.85657400
C	-8.66573200	1.66603300	0.71394700
C	-9.39410600	0.83818500	-1.42673900
C	-8.90110300	0.60774300	-0.14862600
H	-8.24621100	1.48135200	1.70079000
H	-8.67995800	-0.40776700	0.16802900

H	-9.53946400	0.00090200	-2.10221800
C	-10.22688400	2.42144400	-3.24340500
C	-11.74956300	2.58117400	-3.20100400
H	-12.05961400	3.38091600	-2.52109700
H	-12.21730000	1.64883800	-2.86015200
H	-12.14576600	2.81253800	-4.19608800
C	-9.84445600	1.35887900	-4.26706500
H	-9.78240500	3.37482100	-3.56535700
H	-10.12285700	1.68971300	-5.27237700
H	-10.37147200	0.41449800	-4.08333100
H	-8.76883800	1.15758000	-4.25973300
C	-8.59353600	4.13179200	1.24676900
C	-9.40284200	4.07464700	2.54158900
H	-9.16128200	4.93137400	3.18200600
H	-9.18071200	3.16124800	3.10756200
H	-10.48043500	4.09080400	2.34243800
C	-7.09147600	4.15794300	1.54028600
H	-8.84586100	5.07361000	0.74393900
H	-6.84312900	5.01408500	2.18020000
H	-6.50827300	4.23653300	0.61494000
H	-6.77504200	3.25014800	2.06898400
C	-2.20772200	8.51470800	-5.17604800
C	-2.76273800	8.71653300	-6.44299600
C	-2.27100200	10.84810300	-4.69217900
C	-2.77189100	11.08553600	-5.96593100
C	-3.02536000	10.03105800	-6.82813800
H	-2.98496800	12.10377800	-6.27933200
H	-3.45076100	10.22160900	-7.81134800
C	-3.12614600	7.56648800	-7.36359900
C	-4.62928400	7.55829100	-7.65211200
H	-5.21016400	7.48921100	-6.72462500
H	-4.89020200	6.70343100	-8.28876600
H	-4.93661500	8.46831100	-8.18235100
C	-2.32026900	7.61342600	-8.66097200

H	-2.88408200	6.62180700	-6.86123000
H	-2.57537800	6.76052700	-9.30125900
H	-1.24235300	7.58249400	-8.46518100
H	-2.53177900	8.53032000	-9.22541800
C	-1.98539000	9.55243100	-4.26656800
C	-1.43961100	9.25348700	-2.88470900
C	-1.80288200	10.31792000	-1.85601300
H	-1.51860400	9.98273700	-0.85378300
H	-2.87656400	10.52935800	-1.85319200
H	-1.26858000	11.25756900	-2.04288100
C	0.08099600	9.07873600	-2.94022600
H	-1.89070000	8.30396300	-2.56062900
H	0.37720300	8.27693100	-3.62385400
H	0.48331100	8.84197100	-1.94887400
H	0.55507900	10.00686300	-3.28377600
H	-2.11154300	11.68282000	-4.01669500
N	-9.49618800	6.62187900	-1.68931500
C	-8.90050000	7.90645500	-1.90729600
C	-7.81697100	8.30172000	-1.10638800
C	-9.44995300	8.73908200	-2.88957700
C	-7.27505700	9.56344600	-1.34115500
C	-7.81745500	10.41790000	-2.29205900
C	-8.90233000	10.01183700	-3.04899700
H	-6.42591300	9.89132100	-0.75000100
H	-7.38606900	11.40320700	-2.44347300
H	-9.32117200	10.67891400	-3.79843700
C	-10.57601900	8.29402300	-3.80372700
C	-10.25683400	8.58177800	-5.27361900
H	-10.28340800	9.65804200	-5.48008500
H	-11.00332600	8.11165200	-5.92275600
H	-9.26771100	8.20936700	-5.55556200
C	-11.88920300	8.98405300	-3.42569200
H	-10.69996500	7.20813100	-3.69207800
H	-11.77806200	10.07252000	-3.51407700

H	-12.19450800	8.76900400	-2.39668300
H	-12.70165200	8.67535700	-4.09295600
C	-7.30616600	7.45105100	0.04001200
C	-5.81899300	7.64323300	0.31683500
H	-5.23716600	7.55863900	-0.60986800
H	-5.47226500	6.86801300	1.01118600
H	-5.60283400	8.61311600	0.78268300
C	-8.15147000	7.72448800	1.28820900
H	-7.42475700	6.39768100	-0.23536400
H	-8.05730200	8.77240700	1.60149100
H	-7.82893200	7.09176100	2.12568700
H	-9.21549800	7.52311700	1.10576600
H	0.00251000	7.01821700	-5.80579700
H	-0.41089800	4.31279800	-5.30313600
H	-11.71451700	4.64632100	-0.33509700
H	-11.32543700	7.35509000	-0.83908100
C	-2.83429100	3.78476600	-4.21813000
C	-3.92844900	3.40092100	-5.01040900
C	-2.28587900	2.94653000	-3.24006900
C	-4.48275900	2.14571800	-4.76974500
C	-2.84591100	1.67976900	-3.07567900
C	-3.94180300	1.28572000	-3.82289200
H	-5.34067900	1.82689400	-5.35305900
H	-2.42806100	1.00831600	-2.32960400
H	-4.38311900	0.30552300	-3.66701800
C	-1.14767900	3.37943500	-2.33514400
C	-1.45818300	3.09568100	-0.86260800
H	-2.44091200	3.47892300	-0.57296300
H	-0.70144800	3.55788100	-0.21966400
H	-1.44168800	2.01926800	-0.65587700
C	0.15466500	2.67472000	-2.72345800
H	-1.01255500	4.46384100	-2.44814300
H	0.03216700	1.58759900	-2.63352100
H	0.97591800	2.97469100	-2.06303100

H	0.45388800	2.88579000	-3.75508200
C	-4.43774800	4.25604900	-6.15431400
C	-3.59623600	3.98135100	-7.40492000
H	-3.91790500	4.61737800	-8.24025200
H	-3.69650500	2.93459800	-7.72015800
H	-2.53079600	4.17710900	-7.22512800
C	-5.92582600	4.06993200	-6.43035800
H	-4.31457800	5.30864300	-5.87692300
H	-6.27034700	4.84866400	-7.12187400
H	-6.50673300	4.15339500	-5.50301600
H	-6.14532900	3.10229400	-6.89935700
H	-4.62622200	7.65100200	-4.44036800
H	-7.07439500	4.05372200	-1.67365600

62. NHC_Full_CH₃_H (fully optimized)-triplet:

N	-9.80760900	4.41351600	-1.43514000
C	-10.58342200	6.44137800	-1.10020700
C	-10.84694300	5.13668800	-0.88935400
C	-8.84662300	5.25699900	-1.96931900
C	-6.51870600	5.80751200	-3.22505900
C	-5.19455300	5.88143700	-2.89872700
C	-7.04714600	6.67751600	-4.34905300
H	-8.13165400	6.55288000	-4.46805800
H	-6.59442000	6.40558800	-5.31211100
H	-6.83551600	7.74822100	-4.19578000
C	-4.66638000	5.01125600	-1.77474600
H	-4.87733600	3.94051600	-1.92860000
H	-5.11994300	5.28256800	-0.81190700
H	-3.58202600	5.13640900	-1.65491900
N	-2.35056000	5.16554200	-4.38135400
N	-1.90580500	7.27679200	-4.68814400
C	-1.12933900	5.24925200	-5.02362300
C	-0.86624300	6.55408100	-5.23415100
B	-4.20742700	6.87246900	-3.58035600
B	-7.50583000	4.81683300	-2.54300300
C	-2.86653400	6.43285900	-4.15418900
C	-9.53861200	3.06250800	-1.05394900
C	-8.93743700	2.84959000	0.18907300
C	-9.86138300	2.02177200	-1.93004000
C	-8.73084700	1.52904400	0.58940000
C	-9.63334800	0.71931600	-1.49140100
C	-9.08830800	0.47561600	-0.23649400
H	-8.26694100	1.33289000	1.55411700
H	-8.92102700	-0.54770300	0.08817500
H	-9.87171500	-0.11669200	-2.14184500
C	-10.43582800	2.33176900	-3.29740600
C	-11.94235700	2.58836600	-3.20054600
H	-12.17391600	3.41575000	-2.52269100
H	-12.45462000	1.69244400	-2.82752000

H	-12.36139100	2.83081600	-4.18361100
C	-10.15961400	1.23724400	-4.32176700
H	-9.94498500	3.25363600	-3.64555900
H	-10.45642400	1.57344000	-5.32008900
H	-10.73534000	0.32881700	-4.10585100
H	-9.09886300	0.96897300	-4.35323700
C	-8.43826200	3.99399900	1.04899100
C	-9.10050500	4.01775300	2.42390000
H	-8.72423100	4.86149000	3.01469600
H	-8.88677100	3.09901200	2.98434400
H	-10.18881300	4.11699600	2.34430900
C	-6.91437600	3.91155000	1.16276700
H	-8.67614000	4.94046500	0.54871200
H	-6.50697500	4.81963500	1.62904400
H	-6.46224700	3.79963400	0.17074100
H	-6.60978700	3.05403500	1.77689600
C	-2.17530800	8.62778000	-5.06906200
C	-2.77654700	8.84071200	-6.31205700
C	-2.08154000	10.97092400	-4.63113400
C	-2.62666100	11.21466300	-5.88599800
C	-2.98367100	10.16125600	-6.71211400
H	-2.79435400	12.23798000	-6.21045900
H	-3.44764300	10.35741400	-7.67680000
C	-3.27523500	7.69629800	-7.17226200
C	-4.79917500	7.77798900	-7.28590200
H	-5.25132700	7.88917200	-6.29380300
H	-5.20610500	6.86990900	-7.75259900
H	-5.10425700	8.63563300	-7.89960700
C	-2.61311900	7.67329800	-8.54724600
H	-3.03683100	6.74979200	-6.67231100
H	-2.98898300	6.82950300	-9.13822300
H	-1.52474600	7.57464900	-8.46779900
H	-2.82743400	8.59206400	-9.10742600
C	-1.85297300	9.66847300	-4.19275700

C	-1.27843600	9.35846200	-2.82543200
C	-1.55507000	10.45272300	-1.80090300
H	-1.25822800	10.11645200	-0.80261600
H	-2.61591600	10.72063700	-1.76947400
H	-0.97963400	11.36138200	-2.01661900
C	0.22818000	9.10239000	-2.92229200
H	-1.76896600	8.43637800	-2.47741900
H	0.46003400	8.27516900	-3.60024500
H	0.64727400	8.85995600	-1.93924900
H	0.74015100	9.99853300	-3.29519000
H	-1.84352800	11.80689400	-3.98051100
N	-9.36219000	6.52454800	-1.74252000
C	-8.75214000	7.77845500	-2.05877100
C	-7.59416800	8.17483000	-1.36523700
C	-9.33920900	8.57459700	-3.05110600
C	-7.00478200	9.38114500	-1.73836400
C	-7.57923400	10.19447300	-2.70660600
C	-8.74658200	9.80408600	-3.33964100
H	-6.08835700	9.70032300	-1.25377700
H	-7.10722400	11.13715600	-2.96827900
H	-9.19053600	10.44173300	-4.09998200
C	-10.55268800	8.13066300	-3.84780100
C	-10.35636300	8.33775400	-5.35252000
H	-10.36952400	9.40289200	-5.61105000
H	-11.17213600	7.86308700	-5.90821600
H	-9.40920800	7.91904300	-5.70411800
C	-11.80378700	8.89062600	-3.39831300
H	-10.70499400	7.05668500	-3.67361800
H	-11.66163300	9.96740500	-3.55755300
H	-12.02631700	8.74389100	-2.33696300
H	-12.68109800	8.57964900	-3.97647700
C	-7.05319000	7.36539600	-0.20255200
C	-5.61514600	7.71556900	0.16230600
H	-4.95504400	7.68790200	-0.71403800

H	-5.23684000	6.99575900	0.89835000
H	-5.54709700	8.71082000	0.62009000
C	-7.95229000	7.55093800	1.02719800
H	-7.07387400	6.30183000	-0.48711400
H	-7.93147800	8.59634100	1.36066900
H	-7.59798700	6.92696700	1.85917200
H	-8.99586200	7.28187100	0.82955500
H	-0.04322600	7.04501000	-5.72890800
H	-0.58151900	4.35916500	-5.28709100
H	-11.67013000	4.64615600	-0.39448800
H	-11.13098100	7.33170700	-0.83701200
C	-2.96012700	3.91136500	-4.06520900
C	-4.11777900	3.51451000	-4.75898000
C	-2.37287200	3.11546700	-3.07279600
C	-4.70660900	2.30784200	-4.38612700
C	-2.96495500	1.88566300	-2.78447400
C	-4.13193300	1.49471600	-3.41784200
H	-5.62273100	1.98820400	-4.87097600
H	-2.52085900	1.24818200	-2.02407700
H	-4.60349500	0.55174900	-3.15638200
C	-1.15971000	3.55994800	-2.27591800
C	-1.35595500	3.35241300	-0.77125400
H	-2.30336200	3.77048000	-0.41957700
H	-0.54047800	3.82745100	-0.21544400
H	-1.34215300	2.28722900	-0.51294900
C	0.09186700	2.80082100	-2.72550400
H	-1.00803500	4.63405300	-2.44987500
H	-0.04969200	1.72391700	-2.56658300
H	0.96893900	3.11213600	-2.14715900
H	0.31443000	2.94799900	-3.78678300
C	-4.65902700	4.32394800	-5.92154500
C	-3.75971200	4.13917800	-7.15125700
H	-4.11420600	4.76325600	-7.98307500
H	-3.78005100	3.09386700	-7.48504700

H	-2.71627500	4.40863200	-6.95343400
C	-6.09683700	3.97308800	-6.28661700
H	-4.63894400	5.38745300	-5.63669000
H	-6.47550400	4.69285100	-7.02251100
H	-6.75696700	4.00017900	-5.41028300
H	-6.16432200	2.97792100	-6.74466500
H	-4.46012700	8.04338300	-3.71535000
H	-7.25330100	3.64593100	-2.40753300

63. NHC_Full_CH₃_H (twisted)-singlet:

N	-9.38345900	4.86577200	-0.43326200
C	-10.42959800	6.79930700	-0.44980200
C	-10.49947800	5.53844100	0.02115200
C	-8.60041600	5.68992500	-1.22479000
C	-6.33492600	6.23025900	-2.72073300

C	-6.41964200	6.25824900	-4.07608700
C	-5.34817200	7.13591400	-2.01996700
H	-5.84092900	8.04334500	-1.64091300
H	-4.54436000	7.47306300	-2.69268400
H	-4.88497700	6.64707600	-1.14912100
C	-7.40639600	5.35259200	-4.77685100
H	-7.86959700	5.84143000	-5.64769600
H	-8.21020500	5.01544000	-4.10413200
H	-6.91363900	4.44516300	-5.15591000
N	-3.46592200	5.59537500	-5.57297900
N	-3.37110800	7.62273600	-6.36355900
C	-2.32497100	5.68920000	-6.34702600
C	-2.25509000	6.95006700	-6.81797600
B	-5.50210500	7.16455700	-4.97799200
B	-7.25246100	5.32394900	-1.81882700
C	-4.15415100	6.79858100	-5.57203300
C	-9.12748600	3.49432700	-0.13348700
C	-8.72316000	3.16995400	1.17174500
C	-9.32236400	2.52120500	-1.11944000
C	-8.54818900	1.82294100	1.48258700
C	-9.12514200	1.18722900	-0.76035000
C	-8.75153900	0.83836600	0.52624800
H	-8.24040600	1.53953000	2.48419800
H	-8.61225900	-0.20694000	0.78743300
H	-9.27973200	0.41240300	-1.50771100
C	-9.74379200	2.84685700	-2.53904600
C	-11.13266300	2.27825800	-2.83478800
H	-11.88641100	2.66635800	-2.14167700
H	-11.13258900	1.18446000	-2.74824500
H	-11.44373800	2.52964200	-3.85461500
C	-8.71348300	2.31133600	-3.53626700
H	-9.78374800	3.93772600	-2.65322700
H	-8.96713700	2.61521200	-4.55888200
H	-8.67902500	1.21433100	-3.51459600

H	-7.71243500	2.69580700	-3.31039900
C	-8.37662000	4.25120200	2.17877900
C	-8.53002700	3.80359400	3.62942100
H	-8.41790200	4.66139000	4.29976500
H	-7.75590000	3.07970500	3.90994200
H	-9.50629000	3.34547300	3.82086400
C	-6.93936400	4.72153800	1.92515600
H	-9.04509600	5.10993200	2.02200500
H	-6.65172100	5.49358500	2.64819900
H	-6.81094000	5.12572900	0.91146500
H	-6.24674300	3.87752100	2.03724800
C	-3.62707800	8.99418200	-6.66332900
C	-4.03140000	9.31856200	-7.96856100
C	-3.62941500	11.30127900	-6.03645700
C	-4.00301400	11.65014700	-7.32305500
C	-4.20636600	10.66557700	-8.27939800
H	-4.14229100	12.69545500	-7.58423700
H	-4.51414500	10.94899200	-9.28100900
C	-4.37794200	8.23731800	-8.97559900
C	-5.81519700	7.76698000	-8.72197400
H	-5.94361900	7.36279000	-7.70828300
H	-6.10283900	6.99493300	-9.44501700
H	-6.50781800	8.61099700	-8.83406600
C	-4.22453800	8.68493300	-10.42623900
H	-3.70946500	7.37858700	-8.81883000
H	-4.33666700	7.82713900	-11.09658600
H	-3.24827500	9.14305300	-10.61768300
H	-4.99866500	9.40882400	-10.70675500
C	-3.43219700	9.96730100	-5.67737200
C	-3.01077100	9.64164300	-4.25776800
C	-4.04107800	10.17716500	-3.26054400
H	-3.78742300	9.87328700	-2.23793000
H	-5.04212600	9.79269600	-3.48641200
H	-4.07553300	11.27417000	-3.28221300

C	-1.62189800	10.21023500	-3.96202400
H	-2.97081900	8.55077400	-4.14359000
H	-0.86815100	9.82213400	-4.65513600
H	-1.31082400	9.95884700	-2.94219800
H	-1.62196700	11.30403400	-4.04856400
H	-3.47482300	12.07610100	-5.28909400
N	-9.28864600	6.89313100	-1.22384900
C	-8.65606000	8.14511300	-1.50799200
C	-8.01779700	8.80489700	-0.45348600
C	-8.68228800	8.64829000	-2.81560000
C	-7.42663700	10.04152900	-0.72938100
C	-7.40448800	10.54175200	-2.01924600
C	-8.00928300	9.84223400	-3.05941300
H	-6.94985700	10.59651100	0.07503700
H	-6.90315700	11.48375800	-2.22629300
H	-7.96746000	10.24039700	-4.06888000
C	-9.48351500	7.93484200	-3.88385000
C	-9.08946700	8.31788200	-5.30436700
H	-9.38011800	9.35253200	-5.52848800
H	-9.61498200	7.67666900	-6.02022800
H	-8.01394100	8.21751500	-5.47822800
C	-10.97631500	8.22248000	-3.68002700
H	-9.31757200	6.85689600	-3.75018300
H	-11.16782400	9.29911300	-3.77111700
H	-11.33411900	7.89803800	-2.69868500
H	-11.57421600	7.70975600	-4.44200000
C	-7.93702200	8.23180700	0.95108800
C	-6.49594800	8.20980000	1.46039700
H	-5.86811800	7.57416800	0.82598500
H	-6.46017800	7.81811600	2.48287700
H	-6.05612400	9.21313100	1.48188800
C	-8.83525800	9.02883400	1.89869000
H	-8.28706000	7.18895800	0.93393100
H	-8.51428800	10.07758100	1.94052100

H	-8.79134200	8.62373200	2.91581700
H	-9.88027300	9.01490400	1.56929700
H	-1.51277900	7.44799200	-7.42100200
H	-1.67251800	4.84092700	-6.48134000
H	-11.24178900	5.04051800	0.62417900
H	-11.08205200	7.64758000	-0.31549100
C	-4.09850800	4.34339400	-5.28883500
C	-4.73677400	3.68361000	-6.34334100
C	-4.07227900	3.84021600	-3.98122800
C	-5.32793500	2.44697900	-6.06744500
C	-4.74528500	2.64627300	-3.73741300
C	-5.35008300	1.94675600	-4.77758000
H	-5.80471800	1.89199800	-6.87186200
H	-4.78710700	2.24810900	-2.72794700
H	-5.85141500	1.00475000	-4.57053300
C	-3.27105100	4.55366300	-2.91297800
C	-3.66509700	4.17062400	-1.49246100
H	-4.74062200	4.27099200	-1.31859900
H	-3.13958100	4.81183700	-0.77660100
H	-3.37444600	3.13597400	-1.26834000
C	-1.77825100	4.26602400	-3.11680300
H	-3.43699300	5.63160900	-3.04664500
H	-1.58674200	3.18939200	-3.02571300
H	-1.18034800	4.77874800	-2.35483100
H	-1.42044800	4.59046600	-4.09814600
C	-4.81755100	4.25670000	-7.74791500
C	-3.91933100	3.45966100	-8.69552200
H	-3.96324800	3.86476400	-9.71264800
H	-4.24031500	2.41091800	-8.73735300
H	-2.87431400	3.47357700	-8.36613500
C	-6.25862800	4.27872600	-8.25721300
H	-4.46749900	5.29954500	-7.73076200
H	-6.29440000	4.67039900	-9.27969700
H	-6.88644100	4.91437700	-7.62280300

H	-6.69847000	3.27540200	-8.27868700
H	-6.92259300	4.19489900	-1.55159800
H	-5.83196900	8.29360900	-5.24521600

64. NHC_Full_CH₃_H (twisted)-triplet:

N	-9.55557700	4.74385900	-0.74267500
C	-10.53427900	6.71039300	-0.65028000
C	-10.67297700	5.41794900	-0.29382600
C	-8.70132500	5.60087200	-1.41764300
C	-6.34886000	6.17606600	-2.75184000
C	-6.37219600	6.32931700	-4.09937500
C	-5.37833700	6.99424600	-1.92451900
H	-5.87201700	7.88183200	-1.50232100
H	-4.52219900	7.36267000	-2.51010400
H	-4.98647600	6.42342600	-1.06940500

C	-7.32812800	5.51056000	-4.94096200
H	-7.57409800	6.01442800	-5.88969300
H	-8.26671600	5.26941700	-4.42077300
H	-6.87752500	4.54365200	-5.20439400
N	-3.42263600	5.62286900	-5.49138100
N	-3.13208800	7.70870700	-6.04378900
C	-2.21853400	5.71868700	-6.16285800
C	-2.03519200	7.01203300	-6.49852900
B	-5.36994600	7.28025000	-4.84824500
B	-7.34299000	5.22925600	-1.98120000
C	-4.01476900	6.87346900	-5.38489200
C	-9.36477400	3.34231100	-0.55827000
C	-9.04851300	2.88542700	0.73148900
C	-9.53121200	2.47184800	-1.64074800
C	-8.93677700	1.51001800	0.92482000
C	-9.39903600	1.10414900	-1.39717000
C	-9.11475600	0.62550500	-0.12956700
H	-8.69885600	1.12451000	1.91123900
H	-9.02561000	-0.44383100	0.04038800
H	-9.53317700	0.40709300	-2.22113900
C	-9.85603500	2.94144500	-3.04578000
C	-11.24187300	2.45393800	-3.47193300
H	-12.02333400	2.80520500	-2.78997300
H	-11.28189600	1.35755800	-3.48777600
H	-11.48278900	2.80838900	-4.48009000
C	-8.78485900	2.46080500	-4.02819400
H	-9.85458100	4.03914000	-3.05995400
H	-8.96668400	2.86563700	-5.03141300
H	-8.78762600	1.36595600	-4.10751100
H	-7.78695000	2.78346000	-3.71018300
C	-8.72738800	3.85914600	1.85065400
C	-8.96419100	3.28508000	3.24422000
H	-8.86239300	4.07356200	3.99636000
H	-8.22454300	2.51447300	3.49147100

H	-9.96066600	2.84208500	3.34619000
C	-7.26866600	4.31081800	1.71132500
H	-9.36626200	4.74747000	1.74247200
H	-7.00288600	5.01266500	2.51042200
H	-7.07781000	4.79363600	0.74294600
H	-6.60193200	3.44233400	1.78734200
C	-3.42065000	9.06349800	-6.37087800
C	-3.89880300	9.33180700	-7.66000100
C	-3.54464500	11.37243100	-5.77811500
C	-3.97921900	11.67309100	-7.06037700
C	-4.16612200	10.65985900	-7.98917700
H	-4.19005500	12.70335400	-7.33338700
H	-4.54542800	10.89749700	-8.98021500
C	-4.22861600	8.21951200	-8.63774500
C	-5.74469300	7.99990600	-8.66574500
H	-6.13790500	7.78092200	-7.66211700
H	-5.99579500	7.16302000	-9.33109900
H	-6.25547400	8.89637800	-9.04122600
C	-3.70378900	8.48855200	-10.04643800
H	-3.76506000	7.28866000	-8.28517200
H	-3.89252700	7.62199900	-10.69056100
H	-2.62726500	8.68778000	-10.05018300
H	-4.20571000	9.34720900	-10.50769300
C	-3.26750000	10.05876200	-5.40114600
C	-2.84594900	9.75424800	-3.97681900
C	-3.91741000	10.22176700	-2.98792600
H	-3.65545100	9.92352000	-1.96557100
H	-4.89324100	9.78466400	-3.22663100
H	-4.01319000	11.31568700	-3.00055500
C	-1.49730300	10.39999100	-3.65625600
H	-2.74937500	8.66558700	-3.87050100
H	-0.71039800	10.06015600	-4.33746800
H	-1.18858500	10.16518400	-2.63179000
H	-1.56100600	11.49229000	-3.74035100

H	-3.42348400	12.16909600	-5.04724800
N	-9.34845500	6.82580700	-1.35018500
C	-8.66277600	8.07306000	-1.49853500
C	-8.06139300	8.62517000	-0.36381200
C	-8.60365000	8.67810700	-2.76116700
C	-7.41505200	9.85629200	-0.51081900
C	-7.30660400	10.45371300	-1.75444800
C	-7.87953100	9.86118500	-2.87605300
H	-6.96240300	10.32846300	0.35789200
H	-6.76277300	11.38899100	-1.86023800
H	-7.77158300	10.33361800	-3.84819600
C	-9.37665300	8.08349700	-3.91835400
C	-8.88063400	8.52869800	-5.28811200
H	-9.11084500	9.58725300	-5.46618700
H	-9.38909800	7.95493600	-6.07055400
H	-7.80181500	8.38888100	-5.40553700
C	-10.86058600	8.44324300	-3.77384800
H	-9.27974600	6.99252900	-3.84615900
H	-10.98884800	9.53264400	-3.80322300
H	-11.28642500	8.07907500	-2.83408800
H	-11.44352100	8.01374400	-4.59649600
C	-8.07584400	7.94121800	0.99286200
C	-6.66458300	7.81383300	1.56602400
H	-6.03366600	7.19792600	0.91553200
H	-6.69709600	7.34626700	2.55629700
H	-6.18341500	8.79128600	1.68355000
C	-8.98741500	8.70244500	1.95691300
H	-8.46866900	6.91999500	0.87644700
H	-8.62554000	9.72884300	2.09882800
H	-9.01377100	8.21729100	2.93897300
H	-10.01340500	8.76240400	1.57669100
H	-1.22756700	7.50847700	-7.01160500
H	-1.60792800	4.84678300	-6.33521900
H	-11.46515700	4.90001500	0.22271300

H	-11.16418700	7.56877700	-0.47746700
C	-4.09462700	4.37129200	-5.29325600
C	-4.79912500	3.81237500	-6.37155800
C	-4.03367700	3.75945900	-4.03465100
C	-5.36642300	2.54988200	-6.18340000
C	-4.67440300	2.53205100	-3.87737700
C	-5.30363000	1.91779100	-4.95241900
H	-5.90996100	2.08135200	-6.99822700
H	-4.67590100	2.04755000	-2.90596000
H	-5.78080400	0.95071900	-4.81678900
C	-3.26595600	4.40915200	-2.90246200
C	-3.74264100	3.97285000	-1.52161300
H	-4.82817600	4.06512500	-1.41207700
H	-3.26498100	4.58988400	-0.75294900
H	-3.46177100	2.93210000	-1.31512400
C	-1.76967400	4.10820800	-3.04289200
H	-3.41334800	5.49441300	-2.99325900
H	-1.59747500	3.02546700	-2.99437500
H	-1.20457500	4.57465000	-2.22799100
H	-1.35789300	4.47328500	-3.98812700
C	-5.07228700	4.60033500	-7.64405900
C	-3.99518600	4.44643600	-8.72175600
H	-4.24614500	5.07622400	-9.58755200
H	-3.94789000	3.40652900	-9.06945200
H	-3.00013900	4.73785300	-8.37704800
C	-6.42591100	4.24397700	-8.26190400
H	-5.11716100	5.65941600	-7.34421900
H	-6.68556900	4.97428000	-9.03555700
H	-7.22985900	4.23001700	-7.51961300
H	-6.39539100	3.26242100	-8.75083900
H	-7.05670800	4.07386600	-1.78615900
H	-5.63140700	8.44276100	-5.02038000

65. NHC_Full_CH₃_H (planar)-singlet:

N	-9.77787200	4.63661500	-1.15285900
C	-10.82504500	6.55498900	-1.04517800
C	-10.91139700	5.26089500	-0.68456300
C	-8.96725300	5.50698500	-1.85356100
C	-6.53297300	6.04896000	-2.93588400
C	-5.18015800	5.64108000	-3.18760500
C	-7.06447500	7.13484100	-3.85886100
H	-8.15132200	7.06560800	-3.96080200
H	-6.64741600	7.01359900	-4.86827000
H	-6.81635300	8.16164700	-3.54048700
C	-4.64866900	4.55521000	-2.26460500
H	-4.89677700	3.52839700	-2.58296700
H	-5.06575400	4.67646400	-1.25520700
H	-3.56182500	4.62445400	-2.16263700
N	-2.07381200	4.97682200	-4.38171100

N	-1.93523200	7.05339600	-4.97062200
C	-0.88808900	5.13500300	-5.07829000
C	-0.80171500	6.42909300	-5.43891100
B	-4.21933000	6.50467800	-3.93526100
B	-7.49379300	5.18535500	-2.18822400
C	-2.74586900	6.18303800	-4.26992000
C	-9.45379800	3.28774400	-0.80571100
C	-9.00745300	3.04429800	0.49654900
C	-9.58710000	2.27402700	-1.76363000
C	-8.73069500	1.72201900	0.84822000
C	-9.29716600	0.97203200	-1.36517600
C	-8.88169000	0.69648100	-0.06863800
H	-8.36858800	1.50442500	1.85025400
H	-8.65841400	-0.32663600	0.22059500
H	-9.38628300	0.16040300	-2.08014000
C	-10.05072600	2.59746100	-3.17015900
C	-11.57278400	2.77068200	-3.19967400
H	-11.91322900	3.55576700	-2.51716800
H	-12.06412100	1.83397700	-2.90726100
H	-11.91527800	3.02939500	-4.20787600
C	-9.62876800	1.55269100	-4.19659000
H	-9.58187700	3.54983200	-3.45580000
H	-9.85836400	1.90835200	-5.20572500
H	-10.17083400	0.60893400	-4.05857800
H	-8.55574300	1.34380500	-4.14560100
C	-8.71252200	4.15870300	1.48370300
C	-9.34672000	3.91518700	2.85191400
H	-9.16274000	4.77188700	3.51004800
H	-8.92110400	3.03219600	3.34284000
H	-10.42946500	3.76784300	2.77887800
C	-7.19524100	4.32451700	1.61347100
H	-9.12290600	5.10042600	1.09660600
H	-6.95319400	5.14190500	2.30465700
H	-6.73208500	4.53793500	0.64132800

H	-6.74336400	3.40555400	2.00901000
C	-2.25927300	8.40226600	-5.31781300
C	-2.70566000	8.64567300	-6.62006500
C	-2.41580200	10.71800800	-4.75844200
C	-2.83134300	10.99351500	-6.05496800
C	-2.98240600	9.96794400	-6.97177600
H	-3.05461000	12.01662600	-6.34423100
H	-3.34455200	10.18550500	-7.97380400
C	-3.00061800	7.53124500	-7.60718400
C	-4.51790100	7.36544700	-7.73695400
H	-4.98106100	7.15204100	-6.76481000
H	-4.75995400	6.54805500	-8.42813200
H	-4.96976700	8.28441100	-8.13250200
C	-2.36641000	7.77471900	-8.97539800
H	-2.59024700	6.58952700	-7.22006100
H	-2.55041300	6.91801500	-9.63352100
H	-1.28366100	7.92203200	-8.90236100
H	-2.79199600	8.65771700	-9.46633800
C	-2.12588400	9.41602200	-4.35994600
C	-1.66218200	9.09264500	-2.95342800
C	-2.08402100	10.13749400	-1.92702900
H	-1.85439800	9.78187000	-0.91788700
H	-3.15703500	10.34645100	-1.97797400
H	-1.54190100	11.08120900	-2.06511700
C	-0.14012900	8.91936000	-2.92399700
H	-2.13105400	8.14031100	-2.66770400
H	0.20024300	8.13421300	-3.60646700
H	0.20241400	8.66070200	-1.91579800
H	0.35122900	9.85602400	-3.21650300
H	-2.32662100	11.52966500	-4.04351800
N	-9.63932700	6.71319200	-1.74176100
C	-9.08675700	8.03371900	-1.84768000
C	-8.12635500	8.44250800	-0.91282300
C	-9.58990700	8.89395600	-2.83052100

C	-7.67246100	9.75929600	-0.99468800
C	-8.16635100	10.63637200	-1.94780900
C	-9.12001500	10.20482300	-2.85627000
H	-6.93303600	10.10489700	-0.27690900
H	-7.80458200	11.66000200	-1.98344500
H	-9.50043900	10.89033000	-3.60954200
C	-10.58635400	8.42921500	-3.87452300
C	-10.14801700	8.82285500	-5.28691500
H	-10.21430500	9.90704700	-5.43516000
H	-10.80158000	8.35567300	-6.03133100
H	-9.11736700	8.51652800	-5.49037100
C	-11.97763000	8.99752400	-3.58625600
H	-10.63587000	7.33300400	-3.82861100
H	-11.94594200	10.09473700	-3.60008600
H	-12.35492400	8.69146200	-2.60491500
H	-12.69989900	8.67321400	-4.34369900
C	-7.62614200	7.55521300	0.21063000
C	-6.10321600	7.58138200	0.32886400
H	-5.63369200	7.31216200	-0.62575300
H	-5.77313200	6.86363000	1.08843500
H	-5.73326400	8.56708400	0.63617500
C	-8.30752800	7.94463600	1.52435200
H	-7.90363200	6.52196800	-0.01341500
H	-8.06016600	8.97532300	1.81071300
H	-7.98517800	7.28168000	2.33843900
H	-9.39984600	7.87169300	1.44048400
H	-0.04773600	6.97728100	-5.98135100
H	-0.23830500	4.29435600	-5.26095000
H	-11.66536800	4.71268800	-0.14213000
H	-11.47484300	7.39562400	-0.86251300
C	-2.62639700	3.65630100	-4.27579400
C	-3.58681300	3.24752500	-5.21064200
C	-2.12324600	2.79605400	-3.29296200
C	-4.04071500	1.93074000	-5.12878200

C	-2.59315100	1.48519200	-3.26721400
C	-3.54682600	1.05365500	-4.17566900
H	-4.78014600	1.58514800	-5.84656000
H	-2.21272600	0.79967800	-2.51394800
H	-3.90860200	0.03002700	-4.14003600
C	-1.12678600	3.26077800	-2.24896500
C	-1.56512800	2.86715300	-0.83657100
H	-2.59576900	3.17350600	-0.63311300
H	-0.91155100	3.33432100	-0.09215800
H	-1.49886700	1.78296000	-0.68832400
C	0.26447700	2.69243800	-2.53723300
H	-1.07724600	4.35698900	-2.29488200
H	0.23276700	1.59522600	-2.52339500
H	0.98675600	3.01673800	-1.77979400
H	0.64177500	2.99848500	-3.51857700
C	-4.08701800	4.13482000	-6.33409800
C	-3.40564800	3.74536700	-7.64781800
H	-3.72799500	4.40831500	-8.46191300
H	-3.65303000	2.71467900	-7.93415900
H	-2.31332800	3.81829200	-7.56396000
C	-5.60994600	4.10868400	-6.45232600
H	-3.80950700	5.16806000	-6.11006100
H	-5.94001700	4.82646200	-7.21188000
H	-6.07946100	4.37788900	-5.49770200
H	-5.97992100	3.12299800	-6.75966100
H	-4.52600200	7.56741300	-4.39859400
H	-7.18711500	4.12261500	-1.72490500

66. NHC_Full_CH₃_H (planar)-triplet:

N	-9.82483100	4.60050600	-1.18889600
C	-10.83680000	6.54037100	-1.03387700
C	-10.94479400	5.23744600	-0.70843400
C	-8.98664600	5.48414800	-1.85942800
C	-6.50283500	6.06380900	-2.94342800
C	-5.21026200	5.62626100	-3.18013600
C	-7.04408500	7.12221100	-3.89799300
H	-8.12277200	6.99168600	-4.05094100
H	-6.57097700	7.03586400	-4.88536300
H	-6.88306100	8.15721200	-3.55667100
C	-4.66901800	4.56789700	-2.22551700
H	-4.82998400	3.53287700	-2.56680900
H	-5.14217000	4.65425800	-1.23816800
H	-3.59034300	4.69846500	-2.07252700
N	-2.06643200	4.98734200	-4.40438800
N	-1.88828100	7.08959700	-4.93467500
C	-0.87622200	5.14977000	-5.08959900
C	-0.76828300	6.45268800	-5.41509500
B	-4.18298600	6.52554100	-3.92057700
B	-7.53010600	5.16453000	-2.20298600

C	-2.72644700	6.20593600	-4.26414200
C	-9.49476100	3.25859500	-0.83069000
C	-9.01983300	3.02753000	0.46349300
C	-9.64862500	2.23418100	-1.77391700
C	-8.74188100	1.70804900	0.82563700
C	-9.35501600	0.93539300	-1.36821200
C	-8.91531900	0.67287100	-0.07643700
H	-8.36250100	1.50013500	1.82363500
H	-8.69130900	-0.34798400	0.22027900
H	-9.46127600	0.11621300	-2.07242100
C	-10.13848800	2.54911200	-3.17297900
C	-11.66225000	2.70754900	-3.17771700
H	-11.99693800	3.49204500	-2.49175400
H	-12.13976500	1.76731300	-2.87390500
H	-12.02444800	2.95990000	-4.18068800
C	-9.72238200	1.50583100	-4.20335300
H	-9.68521300	3.50764100	-3.46512900
H	-9.96999500	1.85580200	-5.21030900
H	-10.25365300	0.55758300	-4.05470400
H	-8.64702100	1.30565200	-4.16713600
C	-8.70722100	4.15361800	1.43081100
C	-9.35056400	3.94562600	2.80052600
H	-9.14574500	4.80565900	3.44839900
H	-8.95076800	3.05694900	3.30307300
H	-10.43666100	3.82694600	2.72525300
C	-7.18841900	4.29683400	1.56243000
H	-9.10003200	5.09457000	1.02380300
H	-6.93450400	5.12057200	2.24170500
H	-6.72217100	4.49042200	0.58688500
H	-6.74883400	3.37753200	1.97048800
C	-2.21852300	8.43140600	-5.29311300
C	-2.69357500	8.66216200	-6.58730300
C	-2.35852400	10.75468600	-4.75601500
C	-2.79831500	11.01691100	-6.04782000

C	-2.97169300	9.98154200	-6.94968700
H	-3.02245800	12.03768400	-6.34471700
H	-3.35115400	10.18922200	-7.94770300
C	-3.00611700	7.53584700	-7.55437700
C	-4.52490600	7.39254600	-7.68604700
H	-4.99119200	7.19910800	-6.71049100
H	-4.77875100	6.56867300	-8.36518400
H	-4.96451900	8.31175000	-8.09429500
C	-2.36270000	7.74354800	-8.92410100
H	-2.61330000	6.59500200	-7.14712900
H	-2.56748400	6.88338000	-9.57180600
H	-1.27660700	7.86224100	-8.84878900
H	-2.76246500	8.63212600	-9.42685000
C	-2.06474100	9.45600800	-4.35008300
C	-1.57481900	9.14136100	-2.95097700
C	-1.99093200	10.18481900	-1.92078600
H	-1.74328300	9.83504300	-0.91377200
H	-3.06630000	10.38496100	-1.95701400
H	-1.45969200	11.13305400	-2.06962700
C	-0.05105100	8.98298500	-2.94624800
H	-2.02805200	8.18286500	-2.65864400
H	0.28365400	8.19837800	-3.63207400
H	0.31118100	8.73083100	-1.94323900
H	0.42641900	9.92318500	-3.25024100
H	-2.25233800	11.57401100	-4.05196300
N	-9.64660200	6.70276900	-1.71912000
C	-9.07933100	8.00932200	-1.85004800
C	-8.08073400	8.41478700	-0.95239000
C	-9.58447000	8.86047100	-2.84134600
C	-7.58975600	9.71392900	-1.08008300
C	-8.08544900	10.58047700	-2.04255800
C	-9.07868000	10.15621800	-2.91181600
H	-6.81846100	10.05572500	-0.39528900
H	-7.69378100	11.59104400	-2.11621400

H	-9.45842500	10.83453600	-3.67189500
C	-10.61833300	8.39777200	-3.84930800
C	-10.21810100	8.76515700	-5.28001300
H	-10.28021100	9.84726000	-5.44470400
H	-10.89684500	8.29157100	-5.99731300
H	-9.19632900	8.44750200	-5.50935200
C	-11.99131300	8.99365700	-3.52958100
H	-10.68357500	7.30321300	-3.78578500
H	-11.94090500	10.08987100	-3.56076400
H	-12.34566100	8.70849500	-2.53373700
H	-12.74028800	8.67126700	-4.26149100
C	-7.58980200	7.53455200	0.18058700
C	-6.07162400	7.57456800	0.33903400
H	-5.57592500	7.31770400	-0.60552400
H	-5.75507800	6.85169200	1.09927700
H	-5.71426300	8.55871900	0.66526600
C	-8.31004100	7.90928500	1.47771600
H	-7.84998700	6.49876700	-0.05324900
H	-8.08453800	8.94268700	1.77249300
H	-8.00003300	7.24765600	2.29800900
H	-9.39863300	7.82068100	1.36505000
H	-0.00147400	6.99759900	-5.94300600
H	-0.23259400	4.30797400	-5.28853300
H	-11.71162600	4.69254400	-0.18054600
H	-11.48037600	7.38219100	-0.83487800
C	-2.63356300	3.68075700	-4.27321600
C	-3.63220200	3.27504700	-5.17071500
C	-2.12827300	2.82982800	-3.28180300
C	-4.12305700	1.97588500	-5.04275400
C	-2.63394300	1.53404900	-3.21106400
C	-3.62720600	1.10955000	-4.08016700
H	-4.89438900	1.63390600	-5.72741400
H	-2.25407800	0.85589800	-2.45089600
H	-4.01878200	0.09896300	-4.00629900

C	-1.09437800	3.29279400	-2.27399500
C	-1.49450200	2.92567100	-0.84319300
H	-2.51626900	3.24333600	-0.61384600
H	-0.81572600	3.39942100	-0.12603100
H	-1.43234400	1.84360300	-0.67829600
C	0.27861800	2.69692600	-2.59368500
H	-1.02920300	4.38734400	-2.33773700
H	0.22828000	1.60071600	-2.56227200
H	1.02762000	3.01951400	-1.86189100
H	0.63288500	2.98190200	-3.58961200
C	-4.12329600	4.15506700	-6.30378600
C	-3.40295500	3.78033100	-7.60085900
H	-3.71306900	4.44179900	-8.42124000
H	-3.62824800	2.74685000	-7.89551600
H	-2.31438200	3.86915900	-7.48817900
C	-5.64146200	4.11475400	-6.46225900
H	-3.86332400	5.19092600	-6.07004200
H	-5.95812200	4.83753800	-7.22254400
H	-6.13722900	4.37158400	-5.51772500
H	-5.99863900	3.13052300	-6.78844900
H	-4.45771600	7.66089400	-4.18857900
H	-7.25537800	4.02917600	-1.93498300

67. NHC_Full_H_H (fully optimized)-singlet:

N	-9.82517100	4.91108100	-1.37379800
C	-10.32312400	7.01981500	-1.02580100
C	-10.85123700	5.77966200	-1.05535100
C	-8.63857800	5.58630900	-1.53986200
C	-6.10998500	5.78338900	-2.27789700
C	-4.90785900	5.37814400	-2.89938300
N	-2.06923600	5.07667100	-4.73024800
N	-2.35212300	7.15211900	-5.28386900
C	-1.13117700	5.37630900	-5.70239700
C	-1.31508000	6.66557800	-6.05480400
B	-4.01294100	6.40327800	-3.48545600
B	-7.28896800	4.95339500	-1.93432300
C	-2.84088800	6.17386200	-4.44650500
C	-9.99618500	3.49194800	-1.42585800
C	-10.13473300	2.79964300	-0.21663500
C	-10.03789400	2.85728500	-2.67330300
C	-10.35168600	1.42314000	-0.28287200
C	-10.24454300	1.47950800	-2.68663700
C	-10.40850600	0.77163100	-1.50464400
H	-10.46471700	0.85353700	0.63440800
H	-10.57396700	-0.30170800	-1.53691700
H	-10.27656100	0.95225300	-3.63488300
C	-9.90488200	3.65401500	-3.95568700
C	-11.25602800	4.27224800	-4.32737300
H	-11.63953600	4.92385400	-3.53490900

H	-11.99841800	3.48334100	-4.50383200
H	-11.17314200	4.86818800	-5.24316000
C	-9.36409800	2.82651800	-5.11593600
H	-9.18605400	4.46505100	-3.77143400
H	-9.12532600	3.47929700	-5.96164200
H	-10.09964100	2.09479100	-5.47277200
H	-8.45255500	2.28856600	-4.83412400
C	-9.94277400	3.49574700	1.11756800
C	-10.71670400	2.84300400	2.25920900
H	-10.66410900	3.47015100	3.15466600
H	-10.28930000	1.87023000	2.52901700
H	-11.77227300	2.69076400	2.00996800
C	-8.44697100	3.53478600	1.44843800
H	-10.29269300	4.53396800	1.02756700
H	-8.27722400	4.05838600	2.39718200
H	-7.86399600	4.03372000	0.66382700
H	-8.06006600	2.51282400	1.55026900
C	-3.15006800	8.27855800	-5.66779300
C	-4.05477100	8.10266800	-6.71979500
C	-3.82677000	10.54734600	-5.37011300
C	-4.67615900	10.42590200	-6.46341800
C	-4.80107700	9.21247300	-7.12021000
H	-5.26866500	11.27856400	-6.78420600
H	-5.50917900	9.10839400	-7.94015100
C	-4.30801800	6.75147000	-7.36253600
C	-5.72695600	6.28281200	-7.02718600
H	-5.88672200	6.23523500	-5.94011800
H	-5.91072500	5.28696200	-7.45048100
H	-6.47181800	6.96670000	-7.45486300
C	-4.08487400	6.77987500	-8.87306100
H	-3.60930700	6.01675000	-6.94200900
H	-4.24453900	5.78243400	-9.29951300
H	-3.06761400	7.09915200	-9.12427700
H	-4.78340700	7.46573100	-9.36769100

C	-3.04761800	9.47164800	-4.94874500
C	-2.11742900	9.57068500	-3.75909400
C	-2.68888900	10.44773400	-2.65110500
H	-2.06562000	10.37898400	-1.75379700
H	-3.70311800	10.12262400	-2.38855200
H	-2.72332900	11.50532600	-2.93963400
C	-0.74214400	10.06217600	-4.21355200
H	-2.00701000	8.55864900	-3.34788400
H	-0.31143900	9.39366000	-4.96869000
H	-0.04352000	10.11845700	-3.37141000
H	-0.81973600	11.06247400	-4.65854900
H	-3.76738100	11.49281400	-4.83825500
N	-8.98676800	6.90214300	-1.34474900
C	-8.05407800	7.97219700	-1.17153500
C	-7.51082200	8.16001300	0.10021400
C	-7.66144500	8.72253900	-2.28756800
C	-6.59108100	9.19920900	0.25810500
C	-6.20796700	9.97863700	-0.81955500
C	-6.72405800	9.73226800	-2.08672100
H	-6.15193700	9.37538900	1.23748100
H	-5.47789200	10.77177300	-0.68043300
H	-6.36058400	10.30949600	-2.93393600
C	-8.17952700	8.37147600	-3.66760300
C	-7.19068600	8.73923700	-4.76750600
H	-7.10948100	9.82680300	-4.89321600
H	-7.52621700	8.33429900	-5.72883600
H	-6.18527400	8.34389400	-4.56068000
C	-9.53526600	9.03531300	-3.92017000
H	-8.30842700	7.27806900	-3.69013200
H	-9.43531500	10.12748400	-3.88083900
H	-10.28196200	8.73987700	-3.17536800
H	-9.92282000	8.76842200	-4.90982600
C	-7.81580400	7.24800900	1.27419500
C	-6.53418800	6.53326100	1.70943300

H	-6.11032600	5.95587000	0.87900200
H	-6.73288700	5.85418000	2.54592300
H	-5.77923000	7.25621500	2.04176700
C	-8.43542300	8.02469400	2.43548800
H	-8.53650600	6.47827400	0.95683200
H	-7.74615000	8.79262700	2.80742300
H	-8.66248200	7.35396300	3.27151300
H	-9.36279600	8.52610700	2.13768500
H	-0.82341900	7.28317700	-6.78934800
H	-0.42012800	4.63570300	-6.03278800
H	-11.85442100	5.42086800	-0.88982300
H	-10.76180800	7.98148700	-0.81291800
C	-2.20457600	3.77839100	-4.14228600
C	-3.24776700	2.94982400	-4.57906100
C	-1.27478800	3.38157300	-3.17356100
C	-3.33780100	1.67885000	-4.01625000
C	-1.40202800	2.09604900	-2.64729200
C	-2.42050200	1.25451800	-3.06596500
H	-4.14161100	1.01587600	-4.32048900
H	-0.70084300	1.75483800	-1.89208200
H	-2.50752500	0.25929300	-2.63904600
C	-0.23285700	4.34704100	-2.64290400
C	-0.85930100	5.19494400	-1.53033000
H	-1.75788300	5.72062200	-1.87267900
H	-0.14095800	5.93113000	-1.15155700
H	-1.15582600	4.54802300	-0.69507600
C	1.02867700	3.65682000	-2.13276000
H	0.06109100	5.02155600	-3.45885500
H	0.83704200	3.10724700	-1.20385700
H	1.79759800	4.40191900	-1.90572700
H	1.44048900	2.95230500	-2.86333500
C	-4.23280600	3.42317300	-5.63075600
C	-3.66756100	3.18918100	-7.03451200
H	-4.35189100	3.58148400	-7.79882800

H	-3.52996400	2.11719700	-7.22529500
H	-2.69692200	3.68215100	-7.16995400
C	-5.61751800	2.80013800	-5.48722300
H	-4.36709800	4.50096200	-5.48539000
H	-6.31173600	3.28610100	-6.18286600
H	-6.01339000	2.93651900	-4.47255900
H	-5.62090000	1.72922200	-5.72694500
H	-4.27873100	7.57127900	-3.32545000
H	-7.31040000	3.75319700	-2.05048800
H	-6.13553100	6.86797200	-2.15290700
H	-4.77345200	4.29617300	-3.01082300

68. NHC_Full_H_H (fully optimized)-triplet:

N	-9.55561100	4.31858700	-1.20916600
C	-10.22467000	6.23355800	-0.35190600
C	-10.39492300	4.89547900	-0.27702300
C	-8.82032200	5.29130200	-1.86244300
C	-6.84448300	6.16247300	-3.51217700
C	-5.49297000	6.04851800	-3.41018300
N	-2.54115900	5.13500900	-4.29773600
N	-1.93763300	7.16672500	-4.76322900
C	-1.22225800	5.09310900	-4.70628400
C	-0.85111000	6.35617400	-5.00626700
B	-4.41080100	6.97024800	-3.99537900
B	-7.75241900	5.05189000	-2.90797500
C	-3.01443100	6.43539800	-4.31848200
C	-9.11019900	2.96076600	-1.18508900
C	-8.09578400	2.62118500	-0.28518000
C	-9.61438200	2.06208900	-2.13123000
C	-7.63967300	1.30172100	-0.29090900
C	-9.12714100	0.75715400	-2.10492000
C	-8.15952200	0.37672000	-1.18213600
H	-6.85762500	1.00703300	0.40650500
H	-7.79472100	-0.64700900	-1.17528800
H	-9.49525700	0.03055500	-2.82265100
C	-10.64025300	2.52860300	-3.14429400
C	-12.03659000	2.55883300	-2.51659400
H	-12.07564400	3.21138800	-1.63880200
H	-12.33172300	1.55035500	-2.20051400
H	-12.78076600	2.91747600	-3.23641400
C	-10.65480600	1.68424600	-4.41257300
H	-10.36145200	3.55623600	-3.42637800
H	-11.30251200	2.14659300	-5.16379400

H	-11.05040500	0.67861000	-4.22374300
H	-9.65317800	1.58271800	-4.84260800
C	-7.44890900	3.63858900	0.63390500
C	-7.61587400	3.26508500	2.10566500
H	-7.15970700	4.02855300	2.74698600
H	-7.12770500	2.30864900	2.33045700
H	-8.67201600	3.17467100	2.38149000
C	-5.97050600	3.80240800	0.27426700
H	-7.93193800	4.61270400	0.48125200
H	-5.51800500	4.60514400	0.87334600
H	-5.84970600	4.04629400	-0.79128600
H	-5.40620000	2.87997800	0.47464200
C	-2.06512400	8.50655900	-5.22882900
C	-2.41526100	8.69212200	-6.57139500
C	-2.01618700	10.85871400	-4.84117300
C	-2.30870500	11.07601400	-6.17952500
C	-2.51966800	10.00274400	-7.03387800
H	-2.39441900	12.09148100	-6.55624600
H	-2.79032500	10.18085200	-8.07257000
C	-2.76013700	7.52813300	-7.48256300
C	-4.25423000	7.56104300	-7.81682000
H	-4.86491900	7.56604700	-6.90545100
H	-4.53176100	6.68445600	-8.41699600
H	-4.50308500	8.45797700	-8.39867400
C	-1.92004900	7.52184700	-8.75791500
H	-2.56238600	6.58752400	-6.94998700
H	-2.17143500	6.65063500	-9.37393300
H	-0.84800300	7.48538900	-8.53743900
H	-2.10738800	8.41711700	-9.36325200
C	-1.89948800	9.56445200	-4.33386900
C	-1.66401600	9.33979300	-2.85369200
C	-2.84417000	9.89387700	-2.05080600
H	-2.73304100	9.65909200	-0.98545800
H	-3.78809600	9.46392500	-2.40528900

H	-2.90451600	10.98574400	-2.14949300
C	-0.35146500	9.97080400	-2.39058600
H	-1.61834200	8.25726600	-2.67362100
H	0.50774100	9.57603100	-2.94225300
H	-0.18767200	9.78523800	-1.32356100
H	-0.36874400	11.05808200	-2.53589100
H	-1.88920600	11.70554600	-4.17002600
N	-9.25253700	6.47653000	-1.30289300
C	-8.72076200	7.75537700	-1.66232200
C	-7.43854900	8.11284100	-1.20673100
C	-9.45996800	8.55422600	-2.54206900
C	-6.90113500	9.30562100	-1.68580400
C	-7.61374300	10.11217700	-2.56207000
C	-8.88381800	9.74743200	-2.97794300
H	-5.90413900	9.60543000	-1.38072400
H	-7.16767500	11.03204000	-2.92939700
H	-9.42662100	10.38317300	-3.67087800
C	-10.78106900	8.07924500	-3.11562100
C	-10.50214100	7.24020000	-4.36756000
H	-9.98476500	7.85432300	-5.11630200
H	-11.43560000	6.87556900	-4.81210700
H	-9.86122300	6.37801900	-4.14567800
C	-11.73942400	9.21945300	-3.44920200
H	-11.27224200	7.43409800	-2.37482200
H	-11.39326200	9.79482200	-4.31557800
H	-11.86311700	9.91336700	-2.61107900
H	-12.72417400	8.81850600	-3.70958300
C	-6.66089900	7.21415000	-0.26359200
C	-5.17556800	7.54755500	-0.18857500
H	-4.70339000	7.52783900	-1.17953800
H	-4.66727400	6.81200700	0.44596200
H	-5.00171800	8.53334700	0.26431500
C	-7.25417500	7.22783800	1.15003600
H	-6.74056800	6.19365000	-0.66732200

H	-7.13940700	8.21967100	1.60522500
H	-6.72579000	6.50574800	1.78852200
H	-8.31727100	6.96935100	1.16857800
H	0.07901700	6.75859400	-5.37298900
H	-0.68146400	4.16103800	-4.74822800
H	-11.03209900	4.29627800	0.35385300
H	-10.70056700	7.04164300	0.18083600
C	-3.34175300	3.98842400	-3.99545800
C	-4.35464500	3.61958200	-4.89719200
C	-3.17012700	3.36572200	-2.75299000
C	-5.23287800	2.61636300	-4.49538400
C	-4.06799400	2.35454200	-2.40712800
C	-5.10390800	2.00177100	-3.25833900
H	-6.05954000	2.33752700	-5.14001700
H	-3.98197000	1.86267800	-1.44280000
H	-5.82908700	1.25222100	-2.94929100
C	-2.14592100	3.87949500	-1.75635200
C	-2.68286500	5.14676000	-1.08074000
H	-2.87374300	5.96175700	-1.78902400
H	-1.98438500	5.50772600	-0.31596000
H	-3.63729500	4.91663100	-0.58964400
C	-1.78328000	2.85518500	-0.68595400
H	-1.22682400	4.14122600	-2.30026600
H	-2.62046600	2.69966700	0.00721000
H	-0.94025400	3.21746800	-0.08943000
H	-1.51073500	1.88372700	-1.11193600
C	-4.52151900	4.32889400	-6.22743300
C	-3.46134000	3.87734700	-7.23599400
H	-3.54924100	4.45385700	-8.16757200
H	-3.58464100	2.81589800	-7.48531400
H	-2.44378500	4.01789600	-6.85265800
C	-5.92195900	4.18720800	-6.80990600
H	-4.37174400	5.40085900	-6.04255100
H	-6.02950000	4.84732700	-7.67781300

H	-6.68333300	4.46517500	-6.07047100
H	-6.12324200	3.16486800	-7.15466400
H	-4.64172500	8.10384700	-4.31981600
H	-7.54078600	3.89589900	-3.16440000
H	-7.23726400	7.05345700	-4.02829100
H	-5.17931900	5.15461600	-2.84828000

69. NHC_Full_H_H (twisted)-singlet:

N	-9.68077500	4.66411400	-0.70004000
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C	-10.82362300	6.52895300	-0.85251100
C	-10.85808600	5.27765300	-0.34142800
C	-8.89084600	5.50383300	-1.44932500
C	-6.64652800	6.22040300	-2.77823000
C	-6.61126200	6.31109100	-4.11902000
N	-3.62117600	5.84199400	-5.15823300
N	-3.48947300	7.80942500	-6.08820700
C	-2.37439900	5.94567600	-5.74039700
C	-2.28182800	7.17205500	-6.29733500
B	-5.76157700	7.33947400	-4.93452200
B	-7.47992900	5.20988600	-1.92799800
C	-4.34905400	6.99923900	-5.36688700
C	-9.18232800	3.41170900	-0.25062000
C	-8.50732500	3.38887300	0.97405400
C	-9.23762200	2.31126000	-1.11064800
C	-7.94472100	2.17939500	1.37837300
C	-8.64315300	1.12787800	-0.67271000
C	-8.01559600	1.05836800	0.56334400
H	-7.41829800	2.12760000	2.32940100
H	-7.56157600	0.12562800	0.88662300
H	-8.66319800	0.25232700	-1.31814400
C	-9.86499900	2.38794800	-2.49059400
C	-10.92802800	1.30396400	-2.67679900
H	-11.69305400	1.34399100	-1.89472100
H	-10.47982600	0.30333300	-2.65322100
H	-11.42298200	1.41479100	-3.64743000
C	-8.79550300	2.27718900	-3.58397500
H	-10.34895600	3.36864300	-2.59551200
H	-9.26353900	2.27537000	-4.57622300
H	-8.23040400	1.33965700	-3.47867000
H	-8.07945700	3.10878800	-3.53811300
C	-8.30016600	4.64490600	1.80087500
C	-8.89866000	4.51041900	3.19989500
H	-8.74787900	5.43184000	3.77368400

H	-8.42008800	3.69384100	3.75474200
H	-9.97320900	4.30303600	3.16314600
C	-6.80809600	4.98063800	1.87979800
H	-8.79808500	5.48557800	1.29724200
H	-6.65774100	5.95187600	2.36988300
H	-6.36224200	5.02287600	0.87810500
H	-6.26449300	4.22547900	2.46230100
C	-3.66762600	9.22612700	-6.12536300
C	-4.31834900	9.80441600	-7.22020200
C	-3.43534200	11.34880600	-5.05338300
C	-4.03561600	11.95340300	-6.14608900
C	-4.48282200	11.18751000	-7.21574500
H	-4.17570400	13.03082300	-6.15924800
H	-4.98342400	11.67288200	-8.04798800
C	-4.82381500	8.92808800	-8.34801700
C	-5.99189900	9.54658000	-9.10698100
H	-6.78887600	9.87004000	-8.42976900
H	-6.41339400	8.81768500	-9.80621500
H	-5.67446000	10.41264300	-9.70072900
C	-3.68637200	8.59339600	-9.31679600
H	-5.17709900	7.99292800	-7.88713200
H	-4.03964800	7.94318300	-10.12498600
H	-2.85822700	8.08474000	-8.81363100
H	-3.29278100	9.51184500	-9.77029600
C	-3.24715100	9.96647500	-5.01584500
C	-2.66185100	9.31449500	-3.77730500
C	-3.63527800	9.44708800	-2.60191100
H	-3.24053500	8.92244200	-1.71937400
H	-4.61811600	9.01943200	-2.85270900
H	-3.77864200	10.50147800	-2.32830000
C	-1.29568500	9.89590500	-3.41616700
H	-2.52340200	8.24266000	-3.97194400
H	-0.58479700	9.80105000	-4.24366700
H	-0.87848900	9.37507500	-2.54640600

H	-1.36858000	10.95905500	-3.15710200
H	-3.11906400	11.95155600	-4.20449800
N	-9.61914000	6.67374500	-1.51397700
C	-9.10671700	7.88350000	-2.07679300
C	-8.05490400	8.54091600	-1.41847000
C	-9.59998600	8.29514900	-3.32081100
C	-7.47819400	9.63114000	-2.06986000
C	-7.93336700	10.04520700	-3.31225200
C	-8.99167600	9.39249200	-3.92618900
H	-6.64701200	10.15540800	-1.60777800
H	-7.44835800	10.87802300	-3.81362600
H	-9.33071900	9.72650700	-4.90157100
C	-10.68871600	7.50534400	-4.02549400
C	-10.09053300	6.27322600	-4.71422900
H	-9.34932600	6.59000200	-5.45922700
H	-10.87444900	5.70366300	-5.22791500
H	-9.57631800	5.60647500	-4.00976200
C	-11.46835100	8.33377700	-5.04234800
H	-11.40300400	7.15367600	-3.26750100
H	-10.85453700	8.56849100	-5.91976600
H	-11.82808100	9.27769300	-4.61904100
H	-12.33361600	7.76793700	-5.40196000
C	-7.53042500	8.05399500	-0.07813500
C	-6.14436600	8.58733100	0.26815700
H	-5.43278000	8.43587900	-0.55266400
H	-5.75820000	8.05861600	1.14820400
H	-6.16380300	9.65771100	0.51141900
C	-8.50614100	8.36557800	1.06064900
H	-7.43322200	6.95843900	-0.14343900
H	-8.61538500	9.44958000	1.19124100
H	-8.13157000	7.95014700	2.00637300
H	-9.50119600	7.94421700	0.88382200
H	-1.47169700	7.65703200	-6.81780100
H	-1.67148500	5.12870600	-5.69878700

H	-11.60922000	4.76663900	0.23842700
H	-11.53485000	7.33784700	-0.80122000
C	-4.07591500	4.70280800	-4.41573000
C	-4.83472900	3.73494300	-5.07846700
C	-3.85073200	4.66592100	-3.03046700
C	-5.28286600	2.64117200	-4.33657100
C	-4.30387100	3.54703400	-2.33691100
C	-5.00093200	2.53768800	-2.98508500
H	-5.89061500	1.87877200	-4.81582100
H	-4.17761700	3.49384900	-1.26018300
H	-5.38530400	1.69526400	-2.41408300
C	-3.30494000	5.88140400	-2.29993300
C	-3.73327900	5.93250100	-0.83399000
H	-4.81544900	5.78651600	-0.71362100
H	-3.46862900	6.90738400	-0.40629700
H	-3.21654000	5.17143800	-0.23536900
C	-1.78397200	6.03130800	-2.37926600
H	-3.76107200	6.75046100	-2.80046900
H	-1.28440700	5.20660800	-1.85572600
H	-1.47761500	6.96903800	-1.89363600
H	-1.41238300	6.05622300	-3.40745800
C	-5.21670200	3.90414600	-6.53576100
C	-4.13120400	3.33609800	-7.45287400
H	-4.39922300	3.46600000	-8.50758100
H	-4.00477400	2.26205600	-7.26593800
H	-3.16387800	3.82165200	-7.28796100
C	-6.56798100	3.27137000	-6.85994800
H	-5.30690300	4.98461100	-6.72568500
H	-6.90058000	3.58130000	-7.85578600
H	-7.33488400	3.56661200	-6.13293800
H	-6.51116500	2.17596200	-6.86744800
H	-6.01906700	6.96280200	-2.25130400
H	-7.23120900	5.57432000	-4.66319600
H	-6.19321600	8.38456200	-5.34173300

H -7.01712100 4.17298000 -1.53998700

70. NHC_Full_H_H (twisted)-triplet:

N	-9.67971900	4.66582700	-0.69936600
C	-10.82367400	6.52988000	-0.85270800
C	-10.85786500	5.27836300	-0.34204800
C	-8.88957300	5.50620000	-1.44775000
C	-6.64387900	6.22407100	-2.77486200
C	-6.61184000	6.30989700	-4.11654600

N	-3.62185000	5.84057100	-5.15707500
N	-3.49010700	7.80801700	-6.08707700
C	-2.37522200	5.94408400	-5.73951600
C	-2.28271300	7.17038500	-6.29666300
B	-5.76198800	7.33816900	-4.93307800
B	-7.47823300	5.21283500	-1.92530200
C	-4.34953600	6.99810800	-5.36515000
C	-9.18149800	3.41257400	-0.25219200
C	-8.50529100	3.38755000	0.97173200
C	-9.23740100	2.31380300	-1.11435300
C	-7.94141900	2.17757500	1.37283600
C	-8.64174900	1.12986800	-0.67960700
C	-8.01247700	1.05825700	0.55549300
H	-7.41383600	2.12412100	2.32313200
H	-7.55739800	0.12515100	0.87622700
H	-8.66207200	0.25562200	-1.32679900
C	-9.86651400	2.39323300	-2.49337000
C	-10.92815100	1.30816600	-2.68124100
H	-11.69200200	1.34458100	-1.89784100
H	-10.47836500	0.30816500	-2.66149700
H	-11.42479600	1.42122100	-3.65075000
C	-8.79837600	2.28690800	-3.58852800
H	-10.35213300	3.37345800	-2.59507000
H	-9.26786200	2.28661600	-4.58009900
H	-8.23158400	1.35005300	-3.48615800
H	-8.08334800	3.11936800	-3.54174200
C	-8.29805600	4.64195800	1.80096600
C	-8.89358800	4.50376800	3.20088800
H	-8.74280100	5.42418900	3.77626400
H	-8.41276700	3.68673300	3.75310000
H	-9.96792000	4.29505000	3.16597500
C	-6.80614300	4.97894600	1.87774500
H	-8.79781200	5.48318800	1.30003400
H	-6.65572100	5.94973100	2.36873000

H	-6.36211100	5.02273300	0.87530800
H	-6.26095500	4.22345500	2.45836100
C	-3.66812900	9.22468700	-6.12547600
C	-4.31912600	9.80201300	-7.22065600
C	-3.43566300	11.34831400	-5.05540300
C	-4.03597700	11.95197700	-6.14860900
C	-4.48342100	11.18513900	-7.21748100
H	-4.17600100	13.02939200	-6.16272000
H	-4.98418600	11.66978400	-8.05004900
C	-4.82538000	8.92465600	-8.34733600
C	-5.99335200	9.54290900	-9.10667900
H	-6.78994900	9.86767500	-8.42965000
H	-6.41547200	8.81340200	-9.80489900
H	-5.67557600	10.40805600	-9.70158200
C	-3.68850900	8.58820000	-9.31617700
H	-5.17906000	7.99021000	-7.88524800
H	-4.04251900	7.93731800	-10.12350700
H	-2.86046300	8.07959100	-8.81282400
H	-3.29457900	9.50592000	-9.77085700
C	-3.24748300	9.96602200	-5.01668900
C	-2.66302500	9.31491400	-3.77730700
C	-3.63865500	9.44621600	-2.60354900
H	-3.24448000	8.92252600	-1.72019400
H	-4.62047200	9.01700100	-2.85578300
H	-3.78417600	10.50050400	-2.33060600
C	-1.29834000	9.89823800	-3.41371200
H	-2.52275300	8.24325700	-3.97173800
H	-0.58598800	9.80502500	-4.24012500
H	-0.88172800	9.37750700	-2.54361800
H	-1.37324300	10.96108300	-3.15399700
H	-3.11946500	11.95180000	-4.20702100
N	-9.61847900	6.67572900	-1.51255400
C	-9.10649600	7.88549900	-2.07550500
C	-8.05508100	8.54347000	-1.41708100

C	-9.59872900	8.29573200	-3.32038900
C	-7.47780100	9.63293500	-2.06924200
C	-7.93196300	10.04558800	-3.31247700
C	-8.98991300	9.39234000	-3.92652900
H	-6.64677000	10.15753200	-1.60726400
H	-7.44633400	10.87765900	-3.81451300
H	-9.32787600	9.72503100	-4.90273900
C	-10.68589000	7.50434000	-4.02573500
C	-10.08540500	6.27254100	-4.71313700
H	-9.34337500	6.58981700	-5.45712600
H	-10.86799800	5.70197400	-5.22773100
H	-9.57151600	5.60654500	-4.00763900
C	-11.46525600	8.33133100	-5.04397300
H	-11.40062000	7.15229800	-3.26835400
H	-10.85076700	8.56600500	-5.92092500
H	-11.82626900	9.27520400	-4.62166700
H	-12.32964100	7.76445900	-5.40407900
C	-7.53070500	8.05679700	-0.07665600
C	-6.14523300	8.59124200	0.27015800
H	-5.43313900	8.44003700	-0.55029700
H	-5.75909000	8.06301100	1.15050200
H	-6.16547200	9.66168400	0.51308200
C	-8.50697500	8.36644300	1.06215300
H	-7.43231100	6.96132300	-0.14244500
H	-8.61752700	9.45019500	1.19370000
H	-8.13203400	7.95062300	2.00756400
H	-9.50150700	7.94403600	0.88486500
H	-1.47274800	7.65511300	-6.81761700
H	-1.67233400	5.12708800	-5.69798700
H	-11.60930500	4.76674400	0.23686800
H	-11.53548000	7.33829200	-0.80190400
C	-4.07647700	4.70183200	-4.41390100
C	-4.83571200	3.73383500	-5.07593100
C	-3.85136300	4.66586100	-3.02859400

C	-5.28425500	2.64072700	-4.33329800
C	-4.30502600	3.54768600	-2.33424200
C	-5.00234300	2.53806700	-2.98174700
H	-5.89223700	1.87822200	-4.81206600
H	-4.17923100	3.49542500	-1.25740800
H	-5.38723700	1.69630400	-2.41010100
C	-3.30581900	5.88203300	-2.29905600
C	-3.73420500	5.93441200	-0.83322000
H	-4.81646000	5.78897800	-0.71289700
H	-3.46921800	6.90952700	-0.40625200
H	-3.21783500	5.17362700	-0.23392900
C	-1.78489300	6.03226700	-2.37856200
H	-3.76219100	6.75052900	-2.80040100
H	-1.28512800	5.20828700	-1.85407900
H	-1.47881000	6.97061900	-1.89396300
H	-1.41327300	6.05611800	-3.40677700
C	-5.21797800	3.90265900	-6.53320300
C	-4.13259300	3.33469800	-7.45049900
H	-4.40091700	3.46442100	-8.50515100
H	-4.00588200	2.26070600	-7.26348100
H	-3.16533200	3.82048900	-7.28591300
C	-6.56920900	3.26967200	-6.85707700
H	-5.30840800	4.98311200	-6.72322300
H	-6.90178200	3.57908400	-7.85308500
H	-7.33617400	3.56528600	-6.13027800
H	-6.51241100	2.17425700	-6.86398200
H	-6.01969800	6.97073500	-2.25100400
H	-7.22834200	5.56825800	-4.65718700
H	-6.18907300	8.38915900	-5.32928400
H	-7.01987300	4.17035700	-1.54783800

71. NHC_Full_H_H (planar)-singlet:

N	-8.64551500	3.39256100	-1.01817900
C	-6.79158500	2.22558800	-1.11994900
C	-8.04423800	2.21683500	-0.61807800
C	-7.80019300	4.14042000	-1.80252100
C	-7.14724600	6.34725600	-3.15828200
C	-7.37699800	7.65362800	-3.63999300
N	-7.56806400	10.73031000	-4.80127300
N	-5.67790800	10.46958400	-5.82079200
C	-7.25959700	11.93306000	-5.40798100
C	-6.07764000	11.77302500	-6.03672300
B	-6.39343400	8.37656100	-4.48483800

B	-8.08238100	5.56709300	-2.31231000
C	-6.58754800	9.79682400	-5.03752600
C	-10.03794800	3.66354700	-0.86109400
C	-10.88028200	3.46672100	-1.95972400
C	-10.50194700	4.10010900	0.38741500
C	-12.23609400	3.74759700	-1.78553800
C	-11.86586600	4.35306200	0.51329300
C	-12.72343700	4.18654300	-0.56622100
H	-12.91589200	3.61316200	-2.62387300
H	-13.78297300	4.39698900	-0.45036300
H	-12.26489400	4.69087900	1.46438900
C	-9.53478900	4.34349800	1.53201800
C	-10.20146900	4.30077300	2.90309000
H	-10.80153000	3.39563300	3.04583800
H	-10.85520900	5.16777300	3.05565300
H	-9.44133500	4.33439200	3.68969000
C	-8.82020200	5.68607300	1.34180000
H	-8.77257300	3.55111100	1.50691800
H	-8.11558100	5.86453100	2.16241300
H	-9.55377500	6.50173000	1.34098300
H	-8.27425300	5.74012600	0.39344200
C	-10.39405600	2.95448800	-3.30430400
C	-11.10076300	1.64939700	-3.67615300
H	-10.70448500	1.25861600	-4.62018400
H	-12.17738600	1.80719900	-3.81289300
H	-10.97127300	0.88174300	-2.90604200
C	-10.60652100	4.00809100	-4.39310500
H	-9.31597300	2.74409000	-3.24213700
H	-10.26630400	3.62981500	-5.36382400
H	-10.05763000	4.92947500	-4.16929700
H	-11.67188600	4.25420700	-4.48767500
C	-4.32510000	10.03941600	-5.99988300
C	-3.39830500	10.39393900	-5.01606800
C	-2.65916100	8.89631900	-7.26725100

C	-1.70461100	9.27867300	-6.33253900
C	-2.07198800	10.00629900	-5.21280200
H	-0.66775600	8.98461000	-6.47058400
H	-1.32650200	10.26415800	-4.46358300
C	-3.79987600	11.09027100	-3.72885400
C	-3.65335800	10.11806000	-2.55343700
H	-4.25681400	9.21298000	-2.70650500
H	-3.97205200	10.59624700	-1.61793400
H	-2.60525800	9.81446700	-2.43300800
C	-2.99224400	12.36323100	-3.48228200
H	-4.85714900	11.38160700	-3.79320200
H	-3.34120000	12.86157900	-2.57023900
H	-3.08569100	13.06976800	-4.31385600
H	-1.92651500	12.14221500	-3.34787300
C	-3.99425300	9.26093400	-7.11332600
C	-5.07210300	8.83468000	-8.08935500
C	-4.72082900	7.55866500	-8.84529000
H	-5.58652100	7.21342600	-9.41891100
H	-4.42002400	6.75539000	-8.16561500
H	-3.90740900	7.72563000	-9.56224300
C	-5.37624100	9.96235800	-9.07980300
H	-5.97707300	8.63449000	-7.49558800
H	-5.69510100	10.87887400	-8.57371800
H	-6.17085800	9.66764000	-9.77430100
H	-4.48197100	10.19711600	-9.67087700
H	-2.36173300	8.29125400	-8.11811200
N	-6.65132400	3.39274100	-1.83867400
C	-5.45614900	3.76981300	-2.52113600
C	-5.23327800	3.23916000	-3.79713600
C	-4.59796000	4.69642900	-1.92146100
C	-4.09208500	3.65947400	-4.47826600
C	-3.21678000	4.56973800	-3.90362300
C	-3.46462700	5.07747900	-2.63773500
H	-3.89478100	3.28121300	-5.47716800

H	-2.33799800	4.89439500	-4.45329500
H	-2.77902100	5.79919700	-2.20118700
C	-4.87183100	5.30731100	-0.56199900
C	-4.73119800	6.83191300	-0.59460900
H	-3.68074800	7.13456300	-0.69618100
H	-5.10398600	7.26557100	0.34070900
H	-5.30002400	7.26642700	-1.42655900
C	-3.93728600	4.69512100	0.48346900
H	-5.90794000	5.07877100	-0.28133400
H	-2.88943800	4.88737400	0.21834700
H	-4.06811500	3.60918700	0.55532900
H	-4.11790800	5.12842000	1.47357000
C	-6.25033400	2.33332000	-4.46513100
C	-7.22019800	3.18836400	-5.28775200
H	-7.68664200	3.97316500	-4.67974200
H	-8.00866900	2.56438300	-5.72900400
H	-6.68018300	3.68457800	-6.10465400
C	-5.61087200	1.26002600	-5.34231600
H	-6.83070700	1.82422200	-3.68212100
H	-5.15057500	1.69524400	-6.23674500
H	-6.37232700	0.55456600	-5.69042100
H	-4.83994900	0.69542100	-4.80741900
H	-5.47399600	12.45618100	-6.61231000
H	-7.92712300	12.77707100	-5.33563800
H	-8.57315900	1.49098700	-0.02207900
H	-5.98306700	1.51631400	-1.04530100
C	-8.69905400	10.57892300	-3.93715900
C	-8.49380600	10.58625800	-2.55144400
C	-9.96785600	10.45092700	-4.51543900
C	-9.61839100	10.48387100	-1.73576700
C	-11.06201700	10.35503100	-3.65621300
C	-10.88888200	10.37651200	-2.28083000
H	-9.49367200	10.47930900	-0.65715900
H	-12.06073400	10.25328900	-4.06880700

H	-11.75262600	10.29599600	-1.62689700
C	-10.12708200	10.31142100	-6.01701400
C	-9.82389700	8.86214800	-6.41462500
H	-8.82994600	8.54172800	-6.08283900
H	-9.89233800	8.73448500	-7.50129000
H	-10.55499300	8.19111000	-5.94653300
C	-11.50679600	10.71809900	-6.52370300
H	-9.38629900	10.96014800	-6.50543700
H	-12.27475500	10.00105500	-6.21060600
H	-11.51457500	10.73245000	-7.61806200
H	-11.80475900	11.71000400	-6.16697600
C	-7.10553500	10.68635300	-1.95143900
C	-6.72155900	12.14785400	-1.71436500
H	-5.69579500	12.22148200	-1.32769100
H	-7.39199900	12.62189100	-0.98579900
H	-6.77133300	12.72808200	-2.64554500
C	-6.95339800	9.84020500	-0.69039500
H	-6.40396800	10.26591700	-2.67691700
H	-5.89616400	9.79288900	-0.40136700
H	-7.29977900	8.81257300	-0.86829100
H	-7.50404400	10.25527400	0.16299600
H	-8.34484400	8.07579400	-3.33881900
H	-6.19379700	5.93849900	-3.51232000
H	-9.14995200	6.00889100	-1.97325000
H	-5.35520500	7.85290100	-4.80599300

72. NHC_Full_H_H (planar)-triplet:

N	-8.46348500	3.19616400	-1.14532900
C	-6.52021200	2.31857300	-1.67095100
C	-7.67232400	2.07457600	-1.01203200
C	-7.84137100	4.15468700	-1.91871100
C	-7.58089500	6.52306700	-3.10995400
C	-7.81498600	7.80042100	-3.54128200
N	-7.46952900	10.90303300	-4.96269800
N	-5.59834500	10.22848800	-5.86156300
C	-6.92402500	11.97308900	-5.64975400
C	-5.76006600	11.55701800	-6.19318300
B	-6.72433000	8.42603200	-4.43198100
B	-8.38294300	5.55373100	-2.23037400
C	-6.65291900	9.79346200	-5.07524400
C	-9.83384800	3.26557500	-0.76130200
C	-10.81059200	3.06258500	-1.74106300
C	-10.14220300	3.54583800	0.57610200

C	-12.14482800	3.17920000	-1.35089700
C	-11.48938700	3.63418000	0.92060200
C	-12.48054600	3.46415300	-0.03712100
H	-12.92826900	3.03892900	-2.09246200
H	-13.52543400	3.54869900	0.24817500
H	-11.76914300	3.84758300	1.94771100
C	-9.03908000	3.80640700	1.58538000
C	-9.44553900	3.47907700	3.01871300
H	-9.87211700	2.47438300	3.10895400
H	-10.18427900	4.19510200	3.39773300
H	-8.57556000	3.54194100	3.67987100
C	-8.57889000	5.26506000	1.48927600
H	-8.18168300	3.16854300	1.32420900
H	-7.74273900	5.45189900	2.17490400
H	-9.40171300	5.93619800	1.76649300
H	-8.26460000	5.53292300	0.47369300
C	-10.47224500	2.70678700	-3.17741800
C	-11.12487600	1.38118600	-3.57552700
H	-10.82824300	1.09922200	-4.59156400
H	-12.21856000	1.45965100	-3.56393600
H	-10.84229600	0.56894200	-2.89782900
C	-10.89747500	3.82031700	-4.13611600
H	-9.38351800	2.58398100	-3.26363300
H	-10.63496200	3.55749500	-5.16758800
H	-10.41164000	4.77079300	-3.88869900
H	-11.98416900	3.97054300	-4.09529600
C	-4.33975200	9.55318600	-5.89956700
C	-3.41924800	9.82301500	-4.87757100
C	-2.80730900	8.05412500	-6.95731100
C	-1.84097600	8.38634100	-6.01958500
C	-2.15433900	9.24335300	-4.97338300
H	-0.84839300	7.94853400	-6.08415100
H	-1.41435600	9.45201200	-4.20336800
C	-3.79019900	10.62995500	-3.64726900

C	-3.89506800	9.68315400	-2.44346600
H	-4.63561400	8.88676600	-2.61501700
H	-4.18085800	10.23826800	-1.53957500
H	-2.92335900	9.20609200	-2.24957900
C	-2.80256800	11.75863700	-3.35944700
H	-4.77701400	11.08576300	-3.80425200
H	-3.13973200	12.34443600	-2.49630300
H	-2.70344400	12.43688100	-4.21333400
H	-1.80517900	11.37075000	-3.12027200
C	-4.08067300	8.62585600	-6.91061000
C	-5.14199700	8.19593400	-7.90164300
C	-5.39658400	6.69198300	-7.76828000
H	-6.21372300	6.37530800	-8.42623500
H	-5.65933200	6.43507200	-6.73558400
H	-4.50319900	6.11566100	-8.04798600
C	-4.74948500	8.55427000	-9.33468800
H	-6.07462900	8.71497300	-7.64627500
H	-4.58335300	9.62979000	-9.45411000
H	-5.52984000	8.24851400	-10.03997700
H	-3.82373800	8.04091000	-9.62390100
H	-2.57407700	7.34392400	-7.74807400
N	-6.62126300	3.57591700	-2.23130200
C	-5.49815400	4.31083700	-2.72595000
C	-5.16235500	4.20405800	-4.08400000
C	-4.85811300	5.19879900	-1.85541100
C	-4.16522500	5.04891100	-4.56980700
C	-3.53422700	5.96171800	-3.73315600
C	-3.86384600	6.01873500	-2.39008700
H	-3.88849900	5.01930000	-5.62062600
H	-2.78493900	6.63630100	-4.13844600
H	-3.35502700	6.72740000	-1.73996900
C	-5.22169500	5.34711100	-0.38920200
C	-5.63510700	6.79036100	-0.08120900
H	-4.78928400	7.47917800	-0.21814900

H	-5.96924100	6.88353000	0.95890500
H	-6.44531500	7.12077800	-0.74301700
C	-4.05077600	4.92041000	0.49816600
H	-6.07682300	4.69355300	-0.15950900
H	-3.17212500	5.55057800	0.31219800
H	-3.76040400	3.88079100	0.31253800
H	-4.31199900	5.01983100	1.55772200
C	-5.95256100	3.29465900	-5.00783100
C	-7.28967900	3.94866800	-5.38261100
H	-7.94618000	4.09488900	-4.51927400
H	-7.81932100	3.33538200	-6.12207000
H	-7.11537000	4.94125100	-5.82017000
C	-5.19271200	2.93875500	-6.28196600
H	-6.16922600	2.36246000	-4.46302800
H	-5.11560200	3.80962800	-6.94619800
H	-5.73022700	2.16266800	-6.83563300
H	-4.17939800	2.57665700	-6.07756700
H	-5.02901100	12.08064500	-6.78760100
H	-7.42889400	12.92544700	-5.68941400
H	-8.01688900	1.20799000	-0.47104600
H	-5.62748200	1.72602800	-1.79146000
C	-8.65584900	10.97759300	-4.17260900
C	-8.54736400	10.97424700	-2.77365400
C	-9.89220000	11.04326900	-4.83159500
C	-9.72614000	11.06687300	-2.03596400
C	-11.04064500	11.15301900	-4.04958700
C	-10.95764800	11.16896600	-2.66503600
H	-9.67720500	11.05694600	-0.95145400
H	-12.01330200	11.20844200	-4.52814200
H	-11.86355200	11.24673100	-2.07044600
C	-9.97447900	10.86517500	-6.33550600
C	-9.85448200	9.37012400	-6.65681200
H	-8.93456700	8.93319200	-6.25115800
H	-9.87373000	9.20082700	-7.73974400

H	-10.69920200	8.82851800	-6.21295700
C	-11.24900100	11.43244700	-6.95097800
H	-9.12118900	11.38139000	-6.79699600
H	-12.12834800	10.84441800	-6.66288000
H	-11.18653100	11.39477800	-8.04299600
H	-11.42567700	12.47214800	-6.65508400
C	-7.20004900	10.88129100	-2.08555200
C	-6.55418400	12.26478100	-1.97795200
H	-5.55401400	12.19107800	-1.52898200
H	-7.15767600	12.93167500	-1.34891600
H	-6.44587400	12.73610800	-2.96339000
C	-7.26954800	10.18763400	-0.72917100
H	-6.55377700	10.25772700	-2.71295700
H	-6.25644700	9.96188400	-0.37438800
H	-7.81666600	9.23954400	-0.80371700
H	-7.74975500	10.81009300	0.03643200
H	-8.74284100	8.29589700	-3.22787300
H	-6.64179600	6.15150100	-3.51969900
H	-9.44500600	5.81956400	-1.74369300
H	-5.77888500	7.73382700	-4.69440000