

Electronic Supplementary Information

A Theoretical Study on Photomagnetic Fluorescent Protein Chromophore Coupled Diradicals and Their Possible Applications

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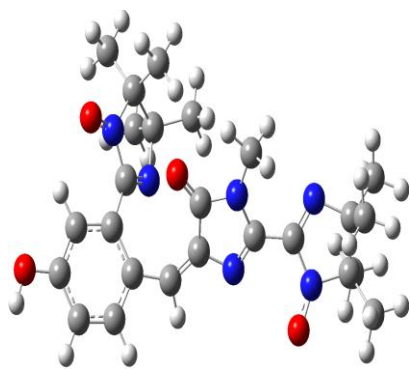
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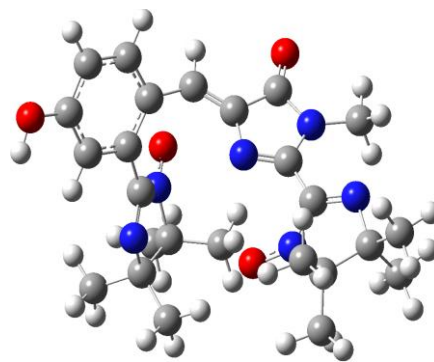
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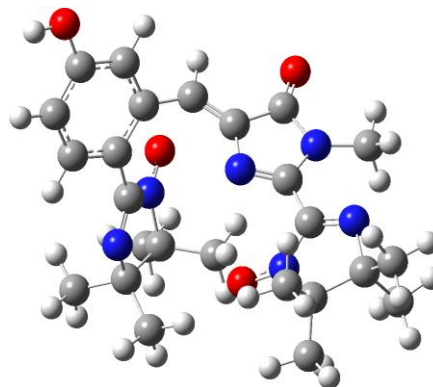
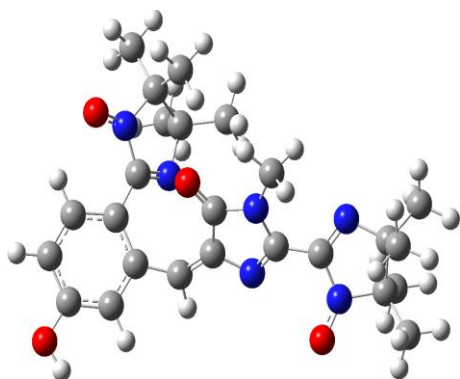
Figures



1(a)



1(b)



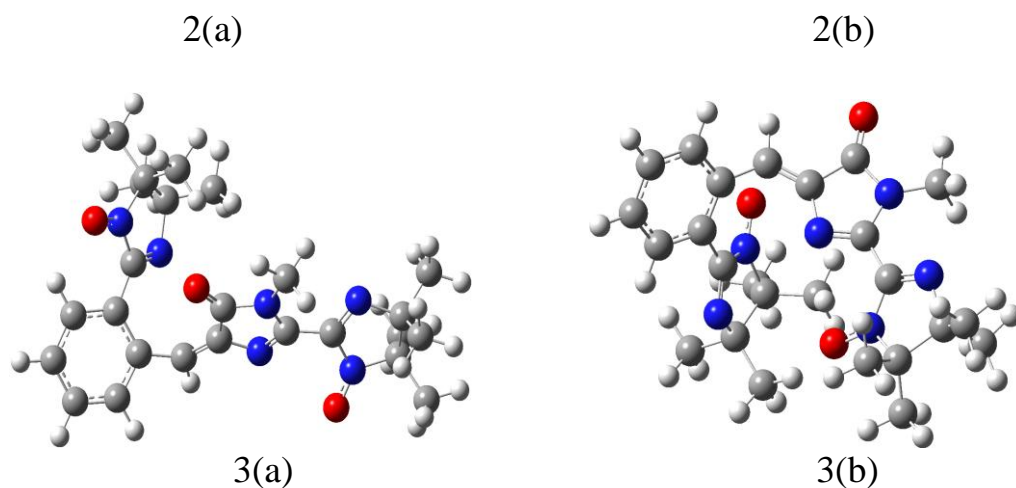
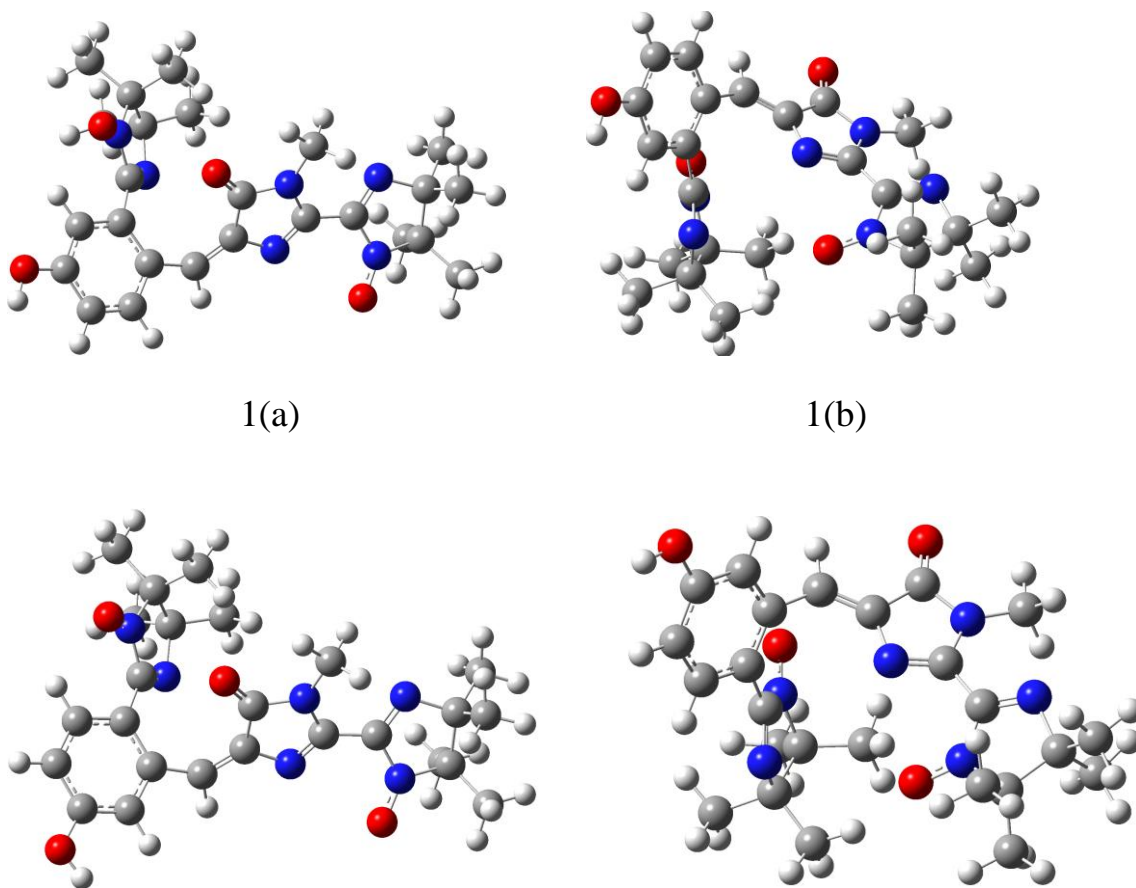


Fig. 1A The gas phase optimized geometries of three trans (1a, 2a, 3a) diradicals and their corresponding cis forms (1b, 2b, 3b) with different GFP variants (*p*-HBDI, *m*-HBDI and BFPF respectively) as coupler. The geometries are optimized using UB3LYP method at 6-31G (d,p) level. The carbon atoms are represented in grey, nitrogen in blue, oxygen in red and hydrogen in white respectively.



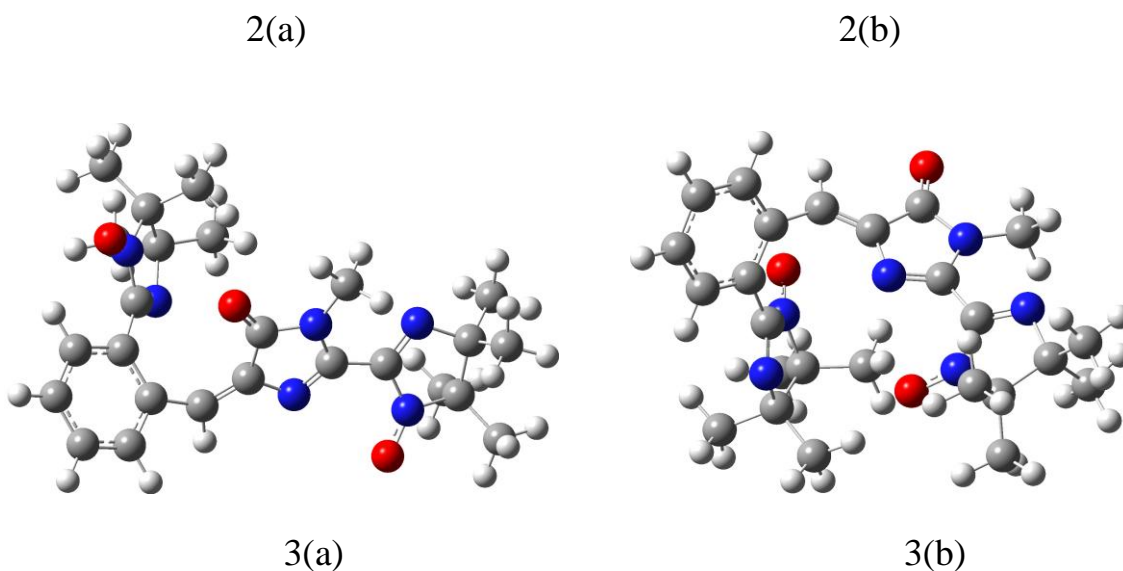
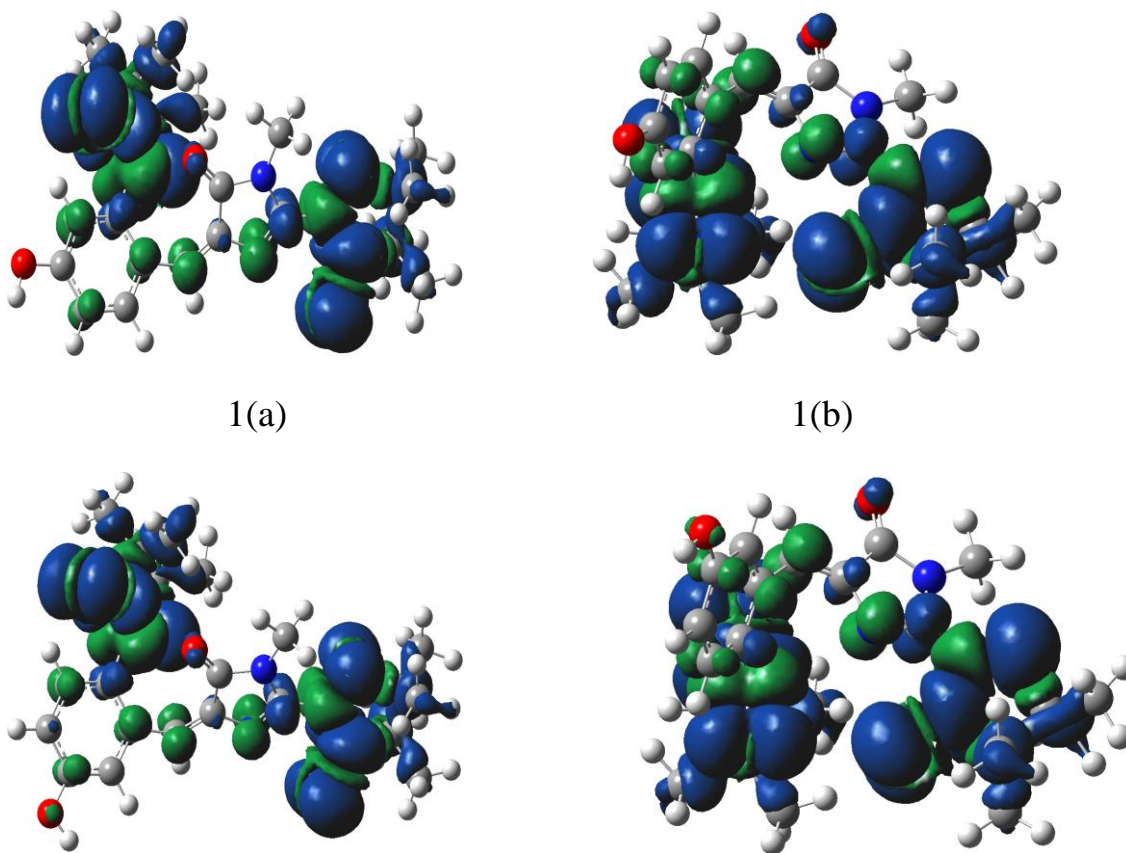


Fig. 2A The PCM optimized geometries of three trans (1a, 2a, 3a) diradicals and their corresponding cis forms (1b, 2b, 3b) with different GFP variants (*p*-HBDI, *m*-HBDI and BFPF respectively) as coupler. The geometries are optimized using PCM method with $\epsilon=58$, at UB3LYP/6-31G (d,p) level of theory. The carbon atoms are represented in grey, nitrogen in blue, oxygen in red and hydrogen in white respectively.



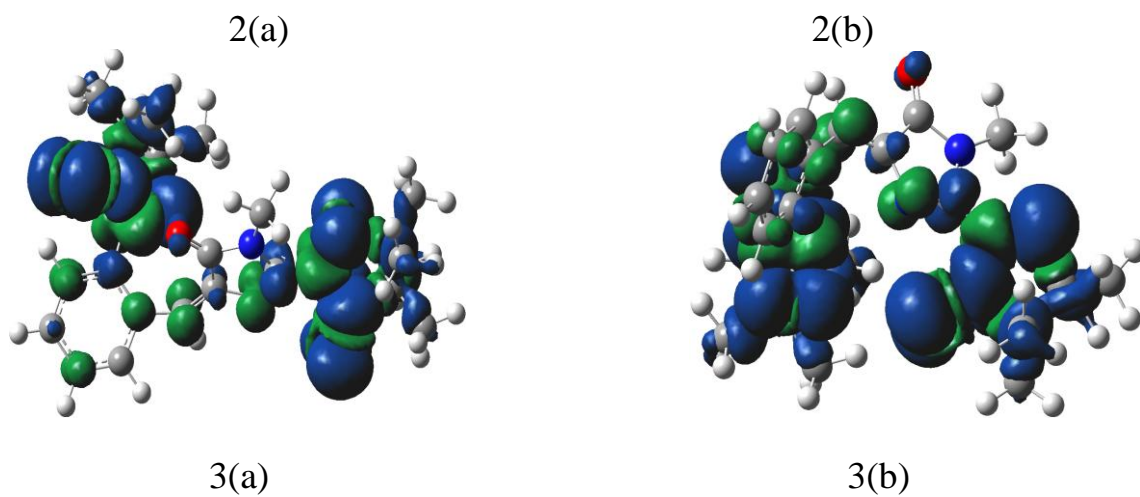
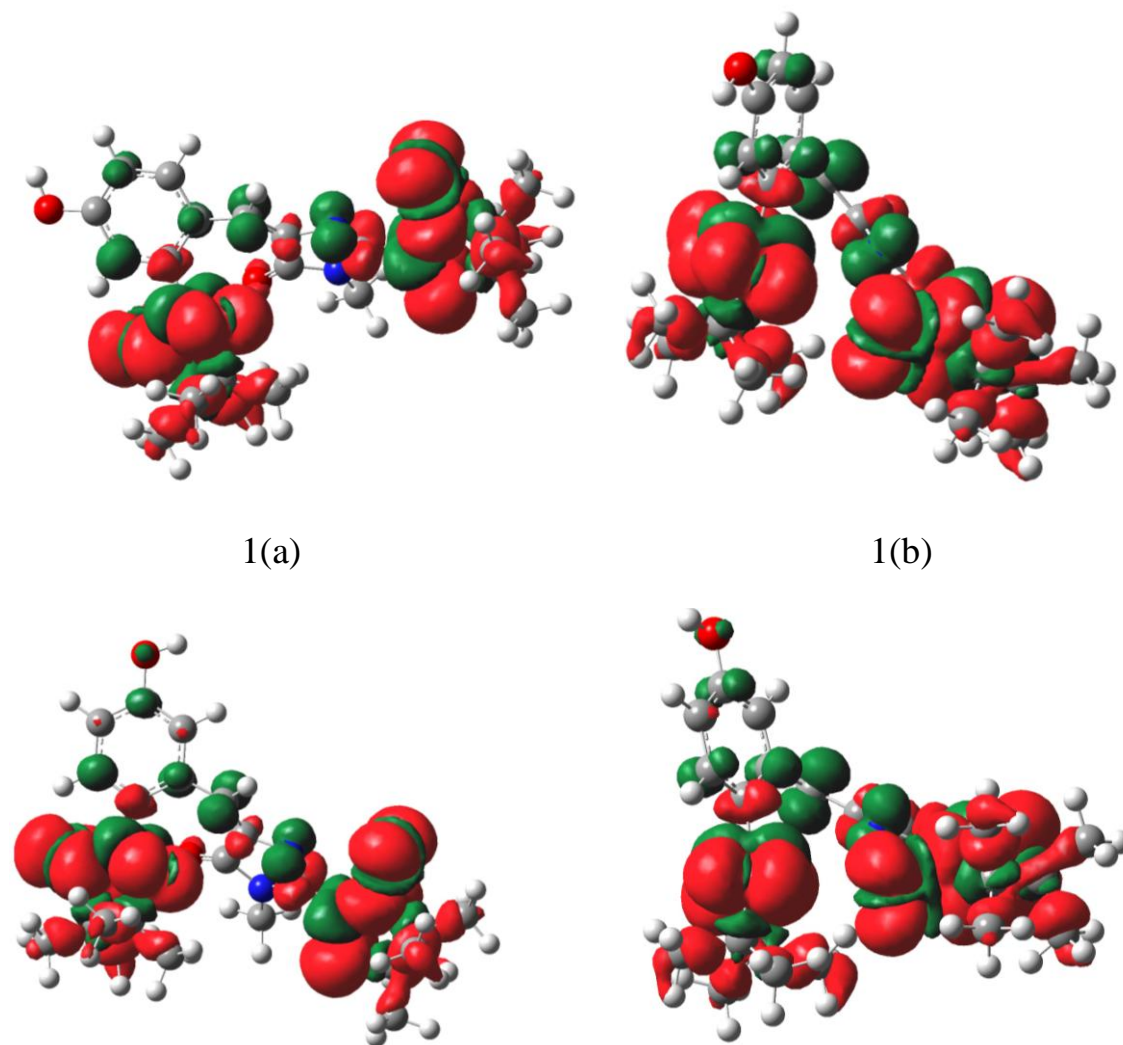


Fig. 1S Gas phase spin-density plots for the diradicals in their triplet optimized states. Different color schemes are used for two different spins.



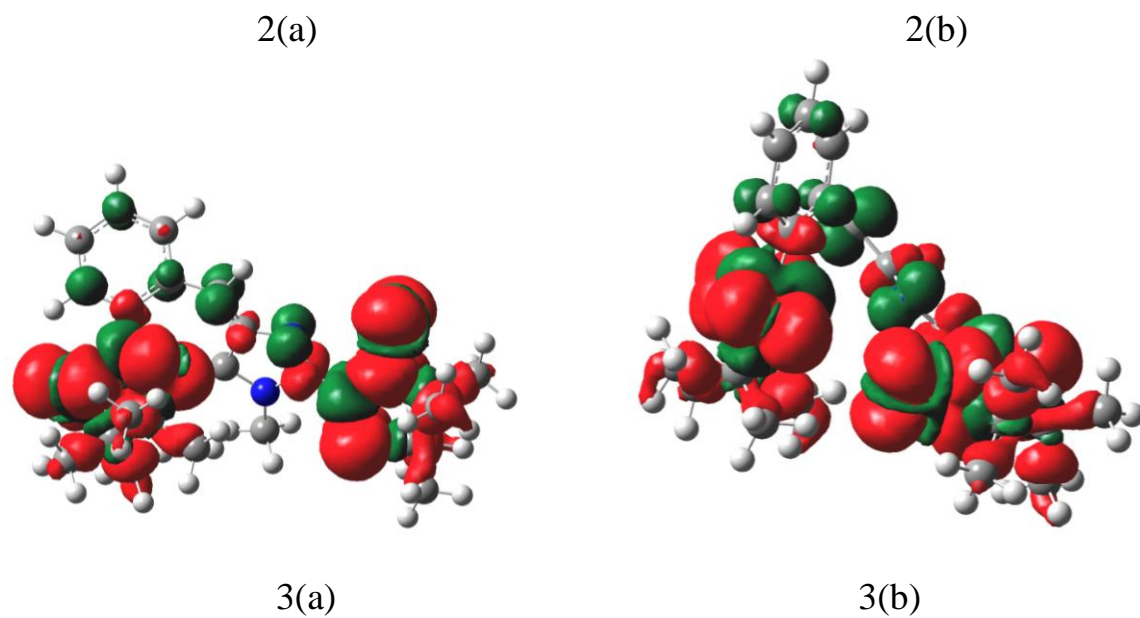


Fig. 2S The spin-density plots for the triplet diradicals optimized using PCM method with $\epsilon=58$. Red and green color schemes are used for the representation of α and β spin respectively.

GAS PHASE OPTIMIZED XYZ CO-ORDINATES

Diradical 1(a)

N	1.34434800	1.26139500	0.52686400
C	2.01644600	0.51277000	-0.29679700
N	1.23447300	-0.11358200	-1.27251900
C	-0.09375300	0.26607400	-1.04863300
C	0.00499100	1.16858000	0.12854300
O	-1.05054100	-0.08885800	-1.72666600
C	1.62683800	-0.95260200	-2.39398100
H	2.35410300	-0.43963000	-3.02821400
H	0.71560600	-1.14448000	-2.96330600
H	2.06803900	-1.88871600	-2.05015000
C	-4.09234400	3.83080600	0.13924400
C	-2.80416700	3.44847100	0.48878900
C	-2.37041700	2.10964200	0.44276700
C	-3.33691100	1.11632100	0.11139600
C	-4.63194700	1.50291000	-0.23769100
C	-5.00860800	2.84979400	-0.24516500
C	5.65069000	0.50288300	0.64616000
C	5.52253600	-0.61846600	-0.45183000
N	4.05831800	-0.76667100	-0.67327400
C	3.46138600	0.27797300	-0.19824600
N	4.31502800	1.17390800	0.46268900
C	-2.42976600	-2.27535800	1.28318800
N	-2.30291300	-0.79744500	1.23422900
C	-3.07534500	-0.32752900	0.31519700
N	-3.75541600	-1.32272200	-0.40883800
C	-3.23263200	-2.67463600	-0.01766300
O	4.03925200	2.30674700	0.95051100
C	-0.94940800	1.92631600	0.72810600
H	-0.54400900	2.60358600	1.47852700
H	-5.36830300	0.75772000	-0.50508900
H	-2.08920900	4.21416400	0.77558900
O	-4.57059100	-1.16665600	-1.36932700
H	-4.38062800	4.87895800	0.16696900
O	-6.29100200	3.13216700	-0.60419700
H	-6.42989300	4.08802400	-0.57068300
C	-1.02455800	-2.88691600	1.37669400
H	-0.40536700	-2.62382800	0.51755000
H	-0.53002400	-2.50657800	2.27436100
H	-1.07435700	-3.97872900	1.44775100
C	-3.18752300	-2.58284700	2.59134300
H	-3.30030200	-3.66062400	2.74416300
H	-2.62303800	-2.17022500	3.43134900
H	-4.17902000	-2.12272700	2.60073400
C	-4.41722200	-3.62789600	0.17076500
H	-4.97832500	-3.68619600	-0.76513700
H	-4.05993800	-4.63051100	0.42394800
H	-5.10217600	-3.29599000	0.95278600
C	-2.36752000	-3.16690900	-1.19180900
H	-1.57260600	-2.45819600	-1.42742300

H	-1.93445400	-4.14654000	-0.97097600
H	-3.00341300	-3.25849200	-2.07652900
C	5.66659700	-0.02996000	2.09099300
H	6.62010500	-0.51359000	2.31958000
H	5.52910400	0.81035000	2.77685700
H	4.86089900	-0.74729900	2.26749400
C	6.76521700	1.53146600	0.46189100
H	6.64889600	2.32453700	1.20418100
H	7.74148300	1.05964100	0.60700200
H	6.74467400	1.99352200	-0.52629500
C	6.11431500	-0.20183700	-1.81452900
H	7.20526200	-0.13070800	-1.76950700
H	5.84899500	-0.95465000	-2.56124800
H	5.71641000	0.75956900	-2.15108800
C	6.10722200	-1.97719500	-0.04970500
H	5.94232800	-2.69322400	-0.85930300
H	7.18557400	-1.90352400	0.12640500
H	5.63506700	-2.37812700	0.84890800

Diradical 1(b)

N	-0.33416600	-1.09810700	-0.10932400
C	-1.55393900	-1.20136300	-0.56041500
N	-1.71085900	-2.07900700	-1.63120100
C	-0.44456800	-2.61817700	-1.91214700
C	0.42649300	-1.96977900	-0.89188800
O	-0.19309300	-3.42777500	-2.78960500
C	-2.89254000	-2.41792500	-2.40822200
H	-2.55810000	-3.12245000	-3.17201000
H	-3.31407400	-1.53088200	-2.88934300
H	-3.65870700	-2.87095600	-1.77887100
C	3.70403000	-0.30311600	1.84692600
C	2.88681500	-0.53576300	0.73315100
C	2.67176700	-1.86300900	0.29139300
C	3.37845800	-2.89382900	0.94394500
C	4.18825800	-2.66029900	2.04448600
C	4.33212600	-1.35169700	2.51765500
H	3.24991100	-3.91284000	0.59052300
H	4.70863200	-3.46864800	2.54648400
O	5.12195900	-1.15613300	3.61111900
H	5.13094300	-0.21474200	3.83045000
C	-3.83758300	0.89646800	1.55483800
C	-4.80797700	-0.01633000	0.71400900
N	-3.91271500	-0.98780700	0.02752600
C	-2.70507000	-0.52756800	0.05620600
N	-2.56680800	0.66355700	0.78370900
C	1.80292600	2.11361000	-1.74687400
N	2.35810400	0.77367400	-1.35858800
C	2.41433300	0.68412300	0.04000300
N	2.17872300	1.80427200	0.63796100
C	2.01628600	2.87449500	-0.38051900
O	2.65951800	-0.12618500	-2.20081100
O	-1.53811700	1.38914400	0.90998500
C	1.73322500	-2.29398500	-0.74462100

H	2.07975500	-3.07593200	-1.41812100
H	3.84875400	0.72517200	2.16561000
C	0.85713400	3.79131800	0.02845400
H	0.71011100	4.58811200	-0.70928700
H	-0.07575300	3.24067200	0.15038500
H	1.09490900	4.25815800	0.98852100
C	-5.83924100	-0.78717400	1.54510200
H	-6.50601900	-0.09925600	2.07548600
H	-6.44684800	-1.40728700	0.88073500
H	-5.36673600	-1.44617300	2.27526200
C	-3.57177400	0.38522000	2.98321700
H	-2.72833400	0.93883200	3.40451700
H	-4.44511100	0.54159100	3.62197900
H	-3.31826100	-0.67795000	2.99268900
C	-4.14680900	2.39241400	1.58873400
H	-5.06167000	2.57421900	2.16016900
H	-3.32365100	2.91992200	2.07620500
H	-4.27050400	2.81451500	0.59018000
C	-5.53681100	0.75136500	-0.40827400
H	-6.06234700	0.03556000	-1.04537400
H	-6.27066100	1.45112300	0.00232900
H	-4.83677900	1.30941600	-1.03633700
C	3.33038600	3.68304000	-0.34298600
H	3.29280800	4.53592800	-1.02765200
H	3.48401800	4.06153300	0.67097400
H	4.19412800	3.06518000	-0.60462900
C	0.32657800	1.89176000	-2.12016100
H	-0.24591000	1.51131700	-1.27285400
H	-0.12667200	2.82577400	-2.46493400
H	0.27814900	1.16380800	-2.93569300
C	2.56799700	2.64127000	-2.96174700
H	2.18025200	3.62210600	-3.25243400
H	3.63884700	2.73221600	-2.77292500
H	2.43382900	1.95306000	-3.79970200

Diradical 2(a)

N	1.25599000	1.19735300	0.52515100
C	1.94432800	0.48291600	-0.31416000
N	1.18641500	-0.10954400	-1.32829900
C	-0.14830800	0.25696600	-1.11922700
C	-0.07593400	1.11851200	0.09563900
O	-1.09030100	-0.08407600	-1.82063700
C	1.60643400	-0.91256300	-2.46633000
H	2.32776500	-0.36879600	-3.08188000
H	0.70453700	-1.10899400	-3.04869900
H	2.06359500	-1.84690000	-2.13976600
C	-4.16694100	3.72828400	-0.02114800
C	-2.87506500	3.35846500	0.35174000
C	-2.46927100	2.01257700	0.37719200
C	-3.42423600	1.00666400	0.08249900
C	-4.72142500	1.40299200	-0.28548400
C	-5.09524600	2.73837700	-0.35082500
C	5.56350600	0.47511000	0.68638800
C	5.45368000	-0.64717800	-0.41343300

N	3.99317800	-0.79414800	-0.66176400
C	3.38937700	0.24946000	-0.19458600
N	4.22987600	1.14465600	0.48200100
C	-2.43355400	-2.36163500	1.25864400
N	-2.33583700	-0.88213900	1.20336500
C	-3.14677300	-0.42549600	0.30964300
N	-3.83039400	-1.43975300	-0.38958300
C	-3.25484500	-2.77658200	-0.02409000
O	3.94337600	2.27711300	0.96418600
C	-1.05025700	1.82400100	0.71654900
H	-0.68331400	2.44982800	1.52873200
H	-5.44724600	0.63834400	-0.52662800
H	-2.14720100	4.12939500	0.59658100
O	-4.67638400	-1.30509200	-1.32738900
H	-6.10099700	3.02633500	-0.63639200
O	-4.57445300	5.02769700	-0.07662800
H	-3.83793900	5.60487800	0.16523500
C	-1.01664300	-2.94908300	1.32405900
H	-0.41963800	-2.67681500	0.45203200
H	-0.51021400	-2.55919800	2.21101200
H	-1.04572000	-4.04157200	1.39729700
C	-3.15974800	-2.68163200	2.58171500
H	-3.24593900	-3.76100800	2.74076500
H	-2.58911400	-2.25326700	3.40964400
H	-4.16086200	-2.24336200	2.60764000
C	-4.39960000	-3.77275200	0.18248800
H	-4.98186100	-3.84137700	-0.73970500
H	-4.00108200	-4.76462100	0.41590300
H	-5.07548500	-3.47276200	0.98500000
C	-2.40037600	-3.22499300	-1.22398400
H	-1.93015400	-4.19247500	-1.02693300
H	-3.05235200	-3.32547200	-2.09593300
H	-1.63310400	-2.48832200	-1.46722800
C	5.55700200	-0.05664500	2.13165300
H	6.50703100	-0.53964800	2.37534400
H	5.40870400	0.78412600	2.81466700
H	4.74891300	-0.77408500	2.29631500
C	6.67987900	1.50439600	0.51837300
H	6.55223800	2.29773900	1.25851100
H	7.65404600	1.03315200	0.67844300
H	6.67413500	1.96580800	-0.47030000
C	6.02949700	-2.00618800	0.00000000
H	5.87870700	-2.72259900	-0.81195200
H	7.10450000	-1.93297600	0.19533100
H	5.54096000	-2.40600700	0.89027000
C	6.06944100	-0.23237700	-1.76604300
H	7.15948700	-0.16276000	-1.70198000
H	5.81645100	-0.98558500	-2.51659800
H	5.67912000	0.72929100	-2.11068600

Diradical 2(b)

N	0.27517300	-1.01950800	0.24906800
C	1.46627000	-1.08075400	0.77404300
N	1.53161600	-1.70617200	2.01719500

C	0.22568600	-2.10057800	2.35012900
C	-0.56757900	-1.65236500	1.16816200
O	-0.10689000	-2.67765700	3.37136100
C	2.66552900	-1.92113500	2.90177400
H	2.27125400	-2.44007300	3.77741700
H	3.10794400	-0.97003900	3.21218900
H	3.43254600	-2.52218000	2.41311800
C	-3.64091200	-0.38691300	-1.98570800
C	-2.89475900	-0.42458500	-0.79860900
C	-2.74170000	-1.66608800	-0.13475000
C	-3.40175100	-2.79474900	-0.63948900
C	-4.14413600	-2.73307600	-1.81931800
C	-4.24960000	-1.52058100	-2.50806600
H	-3.31097400	-3.75089600	-0.13466400
C	3.93367300	0.48249500	-1.58289000
C	4.81966800	-0.36133500	-0.58913300
N	3.84325600	-1.14294400	0.21956100
C	2.67618300	-0.60457000	0.08704900
N	2.63775000	0.46389600	-0.81908600
C	-1.79695600	2.54938700	1.26232200
N	-2.40936300	1.19392300	1.06999400
C	-2.41175500	0.87592000	-0.29773500
N	-2.09351600	1.87239200	-1.05577300
C	-1.92359800	3.08662100	-0.21655200
O	-2.78881400	0.45415200	2.03003500
O	1.67082600	1.23931400	-1.07284300
C	-1.88778200	-1.91018700	1.03888200
H	-2.32751300	-2.47903100	1.85534000
H	-3.74198500	0.56763500	-2.48982700
H	-4.82310200	-1.45913200	-3.43014700
O	-4.73651100	-3.88382700	-2.24789600
H	-5.21370300	-3.70831200	-3.06968500
C	-0.34683600	2.32177500	1.72588700
H	0.23277700	1.77930400	0.97685600
H	0.14478900	3.27749000	1.93018600
H	-0.36263700	1.73824700	2.65154000
C	-0.70809300	3.87785900	-0.71429200
H	-0.55265000	4.77748500	-0.10828000
H	0.20241300	3.27810400	-0.70331000
H	-0.88673600	4.19094600	-1.74684300
C	-3.19615200	3.93016500	-0.44074700
H	-3.14381400	4.88356000	0.09446600
H	-3.29718700	4.13953400	-1.50889200
H	-4.09582900	3.39857200	-0.11792600
C	-2.57115400	3.30497000	2.34359200
H	-2.14263100	4.30173900	2.48413900
H	-3.62972100	3.41203700	2.10104900
H	-2.49828600	2.75995100	3.28782100
C	3.64991600	-0.21921200	-2.92415900
H	2.85914200	0.32580900	-3.44663700
H	4.54225700	-0.22942200	-3.55573900
H	3.31321300	-1.24899400	-2.77973100
C	4.35920100	1.92802600	-1.83379500
H	5.30454000	1.95034100	-2.38381900
H	3.59731000	2.43029300	-2.43434000
H	4.48184200	2.49248600	-0.90809300
C	5.59602100	0.51259700	0.41738400

H	6.05570500	-0.13378600	1.16938200
H	6.38772200	1.08103900	-0.07976100
H	4.93568100	1.21416100	0.93466600
C	5.79346000	-1.32981000	-1.26941300
H	6.51821000	-0.78698300	-1.88513700
H	6.34296300	-1.88531800	-0.50479000
H	5.27609900	-2.05480600	-1.89991000

Diradical 3(a)

N	1.19803600	1.29192300	0.51716400
C	1.83526800	0.52609600	-0.31742000
N	1.03561100	-0.02274200	-1.32482100
C	-0.27073400	0.43201600	-1.11305300
C	-0.13713800	1.29808300	0.09180000
O	-1.23717900	0.14729400	-1.80766900
C	1.39680200	-0.85737000	-2.46036400
H	2.16713400	-0.37545700	-3.06748400
H	0.48672900	-0.97747800	-3.05077700
H	1.77143600	-1.82753200	-2.13246300
C	-4.05449500	4.17242000	-0.04012100
C	-2.79373600	3.72670300	0.34279300
C	-2.46235600	2.35866700	0.36345800
C	-3.47910400	1.41556000	0.05885100
C	-4.74661700	1.87974400	-0.32220800
C	-5.03191100	3.24207100	-0.38566900
C	5.44038800	0.25995200	0.69428600
C	5.26289200	-0.82983300	-0.42845100
N	3.79666800	-0.87683700	-0.68264200
C	3.26108400	0.19666900	-0.19946300
N	4.15695300	1.02239400	0.49468300
C	-2.73845800	-1.99759800	1.28731600
N	-2.54647600	-0.52745500	1.22304000
C	-3.29324900	-0.03332400	0.29489000
N	-4.01230200	-1.00779800	-0.42155700
C	-3.54008900	-2.37512700	-0.01994900
O	3.94561500	2.16286900	0.99620200
C	-1.05995600	2.08065300	0.70115700
H	-0.64765300	2.69698300	1.49861300
H	-5.51233700	1.15667600	-0.56892700
H	-2.02599400	4.44913700	0.60512400
O	-4.81430700	-0.82815800	-1.38929600
H	-4.26897600	5.23649400	-0.06458600
H	-6.02276600	3.56942400	-0.68523500
C	-2.67706200	-2.89788800	-1.18260000
H	-1.85658600	-2.21605700	-1.41065100
H	-2.27751900	-3.88998000	-0.95456900
H	-3.30441600	-2.97119100	-2.07504900
C	-1.36317500	-2.66919400	1.40751700
H	-0.86548500	-2.30190800	2.30884300
H	-1.46142700	-3.75713000	1.48771500
H	-0.72030200	-2.44168200	0.55543800
C	-3.52786400	-2.25685600	2.58724800
H	-3.68687300	-3.32707400	2.75168000
H	-2.95982600	-1.85670700	3.43088900
H	-4.49988100	-1.75672300	2.57576700

C	-4.75617200	-3.28949900	0.15750400
H	-5.30863600	-3.33298200	-0.78433800
H	-4.43380700	-4.30220700	0.41721700
H	-5.43871200	-2.93379900	0.93111000
C	5.38619800	-0.29938200	2.12809300
H	6.29969000	-0.85005400	2.36787700
H	5.28890100	0.53531000	2.82751500
H	4.53039700	-0.96402700	2.27172800
C	6.62551000	1.21399100	0.55532500
H	6.54859200	1.99605700	1.31414600
H	7.56420300	0.67301300	0.70719400
H	6.65661200	1.69845200	-0.42182800
C	5.90967900	-0.42687300	-1.77019600
H	7.00166300	-0.42842500	-1.70097300
H	5.61272400	-1.14624500	-2.53769000
H	5.58332000	0.56498500	-2.09516000
C	5.74949000	-2.23083100	-0.04161500
H	5.55759300	-2.91986500	-0.86846800
H	6.82603800	-2.22915800	0.15880800
H	5.23253600	-2.61640400	0.83880900

Diradical 3(b)

N	-0.22396500	-1.13064500	0.09903500
C	-1.39114600	-1.22072800	-0.47423200
N	-1.46561300	-2.14091800	-1.51771500
C	-0.19484000	-2.72469500	-1.64481600
C	0.58760700	-2.05473900	-0.56551800
O	0.12101800	-3.57698200	-2.45774900
C	-2.57345500	-2.47712700	-2.39780400
H	-2.18807500	-3.22147200	-3.09706300
H	-2.91458500	-1.59847100	-2.95254100
H	-3.41301400	-2.88205300	-1.83237700
C	3.62889700	-0.30639500	2.38973800
C	2.93408500	-0.58452600	1.20228300
C	2.69179800	-1.93193800	0.84538700
C	3.23638700	-2.94676100	1.65357700
C	3.92826700	-2.65546600	2.82442600
C	4.10891200	-1.32533300	3.20563300
H	3.07687700	-3.98188200	1.36526200
H	4.32237700	-3.46240800	3.43486600
C	-3.79544600	1.09817100	1.23933000
C	-4.71318700	0.12182100	0.40871600
N	-3.78594100	-0.92152200	-0.11003000
C	-2.57542900	-0.47896300	-0.01718800
N	-2.46889700	0.76994800	0.60938300
C	2.23920700	1.86815600	-1.59521600
N	2.70375100	0.55573500	-1.03470300
C	2.60015600	0.58740900	0.36440000
N	2.33888900	1.76144800	0.83417000
C	2.33111800	2.74111800	-0.28365300
O	3.05878500	-0.42659600	-1.75623000
O	-1.43691300	1.48783600	0.75098900
C	1.86562200	-2.39091500	-0.27958600
H	2.27281700	-3.19567700	-0.88842900
H	3.79315800	0.73405400	2.64682600

H	4.64268200	-1.08194100	4.11920800
C	-5.82287800	-0.55604500	1.22030200
H	-6.52155700	0.18508100	1.62231600
H	-6.38140800	-1.23428300	0.56983800
H	-5.42443100	-1.14332100	2.04931900
C	-5.33467500	0.78935100	-0.83518800
H	-5.82374200	0.02372800	-1.44273300
H	-6.08352300	1.53490900	-0.55158900
H	-4.57554900	1.27564800	-1.45405600
C	-4.07040900	2.59444600	1.09970700
H	-5.03478700	2.84203000	1.55276500
H	-3.28985700	3.15568600	1.61851200
H	-4.08075400	2.91993200	0.05825400
C	-3.66621100	0.72692200	2.72843000
H	-2.85027800	1.30758300	3.16697100
H	-4.58795000	0.95707700	3.26934900
H	-3.43845300	-0.33350700	2.86362300
C	1.16925900	3.72245900	-0.08887000
H	1.13229200	4.44914500	-0.90802300
H	0.20913200	3.21036000	-0.02156600
H	1.31938400	4.27069800	0.84539800
C	3.66289100	3.51200900	-0.16665900
H	3.73060100	4.30733500	-0.91552200
H	3.72142000	3.96669500	0.82562500
H	4.52566300	2.84989700	-0.28233800
C	0.80344600	1.64989100	-2.10589300
H	0.13091300	1.36047000	-1.29667200
H	0.42087500	2.56072100	-2.57586100
H	0.81690000	0.85418500	-2.85691500
C	3.14505100	2.26715500	-2.76100000
H	2.81718900	3.22260300	-3.18110100
H	4.19118400	2.35770500	-2.46427300
H	3.08364000	1.50542900	-3.54197600

ONIOM OPTIMIZED XYZ CO-ORDINATES

Diradical 1(a)

N	1.26816900	0.15079300	0.69658900	H
C	0.47961300	-0.64751000	1.35178600	H
N	-0.19264200	-1.57431800	0.55389300	H
C	0.19804500	-1.34548600	-0.77034700	H
C	1.14730500	-0.20707200	-0.65165700	H
O	-0.18372000	-1.99254400	-1.73729200	H
C	-1.06711900	-2.66829000	0.94210500	H
H	-0.51633200	-3.43225400	1.49883200	H
H	-1.44408700	-3.10749500	0.01784200	H
H	-1.88413400	-2.30192400	1.56088700	H
C	3.70075800	0.06403600	-4.83338600	H
C	3.35952900	0.30361300	-3.51004700	H
C	2.03580000	0.22231600	-3.03637500	H
C	1.01214400	-0.03118000	-3.99474900	H

C	1.35721400	-0.26363500	-5.32695900	H
C	2.68961800	-0.23597800	-5.74823700	H
C	0.47495600	0.40684400	4.93932900	H
C	-0.79678500	-0.51513000	4.81098800	H
N	-0.90390900	-0.81520700	3.35681600	H
C	0.21749000	-0.51370300	2.78924100	H
N	1.16676400	0.04434500	3.65537400	H
C	-2.38316200	0.95186200	-2.88198200	H
N	-0.90055900	0.96122200	-2.82514900	H
C	-0.42647800	0.11764600	-3.67605400	H
N	-1.41722900	-0.58937700	-4.37725100	H
C	-2.76787000	-0.26951100	-3.80925100	H
O	2.37690900	0.31823000	3.41726200	H
C	1.90078500	0.41365600	-1.59542900	H
H	2.60845500	1.12083600	-1.16627600	H
H	0.58924800	-0.47129600	-6.05816500	H
H	4.14839000	0.53321100	-2.80089100	H
O	-1.25567400	-1.48077100	-5.26548100	H
H	4.73921500	0.11876800	-5.15088900	H
O	2.92731400	-0.47729000	-7.06624300	H
H	3.87779400	-0.42901700	-7.23428300	H
C	-2.91735100	0.84992600	-1.44725100	H
H	-2.57577100	-0.05809500	-0.95016500	H
H	-2.55026600	1.70311800	-0.87293400	H
H	-4.01174500	0.86846700	-1.43009700	H
C	-2.79554000	2.32180200	-3.45530100	H
H	-3.88415200	2.42603800	-3.49644100	H
H	-2.39699300	3.10704000	-2.80903200	H
H	-2.39293400	2.48203800	-4.45750100	H
C	-3.72337200	0.02401000	-4.96936900	H
H	-3.77566700	-0.85751600	-5.61148100	H
H	-4.72747400	0.24134300	-4.59405100	H
H	-3.39101300	0.86397100	-5.58065800	H
C	-3.24301300	-1.53140100	-3.07025300	H
H	-2.53607800	-1.83201300	-2.29630500	H
H	-4.23036200	-1.37329600	-2.62804800	H
H	-3.31107600	-2.34817000	-3.79283900	H
C	0.17246200	1.91280600	4.84088900	H
H	-0.32679700	2.27418100	5.74287500	H
H	1.11536500	2.45173500	4.72227500	H
H	-0.45773400	2.14051000	3.97799700	H
C	1.41377800	0.13717100	6.11290000	H
H	2.31160400	0.74842100	6.00185800	H
H	0.92858400	0.40152200	7.05602500	H
H	1.72496500	-0.90701800	6.16156600	H
C	-0.63260800	-1.86952800	5.52569700	H
H	-0.58225900	-1.73907900	6.61046000	H
H	-1.49110900	-2.50388700	5.29460900	H
H	0.26885500	-2.39169900	5.19707000	H
C	-2.10552500	0.13559200	5.27068600	H
H	-2.93020500	-0.55688300	5.08821900	H
H	-2.07826700	0.35846800	6.34134200	H
H	-2.32112100	1.05803500	4.72970600	H
O	-3.05723800	1.09429700	1.94130800	H
H	-2.14614600	1.47831200	1.98419100	H
H	-2.92501300	0.18199800	1.58124500	H
O	-0.30344700	2.85323400	0.40553700	H

H	-0.10395800	2.78124100	-0.56144800	H
H	0.03574600	3.74644800	0.66436100	H
O	-0.29495600	-5.68809500	-0.86619700	H
H	-0.79323100	-6.18546300	-1.56226100	H
H	-0.02158800	-4.84690500	-1.31090600	H
O	0.51876200	3.78737600	-3.36650700	H
H	1.11255000	3.08007800	-3.01138700	H
H	0.12929300	3.39369900	-4.18682700	H
O	3.08228100	2.93491100	1.87556400	H
H	3.37516700	2.18381000	1.30112300	H
H	2.12155800	2.76084000	2.03902800	H
O	-4.86242200	3.41322800	3.58349700	H
H	-4.10741400	2.88841200	3.95065400	H
H	-5.19533900	2.87145400	2.82458600	H
O	2.15838500	-3.39022600	-4.44676700	H
H	1.59867600	-3.02978900	-3.71406300	H
H	3.04785300	-2.97968300	-4.30452200	H
O	-4.27924500	-2.49809800	3.41116700	H
H	-4.18630300	-1.66881300	2.87902800	H
H	-3.34783800	-2.78301600	3.58652200	H
O	4.27269500	-1.32828500	1.47217700	H
H	4.15391500	-0.38065700	1.21186700	H
H	3.42146000	-1.76315800	1.21510100	H
O	2.55998800	-3.03525800	3.67951500	H
H	2.75887800	-3.99848200	3.79197300	H
H	1.75903800	-3.01394900	3.09829100	H
O	-0.04041300	-5.22721800	3.96785000	H
H	-0.71384800	-4.51176800	3.84716600	H
H	0.30884000	-5.39509200	3.05668900	H
O	2.54357600	4.68452800	-0.80011900	H
H	2.38527900	3.70803800	-0.83740200	H
H	3.51843300	4.77138100	-0.65062900	H
O	1.74747400	3.83084000	7.33131800	H
H	1.76355800	2.88843600	7.63431000	H
H	0.78561200	4.06339400	7.29581100	H
O	4.05450700	-2.57634100	-1.60888900	H
H	3.07201900	-2.46753100	-1.55550400	H
H	4.41492700	-1.67877100	-1.39808500	H
O	-1.16195200	5.85792700	-1.11312500	H
H	-0.19913500	5.72609300	-1.30247200	H
H	-1.57769400	4.98495500	-1.32521200	H
O	-6.02839100	0.64264300	0.80327100	H
H	-6.09704500	0.14007300	-0.04705400	H
H	-5.78257700	-0.04088000	1.47597900	H
O	-4.04526200	3.99884500	0.10338000	H
H	-4.55895300	3.15316800	0.13851800	H
H	-3.20201500	3.79673600	0.58115400	H
O	-6.34292400	-2.40913300	-4.49153400	H
H	-6.15330300	-2.06515100	-5.40036900	H
H	-5.74844400	-3.19497500	-4.39496000	H
O	-4.70051600	-2.55973700	0.03079400	H
H	-4.07732300	-1.79580300	0.11865400	H
H	-4.22114900	-3.31906200	0.44729600	H
O	4.52818900	3.70667200	-3.52199700	H
H	3.67381800	3.31147200	-3.21575300	H
H	5.05951000	2.93321300	-3.83799600	H
O	-5.71009000	0.31214700	4.90307700	H

H	-5.20648600	0.82894100	5.58106200	H
H	-5.19529000	0.43385500	4.06623400	H
O	-3.56514700	-4.96355600	-2.21300800	H
H	-2.90688100	-4.39282100	-1.74282400	H
H	-4.36387900	-4.38760900	-2.31590700	H
O	4.65064500	-1.23632200	5.31084500	H
H	4.65241700	-0.45471600	5.91860100	H
H	4.78889300	-0.85006900	4.40974900	H
O	2.25679200	-4.59126400	0.75424500	H
H	1.85699100	-3.76955100	0.37363200	H
H	3.22920200	-4.40645000	0.77531400	H
O	5.67826800	1.92448500	-0.63819500	H
H	4.86095200	2.41946600	-0.89695100	H
H	5.39025800	0.97851800	-0.58957900	H
O	4.26345600	2.68279000	5.18628800	H
H	3.54573300	3.25964900	4.82253500	H
H	4.42315500	2.00925400	4.47836400	H
O	-2.55273300	-5.75132900	1.67976400	H
H	-2.73354900	-5.51609500	0.73528000	H
H	-2.82873800	-4.95007400	2.19146800	H
O	-1.94521600	4.79632400	3.34979900	H
H	-1.76243300	4.01827000	2.76567900	H
H	-1.80127100	4.45548100	4.26820800	H
O	1.43169600	5.24394900	3.87038100	H
H	0.86810300	5.11181800	4.67369000	H
H	0.93905500	4.78598700	3.14387100	H
O	-1.24407300	1.26836500	9.00914200	H
H	-1.08096800	0.33735200	8.71376900	H
H	-0.90733700	1.82850300	8.26532300	H
O	2.55032300	-6.01413600	-2.53285200	H
H	1.74115100	-5.99515200	-3.10334300	H
H	2.56856500	-5.12448200	-2.09882500	H
O	-0.37991000	2.45566500	-6.86076500	H
H	0.32042800	1.93612400	-7.32969000	H
H	-0.82623700	1.79569700	-6.27344000	H
O	-3.85562600	-1.96765500	7.50625300	H
H	-3.73152000	-2.52632800	6.69827500	H
H	-2.93622700	-1.78056100	7.82258700	H
O	-3.51070600	-5.58583400	5.05934000	H
H	-3.10675800	-4.70608700	5.26611700	H
H	-2.73829000	-6.17172400	4.85816000	H
O	-4.15482800	3.44936600	-6.98812400	H
H	-4.48392400	3.21788400	-6.08341200	H
H	-3.28736900	2.97831100	-7.06533100	H
O	2.82541300	3.18439400	-6.32833700	H
H	2.35600400	2.82683800	-5.53332400	H
H	3.70739300	2.73469600	-6.31946600	H
O	-3.25046800	-3.68102900	-6.50790000	H
H	-3.50889400	-4.12658000	-5.66231000	H
H	-4.05420100	-3.16762600	-6.77364600	H
O	-2.31716900	5.46329600	-4.94778600	H
H	-1.82851300	4.81989600	-5.52010700	H
H	-1.83786800	5.43860900	-4.08182300	H
O	-1.43067200	-4.58431800	7.68919300	H
H	-0.92781600	-3.85124200	8.12515500	H
H	-0.94458100	-4.74947700	6.84256300	H
O	-0.91216100	-4.68457300	-4.21827300	H

H	-1.05223200	-3.87911000	-3.66015200	H
H	-0.60735100	-4.33114100	-5.09138000	H
O	1.25624200	5.99640100	-5.65449700	H
H	0.72934100	5.29132700	-6.10807100	H
H	0.68574200	6.28518900	-4.89845700	H
O	-3.55027900	3.13144000	6.85299900	H
H	-3.61666100	2.24689700	7.29290400	H
H	-2.64215900	3.14534600	6.45909900	H
O	2.02740400	-3.76176600	7.08454100	H
H	1.66650700	-4.33520800	6.36250800	H
H	2.76415200	-3.25805400	6.65587500	H
O	0.42742800	-2.83895000	-7.84567200	H
H	0.91799000	-2.97173700	-6.99605300	H
H	-0.51844700	-3.02131800	-7.61682000	H
O	-5.74400300	0.03038700	-7.73887600	H
H	-5.30274800	-0.85378000	-7.80246400	H
H	-5.00317200	0.68315600	-7.81265500	H
O	-2.13543600	-0.15994900	-8.15201000	H
H	-2.52267400	-1.04772300	-7.94679400	H
H	-1.15942400	-0.28425300	-8.04234000	H

Diradical 1(b)

N	1.68100500	-0.86897800	-0.55114900	H
C	2.96360300	-0.90366500	-0.32255000	H
N	3.55917200	-2.14439000	-0.51840400	H
C	2.54995100	-3.02608900	-0.94363900	H
C	1.34262000	-2.15447800	-0.97309300	H
O	2.70491100	-4.20161000	-1.22903600	H
C	4.94505700	-2.54847500	-0.36115800	H
H	4.96593100	-3.62860800	-0.51275000	H
H	5.31006500	-2.31008000	0.64027300	H
H	5.58205500	-2.05128300	-1.09303500	H
C	-2.57262700	0.10794000	-1.42486300	H
C	-1.59474100	-0.75800400	-0.92317900	H
C	-1.01321400	-1.72356500	-1.77821600	H
C	-1.52940400	-1.83552100	-3.08457100	H
C	-2.50435300	-0.98128400	-3.57569600	H
C	-3.01184300	0.02126500	-2.74388900	H
H	-1.11288100	-2.59333900	-3.74098400	H
H	-2.87348400	-1.06963900	-4.59039100	H
O	-3.95174000	0.86309100	-3.25757800	H
H	-4.21163000	1.49487300	-2.57418300	H
C	4.02929900	2.61297500	0.33019000	H
C	5.37849200	1.86568900	0.00416700	H
N	4.96145400	0.49853400	-0.41864200	H
C	3.74242200	0.30747800	-0.03646000	H
N	3.15787100	1.41738400	0.58783400	H
C	-0.84684100	-1.31768500	2.74448900	H
N	-1.09370300	-1.76281200	1.33301100	H
C	-1.34688000	-0.64324000	0.52985300	H
N	-1.50040700	0.44852800	1.20167900	H
C	-1.44083800	0.14109700	2.65367500	H
O	-1.01460300	-2.97320100	0.96318500	H
C	2.03856200	1.48272300	1.17324900	H
C	0.15382400	-2.55425600	-1.48380000	H

H	0.13893100	-3.57551400	-1.85645900	H
H	-2.98761200	0.84817600	-0.74904000	H
C	-0.60470000	1.21484200	3.35775700	H
H	-0.51433600	1.00408300	4.42833400	H
H	0.39101200	1.29895800	2.92443300	H
H	-1.10153800	2.18147300	3.24275500	H
C	6.19780100	2.49950500	-1.12487300	H
H	6.49011300	3.52335100	-0.87013900	H
H	7.10723300	1.91469700	-1.28537300	H
H	5.64472700	2.51832800	-2.06477500	H
C	3.40185200	3.33889200	-0.87411300	H
H	2.36714700	3.59401400	-0.63036100	H
H	3.94358400	4.25950300	-1.10158000	H
H	3.39338300	2.71149200	-1.76834000	H
C	4.01905000	3.52882600	1.55121900	H
H	4.64452700	4.40713600	1.36949900	H
H	2.99752400	3.86455300	1.73897900	H
H	4.37728900	3.02609800	2.45017800	H
C	6.27581500	1.68395100	1.24343700	H
H	7.11632700	1.03529400	0.98697100	H
H	6.67448700	2.64323200	1.58631100	H
H	5.73080300	1.21940400	2.06883700	H
C	-2.89497100	0.22898300	3.15619700	H
H	-2.95420600	0.07179800	4.23667700	H
H	-3.28673600	1.22301200	2.92970300	H
H	-3.53731000	-0.50534300	2.66475700	H
C	0.67508700	-1.36706100	2.96207700	H
H	1.19641100	-0.69810400	2.27548900	H
H	0.92550400	-1.08744500	3.98869600	H
H	1.01956800	-2.39025000	2.78820100	H
C	-1.53919300	-2.29151000	3.69798400	H
H	-1.33498600	-2.01527600	4.73551500	H
H	-2.61969000	-2.31989200	3.55295900	H
H	-1.15229500	-3.29697400	3.52177900	H
O	0.85403400	1.51659400	-2.39921100	L
H	0.42635800	1.50245200	-1.50659600	L
H	0.59822600	0.65395800	-2.81201400	L
O	-0.29888000	3.85865600	0.99107600	L
H	0.43312700	3.81988700	1.65592000	L
H	-0.26422100	2.98304200	0.53099200	L
O	-3.36931900	3.70846600	0.28502700	L
H	-3.10422300	2.91967600	0.82111200	L
H	-3.85321300	3.33046700	-0.49140400	L
O	-4.47492200	-2.85771500	0.55743700	L
H	-3.89542200	-2.74421700	1.35144800	L
H	-4.01306900	-2.35665100	-0.16043200	L
O	3.89635600	-0.17981600	-3.70883200	L
H	4.01615000	-1.00133500	-3.17036300	L
H	3.50493200	0.47478000	-3.07815100	L
O	-5.28503700	0.92529600	0.82028100	L
H	-5.01499300	-0.01594200	0.67794900	L
H	-5.50438600	1.25805100	-0.08538700	L
O	1.60776800	5.29401100	-3.36328600	L
H	1.67632900	4.31292400	-3.25025800	L
H	2.34381900	5.65932800	-2.81106300	L
O	0.20564300	-5.78205800	-3.68881000	L
H	-0.47625400	-5.12976500	-3.98857600	L

H	-0.05295000	-6.00199100	-2.75871600	L
O	-1.36529100	3.78300800	-2.52700400	L
H	-1.77107700	2.96338300	-2.14826900	L
H	-0.65101100	4.02515900	-1.88595400	L
O	1.52782800	6.56771700	-0.01358900	L
H	0.97726700	5.90744100	-0.50447200	L
H	2.23802000	6.02807100	0.41579800	L
O	0.11492200	-1.25746900	7.06230200	L
H	0.64456000	-1.90562800	6.53342800	L
H	0.03997000	-0.46262300	6.47686800	L
O	4.07056100	-0.96895800	2.98137000	L
H	4.66337800	-1.07942800	3.76602700	L
H	3.63797500	-0.08981200	3.11974300	L
O	-0.71677900	4.60436700	5.06971300	L
H	0.13479800	4.99571500	5.38905600	L
H	-0.61131500	4.55103900	4.08687500	L
O	-2.59860100	-4.71114000	-1.19597200	L
H	-2.38288200	-4.58496100	-2.15349800	L
H	-1.77986500	-5.10903100	-0.80817500	L
O	4.37220200	-6.79415800	-0.37271900	L
H	4.06290400	-6.20212500	0.35816800	L
H	4.96785200	-6.22292600	-0.91991700	L
O	-3.76332300	0.34875400	-6.96470400	L
H	-4.18357000	0.75943600	-6.16776400	L
H	-3.98639900	-0.61350000	-6.89515400	L
O	1.75508000	-2.44794200	-4.65582800	L
H	1.84247100	-3.19991700	-4.01789100	L
H	1.47920000	-1.67863200	-4.09687200	L
O	-2.59167400	2.01068400	6.54444000	L
H	-2.59312500	2.32630500	5.60616000	L
H	-2.11233800	1.14494400	6.51433700	L
O	7.20399100	-0.75969600	-3.36451400	L
H	6.71243500	-1.61723200	-3.42142100	L
H	6.64159600	-0.18988000	-2.78231800	L
O	-4.41453200	4.25713900	-4.00017300	L
H	-4.99631900	3.49396400	-4.24420700	L
H	-4.19709500	4.10810100	-3.04593900	L
O	2.28482300	2.78527800	4.63505300	L
H	2.61726600	2.00445600	4.12577100	L
H	1.74262100	3.29235300	3.98056600	L
O	-2.18987700	6.64924700	-1.18099400	L
H	-1.75017400	6.06008100	-0.51800300	L
H	-2.94972000	6.11401900	-1.52230300	L
O	3.17414100	0.08371400	6.44841400	L
H	2.64476100	-0.13103400	5.63999000	L
H	4.05200100	-0.34618700	6.29092800	L
O	-1.43027800	2.15434100	-5.34779300	L
H	-2.33167800	2.45034500	-5.06519400	L
H	-1.09191500	1.62655900	-4.58179800	L
O	7.30289500	-4.68184600	1.06692700	L
H	6.44693900	-5.15642900	1.21622800	L
H	7.24001100	-3.87332500	1.63491800	L
O	3.75900900	-4.28704700	2.50109800	L
H	4.60841100	-3.84294100	2.74901900	L
H	3.20878700	-3.56580000	2.10502100	L
O	7.59258600	-1.16456800	3.09340500	L
H	6.96131700	-1.27259500	2.33844000	L

H	7.27684300	-0.35432300	3.56704800	L
O	-7.18898100	3.67154400	1.23134300	L
H	-6.29300000	3.70173100	0.81155000	L
H	-7.08246900	3.05434900	1.99819200	L
O	-5.24397900	-3.71596600	-2.88647100	L
H	-5.46912300	-4.03973700	-1.97839300	L
H	-4.53052700	-3.04533400	-2.74047800	L
O	-4.87815700	6.81926900	1.60711000	L
H	-4.87071600	5.82973600	1.58143100	L
H	-4.27629000	7.09036800	0.86915100	L
O	5.62494900	2.25660400	5.01099700	L
H	6.30396900	2.56180700	4.35819500	L
H	5.26523000	1.42050700	4.62177300	L
O	-4.32499500	-4.72505200	4.37800700	L
H	-4.39339500	-4.32959300	3.47293100	L
H	-3.35696900	-4.70538000	4.58536000	L
O	-3.13481600	-3.86761900	-5.70851500	L
H	-2.94185900	-4.13731400	-4.77575200	L
H	-3.91561800	-3.26322300	-5.63518300	L
O	5.03536800	-4.35478200	-3.50843100	L
H	4.56800200	-3.48337000	-3.46063900	L
H	5.84871600	-4.23052400	-2.95753400	L
O	6.21249900	1.93751400	-5.07397600	L
H	5.31692500	2.06692200	-4.67243000	L
H	6.84381700	2.25288900	-4.37943400	L
O	5.36172300	5.01345900	-3.57427700	L
H	4.92539900	5.90209100	-3.56491400	L
H	4.61234400	4.37093500	-3.65041900	L
O	-5.13279500	-6.14727200	0.17651300	L
H	-4.31335000	-6.69983200	0.11648200	L
H	-5.06458600	-5.69691500	1.05568800	L
O	-6.06281100	1.19321200	4.60835100	L
H	-5.18116300	1.42808500	4.99273400	L
H	-5.90025600	1.13210300	3.63372500	L
O	3.77184500	4.78130200	-6.57041300	L
H	4.22902000	3.93022900	-6.35350600	L
H	3.09898500	4.89161600	-5.85247400	L
O	-6.38876000	-0.95707800	-4.87638200	L
H	-6.37510300	-0.00724800	-4.59716700	L
H	-5.50837100	-1.31084900	-4.59414400	L
O	-2.12032600	-6.00375300	2.10475800	L
H	-2.52989300	-5.14829400	1.82130300	L
H	-1.38675200	-5.73755400	2.71381200	L
O	-3.85447100	-6.76816900	-3.74326200	L
H	-2.86889200	-6.69375700	-3.68285400	L
H	-4.17404700	-6.59294300	-2.82260000	L
O	-4.06917000	3.98484000	3.69849500	L
H	-3.14429900	3.83527400	3.37887900	L
H	-4.63667900	3.49744700	3.05007300	L
O	3.25470700	-3.20882400	5.66182400	L
H	2.75987600	-2.76994500	4.92518700	L
H	4.20842500	-3.09953800	5.41951100	L
O	-6.22369400	6.01142900	-1.37592900	L
H	-6.48158900	5.65784600	-2.26408500	L
H	-5.48179500	5.42565000	-1.08185500	L
O	-1.30135200	-8.02805000	-1.01705000	L
H	-2.22704400	-7.77934900	-1.26488200	L

H	-1.19901700	-7.70564600	-0.08656000	L
O	-0.64877400	-0.98051000	-6.60790500	L
H	-0.29251700	-0.58382300	-5.77376800	L
H	-0.91743500	-1.89817000	-6.35081000	L
O	-6.73621300	-1.09018100	-1.59599900	L
H	-6.74285300	-1.58739500	-0.73990600	L
H	-5.78168700	-0.87991000	-1.75310800	L
O	-6.18699800	-1.95460300	3.45580600	L
H	-6.07750900	-1.43889400	2.61790600	L
H	-5.35969000	-1.77357200	3.96858900	L
O	2.28546500	6.33777300	3.44117600	L
H	3.00357400	5.70310400	3.69006100	L
H	1.58245100	5.77068900	3.03590700	L
O	-1.59012900	6.72298100	2.40776000	L
H	-0.70444900	6.65952200	1.96988100	L
H	-2.05402600	5.88700300	2.15050800	L
O	-7.17903200	2.54401400	-2.12493400	L
H	-6.89140300	1.69351300	-2.54210300	L
H	-6.33713100	2.96931400	-1.82443100	L
O	1.92475500	2.08404800	-5.42355700	L
H	1.74391000	1.12565400	-5.25278000	L
H	2.58108900	2.34105900	-4.72813000	L
O	0.98671800	-5.71874000	0.95589600	L
H	1.04826400	-4.78675500	1.28373900	L
H	0.58050000	-5.63799000	0.05672000	L
O	-8.43764600	0.17156600	1.07553700	L
H	-7.96361800	0.45962900	1.89575100	L
H	-8.19977600	0.85373000	0.39827800	L
O	-3.56253100	-1.48163700	6.62846700	L
H	-3.71224000	-2.27463800	6.05493600	L
H	-4.24085500	-0.82628100	6.32715900	L
O	8.46476000	-1.65242500	-0.23019800	L
H	7.84398500	-0.91214400	-0.44608600	L
H	8.17779000	-2.39600600	-0.81772200	L
O	0.71768100	-5.11980100	4.76335900	L
H	0.46307500	-4.32326000	5.29358900	L
H	1.10575100	-4.74990400	3.93106000	L
O	5.11981200	6.79376000	-0.31910300	L
H	4.44298500	6.83374200	-1.04076900	L
H	5.75070800	6.08786200	-0.60921000	L

Diradical 2(a)

N	0.40485200	-0.75856000	0.34509400	H
C	1.19809300	0.20751300	-0.01234900	H
N	0.55724900	1.44107100	-0.18338600	H
C	-0.80304400	1.24351500	0.07939000	H
C	-0.87429900	-0.19954400	0.43730200	H
O	-1.66454500	2.10923300	0.01404200	H
C	1.08334000	2.74708600	-0.54730200	H
H	1.86594900	3.05750800	0.14423400	H
H	0.23881000	3.43617400	-0.49483000	H
H	1.50186800	2.73827900	-1.55468900	H
C	-4.98638100	-0.72159200	2.96477800	H

C	-3.73533000	-1.04816700	2.44376800	H
C	-3.30685700	-0.57725300	1.19022200	H
C	-4.21051300	0.18366000	0.40251800	H
C	-5.46686800	0.49794900	0.94900900	H
C	-5.85286800	0.07261100	2.21261200	H
C	4.71747300	-1.06829000	-0.49175600	H
C	4.82061900	0.49720800	-0.68035400	H
N	3.42309600	0.99661700	-0.62873000	H
C	2.63882000	0.04371100	-0.23910700	H
N	3.28204500	-1.18721200	-0.05403500	H
C	-3.26052300	0.30304500	-3.17205900	H
N	-3.14648200	-0.17918600	-1.77515800	H
C	-3.93760500	0.49943900	-1.01360700	H
N	-4.60346000	1.53628700	-1.70074800	H
C	-4.01362500	1.68141000	-3.07200900	H
O	2.78703000	-2.29085400	0.30716700	H
C	-1.92019700	-0.94299100	0.87029400	H
H	-1.63707700	-1.95613000	1.14957500	H
H	-6.15115400	1.09290000	0.36060900	H
H	-3.05256800	-1.65282300	3.03539900	H
O	-5.43842000	2.37614400	-1.24151400	H
H	-6.82661600	0.32737600	2.61605300	H
O	-5.41111100	-1.14931900	4.18682700	H
H	-4.72333700	-1.69362300	4.59231300	H
C	-1.86230100	0.39350300	-3.79357800	H
H	-1.21300700	1.06578100	-3.23143300	H
H	-1.40353700	-0.59785900	-3.79320900	H
H	-1.91403700	0.74527800	-4.82947800	H
C	-4.06086600	-0.78289400	-3.91830500	H
H	-4.13014100	-0.56484000	-4.98821600	H
H	-3.55137700	-1.74058700	-3.78941100	H
H	-5.07084500	-0.88972900	-3.51631500	H
C	-5.13506400	1.93094800	-4.08214100	H
H	-5.66805600	2.84457200	-3.80852400	H
H	-4.71681200	2.05946000	-5.08486600	H
H	-5.85890800	1.11560400	-4.11042000	H
C	-3.08951600	2.91126900	-3.01443000	H
H	-2.62780300	3.09573700	-3.98787200	H
H	-3.69094000	3.78208200	-2.74359600	H
H	-2.31242900	2.79470600	-2.25737300	H
C	4.84853500	-1.89520700	-1.78085900	H
H	5.88193000	-1.90395800	-2.13499200	H
H	4.54482900	-2.92158900	-1.56364000	H
H	4.21022000	-1.51820700	-2.58211800	H
C	5.59535000	-1.69181900	0.59655700	H
H	5.29264700	-2.73139800	0.73580500	H
H	6.64831800	-1.67037800	0.30498800	H
H	5.48902500	-1.18327100	1.55478400	H
C	5.44211800	0.93687100	-2.01391400	H
H	5.41413700	2.02674800	-2.07910500	H
H	6.48597700	0.61678800	-2.08380300	H
H	4.90090400	0.53976600	-2.87345700	H
C	5.57091200	1.20685100	0.46363500	H
H	6.62157300	0.90581800	0.49304800	H
H	5.52681500	2.28598800	0.30236900	H
H	5.12341600	0.99601900	1.43686700	H
O	-0.25488800	-0.69213600	3.89405500	H

H	0.49838400	-0.70196900	3.25274300	H
H	-0.65798900	-1.59220700	3.81493100	H
O	1.45324000	0.27506900	-3.32011200	H
H	2.41594700	0.04890400	-3.31134900	H
H	1.01406100	-0.49618800	-2.88247200	H
O	-1.00589500	-3.18215700	-1.69736800	H
H	-0.37256500	-3.31197700	-0.94755800	H
H	-0.91191100	-2.22663300	-1.93774900	H
O	-1.64287100	-3.16870100	-5.61316800	H
H	-1.97505200	-2.27431800	-5.87824300	H
H	-1.41250100	-3.07437400	-4.65489400	H
O	0.36412100	-3.93136800	1.97655500	H
H	-0.31276100	-3.98081400	2.69715000	H
H	0.82636500	-3.06992300	2.13078700	H
O	0.97345000	2.60353700	3.26812700	H
H	0.97752800	3.36263300	2.63327200	H
H	0.69764300	1.82658200	2.72101100	H
O	-1.47885200	5.15642500	2.29459600	H
H	-1.23053800	4.41088500	1.69224100	H
H	-1.17621600	4.86315500	3.19055900	H
O	-1.99964600	5.93204100	-0.83949300	H
H	-1.06531500	6.13667200	-0.58417300	H
H	-2.04185100	4.94323600	-0.84978300	H
O	2.40374200	-5.54592000	-0.82206400	H
H	3.24946100	-5.04551200	-0.94232500	H
H	1.77667800	-4.88402200	-0.43623800	H
O	1.54505400	-3.43178000	5.14902600	H
H	1.95438900	-2.72697600	4.58713600	H
H	0.77606600	-2.98578600	5.58511500	H
O	3.90290100	-1.16079300	-5.74296000	H
H	4.21900000	-0.39057600	-5.20743300	H
H	3.25201100	-1.62060300	-5.15566500	H
O	-2.44941100	2.21815300	3.21142400	H
H	-1.87655800	1.42789000	3.04902000	H
H	-3.23632400	2.07744700	2.62845700	H
O	3.53413800	2.80388100	-4.43314000	H
H	3.17503000	2.07038900	-4.99285800	H
H	3.13894600	2.64940300	-3.53874400	H
O	1.80080200	0.00726600	6.25716900	H
H	2.60374200	-0.53752600	6.06021800	H
H	1.76048800	0.66528400	5.51849800	H
O	3.36526500	-0.24404500	3.23791900	H
H	2.89319200	0.44516400	2.70740800	H
H	3.04453400	-1.10473900	2.86954500	H
O	3.83578900	3.99748600	2.01472600	H
H	3.61037500	3.03484800	2.06540700	H
H	3.53939400	4.36800100	2.88359600	H
O	-2.81695900	-4.91439300	1.28257100	H
H	-2.92826600	-4.07003000	1.78704600	H
H	-2.17523300	-4.68985000	0.56296200	H
O	6.78352400	-4.89807900	-1.06530500	H
H	7.17373700	-3.99887000	-0.92562300	H
H	5.98820900	-4.91864000	-0.47588300	H
O	-2.74199600	-0.21590300	6.19406900	H
H	-1.81777800	-0.51838000	6.38044800	H
H	-2.72922500	0.04560800	5.23933600	H
O	-4.52602300	-3.14189900	-1.28566200	H

H	-5.14977000	-2.39697100	-1.09586500	H
H	-3.71367000	-2.92206900	-0.76480100	H
O	0.21100400	2.84810700	-5.50315100	H
H	-0.53664900	3.49338900	-5.43452600	H
H	0.41003000	2.59836800	-4.56612900	H
O	0.45995200	-0.42110200	-6.36788100	H
H	0.55846300	-1.13196500	-5.68584100	H
H	1.23818100	0.17310900	-6.22081300	H
O	-2.74023100	6.30891800	-3.98792600	H
H	-2.22437800	5.66925700	-4.54034100	H
H	-3.68282600	6.02508300	-4.09481400	H
O	0.40974900	5.25383200	-3.06082500	H
H	1.27808100	4.78638700	-3.14902200	H
H	-0.24399200	4.53217800	-2.88126800	H
O	-5.93280100	-4.00355800	2.06494600	H
H	-5.50136600	-3.36618900	1.44236100	H
H	-5.45084500	-3.87838400	2.92065300	H
O	1.80412600	6.11926900	0.55107500	H
H	1.59870400	5.84828200	-0.37874400	H
H	1.24019900	5.52939400	1.11157000	H
O	5.09472300	-2.59686000	4.81770200	H
H	5.32596600	-2.44270100	3.86751000	H
H	4.97264500	-1.68900600	5.19359400	H
O	4.41764300	2.18737400	5.37628400	H
H	4.74057300	1.25491900	5.29487300	H
H	3.75692100	2.28602100	4.64559300	H
O	-2.30859200	-3.88465900	4.83402900	H
H	-3.21494700	-3.95643900	4.44211100	H
H	-2.31437100	-3.01916500	5.31468000	H
O	3.56968100	-4.77329100	2.46292400	H
H	3.46381000	-3.79752000	2.59177400	H
H	4.07494600	-4.85804900	1.61577500	H
O	3.98614100	4.69612200	-1.63839700	H
H	4.02876000	4.02005400	-0.91672600	H
H	4.82541400	4.56787300	-2.14768800	H
O	1.90527900	-3.38788900	-3.25622400	H
H	1.90724500	-2.87826600	-2.40748500	H
H	1.20669200	-2.95191700	-3.80576500	H
O	5.23006700	-4.50860200	-4.01777800	H
H	4.61870700	-4.89117600	-3.33929900	H
H	4.76637100	-3.69469000	-4.33826400	H
O	8.99575300	-0.59720900	-1.41828500	H
H	8.68891700	-0.25090700	-0.54293900	H
H	8.38391500	-1.35009700	-1.61610300	H
O	-0.86081600	2.68688700	6.02964300	H
H	-1.85076200	2.71011200	6.03122700	H
H	-0.63349100	1.84114900	5.56786900	H
O	7.60163200	-4.02806400	2.21410500	H
H	7.61255000	-3.08854100	2.52645400	H
H	6.66650400	-4.32390400	2.34976000	H
O	-7.67761900	0.04170000	-2.05375100	H
H	-7.81694700	-0.25612500	-2.98754100	H
H	-6.86225000	-0.43703500	-1.76088200	H
O	8.36659800	2.81375000	-1.16304100	H
H	7.54861400	3.32411700	-1.38806900	H
H	8.37027700	2.77484200	-0.17373500	H
O	6.34786200	5.56712100	0.58780600	H

H	6.48927600	4.60914600	0.79305000	H
H	6.62047100	5.66013400	-0.35947800	H
O	-7.15347800	-0.60519700	-6.08397500	H
H	-6.27627200	-0.32119300	-6.44486800	H
H	-6.93030500	-1.26294000	-5.37855100	H
O	-8.27803400	-1.86270600	0.71488000	H
H	-7.37067600	-1.92008600	0.32320600	H
H	-8.13650600	-1.98858100	1.68676400	H
O	-5.84498000	5.54667100	-1.58247200	H
H	-4.87850000	5.67790100	-1.41221700	H
H	-5.88979300	5.20982800	-2.51249800	H
O	-5.14343100	-3.72728700	-5.69762500	H
H	-4.74515800	-2.92621100	-6.12194600	H
H	-4.61568100	-3.85883600	-4.87017800	H
O	7.15977300	3.05971300	3.18928000	H
H	7.60723600	2.61657000	2.42526800	H
H	6.21519300	2.77064600	3.12470700	H
O	-4.49605300	4.24562300	1.23748600	H
H	-3.85915100	3.77277100	0.64522700	H
H	-5.19809900	3.57504400	1.43155600	H
O	-5.26629500	2.57465000	4.86201700	H
H	-4.82130800	1.69553200	4.95837900	H
H	-5.56058700	2.60158800	3.91705900	H
O	-7.54327400	-3.31607300	-3.03312800	H
H	-6.69053600	-2.88468500	-3.29122200	H
H	-7.63168800	-3.13009700	-2.06470500	H
O	7.34225200	-1.00709200	-4.49768500	H
H	6.87800900	-0.14825900	-4.66264500	H
H	6.64094000	-1.69537300	-4.61889900	H
O	7.40103700	-0.24819800	3.60420200	H
H	7.70037200	-0.19983600	2.66159200	H
H	6.47284400	0.09601900	3.58809500	H

Diradical 2(b)

N	-1.59340500	0.21563000	-0.33127200	H
C	-1.75745300	0.68440000	0.87387800	H
N	-2.48805700	1.86815600	0.95042600	H
C	-2.83446600	2.22444500	-0.36249700	H
C	-2.26255300	1.10872900	-1.17083900	H
O	-3.46987900	3.21267400	-0.68894600	H
C	-2.86246500	2.67255600	2.10159000	H
H	-3.38580400	3.54343900	1.70307400	H
H	-1.98218300	2.99794800	2.66066600	H
H	-3.51244000	2.11310700	2.77378700	H
C	-0.92813800	-1.94509500	-4.35912700	H
C	-0.97598800	-0.80082900	-3.54915300	H
C	-2.21578600	-0.13452500	-3.39456800	H
C	-3.32814000	-0.59454000	-4.11545100	H
C	-3.25361200	-1.72696400	-4.92559200	H
C	-2.04442200	-2.42013400	-5.03300700	H
H	-4.28222000	-0.08592900	-4.02621500	H
C	-0.02635100	-1.54502500	3.36038400	H
C	-0.99891300	-0.65629200	4.22909700	H
N	-1.82536300	0.09153700	3.24261700	H
C	-1.26288700	0.00907700	2.08220700	H

N	-0.12668800	-0.80921600	2.05404100	H
C	2.03365300	1.14782600	-2.33297800	H
N	0.66108400	1.01118600	-2.92384100	H
C	0.32263800	-0.34564800	-3.01858700	H
N	1.30474200	-1.13983100	-2.75052100	H
C	2.52960300	-0.34494200	-2.49243300	H
O	-0.06512700	2.00515700	-3.23350400	H
O	0.66642500	-1.01185000	1.09055500	H
C	-2.49639800	0.99476000	-2.49705800	H
H	-3.10977000	1.79015800	-2.91282300	H
H	0.02547800	-2.44919400	-4.46235700	H
H	-1.96906800	-3.30484400	-5.66053500	H
O	-4.38696500	-2.10499800	-5.58212500	H
H	-4.20377800	-2.90043800	-6.09921000	H
C	1.84713500	1.60179800	-0.87702200	H
H	1.27218000	0.87647200	-0.29992300	H
H	2.81623700	1.75282500	-0.39402900	H
H	1.31107900	2.55406400	-0.87879900	H
C	3.22997500	-0.91938100	-1.25509600	H
H	4.14024700	-0.35860600	-1.02056800	H
H	2.57768900	-0.91913800	-0.38277600	H
H	3.51196300	-1.95547200	-1.45908400	H
C	3.43932200	-0.55476600	-3.71942800	H
H	4.39837600	-0.04302400	-3.59478000	H
H	3.63289000	-1.62386400	-3.83789000	H
H	2.97071600	-0.19629600	-4.63916300	H
C	2.80044100	2.22031000	-3.10914300	H
H	3.80117600	2.34745600	-2.68802100	H
H	2.89613300	1.97967000	-4.16869200	H
H	2.26817900	3.17060100	-3.02792600	H
C	-0.52888700	-2.97462700	3.09315000	H
H	0.08633900	-3.41953000	2.30758000	H
H	-0.44743400	-3.58982900	3.99247100	H
H	-1.56683800	-2.98754000	2.75563900	H
C	1.43774000	-1.59185600	3.79453900	H
H	1.53035900	-2.13035900	4.74047900	H
H	2.02080600	-2.11873700	3.03671500	H
H	1.86685000	-0.59707500	3.91806500	H
C	-0.26152400	0.41592200	5.05582100	H
H	-0.99599400	1.06943700	5.53171000	H
H	0.35226400	-0.03906200	5.83799700	H
H	0.38119300	1.03678000	4.42740300	H
C	-1.92643900	-1.44959400	5.15568600	H
H	-1.35162600	-2.00269800	5.90480000	H
H	-2.59116700	-0.75835800	5.67961800	H
H	-2.54868400	-2.15601500	4.60498200	H
O	-2.58456000	-2.82438400	-0.42953700	L
H	-1.86426200	-2.60938900	0.21409800	L
H	-2.27908900	-2.43142700	-1.28512200	L
O	4.19728400	0.21342600	1.89197800	L
H	4.36477900	-0.08435500	2.82101500	L
H	3.21359400	0.30793400	1.83617000	L
O	0.79257700	-3.85478400	-0.58280700	L
H	1.53433700	-3.36482600	-0.14794700	L
H	0.31015100	-3.16431100	-1.10234800	L
O	2.03196000	-4.43243000	-3.74753600	L
H	2.36720300	-3.80959800	-3.05517200	L

H	1.11394600	-4.65828900	-3.45351000	L
O	0.92474300	2.83526600	2.17706000	L
H	1.18486100	1.88145100	2.13498700	L
H	0.29797900	2.95500500	1.42055600	L
O	-3.59371400	2.61075100	5.72161100	L
H	-3.54772200	1.66973100	5.41795300	L
H	-2.83570000	3.05527500	5.26567700	L
O	-4.32846300	-2.68471100	2.30847400	L
H	-5.25322300	-2.41742700	2.07757200	L
H	-3.78136200	-1.88317900	2.11344600	L
O	-2.94961600	4.68901800	-3.62870800	L
H	-3.63989700	4.09756100	-4.02120100	L
H	-2.17015100	4.09670700	-3.48182400	L
O	4.16983500	-1.65779800	6.05345700	L
H	3.39185400	-1.10822700	6.32381700	L
H	4.25904300	-1.50016300	5.08003800	L
O	-1.27863000	-6.17343200	0.82894400	L
H	-0.47528000	-6.32138000	0.26953100	L
H	-1.34440900	-5.18923800	0.91359400	L
O	2.75384800	-4.79162200	5.14048000	L
H	3.24721700	-4.18135800	4.53679500	L
H	1.81796200	-4.75508600	4.81948900	L
O	2.92693100	5.08181800	-0.64285300	L
H	2.31271600	4.73326200	0.05109500	L
H	3.56070000	4.33952500	-0.80920800	L
O	2.36672500	5.42162300	3.59765000	L
H	2.71086500	4.54541200	3.90435700	L
H	2.52500100	5.42180400	2.62033900	L
O	4.68467900	-2.94191600	1.61731700	L
H	4.53175300	-2.83364000	2.58949500	L
H	3.82517800	-2.68161400	1.20072100	L
O	-5.17230200	-0.87886200	-0.46671100	L
H	-4.61297400	-0.38828000	0.18605100	L
H	-4.63045600	-0.89181800	-1.29484000	L
O	-2.50561200	2.04229200	-6.01939900	L
H	-2.28489400	1.16237300	-6.41613000	L
H	-1.70153400	2.28595000	-5.49594100	L
O	-6.30244600	2.66782300	0.97243800	L
H	-5.77686200	1.88569400	0.66918200	L
H	-6.05705100	2.77680300	1.92547200	L
O	-5.42418200	-3.45543800	-2.75575500	L
H	-4.45590100	-3.32364600	-2.59659700	L
H	-5.75788300	-2.55930400	-3.01243400	L
O	-4.79156000	-5.22315500	0.04783600	L
H	-5.17645100	-4.31154300	0.01334700	L
H	-4.04705600	-5.15332600	0.69663600	L
O	6.00536100	2.28206200	-4.70674100	L
H	5.56621600	1.58038500	-5.24992500	L
H	5.40094800	3.06333200	-4.77544400	L
O	-5.49452600	0.17244600	3.68516100	L
H	-4.71322100	-0.28357100	4.08715400	L
H	-5.27807400	0.22977900	2.72083000	L
O	-1.64046000	-5.33663500	-2.33127300	L
H	-2.57202500	-5.31037600	-1.99700200	L
H	-1.52089400	-4.47256400	-2.79909900	L
O	1.18057100	-2.89401900	7.56870500	L
H	0.95904400	-1.93601300	7.45360100	L

H	0.68932100	-3.35082800	6.84080900	L
O	2.08669100	-5.65078000	1.86738100	L
H	2.33911300	-4.70913400	2.03930400	L
H	1.26655000	-5.78935000	2.40459600	L
O	6.24944500	1.62425000	-0.96023000	L
H	5.38445600	1.96561500	-0.62054900	L
H	6.03579700	1.24871200	-1.85113900	L
O	4.66795000	3.42368700	1.84240300	L
H	4.90638300	3.06690300	2.73462400	L
H	3.74870400	3.09342100	1.68134500	L
O	-3.17410600	-5.47750400	3.56238700	L
H	-3.27191000	-4.66822100	4.12404600	L
H	-2.19923200	-5.64897700	3.54279700	L
O	-0.31725500	4.98975200	-1.45680000	L
H	0.27424900	4.70141700	-2.19643700	L
H	-0.63655200	4.14517400	-1.05094400	L
O	-0.75772300	5.67139600	1.94665100	L
H	-1.42400500	5.33901100	1.29408500	L
H	0.09555300	5.68292900	1.44457900	L
O	0.00160000	3.96651400	5.44312700	L
H	-0.33249400	3.78682300	4.52872200	L
H	0.82281700	3.41872200	5.51908300	L
O	6.71726300	-1.72789300	-1.65924400	L
H	6.08583900	-1.85829200	-2.41068500	L
H	6.21841300	-2.03189500	-0.85974700	L
O	0.49607900	0.18823300	-6.57316800	L
H	0.69811600	0.87523900	-5.88968800	L
H	1.04433100	-0.59272400	-6.30931200	L
O	4.67349700	-4.75521500	-1.10367300	L
H	3.73040100	-4.63776400	-0.82616100	L
H	4.75262400	-4.23420500	-1.94192100	L
O	3.40511400	1.72035400	5.01917900	L
H	2.89137500	1.86201500	4.18491500	L
H	2.73121500	1.41328900	5.67625500	L
O	0.86901700	4.40774700	-5.28541900	L
H	0.98477200	3.44664500	-5.49236600	L
H	-0.08584800	4.49408800	-5.03874100	L
O	-5.03831500	-2.75208100	6.09751000	L
H	-5.12435700	-2.82304300	5.11368600	L
H	-4.26909900	-3.33387100	6.32197900	L
O	-1.33887000	-5.42988600	6.45419000	L
H	-0.62820100	-5.52177700	5.77086800	L
H	-1.73379400	-4.53826200	6.28317500	L
O	-6.00208000	2.27947400	-2.55063400	L
H	-5.63748500	1.49485400	-2.06943300	L
H	-5.63866500	2.19862000	-3.46813900	L
O	3.34030600	2.13896500	-7.27335200	L
H	3.33494800	2.86909900	-6.60466600	L
H	3.29883300	1.30898000	-6.73530200	L
O	-3.54754100	-5.82169300	-5.13219400	L
H	-2.55770000	-5.84739000	-5.13509300	L
H	-3.77453200	-5.08757200	-4.50803600	L
O	-0.35052100	2.90313600	-8.33569600	L
H	-0.67836500	3.65170800	-7.77660000	L
H	0.59823600	2.79534700	-8.07410600	L

Diradical 3(a)

N	-0.35945500	-0.88474200	-0.09297500	H
C	-1.19002100	0.08247500	0.15721800	H
N	-0.69490000	1.35673700	-0.13852400	H
C	0.60176200	1.19377600	-0.63584600	H
C	0.79547200	-0.28162500	-0.60329600	H
O	1.33276100	2.10324600	-1.00562200	H
C	-1.33442700	2.65916900	-0.05131200	H
H	-2.24457600	2.68816300	-0.65301500	H
H	-0.61269800	3.37721400	-0.44254800	H
H	-1.59684300	2.90161600	0.97757600	H
C	4.41190900	-1.29629700	-3.71877200	H
C	3.33019100	-1.52572500	-2.87670600	H
C	3.05609000	-0.69933200	-1.76975100	H
C	3.97246700	0.34374600	-1.46780300	H
C	5.06164200	0.55968000	-2.32436500	H
C	5.27378100	-0.23692800	-3.44704100	H
C	-4.43642700	-1.28231500	1.47659300	H
C	-4.57231600	0.28210100	1.60968600	H
N	-3.22224900	0.81575200	1.28950400	H
C	-2.53327600	-0.11365400	0.71129600	H
N	-3.18358600	-1.35379800	0.64522500	H
C	3.65712600	1.56177700	2.01616500	H
N	3.43174600	0.60908400	0.90443500	H
C	3.90896000	1.08960800	-0.19211900	H
N	4.46565200	2.37181300	-0.04271200	H
C	4.18271700	2.89016300	1.33696400	H
O	-2.78687500	-2.42142200	0.09918600	H
C	1.81814900	-1.04194900	-1.06476600	H
H	1.61036000	-2.10829200	-1.00798900	H
H	5.74563700	1.36569800	-2.09864100	H
H	2.65234700	-2.34730100	-3.08639100	H
O	4.99723500	3.10033000	-0.93622900	H
H	4.57827900	-1.94049300	-4.57659000	H
H	6.12543900	-0.04030500	-4.09084600	H
C	3.13008500	4.00021700	1.17640100	H
H	2.23744400	3.63206400	0.66919100	H
H	2.85654700	4.41672600	2.14931800	H
H	3.55633800	4.79802800	0.56361700	H
C	2.33968500	1.72345100	2.78903700	H
H	2.01470200	0.74171500	3.14008100	H
H	2.46872600	2.37620300	3.65872300	H
H	1.54644700	2.13305800	2.16287700	H
C	4.68625200	0.88519300	2.94352300	H
H	4.90398600	1.50280900	3.82026300	H
H	4.27852600	-0.06977400	3.28443700	H
H	5.62270000	0.67615700	2.42158000	H
C	5.46939200	3.49245300	1.90997200	H
H	5.81747700	4.28360600	1.24121500	H
H	5.27842600	3.92874000	2.89481000	H
H	6.26911800	2.75689900	2.00708100	H
C	-4.11635300	-2.00848600	2.79420600	H
H	-4.99213100	-2.04426200	3.44744500	H

H	-3.81088400	-3.03147700	2.56191600	H
H	-3.29998100	-1.52491500	3.33436800	H
C	-5.55986500	-2.01563500	0.74450000	H
H	-5.26234500	-3.05455200	0.58986900	H
H	-6.47618800	-2.00062400	1.34151200	H
H	-5.77260400	-1.57998400	-0.23280900	H
C	-5.52298000	0.89682400	0.56249300	H
H	-6.55932700	0.59465600	0.73924100	H
H	-5.46513700	1.98524100	0.62686100	H
H	-5.24520900	0.60597200	-0.45337000	H
C	-4.98267600	0.77040900	3.00392200	H
H	-5.00705900	1.86287100	3.00948400	H
H	-5.97970700	0.40407700	3.26943600	H
H	-4.27872900	0.45167200	3.77429400	H
O	0.44646500	0.03370900	-4.01190900	H
H	-0.35625800	0.03538000	-3.43299900	H
H	1.00575500	0.77230200	-3.66363300	H
O	2.66331700	-2.40437500	2.18326900	H
H	2.05758900	-1.64957200	1.97679900	H
H	2.80391900	-2.85234300	1.31185200	H
O	-0.44647000	-1.61092900	3.36308200	H
H	-0.91369200	-2.06461500	2.61805900	H
H	-0.14645600	-0.75028800	2.97768700	H
O	-0.60098800	-3.10930600	-2.76021800	H
H	0.10103200	-2.72324800	-3.34133400	H
H	-1.12815800	-2.32901500	-2.45535700	H
O	-0.73303000	3.28430900	-3.51879200	H
H	-1.06312700	4.05183500	-2.98780400	H
H	-1.14721400	2.49217000	-3.09355600	H
O	2.80512700	3.44270200	-3.71959200	H
H	3.03774700	2.61071100	-3.23671600	H
H	2.03591700	3.19155400	-4.28966000	H
O	5.60792600	-2.04641100	0.06081000	H
H	5.17749700	-1.65605200	0.86184000	H
H	4.90149300	-2.60111500	-0.35468200	H
O	0.01418100	-4.12284500	1.03804000	H
H	-0.00213900	-3.79268700	0.10505300	H
H	0.80667300	-4.71467700	1.07866300	H
O	-3.97476500	-3.95170700	-2.61016200	H
H	-3.55545100	-3.26765500	-3.19002000	H
H	-4.46759700	-3.42962600	-1.92880900	H
O	-2.48463500	-0.99101700	6.13505500	H
H	-3.44627700	-1.10794400	5.92983100	H
H	-2.14933400	-0.39355200	5.42044400	H
O	3.47513700	1.14024400	-6.18709600	H
H	3.01038300	0.89940500	-5.34691200	H
H	4.07362200	0.37248400	-6.36780200	H
O	-4.21706400	4.45740900	1.69407000	H
H	-3.56672100	3.95692500	2.24778300	H
H	-4.06300900	4.12902200	0.77298700	H
O	-1.82554500	-1.96437500	-5.67976200	H
H	-1.29778900	-1.20327200	-6.02968100	H
H	-2.29531900	-1.59755700	-4.88939400	H
O	-3.07460400	-0.16832900	-2.57876200	H
H	-3.79054700	-0.69856900	-2.14777800	H
H	-3.18103600	0.74261000	-2.20650300	H
O	-4.33007600	3.73942300	-2.33777700	H

H	-4.57669800	3.07189600	-1.64955700	H
H	-3.77571100	3.23478700	-2.98438900	H
O	2.36844300	-5.07339800	-1.34963700	H
H	2.87416000	-4.32468800	-0.94494100	H
H	1.77694800	-4.64156300	-2.01580500	H
O	-3.60539400	-5.61642400	1.05957200	H
H	-3.96016500	-5.26822200	0.20338600	H
H	-2.77447800	-5.10024300	1.21170700	H
O	0.08839500	1.54720600	-6.91389700	H
H	0.37132600	2.05128000	-6.10999400	H
H	0.55637200	0.67774800	-6.83964000	H
O	4.78916500	-5.01541000	1.77137800	H
H	5.27429700	-4.19516600	2.04027400	H
H	4.80702800	-5.00144800	0.78151400	H
O	-1.26535400	1.84389000	3.92602600	H
H	-0.83797500	1.66032500	3.05247000	H
H	-2.15018100	2.22235800	3.69398500	H
O	1.74409600	-0.40371800	5.76336100	H
H	1.98488600	-1.03082400	5.03572600	H
H	0.91176900	0.03253000	5.45091400	H
O	1.75608900	7.38168000	1.56917100	H
H	2.52538200	7.20230000	0.97206300	H
H	1.95056200	6.86036500	2.38815800	H
O	-0.21725300	4.73880200	2.83596800	H
H	0.45477100	4.30262900	3.41762900	H
H	0.14551500	4.63832800	1.92052300	H
O	5.13273300	-4.69815700	-3.24679100	H
H	5.11612700	-4.17767000	-2.40482400	H
H	4.24331800	-4.54143700	-3.65287700	H
O	1.03170500	5.69406000	-1.42436400	H
H	1.46476500	4.83637300	-1.66179900	H
H	0.78268700	5.58923000	-0.47216100	H
O	-6.19794300	-1.79775300	-3.86383800	H
H	-6.18147200	-1.59633800	-2.89451800	H
H	-5.35125800	-1.41908300	-4.21067400	H
O	-3.16247900	1.52577800	-5.37910200	H
H	-2.28371400	1.16184000	-5.10430400	H
H	-3.79785000	0.78171300	-5.22694600	H
O	1.53732200	-2.40827100	-5.96392100	H
H	2.09234700	-3.09864900	-5.52149800	H
H	2.05188200	-1.56941300	-5.85605500	H
O	-1.14826100	-6.10394000	-1.49879500	H
H	-1.72348700	-5.31710200	-1.32506800	H
H	-0.90538300	-6.43681700	-0.59845300	H
O	-2.16994400	6.20340000	-0.39910500	H
H	-2.27818900	5.46898100	-1.05415200	H
H	-1.80508800	5.76322000	0.40923500	H
O	-2.15685000	-4.56290400	4.38174300	H
H	-1.64433600	-4.46183500	3.54066800	H
H	-2.19729200	-3.64830200	4.75893200	H
O	-6.45408900	-4.68985400	2.92354100	H
H	-5.54967000	-4.89615000	3.26982500	H
H	-6.42653200	-4.97157000	1.97475600	H
O	-7.34744300	-4.52878500	-0.96203900	H
H	-6.46750900	-4.97225000	-0.86457900	H
H	-7.15117100	-3.69366800	-1.45643000	H
O	7.79326000	0.97838100	0.17523200	H

H	7.56354400	1.87821300	-0.16780300	H
H	6.92553800	0.50541000	0.23072000	H
O	-7.74838200	3.10381200	2.73957400	H
H	-6.96344400	3.50191700	2.28618200	H
H	-7.91045800	2.25524300	2.25589700	H
O	-7.44703700	3.82341600	-0.87014900	H
H	-7.70277700	2.95246100	-0.47464600	H
H	-6.70029300	4.14381600	-0.30436500	H
O	8.03316100	1.45355500	4.04877100	H
H	7.52339400	0.69107200	4.42189900	H
H	8.19756500	1.20378800	3.10487500	H
O	7.99876800	-1.97996900	-2.34905100	H
H	7.74496600	-1.21847400	-1.76951700	H
H	7.15970300	-2.49213700	-2.46659500	H
O	4.43716800	6.37206300	-1.68493000	H
H	4.04235900	5.56702300	-2.10479300	H
H	5.19189700	6.02570900	-1.14549500	H
O	7.33638000	-1.99425900	2.95052000	H
H	7.50218100	-1.30835700	2.25595800	H
H	6.40397300	-1.83255300	3.24187800	H
O	-6.64839800	1.44183200	-3.10573700	H
H	-5.70751300	1.13707800	-3.15055700	H
H	-7.02997600	0.95612800	-2.33186400	H
O	6.21079800	3.26760300	-4.32211400	H
H	5.74856700	3.80480500	-3.63067000	H
H	5.50608800	2.67735800	-4.68992400	H
O	7.83870100	-4.42194300	0.24069500	H
H	8.10713900	-3.47086900	0.30318300	H
H	7.20106300	-4.45110700	-0.51634900	H

Diradical 3(b)

N	-1.54796100	-0.16187200	-0.61726800	H
C	-2.71128700	0.14137000	-1.12109300	H
N	-2.76970300	0.13815200	-2.51059700	H
C	-1.49195000	-0.21221000	-2.97653600	H
C	-0.72502900	-0.42167500	-1.71518800	H
O	-1.16505600	-0.32249700	-4.14557400	H
C	-3.87780800	0.43997000	-3.40121300	H
H	-3.48266400	0.35910500	-4.41521000	H
H	-4.25029400	1.45403700	-3.23544800	H
H	-4.69738400	-0.26336400	-3.25354200	H
C	2.14882800	-1.34776800	1.72393500	H
C	1.52294900	-0.68282400	0.65890000	H
C	1.32438300	-1.37205700	-0.56086800	H
C	1.86418900	-2.66492800	-0.69170200	H
C	2.49669500	-3.30469200	0.36782600	H
C	2.61688800	-2.65042300	1.59364200	H
H	1.74517800	-3.18289000	-1.63810200	H
H	2.88811700	-4.30836000	0.23655100	H
C	-5.12106400	0.58491500	1.70871800	H
C	-6.04299000	0.34972000	0.45107800	H
N	-5.10126000	-0.00556100	-0.64753500	H
C	-3.90959900	0.34648000	-0.29490700	H
N	-3.82826000	0.87389100	0.99982000	H
C	0.97800200	3.05053200	0.38165200	H

N	1.39500900	1.70446400	-0.13004900	H
C	1.22822600	0.74838500	0.88182900	H
N	0.95460700	1.26217900	2.03428900	H
C	0.99429600	2.74339100	1.92979300	H
O	1.76432100	1.49950000	-1.32628500	H
O	-2.83108700	1.41207200	1.56115300	H
C	0.53866700	-0.90399100	-1.70774400	H
H	0.95021000	-1.10803100	-2.69392200	H
H	2.27346200	-0.80303800	2.65195100	H
H	3.09664600	-3.13985000	2.43472400	H
C	-7.06371300	-0.78088700	0.61329600	H
H	-7.76964700	-0.55677200	1.41903400	H
H	-7.63009800	-0.89233800	-0.31477400	H
H	-6.58377900	-1.73673800	0.82602200	H
C	-6.77194500	1.62882500	-0.00554600	H
H	-7.26872400	1.43700500	-0.95925600	H
H	-7.53018900	1.93311400	0.72182700	H
H	-6.07650500	2.45951200	-0.14969300	H
C	-5.47911500	1.75569700	2.62070000	H
H	-6.41670900	1.55086700	3.14486900	H
H	-4.69014400	1.89020100	3.36381700	H
H	-5.58535200	2.69175100	2.07116000	H
C	-4.86555200	-0.67821900	2.55124600	H
H	-4.03884900	-0.48012300	3.23790000	H
H	-5.74895300	-0.94449500	3.13568200	H
H	-4.59099100	-1.53164600	1.92767200	H
C	-0.18645300	3.33623300	2.70649300	H
H	-0.19536900	4.42890000	2.62849200	H
H	-1.14011400	2.94494400	2.35478700	H
H	-0.08708000	3.07358500	3.76303700	H
C	2.30642800	3.17533500	2.61352600	H
H	2.40407400	4.26410000	2.62958900	H
H	2.30269000	2.81500300	3.64463400	H
H	3.18382200	2.75672000	2.11496400	H
C	-0.42089800	3.32576700	-0.19533200	H
H	-1.14589000	2.58227300	0.13920000	H
H	-0.77034100	4.31883900	0.09957200	H
H	-0.35817000	3.29328600	-1.28691500	H
C	1.96050600	4.10706700	-0.12578000	H
H	1.66431900	5.09723800	0.23249800	H
H	2.98459500	3.91267400	0.19528800	H
H	1.94694800	4.11526000	-1.21812900	H
O	-1.25046800	-1.60763000	2.33193700	L
H	-1.19765200	-0.62463600	2.42948000	L
H	-1.97274000	-1.75170200	1.67143900	L
O	-2.25264400	1.56491100	5.04009600	L
H	-2.02396200	1.03906300	4.23334100	L
H	-1.97636600	0.99002500	5.79722100	L
O	-3.81811500	-2.93613000	-4.27153000	L
H	-3.55541300	-2.72625900	-3.34039800	L
H	-3.20388600	-2.39614000	-4.82966400	L
O	1.42200200	1.81044500	-4.49728600	L
H	1.62940100	0.86581400	-4.28614400	L
H	0.69760500	2.05157800	-3.86712800	L
O	4.06789100	3.27825100	-3.03710900	L
H	4.12501900	2.46338600	-2.47810300	L
H	5.00874200	3.49195800	-3.25930000	L

O	-3.68752500	-2.99762700	-0.37828000	L
H	-2.81715700	-2.86556800	-0.83051600	L
H	-3.46292200	-3.47739900	0.45737000	L
O	-5.79002500	0.28998700	5.90076300	L
H	-5.95481700	-0.67447100	5.74905300	L
H	-4.84597200	0.42478400	5.63503000	L
O	4.79196300	1.02844100	0.69186000	L
H	4.33240100	1.52076000	-0.03316400	L
H	4.44146800	0.10565100	0.62686100	L
O	4.12113700	-0.72447900	-2.16318500	L
H	4.91932400	-0.15422600	-2.03435000	L
H	3.50694500	-0.17126800	-2.70698700	L
O	0.86960000	0.07615700	5.24188100	L
H	0.33895600	-0.29209000	4.49201100	L
H	0.89407200	1.05098200	5.07203900	L
O	-0.74025800	-4.52096500	0.95243600	L
H	-0.18729400	-4.15322000	1.68642200	L
H	-0.70481200	-3.82892200	0.24550000	L
O	-4.44308900	-6.38743600	0.79658500	L
H	-4.84646500	-5.78147400	0.12530800	L
H	-3.50186000	-6.08838600	0.86778200	L
O	0.36612400	-1.40240800	-6.75527300	L
H	0.33997600	-1.98458800	-5.95479900	L
H	0.71904100	-0.53903900	-6.42290500	L
O	4.55465100	-4.58556000	-2.23903000	L
H	4.49732400	-3.59925600	-2.17696100	L
H	3.64085000	-4.87110100	-2.49160200	L
O	3.12586300	-2.37909700	-4.84636100	L
H	2.70894600	-2.64372500	-3.98850500	L
H	2.89041100	-1.42324800	-4.95140900	L
O	1.10989800	5.57227200	5.12801800	L
H	1.49941100	4.69009300	5.35246600	L
H	1.71791700	5.94483700	4.44103700	L
O	0.27413400	-3.24497400	4.80537500	L
H	0.75550400	-2.90834900	4.00868500	L
H	-0.38462300	-3.88840700	4.44207500	L
O	4.02124900	6.49652200	1.61237800	L
H	4.41538000	5.94748300	2.33582300	L
H	3.10155300	6.69211100	1.92286600	L
O	-2.16401400	6.74754300	0.74383700	L
H	-2.91456700	6.12933100	0.55739700	L
H	-1.69642300	6.34437000	1.51797100	L
O	1.15731100	-6.21604000	-1.41542000	L
H	0.48893600	-5.51269500	-1.61157700	L
H	1.19396200	-6.25417000	-0.42675100	L
O	-1.90603700	1.58240000	-6.68804900	L
H	-2.02950700	0.60261000	-6.76053400	L
H	-1.03841700	1.68966100	-6.22313100	L
O	-1.90325100	3.54711800	-4.00530900	L
H	-1.75258700	2.79508000	-3.37964800	L
H	-2.83585100	3.42751800	-4.31555000	L
O	-0.74760400	-3.66022600	-3.56171700	L
H	0.21655200	-3.49106600	-3.70828400	L
H	-0.90086900	-3.42004900	-2.61353400	L
O	-2.76913100	-5.83065100	-2.20637700	L
H	-3.56328800	-5.24069800	-2.24673800	L
H	-2.24131100	-5.48445900	-1.44363100	L

O	-3.61361300	3.54699800	-1.19803900	L
H	-3.64567200	3.59462400	-0.20990700	L
H	-3.21373600	4.40914200	-1.47486800	L
O	-2.86051700	-1.94301700	5.70014900	L
H	-2.30401200	-1.61475700	4.95011400	L
H	-3.73194100	-2.16328200	5.28486900	L
O	-2.94436700	-4.45018000	3.30261100	L
H	-3.71820800	-4.98535300	3.61058500	L
H	-3.32754200	-3.56480800	3.08121300	L
O	-6.45378900	-4.03029600	2.59626400	L
H	-5.76230800	-3.94288300	1.89313600	L
H	-6.07211900	-3.55957900	3.37930400	L
O	5.26415800	0.62914200	-5.09047500	L
H	5.76366500	0.95412900	-4.29972600	L
H	4.34398900	0.97077000	-4.96058000	L
O	4.52166400	0.78717300	3.81949100	L
H	3.61591200	0.66969100	4.20051300	L
H	5.11746000	0.84490400	4.60798100	L
O	-6.46380200	-3.29689200	-2.02277000	L
H	-6.41883700	-3.59909600	-1.08088800	L
H	-5.94433800	-2.45423400	-2.03836900	L
O	5.99630100	-2.06735100	3.13188900	L
H	5.46561600	-2.76498500	3.59204600	L
H	5.34229500	-1.59853300	2.55531400	L
O	-3.50944600	4.67380700	3.21116400	L
H	-3.07169400	4.08497700	3.87576800	L
H	-3.37538900	4.21272300	2.34540800	L
O	-6.22724500	5.29880600	0.34363300	L
H	-5.71587100	5.48646300	-0.48315300	L
H	-5.53509500	5.10182000	1.02343300	L
O	3.38774600	2.05747300	6.91107700	L
H	3.23016900	1.08540100	6.80753600	L
H	2.86544100	2.47303500	6.17984400	L
O	5.12667700	-5.43299700	1.74486200	L
H	4.71754300	-5.23962500	2.62548100	L
H	5.35337300	-4.54259500	1.37615800	L
O	7.90772200	4.96263500	2.84395500	L
H	7.05173200	5.45894000	2.88199000	L
H	7.84168100	4.29742100	3.57439600	L
O	3.38465300	-1.99682000	5.76494500	L
H	4.23154800	-1.48903100	5.83736900	L
H	3.15403600	-1.95761800	4.80314500	L
O	-6.66799800	3.96722300	-2.92998900	L
H	-5.99198200	3.27513100	-2.72063800	L
H	-7.35960900	3.85787100	-2.22991900	L
O	6.07274500	4.07803800	0.30952300	L
H	5.48648600	3.98979000	-0.48328200	L
H	5.49559700	3.82855100	1.07429600	L
O	6.36146700	-2.24294100	-0.21070900	L
H	6.61813500	-1.29726900	-0.06920800	L
H	5.38620200	-2.26332700	-0.04154700	L
O	6.85968000	-2.17816700	-3.49472400	L
H	5.99210200	-2.07357400	-3.96030100	L
H	7.05158900	-1.28099700	-3.12229900	L
O	1.63925600	-5.94453600	3.11512800	L
H	2.16468800	-5.27939500	3.62679500	L
H	1.96538200	-5.85574700	2.18457600	L

O	-8.64072100	-1.02039500	4.27003700	L
H	-8.17405900	-0.18589200	4.01291700	L
H	-8.10723900	-1.74237800	3.85239500	L
O	-7.63941900	0.19143200	-3.62890700	L
H	-7.04941600	0.98540600	-3.58784100	L
H	-7.32716300	-0.38809000	-2.88953200	L
O	7.41283800	1.29339000	-1.45513100	L
H	6.64351800	1.83785300	-1.75813600	L
H	7.43020400	1.41407900	-0.47259500	L
O	5.04066500	3.98867500	4.70907800	L
H	4.23156000	4.55929600	4.70344800	L
H	5.13232400	3.67866400	3.77329700	L
O	7.58804400	1.29097400	2.60385300	L
H	6.89485500	1.98164400	2.45322200	L
H	7.23982100	0.48552700	2.14515400	L

PCM OPTIMIZED XYZ CO-ORDINATES

Diradical 1(a)

N	1.33225400	1.29084800	0.52333400	
C	1.99764300	0.54026800	-0.30675400	
N	1.21052800	-0.06104700	-1.29103600	
C	-0.11011700	0.33399500	-1.06924500	
C	-0.00850600	1.21796100	0.12077400	
O	-1.07045700	0.00930400	-1.76218900	
C	1.60240300	-0.89084900	-2.42242300	
H	2.38894700	-0.40450300	-3.00201300	
H	0.71108900	-1.01058000	-3.03946600	
H	1.96166400	-1.86511500	-2.08956400	
C	-4.14760800	3.82568300	0.16063300	
C	-2.84780700	3.47346900	0.49703400	
C	-2.38444700	2.14311600	0.44769300	
C	-3.33039300	1.12803300	0.12951900	
C	-4.63867600	1.48298200	-0.20181400	
C	-5.04747600	2.82206400	-0.21007100	
C	5.63680400	0.48068700	0.62917300	
C	5.48451000	-0.65972700	-0.44661500	
N	4.01497000	-0.78456100	-0.66022700	
C	3.43971100	0.27997000	-0.20562600	
N	4.31159600	1.17054200	0.43664500	
C	-2.41820200	-2.26372700	1.31358000	
N	-2.32410100	-0.77996000	1.29617700	
C	-3.04015200	-0.31137400	0.33187800	
N	-3.64277100	-1.30557900	-0.45520000	
C	-3.15325700	-2.65958800	-0.03078900	
O	4.05305300	2.32096100	0.89671500	
C	-0.96051400	1.97897600	0.72252000	
H	-0.56028800	2.66106700	1.47126800	
H	-5.36506400	0.71959300	-0.44608800	
H	-2.14882400	4.25604900	0.77645900	
O	-4.36809800	-1.13429800	-1.48455400	
H	-4.46000200	4.86574300	0.18932200	

O	-6.33707600	3.07052600	-0.55564500
H	-6.50832500	4.02265200	-0.52215800
C	-1.00438200	-2.84595500	1.45790000
H	-0.34939500	-2.54743200	0.63748700
H	-0.56206400	-2.48323300	2.38953700
H	-1.03506500	-3.93941100	1.49727000
C	-3.22472600	-2.61547700	2.58060200
H	-3.32761900	-3.69833400	2.69598400
H	-2.69952900	-2.22419000	3.45573400
H	-4.22222300	-2.16924300	2.56302200
C	-4.35504800	-3.60198600	0.10175500
H	-4.85341800	-3.68550000	-0.86722300
H	-4.02046900	-4.59830900	0.40334100
H	-5.08623000	-3.24594400	0.82925600
C	-2.23024400	-3.16953000	-1.15168100
H	-1.41461400	-2.47278100	-1.34869600
H	-1.81908100	-4.14934400	-0.89661100
H	-2.81604600	-3.26825000	-2.06951500
C	5.64976300	-0.02649600	2.08335100
H	6.59654500	-0.52238700	2.31077800
H	5.53620200	0.82726500	2.75690000
H	4.83343600	-0.72669700	2.27819600
C	6.77190900	1.48124200	0.41822700
H	6.70004800	2.27558800	1.16475100
H	7.73594400	0.98036300	0.54161000
H	6.74176600	1.94171700	-0.57042700
C	6.07647400	-0.27835200	-1.81984700
H	7.16785700	-0.22343300	-1.77496100
H	5.80121600	-1.04273000	-2.55101400
H	5.69278100	0.68210600	-2.17473700
C	6.04757400	-2.01964000	-0.01939400
H	5.87698800	-2.74657700	-0.81804800
H	7.12581000	-1.95521100	0.15698000
H	5.56938400	-2.39779600	0.88592700

Diradical 1(b)

N	-0.32675100	-1.11160800	-0.04462200
C	-1.54421300	-1.19115900	-0.50917800
N	-1.69543500	-2.04105700	-1.60491700
C	-0.43841100	-2.58495800	-1.88137000
C	0.43267600	-1.97192600	-0.84229500
O	-0.17921800	-3.37322300	-2.78267300
C	-2.87284800	-2.33703000	-2.41033400
H	-2.52225700	-2.92655900	-3.25858600
H	-3.33788200	-1.41684700	-2.76817700
H	-3.60757200	-2.90478800	-1.83905900
C	3.77313500	-0.29298200	1.81960900
C	2.92133200	-0.54233800	0.73586300
C	2.69289200	-1.87584200	0.31720900
C	3.41501500	-2.90033200	0.96316900
C	4.25557700	-2.65116600	2.03706200
C	4.41992600	-1.33547500	2.48679100
H	3.27714900	-3.92403100	0.62817600
H	4.78710900	-3.45574600	2.53354200
O	5.24385300	-1.13021200	3.54855400

H	5.27803700	-0.18602000	3.75894200
C	-3.86495300	0.88960400	1.59331300
C	-4.81896300	0.00751400	0.70097000
N	-3.91308800	-0.95948100	0.01968600
C	-2.70072900	-0.51903800	0.10115300
N	-2.56741300	0.64505300	0.86904100
C	1.80230600	2.07695200	-1.76359700
N	2.38963900	0.75345000	-1.36325700
C	2.42523700	0.66557800	0.03622100
N	2.14116700	1.77887500	0.62718800
C	1.98018400	2.84693600	-0.39817900
O	2.72681100	-0.14452700	-2.19538200
O	-1.52635100	1.34209200	1.05249000
C	1.73736400	-2.30886300	-0.70074900
H	2.07492800	-3.09477000	-1.37411700
H	3.94188500	0.73697800	2.11781700
C	0.80069500	3.74965200	-0.01826700
H	0.65513500	4.53378700	-0.76865400
H	-0.12732700	3.18768200	0.09170400
H	1.01471400	4.23433300	0.93869600
C	-5.88529300	-0.76783100	1.48175700
H	-6.56070500	-0.07990900	1.99955300
H	-6.47808300	-1.36644700	0.78494900
H	-5.44604800	-1.44390500	2.21711700
C	-3.66812400	0.35260800	3.02336100
H	-2.84135900	0.89129600	3.49412600
H	-4.56947900	0.51114800	3.62051700
H	-3.42861300	-0.71370600	3.02855600
C	-4.15350000	2.38930300	1.63651600
H	-5.10240300	2.56995100	2.14858100
H	-3.36199700	2.89639900	2.19306400
H	-4.20490000	2.83206300	0.64070300
C	-5.50162700	0.80908300	-0.42720100
H	-6.02602600	0.11662700	-1.09057600
H	-6.23170000	1.51331600	-0.01880600
H	-4.77512000	1.36596000	-1.02512900
C	3.28200700	3.67419100	-0.34235600
H	3.23940300	4.52189500	-1.03231200
H	3.41412200	4.06249400	0.67095900
H	4.15880400	3.06846400	-0.58788500
C	0.33509200	1.81746600	-2.15009400
H	-0.24107000	1.43399100	-1.30648200
H	-0.13236600	2.73836200	-2.50889900
H	0.30826500	1.08146100	-2.95904200
C	2.56422300	2.62766000	-2.96970900
H	2.16581200	3.60826700	-3.24420600
H	3.63335300	2.72810200	-2.77624000
H	2.43593200	1.95497900	-3.82123900

Diradical 2(a)

N	1.23154200	1.23728700	0.52476600
C	1.91141400	0.53333100	-0.33251100
N	1.14924800	-0.00869600	-1.36902400
C	-0.17618400	0.37511300	-1.15785500
C	-0.10056300	1.19449000	0.08619100

O	-1.12200800	0.08135700	-1.87958100
C	1.57091700	-0.77328300	-2.53574100
H	2.36107300	-0.24724800	-3.07474300
H	0.69202100	-0.86989100	-3.17415700
H	1.93618400	-1.75915800	-2.24767300
C	-4.24397600	3.71229800	-0.03365600
C	-2.93692600	3.38834400	0.33513400
C	-2.49668600	2.05482100	0.37833300
C	-3.42141000	1.01666500	0.10484100
C	-4.73379700	1.36563800	-0.25457000
C	-5.14725800	2.68876200	-0.33674100
C	5.53069600	0.41045500	0.67576100
C	5.38604500	-0.70661900	-0.42634700
N	3.92017900	-0.80476600	-0.67744300
C	3.35005900	0.25591800	-0.20900300
N	4.21620000	1.11893900	0.47443700
C	-2.40470100	-2.33331500	1.32562000
N	-2.35528100	-0.84770100	1.29752000
C	-3.10121800	-0.40549500	0.34190400
N	-3.68002200	-1.42806500	-0.43150000
C	-3.11951300	-2.75757300	-0.01925800
O	3.95733300	2.25844900	0.96019600
C	-1.07441700	1.88945700	0.71944000
H	-0.72168300	2.50223900	1.54761500
H	-5.44412900	0.57793300	-0.46881600
H	-2.23326400	4.18453800	0.56435900
O	-4.41831400	-1.28806000	-1.45705400
H	-6.16524900	2.94014500	-0.61391300
O	-4.69089500	4.99463200	-0.10939500
H	-3.97432100	5.60535700	0.11500400
C	-0.97752700	-2.87698000	1.48281400
H	-0.32423500	-2.56533400	0.66585500
H	-0.55116100	-2.49914500	2.41602100
H	-0.97997700	-3.97061200	1.52686100
C	-3.21140100	-2.70020900	2.58844300
H	-3.27793800	-3.78471100	2.71498600
H	-2.70931900	-2.28145600	3.46445700
H	-4.22364200	-2.28903800	2.55580500
C	-4.26376500	-3.76881500	0.10365100
H	-4.75722600	-3.87202500	-0.86598100
H	-3.87112900	-4.74688300	0.39539900
H	-5.01357900	-3.46278200	0.83487200
C	-2.16850100	-3.20114600	-1.14560400
H	-1.70853200	-4.16318000	-0.90677900
H	-2.74564000	-3.31237100	-2.06749000
H	-1.38657200	-2.46239600	-1.32806900
C	5.51188400	-0.12491800	2.11964800
H	6.44842200	-0.63693100	2.35339100
H	5.39730300	0.71724800	2.80740500
H	4.68358900	-0.81809700	2.28692100
C	6.68036300	1.40184800	0.50413100
H	6.60610200	2.18109200	1.26617100
H	7.63637600	0.88679400	0.63180900
H	6.67146100	1.88301500	-0.47503400
C	5.91788200	-2.08329700	-0.01315800
H	5.75343700	-2.79234000	-0.82896900
H	6.99279800	-2.03909000	0.18751800

H	5.41418200	-2.47027100	0.87437200
C	6.01484700	-0.30847300	-1.77839100
H	7.10555200	-0.27028900	-1.70754600
H	5.74602600	-1.05530000	-2.52974700
H	5.65317500	0.66375100	-2.12418600

Diradical 2(b)

N	0.27559800	-1.03286900	0.20686600
C	1.46565000	-1.07141500	0.73808100
N	1.52630500	-1.66050700	2.00027400
C	0.22820600	-2.05374100	2.33455800
C	-0.56701900	-1.64638700	1.14059900
O	-0.11249000	-2.59865100	3.37611600
C	2.66013100	-1.82603900	2.90008400
H	2.25560000	-2.21886700	3.83379300
H	3.14867600	-0.86764600	3.08715700
H	3.38995400	-2.52186900	2.48598100
C	-3.67817000	-0.37887000	-1.97725900
C	-2.91270800	-0.42523100	-0.80162500
C	-2.74742000	-1.67338700	-0.15205900
C	-3.40758800	-2.80000700	-0.65987800
C	-4.16692100	-2.72978700	-1.83067400
C	-4.28919200	-1.50923600	-2.50457000
H	-3.30533900	-3.75978200	-0.16399200
C	3.96069500	0.46325500	-1.61593400
C	4.83443500	-0.36518300	-0.59735900
N	3.84715600	-1.13622200	0.21128900
C	2.68054100	-0.60558000	0.05076700
N	2.64823700	0.44070500	-0.87823000
C	-1.82232700	2.52954100	1.29171000
N	-2.45780700	1.18722800	1.07856800
C	-2.42548200	0.86936300	-0.28921800
N	-2.06263300	1.86215000	-1.03374100
C	-1.91384400	3.07648800	-0.18490900
O	-2.87571700	0.44693200	2.02327600
O	1.67167700	1.19339600	-1.16649800
C	-1.88555600	-1.91517600	1.01636200
H	-2.32285700	-2.48110900	1.83601900
H	-3.80153200	0.57908600	-2.46982600
H	-4.87665000	-1.44025600	-3.41598300
O	-4.75721700	-3.87708400	-2.26012800
H	-5.25173900	-3.70460800	-3.07396500
C	-0.38288500	2.27133200	1.77298500
H	0.19915700	1.72675400	1.02713000
H	0.12064600	3.21650600	1.99333700
H	-0.41797600	1.67962300	2.69261100
C	-0.68811800	3.87421400	-0.64423000
H	-0.54528600	4.76096400	-0.01790500
H	0.22306400	3.27487700	-0.62311300
H	-0.84444000	4.20979500	-1.67351600
C	-3.18263500	3.91924700	-0.43183100
H	-3.13909000	4.86862300	0.11015500
H	-3.26245600	4.13747400	-1.50007900
H	-4.08818700	3.38589400	-0.12923400
C	-2.59616500	3.29960400	2.36207100

H	-2.15893900	4.29323000	2.49349000
H	-3.65205600	3.41419500	2.11167600
H	-2.53004100	2.76786400	3.31442100
C	3.71103400	-0.25219900	-2.95651400
H	2.93364800	0.28571500	-3.50568800
H	4.61986200	-0.26141600	-3.56297500
H	3.37691200	-1.28274300	-2.81233100
C	4.38452000	1.90874400	-1.86937500
H	5.34681700	1.92619700	-2.38806100
H	3.64367700	2.39955400	-2.50479000
H	4.47515500	2.48411100	-0.94685700
C	5.59530400	0.52398900	0.40832400
H	6.05540400	-0.11089400	1.16978500
H	6.38656700	1.08983800	-0.09144100
H	4.92706200	1.22744200	0.91243900
C	5.81895600	-1.34089900	-1.25173700
H	6.54669100	-0.80178000	-1.86614800
H	6.36419600	-1.88024600	-0.47255800
H	5.31296000	-2.07703700	-1.87887200

Diradical 3(a)

N	1.18195200	1.32597500	0.50654200
C	1.81443900	0.56066800	-0.33465600
N	1.01413400	0.04076100	-1.35453600
C	-0.28394700	0.50940300	-1.14604600
C	-0.15174900	1.35404600	0.07407100
O	-1.25124000	0.25653400	-1.85584900
C	1.37795500	-0.77921400	-2.50298300
H	2.20292600	-0.32415800	-3.05368400
H	0.49304000	-0.82806100	-3.13862400
H	1.67251100	-1.78190100	-2.19220800
C	-4.11971900	4.16301500	-0.04830300
C	-2.84273200	3.75225200	0.32233600
C	-2.48179800	2.39173100	0.35377500
C	-3.47896600	1.42277000	0.07145100
C	-4.76374800	1.85142700	-0.29270800
C	-5.08227700	3.20639400	-0.36676400
C	5.41553400	0.22286700	0.68825800
C	5.21836600	-0.86133200	-0.43783200
N	3.75098400	-0.87622700	-0.69723800
C	3.23468900	0.20395900	-0.21042400
N	4.14264200	1.00539800	0.49496400
C	-2.71803400	-1.98045800	1.32955700
N	-2.56284700	-0.50252600	1.28636000
C	-3.25983400	-0.02106500	0.31389100
N	-3.90032200	-1.00532700	-0.45708500
C	-3.45226500	-2.36873500	-0.01652800
O	3.94354000	2.14476100	1.00834800
C	-1.07441200	2.13386400	0.68747500
H	-0.67186100	2.74931000	1.49050900
H	-5.52092200	1.10958700	-0.51027700
H	-2.09010700	4.49554100	0.56827300
O	-4.61870600	-0.82371500	-1.48977600
H	-4.35959500	5.22101800	-0.08191600
H	-6.08541100	3.50808800	-0.65095500

C	-2.53199700	-2.91015000	-1.12504900
H	-1.69294100	-2.23953900	-1.31544000
H	-2.15224700	-3.90041500	-0.86181800
H	-3.10979500	-2.99497600	-2.04931300
C	-1.33193200	-2.61816200	1.50267500
H	-0.88724300	-2.25833200	2.43431400
H	-1.40850100	-3.70858800	1.55949200
H	-0.65418200	-2.36054500	0.68673100
C	-3.55513300	-2.27567100	2.59132000
H	-3.70126800	-3.35130100	2.72619300
H	-3.02734400	-1.88748800	3.46628900
H	-4.53451500	-1.79209600	2.55068200
C	-4.67815500	-3.27922900	0.11257500
H	-5.17004400	-3.35898200	-0.86003100
H	-4.37095400	-4.28090200	0.42534100
H	-5.40652200	-2.89898900	0.83056000
C	5.35831500	-0.34093000	2.12026100
H	6.26351600	-0.90920000	2.34731800
H	5.28613800	0.49145400	2.82543600
H	4.49178400	-0.99044100	2.26790600
C	6.61735400	1.15519400	0.54444900
H	6.57723800	1.92219700	1.32129800
H	7.54415900	0.58837000	0.66854800
H	6.64157100	1.65528200	-0.42493200
C	5.87581600	-0.46855500	-1.77769600
H	6.96645700	-0.48786000	-1.69886200
H	5.57470100	-1.18513700	-2.54607000
H	5.56678900	0.52787100	-2.10509500
C	5.67513400	-2.27220100	-0.05085600
H	5.48078400	-2.95506600	-0.88230200
H	6.74931800	-2.28696400	0.15783800
H	5.14566500	-2.65051500	0.82532700

Diradical 3(b)

N	-0.22751500	-1.12337400	0.14147800
C	-1.39116700	-1.19241800	-0.44350800
N	-1.45760500	-2.08256400	-1.51474800
C	-0.19530600	-2.66642800	-1.64431700
C	0.58488100	-2.03479400	-0.54231800
O	0.13195600	-3.49423200	-2.48444100
C	-2.56021000	-2.37598800	-2.42088200
H	-2.15497100	-3.02908600	-3.19481900
H	-2.94059100	-1.45975200	-2.87678500
H	-3.37473000	-2.87626000	-1.89705800
C	3.66813000	-0.30396500	2.37579600
C	2.95338000	-0.58905600	1.20155600
C	2.69264600	-1.93837200	0.86391100
C	3.23134300	-2.95114700	1.67829700
C	3.93970600	-2.65242300	2.83849600
C	4.14461300	-1.31970100	3.19931500
H	3.05705400	-3.98767700	1.40518500
H	4.32917900	-3.45599700	3.45562600
C	-3.83294300	1.09185500	1.27582700
C	-4.73230700	0.11319700	0.42627900
N	-3.78796500	-0.91406200	-0.09698100

C	-2.58283100	-0.46382100	0.01897500
N	-2.49130800	0.77129900	0.67041600
C	2.27849100	1.84075500	-1.62338500
N	2.75697300	0.54037700	-1.04433200
C	2.61589100	0.57345400	0.35125000
N	2.31158800	1.74363400	0.80708000
C	2.32747600	2.72160100	-0.31603700
O	3.14926200	-0.44161700	-1.74819600
O	-1.45799600	1.48139200	0.84764600
C	1.85805100	-2.38959000	-0.25770500
H	2.25962600	-3.19407700	-0.87036200
H	3.85797200	0.73558700	2.61850600
H	4.69410700	-1.07194600	4.10189400
C	-5.84013400	-0.58570000	1.22247200
H	-6.54468600	0.14586000	1.62983900
H	-6.39171100	-1.25697600	0.55885900
H	-5.44178100	-1.18004200	2.04657400
C	-5.35045800	0.78523900	-0.81722800
H	-5.83465400	0.02188200	-1.43146800
H	-6.10419300	1.52293000	-0.52798700
H	-4.59205000	1.28103400	-1.42905800
C	-4.11694200	2.58610600	1.13259700
H	-5.09803400	2.81846000	1.55561300
H	-3.36300400	3.15430100	1.68232900
H	-4.09836200	2.91524700	0.09250400
C	-3.73114400	0.71828800	2.76637900
H	-2.93485400	1.30974400	3.22599300
H	-4.66841100	0.93822900	3.28309000
H	-3.49554100	-0.33968800	2.90656800
C	1.15427400	3.69609900	-0.16185800
H	1.13319600	4.41100900	-0.99088100
H	0.19535500	3.17848000	-0.11458100
H	1.27694100	4.25973400	0.76745700
C	3.65026500	3.50274200	-0.16794900
H	3.72830000	4.29249900	-0.92090300
H	3.67966900	3.96754500	0.82103400
H	4.52118400	2.84748500	-0.25758300
C	0.85607700	1.59556000	-2.15918000
H	0.17185700	1.29723100	-1.36291400
H	0.46846100	2.49925300	-2.63726100
H	0.89254900	0.79943600	-2.90854800
C	3.19849300	2.25706000	-2.77131300
H	2.87240700	3.21777800	-3.17914700
H	4.23992300	2.34682300	-2.45839600
H	3.14741100	1.51108700	-3.56815800