

Electronic Supplementary Material

Regio- and Diastereoselectivity of the 1,3-Dipolar Cycloaddition of α -aryl Nitron with Methacrolein. A Theoretical Investigation

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Z- α -aryl nitron**E=-855.8526317 a.u.**

N	-2.87663800	-0.10128200	-0.00099900
C	-1.88310900	0.76617100	-0.00334700
C	-0.46608500	0.46174400	-0.01625900
C	0.07354000	-0.84262100	-0.03356700
C	1.45235800	-1.02879300	-0.04536700
C	2.32074300	0.06582400	-0.04160000
C	1.80027400	1.36451700	-0.02663300
C	0.42634900	1.55648500	-0.01479700
H	-0.60085300	-1.68723800	-0.04002600
H	1.85751400	-2.03533600	-0.06498500
H	2.47097800	2.21738100	-0.03187000
H	0.02946700	2.56876200	-0.00719300
O	-2.75771600	-1.37025000	-0.01071400
C	-4.29820700	0.40129900	0.01493600
C	-4.97497800	-0.09590800	1.29249100
C	-4.99822400	-0.08012000	-1.25606600
H	-2.18233000	1.80710000	0.00659100
H	-4.24224200	1.49417200	0.02124600
H	-6.01507100	0.24492700	1.31661900
H	-4.95730900	-1.18809000	1.32176400
H	-4.46554800	0.28632400	2.18332500
H	-4.98125400	-1.17185700	-1.29910300
H	-6.03854300	0.26091200	-1.25689400
H	-4.50510600	0.31311200	-2.15127900
C	3.80752900	-0.14930500	0.00791400
F	4.17274100	-1.29895000	-0.60193900
F	4.48373100	0.85927300	-0.58847600
F	4.26212300	-0.22198500	1.28244600

***E*- α -aryl nitron 1**
E=-855.8399629 a.u.

N	-3.10592600	0.61716500	-0.21066100
C	-1.97200200	1.26765300	-0.39925900
C	-0.59467800	0.79636700	-0.28323300
C	-0.13974600	-0.48883900	-0.64505500
C	1.20355900	-0.83164600	-0.53201600
C	2.13512900	0.10429400	-0.07568500
C	1.71136100	1.39553000	0.25232100
C	0.36891400	1.73511700	0.14260700
H	-0.83027400	-1.21477500	-1.06029300
H	1.53409700	-1.82269300	-0.82563600
H	2.43291000	2.13289500	0.58805300
H	0.04879500	2.74098600	0.40003500
O	-4.23607900	1.16136700	-0.42799600
C	-3.18645400	-0.78078200	0.34738700
C	-3.75911000	-1.70490200	-0.72811700
C	-4.05016700	-0.73868300	1.60979600
H	-2.13781800	2.30600800	-0.66806900
H	-2.17236800	-1.07893900	0.61459100
H	-3.87108200	-2.71739500	-0.32715100
H	-4.73871900	-1.33701800	-1.04453000
H	-3.10877100	-1.75400300	-1.60871000
H	-5.05838000	-0.39577400	1.37000500
H	-4.10324000	-1.74278100	2.04327100
H	-3.61938500	-0.06449900	2.35731000
C	3.57548700	-0.28937600	0.09758500
F	3.95824300	-1.21053400	-0.81515200
F	4.40559900	0.77039800	-0.02013200
F	3.80289000	-0.83225200	1.31770000

Methacrolein 2-trans**E=-231.2335429 a.u.**

C	-1.51237000	-0.93857300	-0.00008600
H	-2.54783800	-0.60936300	-0.00025800
H	-1.34298500	-2.01331600	-0.00003300
C	-0.48557800	-0.07556800	0.00006900
C	-0.61361000	1.42203000	0.00001300
H	-1.66128500	1.73532800	-0.00018300
H	-0.11522700	1.85084600	0.87689100
H	-0.11491000	1.85081100	-0.87670100
C	0.88683200	-0.63646400	0.00034900
H	0.93939800	-1.74810500	-0.00030600
O	1.89890000	0.03815700	-0.00018500

Methacrolein 2-cis**E=-231.2288582 a.u.**

C	-0.37832000	1.46091600	-0.00000200
H	-1.27873200	2.06912500	0.00004500
H	0.57952400	1.97286400	-0.00001800
C	-0.42263300	0.12176000	-0.00002300
C	-1.69049700	-0.69285300	0.00001700
H	-2.57692100	-0.05241200	0.00006200
H	-1.74513100	-1.34610900	-0.88094500
H	-1.74506100	-1.34613800	0.88096100
C	0.86462800	-0.63574600	-0.00007600
O	1.97206000	-0.13477500	0.00004000
H	0.75077900	-1.74359100	0.00008400

TS1n-SS-c**E=-1087.056973 a.u.**

C	2.19172500	1.97847200	0.25706100
C	1.75371100	1.28819500	1.39331200
C	1.19050200	-0.55119400	0.76898500
H	2.52774800	0.97549700	2.09069900
H	0.80841300	1.57599300	1.84527800
H	1.36778800	-1.18237000	1.63861600
O	2.14295100	0.08429200	-1.17646400
N	2.11393200	-0.75878400	-0.21225200
C	3.28537300	-1.67230100	0.02977500
H	3.68434500	-1.40548500	1.01575500
C	2.78166300	-3.12257200	0.04792000
H	2.36719600	-3.39845900	-0.92805600
H	3.61505900	-3.79733400	0.27020800
H	2.00823600	-3.28533100	0.80562600
C	4.36320500	-1.45845700	-1.02574400
H	4.78695500	-0.45657000	-0.95806400
H	5.16322300	-2.18624700	-0.85328700
H	3.96376400	-1.61258700	-2.03229500
C	3.62283800	1.94097000	-0.05284100
H	3.92417600	2.53264500	-0.94356500
O	4.46426300	1.32237100	0.59320700
C	1.30268800	2.88549000	-0.54980700
H	1.31138100	3.90899200	-0.14757700
H	1.63466900	2.94080600	-1.59217900
H	0.26494900	2.54115700	-0.54262800
C	-0.25754900	-0.38713600	0.46092000
C	-0.76098500	-0.10363200	-0.81944600
C	-1.16955700	-0.57441500	1.51389500
C	-2.13450900	-0.01591700	-1.03217000
H	-0.07042800	0.03937200	-1.64095600
C	-2.54057300	-0.47206700	1.30492900
H	-0.79959400	-0.81104600	2.50879100
C	-3.02927500	-0.19186300	0.02644100
H	-2.51292100	0.18797400	-2.02864200
H	-3.23086800	-0.62518900	2.12788200
C	-4.50685500	-0.02450200	-0.19590800
F	-4.89795500	1.26037300	-0.01974600
F	-4.87152000	-0.37484400	-1.44932300
F	-5.23316400	-0.77420200	0.66376800

TS1n-RR-c**E=-1087.056973 a.u.**

C	-1.19050200	-0.55119300	0.76898500
N	-2.11393200	-0.75878400	-0.21225200
O	-2.14295100	0.08429200	-1.17646400
C	-2.19172500	1.97847200	0.25706100
C	-1.75371100	1.28819500	1.39331200
C	0.25754900	-0.38713500	0.46092000
C	1.16955700	-0.57441500	1.51389500
C	2.54057300	-0.47206700	1.30492900
C	3.02927500	-0.19186300	0.02644100
C	2.13450900	-0.01591700	-1.03217000
C	0.76098500	-0.10363200	-0.81944600
C	4.50685500	-0.02450200	-0.19590800
F	4.87152000	-0.37484300	-1.44932300
F	5.23316400	-0.77420300	0.66376700
F	4.89795500	1.26037300	-0.01974500
H	-1.36778800	-1.18237000	1.63861600
H	-0.80841300	1.57599300	1.84527800
H	-2.52774800	0.97549700	2.09069900
H	0.79959400	-0.81104600	2.50879100
H	3.23086800	-0.62518900	2.12788200
H	2.51292100	0.18797400	-2.02864200
H	0.07042800	0.03937200	-1.64095600
C	-1.30268800	2.88549000	-0.54980700
H	-1.31138000	3.90899200	-0.14757600
H	-0.26495000	2.54115600	-0.54262900
H	-1.63467000	2.94080700	-1.59217900
C	-3.62283800	1.94097000	-0.05284100
O	-4.46426300	1.32237100	0.59320700
H	-3.92417600	2.53264500	-0.94356500
C	-3.28537300	-1.67230100	0.02977500
H	-3.68434500	-1.40548500	1.01575500
C	-2.78166300	-3.12257200	0.04792000
H	-2.36719600	-3.39845900	-0.92805600
H	-2.00823600	-3.28533100	0.80562600
H	-3.61505900	-3.79733400	0.27020800
C	-4.36320500	-1.45845700	-1.02574400
H	-5.16322300	-2.18624700	-0.85328700
H	-4.78695500	-0.45657000	-0.95806400
H	-3.96376500	-1.61258700	-2.03229500

TS1x-RS-c

E=-1087.047561 a.u.

C	-1.28964500	-0.67169200	0.73973200
N	-2.21359900	-0.80925200	-0.25543100
O	-2.29526200	0.14668500	-1.11293300
C	-2.56126500	1.80899600	0.48632300
C	-1.90164100	1.11281700	1.50867500
C	-1.78319800	2.72522800	-0.36745700
O	-0.58411000	2.93066300	-0.27422800
C	-4.06487500	1.90769100	0.41362400
C	0.15408600	-0.45854800	0.45138100
C	1.07036200	-0.82132500	1.45286800
C	2.44047500	-0.68818400	1.25519100
C	2.91929300	-0.19613800	0.03887200
C	2.01816900	0.16581200	-0.96576400
C	0.64684900	0.04826800	-0.76114000
C	4.39986100	-0.11316800	-0.20801300
F	5.09171400	0.09596700	0.93540500
F	4.71614200	0.88376700	-1.06278700
F	4.88229300	-1.25895800	-0.74945700
H	-1.45126900	-1.38305100	1.54828800
H	-0.90948500	1.46680500	1.77147500
H	-2.49689200	0.73998800	2.34123800
H	-2.38284400	3.24521900	-1.14725300
H	-4.42967900	2.74631800	1.02551000
H	-4.55205700	1.00464000	0.79302800
H	-4.41241000	2.07739400	-0.61061200
H	0.70582200	-1.21653000	2.39839200
H	3.13547900	-0.96737800	2.04015700
H	2.38909600	0.56204800	-1.90519100
H	-0.04842400	0.35502900	-1.53025100
C	-3.41240200	-1.68775500	-0.03660300
H	-3.83952700	-1.41098400	0.93907700
C	-2.96733100	-3.15536900	0.00716900
H	-2.52438400	-3.44828100	-0.95079400
H	-2.23139400	-3.34553700	0.79436200
H	-3.83316500	-3.79831900	0.19792700
C	-4.44712000	-1.45225500	-1.13260400
H	-5.30499700	-2.10853200	-0.95242900
H	-4.79487500	-0.41903000	-1.15337400
H	-4.02988300	-1.68707100	-2.11622900

TS1x-SR-c**E=-1087.047561 a.u.**

C	2.56126500	1.80899600	0.48632300
C	1.90164100	1.11281700	1.50867500
C	1.28964500	-0.67169200	0.73973200
H	2.49689200	0.73998800	2.34123800
H	0.90948500	1.46680500	1.77147500
H	1.45126900	-1.38305100	1.54828800
O	2.29526200	0.14668500	-1.11293300
N	2.21359900	-0.80925200	-0.25543100
C	3.41240200	-1.68775500	-0.03660300
H	3.83952700	-1.41098400	0.93907700
C	2.96733100	-3.15536900	0.00716900
H	2.52438400	-3.44828100	-0.95079400
H	3.83316500	-3.79831900	0.19792700
H	2.23139400	-3.34553700	0.79436200
C	4.44712000	-1.45225500	-1.13260400
H	4.79487500	-0.41903000	-1.15337400
H	5.30499700	-2.10853200	-0.95242900
H	4.02988300	-1.68707100	-2.11622900
C	-0.15408600	-0.45854800	0.45138100
C	-0.64684900	0.04826800	-0.76114000
C	-1.07036200	-0.82132500	1.45286800
C	-2.01816900	0.16581200	-0.96576400
H	0.04842400	0.35502900	-1.53025000
C	-2.44047500	-0.68818500	1.25519100
H	-0.70582200	-1.21653000	2.39839200
C	-2.91929300	-0.19613800	0.03887200
H	-2.38909600	0.56204800	-1.90519100
H	-3.13547900	-0.96737900	2.04015700
C	-4.39986100	-0.11316800	-0.20801300
F	-5.09171400	0.09596800	0.93540500
F	-4.71614200	0.88376700	-1.06278700
F	-4.88229300	-1.25895800	-0.74945700
C	4.06487500	1.90769100	0.41362400
H	4.42967900	2.74631800	1.02551000
H	4.55205700	1.00464000	0.79302800
H	4.41241000	2.07739400	-0.61061100
C	1.78319800	2.72522800	-0.36745700
H	2.38284400	3.24521900	-1.14725300
O	0.58411000	2.93066300	-0.27422800

TS2n-RR-c**E=-1087.054962 a.u.**

C	2.39194900	1.25275000	-1.56626500
C	1.85551200	1.92296100	-0.41822100
C	1.31170800	-0.36418700	0.59553000
H	1.60844200	-0.41362200	1.63663400
O	2.09538600	-0.42633500	-1.53137300
N	2.22051500	-0.82991900	-0.26078100
C	3.58370100	-1.33036800	0.08286700
H	4.26749700	-0.55171700	-0.26741700
C	3.79382500	-1.51235800	1.58348400
H	3.06192500	-2.20111100	2.02276100
H	4.78720600	-1.94429500	1.74119800
H	3.76615500	-0.55182800	2.10435800
C	3.81635300	-2.62635700	-0.70280900
H	3.62330100	-2.47220900	-1.76716300
H	4.85581500	-2.94869800	-0.58095200
H	3.16180700	-3.42759200	-0.34039500
C	-0.12766900	-0.27817300	0.35709400
C	-0.75327000	-0.56904100	-0.87237000
C	-0.94092900	0.06059400	1.45660700
C	-2.13895600	-0.54002400	-0.98063900
H	-0.14329900	-0.81715300	-1.73143000
C	-2.32509800	0.10569000	1.34175800
H	-0.47766700	0.28881000	2.41321400
C	-2.93141700	-0.19992000	0.12062900
H	-2.60960300	-0.77101400	-1.93089500
H	-2.93491000	0.37472800	2.19766500
C	-4.43033900	-0.22140200	0.00154100
F	-4.93075400	-1.46010800	0.22404500
F	-5.02030200	0.60546400	0.89301700
F	-4.84092800	0.14890000	-1.23201000
C	0.56770100	2.70356500	-0.51434800
H	-0.24258500	2.10994000	-0.95375800
H	0.23120900	3.03839700	0.47401700
H	0.67976200	3.60283600	-1.13751300
C	2.74202700	2.15361200	0.69987500
O	3.87203700	1.67443500	0.84749000
H	2.32704800	2.82496900	1.48702900
H	1.91389300	1.45338700	-2.52278800
H	3.47829000	1.23846000	-1.62189700

TS2n-SS-c**E=-1087.054962 a.u.**

C	-1.31170800	-0.36418700	0.59553000
N	-2.22051500	-0.82991900	-0.26078100
O	-2.09538600	-0.42633500	-1.53137300
C	-2.39194900	1.25275000	-1.56626500
C	-1.85551200	1.92296100	-0.41822100
C	0.12766900	-0.27817300	0.35709400
C	0.94092900	0.06059400	1.45660700
C	2.32509800	0.10569000	1.34175800
C	2.93141700	-0.19992000	0.12062900
C	2.13895600	-0.54002400	-0.98063900
C	0.75327000	-0.56904100	-0.87237000
C	4.43033900	-0.22140200	0.00154100
F	4.84092800	0.14890000	-1.23201000
F	5.02030200	0.60546400	0.89301700
H	-1.60844200	-0.41362200	1.63663400
H	0.47766700	0.28881000	2.41321400
H	2.93491000	0.37472800	2.19766500
H	2.60960300	-0.77101400	-1.93089500
H	0.14329900	-0.81715300	-1.73143000
C	-0.56770100	2.70356500	-0.51434800
H	-0.23120900	3.03839700	0.47401700
H	0.24258500	2.10994000	-0.95375800
H	-0.67976200	3.60283600	-1.13751300
C	-2.74202700	2.15361200	0.69987500
O	-3.87203700	1.67443500	0.84749000
H	-2.32704800	2.82496900	1.48702900
H	-3.47829000	1.23846000	-1.62189700
H	-1.91389300	1.45338700	-2.52278800
C	-3.58370100	-1.33036800	0.08286700
H	-4.26749700	-0.55171700	-0.26741700
C	-3.79382500	-1.51235800	1.58348400
H	-3.76615500	-0.55182800	2.10435800
H	-4.78720600	-1.94429500	1.74119800
H	-3.06192500	-2.20111100	2.02276100
C	-3.81635300	-2.62635700	-0.70280900
H	-4.85581400	-2.94869800	-0.58095200
H	-3.62330100	-2.47220900	-1.76716300
H	-3.16180700	-3.42759200	-0.34039500
F	4.93075400	-1.46010800	0.22404500

TS2x-RS-c**E=-1087.045425 a.u.**

C	2.46437000	1.54780400	-1.22852000
C	2.10115700	1.92903600	0.09680300
C	1.44344000	-0.45236300	0.59610100
H	1.71752100	-0.67456700	1.62115200
O	2.28777700	-0.17552900	-1.49350400
N	2.37466600	-0.78126600	-0.30849500
C	3.74459300	-1.27510600	0.00286300
H	4.41172100	-0.41633400	-0.14873900
C	3.89709700	-1.78822100	1.43462000
H	3.18148400	-2.58921900	1.65193100
H	4.90353000	-2.20237700	1.55070700
H	3.78041100	-0.99815600	2.18313300
C	4.09836800	-2.35654900	-1.02548900
H	3.93967000	-1.98421000	-2.03954600
H	5.14937700	-2.64410500	-0.91581500
H	3.47740000	-3.24741100	-0.87839900
C	0.00438800	-0.38515200	0.34884100
C	-0.59299500	-0.33983600	-0.92408700
C	-0.83328600	-0.41566300	1.48256100
C	-1.97806500	-0.35848300	-1.05051000
H	0.03356900	-0.29885600	-1.80432300
C	-2.21501000	-0.41659400	1.35525600
H	-0.39026500	-0.45161300	2.47504300
C	-2.79347900	-0.39430000	0.08198200
H	-2.42791800	-0.33601200	-2.03708100
H	-2.84518700	-0.45290300	2.23786200
C	-4.29055200	-0.34981800	-0.05505600
F	-4.90164300	-1.08612300	0.90323600
F	-4.76909100	0.90989300	0.05982500
F	-4.70387300	-0.82179800	-1.25206800
C	3.15162200	2.16918300	1.16366100
H	2.68403200	2.37632200	2.13387500
H	3.82490900	1.31644800	1.30457700
H	3.78900200	3.03433500	0.92612100
C	0.79864900	2.55342900	0.27005600
H	0.62667600	2.98570500	1.28358100
O	-0.08724700	2.61744800	-0.57742800
H	1.77307300	1.86099900	-2.00555100
H	3.51376900	1.63350800	-1.50502900

TS2x-SR-c**E=-1087.045425 a.u.**

C	-1.44347100	-0.45233400	0.59610600
N	-2.37470500	-0.78125300	-0.30847800
O	-2.28780200	-0.17557300	-1.49351200
C	-2.46426200	1.54780200	-1.22858900
C	-2.10105800	1.92903100	0.09673500
C	-0.00441600	-0.38514900	0.34884200
C	0.83325700	-0.41554100	1.48256500
C	2.21498100	-0.41647900	1.35525700
C	2.79344900	-0.39431100	0.08198000
C	1.97803400	-0.35861400	-1.05051300
C	0.59296400	-0.33996200	-0.92408900
C	4.29052400	-0.34984600	-0.05504300
F	4.70384700	-0.82167400	-1.25211300
F	4.90158800	-1.08629300	0.90315800
F	4.76909000	0.90983900	0.06001900
H	-1.71755700	-0.67450400	1.62116300
H	0.39023800	-0.45138700	2.47505200
H	2.84515900	-0.45269400	2.23786600
H	2.42788800	-0.33624200	-2.03708500
H	-0.03360700	-0.29906800	-1.80432600
C	-3.15153400	2.16926400	1.16356300
H	-3.82488200	1.31657400	1.30446700
H	-2.68395900	2.37638300	2.13378800
H	-3.78885100	3.03445500	0.92599600
C	-0.79851100	2.55335700	0.27000100
H	-0.62652000	2.98561300	1.28353300
O	0.08738900	2.61734000	-0.57747700
H	-1.77291300	1.86091000	-2.00560700
H	-3.51364500	1.63357800	-1.50513700
C	-3.74464300	-1.27504500	0.00289900
H	-4.41175000	-0.41626900	-0.14877300
C	-3.89718000	-1.78805700	1.43469000
H	-3.78049800	-0.99793600	2.18314500
H	-4.90362000	-2.20219100	1.55078900
H	-3.18158100	-2.58904800	1.65207400
C	-4.09842800	-2.35655300	-1.02538300
H	-5.14944400	-2.64408200	-0.91570200
H	-3.93971000	-1.98428500	-2.03946400
H	-3.47747800	-3.24741600	-0.87822500

CA1n-SS-c**E=-1087.103057 a.u.**

C	-2.37735600	-1.44922900	-0.23810800
C	-1.81508800	-1.04268900	1.12794000
C	-1.17651900	0.34623200	0.84913000
H	-2.62788500	-0.96951700	1.85552600
H	-1.08537300	-1.76301200	1.50440600
H	-1.31579300	1.00165300	1.71272500
O	-2.21201700	-0.26992900	-1.09430000
N	-1.93704800	0.89353700	-0.28517600
C	-3.20140700	1.59559900	0.06060800
H	-3.82838200	0.97738200	0.72448800
C	-2.85911100	2.90990900	0.77539800
H	-2.17194300	3.50465600	0.16375900
H	-3.77514800	3.48952700	0.92972300
H	-2.40099200	2.75972500	1.75807900
C	-3.97965400	1.88793400	-1.22539800
H	-4.23822100	0.97072100	-1.75755100
H	-4.90476600	2.42246900	-0.98443900
H	-3.37989100	2.51295800	-1.89665600
C	-3.88139000	-1.74538000	-0.20935800
H	-4.31608900	-1.90863200	-1.21982800
O	-4.57212300	-1.79027700	0.78401300
C	-1.64602200	-2.59440600	-0.93724400
H	-1.74685700	-3.52605400	-0.36903900
H	-2.05175900	-2.75566800	-1.94209800
H	-0.58452500	-2.34810700	-1.03152800
C	0.31844500	0.27165400	0.54989200
C	0.84487700	0.60764700	-0.70172600
C	1.19839000	-0.12963700	1.56485600
C	2.21725200	0.53275200	-0.93655500
H	0.17027200	0.93612300	-1.48366500
C	2.56982600	-0.20237000	1.33823800
H	0.80962800	-0.38035000	2.54962500
C	3.08342900	0.12720600	0.08086900
H	2.61637500	0.79952100	-1.91000000
H	3.24114000	-0.50294500	2.13598600
C	4.55549900	-0.00879000	-0.19175100
F	4.86646400	-1.23957000	-0.66647000
F	4.98332900	0.88252700	-1.11395100
F	5.29639200	0.17569100	0.92467300

CA1n-RR-c

E=-1087.103057 a.u.

C	1.17651900	0.34623200	0.84913000
N	1.93704800	0.89353700	-0.28517600
O	2.21201700	-0.26992900	-1.09430000
C	2.37735600	-1.44922900	-0.23810800
C	1.81508800	-1.04268900	1.12794000
C	-0.31844500	0.27165400	0.54989200
C	-1.19839000	-0.12963700	1.56485600
C	-2.56982600	-0.20237000	1.33823800
C	-3.08342900	0.12720600	0.08086900
C	-2.21725200	0.53275200	-0.93655500
C	-0.84487700	0.60764700	-0.70172600
C	-4.55549900	-0.00879000	-0.19175100
F	-4.98332900	0.88252700	-1.11395100
F	-5.29639200	0.17569100	0.92467300
F	-4.86646400	-1.23957000	-0.66647000
H	1.31579300	1.00165300	1.71272500
H	1.08537300	-1.76301200	1.50440600
H	2.62788500	-0.96951700	1.85552600
H	-0.80962800	-0.38035000	2.54962500
H	-3.24114000	-0.50294500	2.13598600
H	-2.61637500	0.79952100	-1.91000000
H	-0.17027200	0.93612300	-1.48366500
C	1.64602200	-2.59440600	-0.93724400
H	1.74685700	-3.52605400	-0.36903900
H	0.58452500	-2.34810700	-1.03152800
H	2.05175900	-2.75566800	-1.94209800
C	3.88139000	-1.74538000	-0.20935800
O	4.57212300	-1.79027700	0.78401300
H	4.31608900	-1.90863200	-1.21982800
C	3.20140700	1.59559900	0.06060800
H	3.82838200	0.97738200	0.72448800
C	2.85911100	2.90990900	0.77539800
H	2.17194300	3.50465600	0.16375900
H	2.40099200	2.75972500	1.75807900
H	3.77514800	3.48952700	0.92972300
C	3.97965400	1.88793400	-1.22539800
H	4.90476600	2.42246900	-0.98443900
H	4.23822100	0.97072100	-1.75755100
H	3.37989100	2.51295800	-1.89665600

CA1x-RS-c

E=-1087.101302 a.u.

C	-1.37333900	-0.44897000	0.90525400
N	-2.16746700	-0.89873800	-0.25102700
O	-2.48269900	0.33317700	-0.96111600
C	-2.39344000	1.47990200	-0.07791000
C	-1.99345300	0.91459100	1.28998900
C	-1.30261400	2.39572600	-0.65418500
O	-0.81625100	3.31857700	-0.04155000
C	-3.71950600	2.25113900	-0.08433800
C	0.11432500	-0.36649000	0.57474200
C	1.02449100	-0.02099100	1.58364100
C	2.38947800	0.04905800	1.32299900
C	2.86569400	-0.22239100	0.03713600
C	1.96916100	-0.56569600	-0.97605400
C	0.60275800	-0.64021400	-0.70726400
C	4.34388700	-0.20833400	-0.23809700
F	5.00188200	0.64976000	0.57350200
F	4.61678300	0.14790900	-1.51328400
F	4.90011600	-1.42945800	-0.04736900
H	-1.50435800	-1.16672400	1.71955000
H	-1.30440500	1.58284400	1.81055800
H	-2.87685200	0.77003000	1.92059600
H	-1.01776500	2.16037500	-1.70162100
H	-3.62896800	3.15705700	0.52401000
H	-4.52183700	1.62538000	0.31882700
H	-3.99224400	2.54551800	-1.10334400
H	0.66493700	0.19421500	2.58744700
H	3.08385900	0.31935000	2.11160900
H	2.33778300	-0.77083600	-1.97605600
H	-0.09698500	-0.91886400	-1.48659500
C	-3.43218300	-1.60087600	0.08676700
H	-4.00843700	-1.03890600	0.84360700
C	-3.08957600	-2.98818900	0.64726300
H	-2.46622300	-3.53823300	-0.06584300
H	-2.55940300	-2.94874100	1.60415700
H	-4.01236200	-3.55487200	0.81011700
C	-4.28845300	-1.74361800	-1.17449000
H	-5.20624300	-2.29288600	-0.93780700
H	-4.55945800	-0.77014200	-1.58585100
H	-3.73958200	-2.29920300	-1.94320000

CA1x-SR-c**E=-1087.101302 a.u.**

C	2.39346700	1.48001700	-0.07778500
C	1.99342600	0.91463800	1.29003400
C	1.37340100	-0.44893800	0.90519100
H	2.87676000	0.77010400	1.92073500
H	1.30426000	1.58285200	1.81049600
H	1.50442300	-1.16672300	1.71946300
O	2.48282100	0.33335500	-0.96110900
N	2.16756900	-0.89860700	-0.25107800
C	3.43225500	-1.60076200	0.08677400
H	4.00832800	-1.03899000	0.84390100
C	3.08950100	-2.98821600	0.64684700
H	2.46642100	-3.53811100	-0.06661100
H	4.01224800	-3.55489800	0.80992100
H	2.55896800	-2.94897400	1.60354900
C	4.28880900	-1.74319300	-1.17431600
H	4.55996300	-0.76962700	-1.58536400
H	5.20651500	-2.29257000	-0.93755900
H	3.74010400	-2.29854800	-1.94331200
C	-0.11426800	-0.36650200	0.57467300
C	-0.60263900	-0.63970800	-0.70746300
C	-1.02448100	-0.02150900	1.58369700
C	-1.96904900	-0.56519200	-0.97625200
H	0.09712800	-0.91799000	-1.48690600
C	-2.38946800	0.04854900	1.32305200
H	-0.66496400	0.19330500	2.58760100
C	-2.86563000	-0.22239700	0.03706500
H	-2.33763200	-0.76994000	-1.97634700
H	-3.08388000	0.31846000	2.11176900
C	-4.34384800	-0.20836900	-0.23812500
F	-5.00179600	0.64987600	0.57334000
F	-4.61679300	0.14760700	-1.51335700
F	-4.90004600	-1.42946400	-0.04714800
C	3.71951800	2.25128500	-0.08418000
H	3.62917300	3.15694500	0.52459000
H	4.52191200	1.62531800	0.31853800
H	3.99208100	2.54611400	-1.10310700
C	1.30273400	2.39580600	-0.65419800
H	1.01955700	2.16168900	-1.70236900
O	0.81480400	3.31746900	-0.04102200

CA2n-RR-c

E=-1087.093715 a.u.

C	3.52718400	-0.88797800	0.64932000
C	2.14355000	-1.45901400	0.33613600
C	1.48855800	-0.16638100	-0.29512000
H	1.75383000	-0.17504800	-1.36398900
O	3.23679700	0.39736400	1.18994300
N	2.17281600	0.97265300	0.37571000
C	2.78504500	1.93973000	-0.56760600
H	3.47197600	1.41102200	-1.25394400
C	1.68043100	2.61098100	-1.39355500
H	0.97591800	3.13221200	-0.73645500
H	2.12957500	3.34626000	-2.06931000
H	1.11296500	1.90355600	-2.00605000
C	3.57747400	2.98821700	0.21680200
H	4.37916400	2.52656200	0.79584600
H	4.01774900	3.71523200	-0.47471700
H	2.91670800	3.52333400	0.90817400
C	-0.02367600	-0.07855900	-0.18898300
C	-0.64663000	0.57405300	0.88220200
C	-0.82474600	-0.67782600	-1.17014200
C	-2.03568700	0.61233800	0.97780700
H	-0.02867700	1.06634200	1.62501200
C	-2.21464800	-0.64358800	-1.08000600
H	-0.36014400	-1.17170800	-2.02085700
C	-2.82387400	0.00090000	-0.00108600
H	-2.50918600	1.11530100	1.81490600
H	-2.82361600	-1.11451000	-1.84463300
C	-4.32318500	0.09749400	0.07227800
F	-4.78279500	1.22336800	-0.52347000
F	-4.92658700	-0.94451000	-0.54268800
F	-4.76280100	0.12522600	1.35032000
C	1.43402900	-1.96087700	1.60514600
H	1.41212600	-1.17210300	2.36187100
H	0.40483700	-2.27125700	1.40082200
H	1.97332500	-2.81924900	2.02236800
C	2.17755700	-2.57515000	-0.69401000
O	3.17237900	-2.94337700	-1.28039700
H	1.19576300	-3.06436500	-0.88443500
H	4.06732600	-1.44384000	1.42058200
H	4.14860800	-0.83101200	-0.25408700

CA2n-SS-c**E=-1087.093715 a.u.**

C	-1.48855700	-0.16638000	-0.29512000
N	-2.17281600	0.97265400	0.37571000
O	-3.23679400	0.39736400	1.18994500
C	-3.52718300	-0.88797700	0.64932200
C	-2.14355000	-1.45901400	0.33613600
C	0.02367600	-0.07855900	-0.18898400
C	0.82474600	-0.67782600	-1.17014300
C	2.21464800	-0.64358800	-1.08000700
C	2.82387400	0.00090000	-0.00108700
C	2.03568700	0.61233700	0.97780700
C	0.64663100	0.57405300	0.88220100
C	4.32318500	0.09749300	0.07227800
F	4.76280100	0.12521300	1.35032100
F	4.92658900	-0.94450300	-0.54269800
H	-1.75383000	-0.17504700	-1.36399000
H	0.36014400	-1.17170800	-2.02085800
H	2.82361600	-1.11451000	-1.84463400
H	2.50918600	1.11530100	1.81490600
H	0.02867700	1.06634200	1.62501100
C	-1.43402700	-1.96087900	1.60514400
H	-0.40483500	-2.27125800	1.40081800
H	-1.41212200	-1.17210500	2.36186900
H	-1.97332300	-2.81925100	2.02236500
C	-2.17755900	-2.57514900	-0.69401200
O	-3.17238300	-2.94337700	-1.28039500
H	-1.19576500	-3.06436200	-0.88444200
H	-4.14860800	-0.83101000	-0.25408400
H	-4.06732400	-1.44384000	1.42058500
C	-2.78504600	1.93973000	-0.56760600
H	-3.47197700	1.41102100	-1.25394200
C	-1.68043400	2.61098100	-1.39355600
H	-1.11296800	1.90355600	-2.00605200
H	-2.12957800	3.34626000	-2.06931100
H	-0.97592000	3.13221200	-0.73645700
C	-3.57747400	2.98821700	0.21680300
H	-4.01775200	3.71523000	-0.47471600
H	-4.37916300	2.52656200	0.79585000
H	-2.91670800	3.52333600	0.90817300
F	4.78279500	1.22337500	-0.52345800

CA2x-RS-c

E=-1087.093189 a.u.

C	-3.55851500	-1.09649600	-0.00181300
C	-2.14153400	-1.49220400	0.40217500
C	-1.51461200	-0.06584900	0.57982100
H	-1.73255200	0.22551700	1.61961600
O	-3.36468300	0.00071100	-0.88376600
N	-2.26531700	0.80653000	-0.35906100
C	-2.84554700	2.01197600	0.27761100
H	-3.47687500	1.71462400	1.13632600
C	-1.71355900	2.91309200	0.78685800
H	-1.05740100	3.20515700	-0.04005800
H	-2.14145500	3.82121100	1.22440100
H	-1.09822800	2.43424300	1.55473100
C	-3.71182000	2.76235700	-0.73685000
H	-4.52969500	2.13615600	-1.09747200
H	-4.13453000	3.66056500	-0.27286400
H	-3.10738500	3.06853400	-1.59819700
C	-0.01045500	0.02928300	0.37360000
C	0.53748900	0.31590200	-0.88385100
C	0.85653100	-0.18781600	1.45280000
C	1.91812000	0.36465100	-1.06064800
H	-0.13231600	0.51954800	-1.71245000
C	2.23878100	-0.14010100	1.28194100
H	0.44897600	-0.38064100	2.44252600
C	2.77283300	0.13405300	0.02115700
H	2.33340600	0.59407200	-2.03659000
H	2.90001400	-0.29856600	2.12753900
C	4.26367000	0.13484000	-0.18027200
F	4.92225700	0.52049800	0.93608500
F	4.72561200	-1.09753700	-0.49991400
F	4.63734100	0.96405000	-1.17957400
C	-2.05452600	-2.33352200	1.68794100
H	-1.01376300	-2.54811100	1.95578000
H	-2.51918800	-1.80354900	2.52711700
H	-2.57003200	-3.29148300	1.55966700
C	-1.47920600	-2.32148700	-0.70484900
H	-0.37747700	-2.42006500	-0.62121700
O	-2.08774900	-2.90586000	-1.57190300
H	-4.06788700	-1.87557300	-0.57281000
H	-4.15971600	-0.82131300	0.87965400

CA2x-SR-c**E=-1087.093189 a.u.**

C	1.51461200	-0.06584900	0.57982100
N	2.26531700	0.80653000	-0.35906200
O	3.36468300	0.00071000	-0.88376700
C	3.55851500	-1.09649700	-0.00181300
C	2.14153400	-1.49220400	0.40217500
C	0.01045500	0.02928300	0.37360000
C	-0.85653100	-0.18781600	1.45280000
C	-2.23878100	-0.14010100	1.28194100
C	-2.77283300	0.13405300	0.02115700
C	-1.91812000	0.36465000	-1.06064900
C	-0.53748900	0.31590100	-0.88385100
C	-4.26367000	0.13484000	-0.18027200
F	-4.63734100	0.96405200	-1.17957300
F	-4.92225700	0.52049600	0.93608500
F	-4.72561200	-1.09753600	-0.49991600
H	1.73255200	0.22551700	1.61961600
H	-0.44897600	-0.38064000	2.44252600
H	-2.90001400	-0.29856500	2.12753900
H	-2.33340600	0.59407100	-2.03659000
H	0.13231600	0.51954700	-1.71245100
C	2.05452700	-2.33352100	1.68794200
H	2.51918800	-1.80354800	2.52711700
H	1.01376400	-2.54811100	1.95578100
H	2.57003200	-3.29148300	1.55966800
C	1.47920600	-2.32148800	-0.70484900
H	0.37747700	-2.42006700	-0.62121500
O	2.08774800	-2.90585900	-1.57190300
H	4.06788700	-1.87557400	-0.57281000
H	4.15971600	-0.82131300	0.87965300
C	2.84554800	2.01197600	0.27761000
H	3.47687600	1.71462400	1.13632500
C	1.71356000	2.91309200	0.78685900
H	1.09823100	2.43424300	1.55473200
H	2.14145700	3.82121100	1.22440000
H	1.05740100	3.20515700	-0.04005600
C	3.71182000	2.76235700	-0.73685100
H	4.13453200	3.66056400	-0.27286400
H	4.52969300	2.13615500	-1.09747500
H	3.10738400	3.06853700	-1.59819600

TS1n-SS-t**E=-1087.053972 a.u.**

C	-2.20156300	1.74302900	-0.60333400
C	-1.83295900	0.85446800	-1.62194500
C	-1.17295700	-0.85309200	-0.67288600
H	-2.62958300	0.41261100	-2.22093900
H	-0.91359600	1.04042900	-2.17003700
H	-1.30385300	-1.63745700	-1.41142200
O	-2.16635800	0.17900600	1.06090700
N	-2.10940100	-0.87376100	0.31419600
C	-3.39188400	-1.63654800	0.18925800
H	-4.08754600	-0.95636800	-0.32397200
C	-3.24687700	-2.92693700	-0.62019500
H	-2.45511800	-3.56521000	-0.21219500
H	-4.18756300	-3.48344000	-0.56295800
H	-3.04376300	-2.74882900	-1.68084300
C	-3.92471900	-1.90947400	1.59860600
H	-3.98344700	-0.98357800	2.17206600
H	-4.92448600	-2.35014200	1.53215800
H	-3.27139200	-2.61113700	2.12985100
C	-3.63393600	1.94595900	-0.32465100
H	-4.31439300	1.21932700	-0.82758000
O	-4.08606000	2.85274200	0.35239000
C	-1.25726700	2.75320800	-0.01564200
H	-1.42717400	3.73667700	-0.47357500
H	-1.43907000	2.86852300	1.05629400
H	-0.21369800	2.47310700	-0.17700200
C	0.25973500	-0.57258800	-0.38829700
C	0.73492700	-0.05218000	0.82679000
C	1.19161100	-0.90422600	-1.38705200
C	2.10145600	0.12115200	1.03041700
H	0.02795400	0.20890700	1.60370700
C	2.55523300	-0.71506600	-1.19050100
H	0.84403700	-1.32448400	-2.32811800
C	3.01590800	-0.20159600	0.02423100
H	2.45891200	0.50866700	1.97894600
H	3.26116800	-0.98189900	-1.96989700
C	4.48409500	0.05261500	0.22823100
F	4.83064900	1.30988800	-0.13654500
F	4.84504000	-0.09203000	1.52250200
F	5.24686100	-0.79071400	-0.50355800

TS1n-RR-t
E=-1087.053972 a.u.

C	1.17298000	-0.85307600	-0.67286600
N	2.10941200	-0.87374000	0.31422800
O	2.16637000	0.17903200	1.06093200
C	2.20156700	1.74303800	-0.60333300
C	1.83300300	0.85444500	-1.62193100
C	-0.25971700	-0.57257000	-0.38829000
C	-1.19158800	-0.90426200	-1.38703100
C	-2.55521300	-0.71511300	-1.19048900
C	-3.01589400	-0.20159700	0.02422100
C	-2.10144600	0.12121000	1.03039200
C	-0.73491500	-0.05211400	0.82677300
C	-4.48408400	0.05259900	0.22821700
F	-4.84503000	-0.09204800	1.52248700
F	-5.24684300	-0.79073700	-0.50357300
F	-4.83064800	1.30987000	-0.13656000
H	1.30387600	-1.63746200	-1.41137800
H	0.91366400	1.04039700	-2.17006900
H	2.62965200	0.41258100	-2.22088700
H	-0.84400800	-1.32455800	-2.32807900
H	-3.26114400	-0.98199000	-1.96987400
H	-2.45890800	0.50876300	1.97890400
H	-0.02794500	0.20901400	1.60367900
C	1.25723900	2.75322200	-0.01569900
H	1.42718100	3.73669000	-0.47362200
H	0.21367900	2.47312600	-0.17712300
H	1.43897700	2.86853800	1.05624800
C	3.63392600	1.94598600	-0.32459200
O	4.08601200	2.85279300	0.35244400
H	4.31441100	1.21934900	-0.82747400
C	3.39189000	-1.63653700	0.18934800
H	4.08766300	-0.95624200	-0.32357800
C	3.24703300	-2.92671900	-0.62045900
H	2.45511300	-3.56505000	-0.21286400
H	3.04425100	-2.74832000	-1.68112300
H	4.18766600	-3.48329700	-0.56308000
C	3.92444100	-1.90979200	1.59874300
H	4.92422100	-2.35045100	1.53240200
H	3.98306100	-0.98401900	2.17241500
H	3.27100100	-2.61156800	2.12970000

TS1x-RS-t

E=-1087.049825 a.u.

C	-1.19507700	-0.86090500	0.70585800
N	-2.12987000	-0.89554700	-0.28735400
O	-2.20953400	0.15636700	-1.02734500
C	-2.47310500	1.63913500	0.68554200
C	-1.81660900	0.84129300	1.63864200
C	-1.68709800	2.66015900	-0.02811200
O	-2.17304500	3.56699200	-0.68216300
C	-3.97126900	1.78618600	0.63310900
C	0.23956300	-0.59747900	0.41517700
C	1.18217800	-1.01520400	1.37047400
C	2.54485400	-0.82605000	1.16649300
C	2.99308500	-0.22224900	-0.01090800
C	2.06750200	0.19064800	-0.97264600
C	0.70223800	0.01547100	-0.76136000
C	4.46159900	0.02996700	-0.21500400
F	4.79660300	0.02834000	-1.52405800
F	5.22133800	-0.90450400	0.40087700
H	-1.33664500	-1.64953200	1.44268100
H	-0.82564100	1.15279500	1.96004400
H	-2.41864700	0.40192800	2.43319700
H	-0.58474900	2.55575000	0.07236400
H	-4.28366600	2.64396300	1.24508600
H	-4.48158800	0.90014900	1.02279600
H	-4.31293000	1.98417700	-0.38522000
H	0.84419300	-1.50364800	2.28152800
H	3.25980500	-1.16127400	1.91058500
H	2.41472200	0.65047000	-1.89213200
H	-0.01234600	0.33994400	-1.50708200
C	-3.35310700	-1.75144200	-0.12629600
H	-3.78419500	-1.50999200	0.85732100
C	-2.95354300	-3.23193400	-0.15436700
H	-2.50670500	-3.48877000	-1.12083000
H	-2.23682700	-3.48960000	0.63141900
H	-3.84216300	-3.85518500	-0.00937000
C	-4.36745300	-1.42597600	-1.21874400
H	-5.25006200	-2.05871600	-1.07837400
H	-4.67601500	-0.38086800	-1.19077300
H	-3.94909900	-1.62843600	-2.20943300
F	4.83869600	1.23050600	0.28502400

TS1x-SR-t

E= -1087.049825 a.u.

C	2.47321000	1.63890800	0.68586300
C	1.81648200	0.84092300	1.63869600
C	1.19494000	-0.86099700	0.70548600
H	2.41836100	0.40132700	2.43324200
H	0.82551100	1.15248400	1.96003700
H	1.33630600	-1.64980600	1.44214600
O	2.20976400	0.15653200	-1.02734800
N	2.12990900	-0.89551800	-0.28758000
C	3.35312600	-1.75143200	-0.12640800
H	3.78423400	-1.50984000	0.85716600
C	2.95358600	-3.23193300	-0.15425700
H	2.50667700	-3.48891200	-1.12064800
H	3.84224300	-3.85513100	-0.00925400
H	2.23695900	-3.48954100	0.63162700
C	4.36745900	-1.42613000	-1.21892200
H	4.67597700	-0.38100500	-1.19114700
H	5.25009200	-2.05881200	-1.07844000
H	3.94910600	-1.62879900	-2.20957000
C	-0.23963300	-0.59743700	0.41459900
C	-0.70199500	0.01709200	-0.76118100
C	-1.18255100	-1.01666200	1.36902400
C	-2.06725300	0.19256500	-0.97264300
H	0.01277300	0.34261500	-1.50626300
C	-2.54512500	-0.82746000	1.16479400
H	-0.84479900	-1.50635100	2.27949400
C	-2.99305500	-0.22187400	-0.01188600
H	-2.41421200	0.65382700	-1.89147000
H	-3.26031500	-1.16399500	1.90810900
C	-4.46173900	0.03014700	-0.21500900
F	-4.84219900	1.22264100	0.30146900
F	-4.79493500	0.04600700	-1.52434500
F	-5.22031000	-0.91445300	0.38684800
C	3.97140700	1.78575700	0.63362000
H	4.28385500	2.64339300	1.24576800
H	4.48156000	0.89958400	1.02320700
H	4.31320700	1.98386800	-0.38463900
C	1.68745700	2.66027500	-0.02757800
H	0.58508100	2.55610300	0.07285000
O	2.17362400	3.56714700	-0.68141400

TS2n-RR-t**E=-1087.051335 a.u.**

C	-2.49016700	0.90243200	1.77007800
C	-1.90764300	1.72185800	0.76216900
C	-1.38359500	-0.27256100	-0.58499600
H	-1.67946000	-0.09764600	-1.61249700
O	-2.16513500	-0.81684500	1.46583300
N	-2.26231600	-0.97900900	0.14446900
C	-3.63523300	-1.33016500	-0.31490100
H	-4.29504600	-0.54238500	0.07561100
C	-3.76406400	-1.37779600	-1.83787300
H	-3.03308600	-2.06459200	-2.27955500
H	-4.76288000	-1.74656300	-2.09114900
H	-3.65436400	-0.39383700	-2.30365100
C	-4.02347300	-2.66523500	0.32955700
H	-3.87654600	-2.62704800	1.41070600
H	-5.07679600	-2.88262600	0.12404800
H	-3.41557200	-3.48125800	-0.07725100
C	0.06122800	-0.24555800	-0.35034500
C	0.69405800	-0.83303700	0.76264100
C	0.86288200	0.35761700	-1.33816300
C	2.08015500	-0.83130800	0.86386600
H	0.09008800	-1.28665500	1.53829000
C	2.24871600	0.37506900	-1.22535700
H	0.39058100	0.82018800	-2.20088800
C	2.86372100	-0.22538200	-0.12438600
H	2.55851000	-1.29198900	1.72215700
H	2.85135600	0.85289500	-1.99041900
C	4.36376100	-0.27421800	-0.02773900
F	4.86271300	-1.40635800	-0.57956000
F	4.94571200	0.76313100	-0.66882700
F	4.78531300	-0.24824300	1.25637100
C	-0.60327000	2.44113600	1.00238800
H	0.08681600	1.84272900	1.60509400
H	-0.11686600	2.69698100	0.05734400
H	-0.77932700	3.38732500	1.53267900
C	-2.76750500	2.24103300	-0.29337200
O	-2.45735300	3.09545400	-1.11501700
H	-3.79168300	1.79122700	-0.31698900
H	-2.04305100	0.91917000	2.76038200
H	-3.57761200	0.84819600	1.79501700

TS2n-SS-t**E=-1087.051335 a.u.**

C	1.38359500	-0.27254700	-0.58498900
N	2.26229700	-0.97902000	0.14446700
O	2.16510900	-0.81687000	1.46582800
C	2.49015700	0.90243000	1.77008600
C	1.90765200	1.72184300	0.76215700
C	-0.06123500	-0.24555300	-0.35035000
C	-0.86289200	0.35758600	-1.33818600
C	-2.24872600	0.37503900	-1.22537800
C	-2.86372600	-0.22537400	-0.12438300
C	-2.08015700	-0.83126300	0.86388700
C	-0.69405900	-0.83299000	0.76266000
C	-4.36376600	-0.27421300	-0.02773600
F	-4.78531800	-0.24827100	1.25637000
F	-4.94571100	0.76315700	-0.66879400
H	1.67945700	-0.09764100	-1.61249400
H	-0.39059300	0.82012800	-2.20092800
H	-2.85136900	0.85283800	-1.99045400
H	-2.55851000	-1.29190800	1.72220000
H	-0.09008300	-1.28657400	1.53832300
C	0.60328700	2.44114800	1.00234900
H	0.11691300	2.69700800	0.05729400
H	-0.08682700	1.84275400	1.60503500
H	0.77935100	3.38732900	1.53265000
C	2.76754600	2.24101300	-0.29336600
O	2.45743000	3.09545300	-1.11499900
H	3.79171100	1.79118000	-0.31697400
H	3.57760000	0.84818200	1.79503700
H	2.04302700	0.91917600	2.76038300
C	3.63521800	-1.33017800	-0.31489300
H	4.29502600	-0.54239500	0.07562200
C	3.76406100	-1.37780000	-1.83786500
H	3.65443400	-0.39382500	-2.30363000
H	4.76285200	-1.74663700	-2.09113700
H	3.03303900	-2.06453800	-2.27956500
C	4.02345500	-2.66525000	0.32956400
H	5.07679300	-2.88261300	0.12410600
H	3.87646900	-2.62708200	1.41070500
H	3.41559200	-3.48127900	-0.07729100
F	-4.86271900	-1.40632800	-0.57959000

TS2x-RS-t**E=-1087.048214 a.u.**

C	2.34434800	1.01003200	-1.76149400
C	2.08910700	1.73363300	-0.56464700
C	1.43481000	-0.22564300	0.58560300
H	1.73010700	-0.05343900	1.61431700
O	2.20145200	-0.77391900	-1.46215100
N	2.31415800	-0.93206500	-0.14638900
C	3.68793200	-1.30248200	0.29409100
H	4.35896100	-0.56278700	-0.16207200
C	3.86353300	-1.27937200	1.81235600
H	3.13577400	-1.93080500	2.30946900
H	4.86315100	-1.65392400	2.05401500
H	3.78134200	-0.27210500	2.23155400
C	4.01042400	-2.68185600	-0.29278600
H	3.83407600	-2.68800000	-1.37042300
H	5.06072200	-2.92956700	-0.10607300
H	3.38462800	-3.45407300	0.16880900
C	-0.02057900	-0.25998600	0.36361700
C	-0.63348600	-0.91281900	-0.72262600
C	-0.83912000	0.34337500	1.33556600
C	-2.01884900	-0.96149600	-0.82053300
H	-0.01628300	-1.37863800	-1.48056200
C	-2.22513100	0.31007000	1.22567900
H	-0.38348300	0.85292600	2.17984400
C	-2.82091900	-0.34647700	0.14718200
H	-2.48263300	-1.48240400	-1.65225200
H	-2.84218700	0.78447700	1.98087300
C	-4.31613100	-0.35072800	-0.01318000
F	-4.95347500	-0.15990700	1.16291600
F	-4.73248100	0.62749800	-0.85125500
F	-4.75996800	-1.51956600	-0.53064200
C	3.21565000	2.25624800	0.30561100
H	2.88099200	2.41507200	1.33487400
H	4.07967600	1.58494900	0.31451400
H	3.56322900	3.23349800	-0.05708100
C	0.82780000	2.46916100	-0.48033600
H	0.06640900	2.18061000	-1.23896100
O	0.58024500	3.33613900	0.34673400
H	1.58823400	1.04870600	-2.54178300
H	3.36158900	0.98999900	-2.14480800

TS2x-SR-t**E=-1087.048214 a.u.**

C	-1.43483100	-0.22560800	0.58561400
N	-2.31419000	-0.93201500	-0.14638400
O	-2.20147400	-0.77387600	-1.46214300
C	-2.34437300	1.01007600	-1.76149200
C	-2.08905800	1.73368300	-0.56466800
C	0.02055800	-0.25998900	0.36363400
C	0.83911400	0.34345100	1.33552300
C	2.22512200	0.31009800	1.22563900
C	2.82089800	-0.34658400	0.14721300
C	2.01881300	-0.96168300	-0.82043700
C	0.63345000	-0.91295200	-0.72253800
C	4.31610500	-0.35075400	-0.01318200
F	4.75993300	-1.51930700	-0.53128800
F	4.95347900	-0.16056100	1.16300000
F	4.73242900	0.62793800	-0.85072600
H	-1.73013000	-0.05338900	1.61432500
H	0.38348900	0.85309900	2.17974800
H	2.84219100	0.78455900	1.98078900
H	2.48258300	-1.48269900	-1.65209400
H	0.01623800	-1.37883600	-1.48042800
C	-3.21553100	2.25629100	0.30567900
H	-4.07946300	1.58488000	0.31481200
H	-2.88072100	2.41531300	1.33486200
H	-3.56330600	3.23344200	-0.05709900
C	-0.82772200	2.46916200	-0.48041000
H	-0.06638300	2.18059700	-1.23908300
O	-0.58008900	3.33611000	0.34666700
H	-1.58829800	1.04873200	-2.54181900
H	-3.36163400	0.99004700	-2.14475500
C	-3.68795900	-1.30247400	0.29408000
H	-4.35900700	-0.56281200	-0.16210800
C	-3.86360900	-1.27934200	1.81233800
H	-3.78141600	-0.27206900	2.23152200
H	-4.86324300	-1.65387300	2.05396400
H	-3.13588200	-1.93078100	2.30948800
C	-4.01038900	-2.68186400	-0.29279100
H	-5.06068400	-2.92960600	-0.10610300
H	-3.83401400	-2.68801200	-1.37042400
H	-3.38458000	-3.45405600	0.16882500

CA1n-SS-t
E=-1087.101744 a.u.

C	-2.37329800	-1.38952200	0.01741700
C	-1.85363300	-0.79709400	1.33845200
C	-1.18169800	0.53016600	0.88744200
H	-2.67834200	-0.57696900	2.02726200
H	-1.16327000	-1.47347700	1.84691300
H	-1.27857000	1.27863300	1.67856300
O	-2.34770900	-0.26803400	-0.92526300
N	-1.96857300	0.96566600	-0.27195000
C	-3.17675100	1.77190500	0.03519700
H	-3.78863800	1.28442100	0.81639800
C	-2.73693500	3.15403700	0.53737400
H	-2.08466400	3.63304200	-0.20061300
H	-3.61915100	3.78632000	0.68165000
H	-2.20312600	3.11739600	1.49233500
C	-4.02328800	1.92113500	-1.23187500
H	-4.36234400	0.95401400	-1.60639600
H	-4.90088800	2.54104100	-1.01892900
H	-3.43798200	2.40597800	-2.02115700
C	-3.84424200	-1.79322400	0.14168100
H	-4.50872800	-0.96650800	0.48131400
O	-4.28644200	-2.88753800	-0.11869100
C	-1.52916900	-2.51736800	-0.56221100
H	-1.60042900	-3.40777600	0.06957400
H	-1.89202700	-2.78385800	-1.55849100
H	-0.48320700	-2.21025600	-0.63613100
C	0.30106500	0.38088600	0.56034200
C	0.79208900	0.53157900	-0.74015900
C	1.20556600	0.10706400	1.59595700
C	2.15534600	0.39809000	-1.00279300
H	0.09761100	0.76165800	-1.53980900
C	2.56765700	-0.02160400	1.34128100
H	0.84488900	0.00370900	2.61729500
C	3.04628300	0.12126700	0.03569500
H	2.52734400	0.51872800	-2.01498000
H	3.25969700	-0.22077300	2.15312100
C	4.50937900	-0.07794100	-0.24896100
F	4.80647400	-1.38336800	-0.45560900
F	4.90804700	0.59320600	-1.35191600
F	5.28268200	0.33720000	0.78067300

CA1n-RR-t
E=-1087.101744 a.u.

C	1.18169900	0.53016700	0.88744200
N	1.96857300	0.96566600	-0.27195100
O	2.34770800	-0.26803500	-0.92526300
C	2.37329700	-1.38952200	0.01741800
C	1.85363300	-0.79709300	1.33845300
C	-0.30106500	0.38088700	0.56034200
C	-1.20556600	0.10706900	1.59595800
C	-2.56765700	-0.02159900	1.34128200
C	-3.04628300	0.12126800	0.03569600
C	-2.15534600	0.39808700	-1.00279300
C	-0.79208900	0.53157600	-0.74016000
C	-4.50937800	-0.07794100	-0.24896100
F	-4.90804800	0.59321400	-1.35191000
F	-5.28268200	0.33718900	0.78067700
F	-4.80647000	-1.38336700	-0.45562100
H	1.27857100	1.27863500	1.67856200
H	1.16327000	-1.47347500	1.84691400
H	2.67834200	-0.57696800	2.02726200
H	-0.84488900	0.00371700	2.61729600
H	-3.25969700	-0.22076600	2.15312200
H	-2.52734400	0.51872200	-2.01498000
H	-0.09761100	0.76165300	-1.53981000
C	1.52916700	-2.51736900	-0.56220900
H	1.60042800	-3.40777600	0.06957700
H	0.48320600	-2.21025600	-0.63612700
H	1.89202500	-2.78385900	-1.55848900
C	3.84424100	-1.79322500	0.14168200
O	4.28644000	-2.88754000	-0.11868900
H	4.50872800	-0.96650900	0.48131200
C	3.17675200	1.77190400	0.03519400
H	3.78864200	1.28441700	0.81639200
C	2.73693900	3.15403500	0.53737700
H	2.08466100	3.63304000	-0.20060400
H	2.20313900	3.11739200	1.49234300
H	3.61915600	3.78631900	0.68164600
C	4.02328500	1.92113700	-1.23188100
H	4.90088700	2.54103900	-1.01893600
H	4.36233400	0.95401600	-1.60640800
H	3.43797700	2.40598600	-2.02115800

CA1x-RS-t

E=-1087.101181 a.u.

C	-1.15099800	0.00395200	-0.89923800
N	-1.93768100	0.59724100	0.19954100
O	-3.30039700	0.19843000	-0.14868000
C	-3.19154100	-1.20084800	-0.35051900
C	-1.78922400	-1.40631400	-0.99947800
C	-3.27139500	-1.95560900	0.98526700
O	-3.57202700	-1.46396100	2.04406300
C	-4.36275800	-1.63997300	-1.23297600
C	0.33127400	0.00023200	-0.58900200
C	1.26193600	0.29396700	-1.59159400
C	2.63095200	0.25209700	-1.33213300
C	3.08473000	-0.07549600	-0.05335200
C	2.16455800	-0.35968700	0.96091200
C	0.79919800	-0.32408800	0.69336400
C	4.55993200	-0.17761600	0.22211700
F	4.86010200	0.16823000	1.49404500
F	5.28387400	0.61786300	-0.59688700
H	-1.32001100	0.52983800	-1.85138000
H	-1.19495000	-2.14895300	-0.45629200
H	-1.86103100	-1.73640500	-2.04007700
H	-3.04799100	-3.04685900	0.89441700
H	-4.35415900	-2.72549900	-1.38090200
H	-4.29356200	-1.15502100	-2.21153200
H	-5.31409600	-1.35990300	-0.76961000
H	0.91377500	0.56074100	-2.58650600
H	3.34353000	0.48526200	-2.11633700
H	2.51817500	-0.59992000	1.95847100
H	0.08106800	-0.52834700	1.48133900
C	-1.93228100	2.06605400	0.33125700
H	-0.86819600	2.30749500	0.45370100
C	-2.66777800	2.44055800	1.62242400
H	-3.72861300	2.18349900	1.54897000
H	-2.24773300	1.89578300	2.47285400
H	-2.58192500	3.51607900	1.81292400
C	-2.47983400	2.83737500	-0.88148600
H	-2.39787100	3.91419700	-0.69826700
H	-1.92398800	2.61947400	-1.79992900
H	-3.53300300	2.59750900	-1.05263600
F	5.01525800	-1.44087300	0.04368400

CA1x-SR-t
E=-1087.101181 a.u.

C	3.19154600	-1.20072300	-0.35076300
C	1.78938500	-1.40600600	-1.00009800
H	1.86147200	-1.73563200	-2.04083000
H	1.19504600	-2.14894500	-0.45738800
O	3.30039100	0.19851800	-0.14862000
N	1.93762800	0.59719300	0.19958100
C	1.93217300	2.06595800	0.33172200
H	0.86805000	2.30736100	0.45396400
C	2.66733800	2.44005400	1.62319600
H	3.72814900	2.18281100	1.55000300
H	2.58161000	3.51554900	1.81390800
H	2.24692600	1.89515700	2.47337000
C	2.48005600	2.83763400	-0.88065100
H	1.92447600	2.61994800	-1.79930800
H	2.39799700	3.91440400	-0.69716300
H	3.53328700	2.59784900	-1.05156500
C	4.36297800	-1.63969200	-1.23300700
H	4.35438400	-2.72518600	-1.38120100
H	4.29406400	-1.15450000	-2.21146700
H	5.31420300	-1.35977100	-0.76931100
C	3.27108300	-1.95575300	0.98489400
H	3.04748800	-3.04695600	0.89381700
O	3.57166500	-1.46435800	2.04382400
C	1.15104100	0.00417400	-0.89943800
H	1.32003300	0.53035100	-1.85142400
C	-0.33123200	0.00032400	-0.58920600
C	-0.79912800	-0.32499700	0.69293000
C	-1.26191000	0.29500500	-1.59149300
C	-2.16446900	-0.36066400	0.96052300
H	-0.08098100	-0.52994300	1.48071900
C	-2.63093000	0.25309400	-1.33198800
H	-0.91377500	0.56254200	-2.58621400
C	-3.08467500	-0.07551600	-0.05346100
H	-2.51806500	-0.60170200	1.95790100
H	-3.34351800	0.48699300	-2.11596900
C	-4.55986200	-0.17767900	0.22208700
F	-5.01520500	-1.44090300	0.04342600
F	-4.85992700	0.16789100	1.49412100
F	-5.28387400	0.61798300	-0.59666100

CA2n-RR-t

E=-1087.095235 a.u.

C	-3.54727000	0.94718900	0.60073700
C	-2.15000500	1.48516700	0.24278300
C	-1.53424500	0.15295100	-0.33484200
H	-1.77990700	0.13091900	-1.40926200
O	-3.28251000	-0.32998400	1.16595400
N	-2.25560400	-0.95497600	0.34895900
C	-2.90870800	-1.90684400	-0.58207800
H	-3.56658300	-1.35980000	-1.28347400
C	-1.82910400	-2.63940600	-1.38879400
H	-1.15750000	-3.18518000	-0.71759600
H	-2.30547100	-3.36019500	-2.06150100
H	-1.22148300	-1.96626300	-2.00137100
C	-3.75370800	-2.90568100	0.21183100
H	-4.54108800	-2.40065700	0.77422200
H	-4.21687400	-3.62599800	-0.47161400
H	-3.12387300	-3.45526600	0.92032500
C	-0.02525100	0.04150900	-0.20329000
C	0.56970200	-0.66312600	0.84973200
C	0.79837300	0.67313400	-1.14441300
C	1.95660100	-0.72996500	0.96214100
H	-0.06739200	-1.16885800	1.56671800
C	2.18557900	0.61106600	-1.03620300
H	0.35545900	1.22295900	-1.97176600
C	2.76844900	-0.09274000	0.02022400
H	2.40944400	-1.27455100	1.78452900
H	2.81313500	1.10865400	-1.76801900
C	4.26429900	-0.22207500	0.10860900
F	4.70754200	-1.34206200	-0.51151900
F	4.89759000	0.82201600	-0.47097000
F	4.68781000	-0.29408100	1.39049900
C	-1.43029300	2.05273000	1.46728400
H	-1.41791100	1.31752500	2.27651400
H	-0.40210900	2.33428000	1.22990700
H	-1.94686700	2.95231400	1.81582400
C	-2.24286300	2.50853800	-0.87789300
O	-1.76033200	3.61709300	-0.85125200
H	-2.81261100	2.15854700	-1.77164900
H	-4.05490700	1.53851000	1.36750800
H	-4.19731100	0.87347500	-0.28668200

CA2n-SS-t**E=-1087.095235 a.u.**

C	1.53434400	0.15293100	-0.33492900
N	2.25575400	-0.95489800	0.34898400
O	3.28351600	-0.32972500	1.16508600
C	3.54759900	0.94746900	0.59965400
C	2.15003200	1.48515700	0.24257900
C	0.02535400	0.04141000	-0.20337800
C	-0.79827500	0.67280900	-1.14465300
C	-2.18548800	0.61081200	-1.03641400
C	-2.76835900	-0.09271200	0.02018800
C	-1.95652300	-0.72973900	0.96224900
C	-0.56961900	-0.66295900	0.84982000
C	-4.26422300	-0.22194400	0.10869000
F	-4.68766100	-0.29336600	1.39063400
F	-4.89745800	0.82193600	-0.47132100
H	1.78005000	0.13083900	-1.40935500
H	-0.35536200	1.22239900	-1.97216600
H	-2.81302800	1.10824800	-1.76835100
H	-2.40937700	-1.27412000	1.78477100
H	0.06746700	-1.16848800	1.56695600
C	1.43089700	2.05229400	1.46761500
H	0.40247400	2.33357700	1.23093600
H	1.41925100	1.31691200	2.27669500
H	1.94740500	2.95197600	1.81599800
C	2.24217900	2.50885400	-0.87789400
O	1.75996700	3.61752600	-0.85049100
H	2.81113800	2.15899400	-1.77221600
H	4.19709900	0.87387800	-0.28817600
H	4.05560600	1.53893800	1.36608000
C	2.90825200	-1.90725500	-0.58196300
H	3.56609200	-1.36057900	-1.28368400
C	1.82822200	-2.63973500	-1.38819900
H	1.22063700	-1.96657800	-2.00080200
H	2.30421500	-3.36084000	-2.06083100
H	1.15662900	-3.18514800	-0.71669100
C	3.75315400	-2.90612300	0.21201400
H	4.21577800	-3.62691400	-0.47130100
H	4.54095100	-2.40119400	0.77391500
H	3.12333900	-3.45515100	0.92096200
F	-4.70752300	-1.34218000	-0.51094100

CA2x-RS-t
E=-1087.094966 a.u.

C	3.57512600	1.17458500	-0.11584800
C	2.13141800	1.56027900	0.24785900
C	1.57299600	0.11733400	0.52053100
H	1.81612500	-0.09487400	1.57374600
O	3.43255200	0.02143500	-0.92979500
N	2.34387300	-0.78479600	-0.37236000
C	2.95111900	-1.94302800	0.32399600
H	3.57719500	-1.58708100	1.16368200
C	1.83827000	-2.83801900	0.88375700
H	1.18652700	-3.18728700	0.07584800
H	2.28609500	-3.71241000	1.36754400
H	1.21521700	-2.33093900	1.62667600
C	3.83037800	-2.72835300	-0.65211900
H	4.63355900	-2.10553600	-1.05010000
H	4.27501700	-3.58981200	-0.14152800
H	3.22997200	-3.09551200	-1.49211800
C	0.06992200	-0.02830800	0.34166300
C	-0.49063300	-0.41897700	-0.88152000
C	-0.78542300	0.25485500	1.41457600
C	-1.87239400	-0.50572800	-1.03239300
H	0.16847200	-0.67982200	-1.70227700
C	-2.16849000	0.17090600	1.26904900
H	-0.36762800	0.53238800	2.37924400
C	-2.71547700	-0.20785900	0.04144800
H	-2.29683000	-0.81773200	-1.98113400
H	-2.82009800	0.38384600	2.10996800
C	-4.20825300	-0.25444400	-0.13903900
F	-4.84856700	-0.52313500	1.02139600
F	-4.69602000	0.92410800	-0.59163600
F	-4.57671800	-1.19897400	-1.03370400
C	2.00620700	2.49395900	1.44923200
H	0.95613100	2.67881100	1.69219400
H	2.50267100	2.06740700	2.32806500
H	2.45798300	3.46611100	1.23086300
C	1.48627600	2.17993600	-0.99256500
H	1.62425100	1.60338400	-1.92976900
O	0.89871400	3.23874600	-0.99001500
H	4.10186500	1.92238800	-0.71835700
H	4.16172500	0.97797600	0.79618400

CA2x-SR-t

E=-1087.094966 a.u.

C	-1.57299500	0.11733400	0.52053000
N	-2.34387300	-0.78479600	-0.37236100
O	-3.43254800	0.02143700	-0.92979900
C	-3.57512400	1.17458600	-0.11585100
C	-2.13141700	1.56028000	0.24785900
C	-0.06992200	-0.02830900	0.34166200
C	0.78542400	0.25485600	1.41457400
C	2.16849100	0.17090500	1.26904700
C	2.71547700	-0.20786200	0.04144500
C	1.87239400	-0.50573100	-1.03239400
C	0.49063300	-0.41897900	-0.88152100
C	4.20825300	-0.25444600	-0.13903900
F	4.57671900	-1.19895400	-1.03372600
F	4.84856300	-0.52316800	1.02139200
F	4.69602500	0.92411700	-0.59160400
H	-1.81612400	-0.09487400	1.57374600
H	0.36763000	0.53239000	2.37924200
H	2.82009900	0.38384500	2.10996500
H	2.29683000	-0.81773600	-1.98113500
H	-0.16847200	-0.67982500	-1.70227800
C	-2.00620800	2.49395800	1.44923300
H	-2.50267300	2.06740500	2.32806500
H	-0.95613300	2.67881000	1.69219600
H	-2.45798400	3.46611000	1.23086400
C	-1.48627300	2.17993800	-0.99256400
H	-1.62424800	1.60338800	-1.92976900
O	-0.89870800	3.23874600	-0.99001000
H	-4.10186200	1.92239000	-0.71836100
H	-4.16172500	0.97797600	0.79617900
C	-2.95112300	-1.94302500	0.32399700
H	-3.57719800	-1.58707500	1.16368300
C	-1.83827600	-2.83801900	0.88375900
H	-1.21522100	-2.33093900	1.62667600
H	-2.28610300	-3.71240800	1.36754700
H	-1.18653500	-3.18729000	0.07584900
C	-3.83038400	-2.72834900	-0.65211700
H	-4.27502500	-3.58980600	-0.14152400
H	-4.63356500	-2.10553000	-1.05009700
H	-3.22998100	-3.09550900	-1.49211700

Structure corresponding to P-I (ELF analysis)

E=-1087.064460 a.u.

C	-2.08000600	1.56992800	-1.50913800
C	-2.01247600	1.56762500	-0.04881800
C	-0.39197400	1.54538500	0.45726700
H	-2.43226400	2.48623200	0.36740100
H	-2.46805100	0.68659200	0.40796200
H	-0.34832000	2.04103600	1.43137800
O	0.06391500	1.92048500	-1.71128000
N	0.30378900	2.32418700	-0.50137100
C	0.64730100	3.75591000	-0.21970900
H	-0.19787900	4.19707200	0.32482300
C	1.89924800	3.78252400	0.67205200
H	2.75605100	3.35062000	0.14343900
H	2.14158700	4.81708000	0.93816600
H	1.75608900	3.22255300	1.60269400
C	0.86419700	4.52981100	-1.51549600
H	-0.06067400	4.60629100	-2.08758600
H	1.20152200	5.54119800	-1.26504900
H	1.63004200	4.05287300	-2.13506600
C	-2.26550700	2.85457800	-2.17492400
H	-2.34851200	2.79850400	-3.28093500
O	-2.30461300	3.94065300	-1.60057900
C	-2.27299100	0.30941900	-2.30530600
H	-3.34061100	0.06718200	-2.41785700
H	-1.85598100	0.41721000	-3.31274700
H	-1.79169400	-0.54620000	-1.82419100
C	0.06176500	0.10405700	0.61229300
C	0.67184700	-0.64540300	-0.40504000
C	-0.18701400	-0.51745800	1.84378100
C	0.99747900	-1.98500300	-0.19576600
H	0.88203400	-0.17710500	-1.35866300
C	0.12821200	-1.85663000	2.05342100
H	-0.64012200	0.05278900	2.65167400
C	0.71763700	-2.59854600	1.02801700
H	1.47261000	-2.55489100	-0.98783300
H	-0.07203000	-2.32077800	3.01344100
C	0.99947300	-4.06243500	1.22634900
F	-0.05383300	-4.83090300	0.85795500
F	2.05832900	-4.47649700	0.49576200
F	1.25913000	-4.35341500	2.52112100

Structure corresponding to P-II (ELF analysis)**E=-1087.075230 a.u.**

C	-1.92606200	1.59626600	-1.52815300
C	-1.94419600	1.58559600	-0.03723000
C	-0.41534100	1.53857600	0.46516400
H	-2.39675500	2.50565200	0.34184200
H	-2.47472500	0.72012600	0.36734400
H	-0.34760600	2.03409000	1.43900700
O	-0.07736600	1.90218300	-1.72439300
N	0.32787600	2.29670500	-0.50460300
C	0.62959200	3.73834400	-0.22825900
H	-0.21747800	4.18869100	0.30913400
C	1.87970700	3.77506300	0.66963500
H	2.74012600	3.35286200	0.13936200
H	2.11164200	4.80970300	0.94595100
H	1.74077000	3.20524600	1.59514800
C	0.86342600	4.52001400	-1.51834000
H	-0.05257500	4.61314000	-2.10177100
H	1.20960200	5.52694500	-1.26151900
H	1.63006500	4.03893000	-2.13473800
C	-2.26204300	2.87648300	-2.18364300
H	-2.39268900	2.81705500	-3.28479600
O	-2.32693700	3.94788800	-1.60106400
C	-2.23461200	0.33289900	-2.29840200
H	-3.31840600	0.15120200	-2.32086900
H	-1.89134200	0.41368700	-3.33545600
H	-1.75842600	-0.53806500	-1.84162400
C	0.05053900	0.09878100	0.62390900
C	0.66954900	-0.64079300	-0.39489500
C	-0.19504900	-0.52584500	1.85186900
C	0.99947500	-1.98026700	-0.19213100
H	0.88342700	-0.16436400	-1.34387800
C	0.13013300	-1.86250300	2.05876500
H	-0.65192100	0.04060500	2.66045900
C	0.72061800	-2.59823600	1.02999900
H	1.47867500	-2.54598000	-0.98485600
H	-0.06527200	-2.33075300	3.01775100
C	1.00148000	-4.06172700	1.22595000
F	-0.05311400	-4.82934200	0.85727700
F	2.05946700	-4.47713000	0.49501100
F	1.26019100	-4.35462700	2.52067300

Structure corresponding to P-III (ELF analysis)**E=-1087.091525 a.u.**

C	-1.76948000	1.62854800	-1.53978400
C	-1.90846900	1.59961000	-0.02661600
C	-0.41993600	1.53470800	0.47902500
H	-2.37773800	2.52116100	0.32675600
H	-2.48491200	0.74283600	0.32645100
H	-0.33434600	2.03871800	1.44674500
O	-0.22158700	1.88508100	-1.74419200
N	0.35793900	2.26319900	-0.50719200
C	0.61168000	3.71717800	-0.24008900
H	-0.24397700	4.16933500	0.28515100
C	1.85737900	3.77018700	0.66639500
H	2.72235800	3.35707600	0.13709500
H	2.07556600	4.80723000	0.94559100
H	1.72342700	3.19665100	1.59031400
C	0.86303700	4.50607600	-1.52429600
H	-0.04265000	4.60748000	-2.12250000
H	1.20866900	5.51142500	-1.26015700
H	1.63705700	4.02511200	-2.13201700
C	-2.26094400	2.89925100	-2.18929400
H	-2.43211000	2.83050100	-3.28518100
O	-2.35542600	3.95819200	-1.60455900
C	-2.18528600	0.36510500	-2.29129300
H	-3.27609000	0.25072500	-2.25025800
H	-1.89062600	0.42043000	-3.34503300
H	-1.73012600	-0.52398200	-1.84885700
C	0.04689400	0.09521600	0.63817700
C	0.67010400	-0.63692300	-0.38388800
C	-0.20065300	-0.53439700	1.86129700
C	0.99997700	-1.97751800	-0.18866900
H	0.89231600	-0.15231100	-1.32706900
C	0.12974400	-1.86983800	2.06366700
H	-0.66039600	0.02843800	2.67089000
C	0.72202900	-2.59943600	1.03186300
H	1.48122500	-2.53984500	-0.98263900
H	-0.06358900	-2.34283500	3.02070600
C	1.00309600	-4.06215300	1.22557900
F	-0.05238000	-4.82899600	0.85663700
F	2.06060900	-4.47800200	0.49425700
F	1.26153800	-4.35655300	2.52024000

Structure corresponding to P-IV (ELF analysis)**E=-1087.095202 a.u.**

C	-1.72722300	1.64619600	-1.54259600
C	-1.89233000	1.60882500	-0.02448200
C	-0.41694100	1.53091800	0.48403600
H	-2.36257500	2.53230400	0.32418500
H	-2.48619800	0.75580500	0.31177900
H	-0.32281900	2.04361600	1.44636700
O	-0.25872200	1.88474100	-1.75385200
N	0.37284800	2.24461700	-0.51359700
C	0.60357300	3.70234300	-0.24905700
H	-0.26122800	4.14783000	0.26716100
C	1.84220600	3.76714500	0.66534900
H	2.71316500	3.36195800	0.13987200
H	2.04932700	4.80623100	0.94498900
H	1.71011700	3.19272600	1.58889600
C	0.86274500	4.49451300	-1.52999500
H	-0.03723200	4.59562600	-2.13683500
H	1.20330700	5.50035700	-1.26098100
H	1.64374000	4.01676300	-2.13131700
C	-2.26780800	2.91000900	-2.18941300
H	-2.45590400	2.83479600	-3.28247100
O	-2.37482800	3.96715400	-1.60651700
C	-2.15983600	0.38403100	-2.28732000
H	-3.25043600	0.28238600	-2.23075600
H	-1.87809900	0.43447700	-3.34477700
H	-1.70743700	-0.50835200	-1.84870400
C	0.04569000	0.09232700	0.64797500
C	0.67116600	-0.63488100	-0.37572800
C	-0.20428100	-0.53995200	1.86863300
C	1.00057800	-1.97593600	-0.18565000
H	0.89728800	-0.14546800	-1.31551600
C	0.12890600	-1.87511800	2.06719200
H	-0.66602100	0.02027100	2.67887200
C	0.72257700	-2.60063400	1.03337800
H	1.48281400	-2.53578200	-0.98076900
H	-0.06390500	-2.35153900	3.02257300
C	1.00406100	-4.06309600	1.22529900
F	-0.05181800	-4.82920900	0.85616600
F	2.06138000	-4.47860800	0.49365900
F	1.26258400	-4.35818000	2.51986000