Supporting Information

Exploring the structure-aromaticity relationships in Hückel and Möbius N-fused pentaphyrins using DFT

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This PDF files includes:

I. Effect of the dispersion correction on the geometries of unsubstituted N-fused [24] and [22]pentaphyrins

Table S1. Root mean square deviations (RMSD in Å) of the optimized geometries computed with B3LYP and B3LYP-D methods for **1** and **2**.[a]

[22]NFP 1	**1a**	**1b**	**1c**	**1d**	**[24]NFP 2**	**2a**	**2b**	**2c**
$RMSD_{30}$	0.009	0.041	0.024	0.090	$RMSD_{30}$	0.0379	0.129	0.044

[a] Considering the geometry of the macrocycle (30 atoms).

Table S2. Relative energies (E_{rel}), ring strain descriptors (Φ_P and ψ_{MAX}), torsional π-conjugation index (Π), and bond-length parameters ($\Delta r_{C\text{-}N}$, $\Delta r_{C\text{-}C}$, HOMA) of Hückel and Möbius conformations of unsubstituted [22]NFP **1** calculated with different methods.

Conformer	E_{rel}	Φ_p	ψ_{MAX}	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$	HOMA
		B3LYP					
1a (H)	0.0	0.0	0.0	1.00	0.044	0.072	0.871
1c (H)	2.8	23.6	29.5	0.63	0.049	0.062	0.864
1d (M**)**	18.2	35.8	82.6	-0.07	0.101	0.127	0.589
		B3LYP-D					
1a (H)	1.4	0.0	0.0	1.00	0.047	0.069	0.874
1c (H)	0.0	22.2	27.9	0.65	0.049	0.060	0.859
1d (M**)**	17.8	36.7	83.1	-0.07	0.100	0.126	0.609

Table S3. Relative energies (E_{rel}), ring strain descriptors (Φ_P and ψ_{MAX}), torsional π-conjugation index (Π), and bond-length parameters ($\Delta r_{C\text{-}N}$, $\Delta r_{C\text{-}C}$, HOMA) of Hückel and Möbius conformations of unsubstituted [24]NFP **2** calculated with different methods.

Conformer	E_{rel}	Φ_p	ψ_{MAX}	Π	$\Delta r_{C\text{-}N}$	$\Delta r_{C\text{-}C}$	HOMA
		B3LYP					
2a (H)	3.7	10.7	16.0	0.91	0.045	0.112	0.670
2b (M)	3.9	39.1	49.1	-0.26	0.019	0.083	0.720
2c (H**)**	0.0	23.6	43.1	0.52	0.044	0.107	0.622
		B3LYP-D					
2a (H)	7.2	11.8	17.3	0.89	0.043	0.111	0.680
2b (M)	3.8	38.0	42.5	-0.29	0.008	0.076	0.775
2c (H**)**	0.0	21.6	38.5	0.58	0.042	0.104	0.646

II. Mutual relationships between aromaticity indices of N-fused [24] and [22]pentaphyrins.

Table S4. Correlation coefficients (*R*) between energetic, magnetic, reactivity and structural descriptors of aromaticity for unsubstituted [24]- and [22] N-fused pentaphyrins (n = 6).

	ISE	ISE_{corr}	Λ	Δη	NICS	NICS(1)	NICSzz(1)	HOMA
ISE	1							
ISEcorr		1						
Λ	-0.694	**-0.916**	1					
Δη	0.621	**0.943**	**-0.991**	1				
NICS(0)	-0.648	**-0.826**	**0.980**	**-0.958**	1			
NICS(1)	-0.644	**-0.888**	**0.993**	**-0.983**	**0.992**	1		
NICSzz(1)	-0.666	**-0.900**	**0.997**	**-0.989**	**0.992**	**0.998**	1	
HOMA	0.702	0.855	-0.692	0.711	-0.565	-0.649	-0.672	1

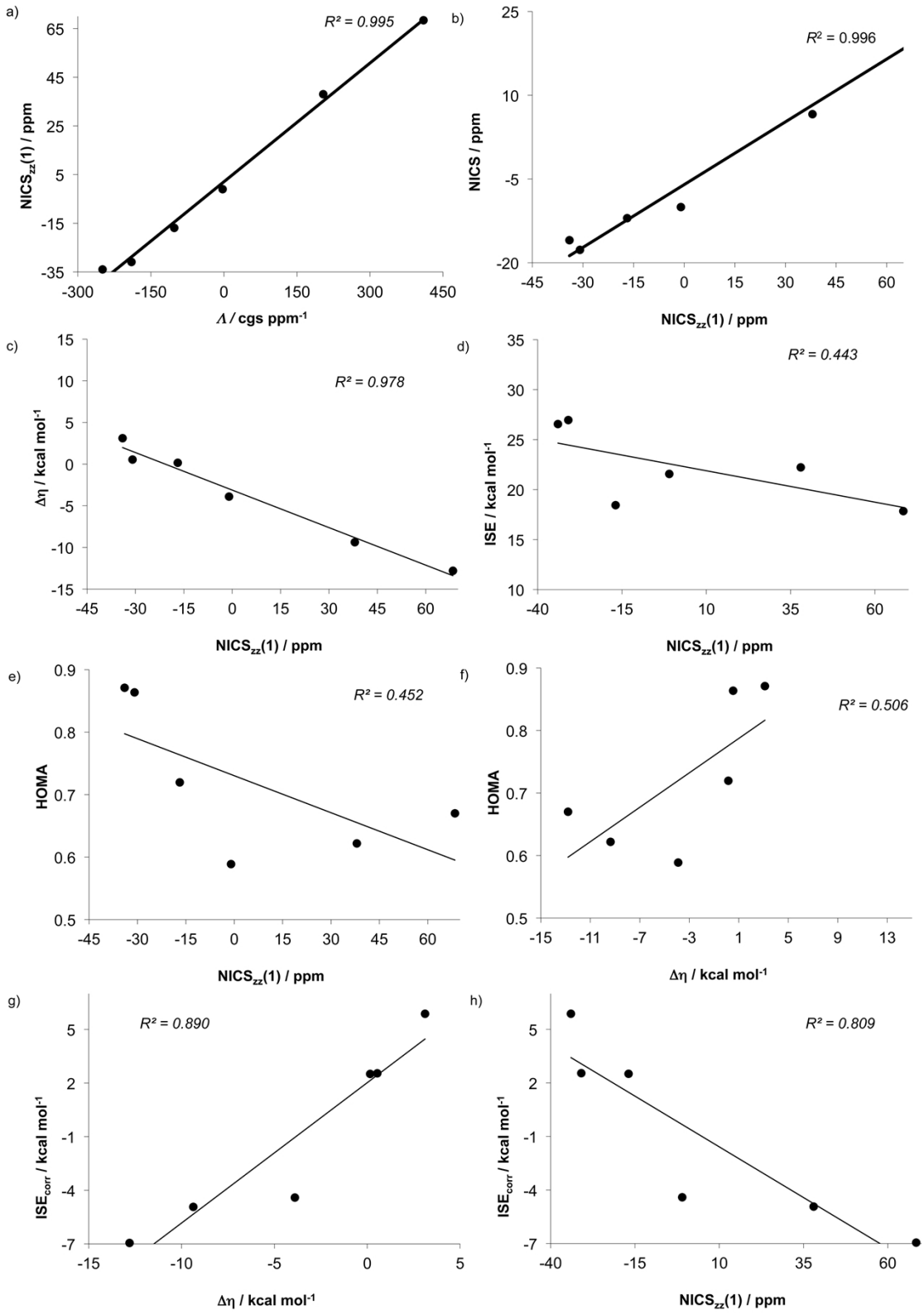


Figure S1. Dependence between the different aromaticity descriptors computed for quantifying the aromaticity of N-fused pentaphyrins *(n* = 6). The aromaticity descriptors of **1a-d** and **2a-c** are collected in Table 2.

III. *Syn-anti* corrections for the isomerization stabilization energies (ISE)

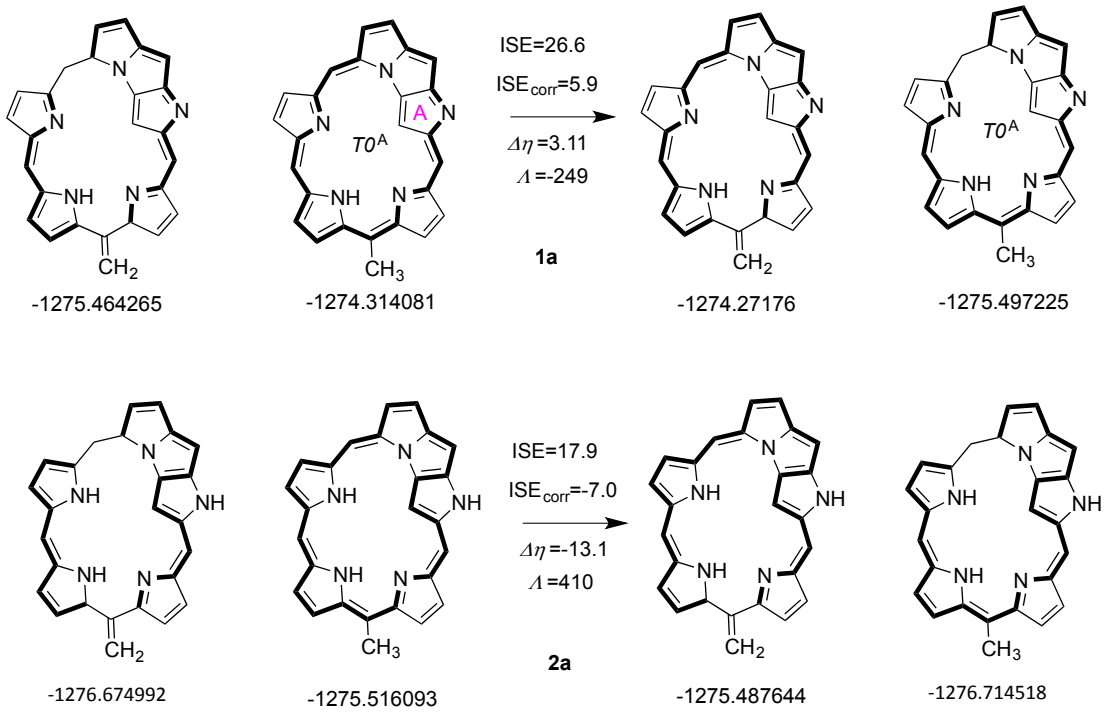


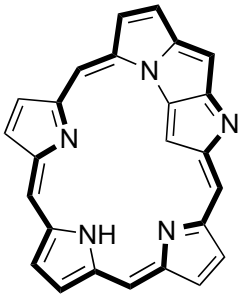
Figure S2. *Syn-anti* corrections applied for the ISE values computed for N-fused [22] and [24]pentaphyrins. Zero-point corrected energies in hartrees evaluated at B3LYP/6-31G(d,p) level of theory.

IV. Cartesian coordinates of B3LYP/6-31G(d,p) optimized geometries

Unsubstituted N-fused [22]pentaphyrin (R=H) **1**

1a

T0[A]



Sum of electronic and zero-point Energies= -1235.022890

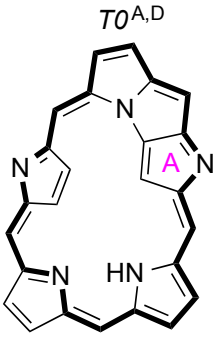
N	-2.47056200	-1.71771900	0.00001700
N	-2.79822200	1.04412700	-0.00013900
N	0.61140100	2.14721900	-0.00006300
N	3.34891200	-0.41422500	0.00002800
N	1.70091400	-3.50915400	-0.00003700
C	-1.98050000	-2.99602900	-0.00000600
C	-3.11237600	-3.87186200	-0.00001000
C	-4.25236200	-3.10228300	0.00001400
C	-3.84482100	-1.73601500	0.00002800
C	-4.62705400	-0.57885500	0.00007800
C	-4.13301600	0.72421400	0.00004300
C	-4.96832500	1.91586300	0.00006000
C	-4.10900000	2.96217000	0.00004400
C	-2.75555500	2.39456000	0.00003300
C	-1.65456200	3.27584900	0.00008200
C	-0.25988900	3.20870500	0.00002500
C	0.46282500	4.48741700	0.00002300
C	1.77312000	4.17842200	-0.00003100
C	1.84168000	2.71014100	-0.00007500
C	3.13999800	2.14738900	-0.00009500
C	3.77150100	0.91200200	-0.00005100
C	5.21334700	0.84569700	-0.00004700
C	5.63288700	-0.46244700	0.00002400
C	4.46989900	-1.26863600	0.00006100
C	4.09457700	-2.61639000	0.00005700
C	2.69120800	-2.62118600	0.00000900
C	2.20569900	-1.23211300	-0.00002200
C	0.85471500	-1.26867000	-0.00007200
C	0.55988400	-2.73892400	-0.00000600
C	-0.64472800	-3.42443500	-0.00000300
H	-3.04129400	-4.95055900	-0.00002300
H	-5.27960400	-3.43913400	0.00002500
H	-6.05048100	1.92701000	0.00011100
H	-4.33855200	4.02008800	0.00008700
H	-0.00317900	5.46432800	0.00007400
H	2.62714400	4.84359600	-0.00003300
H	5.83893700	1.72791800	-0.00008800
H	6.65021300	-0.82708500	0.00004400
H	0.17336900	-0.42810900	-0.00010100
H	-5.70389400	-0.71444200	0.00012900
H	-0.52044200	-4.50319900	0.00000100
H	4.76748400	-3.46144200	0.00007900
H	3.89299900	2.93099700	-0.00013500
H	-1.99232300	4.31005500	0.00016300
H	-1.98239600	-0.81926400	0.00004900

1b

Sum of electronic and zero-point Energies= -1235.000956

N	2.49003200	-3.27828900	-0.40238100
C	1.24182400	-2.82389700	-0.04683400
C	0.11031700	-3.61724100	-0.19245800
C	-1.25291800	-3.28348200	-0.07147200
C	-2.30404600	-4.25255600	-0.05149200
C	-3.50314200	-3.59487900	0.06862900
C	-3.23593900	-2.19306600	0.09414800
C	-4.19738400	-1.17817200	0.11011100
C	-4.04284000	0.21041700	0.04159200
N	-2.85536900	0.87789900	0.00305600
C	-3.18823700	2.18817100	-0.15208400
C	-2.32544900	3.29753600	-0.27790900
C	-0.95047800	3.37977300	-0.05005800
N	-0.22902500	2.41248800	0.55599100
C	1.07136400	2.77451200	0.42267200
C	1.96994200	1.76987600	0.81099600
C	3.24344000	1.35855900	0.43875700
C	4.46234600	1.87985000	-0.09278800
C	5.31870000	0.82183000	-0.38728200
C	4.64048400	-0.39590100	-0.09865300
C	4.60390900	-1.77029000	-0.46410200
C	3.29180600	-2.21473700	-0.20039000
C	2.54846100	-1.08459200	0.35820200
C	1.25155100	-1.43241300	0.46451400
N	-1.86467500	-2.04547300	0.02760400
C	-5.18003000	1.12356800	-0.07321100
C	-4.64373000	2.35723500	-0.22558100
N	3.43944400	-0.02542000	0.49427700
C	-0.07058400	4.46652100	-0.51541900
C	1.20060500	4.06699700	-0.25152800
H	-2.13688000	-5.31941300	-0.10234500
H	-4.49244700	-4.02736000	0.12402400
H	-6.22386700	0.83692000	-0.06095800
H	-5.15670600	3.30238800	-0.35121000
H	-0.39170000	5.37316800	-1.01355200
H	2.12241300	4.58690300	-0.47709900
H	4.68666400	2.93156100	-0.20672300
H	6.31132500	0.90550300	-0.80805100
H	0.41113200	-0.86766700	0.83581300
H	-5.22163000	-1.53932600	0.13986800
H	0.30046700	-4.65335600	-0.45737300
H	5.40437200	-2.31031200	-0.94910400
H	1.41778100	0.98532900	1.31536100
H	-2.80550400	4.20967100	-0.62733700
H	-1.44811500	-1.12415500	-0.06131700

1c



Sum of electronic and zero-point Energies= -1235.018438

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N	-2.94224500	-1.06949100	0.02635400
N	0.55405300	-3.31345600	-0.29241900
N	3.44852200	-0.08982400	-0.01053900
N	2.10763200	3.15830500	-0.00585500
C	-1.63928800	2.90065700	-0.03407700
C	-2.69051600	3.86947700	-0.02028900
C	-3.89671900	3.20681500	0.00233500
C	-3.62233600	1.80950700	0.00879500

C	-4.54188700	0.74943300	-0.01215900
C	-4.22687500	-0.60841300	-0.04335700
C	-5.15806900	-1.70593500	-0.27897500
C	-4.39403600	-2.82425200	-0.40574700
C	-3.01296800	-2.40561100	-0.18408700
C	-1.86354400	-3.22823500	-0.25545900
C	-0.62178700	-2.84594500	0.23637500
C	-0.37614800	-1.83211200	1.26798700
C	0.96156000	-1.63089700	1.27157900
C	1.50159500	-2.51167500	0.23162800
C	2.84010000	-2.51996600	-0.23139900
C	3.71893900	-1.45125000	-0.22083400
C	5.14484000	-1.52925800	-0.39332400
C	5.70666200	-0.28108200	-0.24086500
C	4.64893400	0.64393200	-0.03291700
C	4.41174300	2.02403400	0.02203000
C	3.01095700	2.17860700	0.01354200
C	2.39606100	0.84105000	-0.05601800
C	1.05966900	1.02441100	-0.17337000
C	0.89769800	2.49768700	-0.09672900
C	-0.27010200	3.24460600	-0.05841000
H	-2.52446800	4.93759900	-0.03489000
H	-4.88799700	3.63817000	0.01042000
H	-6.23352000	-1.61673700	-0.36468200
H	-4.71985700	-3.83799600	-0.59962300
H	-1.13205800	-1.38538200	1.89575100
H	1.53986900	-0.98113100	1.91255300
H	5.66895000	-2.46143400	-0.55644500
H	6.75700200	-0.02990400	-0.28756400
H	0.27787000	0.29347900	-0.28346300
H	-1.84661800	0.73181900	0.00585600
H	-1.92609200	-4.15702000	-0.81702400
H	3.20438800	-3.43856400	-0.68294500
H	5.16784200	2.79553600	0.01514200
H	-0.09164200	4.31543500	-0.01530000
H	-5.58987900	1.03095200	-0.05267300

$TS1_{1a\text{-}1b}$

Sum of electronic and zero-point Energies= -1234.995318

C	2.89441900	2.08771600	0.65283200
C	2.25739500	0.81950800	0.25878300
C	0.91355400	0.98703000	0.31982800
C	0.77007100	2.39139600	0.74453500
C	-0.33796300	3.19578200	0.73729800
C	-1.66953900	2.92422300	0.29281900
N	-2.21101200	1.70594100	0.00099800
C	-3.48257700	1.85493600	-0.51164900
C	-4.31439900	0.75939600	-0.83940800
C	-4.00608300	-0.57159000	-0.62697700
C	-4.89233100	-1.71462900	-0.73907600
C	-4.22010800	-2.76726600	-0.18877200
C	-2.91213300	-2.25570300	0.19665100
C	-1.88622900	-2.96304500	0.93891900
C	-0.53965800	-2.85717200	0.76872400
C	0.46886300	-3.28547100	1.73807900
C	1.66439400	-2.93676600	1.20811900
C	1.36907900	-2.38883900	-0.13123200
C	2.45251900	-2.13634500	-1.10202600
C	3.37441300	-1.15460400	-0.98228100
C	4.71950000	-1.07117900	-1.55712700
C	5.38282000	0.00080600	-1.04254300
C	4.46886300	0.73591100	-0.20026100
C	4.30619800	1.98089200	0.36187400
N	-2.79061400	-0.96067500	-0.07714100
N	0.08342300	-2.31435300	-0.37534700
N	3.27021800	-0.02784300	-0.15521400
N	2.02619700	3.01147100	0.98814400
C	-2.64521500	3.90034300	-0.03738800
C	-3.75618200	3.24206700	-0.55093500
H	-2.50446500	4.96680200	0.07217500
H	-4.67361700	3.68531600	-0.91395000
H	-5.89385500	-1.70368000	-1.15041500
H	-4.55925800	-3.78842500	-0.07402300

H	0.26325500	-3.71780200	2.70960900
H	2.65294600	-3.04280200	1.63618200
H	5.11932300	-1.81438900	-2.23528500
H	6.40263600	0.29327600	-1.25373800
H	0.14310300	0.28732100	0.03428200
H	-5.29549100	1.00219700	-1.23859000
H	-0.14980100	4.23134700	1.00408900
H	5.05456400	2.75702900	0.42956600
H	2.60850700	-2.88746400	-1.87207500
H	-2.23607300	-3.59797700	1.75311500
H	-1.85729500	0.76307900	0.17626300

	1	2	3
	A	A	A
Frequencies --	-37.5606	43.2485	52.1911
Red. masses --	4.7111	5.6890	5.8868
Frc consts --	0.0039	0.0063	0.0094
IR Inten --	2.3073	0.2979	2.0178

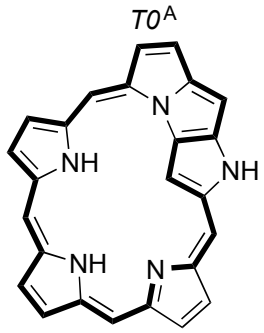
TS2

N	2.09192400	3.18332600	0.60339600
C	0.92190600	2.62065400	0.26789900
C	-0.26913000	3.39868700	0.29190800
C	-1.58040500	3.03407300	0.08299800
C	-2.67577300	3.98101000	-0.02079400
C	-3.82689000	3.29907800	-0.25117200
C	-3.51553100	1.88447400	-0.26449900
C	-4.40163700	0.83436100	-0.36559800
C	-4.07338300	-0.54472000	-0.23620200
N	-2.83872200	-1.02923200	-0.09545500
C	-3.00064900	-2.40160900	0.11701100
C	-2.01534700	-3.30366600	0.37590900
C	-0.57617900	-3.04886500	0.33708000
N	0.05489500	-2.67769300	-0.74689900
C	1.38765900	-2.44816900	-0.33676000
C	2.29498300	-1.92763900	-1.19112900
C	3.52782400	-1.26450100	-0.73880100
C	4.88285500	-1.54623300	-0.68331600
C	5.56325000	-0.38524700	-0.18275400
C	4.60707700	0.58922000	0.05583800
C	4.37357000	1.96189300	0.49679200
C	3.01907700	2.18465800	0.40477400
C	2.37065500	0.96826300	-0.08240100
C	1.04639800	1.19833300	-0.17703300
N	-2.15190300	1.77907200	-0.08624900
C	-5.09659700	-1.60395200	-0.15341500
C	-4.43072200	-2.74923000	0.09476500
N	3.38025600	0.03105000	-0.28088000
C	0.32281200	-3.16651900	1.50950000
C	1.53878100	-2.75256200	1.09305000
H	-2.54356900	5.05161500	0.05630800
H	-4.82099800	3.70116100	-0.38968700
H	-6.16407400	-1.45299100	-0.25377500
H	-4.82903300	-3.74665200	0.22956000
H	0.02500300	-3.48248300	2.50124600
H	2.45496000	-2.66600000	1.66090900
H	5.33995900	-2.48078300	-0.97424000
H	6.62907300	-0.29211100	-0.02862200
H	0.26464200	0.54379400	-0.53228000
H	-5.44893900	1.09006300	-0.48407100
H	-0.10435100	4.45371800	0.48683300
H	5.14296600	2.64892700	0.82187700
H	1.98918300	-1.80291300	-2.22920500
H	-2.32367200	-4.30204600	0.68285800
H	-1.73391400	0.86027800	0.03298400

Sum of electronic and zero-point Energies= -1234.985857

	1	2	3
	A	A	A
Frequencies --	-88.3184	36.5375	49.9527
Red. masses --	4.3919	5.7622	6.0806
Frc consts --	0.0202	0.0045	0.0089
IR Inten --	0.3240	0.5827	0.0416

2a



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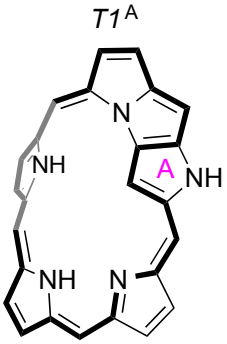
N	0.53922700	2.26524900	0.00499700
N	3.37477400	-0.37178900	-0.09380100
N	1.74959900	-3.40258200	-0.09651600
C	-1.94718400	-3.01670900	0.26666300
C	-3.07001300	-3.94180400	0.34016600
C	-4.19372100	-3.18865700	0.23183700
C	-3.74128200	-1.80715400	0.09550700
C	-4.61550900	-0.69733200	-0.09231400
C	-4.20523300	0.60514700	-0.22394300
C	-5.02720400	1.78230900	-0.41080300
C	-4.21174500	2.86387200	-0.43359600
C	-2.83349800	2.42650900	-0.25811500
C	-1.80064400	3.32196100	-0.16520300
C	-0.38820900	3.29756500	0.07113500
C	0.31961000	4.45719800	0.42103000
C	1.66498000	4.12588000	0.54335800
C	1.81520000	2.75925700	0.26598700
C	3.11710500	2.16704100	0.21689600
C	3.76427800	0.97455700	0.05035000
C	5.22579100	0.95460900	-0.07134500
C	5.67021800	-0.30546100	-0.30145300
C	4.52194300	-1.17155400	-0.30561600
C	4.19252500	-2.51130200	-0.39030600
C	2.78643200	-2.53392300	-0.19823400
C	2.27686400	-1.22672500	-0.00747900
C	0.88801800	-1.31816800	0.20370600
C	0.56522400	-2.69065400	0.13430800
C	-0.63727000	-3.43266600	0.25346700
H	-2.98870300	-5.01629700	0.44779700
H	-5.22575100	-3.51543300	0.22990500
H	-6.10443200	1.75942200	-0.50217600
H	-4.49185000	3.90243400	-0.54854400
H	-0.13686500	5.42463100	0.57491000
H	2.48087400	4.78416100	0.80768600
H	5.82076800	1.85616700	-0.01099400
H	6.69120300	-0.62834200	-0.44833100
H	0.16998500	-0.55802800	0.46382100
H	-2.15913700	0.35436000	-0.00967300
H	0.35489100	1.35450900	-0.38750000
H	1.79019700	-4.39891600	-0.23670300
H	-5.68145800	-0.89121500	-0.13905200
H	-0.49988100	-4.51212500	0.30501400
H	4.87299800	-3.33529400	-0.54055000
H	3.84970200	2.96128700	0.33427700
H	-2.15101000	4.34828000	-0.22432400

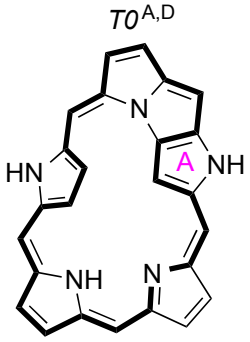
2b



Sum of electronic and zero-point Energies= -1236.228209

N	-2.42513600	1.39855500	0.39444100
N	-2.86303000	-1.18827700	-0.15091700
N	1.02402100	-2.34985200	-0.20857900
N	3.36539400	0.07329600	-0.30636300
N	1.64608700	3.06184500	-0.49416100
C	-1.94975900	2.68280900	0.49404300
C	-3.05907800	3.61633800	0.66559500
C	-4.19759100	2.87594700	0.62041300
C	-3.77596400	1.49420800	0.41381700
C	-4.64715800	0.42059900	0.08591000
C	-4.17764900	-0.82670300	-0.29550500
C	-4.80908400	-1.88653800	-1.05350500
C	-3.83840600	-2.76541800	-1.44497300
C	-2.57889400	-2.33705900	-0.86843900
C	-1.31700900	-2.87520500	-0.93442200
C	-0.31509900	-2.54586600	0.04953900
C	-0.44748100	-2.55753500	1.44943200
C	0.83028300	-2.43538700	2.01167700
C	1.74674300	-2.27053500	0.96781800
C	3.17075100	-2.05687200	0.99053000
C	3.86976300	-1.10085200	0.31101400
C	5.30340300	-1.05910400	0.09808900
C	5.63547900	0.07804100	-0.58704100
C	4.44242800	0.83837600	-0.79065700
C	4.04077600	2.15298500	-1.04583100
C	2.69347900	2.19982800	-0.64453600
C	2.26225900	0.92828400	-0.17928200
C	0.92498900	1.01550400	0.21682000
C	0.54043700	2.37127800	0.02450200
C	-0.64150700	3.09971200	0.29365500
H	-2.96303000	4.68945100	0.77618600
H	-5.22265000	3.21860900	0.68400700
H	-5.86253600	-1.92362000	-1.29710300
H	-3.96546700	-3.66215200	-2.03666400
H	-1.38132500	-2.70406500	1.97208800
H	1.08253200	-2.42224700	3.06286400
H	5.96676100	-1.85885600	0.39865100
H	6.62556100	0.38259700	-0.89843100
H	0.28934500	0.26183700	0.65260200
H	-2.19524400	-0.45457200	0.11372000
H	1.43151000	-2.27907600	-1.12822500
H	1.61175000	4.01851200	-0.80562300
H	-5.70689100	0.62856700	-0.01251400
H	-0.51577600	4.18178700	0.26786300
H	4.67225900	2.95388200	-1.40076200
H	3.76170400	-2.72281900	1.61499900
H	-1.09652600	-3.61782000	-1.69660200

2c



Sum of electronic and zero-point Energies= -1236.234370

N	2.12303500	3.06471800	0.06016600
N	3.49694000	-0.08813800	-0.09156400
N	0.44224000	-3.14726200	-0.25273700
N	-3.06301500	-1.05692300	0.00236000
N	-2.22647200	1.65991100	0.02816200
C	0.86803800	2.43382400	0.07010000
C	1.07939100	1.03994500	0.01151100
C	2.46911600	0.85363100	-0.03086400
C	3.10104700	2.12037100	-0.01906700
C	4.51129800	1.97840800	-0.11878900
C	4.71544600	0.60810900	-0.18651200
H	2.25506300	4.06287500	0.06075000
C	5.74902600	-0.36824900	-0.42672200
H	0.49219800	-3.60702700	-1.14903300
C	5.16127100	-1.59122800	-0.50643300
H	-2.24187200	-0.46777900	0.11609800
C	3.72115400	-1.47007000	-0.26922400
H	0.28786100	0.31303800	-0.00916100
C	2.84298000	-2.50550500	-0.18624300
H	6.80113800	-0.14189500	-0.53262400
C	1.49196100	-2.44486900	0.31821100
H	5.65039900	-2.54370500	-0.66031500
C	0.96754900	-1.75287900	1.40551500
H	1.54421600	-1.15518500	2.09565500
C	-0.42152100	-1.99307400	1.44460300
H	-1.12695800	-1.61842700	2.17200300
C	-0.74399300	-2.83739500	0.38400800
H	-4.86185600	-3.74527200	-0.66650100
C	-2.04353300	-3.28699400	-0.07637700
H	-6.26258900	-1.46427800	-0.69047000
C	-3.10538600	-2.43438300	-0.17400600
H	-4.85523800	3.73464700	-0.10972300
C	-4.49426300	-2.74340200	-0.48926300
H	-2.48816000	5.01838900	0.09378800
C	-5.20595400	-1.58715300	-0.49362500
C	-4.29624400	-0.48680400	-0.21613400
C	-4.54569600	0.86364400	-0.20765900
C	-3.54983900	1.88107500	-0.06589300
C	-3.86221900	3.30777400	-0.04780600
C	-2.67264900	3.95179400	0.05684900
C	-1.64345300	2.91880600	0.08854000
C	-0.29985200	3.23706800	0.11405200
H	3.22985800	-3.47626600	-0.49153200
H	5.26978700	2.74502200	-0.16784600
H	-0.10149900	4.30811100	0.15008400
H	-5.57059900	1.18484700	-0.35912600
H	-2.19292500	-4.32790000	-0.34938800

$TS1_{2a\text{-}2b}$

Sum of electronic and zero-point Energies= -1236.223498

	1	2	3
	A	A	A
Frequencies --	-61.8532	32.4282	39.3236
Red. masses --	4.4451	5.4561	6.0073

```
 Frc consts  --     0.0100                0.0034                0.0055
 IR Inten    --     0.8061                0.0502                0.2614

C                  2.72468600    2.38376100   -0.46406800
 C                  2.25637100    1.08709800   -0.12755400
 C                  0.90792200    1.17470100    0.24292900
 C                  0.56269300    2.54523500    0.15826300
 C                 -0.61828000    3.27568300    0.43595000
 C                 -1.92686700    2.85446500    0.55320300
 N                 -2.39101000    1.56831000    0.34715800
 C                 -3.73147600    1.66556300    0.33182900
 C                 -4.59670500    0.59244700   -0.04415300
 C                 -4.14958000   -0.66113800   -0.37699400
 C                 -4.87176100   -1.75162000   -1.01228900
 C                 -3.99224200   -2.74777800   -1.27543300
 C                 -2.68326000   -2.36879700   -0.74093900
 C                 -1.57493800   -3.15394500   -0.69693300
 C                 -0.38643100   -2.96825000    0.15267500
 C                 -0.10463400   -3.65608300    1.32856500
 C                  1.23374700   -3.39662900    1.67619500
 C                  1.76460200   -2.51783200    0.73226500
 C                  3.14332200   -2.12588100    0.62087100
 C                  3.80063600   -1.04487000    0.11524500
 C                  5.24145700   -1.02004100   -0.11038200
 C                  5.61541900    0.18227200   -0.62776700
 C                  4.44443400    1.00888400   -0.70284100
 C                  4.08556100    2.34488200   -0.84188100
 N                  1.69794000    3.25329400   -0.26300000
 N                  3.34193800    0.22543500   -0.30627900
 N                  0.74780800   -2.25105600   -0.17564000
 N                 -2.84973200   -1.09647700   -0.21827000
 C                 -4.17446700    3.02960000    0.60051000
 C                 -3.04415000    3.77098700    0.73922800
 H                  1.69780900    4.23632900   -0.48090900
 H                  0.86758400   -1.74455700   -1.03998800
 H                 -2.13848400   -0.42756600    0.07260800
 H                  0.24216800    0.40402800    0.59469700
 H                  6.61240900    0.49238100   -0.90864200
 H                  5.87376000   -1.87864300    0.07249400
 H                  1.77668100   -3.78630500    2.52647600
 H                 -0.80378500   -4.29728300    1.84587600
 H                 -4.19272300   -3.70203900   -1.74381900
 H                 -5.92868800   -1.72504800   -1.24152600
 H                 -5.20431300    3.36030200    0.64585500
 H                 -2.95818700    4.83460500    0.92395300
 H                  3.82049200   -2.87964500    1.01609100
 H                  4.73984400    3.15910000   -1.11438200
 H                 -0.47894400    4.35426200    0.50370300
 H                 -5.65327600    0.80514000   -0.16474900
 H                 -1.65730700   -4.11788500   -1.19448700
```

$TS1_{2b\text{-}2c}$

```
Sum of electronic and zero-point Energies=          -1236.227799

                     1                     2                     3
                     A                     A                     A
 Frequencies --   -39.6286              46.9272              60.3599
 Red. masses --     4.5203               5.7976               4.9688
 Frc consts  --     0.0042               0.0075               0.0107
 IR Inten    --     1.0275               0.0990               0.4684

C                  2.77528000    2.20808800   -0.53268000
 C                  2.31265900    0.92398900   -0.14897900
 C                  0.95655500    1.01128700    0.19355400
 C                  0.59844400    2.37575900    0.04513700
 C                 -0.58862700    3.11792100    0.27459900
 C                 -1.90771600    2.72741400    0.41768500
 N                 -2.41180300    1.45012600    0.31336700
 C                 -3.75645000    1.57939600    0.30002400
 C                 -4.65407100    0.51606500    0.00282300
 C                 -4.22113800   -0.76187400   -0.30048300
 C                 -4.90524800   -1.86132600   -0.95456500
 C                 -3.98133700   -2.81751500   -1.25683200
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C	-2.69492000	-2.39268400	-0.73236800
C	-1.47495700	-3.01235000	-0.75376600
C	-0.40314000	-2.61411900	0.13312300
C	-0.45189000	-2.37363600	1.51110500
C	0.86911800	-2.21669600	1.97657500
C	1.72073900	-2.30586100	0.88086900
C	3.17225600	-2.19324100	0.77378500
C	3.87099200	-1.18740500	0.19078300
C	5.31318300	-1.17890900	-0.05133800
C	5.68042700	0.01207700	-0.59945400
C	4.50977200	0.83587100	-0.70275100
C	4.14010300	2.16312000	-0.89292800
N	-2.92042600	-1.16268800	-0.13547000
N	0.92881700	-2.55812200	-0.22207000
N	3.41186900	0.06624100	-0.27683100
N	1.73409900	3.07579700	-0.38808400
C	-3.00043600	3.68862400	0.54700000
C	-4.15275400	2.97475300	0.47490200
H	-2.88191300	4.76011500	0.65145800
H	-5.17142000	3.34014000	0.50706700
H	-5.96118800	-1.87156000	-1.18968400
H	-4.15218400	-3.76130800	-1.75736600
H	-1.35707600	-2.36629400	2.10059500
H	1.18423700	-2.02415300	2.99238900
H	5.94669400	-2.02996100	0.15802600
H	6.67724200	0.31511800	-0.89038900
H	0.29451500	0.24333900	0.55922200
H	-2.22047300	-0.45165200	0.09776400
H	1.28199900	-2.66159800	-1.16076700
H	1.72737700	4.04831200	-0.64814300
H	-5.70730600	0.74713100	-0.11112000
H	-0.44238400	4.19779000	0.27420700
H	4.78862300	2.97020900	-1.19982500
H	3.77366700	-2.99162200	1.20492300
H	-1.33935600	-3.87598000	-1.39965900

3 (R=CH_3)

***T1*^{A}**

Sum of electronic and zero-point Energies= -1431.458854

C	3.07983400	1.64520900	-0.66564100
N	2.35139900	2.68367800	-1.00091600
C	1.02659500	2.29019300	-0.65930200
C	0.01299100	3.21886100	-0.67404000
C	-1.32894000	2.99132000	-0.13603000
C	-2.17515400	4.08732100	0.33169700
C	-3.30448500	3.52156900	0.83195600
C	-3.16621100	2.08887300	0.63152500
C	-4.12107700	1.11942900	0.90557800
C	-3.98182800	-0.25972600	0.54038500
N	-2.85600600	-0.78807200	-0.04002100
C	-3.07937600	-2.07259000	-0.44266400
C	-2.11017100	-2.82485700	-1.22003500
C	-0.76637900	-2.79303700	-0.94580700
N	-0.24293200	-2.34523500	0.28479200
C	1.06306500	-2.45424200	0.16963400
C	2.04974700	-2.35589400	1.26512500
C	3.13416400	-1.54254200	1.11709300
C	4.48955300	-1.62547300	1.65608400
C	5.29077200	-0.70255400	1.04735400

C	4.47244100	0.11144900	0.18179600
C	4.48033400	1.34987600	-0.43294600
C	2.28096000	0.51886000	-0.17246900
C	0.98464700	0.90842700	-0.14717500
N	-1.93099900	1.81553500	0.03743500
C	-4.95288900	-1.28455600	0.55186600
C	-4.40231300	-2.39721400	-0.08552900
C	0.32058100	-3.19875700	-1.83157400
C	1.46780400	-2.93373100	-1.16010200
N	3.17507300	-0.46644800	0.21785000
H	-1.93005000	5.13923800	0.30199800
H	-4.14728200	4.03789300	1.26881600
H	-5.95013300	-1.20317600	0.95879600
H	-4.87839200	-3.35342900	-0.24760100
H	0.22112100	-3.56866200	-2.84286200
H	2.48795300	-3.07493300	-1.49156300
H	4.81221000	-2.38380800	2.35701300
H	6.35268100	-0.57125500	1.20481600
H	0.11488900	0.39670100	0.22429500
C	0.30700100	4.61796500	-1.16323700
H	0.29923400	5.33577800	-0.33349600
H	1.29011800	4.65207300	-1.62820800
H	-0.45378700	4.94780900	-1.87941400
C	-5.43205100	1.49310200	1.55605900
H	-6.26077700	1.39898900	0.84459600
H	-5.64831900	0.82190100	2.39309200
H	-5.42876200	2.51243200	1.93734800
C	-2.66866600	-3.60345800	-2.38370800
H	-1.91194100	-4.22012600	-2.86904700
H	-3.46846600	-4.26879900	-2.03750700
H	-3.11954400	-2.93701300	-3.12819700
C	1.87992100	-3.29899600	2.42569600
H	1.86230900	-4.34651900	2.09951500
H	2.66625400	-3.17756500	3.17489400
H	0.91520100	-3.10620300	2.90970000
C	5.63721600	2.27011400	-0.64940600
H	5.83581600	2.41477700	-1.71842700
H	5.42670700	3.26100000	-0.23176600
H	6.55219600	1.88756800	-0.18838300
H	-2.04350300	-0.20053000	-0.22548500

***TO*^{A,D}**

Sum of electronic and zero-point Energies= -1431.474123

C	3.04845300	2.02139800	0.02087300
C	2.37251200	0.72085800	-0.03643400
C	1.04523100	0.98051200	-0.17849900
C	0.95535500	2.46312600	-0.15984700
C	-0.16931500	3.28870000	-0.20329300
C	-1.56946400	2.92607300	-0.18386200
N	-2.14891400	1.70919600	-0.04599300
C	-3.51657500	1.93894800	-0.02348500
C	-4.52446900	0.96846000	0.08522000
C	-4.29209300	-0.42833400	0.12327500
C	-5.22668900	-1.50005200	0.04710800
C	-4.51358800	-2.68062200	-0.04944700
C	-3.13043900	-2.36633600	0.01489300
C	-2.00755200	-3.23107400	-0.09862100
C	-0.75005800	-2.82488700	0.34332600
C	-0.45580800	-1.79530800	1.34077800
C	0.89222800	-1.64651200	1.33074600
C	1.39272300	-2.56566500	0.31192900
C	2.74638400	-2.68820700	-0.12633700
C	3.64447300	-1.63073000	-0.08934100
C	5.08018000	-1.74506300	-0.16772200
C	5.66342100	-0.51094600	-0.02165500
C	4.61947500	0.44471300	0.09202400
C	4.44928000	1.83276000	0.09729500
N	2.21260400	3.04530200	-0.05607200
C	-2.59095600	3.97087700	-0.26782500
C	-3.79289200	3.35906600	-0.16130900
N	-3.04378000	-0.99677500	0.12802600
N	0.40864600	-3.32709900	-0.19386700
N	3.39359800	-0.25376300	0.06764400

H	-2.41625700	5.02801300	-0.39327400
H	-4.76468500	3.82942200	-0.19193500
H	-6.30149200	-1.39779000	0.04059300
H	-4.91589500	-3.68065300	-0.12307600
H	1.49382500	-1.00586000	1.95886100
H	5.59742700	-2.68947800	-0.25687500
H	6.72137100	-0.28932200	-0.00468000
H	0.20404800	0.31902900	-0.27287100
H	-2.21407400	-0.40698300	0.06956300
C	0.11106600	4.78284300	-0.24536300
C	5.51288800	2.88148100	0.12548300
C	3.17369100	-4.03210700	-0.66901500
C	-2.17797100	-4.55824700	-0.79092500
C	-5.97572300	1.40565800	0.08728400
H	-1.17061600	-1.31103000	1.99131700
H	-0.30036600	5.22800200	-1.15816800
H	1.18248200	4.95996000	-0.22249000
H	-0.35061800	5.29609000	0.60460600
H	5.37711400	3.59365900	-0.69543200
H	5.46885000	3.46046400	1.05559100
H	6.51342200	2.44851500	0.04434000
H	4.05362500	-3.96852400	-1.31131800
H	3.38272600	-4.74041100	0.14274100
H	-1.19868800	-5.00158300	-0.97151500
H	2.34493200	-4.44992200	-1.24562100
H	-2.71055300	-4.45601400	-1.74155400
H	-2.75870500	-5.24746300	-0.16377200
H	-6.37161000	1.48219500	-0.93288400
H	-6.60201000	0.69640500	0.63101800
H	-6.10194100	2.37694700	0.56513600

4 (R=CH_3)

***T1*^{A}**

Sum of electronic and zero-point Energies= -1432.679329

C	-2.51384400	2.06016100	-0.73569300
C	-2.12235100	0.84326800	-0.12148900
C	-0.80930300	0.97251800	0.34393900
C	-0.40584400	2.30906100	0.05787700
C	0.73717700	3.08406200	0.41729000
C	2.02752400	2.59409200	0.66847500
N	2.44999000	1.30980700	0.41617700
C	3.80207300	1.30878600	0.54152000
C	4.65398400	0.23500800	0.13436700
C	4.11264300	-0.95079300	-0.36112000
C	4.69307700	-2.01382500	-1.15102700
C	3.68221400	-2.82874000	-1.58698400
C	2.44304400	-2.35908200	-1.01005000
C	1.15098500	-2.85431800	-1.05136300
C	0.26162100	-2.51263000	0.03147200
C	0.53103800	-2.53314900	1.41574100
C	-0.67873600	-2.39671900	2.10148000
C	-1.69786100	-2.21867000	1.15313300
C	-3.11056000	-1.99304400	1.30228400
C	-3.79553300	-1.09971400	0.51019200
C	-5.21194200	-1.04422100	0.23542000
C	-5.48313900	0.01349000	-0.59729100
C	-4.26619300	0.71347600	-0.83718500
C	-3.83785800	1.99970400	-1.20750700
N	-1.47739700	2.94032400	-0.59530300
C	3.17307300	3.41325500	1.05588800
C	4.27083800	2.61521100	0.97865800
N	2.77408600	-1.23979300	-0.26946200
N	-1.09514500	-2.31194000	-0.08793200
N	-3.22953200	-0.01536100	-0.22342000
H	3.16151600	4.45480600	1.34402700
H	5.29674800	2.89389000	1.17832500
H	5.74401700	-2.11808200	-1.38173100
H	3.78679700	-3.71991300	-2.19051400
H	1.51048800	-2.68634100	1.84369600
H	-0.81680500	-2.38190000	3.17341800
H	-5.91549100	-1.79329000	0.57045900
H	-6.45195200	0.29254000	-0.98940500
H	-0.20918100	0.26735400	0.89600900

H	2.14008000	-0.48104200	0.00930300
H	-1.59298000	-2.20882900	-0.95850000
H	-1.41578500	3.84725500	-1.02489000
C	-3.83494900	-2.80727700	2.34847100
H	-4.84308800	-2.43039200	2.53194200
H	-3.89870100	-3.86715800	2.07134700
H	-3.29171400	-2.76662300	3.29971500
C	0.52205400	4.58802300	0.40975100
H	0.52307900	4.99255300	-0.61365200
H	-0.43502800	4.85612800	0.86880800
H	1.30684600	5.11677500	0.94680600
C	6.15075300	0.44545300	0.12555700
H	6.45619100	1.23083200	-0.57678200
H	6.51459600	0.74281900	1.11592600
H	6.68315900	-0.46808000	-0.14677000
C	0.67228100	-3.75943900	-2.15722700
H	1.49111000	-4.03263200	-2.82711900
H	0.21769500	-4.67879300	-1.76914300
H	-0.08721600	-3.26708400	-2.78235400
C	-4.65165500	3.06844500	-1.86960400
H	-4.57869300	4.02122600	-1.33108900
H	-4.32824800	3.25567800	-2.90187300
H	-5.70909500	2.79269600	-1.90626000

TO^{A,D}

Sum of electronic and zero-point Energies= -1432.676315

C	3.16861700	1.91262600	0.00333300
C	2.45481500	0.69445800	-0.04575100
C	1.07811400	0.98919600	-0.02148100
C	0.96178500	2.39784900	0.06804500
C	-0.14196000	3.31412400	0.13073100
C	-1.50765200	3.03607400	0.05559900
N	-2.12835900	1.78633100	-0.02334800
C	-3.44719900	2.03433600	-0.14711300
C	-4.51245400	1.06638200	-0.27285600
C	-4.32225300	-0.29692900	-0.19057700
C	-5.29418500	-1.36688000	-0.36274300
C	-4.65896800	-2.55798500	-0.24373400
C	-3.24993300	-2.31397300	0.02662800
C	-2.24038000	-3.22344500	0.18757100
C	-0.90672300	-2.76033100	0.55821500
C	-0.48406200	-1.90449200	1.57060600
C	0.91315300	-1.73997900	1.44735400
C	1.33988900	-2.48758900	0.35388400
C	2.66291000	-2.69752000	-0.20210300
C	3.60161900	-1.70643400	-0.27655400
C	5.04194300	-1.88340900	-0.47444600
C	5.68004300	-0.68853300	-0.36306700
C	4.68784100	0.32612000	-0.14338700
C	4.57288200	1.70774000	-0.06404400
N	2.26626100	2.92349700	0.09180300
C	-2.52307700	4.08390700	-0.01065600
C	-3.71897500	3.46624200	-0.15139800
N	-3.12065200	-0.92578400	0.06620000
N	0.22221600	-3.14300000	-0.13566700
N	3.43237000	-0.31037100	-0.08898900
H	2.48972300	3.90243900	0.09379000
H	0.19502400	-3.63933500	-1.01213000
H	-2.26575800	-0.38645000	0.16188900
H	0.23415100	0.32479900	-0.06560900
H	6.74543600	-0.51398700	-0.42691300
H	5.51591000	-2.84490900	-0.60432500
H	1.55605400	-1.15576700	2.08837900
H	-1.12621700	-1.47021400	2.32327300
H	-5.11007000	-3.53686900	-0.31751000
H	-6.34538000	-1.22357000	-0.56413500
H	-4.68669100	3.93718700	-0.24594000
H	-2.36737000	5.15185800	0.00832600
C	-2.44376300	-4.70628200	-0.00671200
H	-3.45568900	-4.94807300	-0.33604000
H	-1.75913300	-5.11390300	-0.76369300
H	-2.24368800	-5.26183200	0.91851500
C	2.98653600	-4.10498400	-0.65485000
H	2.88237100	-4.82200000	0.16782000

H	2.29671400	-4.43144300	-1.44481400
H	3.98972500	-4.19272100	-1.07130900
C	5.67099200	2.72496200	-0.07967400
H	5.56636400	3.42727100	-0.91668500
H	5.68920100	3.32206700	0.84117900
H	6.64911300	2.24618300	-0.17586100
C	0.28291400	4.76994900	0.27396600
H	0.95097300	4.89491600	1.13457000
H	0.81709000	5.12470700	-0.61772400
H	-0.55319700	5.44135400	0.43569800
C	-5.90708000	1.60989500	-0.50937000
H	-6.23973200	2.24199400	0.32301100
H	-5.95411900	2.22461000	-1.41608800
H	-6.64597600	0.81641000	-0.62016600

5 (R=CF_3)

***T1*^{A}**

Sum of electronic and zero-point Energies= -2920.113951

C	-3.19483200	1.32813400	0.42572200
N	-2.62077700	2.43854200	0.80718800
C	-1.25376400	2.20606000	0.55309100
C	-0.34183600	3.22897900	0.64337200
C	0.98889600	3.19175400	0.05642000
C	1.63610500	4.36261900	-0.54222100
C	2.78653600	3.92055700	-1.10171900
C	2.86406000	2.49128700	-0.80329100
C	3.88796000	1.59292700	-1.06485000
C	3.93225300	0.25168200	-0.56955800
N	2.89471800	-0.34671800	0.10282200
C	3.28886200	-1.55274800	0.60621900
C	2.44638800	-2.46328200	1.33986200
C	1.11977100	-2.73984800	1.09785300
N	0.37792400	-2.18375300	0.03326800
C	-0.70058500	-2.93085900	-0.05188000
C	-1.79727700	-2.88867600	-1.04490200
C	-2.85817300	-2.02784300	-1.07529300
C	-4.20831000	-2.33907900	-1.56822800
C	-5.09378400	-1.40896300	-1.12081200
C	-4.35301200	-0.40271500	-0.41597500
C	-4.51958100	0.84495600	0.15201500
C	-2.23943700	0.29077800	-0.00796700
C	-1.00698300	0.83353000	0.03316300
N	1.72585800	2.09828400	-0.09868500
C	5.02286400	-0.65332300	-0.53706500
C	4.63653900	-1.74775700	0.21800700
C	0.36692100	-3.83487300	1.71863000
C	-0.74589000	-3.98841900	0.97161600
N	-2.99753800	-0.80045700	-0.42477700
H	1.24185200	5.36690500	-0.55068500
H	3.51426700	4.50543300	-1.63750500
H	5.98453200	-0.49537700	-0.99701700
H	5.23055500	-2.61878600	0.44461200
H	0.67843200	-4.42338600	2.56633200
H	-1.53338800	-4.72099000	1.07815400
H	-4.44648100	-3.23132900	-2.12508300
H	-6.16278700	-1.39536100	-1.26942500
H	-0.06201700	0.41593400	-0.26126400
C	-0.76924600	4.58261100	1.20445500
C	5.13369500	2.00640800	-1.83602400
C	3.14243100	-3.30523100	2.41182000
C	-1.93065200	-4.18347300	-1.82442700
C	-5.80758700	1.56843600	0.33950900
H	2.03441100	0.16832800	0.28588600
F	0.30561600	5.21781000	1.74180600
F	-1.24961000	5.38920300	0.22878400
F	-1.68265000	4.50552300	2.17310400
F	-5.82231700	2.74559200	-0.31354000
F	-6.84859400	0.83015900	-0.12558300
F	-6.04721200	1.82835500	1.63970900
F	-2.44592100	-3.99024500	-3.05960000
F	-0.73725700	-4.78271800	-1.97733900
F	-2.74755200	-5.08074500	-1.20369100
F	3.27390600	-4.59445400	2.02872700

F	4.37232900	-2.85193200	2.71224900
F	2.43991600	-3.29958400	3.56732500
F	5.01877600	3.17826600	-2.48551400
F	6.19987400	2.10976200	-1.01086600
F	5.44462200	1.08229300	-2.77312500

***T0*^{A,D}**

Sum of electronic and zero-point Energies= -2920.115617

C	3.03973100	-1.79907200	-0.08102600
C	2.32469800	-0.50962400	-0.15599100
C	1.02328300	-0.77835900	0.10934700
C	1.00486400	-2.24856300	0.36733000
C	-0.08369300	-3.07829500	0.62904500
C	-1.47226700	-2.87186600	0.29994600
N	-2.12224300	-1.70998500	0.08008300
C	-3.41946100	-2.06348000	-0.25836200
C	-4.48017900	-1.16644700	-0.45152100
C	-4.38367800	0.24344500	-0.33538500
C	-5.37089100	1.27732700	-0.25922100
C	-4.72196800	2.46814600	-0.01964000
C	-3.32016200	2.21211500	0.00052000
C	-2.20197200	3.07537100	0.11528300
C	-0.96156400	2.73074500	-0.42126900
C	-0.70563800	1.77723300	-1.51106200
C	0.64208400	1.70475300	-1.62381600
C	1.17712700	2.60816300	-0.60026300
C	2.56385200	2.84195600	-0.33713500
C	3.53047300	1.85380600	-0.44777400
C	4.96495300	2.00188800	-0.57358300
C	5.55986300	0.77252400	-0.67875100
C	4.53730700	-0.20449200	-0.56753200
C	4.40434000	-1.57900800	-0.36519900
N	2.26396500	-2.80987700	0.25703500
C	-2.36090600	-4.02028200	0.06114000
C	-3.55612800	-3.51698100	-0.30421000
N	-3.16772100	0.85714800	-0.19023600
N	0.20797100	3.25876400	0.05087100
N	3.30106400	0.46190800	-0.48138900
H	-2.08729700	-5.05950900	0.13139800
H	-4.44290500	-4.06902900	-0.56861600
H	-6.43341800	1.14072000	-0.35596200
H	-5.17236400	3.44158200	0.07885100
H	-1.44945800	1.29834100	-2.13105000
H	1.22091600	1.14342800	-2.34353200
H	5.46140800	2.95516600	-0.62478200
H	6.61046700	0.55959000	-0.80328700
H	0.16492100	-0.13634500	0.16880400
H	-2.32586000	0.29288200	-0.05628300
C	0.23972700	-4.47213800	1.19774300
C	5.50473000	-2.58609000	-0.36933400
C	2.90375400	4.23377100	0.17902200
C	-2.30203500	4.35543500	0.93188400
C	-5.83286000	-1.79369900	-0.76445700
F	-1.74940500	4.19421300	2.14668700
F	-3.59227400	4.72529500	1.13204400
F	-1.69328700	5.38395500	0.32470000
F	2.56998900	4.35384900	1.47603200
F	2.25091400	5.18301100	-0.51081700
F	4.22445100	4.53592300	0.08911800
F	6.69671200	-2.00032900	-0.64968200
F	5.29651300	-3.54113100	-1.29563900
F	5.62472400	-3.19967400	0.82224600
F	1.33900900	-4.50456100	1.95368900
F	0.36582700	-5.40127900	0.22343500
F	-0.76906400	-4.88485900	2.01115600
F	-5.75589800	-2.59191200	-1.85407700
F	-6.27498200	-2.55661100	0.25832900
F	-6.80122700	-0.89391600	-1.02771800

6 (R=CF_3)

***T1*^{A}**

Sum of electronic and zero-point Energies= -2921.367135

C	-2.27964600	1.93921000	-0.69815900
C	-1.97016300	0.74790300	-0.00344800
C	-0.68413800	0.86971700	0.53809800
C	-0.23624000	2.17566900	0.20342100
C	0.90158400	2.93617100	0.65835100
C	2.18481800	2.44222300	0.87755100
N	2.57070100	1.16785300	0.49852500
C	3.90966100	1.11457100	0.63524000
C	4.71606900	0.03251700	0.14978500
C	4.15269500	-1.11151000	-0.41559500
C	4.69041000	-2.17469900	-1.24984200
C	3.65359300	-2.94913300	-1.67656300
C	2.43861600	-2.46060600	-1.05440000
C	1.14462900	-2.93846300	-1.02257700
C	0.28115600	-2.60940100	0.08852000
C	0.59083600	-2.60147300	1.46235500
C	-0.59967600	-2.42742700	2.17437900
C	-1.63614900	-2.27439100	1.24211400
C	-3.05172700	-2.02735000	1.38751800
C	-3.72721000	-1.13721900	0.58751400
C	-5.13098300	-1.07023900	0.22460200
C	-5.32714500	-0.03964300	-0.65303600
C	-4.08072100	0.63361600	-0.83098400
C	-3.57866500	1.87190300	-1.24197800
N	-1.22585900	2.78646100	-0.56858100
C	3.36066500	3.17822300	1.36349100
C	4.42418000	2.35902200	1.20821700
N	2.81100500	-1.35778000	-0.30977000
N	-1.07043900	-2.39552300	-0.00860600
N	-3.10353900	-0.07830300	-0.12771200
H	3.37678600	4.17968400	1.75507000
H	5.45575400	2.57425900	1.43950800
H	5.73052800	-2.29551600	-1.50210100
H	3.71147500	-3.82167600	-2.30795200
H	1.57748000	-2.75766300	1.87219200
H	-0.72179500	-2.39039300	3.24559800
H	-5.86488100	-1.78892100	0.55129700
H	-6.25580800	0.24685400	-1.12566900
H	-0.14146800	0.18322600	1.16711100
H	2.19796000	-0.60446300	0.02593000
H	-1.58065900	-2.38794000	-0.87915000
H	-1.15167700	3.70857300	-0.96821000
C	-3.76235100	-2.87698900	2.40956600
C	0.58696500	4.41601800	0.81826100
C	6.20701200	0.22852100	0.18012200
C	0.60856200	-3.88074700	-2.05684500
F	-0.53925000	-3.37668800	-2.61080600
F	0.27262900	-5.08215100	-1.53951900
F	1.46238800	-4.10265600	-3.07374300
F	-3.15525600	-2.77428600	3.61848100
F	-5.05379600	-2.53397600	2.59290600
F	-3.74015800	-4.18663600	2.07544200
F	-0.55033500	4.60131500	1.52330100
F	1.53048700	5.15750700	1.41680300
F	0.37276600	4.99711900	-0.40769300
F	6.64770200	0.48113000	1.43981300
F	6.60547800	1.27933200	-0.57727200
F	6.89960700	-0.84853800	-0.25400500
C	-4.33338500	2.95655600	-1.91467100
F	-5.28711400	2.46705600	-2.73713500
F	-4.95727600	3.78205600	-1.04038600
F	-3.49968100	3.73493900	-2.64914700

***TO*^{A,D}**

Sum of electronic and zero-point Energies= -2921.360203

C	-3.40152600	-1.22291100	-0.04261700
C	-2.45044200	-0.18093700	-0.07911800
C	-1.17691900	-0.74598300	0.08198100
C	-1.37591900	-2.13579100	0.26992700
C	-0.46402800	-3.21955900	0.52573300
C	0.90842200	-3.25167800	0.30268800
N	1.69550100	-2.14933500	-0.04915900
C	2.90424800	-2.64546100	-0.34181600
C	4.07610800	-1.86450600	-0.68792300

C	4.22914400	-0.52806300	-0.38346700
C	5.41038700	0.33083100	-0.46752700
C	5.09259800	1.55098800	0.01380400
C	3.67864400	1.55250500	0.38829800
C	2.88654900	2.57402500	0.82393900
C	1.43833500	2.39743800	1.01150200
C	0.68961100	1.72921100	1.97253200
C	-0.67200200	1.88207300	1.63195500
C	-0.73997100	2.63683100	0.46076100
C	-1.89266900	3.11816600	-0.28263700
C	-3.04012400	2.39299900	-0.45982400
C	-4.39235500	2.87117000	-0.77855800
C	-5.27552700	1.84277900	-0.69985900
C	-4.53823500	0.65254300	-0.38953000
C	-4.71114600	-0.71599300	-0.24176300
N	-2.75392700	-2.38470400	0.19126500
C	1.72233500	-4.46976000	0.24218700
C	2.94290900	-4.09907400	-0.19873700
N	3.23125600	0.25823300	0.14712000
N	0.55849600	2.94853900	0.11495900
N	-3.18978100	1.00223900	-0.24729700
H	-3.18673900	-3.29327400	0.22699500
H	0.82488200	3.52913000	-0.66553700
H	2.29845000	-0.11569700	0.30187800
H	-0.21224700	-0.27417800	0.08291600
H	-6.34592400	1.88490400	-0.83902400
H	-4.63029900	3.90378800	-0.96544500
H	-1.52113200	1.50207400	2.17955300
H	1.09153300	1.21001500	2.83047800
H	5.74415000	2.40392300	0.09971300
H	6.37224600	0.01500900	-0.83239900
H	3.79025500	-4.73826200	-0.38836900
H	1.39745300	-5.47551300	0.43937400
C	3.36531600	3.98978900	0.96076300
C	-1.77539900	4.54440800	-0.77196000
C	-5.96769400	-1.48559600	-0.38987800
C	-1.16905900	-4.45829800	1.08105800
C	5.21765800	-2.64028900	-1.29997600
F	2.85609300	4.57205200	2.06511900
F	2.94390900	4.74657800	-0.09823400
F	4.70721600	4.12998600	1.02173300
F	6.15148600	-1.86110400	-1.89295500
F	5.87639000	-3.40227100	-0.38760100
F	4.77633700	-3.48745100	-2.25862900
F	-1.97924600	-5.03203700	0.14099100
F	-1.97608200	-4.11264500	2.11357000
F	-0.37840600	-5.43228500	1.55039200
F	-6.18493500	-1.89985400	-1.66170800
F	-7.04809700	-0.75877900	-0.02770100
F	-5.93496800	-2.60558700	0.37638400
F	-2.82563000	4.99551400	-1.48153600
F	-0.69125300	4.66506000	-1.60126400
F	-1.57380500	5.40639200	0.24366200

7 (R=C_6F_5)

***TO*[A]**

Sum of electronic and zero-point Energies= -4870.706790

C	-3.09841600	-0.63260700	0.47318600
N	-2.78292700	-1.91580100	0.18976500
C	-1.56599300	-1.83974800	-0.38248400
C	-0.95409300	-3.04184200	-0.83799300
C	0.41323400	-3.24985400	-1.00945400
C	1.04493800	-4.46236400	-1.47283900
C	2.38890600	-4.34973000	-1.28225400
C	2.64651700	-3.05688500	-0.70037800
C	3.83646400	-2.56337000	-0.16959100
C	3.94161500	-1.26357400	0.40445500
N	3.01540800	-0.30056000	0.24315800
C	3.54834600	0.82824100	0.83358700
C	3.12420200	2.13150800	0.63592600
C	1.99787500	2.63076000	-0.13624400
N	0.70805700	2.30543400	-0.04076700
C	0.05385800	3.20401100	-0.87427600
C	-1.30356500	3.50992100	-0.83154900

C	-2.35434600	2.90637100	-0.07860300
C	-3.50015200	3.60208900	0.37600600
C	-4.34441200	2.72095100	1.05316200
C	-3.75161900	1.45962200	0.98172700
C	-4.12294200	0.07063200	1.10083300
C	-2.05963400	0.29586400	0.03346800
C	-1.05180600	-0.43781700	-0.48993800
N	1.43600800	-2.41083700	-0.61782100
C	5.08502300	-0.79124000	1.19234400
C	4.82321400	0.49702900	1.49062000
C	2.22844100	3.71089500	-1.10580900
C	1.01665000	4.02367700	-1.61226700
N	-2.51177300	1.59039700	0.35168000
H	0.51147000	-5.30550200	-1.88459500
H	3.14495700	-5.08832400	-1.50124600
H	5.94767900	-1.37339300	1.48043900
H	5.42997400	1.17406600	2.07331500
H	3.19229800	4.11298800	-1.38521700
H	0.78677400	4.74709000	-2.38045200
H	-3.65229500	4.66383600	0.25414300
H	-5.28397300	2.95651400	1.52903500
H	-0.11805100	-0.09935200	-0.91127600
C	5.03100700	-3.45699000	-0.18755300
C	5.53950600	-4.03613500	0.98050300
C	5.69255300	-3.76381900	-1.38236800
C	6.65656200	-4.86737100	0.97091800
C	6.80482100	-4.60148400	-1.41987300
C	7.28959700	-5.15333600	-0.23656400
C	4.00148900	3.24035200	1.13349300
C	5.28641000	3.48508400	0.63292300
C	3.52380600	4.12893700	2.10632200
C	6.06945900	4.54270300	1.08838200
C	4.29016100	5.18992000	2.58107500
C	5.56861300	5.39674800	2.06830700
C	-1.75790600	4.71583800	-1.59989800
C	-2.61020100	4.57329100	-2.70157300
C	-1.38553000	6.01827300	-1.24818900
C	-3.05905300	5.66750900	-3.43559600
C	-1.82652500	7.12882600	-1.96475000
C	-2.66548100	6.95099200	-3.06242700
C	-5.34993900	-0.44290700	1.70594700
C	-5.90225100	0.13065400	2.86398700
C	-6.03639000	-1.54792900	1.16946200
C	-7.05312100	-0.36325000	3.46614500
C	-7.18713700	-2.05910100	1.76211700
C	-7.69785500	-1.46845800	2.91525400
C	-1.86725100	-4.20371400	-1.03001500
C	-1.77732900	-5.36352800	-0.25286800
C	-2.90500100	-4.15009600	-1.96905000
C	-2.65996400	-6.42913600	-0.41000800
C	-3.79847300	-5.20117300	-2.14312000
C	-3.67548800	-6.34584700	-1.35820500
F	5.79056000	2.70781700	-0.33598000
F	2.30197700	3.95721400	2.62200900
F	3.81023400	6.00651100	3.52432600
F	6.31210600	6.41094100	2.51396000
F	7.29062100	4.75044600	0.58337000
F	4.95272000	-3.78486800	2.15969900
F	7.11606800	-5.40029800	2.10780500
F	8.35663200	-5.95437700	-0.25924100
F	7.41070100	-4.87346100	-2.58043700
F	5.25179900	-3.25267000	-2.54039600
F	-3.04858800	-3.06942900	-2.74458600
F	-4.76858400	-5.12422800	-3.06082200
F	-4.52493500	-7.36278700	-1.52062800
F	-2.54222300	-7.52463800	0.34986300
F	-0.82662700	-5.47593200	0.68681700
F	-5.30767400	1.18875400	3.43878300
F	-5.61956200	-2.12202500	0.04011600
F	-7.81723500	-3.10395600	1.21668600
F	-8.80263900	-1.95184000	3.48436200
F	-7.53604400	0.20918000	4.57389700
F	-3.00481700	3.35271600	-3.08479400
F	-3.86082200	5.49604800	-4.49117900
F	-3.09180200	8.00797200	-3.75524400
F	-1.45691700	8.36102200	-1.60088600
F	-0.59470000	6.23043300	-0.18939900

H	1.38713700	-1.47961000	-0.20565500

***T1*[A]**

Sum of electronic and zero-point Energies= -4870.715680

C	-2.33788500	1.83005300	0.03608800
C	-1.90394700	0.48039600	-0.37069900
C	-0.57342000	0.55747700	-0.65002900
C	-0.24698500	1.98006400	-0.42131200
C	0.91619000	2.68549600	-0.64604000
C	2.23926500	2.14601200	-0.93289700
N	2.65143200	0.92906500	-0.58871400
C	4.01559200	0.87973100	-0.87830200
C	4.83385300	-0.17691500	-0.48584400
C	4.33548200	-1.34036100	0.17849900
C	4.96657000	-2.44273200	0.80536600
C	3.96643600	-3.24397100	1.36091000
C	2.72666600	-2.65692900	1.03235300
C	1.33494200	-3.02970300	1.21754600
C	0.48494300	-2.87722100	0.13856200
C	0.86859100	-2.90574500	-1.27690800
C	-0.29558200	-2.88881500	-1.97423800
C	-1.35652900	-2.75577300	-0.97316000
C	-2.79246500	-2.61852300	-1.25625100
C	-3.52013400	-1.55348400	-0.79631400
C	-4.97228300	-1.47195700	-0.66444300
C	-5.33308500	-0.27660300	-0.12872800
C	-4.14014500	0.50339800	0.04004200
C	-3.76149900	1.80771800	0.30466300
N	-1.37905100	2.70979700	0.01857200
C	3.32876900	2.92429600	-1.51786300
C	4.43159500	2.13143000	-1.48673800
N	2.98862900	-1.52382600	0.32886600
N	-0.89876300	-2.77322400	0.26235200
N	-3.04350600	-0.32003200	-0.33159800
F	6.80725700	0.02039700	1.56805300
F	9.45951400	0.13162900	1.07950900
F	10.38458300	0.07198200	-1.48589300
F	8.62786600	-0.10533800	-3.56666100
F	5.97431700	-0.22469300	-3.09386300
F	2.08852500	-1.82087100	3.68627600
F	1.21505200	-2.67611600	6.08103400
F	-0.50225700	-4.78934400	6.23948400
F	-1.31744300	-6.06211500	3.97316400
F	-0.42842900	-5.26367500	1.57499900
F	-2.39685000	-5.39289800	-0.74095100
F	-3.45884700	-7.35418500	-2.23718200
F	-5.08889000	-6.75417200	-4.34213200
F	-5.62625900	-4.14672900	-4.94690400
F	-4.54694400	-2.16553800	-3.49678700
F	-5.91278100	1.54273300	2.15450500
F	-7.43227800	3.60947300	2.95522200
F	-6.97619400	6.12004100	1.97562200
F	-4.98739000	6.52223200	0.14932300
F	-3.49371300	4.46806800	-0.70921600
F	-0.76175000	4.31624800	-2.31268000
F	-0.90534300	6.99334700	-2.10754600
F	0.61733600	8.31584600	-0.27131500
F	2.29156100	6.92034800	1.37486300
F	2.43206900	4.23128200	1.19583500
C	6.30006900	-0.10422700	-0.74620100
C	7.22852500	-0.01672200	0.29736000
C	8.59956400	0.04217800	0.06075600
C	9.07359400	0.01479800	-1.24881900
C	8.17525000	-0.07271200	-2.30967200
C	6.80839800	-0.13219600	-2.04995900
C	0.85204900	-3.49150800	2.52790600
C	1.26507500	-2.87557800	3.72236200
C	0.81572600	-3.29885000	4.96771700
C	-0.06723400	-4.37342100	5.05029500
C	-0.48977900	-5.01581800	3.88873600
C	-0.03500700	-4.57734900	2.64924200
C	-3.43328700	-3.69333200	-2.04360000
C	-3.17525400	-5.05014100	-1.77372200
C	-3.71992200	-6.07782600	-2.53716300
C	-4.55636000	-5.77497900	-3.60909100

C	-4.83575900	-4.44411000	-3.90966800
C	-4.27351100	-3.42996800	-3.14055200
C	-4.61479600	2.92308900	0.71309000
C	-5.65716200	2.75942600	1.63994400
C	-6.45374200	3.81559600	2.06603100
C	-6.21951700	5.09673500	1.57259800
C	-5.19951200	5.29935100	0.64674100
C	-4.42112400	4.22627600	0.22171500
C	0.83468300	4.17389500	-0.55790000
C	-0.01466800	4.92079300	-1.38427600
C	-0.09313500	6.30719300	-1.29541600
C	0.68607500	6.98530100	-0.36119500
C	1.54278400	6.27285000	0.47367400
C	1.60674300	4.88695400	0.36606600
H	3.25266000	3.93457700	-1.89330200
H	5.42909600	2.37792700	-1.82098300
H	6.03069600	-2.62333300	0.84200100
H	4.09855100	-4.17533900	1.89227800
H	1.87325200	-3.00712900	-1.66117100
H	-0.43399000	-2.93376200	-3.04648600
H	-5.63046100	-2.29497400	-0.90276400
H	-6.32790700	0.05074600	0.13218100
H	0.10596700	-0.18921600	-1.02575800
H	2.34436400	-0.76171100	0.07923200

***TO*^{A,D}**

Sum of electronic and zero-point Energies= -4870.722092

N	-3.60913900	0.43924800	-0.00400600
C	-2.32885000	0.94448300	0.09803300
C	-2.16718600	2.32311200	0.25999900
C	-0.97390100	3.11793300	0.27431900
C	-1.03548000	4.54310200	0.61023500
C	0.22153800	5.02452100	0.49488900
C	1.04947600	3.89651600	0.09027600
C	2.43429700	4.00072600	-0.12578500
C	3.29735500	2.92699300	-0.42798700
N	2.87805200	1.63142500	-0.57211400
C	3.95878300	0.78498900	-0.69681900
C	3.84615700	-0.62302600	-0.76114200
C	2.64483200	-1.24290700	-1.12380400
N	2.30795700	-2.48536300	-0.67996900
C	1.01955000	-2.64736700	-1.03749400
C	0.25590100	-3.75342200	-0.58154200
C	-1.13251900	-3.74589700	-0.45752300
C	-1.98375400	-4.90106500	-0.38981500
C	-3.30328700	-4.51084300	-0.39151300
C	-3.32843900	-3.09447300	-0.39532400
C	-4.24190000	-2.02154000	-0.29310000
C	-3.43494700	-0.86069200	-0.19709800
N	0.29715800	2.74772000	-0.02361100
C	4.72219800	2.91435600	-0.52940800
C	5.12515600	1.60503800	-0.66181600
C	1.57100400	-0.66119500	-1.93785000
C	0.55589500	-1.55718700	-1.89651900
N	-1.99848000	-2.64361800	-0.43747600
C	-2.01909500	-1.24667500	-0.23216700
C	-1.29831400	-0.12006900	-0.00690600
C	3.07215900	5.34710800	0.00215900
C	3.89769500	5.67094500	1.08408300
C	4.49872400	6.92159000	1.20522200
C	4.27546500	7.88837000	0.22730800
C	3.45741100	7.59764800	-0.86229300
C	2.87013300	6.33885900	-0.96400200
C	4.99568200	-1.46193200	-0.31137900
C	4.96809200	-2.14645300	0.90857000
C	6.01957000	-2.96924500	1.30572000
C	7.13558300	-3.11282900	0.48463000
C	7.19622400	-2.43212000	-0.72848100
C	6.12925400	-1.62414400	-1.11073900
C	1.00726000	-4.97790000	-0.16640500
C	1.68462000	-5.02410500	1.05575700
C	2.44440700	-6.13016600	1.42809700
C	2.53500300	-7.22539300	0.57180700
C	1.86741400	-7.20877700	-0.65002600
C	1.12295900	-6.08718200	-1.00591200

C	-5.70336700	-2.08903200	-0.24639800
C	-6.49108000	-1.14381800	-0.92669100
C	-7.88142400	-1.16246100	-0.86965200
C	-8.53281900	-2.14464000	-0.12771400
C	-7.78467400	-3.10365700	0.55116600
C	-6.39670600	-3.06371700	0.48803500
C	-3.45418800	3.08146800	0.40549900
C	-3.92410500	3.91223600	-0.61376200
C	-5.13036900	4.59969400	-0.50915600
C	-5.90168800	4.45828800	0.64117600
C	-5.45923900	3.63651500	1.67525100
C	-4.25096700	2.95862500	1.54632300
H	-1.91937500	5.08282800	0.91307900
H	0.56360200	6.03166900	0.68147300
H	5.35457500	3.78852400	-0.49573200
H	6.13498500	1.24023000	-0.77161400
H	1.62386400	0.25457700	-2.50982700
H	-0.38786900	-1.51340300	-2.41913600
H	-1.61506100	-5.91564800	-0.40445400
H	-4.17047200	-5.15218100	-0.36783000
H	-0.23881200	0.03903300	0.07336600
F	-5.71863800	-3.99653200	1.17941300
F	-5.91453700	-0.20966800	-1.68638100
F	-8.59511900	-0.25371400	-1.54108700
F	-9.86510400	-2.17262600	-0.07370600
F	-8.40151400	-4.04686000	1.27097700
F	-7.05934000	5.11486700	0.75617000
F	-5.55125700	5.38967600	-1.50426300
F	-3.20544900	4.06648600	-1.73582500
F	-6.19746000	3.50425200	2.78410500
F	-3.85521500	2.17977000	2.56035500
F	4.12906600	4.76507000	2.04377200
F	2.09385200	6.08932100	-2.02535900
F	5.28061500	7.19946800	2.25291000
F	4.84503900	9.08963900	0.33300800
F	3.24655600	8.52241900	-1.80353700
F	3.92959000	-2.01255800	1.73692200
F	6.21626900	-0.97191000	-2.28331100
F	8.26855300	-2.56073200	-1.51810600
F	8.14947500	-3.89360600	0.86477000
F	5.96937700	-3.61278200	2.47642200
F	1.61102500	-3.99449300	1.90351900
F	0.48575800	-6.09813000	-2.18888900
F	1.94747000	-8.26099000	-1.47291400
F	3.25404000	-8.29314900	0.92613400
F	3.08137800	-6.15065600	2.60339500
H	1.89687800	1.39030900	-0.43952100

8 (R=C_6F_5)

***T1*^{A}**

Sum of electronic and zero-point Energies= -4871.954526

C	-2.27007900	1.85213900	0.38973900
C	-1.91504700	0.58951900	-0.14794100
C	-0.60442500	0.64578300	-0.62384100
C	-0.16685600	1.98557500	-0.41600900
C	1.00829700	2.69039200	-0.81081200
C	2.28105300	2.15315400	-1.04120200
N	2.67560700	0.88016200	-0.71717300
C	4.02083600	0.84208800	-0.88695000
C	4.84253200	-0.23434700	-0.43197700
C	4.29002500	-1.36861300	0.17205300
C	4.88518300	-2.44185800	0.93413700
C	3.87513000	-3.21236500	1.44405400
C	2.62390800	-2.69562400	0.94643100
C	1.31538700	-3.16939000	1.03364300
C	0.42426300	-2.85916800	-0.06068200
C	0.69171900	-2.94952100	-1.44296300
C	-0.51410000	-2.80931000	-2.12907500
C	-1.52217700	-2.56361900	-1.18318200
C	-2.92816300	-2.31615400	-1.35114600
C	-3.61063900	-1.36698600	-0.60889600
C	-5.01328500	-1.29996900	-0.30873400
C	-5.26739700	-0.18925400	0.45968800
C	-4.04481900	0.51865900	0.63031000
C	-3.58378100	1.82954900	0.92021800

N	-1.19970000	2.67596900	0.22260000
C	3.42748600	2.92261900	-1.51637700
C	4.50813100	2.10781500	-1.42301900
N	2.94070700	-1.59243800	0.18723100
N	-0.91868100	-2.59560100	0.05675000
N	-3.03200300	-0.24079500	0.03116700
F	6.58108200	-0.02629600	1.84387600
F	9.25867700	0.18533000	1.65309800
F	10.46423800	0.23863600	-0.79800800
F	8.95032200	0.06586700	-3.06264800
F	6.26901700	-0.16837000	-2.88831100
F	2.02570700	-2.70600100	3.77715900
F	1.20637600	-4.26041400	5.79624400
F	-0.43582400	-6.39130000	5.32854200
F	-1.23018600	-6.95850100	2.77900200
F	-0.38880700	-5.45534200	0.72597300
F	-2.76286100	-5.15916800	-1.46576800
F	-4.02024800	-6.65105600	-3.31550600
F	-5.62501200	-5.46851000	-5.17854700
F	-5.93991000	-2.75857100	-5.18454000
F	-4.66257600	-1.23937300	-3.37738800
F	-5.65594500	1.39417100	2.85659200
F	-6.99657900	3.37356800	4.04452300
F	-6.42174000	5.98794300	3.47930900
F	-4.45849600	6.56900000	1.66023000
F	-3.12878800	4.61503300	0.41785400
F	-0.64027200	3.96938400	-2.74467200
F	-0.90208000	6.64560900	-2.97063900
F	0.44505300	8.30150400	-1.27191600
F	2.05722500	7.25389500	0.66372700
F	2.32431800	4.58540500	0.90808800
C	6.32308800	-0.10985100	-0.51648200
C	7.13355200	-0.01364700	0.62151600
C	8.51982200	0.09653200	0.54084000
C	9.13626400	0.12829800	-0.70709300
C	8.36143700	0.04318900	-1.86127900
C	6.97884400	-0.07938800	-1.75413400
C	0.86662000	-4.01288400	2.15148500
C	1.24782700	-3.75758500	3.48416700
C	0.82393300	-4.54824700	4.54740100
C	-0.02057500	-5.63066700	4.31379900
C	-0.42995700	-5.91256500	3.01234100
C	0.01435800	-5.11988700	1.95961800
C	-3.65701400	-3.13552000	-2.34322100
C	-3.51828600	-4.53475500	-2.37839200
C	-4.16767800	-5.32206000	-3.32339400
C	-4.99360800	-4.72151900	-4.27138100
C	-5.15919700	-3.33872100	-4.26661100
C	-4.49581100	-2.56650900	-3.31735300
C	-4.33155100	2.90338900	1.56903300
C	-5.34185600	2.65637000	2.51741900
C	-6.04793200	3.67305700	3.15117500
C	-5.75305900	5.00505100	2.87259500
C	-4.75251000	5.29714900	1.94973200
C	-4.07227100	4.26235700	1.31922200
C	0.86323100	4.17634900	-0.92057300
C	0.03341500	4.75281800	-1.89370000
C	-0.11259700	6.13111200	-2.02231700
C	0.57777000	6.97886700	-1.15816400
C	1.40405400	6.44191500	-0.17439300
C	1.53474400	5.05882700	-0.06319700
H	3.40527700	3.94352400	-1.87006900
H	5.53374400	2.34662200	-1.66531600
H	5.94547800	-2.58646600	1.07981100
H	3.97653600	-4.10249400	2.04827600
H	1.66318400	-3.15576700	-1.86663700
H	-0.66496900	-2.84457900	-3.19857700
H	-5.72014900	-2.06826900	-0.58751400
H	-6.22082800	0.10959500	0.86737100
H	-0.02565400	-0.11167500	-1.12638400
H	2.31723800	-0.83694600	-0.12609300
H	-1.41500200	-2.49811600	0.92944100
H	-1.18004100	3.65600300	0.44844700

***TO*^{A,D}**

Sum of electronic and zero-point Energies= -4871.952173

C	-3.53064300	-0.84881900	-0.13796900
C	-2.17183200	-1.22832300	-0.15053400
C	-1.38176800	-0.06746300	-0.15221500
C	-2.28176300	1.02384800	-0.15690300
C	-2.11112800	2.44436500	-0.15109000
C	-0.94983100	3.20881400	-0.11878900
N	0.37181400	2.76701800	-0.07892300
C	1.11814800	3.88151300	0.00156400
C	2.56049900	3.92636900	0.07960700
C	3.37921600	2.82517600	-0.06225400
C	4.82652200	2.75192900	0.06757700
C	5.20902300	1.46564800	-0.10979000
C	4.02289600	0.66023800	-0.36846900
C	3.93683600	-0.69323700	-0.55768000
C	2.64826200	-1.30805000	-0.88447100
C	1.73281000	-0.97275500	-1.88119800
C	0.62248600	-1.83127500	-1.75348400
C	0.86353200	-2.68096100	-0.67563600
C	0.07194700	-3.75600500	-0.11485500
C	-1.29809300	-3.73046400	-0.03485700
C	-2.17289300	-4.88364100	0.13392800
C	-3.47289200	-4.49671000	0.04173300
C	-3.49727600	-3.07154400	-0.14038000
C	-4.39227200	-1.99228800	-0.14341500
N	-3.58351700	0.50402200	-0.16848200
C	-0.98626300	4.66814900	-0.08711900
C	0.29694100	5.08732200	-0.00530100
N	2.95406600	1.54733100	-0.34198900
N	2.11706700	-2.36711900	-0.18869000
N	-2.16658000	-2.62923200	-0.19188300
C	1.32910700	-6.58415100	2.12046100
C	0.62733100	-5.47199000	1.66169100
C	5.16277000	-1.53945700	-0.50463800
C	5.35706000	-2.51720100	0.47677000
C	6.47304900	-3.34620700	0.50936900
C	7.46084000	-3.19865100	-0.46159100
C	7.31298400	-2.23035100	-1.45129600
C	6.17625300	-1.42478100	-1.46642600
C	3.20981600	5.24525400	0.32472800
C	4.02867400	5.85802900	-0.63221700
C	4.63664500	7.09191600	-0.41156200
C	4.42268300	7.75813200	0.79199400
C	3.60939400	7.18208500	1.76539500
C	3.02285600	5.94245200	1.52575200
C	-3.40069400	3.22288800	-0.17548600
C	-4.06636300	3.48674500	-1.37691200
C	-5.25456500	4.21339500	-1.41725300
C	-5.80754900	4.69131100	-0.23100700
C	-5.17177500	4.44004400	0.98273800
C	-3.98472200	3.70952600	0.99842400
H	-4.41839500	1.04934900	-0.03342800
H	2.52933400	-2.74904800	0.64906200
H	1.96272500	1.33206400	-0.40291200
H	-0.31207700	0.03429600	-0.14403900
H	-4.34424000	-5.13107100	0.08052100
H	-1.80735600	-5.89528800	0.22978600
H	-0.25239000	-1.85778900	-2.38545000
H	1.88193500	-0.20901000	-2.63069900
H	6.21323400	1.07131500	-0.06395900
H	5.46216000	3.59520900	0.29314200
H	0.65696900	6.10519100	0.02874900
H	-1.87195400	5.28475300	-0.12301900
C	-5.85262300	-2.03200500	-0.14440900
C	-6.63053000	-1.00526700	0.41864700
C	-8.02018600	-1.00340800	0.40280300
C	-8.70544500	-2.06350800	-0.18392000
C	-7.97824400	-3.10492200	-0.75440100
C	-6.58808700	-3.07348700	-0.74035500
C	0.79677200	-4.96318500	0.36348100
C	1.72594200	-5.63040100	-0.45264100
C	2.44184200	-6.73847500	-0.01086900
C	2.24115000	-7.21931000	1.28168600

F	4.43601200	-2.68139600	1.45567700
F	6.07292200	-0.51375800	-2.44317600
F	8.25598000	-2.08737400	-2.38782400
F	8.54285500	-3.97916800	-0.44099100
F	6.60956400	-4.26481800	1.47159600
F	-0.21892900	-4.88109800	2.51558700
F	1.14228900	-7.03480300	3.36516600
F	2.91919900	-8.28368400	1.71246300
F	3.30827100	-7.35301100	-0.82264700
F	1.93462600	-5.21464300	-1.70751200
F	-5.95106100	-4.09245200	-1.34304700
F	-6.02778300	0.04397600	1.02164200
F	-8.69710800	0.00470600	0.96255400
F	-10.03997600	-2.08174100	-0.19864100
F	-8.61905100	-4.12361400	-1.33686700
F	-3.39811500	3.48578900	2.17994800
F	-5.70331800	4.89660500	2.12084300
F	-6.94561400	5.38726900	-0.25774100
F	-5.86548500	4.45357200	-2.58215100
F	-3.55897300	3.04107900	-2.53292000
F	2.25694200	5.41539800	2.49025200
F	3.41007400	7.81574700	2.92700000
F	4.99698200	8.94337600	1.01435400
F	5.41379200	7.64368600	-1.35108700
F	4.25357400	5.25533200	-1.80911500

9 (R=$C_6H_3Cl_2$)

TO[A]

Sum of electronic and zero-point Energies= -6985.888627

C	3.37798600	-0.73391400	0.27037900
N	2.98437700	-1.94005100	0.61248500
C	1.59325000	-1.87508600	0.52872400
C	0.91073500	-3.07771000	0.59992000
C	-0.44949100	-3.33849500	0.24635900
C	-1.00357500	-4.62174700	-0.02343200
C	-2.28505800	-4.44277800	-0.50838700
C	-2.54744800	-3.05057500	-0.51005000
C	-3.72241300	-2.35886200	-0.88632100
C	-3.90729900	-0.98947900	-0.71671300
N	-2.96431200	-0.16034900	-0.12763700
C	-3.58441700	1.00769600	0.05917900
C	-3.06668300	2.15107900	0.78232600
C	-1.78519800	2.65914000	0.85815100
N	-0.68033900	2.30221100	0.07156000
C	0.19854300	3.28021600	0.25303200
C	1.45219200	3.53205900	-0.45733900
C	2.53931200	2.73073900	-0.71934200
C	3.79841200	3.25597000	-1.24567100
C	4.79877100	2.34569900	-1.08748700
C	4.22233400	1.17584500	-0.51501800
C	4.59976900	-0.09364500	-0.09731300
C	2.26369200	0.19880100	0.04691100
C	1.11462800	-0.50251200	0.19525500
N	-1.41837100	-2.42004600	-0.04390100
C	-5.14230700	-0.26935200	-0.96333900
C	-4.95515200	0.97282900	-0.45061900
C	-1.48745400	3.87083300	1.62868500
C	-0.26997900	4.28222000	1.22792400
N	2.83700500	1.40878900	-0.36107900
H	-0.47633600	-5.55522700	0.09693300
H	-2.97655900	-5.20704800	-0.83025900
H	-6.02827000	-0.66986100	-1.43512300
H	-5.65703700	1.79362500	-0.43579900
H	-2.13844700	4.33677100	2.35338500
H	0.28386100	5.14434000	1.56799200
H	3.89976600	4.25073700	-1.65072100
H	5.83957200	2.46151900	-1.35249500
H	0.10820700	-0.13167800	0.07137600
C	-4.83657100	-3.17872200	-1.46079300
C	-4.93720000	-3.41442600	-2.84386000
C	-5.82963100	-3.75934500	-0.65132700
C	-5.96533500	-4.17714400	-3.39615700
C	-6.86635300	-4.52655200	-1.18132500
C	-6.92860300	-4.73137300	-2.55723500
C	-4.13798700	2.91405800	1.51979800

C	-4.60848200	2.47967400	2.77267700
C	-4.74152700	4.07300400	0.99747800
C	-5.60591500	3.15618200	3.47329100
C	-5.74588100	4.76289200	1.67579600
C	-6.17347400	4.29954400	2.91726200
C	1.58819400	4.97829400	-0.86340600
C	2.31951600	5.93056600	-0.12536500
C	0.94063200	5.46113900	-2.01843300
C	2.40654100	7.26959200	-0.50434900
C	1.01498800	6.79455400	-2.41879100
C	1.74971700	7.69702100	-1.65516300
C	5.95800900	-0.66883000	-0.10025400
C	6.66357800	-0.94842900	-1.28772000
C	6.61875100	-0.99398800	1.10210700
C	7.93755700	-1.51322700	-1.28634700
C	7.88981200	-1.56353300	1.12690400
C	8.54663800	-1.82154000	-0.07320700
C	1.71627500	-4.29222900	0.96457800
C	2.42643100	-5.04515900	0.01443800
C	1.77527100	-4.74563800	2.29186300
C	3.16339300	-6.17551400	0.36209900
C	2.50602600	-5.87195300	2.66605700
C	3.20124200	-6.58414700	1.69300100
H	-1.44204500	-1.40975500	0.10836900
H	-5.92628200	2.78458200	4.43953400
H	-6.95274700	4.83180900	3.45342300
H	-6.18094200	5.64918600	1.22902500
H	2.52504400	-6.17696300	3.70571900
H	3.77501100	-7.46217900	1.97242500
H	3.69944000	-6.72061600	-0.40593400
H	-7.60921100	-4.95294200	-0.51752000
H	-7.73255900	-5.32684600	-2.97806900
H	-6.00176200	-4.32913400	-4.46843900
H	8.35330300	-1.79296000	2.07910900
H	9.53736000	-2.26476600	-0.06324500
H	8.43372300	-1.71418300	-2.22846700
H	2.98052900	7.96061400	0.10172800
H	1.81155400	8.73753200	-1.95767000
H	0.50182900	7.11090000	-3.31927400
Cl	-3.91141500	1.05003200	3.51393100
Cl	-4.25113000	4.68443900	-0.57484300
Cl	-5.78517600	-3.52667100	1.08742600
Cl	-3.74090300	-2.73404300	-3.93218500
Cl	0.90920100	-3.87336100	3.54880400
Cl	2.39755500	-4.57357900	-1.67563400
Cl	5.85003500	-0.64797300	2.64023500
Cl	5.93092200	-0.61348500	-2.85120400
Cl	3.15550000	5.45614100	1.34872400
Cl	0.02258100	4.35709800	-3.02364100

TO^{A,D}

Sum of electronic and zero-point Energies= -6985.907822

N	3.08100600	-1.97163900	0.01182100
C	1.70597300	-1.88435100	0.07976700
C	0.96917300	-3.06535900	0.17982100
C	-0.44769900	-3.27846000	0.15871200
C	-0.99848100	-4.62858600	0.31498100
C	-2.34175100	-4.51313800	0.22351700
C	-2.61074200	-3.09734800	0.01191300
C	-3.90661600	-2.57636100	-0.12339600
C	-4.22675200	-1.21510300	-0.30486000
N	-3.29140400	-0.22205000	-0.41933000
C	-3.90013700	1.01335400	-0.44314600
C	-3.19802000	2.23975800	-0.46948400
C	-1.86113000	2.30843900	-0.87653500
N	-1.00411400	3.25348800	-0.39386800
C	0.21222800	2.87029800	-0.82690400
C	1.40143300	3.51183000	-0.38706000
C	2.64451100	2.88776800	-0.32291300
C	3.91609400	3.55572800	-0.26041900
C	4.93399100	2.63063700	-0.29312400
C	4.33639800	1.34656500	-0.31671200
C	4.69962700	-0.00870200	-0.22411900
C	3.48007900	-0.71539200	-0.14100900

N	-1.43972800	-2.37147400	-0.02150200
C	-5.50682300	-0.58293700	-0.31010300
C	-5.30401100	0.77844400	-0.36681700
C	-1.17344300	1.37249000	-1.77152700
C	0.13051500	1.73977200	-1.75078300
N	2.94300700	1.51770100	-0.34780700
C	2.36276600	0.24076400	-0.17544800
C	1.22740600	-0.47857200	-0.00098300
Cl	-4.94032600	-3.75911900	-2.76608100
Cl	-3.53888500	2.45074000	2.59008000
Cl	-4.12745800	4.32148300	-2.53204300
Cl	1.43905500	4.01486300	2.66127400
Cl	1.18277200	5.67827300	-2.56007900
Cl	5.68163300	-1.47851100	-2.72569200
Cl	6.30925000	0.44797600	2.37298000
Cl	1.72229500	-4.52375900	-2.42934100
Cl	1.78241400	-3.93998200	3.01456800
C	-5.06862700	-3.52000100	-0.03870700
C	-5.67302300	-3.85078400	1.18816300
C	-6.75656600	-4.72435800	1.27385100
C	-7.26789300	-5.29262800	0.11000800
C	-6.70462800	-4.99073800	-1.12714900
C	-5.62211600	-4.11414300	-1.18762200
C	-3.87352300	3.45904100	0.06079500
C	-4.09022600	3.65319900	1.43766100
C	-4.71119400	4.79564000	1.93879500
C	-5.14169200	5.78175000	1.05520700
Cl	-5.06221200	-3.15218700	2.67747700
C	-4.95164200	5.63023600	-0.31579000
C	-4.32270300	4.48235200	-0.79354700
C	1.30077300	4.92880100	0.07633900
C	1.30713200	5.26986300	1.44170000
C	1.18867500	6.58775600	1.88020600
C	1.06297400	7.61042400	0.94419000
C	1.05466000	7.32046400	-0.41777200
C	1.16975200	5.99531800	-0.83187200
C	6.07205600	-0.55172700	-0.17464300
C	6.61882900	-1.26695300	-1.25839400
C	7.90385700	-1.80441500	-1.22468400
C	8.68690600	-1.63201400	-0.08649200
C	8.19059200	-0.92944200	1.00813300
C	6.90135000	-0.40334700	0.95393300
C	1.81165300	-4.30824300	0.29987800
C	2.20917100	-5.04877000	-0.82468300
C	2.98750000	-6.20022200	-0.72460100
C	3.38970200	-6.64296800	0.53283500
C	3.01628700	-5.94133300	1.67604200
C	2.23841900	-4.79230700	1.54664800
H	-0.42475600	-5.52828400	0.47641500
H	-3.08295400	-5.29607000	0.29149300
H	-6.45218100	-1.10231700	-0.25986000
H	-6.05471200	1.55490100	-0.38508900
H	-1.63802500	0.60407300	-2.37351800
H	0.94757900	1.32275100	-2.32090600
H	4.01800000	4.63121300	-0.25144200
H	5.99655700	2.82566600	-0.28800900
H	0.19860800	-0.17576000	0.05805800
H	-7.18645900	-4.94975300	2.24270500
H	-8.11047100	-5.97437100	0.16739900
H	-7.09297900	-5.42558100	-2.04057200
H	-4.84618300	4.90473800	3.00841300
H	-5.62748900	6.67402300	1.43733800
H	-5.28518200	6.38796000	-1.01490800
H	0.96213000	8.10671300	-1.15760000
H	0.97101100	8.63928600	1.27764300
H	1.19072400	6.79917600	2.94295600
H	8.27886600	-2.34568100	-2.08524200
H	9.68889100	-2.04781500	-0.05203200
H	8.78658300	-0.79287700	1.90270200
H	3.27135300	-6.73396600	-1.62400800
H	3.99682700	-7.53830900	0.62218700
H	3.32145800	-6.27268500	2.66166100
H	-2.29994900	-0.43735000	-0.32518400

10 (R=$C_6H_3Cl_2$)

***TO*^{A,D}**

Sum of electronic and zero-point Energies= -6987.130283

C	3.60047700	-0.48794900	-0.09256800
C	2.46132000	0.34682700	-0.08967600
C	1.31421700	-0.46231600	-0.12471100
C	1.77178800	-1.79984200	-0.16669900
C	1.10675000	-3.06630400	-0.19724200
C	-0.25203200	-3.36334900	-0.17336200
N	-1.32556700	-2.47594600	-0.13268000
C	-2.42331000	-3.24766400	-0.04948800
C	-3.78245900	-2.77232500	0.03975000
C	-4.15167300	-1.44809800	-0.05049200
C	-5.47907800	-0.86894800	0.08955400
C	-5.37574000	0.47593900	-0.03688600
C	-3.97928700	0.81275000	-0.27835500
C	-3.42391600	2.04995100	-0.45314600
C	-2.01085000	2.18376500	-0.79919400
C	-1.26681000	1.55899300	-1.79787500
C	0.07579300	1.96015800	-1.65049900
C	0.14596500	2.82266100	-0.55808300
C	1.27413300	3.51987300	0.02237400
C	2.53299400	2.99542600	0.11985300
C	3.76216500	3.75105500	0.35107000
C	4.83699500	2.92471100	0.25411800
C	4.34950200	1.59492300	0.01013000
C	4.80476900	0.27707500	-0.03585800
N	3.17524100	-1.77190500	-0.16698400
C	-0.74186300	-4.73822600	-0.13626200
C	-2.09048200	-4.66801300	-0.04845300
N	-3.29654800	-0.39735000	-0.28681800
N	-1.14415500	2.98126800	-0.08695400
N	2.95126600	1.65959800	-0.07016700
Cl	5.60362300	-1.69320200	2.20988000
C	0.63568100	6.52324100	2.31881300
Cl	6.70614100	1.33700000	-2.26247000
C	0.87661300	5.22703000	1.86369000
Cl	1.16276600	5.74223900	-2.11432700
C	-4.25555600	3.28277300	-0.30854200
Cl	0.93736500	3.94267900	3.06445000
C	-4.47465400	3.90746400	0.93406500
Cl	-3.74590900	3.22767300	2.38885500
C	-5.23307400	5.06817900	1.07704000
Cl	-4.63553300	3.23095700	-3.02258400
C	-5.79900700	5.65094700	-0.05364500
Cl	-5.21705900	-3.87878200	-2.46264600
C	-5.60510600	5.08026700	-1.30897600
Cl	-4.39739400	-3.57854000	2.95121300
C	-4.84293700	3.91850500	-1.42130400
Cl	1.94170500	-4.08318000	-2.98493600
C	-4.86682900	-3.78004100	0.25706800
Cl	2.04804900	-4.26779700	2.49244400
C	-5.58683100	-4.35093400	-0.81053800
C	-6.59617200	-5.29459000	-0.62070500
C	-6.91459100	-5.69974900	0.67263400
C	-6.23168900	-5.16718400	1.76290600
C	-5.22703000	-4.22514500	1.54427400
C	2.03501500	-4.25350500	-0.24992300
C	2.47902000	-4.79234300	-1.47272200
C	3.33946100	-5.88820900	-1.53891300
C	3.79010000	-6.47405800	-0.35876200
C	3.38774700	-5.96874400	0.87462900
C	2.52599400	-4.87219800	0.91596000
H	3.75766100	-2.58947900	-0.09110400
H	-1.38260700	3.42608900	0.78771200
H	-2.29480600	-0.55067000	-0.36019400
H	0.27655800	-0.18300700	-0.11147600
H	5.87950100	3.19457500	0.34162400
H	3.77574100	4.82044200	0.50261100
H	0.90903800	1.68349400	-2.27865500
H	-1.67369300	0.91074200	-2.56020500
H	-6.17099000	1.20551500	0.01518400
H	-6.37463100	-1.44427100	0.27413800
H	-2.79508100	-5.48542300	0.00715900
H	-0.13275400	-5.62990000	-0.16015500

H	8.30388300	-2.24733500	1.75502300
H	9.93383100	-1.42782800	0.05319900
H	9.17496400	0.17918800	-1.69440700
H	0.65360000	8.11267600	-0.69053100
H	0.36786100	8.57601100	1.74162000
H	0.51137500	6.70353300	3.38002700
H	-5.36969900	5.50343600	2.05999800
H	-6.39174300	6.55500600	0.04349100
C	6.20265300	-0.18274200	-0.01270900
H	-6.03876500	5.52369500	-2.19769000
C	6.68148500	-1.09738700	0.95260300
H	-7.11784400	-5.70137100	-1.47905400
C	7.99838500	-1.54973100	0.98405300
H	-7.69821600	-6.43390900	0.83165400
C	8.90415100	-1.08560700	0.03477700
H	-6.46905400	-5.47228000	2.77532200
C	8.48717400	-0.18388500	-0.93985100
H	3.64538000	-6.26988600	-2.50591200
C	7.16212000	0.24687800	-0.95956300
H	4.45899200	-7.32782900	-0.40054500
C	1.04583100	4.92169200	0.49906800
H	3.73160500	-6.41312300	1.80123300
C	0.94855400	6.00762900	-0.39368700
C	0.71053300	7.31153300	0.03693800
C	0.55431700	7.56358500	1.39785000

***T1*[A]**

Sum of electronic and zero-point Energies= -6987.128134

C	-2.50440100	-1.72898900	0.48199400
C	-2.02304300	-0.49913700	-0.03606000
C	-0.72020100	-0.68155100	-0.50310600
C	-0.41833200	-2.06119400	-0.31132900
C	0.68507600	-2.87359700	-0.70285200
C	2.00297900	-2.47466700	-0.94566500
N	2.52661700	-1.23546800	-0.67145100
C	3.86940100	-1.35331400	-0.80838800
C	4.79813300	-0.35487700	-0.38397200
C	4.36876400	0.86212700	0.14261100
C	5.06295600	1.85208800	0.93581800
C	4.13925000	2.74375700	1.40668600
C	2.85151000	2.39237500	0.84919800
C	1.61200600	2.99734500	0.93621600
C	0.64294100	2.75626000	-0.10858400
C	0.85563100	2.80860600	-1.50179300
C	-0.38877700	2.77056500	-2.13298200
C	-1.37073600	2.62201000	-1.14124900
C	-2.79822700	2.48878300	-1.24912600
C	-3.54043100	1.60352800	-0.49823700
C	-4.95120200	1.65123600	-0.20808100
C	-5.30108300	0.56278000	0.55135700
C	-4.14085200	-0.24327800	0.72458100
C	-3.81336800	-1.58881200	0.99361000
N	-1.52534500	-2.65648700	0.30473800
C	3.06804000	-3.38453400	-1.36071400
C	4.22870000	-2.68572700	-1.27874500
N	3.06168600	1.26261600	0.08327000
N	-0.71294900	2.62339300	0.07276500
N	-3.05838900	0.43271600	0.14654200
H	2.94024600	-4.41638700	-1.65620400
H	5.23013900	-3.03592400	-1.48750600
H	6.12503800	1.84518500	1.13599800
H	4.32221500	3.60754800	2.02997000
H	1.82309200	2.92452100	-1.96700400
H	-0.58469000	2.80830400	-3.19505400
H	-5.58852900	2.47429800	-0.49795700
H	-6.28207900	0.32961900	0.94072900
H	-0.06515800	0.01980500	-0.99332500
H	2.35901200	0.57190500	-0.20679400
H	-1.17056600	2.54613200	0.96880400
H	-1.58487700	-3.63337400	0.53925100
C	6.26017100	-0.65821500	-0.38886400
C	6.89334700	-1.34870000	0.66355300
C	7.09513200	-0.26649400	-1.45356000

C	8.25847100	-1.63394600	0.66263700
C	8.46233900	-0.53907200	-1.47995400
C	9.03944800	-1.22591900	-0.41531900
H	8.69443700	-2.16735900	1.49917400
H	9.05732200	-0.21554800	-2.32591300
H	10.10280000	-1.44390700	-0.42555300
C	1.30097100	3.95357300	2.03980900
C	1.54015800	5.33764200	1.92956300
C	0.73201200	3.52487600	3.25428100
C	1.25193300	6.23285500	2.95898100
C	0.43010900	4.39784300	4.29793500
C	0.69682000	5.75568300	4.14351200
H	1.46117800	7.28770400	2.82503000
H	-0.00686500	4.01244000	5.21163100
H	0.46815900	6.44611200	4.94918300
C	-3.50203800	3.36827100	-2.22798600
C	-4.04098900	2.87047500	-3.43223400
C	-3.64561900	4.75432300	-2.01577600
C	-4.67934600	3.69116100	-4.36160100
C	-4.28150400	5.59370400	-2.92758500
C	-4.79707800	5.05390700	-4.10343900
H	-5.06959900	3.25988100	-5.27594000
H	-4.37151200	6.65153000	-2.71033800
H	-5.29245600	5.69906000	-4.82210900
C	-4.69378600	-2.59773200	1.60426100
C	-5.27538100	-2.42167300	2.88151800
C	-5.01526000	-3.81444300	0.96109100
C	-6.11142300	-3.36983100	3.46735800
C	-5.84029100	-4.78033200	1.53245300
C	-6.39189200	-4.55282900	2.78973300
H	-6.52337600	-3.17933800	4.45138300
H	-6.05268100	-5.69104200	0.98485300
H	-7.03928700	-5.29725500	3.24181900
C	0.40131900	-4.34773500	-0.79486100
C	0.66528700	-5.23539100	0.26654200
C	-0.16011000	-4.91982900	-1.95342800
C	0.40163100	-6.60335200	0.18351100
C	-0.42744200	-6.28367700	-2.06230000
C	-0.14362800	-7.12238700	-0.98724000
H	0.62531700	-7.24332300	1.02895600
H	-0.85126700	-6.67422800	-2.98002100
H	-0.34960300	-8.18543000	-1.06234900
Cl	2.23928300	5.98748600	0.45547200
Cl	0.35410100	1.81977100	3.47384200
Cl	-3.04480300	5.47599600	-0.52974000
Cl	-3.88650000	1.16686500	-3.83177500
Cl	-4.92660000	-0.98109300	3.82863700
Cl	-4.39490000	-4.14934400	-0.65140700
Cl	-0.52932200	-3.90216400	-3.33441100
Cl	1.33812900	-4.62554500	1.77062400
Cl	5.95388400	-1.87451700	2.05107800
Cl	6.41164900	0.59692300	-2.82375500