

Z-matrix TS endo 6a'

O 2

C

C,1,R1

F,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

O,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

C,2,R12,1,A11,5,B10,0

F,13,R13,8,A12,11,B11,0

F,13,R14,8,A13,12,B12,0

R1=1.35648431

R2=1.34069498

R3=1.31646106

R4=1.31590492

R5=1.36734536

R6=1.39576604

R7=1.54441432

R8=1.35054258

R9=1.33417597

R10=1.3553755

R11=1.35833338

R12=2.35565391

R13=1.33199079

R14=1.33133009

A1=118.98734505

A2=122.51180786

A3=122.75809211

A4=119.06723484

A5=116.9760892

A6=110.73773879

A7=110.35105782

A8=106.61482216

A9=95.25991035

A10=109.26976666

A11=105.04719959

A12=115.07670975

A13=114.06518837

B1=16.34957606

B2=185.03685341

B3=-23.67527712

B4=126.66429853

B5=316.06271821

B6=120.46901179

B7=-121.47653433

B8=84.91300011

B9=-212.26563565

B10=79.50141184

B11=328.74335049

B12=319.04708056

Z-matrix cyclized product radical 6a' (endo addition)

0 2
C
C,1,R1
F,2,R2,1,A1
F,1,R3,2,A2,3,B1,0
F,1,R4,2,A3,3,B2,0
O,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
F,7,R8,6,A7,8,B6,0
F,7,R9,6,A8,8,B7,0
F,8,R10,2,A9,6,B8,0
F,8,R11,11,A10,6,B9,0
C,2,R12,1,A11,5,B10,0
F,13,R13,8,A12,11,B11,0
F,13,R14,8,A13,12,B12,0

R1=1.51290378
R2=1.35908182
R3=1.32684673
R4=1.32893908
R5=1.40922747
R6=1.39052192
R7=1.54527421
R8=1.34928011
R9=1.33450986
R10=1.35177868
R11=1.34148671
R12=1.57276285
R13=1.3482514
R14=1.34670932
A1=107.95048008
A2=114.33297682
A3=114.09612944
A4=108.01087084
A5=112.99336989
A6=105.55017048
A7=110.82356246
A8=108.58508043
A9=104.00733932
A10=109.91201982
A11=115.33944168
A12=112.47291684
A13=109.45472027
B1=50.77344102
B2=181.80932109
B3=-58.68771291
B4=131.83424454
B5=334.10742415
B6=118.92325461
B7=-121.83721083
B8=90.33355385
B9=-199.98462905
B10=59.44137527
B11=327.39695525
B12=328.41756825

Z-matrix starting radical 6a' (exo)

0 2
C
C,1,R1
F,2,R2,1,A1
F,1,R3,2,A2,3,B1,0
F,1,R4,2,A3,3,B2,0
O,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
F,7,R8,6,A7,8,B6,0
F,7,R9,6,A8,8,B7,0
F,8,R10,2,A9,6,B8,0
F,8,R11,11,A10,6,B9,0
C,1,R12,2,A11,5,B10,0
F,13,R13,8,A12,11,B11,0
F,13,R14,8,A13,12,B12,0

R1=1.32961574
R2=1.33492468
R3=1.31911558
R4=1.32245506
R5=1.35903572
R6=1.39726959
R7=1.55139477
R8=1.34982925
R9=1.33647843
R10=1.35167487
R11=1.36625845
R12=3.26422949
R13=1.32637092
R14=1.32880747
A1=121.0249665
A2=123.51041038
A3=123.2431878
A4=122.69055196
A5=118.6500556
A6=112.52167814
A7=111.09608017
A8=106.05458506
A9=97.3532219
A10=108.64441313
A11=77.45615082
A12=114.06981565
A13=114.25204789
B1=1.44883987
B2=180.92237029
B3=-7.00518246
B4=106.68604741
B5=272.66793865
B6=122.5439543
B7=-118.74106104
B8=63.75027339
B9=-219.91073224
B10=306.5573487
B11=321.23280076
B12=309.17732692

E(B3LYP)=-1164.16608 E(PMP2)=-1161.33234

Z-matrix TS exo 6a'

0 2

C

C,1,R1

F,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

O,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

C,1,R12,2,A11,5,B10,0

F,13,R13,8,A12,11,B11,0

F,13,R14,8,A13,12,B12,0

R1=1.36214384

R2=1.33133047

R3=1.31958315

R4=1.32482401

R5=1.35442733

R6=1.40822384

R7=1.55369188

R8=1.34847243

R9=1.33313404

R10=1.35433699

R11=1.36403729

R12=2.35513865

R13=1.33298971

R14=1.3369145

A1=120.25174214

A2=121.23089819

A3=121.62927991

A4=120.69543808

A5=115.62785432

A6=113.17393111

A7=110.15034592

A8=105.80685456

A9=100.02571426

A10=108.42698063

A11=92.40606612

A12=112.66832942

A13=112.74964153

B1=-14.14924257

B2=190.84157909

B3=29.40255418

B4=81.34978791

B5=298.46271047

B6=122.22840553

B7=-119.76708244

B8=73.07326955

B9=-216.720324

B10=266.06660238

B11=310.37399221

B12=302.37222596

Z-matrix cyclized radical product '6a' (exo addition)

O 2

C

C,1,R1

F,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

O,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

C,1,R12,2,A11,5,B10,0

F,13,R13,8,A12,11,B11,0

F,13,R14,8,A13,12,B12,0

R1=1.51410311

R2=1.33283861

R3=1.34771976

R4=1.35880921

R5=1.36073846

R6=1.40568279

R7=1.55231003

R8=1.34786482

R9=1.33195611

R10=1.35255503

R11=1.34908207

R12=1.55140001

R13=1.34691111

R14=1.35707796

A1=115.21925932

A2=110.64367548

A3=108.854625

A4=115.71079282

A5=117.66008165

A6=111.3470002

A7=110.08538603

A8=106.62823679

A9=102.91051412

A10=109.29456401

A11=110.51321942

A12=109.81792143

A13=108.08579315

B1=-32.55030132

B2=206.9602774

B3=68.97873311

B4=54.07244853

B5=306.7375908

B6=121.08961967

B7=-120.45855582

B8=75.67338632

B9=-210.76238748

B10=241.9381647

B11=307.38679763

B12=307.61959749

Z-matrix starting radical 6b

O 2

C

C,1,R1

H,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,2,R14,1,A13,5,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

R1=1.33020195

R2=1.08196154

R3=1.31927833

R4=1.31381153

R5=1.49345278

R6=1.55330886

R7=1.54913817

R8=1.36268572

R9=1.35095399

R10=1.35443119

R11=1.36778361

R12=1.36972976

R13=1.36032966

R14=3.04611821

R15=1.33163034

R16=1.32734645

A1=117.73789058

A2=122.80660379

A3=126.62825009

A4=124.86247257

A5=113.72392086

A6=116.64791206

A7=107.75031379

A8=108.3926597

A9=103.00069327

A10=108.06841904

A11=109.83993478

A12=112.15425859

A13=107.12675618

A14=114.88088103

A15=114.04066519

B1=1.71321249

B2=-179.10353811

B3=-3.08498857

B4=137.28675722

B5=-66.55557515

B6=121.58222782

B7=-120.90910925

B8=69.03937189

B9=143.31696871

B10=117.76082993
B11=-122.79478414
B12=88.58685112
B13=-61.47746688
B14=-48.07558964

E(B3LYP)=-1227.51352 E(PMP2)=-1224.50806

Z-matrix TS endo 6b

O 2

C

C,1,R1

H,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,2,R14,1,A13,5,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

R1=1.36105078

R2=1.08436866

R3=1.32106974

R4=1.31529984

R5=1.50890905

R6=1.54783884

R7=1.54198844

R8=1.36279112

R9=1.34528098

R10=1.35446588

R11=1.35773281

R12=1.36303867

R13=1.35950653

R14=2.2500

R15=1.33605394

R16=1.33186051

A1=115.62290489

A2=122.02756618

A3=125.99035371

A4=122.63695431

A5=110.51034637

A6=109.7376889

A7=107.63771831

A8=111.10199941

A9=103.76939225

A10=109.13019863

A11=110.74120135

A12=111.7139233

A13=111.45216137

A14=113.33484171

A15=115.15136351

B1=17.17679586

B2=187.8730481

B3=-21.93477921

B4=144.95559354

B5=309.60574791

B6=116.79088421

B7=-123.62065534

B8=75.65849786

B9=-207.16421024

B10=119.74589384
B11=-120.04625943
B12=87.00321803
B13=325.74067537
B14=334.30011346

Z-matrix cyclized radical product 6b (endo addition)

O 2

C

C,1,R1

H,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,2,R14,1,A13,5,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

R1=1.49931644

R2=1.09307297

R3=1.33647219

R4=1.33015391

R5=1.54066754

R6=1.54550649

R7=1.54399857

R8=1.36021106

R9=1.34141797

R10=1.35231327

R11=1.34406707

R12=1.35150556

R13=1.35829836

R14=1.56579483

R15=1.3559912

R16=1.35097673

A1=107.60705276

A2=113.98444375

A3=116.73708666

A4=114.28632367

A5=104.6496734

A6=103.70256419

A7=108.15831839

A8=113.31264819

A9=110.19395137

A10=109.65046887

A11=112.05896152

A12=111.57378773

A13=116.04120783

A14=109.17133271

A15=110.21937265

B1=45.84636751

B2=177.54142282

B3=-64.08944534

B4=156.46456205

B5=320.60795623

B6=114.81667167

B7=-123.24148827

B8=78.24252072

B9=-198.33515881

B10=121.38537729

B11=-116.7173887

B12=58.87802979

B13=338.80029143

B14=335.7882724

Z-matrix TS exo 6b

O 2

C

C,1,R1

H,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,1,R14,2,A13,5,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

R1=1.36342145

R2=1.08235916

R3=1.32347374

R4=1.32544058

R5=1.49301324

R6=1.55698044

R7=1.55008058

R8=1.36060419

R9=1.35007199

R10=1.35474436

R11=1.36233881

R12=1.36038613

R13=1.36198491

R14=2.25001

R15=1.3330689

R16=1.33100212

A1=117.90871857

A2=121.32850889

A3=124.05380029

A4=120.3015275

A5=111.53446395

A6=114.6865881

A7=107.47012867

A8=109.78675202

A9=101.21674623

A10=108.45921017

A11=109.99259849

A12=112.20596245

A13=96.10903361

A14=113.30483033

A15=112.96452342

B1=-14.89626608

B2=189.31845985

B3=33.39261034

B4=73.20470844

B5=305.1822043

B6=119.74902211

B7=-121.96219329

B8=75.40701687

B9=-214.00942505

B10=118.4799748
B11=-120.69261049
B12=262.26701599
B13=303.6955497
B14=313.09176539

Z-matrix cyclized product radical 6b (exo addition)

O 2

C

C,1,R1

H,2,R2,1,A1

F,1,R3,2,A2,3,B1,0

F,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,1,R14,2,A13,5,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

R1=1.4902631

R2=1.08344652

R3=1.35704229

R4=1.37112043

R5=1.49028318

R6=1.55095457

R7=1.5474296

R8=1.3570395

R9=1.34820293

R10=1.35549233

R11=1.34990248

R12=1.35711855

R13=1.37102576

R14=1.55091058

R15=1.35702328

R16=1.34822636

A1=119.73462654

A2=110.41034214

A3=110.06721669

A4=119.50668859

A5=112.48812979

A6=112.38550061

A7=107.87192314

A8=109.94311245

A9=100.11651164

A10=109.15045056

A11=110.39765253

A12=110.08352865

A13=112.49346358

A14=108.32577387

A15=109.20654143

B1=25.55865281

B2=266.57909145

B3=74.99029358

B4=44.71625081

B5=313.3240079

B6=119.33692842

B7=-121.86390599

B8=79.66956197

B9=-210.07244158

B10=121.26549888
B11=-119.75640112
B12=240.284647
B13=305.67982829
B14=305.53972605

Z-matrix strarting radical 6c

0 2
C
C,1,R1
H,2,R2,1,A1
H,1,R3,2,A2,3,B1,0
H,1,R4,2,A3,3,B2,0
C,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
F,7,R8,6,A7,8,B6,0
F,7,R9,6,A8,8,B7,0
F,8,R10,2,A9,6,B8,0
F,8,R11,11,A10,6,B9,0
F,6,R12,2,A11,7,B10,0
F,6,R13,2,A12,7,B11,0
C,2,R14,1,A13,5,B12,0
F,15,R15,8,A14,12,B13,0
F,15,R16,8,A15,11,B14,0

R1=1.33175938
R2=1.08651995
R3=1.08553012
R4=1.08522865
R5=1.50060975
R6=1.55275028
R7=1.54933908
R8=1.36369216
R9=1.35127224
R10=1.35547091
R11=1.36578235
R12=1.37022686
R13=1.36113569
R14=3.10137809
R15=1.32908549
R16=1.32879549
A1=122.30177498
A2=121.06302643
A3=121.61505121
A4=123.0152315
A5=114.90975041
A6=116.23188733
A7=107.61382183
A8=108.50363879
A9=90.46876644
A10=108.35083152
A11=109.19846874
A12=111.66267868
A13=101.68810346
A14=114.61476179
A15=114.07549887
B1=0.34021178
B2=180.09037157

B3=-1.95166713
B4=120.83575816
B5=301.81193893
B6=120.69268516
B7=-121.88493453
B8=83.21018066
B9=-219.78083768
B10=117.98358363
B11=-123.12703574
B12=87.6540863
B13=311.47488511
B14=324.20164874

E(B3LYP)=-1029.04839 E(PMP2)=-1026.47024

Z-matrix TS endo 6c

0 2
C
C,1,R1
H,2,R2,1,A1
H,1,R3,2,A2,3,B1,0
H,1,R4,2,A3,3,B2,0
C,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
F,7,R8,6,A7,8,B6,0
F,7,R9,6,A8,8,B7,0
F,8,R10,2,A9,6,B8,0
F,8,R11,11,A10,6,B9,0
F,6,R12,2,A11,7,B10,0
F,6,R13,2,A12,7,B11,0
C,2,R14,1,A13,5,B12,0
F,15,R15,8,A14,12,B13,0
F,15,R16,8,A15,11,B14,0

R1=1.36149933
R2=1.08707372
R3=1.08470103
R4=1.08415593
R5=1.51309602
R6=1.54615333
R7=1.54020513
R8=1.36269803
R9=1.34693348
R10=1.35490729
R11=1.35848029
R12=1.36458651
R13=1.36262483
R14=2.29000
R15=1.33475454
R16=1.32836276
A1=120.75838077
A2=120.81886552
A3=121.40898273
A4=121.42246183
A5=112.0716237
A6=109.89438185
A7=107.71836812
A8=111.41077768
A9=101.55843031
A10=109.04479484
A11=110.22667696
A12=111.15493949
A13=108.72840272
A14=113.53001951
A15=115.26321775
B1=13.00387192
B2=188.98631275
B3=-14.5661023
B4=137.48880002
B5=311.69914043
B6=116.73166791
B7=-123.59749658
B8=78.43839671
B9=-207.4190327

B10=119.9778283
B11=-120.53373251
B12=90.62857554
B13=322.42073523
B14=331.82513787

Z-matrix cyclized radical product 6c (endo addition)

0 2

C

C,1,R1

H,2,R2,1,A1

H,1,R3,2,A2,3,B1,0

H,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,2,R14,1,A13,5,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

R1=1.48464678

R2=1.09583718

R3=1.08208195

R4=1.08241113

R5=1.54423144

R6=1.54415284

R7=1.5594301

R8=1.3590945

R9=1.34387096

R10=1.34814632

R11=1.34891019

R12=1.35028053

R13=1.36260598

R14=1.54937736

R15=1.35320738

R16=1.35754336

A1=111.45116372

A2=120.6460441

A3=120.04654417

A4=115.24397307

A5=104.60068367

A6=104.45477984

A7=108.07952927

A8=113.33273157

A9=128.1675241

A10=109.2414199

A11=112.9555692

A12=110.45964681

A13=115.12932345

A14=110.56956629

A15=108.61919

B1=-7.32065331

B2=175.25391029

B3=-64.39096532

B4=166.5511003

B5=323.1625922

B6=115.82553324

B7=-122.70893303

B8=76.52893274

B9=-197.8761098

B10=122.1193163
B11=-115.9461412
B12=53.86746658
B13=370.02666044
B14=367.29071554

Z-matrix TS exo 6c

0 2
C
C,1,R1
H,2,R2,1,A1
H,1,R3,2,A2,3,B1,0
H,1,R4,2,A3,3,B2,0
C,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
F,7,R8,6,A7,8,B6,0
F,7,R9,6,A8,8,B7,0
F,8,R10,2,A9,6,B8,0
F,8,R11,11,A10,6,B9,0
F,6,R12,2,A11,7,B10,0
F,6,R13,2,A12,7,B11,0
C,1,R14,2,A13,5,B12,0
F,15,R15,8,A14,12,B13,0
F,15,R16,8,A15,11,B14,0

R1=1.35558297
R2=1.08497069
R3=1.08586555
R4=1.08584166
R5=1.49531986
R6=1.55597437
R7=1.55207729
R8=1.36122912
R9=1.35203985
R10=1.35914365
R11=1.3645011
R12=1.36119177
R13=1.36649141
R14=2.37001
R15=1.33345413
R16=1.33441994
A1=122.63361063
A2=120.92162078
A3=121.01796601
A4=119.15180577
A5=111.14735119
A6=115.42449624
A7=107.60702686
A8=109.47320059
A9=99.63502352
A10=108.0464905
A11=111.40006245
A12=111.73992891
A13=95.8389123
A14=113.49733333
A15=112.42362195
B1=-9.57017837
B2=185.50543587
B3=22.27318205
B4=75.0822053
B5=303.71980248
B6=120.48453122
B7=-121.52206484
B8=75.73203356
B9=-215.97323136

B10=119.19010102
B11=-119.60739336
B12=271.86875643
B13=300.66131944
B14=310.38683224

Z-matrix cyclized radical product 6c (exo addition)

0 2
C
C,1,R1
H,2,R2,1,A1
H,1,R3,2,A2,3,B1,0
H,1,R4,2,A3,3,B2,0
C,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
F,7,R8,6,A7,8,B6,0
F,7,R9,6,A8,8,B7,0
F,8,R10,2,A9,6,B8,0
F,8,R11,11,A10,6,B9,0
F,6,R12,2,A11,7,B10,0
F,6,R13,2,A12,7,B11,0
C,1,R14,2,A13,5,B12,0
F,15,R15,8,A14,12,B13,0
F,15,R16,8,A15,11,B14,0

R1=1.49364933
R2=1.08315642
R3=1.09356019
R4=1.10152594
R5=1.48615672
R6=1.54980595
R7=1.5463137
R8=1.35796372
R9=1.35072488
R10=1.36189792
R11=1.3501678
R12=1.35855606
R13=1.37953061
R14=1.52886979
R15=1.36357139
R16=1.35981774
A1=122.24572127
A2=111.76450058
A3=110.88157425
A4=118.79326005
A5=112.24435095
A6=112.07865021
A7=108.02595937
A8=110.33412927
A9=99.94583156
A10=108.86317788
A11=111.22380571
A12=110.36293816
A13=111.51692986
A14=107.85309939
A15=108.36912447
B1=21.25553901
B2=261.29986788
B3=70.95643894
B4=46.92949683
B5=313.40708515
B6=119.28880491
B7=-121.92444077
B8=79.39375912
B9=-210.02073293

B10=121.76472529
B11=-119.0509424
B12=240.83006606
B13=306.1812043
B14=304.05317032

Z-matrix starting radical 7c

O 2

C

C,1,R1

H,2,R2,1,A1

H,1,R3,2,A2,3,B1,0

H,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,8,R14,7,A13,6,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

C,1,R17,2,A16,5,B15,0

F,18,R18,15,A17,8,B16,0

F,18,R19,15,A18,8,B17,0

R1=1.33081202

R2=1.08514839

R3=1.08548033

R4=1.08524838

R5=1.50141926

R6=1.5577996

R7=1.55955341

R8=1.36069054

R9=1.35464539

R10=1.35570243

R11=1.35466163

R12=1.36828896

R13=1.36772058

R14=1.5524955

R15=1.3578341

R16=1.36463607

R17=3.2741794

R18=1.32992611

R19=1.32693193

A1=122.08254018

A2=120.93840039

A3=121.88833842

A4=123.02981139

A5=115.69930264

A6=118.88871664

A7=108.12944869

A8=108.08107544

A9=112.01883667

A10=108.56545992

A11=108.55831219

A12=111.69141081

A13=118.24770576

A14=108.9280474

A15=107.19581376

A16=80.75812604

A17=113.69668566

A18=114.50067478

B1=0.49594442
B2=-179.4219229
B3=-3.22627245
B4=133.69660754
B5=-81.90238352
B6=123.53720657
B7=-119.48496098
B8=51.65229792
B9=143.02987934
B10=118.20899599
B11=-123.46510016
B12=54.13426732
B13=-77.81267442
B14=-77.96191477
B15=-63.31940936
B16=160.16463415
B17=-69.58550874

E(B3LYP)=-1266.82472 E(PMP2)=-1263.67590

Z-matrix TS endo 7c

0 2

C

C,1,R1

H,2,R2,1,A1

H,1,R3,2,A2,3,B1,0

H,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,8,R14,7,A13,6,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

C,2,R17,1,A16,5,B15,0

F,18,R18,15,A17,8,B16,0

F,18,R19,15,A18,8,B17,0

R1=1.35417353

R2=1.08611125

R3=1.08481728

R4=1.08507194

R5=1.50965305

R6=1.55172165

R7=1.55127202

R8=1.36216154

R9=1.35231192

R10=1.35501451

R11=1.35336498

R12=1.36866458

R13=1.36415647

R14=1.54567272

R15=1.35809569

R16=1.36346585

R17=2.3850003

R18=1.33105943

R19=1.33015536

A1=121.05184415

A2=120.93499515

A3=121.41298455

A4=120.38166396

A5=115.90326979

A6=117.54522133

A7=107.50339662

A8=108.25875918

A9=104.23588274

A10=108.84415546

A11=109.15358644

A12=110.77214434

A13=115.65561227

A14=108.81752413

A15=107.66694021

A16=102.28973769

A17=113.76573333

A18=114.263574

B1=10.78094034
B2=186.97169663
B3=-13.81636826
B4=162.8676098
B5=292.17201419
B6=121.97006945
B7=-120.81972223
B8=67.54182444
B9=-215.66032709
B10=118.43180131
B11=-123.59345694
B12=58.63132409
B13=300.89525969
B14=300.44817312
B15=90.95501662
B16=165.16824429
B17=294.77113856

Z-matrix cyclized radical product 7c (endo addition)

0 2

C

C,1,R1

H,2,R2,1,A1

H,1,R3,2,A2,3,B1,0

H,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,8,R14,7,A13,6,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

C,2,R17,1,A16,5,B15,0

F,18,R18,15,A17,8,B16,0

F,18,R19,15,A18,8,B17,0

R1=1.49322669

R2=1.09549656

R3=1.08207533

R4=1.08255824

R5=1.53875367

R6=1.54733162

R7=1.54619114

R8=1.36052554

R9=1.34876994

R10=1.35431851

R11=1.35070369

R12=1.3582551

R13=1.36232699

R14=1.54609669

R15=1.36052754

R16=1.34904823

R17=1.54768861

R18=1.35866983

R19=1.35958279

A1=110.65990352

A2=120.19624014

A3=120.05780082

A4=111.48181825

A5=113.54304032

A6=112.81373286

A7=107.74686246

A8=109.93815104

A9=104.05733825

A10=109.10759743

A11=109.49354687

A12=110.35157326

A13=111.92985387

A14=108.08641332

A15=109.24745449

A16=111.65000755

A17=107.74210243

A18=107.70972704

B1=24.54258877
B2=198.36319716
B3=-43.04565735
B4=177.32114909
B5=307.50603399
B6=119.1808664
B7=-122.18676315
B8=75.13758294
B9=-209.59249684
B10=120.30515935
B11=-120.98161603
B12=50.18677936
B13=307.41496691
B14=306.89948226
B15=80.70796897
B16=173.69554444
B17=290.18260008

Z-matrix TS exo 7c

0 2
C
C,1,R1
H,2,R2,1,A1
H,1,R3,2,A2,3,B1,0
H,1,R4,2,A3,3,B2,0
C,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
F,7,R8,6,A7,8,B6,0
F,7,R9,6,A8,8,B7,0
F,8,R10,2,A9,6,B8,0
F,8,R11,11,A10,6,B9,0
F,6,R12,2,A11,7,B10,0
F,6,R13,2,A12,7,B11,0
C,8,R14,7,A13,6,B12,0
F,15,R15,8,A14,12,B13,0
F,15,R16,8,A15,11,B14,0
C,1,R17,2,A16,5,B15,0
F,18,R18,15,A17,8,B16,0
F,18,R19,15,A18,8,B17,0

R1=1.34983612
R2=1.08511477
R3=1.08538086
R4=1.08505552
R5=1.49308472
R6=1.55277715
R7=1.56104692
R8=1.35863511
R9=1.3552162
R10=1.35721204
R11=1.35467158
R12=1.36563288
R13=1.36509168
R14=1.56389911
R15=1.35689759
R16=1.36441986
R17=2.4000003
R18=1.33574683
R19=1.33335891
A1=122.60633527
A2=120.80027882
A3=120.95858497
A4=121.09844173
A5=113.55384892
A6=118.23630269
A7=107.92796137
A8=107.94289971
A9=100.28179138
A10=108.60687657
A11=110.48519058
A12=111.46961
A13=119.55434427
A14=109.30869158
A15=106.53123991
A16=103.56279604
A17=111.28993055
A18=113.75980739

B1=-8.29173189
B2=184.81649302
B3=14.92512205
B4=100.18721996
B5=297.47020525
B6=123.27416984
B7=-119.73388541
B8=72.80680321
B9=-220.00492297
B10=118.70911706
B11=-121.08956453
B12=65.19434355
B13=279.70240143
B14=279.68473198
B15=268.04084829
B16=171.9291515
B17=297.89556167

Z-matrix cyclized radical product 7c (endo addition)

O 2

C

C,1,R1

H,2,R2,1,A1

H,1,R3,2,A2,3,B1,0

H,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

F,7,R8,6,A7,8,B6,0

F,7,R9,6,A8,8,B7,0

F,8,R10,2,A9,6,B8,0

F,8,R11,11,A10,6,B9,0

F,6,R12,2,A11,7,B10,0

F,6,R13,2,A12,7,B11,0

C,8,R14,7,A13,6,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

C,1,R17,2,A16,5,B15,0

F,18,R18,15,A17,8,B16,0

F,18,R19,15,A18,8,B17,0

R1=1.4906358

R2=1.0836627

R3=1.09493652

R4=1.09272223

R5=1.48835789

R6=1.55912123

R7=1.55615164

R8=1.3546299

R9=1.35410247

R10=1.36383029

R11=1.35034381

R12=1.36049615

R13=1.37228825

R14=1.55971805

R15=1.36034643

R16=1.35073756

R17=1.54036817

R18=1.36424429

R19=1.35947958

A1=122.36058871

A2=111.31529787

A3=109.80601059

A4=118.83180445

A5=114.49616733

A6=115.67953345

A7=108.30027723

A8=108.82466045

A9=93.86184386

A10=108.70705381

A11=110.77175375

A12=110.09404295

A13=117.51201163

A14=108.55017203

A15=107.63445317

A16=114.48533576

A17=105.77729833

A18=108.11765

B1=-40.67432684
B2=199.35386306
B3=30.87727208
B4=75.29746407
B5=313.84146235
B6=122.17699
B7=-120.22602643
B8=84.43384885
B9=-216.92134405
B10=120.74494862
B11=-119.67955061
B12=61.84405077
B13=278.3321859
B14=278.27388792
B15=239.90887864
B16=163.60261142
B17=278.54786223

cartesian coordinate starting radical 7d

O 2
C,0,-2.4999843453,1.6244873913,0.2021035819
C,0,-2.2132361298,0.3801863964,0.59231776
H,0,-1.9925869083,0.1918879696,1.6444568487
H,0,-2.5142079119,2.454146267,0.9035333376
H,0,-2.7239727003,1.861575815,-0.8360802116
C,0,-2.2330820515,-0.8352285117,-0.2993946267
C,0,-1.0985695926,-1.8569800695,-0.0762503752
C,0,0.2928877639,-1.5214307345,-0.6414911128
H,0,-1.0033092826,-2.0736468556,0.9947594868
H,0,-1.4029070701,-2.7985209339,-0.5489443921
H,0,0.2287095383,-1.2106450623,-1.6901903978
H,0,0.9086100313,-2.4275709673,-0.6154344613
H,0,-3.1771032322,-1.3702139684,-0.1127935151
H,0,-2.2636277461,-0.5255171718,-1.3525829677
C,0,1.108511646,-0.4803363962,0.1098913317
F,0,1.0577813161,-0.7095179986,1.4611315
F,0,2.435965951,-0.6221844672,-0.2577511461
C,0,0.7093833893,0.9565383245,-0.1130903149
F,0,1.4635291611,1.8494989649,0.5256059633
F,0,0.5477159276,1.2927686682,-1.3991242273

E (B3LYP)=-671.43145 E (PMP2)=-669.55247

Z-matrix TS endo 7d

O 2

C

C,1,R1

H,2,R2,1,A1

H,1,R3,2,A2,3,B1,0

H,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

H,7,R8,6,A7,8,B6,0

H,7,R9,6,A8,8,B7,0

H,8,R10,2,A9,6,B8,0

H,8,R11,11,A10,6,B9,0

H,6,R12,2,A11,7,B10,0

H,6,R13,2,A12,7,B11,0

C,8,R14,7,A13,6,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

C,2,R17,1,A16,5,B15,0

F,18,R18,15,A17,8,B16,0

F,18,R19,15,A18,8,B17,0

R1=1.35599853

R2=1.09012371

R3=1.0858076

R4=1.08762105

R5=1.51863018

R6=1.53963257

R7=1.53665478

R8=1.09719144

R9=1.09627609

R10=1.09575228

R11=1.09570361

R12=1.09954781

R13=1.09823353

R14=1.51619939

R15=1.37426645

R16=1.3798221

R17=2.37870002

R18=1.33460986

R19=1.34361008

A1=118.42687183

A2=121.48636887

A3=121.62280855

A4=123.16627493

A5=115.72567622

A6=115.83919829

A7=109.35099126

A8=108.49554567

A9=102.42469182

A10=107.41493627

A11=107.6371602

A12=109.43660969

A13=113.68020551

A14=110.33894488

A15=109.5213482

A16=102.19768279

A17=114.75143861

A18=112.96357074

B1=9.63710183
B2=185.61870199
B3=-12.87615616
B4=164.10504888
B5=289.85106525
B6=123.35661738
B7=-121.13324207
B8=70.38371036
B9=-212.40276962
B10=120.01903075
B11=-125.18109672
B12=62.85038451
B13=293.68996323
B14=295.57819257
B15=92.15107796
B16=174.56302596
B17=302.63094481

Z-matrix cyclized radical product 7d (endo addition)

0 2
C
C,1,R1
H,2,R2,1,A1
H,1,R3,2,A2,3,B1,0
H,1,R4,2,A3,3,B2,0
C,2,R5,1,A4,5,B3,0
C,6,R6,2,A5,1,B4,0
C,7,R7,6,A6,2,B5,0
H,7,R8,6,A7,8,B6,0
H,7,R9,6,A8,8,B7,0
H,8,R10,2,A9,6,B8,0
H,8,R11,11,A10,6,B9,0
H,6,R12,2,A11,7,B10,0
H,6,R13,2,A12,7,B11,0
C,8,R14,7,A13,6,B12,0
F,15,R15,8,A14,12,B13,0
F,15,R16,8,A15,11,B14,0
C,2,R17,1,A16,5,B15,0
F,18,R18,15,A17,8,B16,0
F,18,R19,15,A18,8,B17,0

R1=1.49349629
R2=1.09895037
R3=1.08409902
R4=1.08520109
R5=1.54593211
R6=1.5375262
R7=1.53745604
R8=1.09710855
R9=1.09558825
R10=1.09537581
R11=1.09516126
R12=1.09532287
R13=1.09805356
R14=1.51648413
R15=1.37722825
R16=1.36390198
R17=1.54121135
R18=1.36258388
R19=1.37417356
A1=109.39839234
A2=120.63556082
A3=120.36912303
A4=113.01766843
A5=112.61455312
A6=111.85141673
A7=109.63392848
A8=109.97560374
A9=102.67859624
A10=107.90846869
A11=108.78694206
A12=108.38160145
A13=110.53997736
A14=109.74609031
A15=110.96196113
A16=111.54635512
A17=109.14545325
A18=107.06152531

B1=36.55588108
B2=205.93806333
B3=-32.2397722
B4=179.055068
B5=304.4695693
B6=120.94787829
B7=-121.89768879
B8=76.75179888
B9=-206.60946023
B10=122.43532243
B11=-121.69662062
B12=54.09883825
B13=301.99419647
B14=304.01934109
B15=90.91315248
B16=178.99817789
B17=295.00350405

Z-matrix TS exo 7d

O 2

C

C,1,R1

H,2,R2,1,A1

H,1,R3,2,A2,3,B1,0

H,1,R4,2,A3,3,B2,0

C,2,R5,1,A4,5,B3,0

C,6,R6,2,A5,1,B4,0

C,7,R7,6,A6,2,B5,0

H,7,R8,6,A7,8,B6,0

H,7,R9,6,A8,8,B7,0

H,8,R10,2,A9,6,B8,0

H,8,R11,11,A10,6,B9,0

H,6,R12,2,A11,7,B10,0

H,6,R13,2,A12,7,B11,0

C,8,R14,7,A13,6,B12,0

F,15,R15,8,A14,12,B13,0

F,15,R16,8,A15,11,B14,0

C,1,R17,2,A16,5,B15,0

F,18,R18,15,A17,8,B16,0

F,18,R19,15,A18,8,B17,0

R1=1.35480487

R2=1.08949972

R3=1.08653121

R4=1.08764275

R5=1.50040522

R6=1.54652865

R7=1.54032742

R8=1.09583293

R9=1.09723627

R10=1.09605532

R11=1.09549494

R12=1.09870467

R13=1.09852822

R14=1.52973292

R15=1.36976176

R16=1.38373857

R17=2.3750002

R18=1.3397222

R19=1.34892943

A1=119.27052479

A2=121.4614791

A3=120.94226115

A4=123.00203592

A5=112.44595292

A6=116.35890556

A7=109.56284892

A8=108.21443763

A9=97.80772459

A10=106.66573198

A11=110.36887966

A12=109.88080981

A13=117.13336259

A14=110.90093708

A15=108.02639626

A16=103.25463727

A17=112.70760251

A18=111.8942578