

Supplementary Material

Study of the Electrochemical Behavior of N-Substituted-4-Piperidones Curcumin Analogs: A Combined Experimental and Theoretical Approach

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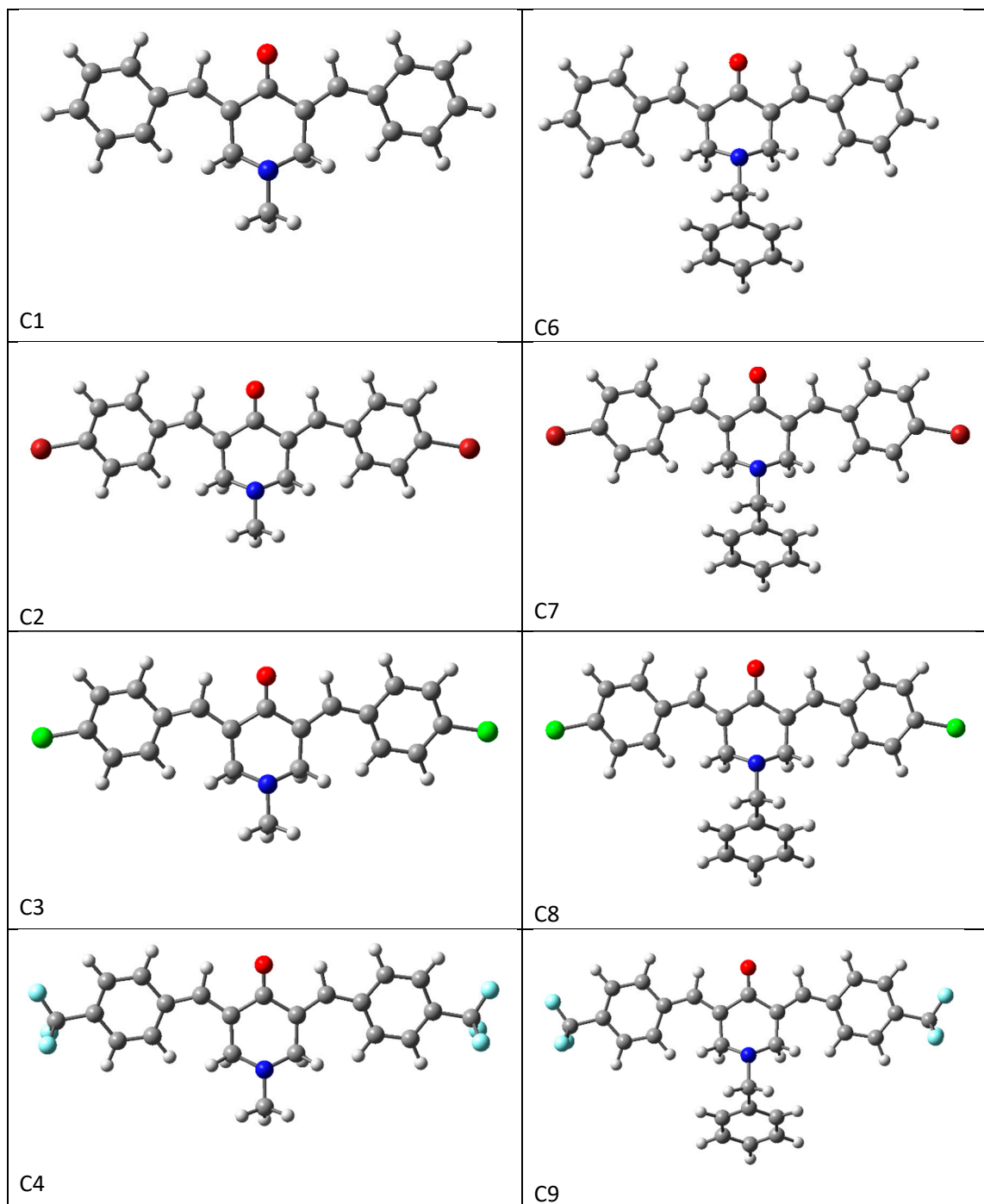
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Table S1. Optimized geometries for triplet dications of compounds 1 -10 at DFT M06/6-311+G(d,p) level



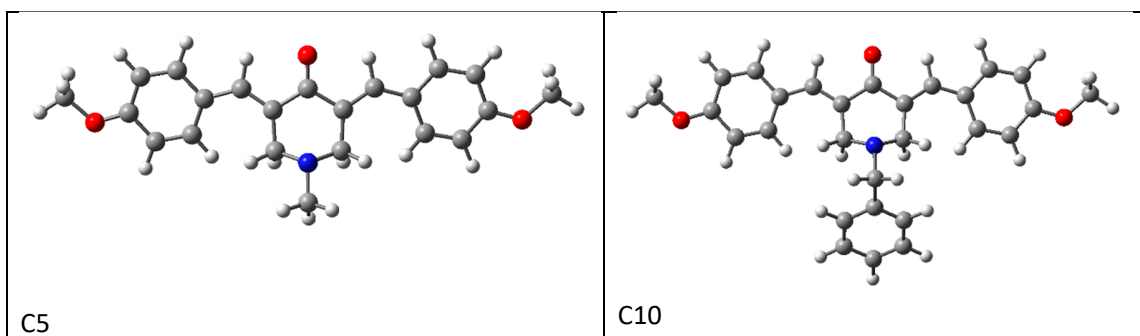
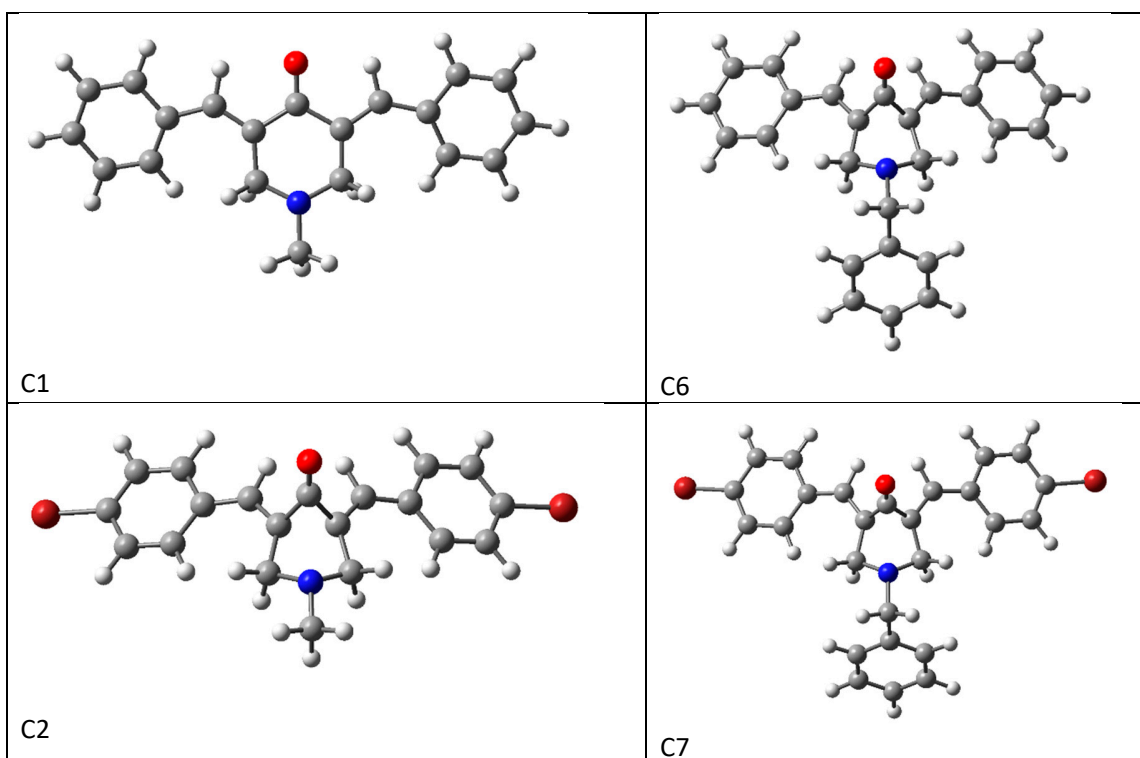
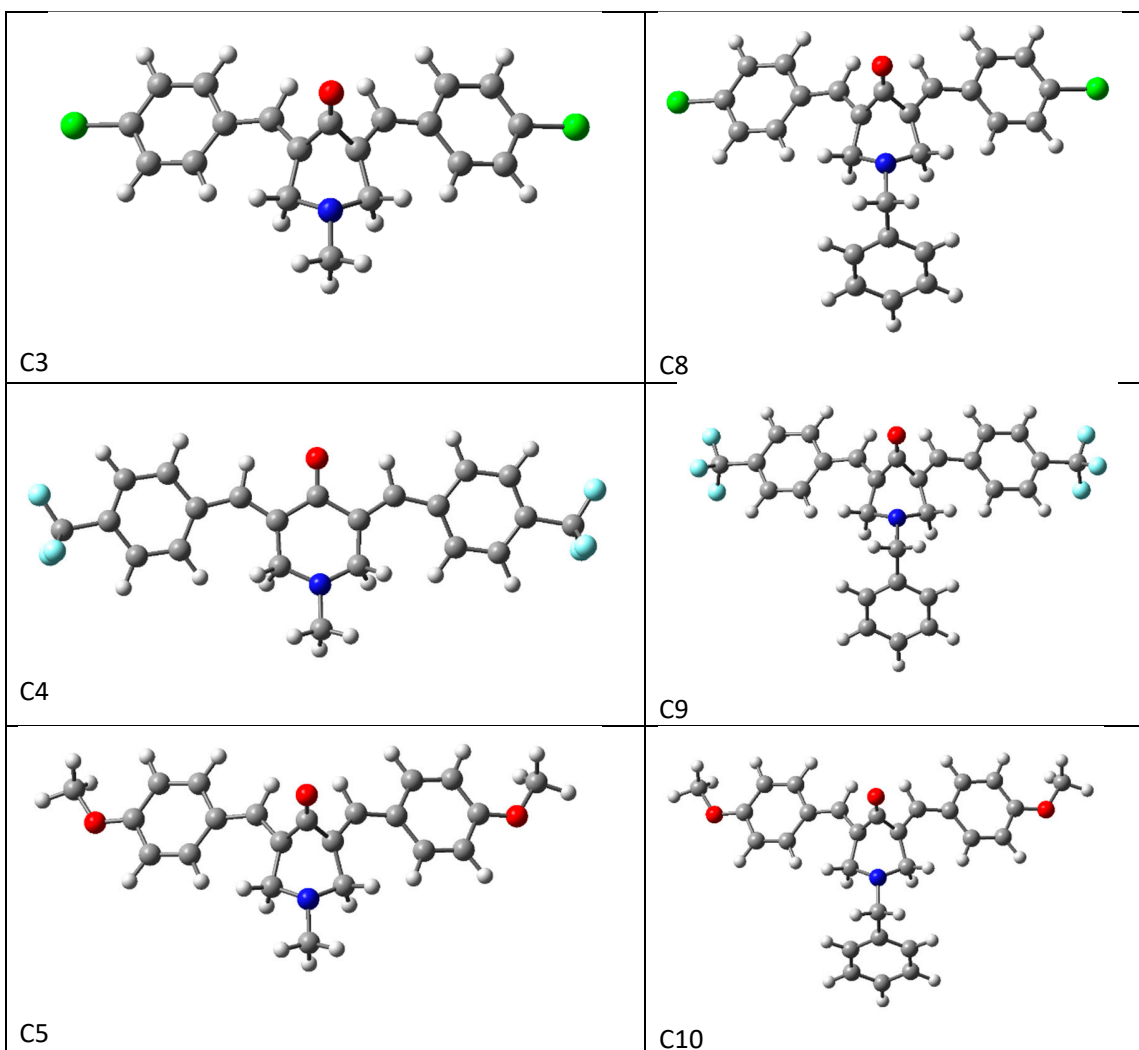


Table S2. Optimized geometries for singlet dications of compounds 1 -10 at DFT M06/6-311+G(d,p) level





- Optimized geometry cartesian coordinates of all compounds (neutral, singlet dication and triplet dication)

Neutral species at DFT M06/6-311+G(d,p) level

C1

O 1

C	1.18769500	1.18271000	0.07836400
C	0.00000100	-1.09136500	0.03158700
C	-1.18770100	1.18270600	0.07835900
H	1.19850000	1.63750400	-0.94091100
H	2.06889300	1.57420900	0.60169100
H	-1.19850200	1.63749700	-0.94091700
H	-2.06890400	1.57420300	0.60167900
O	0.00000400	-2.30782900	0.05792300
N	-0.00000600	1.60220900	0.79306900
C	-0.00000900	3.03078500	1.00231700
H	0.88636000	3.32610200	1.57159400
H	-0.00000800	3.59403600	0.04704800
H	-0.88638200	3.32609900	1.57159000
C	-1.27114800	-0.31104700	-0.00442400
C	1.27114700	-0.31104200	-0.00442200
C	-2.40968700	-1.02089400	-0.07490100
H	-2.27155500	-2.10227600	-0.04657400
C	2.40968800	-1.02088700	-0.07489900
H	2.27155700	-2.10226900	-0.04656600
C	-3.79152600	-0.56669700	-0.13737600
C	-4.78707100	-1.42537700	0.34694200
C	-4.18969600	0.66031600	-0.68208400
C	-6.12100500	-1.05712800	0.33078900
H	-4.49399800	-2.39215100	0.74831400

C	-5.52728700	1.02308200	-0.71067400
H	-3.45294200	1.32090600	-1.12578300
C	-6.49604300	0.17233100	-0.19627500
H	-6.87365000	-1.73447400	0.72243600
H	-5.81662700	1.97420600	-1.14735000
H	-7.54243700	0.46046400	-0.21824400
C	3.79152800	-0.56669200	-0.13737400
C	4.78706900	-1.42536900	0.34695400
C	4.18970300	0.66031400	-0.68209600
C	6.12100500	-1.05712400	0.33080100
H	4.49399300	-2.39213800	0.74833600
C	5.52729500	1.02307600	-0.71068700
H	3.45295300	1.32090000	-1.12580600
C	6.49604700	0.17232900	-0.19627600
H	6.87364700	-1.73446700	0.72245700
H	5.81663900	1.97419400	-1.14737300
H	7.54244200	0.46045900	-0.21824500

C2

O 1

C	0.95964500	0.20247300	1.18748300
C	-1.31177200	0.08139000	0.00000000
C	0.95964500	0.20247300	-1.18748300
H	1.45086900	-0.79967400	1.19857400
H	1.33187700	0.74069800	2.06801400
H	1.45086900	-0.79967400	-1.19857400
H	1.33187700	0.74069800	-2.06801400
O	-2.52805600	0.07049900	0.00000000
N	1.35240400	0.93194100	0.00000000

C	2.77199800	1.19740000	0.00000000
H	3.04437700	1.77819100	0.88613900
H	3.37287700	0.26551100	0.00000000
H	3.04437700	1.77819100	-0.88613900
C	-0.53028300	0.06817200	-1.27095900
C	-0.53028300	0.06817200	1.27095900
C	-1.23745800	-0.02810100	-2.40904500
H	-2.31936800	-0.03310100	-2.27271500
C	-1.23745800	-0.02810100	2.40904500
H	-2.31936800	-0.03310100	2.27271500
C	-0.77748000	-0.08202900	-3.78857400
C	-1.64153200	0.37788800	-4.79058500
C	0.46262100	-0.59896400	-4.18171000
C	-1.27426900	0.36852900	-6.12404100
H	-2.61927400	0.75896700	-4.50771200
C	0.83709000	-0.62904600	-5.51516500
H	1.13363500	-1.02430800	-3.44360400
C	-0.03015900	-0.13450400	-6.47755900
H	-1.94946500	0.74011900	-6.88726200
H	1.79497600	-1.04473000	-5.80905400
C	-0.77748000	-0.08202900	3.78857400
C	-1.64153200	0.37788800	4.79058500
C	0.46262100	-0.59896400	4.18171000
C	-1.27426900	0.36852900	6.12404100
H	-2.61927400	0.75896700	4.50771200
C	0.83709000	-0.62904600	5.51516500
H	1.13363500	-1.02430800	3.44360400
C	-0.03015900	-0.13450400	6.47755900
H	-1.94946500	0.74011900	6.88726200

H	1.79497600	-1.04473000	5.80905400
Br	0.48100100	-0.16844500	-8.30196000
Br	0.48100100	-0.16844500	8.30196000
C3			
O 1			
C	1.07314600	0.13969300	1.18789700
C	-1.19990700	0.05895300	0.00000000
C	1.07314600	0.13969300	-1.18789700
H	1.54449000	-0.87203900	1.20055200
H	1.45580000	0.67147600	2.06797800
H	1.54449000	-0.87203900	-1.20055200
H	1.45580000	0.67147600	-2.06797800
O	-2.41636300	0.06767000	0.00000000
N	1.48106400	0.86020100	0.00000000
C	2.90590500	1.09563400	0.00000000
H	3.19050900	1.67054000	0.88613400
H	3.48677000	0.15116300	0.00000000
H	3.19050900	1.67054000	-0.88613400
C	-0.41905500	0.03402700	-1.27097400
C	-0.41905500	0.03402700	1.27097400
C	-1.12894700	-0.04645400	-2.40875200
H	-2.21047900	-0.03258600	-2.27009100
C	-1.12894700	-0.04645400	2.40875200
H	-2.21047900	-0.03258600	2.27009100
C	-0.67473500	-0.10472400	-3.78968600
C	-1.53991100	0.36279600	-4.78749000
C	0.55938700	-0.63145800	-4.18953400
C	-1.17987800	0.35147000	-6.12232700

H	-2.51294700	0.75167600	-4.49944800
C	0.92738800	-0.66330000	-5.52428600
H	1.23042200	-1.06306700	-3.45533900
C	0.05828300	-0.16111600	-6.48011900
H	-1.85177000	0.72769500	-6.88609400
H	1.87960500	-1.08437300	-5.82872800
C	-0.67473500	-0.10472400	3.78968600
C	-1.53991100	0.36279600	4.78749000
C	0.55938700	-0.63145800	4.18953400
C	-1.17987800	0.35147000	6.12232700
H	-2.51294700	0.75167600	4.49944800
C	0.92738800	-0.66330000	5.52428600
H	1.23042200	-1.06306700	3.45533900
C	0.05828300	-0.16111600	6.48011900
H	-1.85177000	0.72769500	6.88609400
H	1.87960500	-1.08437300	5.82872800
Cl	0.52003800	-0.19268600	-8.16096300
Cl	0.52003800	-0.19268600	8.16096300

C4

O 1

C	1.18681400	-0.92930900	-0.24560000
C	0.00000400	1.34124400	-0.10445800
C	-1.18685800	-0.92928400	-0.24554100
H	1.19417100	-1.43303500	0.75003000
H	2.06770200	-1.29631000	-0.78635900
H	-1.19416200	-1.43298500	0.75010100
H	-2.06778200	-1.29628900	-0.78623900
O	0.00002100	2.55623800	-0.09070400

N	-0.00004400	-1.30813700	-0.98303600
C	-0.00006500	-2.72309600	-1.27537300
H	0.88591400	-2.98432900	-1.86124200
H	-0.00004900	-3.34103800	-0.35502000
H	-0.88607700	-2.98431200	-1.86120000
C	-1.27209800	0.55875300	-0.09118200
C	1.27208600	0.55872300	-0.09120200
C	-2.40797800	1.26500600	0.02480400
H	-2.27455400	2.34702000	0.04342100
C	2.40797800	1.26495700	0.02480000
H	2.27456200	2.34697300	0.04342500
C	-3.78634700	0.79737700	0.08198400
C	-4.79288300	1.65296100	-0.37820400
C	-4.16456900	-0.44698800	0.60378100
C	-6.12334400	1.27134500	-0.36388700
H	-4.51676800	2.63119800	-0.76182900
C	-5.49284400	-0.82699400	0.63398000
H	-3.41748500	-1.10847200	1.02750700
C	-6.47286000	0.02730100	0.14058700
H	-6.88984300	1.94154900	-0.73700300
H	-5.77556600	-1.78897600	1.05172500
C	3.78634900	0.79733100	0.08197600
C	4.79287900	1.65294100	-0.37817800
C	4.16458500	-0.44704600	0.60373800
C	6.12334500	1.27134000	-0.36387100
H	4.51675500	2.63118700	-0.76177400
C	5.49286400	-0.82703800	0.63392600
H	3.41751200	-1.10855100	1.02744600
C	6.47287200	0.02728000	0.14055600

H	6.88983600	1.94156400	-0.73696600
H	5.77559700	-1.78903000	1.05164100
C	7.89904400	-0.42362100	0.19185800
C	-7.89902400	-0.42363000	0.19186000
F	8.73985800	0.47007800	-0.32966700
F	8.07261500	-1.57225000	-0.47735300
F	8.29421600	-0.65481700	1.45210100
F	-8.73987000	0.47015100	-0.32947000
F	-8.07259700	-1.57213800	-0.47756200
F	-8.29414700	-0.65507100	1.45207200

C5

O 1

C	1.18818500	1.18642600	0.12630200
C	0.00000900	-1.08699500	0.09221500
C	-1.18825900	1.18638200	0.12628100
H	1.20527400	1.64257400	-0.89266100
H	2.06757600	1.57555200	0.65501200
H	-1.20534100	1.64252100	-0.89268600
H	-2.06768000	1.57547600	0.65496500
O	0.00003400	-2.30501800	0.13035800
N	-0.00005200	1.61150200	0.83668200
C	-0.00008100	3.04079500	1.03673600
H	0.88634900	3.33999600	1.60413500
H	-0.00008200	3.59862200	0.07809200
H	-0.88653300	3.33996300	1.60411800
C	-1.26865600	-0.30770400	0.04622600
C	1.26864400	-0.30765800	0.04623200
C	-2.40842300	-1.01735300	-0.03290100

H	-2.26616300	-2.09813200	0.00245700
C	2.40842900	-1.01728500	-0.03288100
H	2.26617900	-2.09806300	0.00254800
C	-3.78870000	-0.57485900	-0.12104300
C	-4.79162500	-1.45540200	0.29356100
C	-4.19802600	0.66899400	-0.63010900
C	-6.13458600	-1.11608800	0.25552100
H	-4.50449100	-2.43529700	0.66663600
C	-5.53037300	1.01577300	-0.68863300
H	-3.46329300	1.36150500	-1.02540800
C	-6.51075900	0.13156200	-0.23588200
H	-6.87456700	-1.82958700	0.59939800
H	-5.84816700	1.97047400	-1.09549700
C	3.78871300	-0.57480500	-0.12105400
C	4.79161300	-1.45529800	0.29371700
C	4.19808100	0.66895400	-0.63032300
C	6.13458000	-1.11601200	0.25567000
H	4.50445200	-2.43512800	0.66694200
C	5.53043600	1.01570000	-0.68885900
H	3.46338200	1.36140300	-1.02578500
C	6.51079200	0.13155100	-0.23592100
H	6.87453900	-1.82946800	0.59968900
H	5.84826000	1.97032400	-1.09587900
C	-8.81470700	-0.29722100	0.09378700
H	-8.72066300	-0.54374700	1.15910700
H	-9.75147100	0.23615000	-0.06748600
H	-8.82537500	-1.22644200	-0.49023900
C	8.81472000	-0.29721600	0.09390200
H	8.82539200	-1.22653600	-0.48996800

H	9.75149900	0.23611100	-0.06742800
H	8.72063400	-0.54356200	1.15925900
O	-7.78656100	0.56511600	-0.32898100
O	7.78660400	0.56506700	-0.32904800

- Singlet dication species at DFT M06/6-311+G(d,p) level

C1

2 1

C	1.24075200	1.34047000	0.13235100
C	0.00000200	-0.88826000	0.12104800
C	-1.24076000	1.34046500	0.13235600
H	1.57527900	1.70705500	-0.87067700
H	2.00430500	1.74326500	0.81741200
H	-1.57529800	1.70705300	-0.87066700
H	-2.00431100	1.74325100	0.81742500
O	0.00000500	-2.09246100	0.21879400
N	-0.00000500	1.97265400	0.41809700
C	-0.00000800	3.41961700	0.53349800
H	0.88646200	3.74715200	1.08034900
H	-0.00001300	3.90118200	-0.45537900
H	-0.88647800	3.74714700	1.08035400
C	-1.29193200	-0.13272300	0.07731800
C	1.29193100	-0.13271800	0.07731800
C	-2.42936500	-0.89808400	0.01129400
H	-2.21628000	-1.96597700	0.07440600
C	2.42936700	-0.89807700	0.01130100
H	2.21628300	-1.96596900	0.07443000
C	-3.81226700	-0.57612700	-0.09298000
C	-4.72158400	-1.64830300	0.14284500

C	-4.34319400	0.69509600	-0.41922500
C	-6.08137800	-1.44820000	0.10804000
H	-4.32121600	-2.63198700	0.37087700
C	-5.70065400	0.88668100	-0.46725500
H	-3.69454800	1.52490100	-0.67294700
C	-6.57637000	-0.18147400	-0.19410300
H	-6.76252100	-2.26809500	0.30479800
H	-6.10796800	1.85653200	-0.73072200
H	-7.64842600	-0.01600600	-0.23771100
C	3.81226900	-0.57612300	-0.09297900
C	4.72158500	-1.64829000	0.14288800
C	4.34319900	0.69508900	-0.41926900
C	6.08137900	-1.44818900	0.10808300
H	4.32121500	-2.63196600	0.37095300
C	5.70065900	0.88667100	-0.46730100
H	3.69455500	1.52488300	-0.67303200
C	6.57637300	-0.18147500	-0.19410400
H	6.76252100	-2.26807800	0.30487300
H	6.10797500	1.85651100	-0.73080500
H	7.64843000	-0.01600900	-0.23771400

C2

2 1

C	0.43045800	2.51849300	1.16066700
C	-1.65755000	1.82917500	0.00000000
C	0.43045800	2.51849300	-1.16066700
H	1.46746200	2.16175800	1.32386100
H	0.08717700	3.05722800	2.05074100
H	1.46746200	2.16175800	-1.32386100

H	0.08717700	3.05722800	-2.05074100
O	-2.79878100	2.07118600	0.00000000
N	0.30273900	3.36979700	0.00000000
C	1.17010100	4.53410000	0.00000000
H	0.96704100	5.14280600	0.88341400
H	2.23519400	4.24904100	0.00000000
H	0.96704100	5.14280600	-0.88341400
C	-0.47795200	1.35996800	-0.82478400
C	-0.47795200	1.35996800	0.82478400
C	-0.72177200	0.17278800	-1.58345100
H	-1.33360300	-0.57777200	-1.07940600
C	-0.72177200	0.17278800	1.58345100
H	-1.33360300	-0.57777200	1.07940600
C	-0.38693700	-0.15138200	-2.88695900
C	-0.88838400	-1.39265200	-3.39651600
C	0.41057400	0.65586700	-3.75768400
C	-0.62537400	-1.79711900	-4.67251100
H	-1.49897300	-2.01800300	-2.75107300
C	0.67758400	0.25123700	-5.03150800
H	0.81945100	1.59832200	-3.41684500
C	0.15970100	-0.97523400	-5.50066200
H	-1.01297200	-2.73498900	-5.05457900
H	1.28322600	0.86078700	-5.69293200
C	-0.38693700	-0.15138200	2.88695900
C	-0.88838400	-1.39265200	3.39651600
C	0.41057400	0.65586700	3.75768400
C	-0.62537400	-1.79711900	4.67251100
H	-1.49897300	-2.01800300	2.75107300
C	0.67758400	0.25123700	5.03150800

H	0.81945100	1.59832200	3.41684500
C	0.15970100	-0.97523400	5.50066200
H	-1.01297200	-2.73498900	5.05457900
H	1.28322600	0.86078700	5.69293200
Br	0.52097400	-1.50386600	-7.22930800
Br	0.52097400	-1.50386600	7.22930800

C3

2 1

C	2.24111900	-0.36006200	1.16007000
C	1.39234000	1.66773400	0.00000000
C	2.24111900	-0.36006200	-1.16007000
H	1.96893100	-1.42278400	1.31988100
H	2.75022800	0.02318900	2.05126400
H	1.96893100	-1.42278400	-1.31988100
H	2.75022800	0.02318900	-2.05126400
O	1.54638600	2.82365800	0.00000000
N	3.07984200	-0.16231600	0.00000000
C	4.31070100	-0.93243600	0.00000000
H	4.90111400	-0.68122100	0.88348500
H	4.11225200	-2.01705400	0.00000000
H	4.90111400	-0.68122100	-0.88348500
C	1.01440700	0.45460800	-0.82476500
C	1.01440700	0.45460800	0.82476500
C	-0.18555400	0.60710600	-1.58673200
H	-0.98262900	1.16090700	-1.08688100
C	-0.18555400	0.60710600	1.58673200
H	-0.98262900	1.16090700	1.08688100
C	-0.47719300	0.24696600	-2.89127800

C	-1.74874800	0.65413500	-3.41057800
C	0.39358500	-0.49122400	-3.75329600
C	-2.12322200	0.35860200	-4.68825500
H	-2.42225300	1.21861700	-2.77177600
C	0.02030600	-0.79186800	-5.02859600
H	1.35998700	-0.82890200	-3.40222000
C	-1.23796200	-0.36655700	-5.50519800
H	-3.08238400	0.67241600	-5.08458200
H	0.67279200	-1.35318600	-5.68801900
C	-0.47719300	0.24696600	2.89127800
C	-1.74874800	0.65413500	3.41057800
C	0.39358500	-0.49122400	3.75329600
C	-2.12322200	0.35860200	4.68825500
H	-2.42225300	1.21861700	2.77177600
C	0.02030600	-0.79186800	5.02859600
H	1.35998700	-0.82890200	3.40222000
C	-1.23796200	-0.36655700	5.50519800
H	-3.08238400	0.67241600	5.08458200
H	0.67279200	-1.35318600	5.68801900
Cl	-1.68685100	-0.74018600	-7.08928600
Cl	-1.68685100	-0.74018600	7.08928600

C4

2 1

C	-1.24232300	1.30062800	-0.18657300
C	0.00000000	-0.92770600	-0.16358500
C	1.24233400	1.30062200	-0.18655900
H	-1.60696700	1.67288200	0.80371300
H	-1.99015700	1.70026400	-0.89273900

H	1.60696700	1.67287500	0.80373200
H	1.99017900	1.70025600	-0.89271400
O	-0.00000200	-2.13312200	-0.24176900
N	0.00000800	1.94155500	-0.43722900
C	0.00000900	3.38979600	-0.54545700
H	-0.88707400	3.72089800	-1.08915900
H	-0.00003700	3.86296000	0.44734800
H	0.88713900	3.72090300	-1.08907800
C	1.29141500	-0.17137600	-0.13008900
C	-1.29141200	-0.17137100	-0.13009600
C	2.42915000	-0.93763300	-0.06862200
H	2.21300400	-2.00547200	-0.11901300
C	-2.42915100	-0.93762200	-0.06862600
H	-2.21300800	-2.00546200	-0.11900800
C	3.81522600	-0.61892300	0.02040200
C	4.71433400	-1.70265600	-0.18520600
C	4.35700900	0.65734000	0.30197300
C	6.07925000	-1.51677200	-0.15898800
H	4.30872700	-2.69083800	-0.38184600
C	5.71430400	0.83920000	0.34123700
H	3.72005700	1.50426400	0.52519200
C	6.57866500	-0.24799500	0.10222000
H	6.75613300	-2.34615200	-0.32921700
H	6.13831700	1.81218300	0.56997100
C	-3.81522600	-0.61891000	0.02039100
C	-4.71433200	-1.70265500	-0.18517300
C	-4.35701400	0.65736100	0.30191400
C	-6.07924900	-1.51677600	-0.15895100
H	-4.30872300	-2.69084200	-0.38178100

C	-5.71431000	0.83921700	0.34118000
H	-3.72006700	1.50429900	0.52509100
C	-6.57866800	-0.24799100	0.10221300
H	-6.75612900	-2.34616500	-0.32914500
H	-6.13832400	1.81220900	0.56987300
C	-8.06820300	0.02130400	0.14436400
C	8.06819900	0.02130700	0.14436100
F	-8.77228000	-1.08531500	0.00262200
F	-8.38369200	0.86354600	-0.83482100
F	-8.38423600	0.58979800	1.30218800
F	8.77228000	-1.08530800	0.00261000
F	8.38367200	0.86355200	-0.83482900
F	8.38424200	0.58980300	1.30218000

C5

2 1

C	1.15900800	2.33720100	-0.34634700
C	0.00000000	1.44106700	1.67340000
C	-1.15900600	2.33720100	-0.34634900
H	1.32292000	2.06633800	-1.40946800
H	2.05004100	2.84632200	0.03792900
H	-1.32291700	2.06633900	-1.40946900
H	-2.05004000	2.84632400	0.03792700
O	0.00000000	1.54783200	2.83896100
N	0.00000100	3.17811000	-0.15740800
C	0.00000200	4.39269100	-0.95055500
H	0.88326200	4.98855200	-0.71099200
H	0.00000300	4.17491300	-2.03200200
H	-0.88325800	4.98855300	-0.71099400

C	-0.82606900	1.10544300	0.46167600
C	0.82606900	1.10544200	0.46167700
C	-1.59122200	-0.10472600	0.57148400
H	-1.09638600	-0.91116500	1.11563200
C	1.59122100	-0.10472700	0.57148300
H	1.09638400	-0.91116800	1.11562900
C	-2.88263000	-0.38630000	0.18850700
C	-3.41188900	-1.66944200	0.55796800
C	-3.75157900	0.50292800	-0.53215000
C	-4.68488600	-2.04095700	0.26200800
H	-2.77050400	-2.35711400	1.10253900
C	-5.01876000	0.14050600	-0.83703600
H	-3.39902700	1.47717100	-0.84433600
C	-5.51871100	-1.13348200	-0.44056900
H	-5.05772800	-3.01253600	0.56263900
H	-5.69196800	0.79553700	-1.37925700
C	2.88262900	-0.38630100	0.18850600
C	3.41188700	-1.66944400	0.55796500
C	3.75157900	0.50292800	-0.53214800
C	4.68488500	-2.04095900	0.26200600
H	2.77050100	-2.35711800	1.10253400
C	5.01876000	0.14050700	-0.83703300
H	3.39902700	1.47717200	-0.84433100
C	5.51871100	-1.13348200	-0.44056800
H	5.05772700	-3.01253900	0.56263500
H	5.69196900	0.79553900	-1.37925200
C	-7.40102800	-2.60784400	-0.42427100
H	-7.42102800	-2.73090700	0.66103600
H	-8.41398600	-2.51481200	-0.80723200

H	-6.89398200	-3.44553500	-0.90887900
C	7.40102700	-2.60784500	-0.42427200
H	6.89398100	-3.44553400	-0.90888200
H	8.41398500	-2.51481300	-0.80723300
H	7.42102700	-2.73091100	0.66103500
O	-6.74865000	-1.37065500	-0.76808400
O	6.74865000	-1.37065500	-0.76808300

C6

2 1

C	1.13690700	0.77539400	0.82365500
C	0.07378500	-1.13061300	1.97824600
C	-1.18069000	0.65320700	0.83357900
H	1.24710500	1.21566300	-0.18478700
H	2.02717100	0.99593900	1.42341900
H	-1.34849100	1.07998100	-0.17286400
H	-2.08214200	0.77916200	1.44382400
O	0.10201700	-1.67529200	3.00645500
N	-0.04629400	1.23419500	1.52365300
C	-0.76552200	-0.79545400	0.74882200
C	0.87652000	-0.70796000	0.74845100
C	-1.46580200	-1.90319100	0.19440800
H	-0.91459800	-2.84551900	0.18257500
C	1.69342800	-1.74539900	0.21999300
H	1.25579500	-2.74544200	0.25543200
C	-2.77702800	-2.00753300	-0.25703500
C	-3.22068500	-3.31062200	-0.64014000
C	-3.69081000	-0.91695800	-0.36130900
C	-4.50103500	-3.51280100	-1.08696200

H	-2.53013900	-4.14605100	-0.56444300
C	-4.96601800	-1.13226900	-0.81112600
H	-3.38394900	0.08724200	-0.09840000
C	-5.37336800	-2.42521900	-1.16967900
H	-4.83660000	-4.50346100	-1.37143100
H	-5.66441000	-0.30729000	-0.89369400
C	3.00320200	-1.71445000	-0.24685900
C	3.60268600	-2.97342700	-0.55896700
C	3.76993200	-0.52638100	-0.43649500
C	4.89341800	-3.04202400	-1.01654200
H	3.02428100	-3.88235000	-0.41775500
C	5.05457600	-0.60854900	-0.90256000
H	3.34048400	0.44638100	-0.23303200
C	5.61860300	-1.86068000	-1.18710600
H	5.34868700	-3.99908000	-1.24398300
H	5.64054800	0.29073900	-1.05467400
C	-0.12334700	2.67799400	1.81414900
H	0.75786400	2.92520900	2.41593800
H	-1.00039200	2.82351400	2.45375000
C	-0.20177300	3.53370500	0.58238900
C	-1.43978000	3.86431300	0.03221100
C	0.95799300	3.99741600	-0.03737200
C	-1.51756500	4.63041600	-1.12185300
H	-2.35389700	3.55786000	0.53898000
C	0.88288400	4.76447500	-1.19143300
H	1.92828900	3.79576200	0.41450900
C	-0.35528600	5.07578000	-1.73773400
H	-2.48580800	4.90267100	-1.52933200
H	1.78986100	5.14136300	-1.65297700

H	-0.41514100	5.68841600	-2.63114400
H	-6.38875200	-2.58209300	-1.52242100
H	6.64081400	-1.91067100	-1.55107100

C7

2 1

C	1.16112300	1.49132800	1.07623800
C	-0.00003200	-0.19669700	2.46488700
C	-1.16111800	1.49135700	1.07618600
H	1.31255600	1.76676000	0.01522100
H	2.05508100	1.75294100	1.65463600
H	-1.31250700	1.76680800	0.01516700
H	-2.05509100	1.75298200	1.65455500
O	-0.00008700	-0.60577000	3.55703900
N	-0.00000200	2.11706200	1.67402500
C	-0.82183300	0.02681400	1.20667400
C	0.82180000	0.02679300	1.20673200
C	-1.58008800	-1.11000200	0.79577700
H	-1.07656000	-2.07081900	0.91856100
C	1.58005000	-1.11004000	0.79583200
H	1.07651000	-2.07085000	0.91862600
C	-2.89166500	-1.20975500	0.35975300
C	-3.41303300	-2.52841900	0.16857800
C	-3.75808300	-0.10256800	0.10380500
C	-4.70374300	-2.73329100	-0.22484700
H	-2.76772800	-3.38213800	0.35616400
C	-5.04623000	-0.30553900	-0.29567200
H	-3.39973600	0.91308200	0.21493800
C	-5.53103800	-1.62076600	-0.45518800

H	-5.09766100	-3.73454400	-0.35711800
H	-5.70620300	0.53189800	-0.49259100
C	2.89161500	-1.20980800	0.35979500
C	3.41296200	-2.52848100	0.16859900
C	3.75805200	-0.10262900	0.10385400
C	4.70366300	-2.73336800	-0.22484000
H	2.76764400	-3.38219000	0.35618000
C	5.04619000	-0.30561700	-0.29563500
H	3.39972500	0.91302500	0.21500800
C	5.53097600	-1.62085300	-0.45517400
H	5.09756400	-3.73462600	-0.35712800
H	5.70617800	0.53180900	-0.49254600
C	0.00001500	3.58905300	1.72792600
H	0.88022700	3.88266500	2.31040800
H	-0.88023900	3.88268600	2.31033300
C	0.00008100	4.24558000	0.37718300
C	-1.20043100	4.54636400	-0.26485300
C	1.20065800	4.54637700	-0.26472800
C	-1.20197400	5.11912300	-1.52897500
H	-2.14457400	4.37102000	0.24931700
C	1.20232900	5.11913500	-1.52884900
H	2.14474700	4.37104300	0.24954400
C	0.00020900	5.39792800	-2.16519100
H	-2.14168500	5.37009500	-2.01037000
H	2.14208800	5.37011700	-2.01014500
H	0.00025800	5.85797200	-3.14781900
Br	-7.28162600	-1.88173400	-0.97817900
Br	7.28155100	-1.88184200	-0.97818200

C8

2 1

C	1.16080800	1.12407800	1.03789800
C	-0.00003200	-0.65168800	2.32054800
C	-1.16082600	1.12410100	1.03788100
H	1.31346800	1.45924400	-0.00584200
H	2.05391100	1.35250500	1.63149600
H	-1.31346300	1.45926900	-0.00586200
H	-2.05393400	1.35254800	1.63146400
O	-0.00004400	-1.12550100	3.38594300
N	-0.00000800	1.71692100	1.66803600
C	-0.82324800	-0.34606700	1.08185100
C	0.82319900	-0.34608400	1.08186100
C	-1.57998900	-1.45224200	0.59133100
H	-1.08022800	-2.42074200	0.65523300
C	1.57992000	-1.45227400	0.59133800
H	1.08013700	-2.42076300	0.65523100
C	-2.88551400	-1.51748600	0.13172500
C	-3.40523800	-2.81661500	-0.16979200
C	-3.74529500	-0.39078700	-0.05463000
C	-4.68566100	-2.98664500	-0.60897700
H	-2.76554000	-3.68421100	-0.03419400
C	-5.02385300	-0.55731500	-0.49669700
H	-3.38936300	0.61195500	0.14417100
C	-5.50299800	-1.85506400	-0.77103400
H	-5.08306600	-3.97083800	-0.83029000
H	-5.68364900	0.29054700	-0.64267700
C	2.88544500	-1.51754500	0.13173500
C	3.40513500	-2.81668600	-0.16979200

C	3.74525800	-0.39086800	-0.05460700
C	4.68555400	-2.98674700	-0.60897600
H	2.76541300	-3.68426600	-0.03420400
C	5.02381200	-0.55742800	-0.49667300
H	3.38935400	0.61188100	0.14420200
C	5.50292200	-1.85518700	-0.77102100
H	5.08293200	-3.97094800	-0.83029900
H	5.68363200	0.29041700	-0.64264300
C	0.00001000	3.18565500	1.78822700
H	0.88034300	3.45318100	2.38281100
H	-0.88035200	3.45321300	2.38275400
C	0.00007200	3.89918300	0.46627200
C	-1.20044000	4.22299200	-0.16472500
C	1.20064900	4.22294700	-0.16462600
C	-1.20192700	4.83741100	-1.40924400
H	-2.14461700	4.03076500	0.34337000
C	1.20226500	4.83736500	-1.40914500
H	2.14477600	4.03067700	0.34354800
C	0.00020100	5.13627800	-2.03632100
H	-2.14156200	5.10502800	-1.88175100
H	2.14194900	5.10494400	-1.88157400
H	0.00025000	5.62810900	-3.00345800
Cl	-7.09329600	-2.04864400	-1.30976400
Cl	7.09321600	-2.04880500	-1.30975000

C9

2 1

C	1.16158400	1.46533800	0.98433900
C	-0.00017000	-0.16791000	2.39778800

C	-1.16160000	1.46547100	0.98418700
H	1.29427600	1.76664000	-0.07078500
H	2.05981000	1.71847100	1.55858200
H	-1.29412100	1.76678500	-0.07095700
H	-2.05986600	1.71870700	1.55832000
O	-0.00027200	-0.55436000	3.49350900
N	-0.00001500	2.06600400	1.61410100
C	-0.81801300	0.00243100	1.10616900
C	0.81781200	0.00233900	1.10628200
C	-1.57875000	-1.14380700	0.76113400
H	-1.07519100	-2.10138000	0.90894000
C	1.57846100	-1.14398100	0.76128300
H	1.07481500	-2.10150800	0.90909300
C	-2.90688900	-1.25777100	0.35000600
C	-3.42468000	-2.58007700	0.23230400
C	-3.75995000	-0.15890700	0.04165600
C	-4.72410800	-2.79718200	-0.15720600
H	-2.78208500	-3.42465300	0.46459000
C	-5.05075300	-0.38454700	-0.35114900
H	-3.39504100	0.85874400	0.09793100
C	-5.53110400	-1.69975300	-0.44686700
H	-5.12229100	-3.80206900	-0.24120800
H	-5.70887700	0.44399000	-0.59362400
C	2.90658800	-1.25805700	0.35016300
C	3.42427000	-2.58040800	0.23245400
C	3.75973300	-0.15926100	0.04179300
C	4.72366800	-2.79761900	-0.15709800
H	2.78161300	-3.42493100	0.46476000
C	5.05050100	-0.38500800	-0.35105900

H	3.39491200	0.85842100	0.09808300
C	5.53074000	-1.70025400	-0.44679700
H	5.12176900	-3.80253700	-0.24111100
H	5.70868500	0.44347600	-0.59355800
C	0.00005500	3.53679800	1.74245300
H	0.88119100	3.80060400	2.33688700
H	-0.88133700	3.80069400	2.33646500
C	0.00041800	4.24051900	0.41643900
C	-1.20123900	4.55965000	-0.21564500
C	1.20245200	4.55997000	-0.21477700
C	-1.20186500	5.16978400	-1.46195400
H	-2.14565500	4.37067700	0.29306200
C	1.20382800	5.17010400	-1.46108400
H	2.14654400	4.37125200	0.29462400
C	0.00117100	5.46638800	-2.08918300
H	-2.14106400	5.43605800	-1.93581600
H	2.14330100	5.43663300	-1.93426000
H	0.00145700	5.95433700	-3.05822900
C	-6.96897000	-1.88759200	-0.89829700
C	6.96857000	-1.88821300	-0.89829500
F	-7.31045000	-3.16181700	-0.92363400
F	-7.10885600	-1.37717000	-2.11559400
F	-7.77676000	-1.23815200	-0.07090100
F	7.30993900	-3.16246600	-0.92365100
F	7.77645200	-1.23884400	-0.07093500
F	7.10843900	-1.37779900	-2.11559600

C10

2 1

C	1.16072100	1.22032800	1.06946200
C	0.00011200	-0.55585400	2.37748800
C	-1.16068100	1.22022800	1.06949300
H	1.32539200	1.51449100	0.01468900
H	2.05106700	1.46889400	1.65986700
H	-1.32540900	1.51439100	0.01472700
H	-2.05103100	1.46871000	1.65992600
O	0.00014300	-1.03513800	3.44512600
N	0.00000000	1.84448800	1.66459400
C	-0.82486400	-0.24918300	1.15518800
C	0.82503600	-0.24911300	1.15517100
C	-1.58265800	-1.35659900	0.64862000
H	-1.08334800	-2.32481100	0.71761800
C	1.58291100	-1.35646600	0.64858400
H	1.08367800	-2.32471700	0.71758600
C	-2.87493900	-1.41615000	0.17715500
C	-3.39734500	-2.71369200	-0.14475800
C	-3.74938300	-0.29027900	0.00140400
C	-4.67152000	-2.89421500	-0.58223400
H	-2.75019000	-3.57783100	-0.02126400
C	-5.01865400	-0.45901600	-0.43628100
H	-3.39954900	0.71128400	0.21504900
C	-5.51240200	-1.76215400	-0.72998500
H	-5.03836000	-3.88789600	-0.80898600
H	-5.69766100	0.37533200	-0.57397600
C	2.87519200	-1.41592300	0.17710200
C	3.39768000	-2.71342800	-0.14482100

C	3.74956100	-0.28999400	0.00134900
C	4.67186400	-2.89386800	-0.58230400
H	2.75058200	-3.57761000	-0.02132400
C	5.01884200	-0.45864700	-0.43634400
H	3.39966700	0.71154500	0.21500300
C	5.51267300	-1.76175200	-0.73005500
H	5.03876700	-3.88752400	-0.80906100
H	5.69779500	0.37574500	-0.57403600
C	-0.00010200	3.31518200	1.70680700
H	0.87976700	3.61437300	2.28735200
H	-0.87997100	3.61417700	2.28745000
C	-0.00029400	3.97006900	0.35427300
C	-1.20017800	4.26920700	-0.28951800
C	1.19940100	4.26989100	-0.28956100
C	-1.20232100	4.83675500	-1.55608300
H	-2.14432400	4.09374700	0.22460900
C	1.20117600	4.83744500	-1.55612400
H	2.14366700	4.09500900	0.22454300
C	-0.00066200	5.11341000	-2.19392800
H	-2.14243700	5.08458900	-2.03851100
H	2.14113400	5.08583200	-2.03857900
H	-0.00080900	5.56904900	-3.17867400
O	-6.74500500	-1.80918700	-1.12702500
O	6.74527800	-1.80870400	-1.12709600
C	-7.39154900	-3.05423500	-1.44897500
H	-7.41179700	-3.70425000	-0.57100900
H	-8.40521700	-2.78661600	-1.73578000
H	-6.88188400	-3.53664200	-2.28642500
C	7.39190400	-3.05370800	-1.44905100

H	8.40555400	-2.78602100	-1.73585600
H	7.41219600	-3.70372400	-0.57108700
H	6.88227100	-3.53614700	-2.28650300

- Triplet dication species at DFT M06/6-311+G(d,p) level

C1

2 3

C	1.21703800	1.36489200	0.17203600
C	-0.00000800	-0.87357900	0.37211000
C	-1.21699500	1.36492100	0.17202700
H	1.36557800	1.67668400	-0.89269600
H	2.06069500	1.79998200	0.72298200
H	-1.36551700	1.67671800	-0.89270500
H	-2.06064300	1.80003200	0.72296800
O	-0.00002800	-2.06431600	0.60171400
N	0.00002700	1.92720200	0.67939900
C	0.00004500	3.37602000	0.78171600
H	0.88345400	3.70436300	1.33329900
H	0.00005400	3.86236700	-0.20697500
H	-0.88335900	3.70438500	1.33329400
C	-1.27464200	-0.11670700	0.20728300
C	1.27464800	-0.11673600	0.20729400
C	-2.41485400	-0.90150400	0.12345500
H	-2.20871700	-1.95819500	0.30176600
C	2.41484800	-0.90154700	0.12345700
H	2.20870600	-1.95824100	0.30174500
C	-3.76977400	-0.58433000	-0.11063700
C	-4.71167400	-1.63727200	0.12272900
C	-4.25876500	0.67382300	-0.56713600

C	-6.05689800	-1.42846600	-0.03425900
H	-4.34051500	-2.60456300	0.44896500
C	-5.60138800	0.86942300	-0.73665800
H	-3.57424200	1.47345400	-0.82066200
C	-6.50741300	-0.17492500	-0.46117700
H	-6.76649700	-2.22405300	0.16189400
H	-5.97735800	1.82123100	-1.09503800
H	-7.57165400	-0.00469500	-0.59701100
C	3.76976300	-0.58436300	-0.11063600
C	4.71167700	-1.63730200	0.12268900
C	4.25873300	0.67381300	-0.56709300
C	6.05689600	-1.42847400	-0.03430500
H	4.34053200	-2.60460900	0.44889500
C	5.60135200	0.86943500	-0.73662000
H	3.57419400	1.47344600	-0.82057500
C	6.50739100	-0.17491200	-0.46118600
H	6.76650700	-2.22405900	0.16181400
H	5.97730600	1.82126100	-1.09496700
H	7.57162900	-0.00466400	-0.59702300

C2

2 3

C	1.29222700	0.38223600	1.20089300
C	-0.95098400	0.57090800	0.00000000
C	1.29222700	0.38223600	-1.20089300
H	1.64282700	-0.67717000	1.27124500
H	1.72352500	0.90422500	2.06368700
H	1.64282700	-0.67717000	-1.27124500
H	1.72352500	0.90422500	-2.06368700

O	-2.14246100	0.79227300	0.00000000
N	1.77448900	1.01824100	0.00000000
C	3.22234600	1.15375000	0.00000000
H	3.53957700	1.71444800	0.88212100
H	3.73411100	0.17558400	0.00000000
H	3.53957700	1.71444800	-0.88212100
C	-0.19411100	0.40089300	-1.27967000
C	-0.19411100	0.40089300	1.27967000
C	-0.97661100	0.30560300	-2.40634200
H	-2.03836800	0.45825400	-2.20961700
C	-0.97661100	0.30560300	2.40634200
H	-2.03836800	0.45825400	2.20961700
C	-0.64072400	0.08568800	-3.76677800
C	-1.67717100	0.30915500	-4.72346400
C	0.62718500	-0.35881600	-4.23919500
C	-1.45760200	0.15556000	-6.06148200
H	-2.65396500	0.62603100	-4.37021500
C	0.85378700	-0.52991900	-5.57420500
H	1.41862100	-0.60160300	-3.54141300
C	-0.18396900	-0.26169800	-6.49889300
H	-2.24253400	0.34367000	-6.78560900
H	1.81437700	-0.87778700	-5.93857700
C	-0.64072400	0.08568800	3.76677800
C	-1.67717100	0.30915500	4.72346400
C	0.62718500	-0.35881600	4.23919500
C	-1.45760200	0.15556000	6.06148200
H	-2.65396500	0.62603100	4.37021500
C	0.85378700	-0.52991900	5.57420500
H	1.41862100	-0.60160300	3.54141300

C	-0.18396900	-0.26169800	6.49889300
H	-2.24253400	0.34367000	6.78560900
H	1.81437700	-0.87778700	5.93857700
Br	0.13188200	-0.48048500	-8.29631300
Br	0.13188200	-0.48048500	8.29631300

C3

2 3

C	1.33333300	0.29452800	1.20337900
C	-0.90496400	0.51288400	0.00000000
C	1.33333300	0.29452800	-1.20337900
H	1.66135900	-0.77176700	1.28708000
H	1.77176400	0.81419600	2.06418700
H	1.66135900	-0.77176700	-1.28708000
H	1.77176400	0.81419600	-2.06418700
O	-2.09388300	0.75200500	0.00000000
N	1.84001800	0.90209800	0.00000000
C	3.29080200	1.00478600	0.00000000
H	3.61963700	1.55873800	0.88202100
H	3.78107100	0.01624900	0.00000000
H	3.61963700	1.55873800	-0.88202100
C	-0.15134300	0.33352400	-1.27818400
C	-0.15134300	0.33352400	1.27818400
C	-0.93757400	0.24697000	-2.40928400
H	-1.99548500	0.42315300	-2.21050800
C	-0.93757400	0.24697000	2.40928400
H	-1.99548500	0.42315300	2.21050800
C	-0.61006400	0.00851300	-3.76378200
C	-1.64912800	0.23262400	-4.72125500

C	0.65271000	-0.45505800	-4.23736600
C	-1.43577600	0.06327300	-6.05743700
H	-2.62122500	0.56363400	-4.36789300
C	0.87167100	-0.64244000	-5.56973200
H	1.44473500	-0.69934800	-3.54088300
C	-0.16798600	-0.37200300	-6.49272900
H	-2.21667700	0.25046700	-6.78605500
H	1.82405500	-1.00532500	-5.94061000
C	-0.61006400	0.00851300	3.76378200
C	-1.64912800	0.23262400	4.72125500
C	0.65271000	-0.45505800	4.23736600
C	-1.43577600	0.06327300	6.05743700
H	-2.62122500	0.56363400	4.36789300
C	0.87167100	-0.64244000	5.56973200
H	1.44473500	-0.69934800	3.54088300
C	-0.16798600	-0.37200300	6.49272900
H	-2.21667700	0.25046700	6.78605500
H	1.82405500	-1.00532500	5.94061000
Cl	0.11554100	-0.59528500	-8.13935200
Cl	0.11554100	-0.59528500	8.13935200

C4

2 3

C	-1.23475200	1.31779200	-0.29707300
C	0.00000100	-0.92963600	-0.41329000
C	1.23475000	1.31779300	-0.29706100
H	-1.47854100	1.66234600	0.73793000
H	-2.03732600	1.72795600	-0.92603400
H	1.47852900	1.66234900	0.73794400

H	2.03732900	1.72796000	-0.92601100
O	0.00000000	-2.12973400	-0.57539900
N	0.00000000	1.91455300	-0.69932800
C	-0.00000100	3.35427800	-0.87068300
H	-0.88598700	3.65942100	-1.43127100
H	-0.00001500	3.87729000	0.09807700
H	0.88599700	3.65942500	-1.43124900
C	1.27353500	-0.16362300	-0.29510300
C	-1.27353500	-0.16362400	-0.29510900
C	2.41649000	-0.94124400	-0.21621300
H	2.20064300	-2.00312300	-0.34631100
C	-2.41648900	-0.94124500	-0.21622100
H	-2.20064100	-2.00312500	-0.34630700
C	3.78446800	-0.62589700	-0.03947100
C	4.70240800	-1.69710400	-0.26080100
C	4.30506200	0.64070200	0.34432400
C	6.05947100	-1.50588000	-0.15998900
H	4.31107700	-2.67327100	-0.53228100
C	5.65443700	0.82331900	0.46054800
H	3.64651400	1.46497000	0.58702800
C	6.53503700	-0.24668200	0.19809000
H	6.75241000	-2.31874000	-0.34507100
H	6.06281900	1.78128000	0.76763800
C	-3.78446700	-0.62589700	-0.03948300
C	-4.70240700	-1.69711100	-0.26078200
C	-4.30506200	0.64071400	0.34427200
C	-6.05947000	-1.50588800	-0.15996500
H	-4.31107600	-2.67328400	-0.53223900
C	-5.65443800	0.82333200	0.46049500

H	-3.64651800	1.46499600	0.58694000
C	-6.53503800	-0.24668100	0.19807900
H	-6.75240800	-2.31875400	-0.34502100
H	-6.06281800	1.78130400	0.76755100
C	-8.02129900	0.02796400	0.32196800
C	8.02129900	0.02796500	0.32196400
F	-8.73857900	-1.06539700	0.15374200
F	-8.36884600	0.92222500	-0.59688600
F	-8.27648500	0.53522000	1.52128700
F	8.73857600	-1.06540600	0.15378500
F	8.36884000	0.92218100	-0.59693800
F	8.27649600	0.53527900	1.52125500

C5

2 3

C	1.19699300	1.40858700	0.21592200
C	-0.00000200	-0.82577800	0.49737500
C	-1.19698000	1.40859700	0.21592700
H	1.25042800	1.72632300	-0.85391300
H	2.06271100	1.85978900	0.71574200
H	-1.25041800	1.72633600	-0.85390700
H	-2.06269000	1.85980500	0.71575300
O	-0.00000700	-2.01175200	0.75615400
N	0.00001000	1.89735000	0.85807000
C	0.00001600	3.34703800	0.96285500
H	0.88244600	3.67716300	1.51586200
H	0.00001600	3.83790000	-0.02668700
H	-0.88240800	3.67717000	1.51586600
C	-1.27773900	-0.07760900	0.29800900

C	1.27774100	-0.07761900	0.29800700
C	-2.40953600	-0.85941900	0.24089800
H	-2.21957700	-1.91334800	0.44631400
C	2.40953400	-0.85943300	0.24089400
H	2.21957200	-1.91336300	0.44630500
C	-3.76003700	-0.52228900	-0.00510600
C	-4.73498900	-1.54178200	0.24515900
C	-4.22342900	0.73266100	-0.50352300
C	-6.06781800	-1.32927500	0.07280600
H	-4.38889200	-2.50785100	0.60107500
C	-5.54794900	0.95811900	-0.69398100
H	-3.51783800	1.50932300	-0.76903500
C	-6.50196500	-0.06273200	-0.39836700
H	-6.78259000	-2.11505300	0.28686900
H	-5.92585500	1.89811800	-1.08182200
C	3.76003400	-0.52230200	-0.00510800
C	4.73498800	-1.54179500	0.24514500
C	4.22342200	0.73265600	-0.50350800
C	6.06781700	-1.32928200	0.07279300
H	4.38889400	-2.50787000	0.60104900
C	5.54794100	0.95812000	-0.69396400
H	3.51782700	1.50932100	-0.76900600
C	6.50196000	-0.06273200	-0.39836500
H	6.78259100	-2.11506200	0.28684500
H	5.92584500	1.89812500	-1.08179200
C	-8.82044900	-0.65957400	-0.37414100
H	-8.84989700	-0.93790900	0.68179700
H	-9.72311400	-0.11751600	-0.64351300
H	-8.70437500	-1.53850200	-1.01222000

C	8.82044600	-0.65956900	-0.37414900
H	8.70437400	-1.53848800	-1.01224100
H	9.72310900	-0.11750500	-0.64351200
H	8.84989400	-0.93791900	0.68178500
O	-7.73807300	0.26287600	-0.60855300
O	7.73806700	0.26288200	-0.60854700

C6

2 3

C	1.22467300	0.19179500	0.65222500
C	0.04216800	-2.00085300	0.09353300
C	-1.19636400	0.15492200	0.67408300
H	1.32573800	0.84741300	-0.25532700
H	2.08050800	0.44827100	1.28974300
H	-1.33789800	0.81600300	-0.22380500
H	-2.04870200	0.37601500	1.32972000
O	0.05745200	-3.19657000	-0.10600000
N	0.01460100	0.53031100	1.34533500
C	-1.23929900	-1.24854800	0.21202100
C	1.30448500	-1.21428600	0.20172800
C	-2.37750300	-1.97259400	-0.10663600
H	-2.16933500	-3.02773800	-0.29055500
C	2.45902200	-1.91240300	-0.11509100
H	2.27487200	-2.97296000	-0.29351100
C	-3.73550300	-1.59881000	-0.19980900
C	-4.67976700	-2.66826500	-0.28897000
C	-4.22247000	-0.26087100	-0.22798900
C	-6.02729700	-2.41802800	-0.33860600
H	-4.31070100	-3.68978900	-0.29450800

C	-5.56763900	-0.01995500	-0.29719200
H	-3.53423100	0.57625000	-0.23749900
C	-6.47638200	-1.09466300	-0.33953300
H	-6.73873800	-3.23454100	-0.38506500
H	-5.94249100	0.99685800	-0.33193400
C	3.80869500	-1.50989200	-0.20732300
C	4.77472300	-2.56073900	-0.28727000
C	4.26876800	-0.16255300	-0.23837800
C	6.11731200	-2.28425200	-0.32912900
H	4.42596700	-3.58935100	-0.29131500
C	5.60940500	0.10463800	-0.29891000
H	3.56357400	0.66029900	-0.25589800
C	6.53978400	-0.95221200	-0.33081400
H	6.84512900	-3.08657900	-0.36829600
H	5.96436200	1.12852700	-0.33424500
C	-0.00414400	1.91012300	1.84818700
H	0.89006300	2.04126400	2.46735000
H	-0.86922300	1.99922800	2.51483400
C	-0.05997900	2.96182000	0.76820000
C	-1.28966800	3.43578300	0.30299300
C	1.11521200	3.46858000	0.20707000
C	-1.34416700	4.36785700	-0.72284500
H	-2.20999000	3.10481300	0.78194800
C	1.06156400	4.40005600	-0.81954200
H	2.08010600	3.16491500	0.61066500
C	-0.16838100	4.84708100	-1.28806700
H	-2.30242700	4.74222400	-1.06753200
H	1.97882800	4.79920600	-1.23971300
H	-0.21006800	5.59129500	-2.07624800

H	7.60097700	-0.72488300	-0.37269500
H	-7.54162200	-0.88874600	-0.38907500
C7			
2 3			
C	1.21466100	0.39872300	0.69397200
C	0.02429600	-1.82839600	0.32297900
C	-1.18790000	0.38232900	0.71317900
H	1.27899000	0.99494400	-0.25106500
H	2.08023000	0.69423400	1.29979800
H	-1.27677300	0.98459700	-0.22599000
H	-2.04826200	0.66224300	1.33387800
O	0.03034600	-3.03666000	0.22884600
N	0.01676200	0.71387200	1.43311800
C	-1.25598500	-1.05819300	0.36307300
C	1.29718900	-1.04431200	0.35361700
C	-2.38520100	-1.79412500	0.08619800
H	-2.18888200	-2.86066000	-0.02797000
C	2.43199600	-1.77253900	0.08017700
H	2.24358200	-2.84128600	-0.02650700
C	-3.74520700	-1.41450200	-0.03747800
C	-4.70037600	-2.47411300	-0.06604600
C	-4.22038000	-0.07764300	-0.15991200
C	-6.04021900	-2.22557100	-0.15226300
H	-4.34554400	-3.49822500	0.00177300
C	-5.55748800	0.18013500	-0.26495100
H	-3.52406000	0.75150700	-0.21067300
C	-6.47959900	-0.89182100	-0.24895200
H	-6.76284500	-3.03384900	-0.15313200

H	-5.92468200	1.19514000	-0.37155200
C	3.78970200	-1.38502100	-0.04458300
C	4.75125100	-2.43919000	-0.06130100
C	4.25711400	-0.04638200	-0.17678500
C	6.08983600	-2.18337500	-0.14426000
H	4.40218900	-3.46478900	0.01353500
C	5.59300000	0.21873000	-0.27840300
H	3.55531800	0.77743600	-0.23752700
C	6.52157500	-0.84764600	-0.24953000
H	6.81732300	-2.98724900	-0.13568300
H	5.95459600	1.23503900	-0.39177800
C	0.00685900	2.09563000	1.94151500
H	0.90397500	2.21711700	2.55862000
H	-0.85321000	2.18202700	2.61517000
C	-0.05102800	3.15726900	0.87572200
C	-1.27991600	3.64607700	0.42315800
C	1.12088000	3.66627900	0.30888500
C	-1.33804300	4.59869200	-0.58200100
H	-2.19862600	3.30497000	0.89830300
C	1.06651500	4.61864600	-0.69699500
H	2.08667700	3.34263200	0.69414800
C	-0.16398300	5.08236000	-1.14804900
H	-2.29671500	4.98496000	-0.91242000
H	1.98294000	5.01994300	-1.11718400
H	-0.20742000	5.83935400	-1.92393000
Br	-8.28170700	-0.53529300	-0.37972400
Br	8.32181600	-0.48116800	-0.37451000

C8

2 3

C	1.20342100	0.29318200	0.67041400
C	0.00009200	-1.91117100	0.22046300
C	-1.20333000	0.29312000	0.67045900
H	1.29112200	0.91427000	-0.25849300
H	2.06481100	0.56367600	1.29400600
H	-1.29110200	0.91422300	-0.25843100
H	-2.06471300	0.56355500	1.29408800
O	0.00011700	-3.11635700	0.08731100
N	0.00005000	0.62164700	1.39029900
C	-1.27489000	-1.13637700	0.28397100
C	1.27504300	-1.13632100	0.28395700
C	-2.41244800	-1.86124400	-0.00887200
H	-2.21958000	-2.92599800	-0.14509300
C	2.41263000	-1.86115100	-0.00886000
H	2.21980200	-2.92591400	-0.14506900
C	-3.76716300	-1.47387600	-0.12353400
C	-4.72916600	-2.52893200	-0.17688100
C	-4.23742200	-0.13116700	-0.21038800
C	-6.06786100	-2.27185300	-0.24710400
H	-4.37907500	-3.55622500	-0.13899400
C	-5.57255800	0.13496900	-0.29893200
H	-3.53791900	0.69587100	-0.24630400
C	-6.49879200	-0.93382300	-0.30271800
H	-6.79950200	-3.07188400	-0.26611900
H	-5.94254800	1.15123500	-0.37764200
C	3.76733600	-1.47374000	-0.12349100
C	4.72937300	-2.52876700	-0.17680000

C	4.23755500	-0.13101600	-0.21033400
C	6.06806300	-2.27164600	-0.24697600
H	4.37931300	-3.55607000	-0.13891900
C	5.57268500	0.13516100	-0.29883100
H	3.53802500	0.69599900	-0.24627600
C	6.49895300	-0.93360200	-0.30258000
H	6.79973000	-3.07165400	-0.26596100
H	5.94264600	1.15143800	-0.37752900
C	0.00001500	2.00436800	1.89417500
H	0.87929300	2.11058500	2.53935100
H	-0.87915100	2.11047600	2.53952200
C	-0.00016400	3.06421900	0.82374700
C	-1.20247300	3.56335400	0.31404200
C	1.20196800	3.56343000	0.31369900
C	-1.20422700	4.51385300	-0.69505200
H	-2.14585000	3.23435800	0.74737400
C	1.20336900	4.51392800	-0.69539800
H	2.14549100	3.23449600	0.74675900
C	-0.00051700	4.98701200	-1.20492800
H	-2.14290300	4.90724600	-1.07115800
H	2.14191300	4.90737900	-1.07177400
H	-0.00065300	5.74392400	-1.98206300
Cl	-8.15041800	-0.59140400	-0.39602000
Cl	8.15057100	-0.59113200	-0.39582400

C9

2 3

C	1.20241800	0.30720300	0.77708700
C	-0.02225400	-1.85409100	0.17110100

C	-1.22889600	0.32393800	0.74987800
H	1.36175500	0.98136100	-0.11014300
H	2.04312900	0.52553900	1.44932000
H	-1.35180900	0.98537600	-0.15210500
H	-2.08087100	0.56793800	1.39799900
O	-0.02725500	-3.04556200	-0.04522500
N	-0.01765900	0.69815900	1.41654100
C	-1.29122400	-1.07915800	0.29088300
C	1.25189500	-1.09092700	0.30266500
C	-2.44047200	-1.78407600	-0.02505500
H	-2.24609200	-2.84098300	-0.21493700
C	2.39677600	-1.80195600	-0.01510700
H	2.19572300	-2.85574900	-0.21480700
C	-3.79724700	-1.39403300	-0.10611000
C	-4.75047800	-2.45232200	-0.18397800
C	-4.27119200	-0.05341300	-0.12846400
C	-6.10019600	-2.19319800	-0.21704800
H	-4.39415100	-3.47823500	-0.19479200
C	-5.61327700	0.20041300	-0.18133500
H	-3.57828000	0.77945300	-0.14714600
C	-6.53061700	-0.86909700	-0.21216800
H	-6.82342900	-2.99995400	-0.25627500
H	-5.98636400	1.21940400	-0.21237600
C	3.75635000	-1.41990600	-0.09302900
C	4.70289900	-2.48255600	-0.18508400
C	4.23832800	-0.08217100	-0.10313100
C	6.05404300	-2.23086500	-0.22274300
H	4.34075400	-3.50631200	-0.20424700
C	5.58166600	0.16446900	-0.16110600

H	3.55083100	0.75525000	-0.10885700
C	6.49247200	-0.90953300	-0.20819400
H	6.77198100	-3.04166200	-0.27344700
H	5.96004900	1.18172600	-0.18399300
C	-0.01118800	2.07923700	1.90893800
H	0.85070200	2.18254600	2.57764900
H	-0.91034100	2.21229900	2.52025600
C	0.04356300	3.11869400	0.81437600
C	-1.13265700	3.61645200	0.24922900
C	1.27454600	3.58485700	0.34357700
C	-1.07840500	4.53063000	-0.79364200
H	-2.09748800	3.32126800	0.65917700
C	1.32824000	4.49920700	-0.69894500
H	2.19477400	3.26590100	0.83075800
C	0.15197200	4.96939100	-1.27019200
H	-1.99571600	4.92273000	-1.22021900
H	2.28630400	4.86812500	-1.04980600
H	0.19291400	5.70181100	-2.06936200
C	-8.00558400	-0.52254600	-0.25008000
C	7.96893200	-0.57078400	-0.25480300
F	8.71894000	-1.65137600	-0.35232600
F	8.29907100	0.08686600	0.85145600
F	8.20649100	0.21706600	-1.29742800
F	-8.76153000	-1.59950100	-0.34089600
F	-8.32434300	0.13816900	0.85768300
F	-8.24587500	0.26504200	-1.29201800

C10

C	1.19909700	0.38949300	0.58599000
C	0.00009100	-1.83501400	0.23639600
C	-1.19901200	0.38942900	0.58604600
H	1.26955500	0.97948000	-0.35984100
H	2.06165500	0.68393500	1.19654000
H	-1.26954600	0.97942500	-0.35977300
H	-2.06156000	0.68381800	1.19663700
O	0.00011900	-3.04580600	0.14491000
N	0.00005100	0.69878400	1.32811000
C	-1.27569100	-1.06028800	0.26470500
C	1.27583900	-1.06022700	0.26466900
C	-2.41263100	-1.79497300	0.00809400
H	-2.22615500	-2.86521200	-0.08396400
C	2.41280500	-1.79487200	0.00806300
H	2.22636700	-2.86512000	-0.08397500
C	-3.76382200	-1.40294300	-0.11679000
C	-4.73599300	-2.45373300	-0.13381100
C	-4.23473200	-0.06079800	-0.24747300
C	-6.07245700	-2.20664600	-0.20717200
H	-4.38532200	-3.47941600	-0.06519900
C	-5.56348700	0.20181900	-0.33755400
H	-3.53328700	0.76267700	-0.31247800
C	-6.51354200	-0.86265000	-0.30220700
H	-6.78291800	-3.02435400	-0.19756200
H	-5.94827600	1.20995100	-0.44846900
C	3.76398400	-1.40280300	-0.11682400
C	4.73618600	-2.45356600	-0.13381400
C	4.23485900	-0.06064700	-0.24752800
C	6.07264300	-2.20644400	-0.20715800

H	4.38554100	-3.47925700	-0.06518800
C	5.56360900	0.20200500	-0.33759200
H	3.53339200	0.76280600	-0.31256000
C	6.51369200	-0.86243700	-0.30220900
H	6.78312600	-3.02413200	-0.19752300
H	5.94837100	1.21014600	-0.44852000
C	0.00002000	2.07145600	1.86436800
H	0.87926900	2.16095700	2.51222900
H	-0.87911300	2.16084900	2.51240300
C	-0.00015700	3.15170400	0.81736700
C	-1.20000300	3.65648500	0.31300300
C	1.19951500	3.65655300	0.31265700
C	-1.20253900	4.62563800	-0.67928400
H	-2.14401900	3.31463000	0.73550200
C	1.20170600	4.62570600	-0.67963300
H	2.14367300	3.31475000	0.73488000
C	-0.00050300	5.10702700	-1.18197600
H	-2.14203500	5.02380100	-1.04881200
H	2.14107300	5.02392000	-1.04943400
H	-0.00063600	5.87407800	-1.94918900
O	-7.75533000	-0.49492200	-0.37726000
O	7.75547200	-0.49467600	-0.37724400
C	-8.83324500	-1.44988200	-0.36230300
H	-8.80927800	-2.02724800	0.56495600
H	-9.74325200	-0.85758100	-0.40983200
H	-8.76467800	-2.10294300	-1.23544200
C	8.83341200	-1.44960700	-0.36224700
H	9.74340400	-0.85728200	-0.40976900

H	8.80944200	-2.02695500	0.56502200
H	8.76488100	-2.10268600	-1.23537500