

Supplementary Material

Experimental and DFT study of 2-ferrocenylpropan-2-ol cyclodimerization products

Jasmina Lapić,^a Mario Cetina,^b Davor Šakić,^c Senka Djaković,^{a,*} Valerije Vrčec,^{c,*} and
Vladimir Rapić^a

^a Department of Chemistry and Biochemistry, Faculty of Food Technology and Biotechnology,
University of Zagreb, Pierottijeva 6, HR-10000 Zagreb, Croatia

^b Department of Applied Chemistry, Faculty of Textile Technology, University of
Zagreb, Prilaz baruna Filipovića 28a, HR-10000 Zagreb, Croatia

^c Department of Organic Chemistry, Faculty of Pharmacy and Biochemistry, University
of Zagreb, A. Kovačića 1, HR-10000 Zagreb, Croatia

E-mail: sdjakov@pbf.hr, valerije@pharma.hr

Redundant internal coordinates for **3**
(optimized at BP86/AE1 level):

H,0,-5.5346982663,-0.1841000516,1.3048254419
H,0,-3.343657383,1.1969678285,2.1024610592
C,0,-4.7814516381,0.2515447683,0.6452871432
H,0,5.6494696601,-1.618916822,0.2457638126
H,0,4.0384774328,-1.0989178592,2.3789193693
C,0,-3.6197132985,0.9921455897,1.0653189248
H,0,3.378312063,-2.432543812,-1.8465136103
H,0,-1.8015731632,2.830553099,-2.1742453438
H,0,1.70795248,-2.4843171889,0.2880472367
H,0,-1.9729323923,-1.6266060796,2.4108620353
C,0,5.1484069622,-0.6718150427,0.455884074
C,0,4.2922885001,-0.3987880555,1.5807757263
H,0,-0.8263766194,1.3340295539,-2.0889255938
C,0,2.7321586576,-1.615302835,-1.5194820126
C,0,-4.7602589281,0.1718538713,-0.7902009746
H,0,-5.4940782659,-0.3362947531,-1.4187780484
C,0,1.8564069977,-1.6341163322,-0.3804862849
C,0,-1.03607422,2.2928314167,-1.5862368221
H,0,-3.6673598044,-3.2241375509,1.0400867992
C,0,-1.9700077769,-1.7619457158,1.3281695306
C,0,-2.8502580069,1.360454377,-0.1082671103
H,0,-2.4944738241,4.0738210445,-0.1311041956
H,0,-0.1177665302,2.9069092404,-1.6121257754
Fe,0,-3.0348958965,-0.641025337,0.0032015189
C,0,-2.8789476121,-2.6085808827,0.6023266534

C,0,-3.5878088132,0.8643519756,-1.2542726772
Fe,0,3.2682985188,-0.1467317738,-0.1923439379
C,0,-1.5118887237,2.1013344336,-0.129949999
C,0,5.2078982056,0.5150038972,-0.3573323556
C,0,3.8279253945,0.9589376021,1.4634456589
C,0,-1.0986442141,-1.0857991394,0.383554083
C,0,2.6326246116,-0.3152324104,-2.1262347379
H,0,5.7586275308,0.6238022047,-1.2938452867
C,0,-1.7475259015,3.5220146097,0.4670569489
H,0,3.191462561,0.0370777474,-2.99580992
H,0,3.1713767069,1.4792866979,2.162901835
C,0,1.1815663353,-0.3568122597,-0.2757713002
H,0,-0.809690767,4.1084736246,0.4712498779
H,0,-2.1204931695,3.4679149753,1.5055283841
C,0,4.3881853139,1.5221144178,0.2633044451
C,0,0.0339638984,-0.0898113738,0.7190222362
C,0,-2.5739940337,-2.4855810657,-0.7977764353
C,0,1.6925692196,0.4584797033,-1.3562020856
C,0,-0.4330976149,1.4234288308,0.7953260853
C,0,-1.4767950209,-1.5631316087,-0.9324427544
H,0,0.482599183,2.0472438188,0.7496346941
H,0,-3.0888353539,-2.9904227781,-1.6177148612
H,0,4.2156661685,2.531949293,-0.1139123648
H,0,0.9491923491,-1.4447301793,2.2145622692
H,0,-0.8171789832,1.5515811102,1.8257827451
H,0,-1.0148721052,-1.2521766727,-1.871638731
H,0,1.4332368073,1.4967394016,-1.5530279458
C,0,0.5437793554,-0.4210079949,2.1541062124
H,0,-0.2739526323,-0.3312634696,2.8906281902
H,0,1.3420140923,0.2805089511,2.4441527942
H,0,-3.2801690463,0.9488039604,-2.2975136208

Redundant internal coordinates for **3**
(optimized at B3LYP/AE1 level):

H,0,-5.4829805666,-0.1301921198,1.4503158205
H,0,-3.2516596384,1.199443353,2.1332013137
C,0,-4.7653634573,0.2956026617,0.7608409689
H,0,5.5455835298,-1.7006396115,0.5141016046
H,0,3.8592303504,-0.9400832105,2.4793892156
C,0,-3.5815255546,1.0082856187,1.119774887
H,0,3.3708289707,-2.3540730868,-1.9455231631
H,0,-1.8659123211,2.7672068103,-2.1975138592
H,0,1.6815873618,-2.4868116283,0.141321745
H,0,-1.8889989613,-1.7157954078,2.3575008868
C,0,5.1040165793,-0.7191034843,0.6291271555
C,0,4.2103816075,-0.3176462878,1.6669579947
H,0,-0.9085054029,1.2780936122,-2.1169680085
C,0,2.7256673385,-1.5563804755,-1.600083485
C,0,-4.8211132093,0.2266943992,-0.6618575791
H,0,-5.5889274319,-0.2605263931,-1.248866341

C,0,1.8409457084,-1.618493787,-0.4845144237
C,0,-1.0942514844,2.2377508193,-1.6276086737
H,0,-3.5959421282,-3.2789242466,1.0096275636
C,0,-1.9188429982,-1.8197186608,1.2817173539
C,0,-2.8750520361,1.36904802,-0.0797333802
H,0,-2.4706067226,4.0580578944,-0.1597102513
H,0,-0.1807468195,2.8386192304,-1.6922285296
Fe,0,-3.049392097,-0.6461147725,0.0279436056
C,0,-2.8337895325,-2.649932437,0.5679068905
C,0,-3.6734481347,0.898578644,-1.178641717
Fe,0,3.2821698588,-0.138390651,-0.1943743694
C,0,-1.5274802778,2.0800069692,-0.158737454
C,0,5.2915025994,0.3926502868,-0.2465976255
C,0,3.8473112246,1.0430193582,1.4322100543
C,0,-1.0898547709,-1.1173301208,0.3374025138
C,0,2.6361225379,-0.2449835723,-2.1515082179
H,0,5.89882019,0.4009719942,-1.1425894447
C,0,-1.7163391976,3.5104223223,0.416328113
H,0,3.2008481482,0.13759625,-2.9920832679
H,0,3.1793782522,1.6405851698,2.0382887794
C,0,1.1723501684,-0.3563952186,-0.3412726549
H,0,-0.7782016969,4.0775885197,0.3742043206
H,0,-2.0489848974,3.4826468841,1.459751421
C,0,4.5140431394,1.4816761169,0.2492647783
C,0,0.0316401894,-0.1116399804,0.6613562077
C,0,-2.5744718523,-2.489658103,-0.8249850829
C,0,1.6928448597,0.4924525368,-1.3719712089
C,0,-0.4401857805,1.3969180716,0.7457596845
C,0,-1.4998668809,-1.56097748,-0.9663816675
H,0,0.4661114234,2.0154440191,0.6916455144
H,0,-3.1049524267,-2.9735859449,-1.6349471178
H,0,4.4309831213,2.4620129115,-0.2019518401
H,0,0.9662795814,-1.4499912426,2.1421652918
H,0,-0.8090404456,1.5222346303,1.7708171342
H,0,-1.0769998921,-1.2235174453,-1.9033199444
H,0,1.4375006543,1.5277082206,-1.5313632807
C,0,0.5585214626,-0.4367409288,2.0865896248
H,0,-0.243743935,-0.3520774289,2.8267298607
H,0,1.348479534,0.2637138322,2.3658652371
H,0,-3.4228238413,0.9853015692,-2.2268589537

Redundant internal coordinates for **4a**
(optimized at BP86/AE1 level):

H,0,-0.1236044255,3.1774387635,2.2877710752
H,0,0.9595430105,4.0221537802,-0.0577187201
C,0,0.1289334237,2.5397325638,1.4369210349
H,0,-5.2451752106,-1.9526596437,0.4618157534
H,0,-3.465059646,-0.5465848645,1.9681223491
C,0,0.7096017177,2.9880299479,0.1898474287
H,0,-4.152344346,-0.4068352779,-2.0613399299

H,0,0.1001849697,3.0476757819,-3.0217773303
H,0,-2.1503760258,0.8490266499,-0.7068927232
H,0,3.2773493039,3.8058546668,2.4728827428
C,0,-4.2431290678,-2.2817047486,0.7442251763
C,0,-3.3014623077,-1.5368457223,1.5385320368
H,0,-0.7790604814,1.5077425648,-2.7904794563
C,0,-3.1387703953,-0.7862066927,-1.9158811664
C,0,-0.0100062642,1.100323043,1.3913896197
H,0,-0.3968111984,0.4729429589,2.1965922525
C,0,-2.0799915519,-0.121078754,-1.2021874229
C,0,0.2011551836,1.946900251,-3.0397414636
H,0,2.4013039091,1.7003257878,3.9617993654
C,0,3.365362347,2.7505303254,2.2068904543
C,0,0.9110453166,1.8235259176,-0.6278046968
H,0,2.6129355277,3.1861277138,-2.5215234673
H,0,0.4568734142,1.6457350509,-4.0729541805
Fe,0,1.9544973943,1.6709270012,1.1698600518
C,0,2.9032235429,1.6378092546,2.9941308996
C,0,0.4711118239,0.6694215646,0.1070987738
Fe,0,-2.5268475216,-1.9259795677,-0.3294174751
C,0,1.3077660206,1.4787014968,-2.0564335596
C,0,-3.6210184109,-3.5230316049,0.3624332107
H,0,4.3625734073,2.8223119149,0.1810423346
C,0,-2.0991169573,-2.3206251084,1.651162944
C,0,3.9358497,2.2297263781,0.9920081009
C,0,-2.6339840551,-2.0546584105,-2.3712182373
H,0,-4.0691235243,-4.300377315,-0.2597078976
C,0,2.6549500246,2.0811289186,-2.5070640966
H,0,-3.1951835729,-2.8108110278,-2.9243529858
H,0,-1.1988262661,-2.0350943792,2.1983158263
C,0,-0.9041247255,-0.9640664534,-1.2170119574
H,0,2.9091750961,1.74400863,-3.5296734772
H,0,3.4704606628,1.7784055209,-1.8286148885
C,0,-2.2941740042,-3.5466233275,0.9215619765
C,0,0.5075168877,-0.5955535096,-0.7418433959
C,0,3.1886162638,0.4289816667,2.2663364468
C,0,-1.2668691945,-2.1671708965,-1.9355608214
C,0,1.3795704839,-0.0902335465,-1.9710335417
C,0,3.827871217,0.7954030879,1.029820378
H,0,1.066399473,-0.5707973809,-2.9153184003
H,0,2.9496310797,-0.5853587955,2.5914178593
H,0,-1.562753534,-4.3487214863,0.8048876399
H,0,0.6113974157,-2.1625310605,0.7959644365
H,0,2.428084949,-0.3864627689,-1.7814011162
H,0,4.1726073837,0.1060224309,0.2561547859
H,0,-0.6152086356,-3.0247108127,-2.1156987058
C,0,1.1932543487,-1.8047909186,-0.069509313
H,0,2.2020406129,-1.5217313013,0.2742973654
H,0,1.2949817596,-2.6474777086,-0.7775303509

Redundant internal coordinates for **4a**
(optimized at B3LYP/AE1 level):

H,0,-0.0048686586,0.0348829895,0.0626154569
H,0,0.0209630513,0.0079166785,2.7579294205
C,0,0.8813866185,0.0296597875,0.6854684272
H,0,5.587976499,4.6724054157,-2.1185833673
H,0,3.68691507,2.7643382529,-2.2948070928
C,0,0.8957189822,0.0097991547,2.1197212661
H,0,4.8336831449,4.8293154162,1.0306738192
H,0,1.9332751274,1.7345369374,4.6771127102
H,0,3.2074060703,2.6769885664,1.0409382824
H,0,-0.6378563451,-3.1722634975,1.3424788149
C,0,5.7520837951,3.6040639177,-2.0606235522
C,0,4.7465112237,2.5954855054,-2.1528528321
H,0,3.2683559518,2.2692850437,3.6412739526
C,0,5.1370925158,3.8040912681,1.2000284646
C,0,2.2350119379,-0.0104332635,0.2130163657
H,0,2.5404912988,-0.024835233,-0.8249544285
C,0,4.2763453428,2.6649092143,1.2055685591
C,0,2.9640232119,1.5159259022,4.37278134
H,0,0.8683940484,-3.1859819124,-0.8976455684
C,0,0.4377735683,-3.2859353816,1.2994026201
C,0,2.2612355613,-0.0286143129,2.5262682586
H,0,1.6447201913,-0.7350900469,5.2422004572
H,0,3.6053944835,1.6236358776,5.2564845574
Fe,0,1.7869417054,-1.7013269752,1.3362486169
C,0,1.233867078,-3.2935355001,0.115526278
C,0,3.0797832964,-0.0404028183,1.3619213955
Fe,0,5.6968305614,2.4968356272,-0.3021114874
C,0,3.073710775,0.0819760681,3.8026650771
C,0,7.0077662102,2.958501465,-1.8487675636
H,0,1.0121599105,-3.4361406711,3.4594385046
C,0,5.3818213547,1.3262718251,-2.0006742293
C,0,1.3114534905,-3.4218391003,2.4198078413
C,0,6.469600192,3.3458780773,1.4211971707
H,0,7.9625013992,3.4517265942,-1.7193749689
C,0,2.6727610414,-0.9140869449,4.9037237472
H,0,7.360631856,3.9601019448,1.4502609293
H,0,4.888484116,0.3636899887,-2.0213035029
C,0,5.0639449244,1.4903976578,1.4414311884
H,0,3.3302891476,-0.8097462098,5.7760173117
H,0,2.7369927661,-1.9465943424,4.5479575141
C,0,6.7790632303,1.5498902838,-1.8107986
C,0,4.55723266,0.0697164768,1.7000860736
C,0,2.6000778447,-3.4347567799,0.5031167447
C,0,6.4255169264,1.9261467087,1.5611204248
C,0,4.5138806005,-0.2136595919,3.257761455
C,0,2.6476871264,-3.5145582916,1.9275679506
H,0,5.2790042478,0.3587808987,3.7924266017
H,0,3.4501676904,-3.4605314949,-0.1659005403
H,0,7.5303148783,0.7872025153,-1.6514846547

H,0,5.4584978749,-0.8216588014,-0.0837870948
H,0,4.7354116424,-1.2760996128,3.4122358018
H,0,3.5408671565,-3.620631229,2.5293996887
H,0,7.2830987981,1.2872040747,1.7279097055
C,0,5.4554303367,-0.9669432172,0.999828916
H,0,5.1018643083,-1.9792567086,1.213814402
H,0,6.4914488381,-0.8892010737,1.3490666462

Redundant internal coordinates for **4b**
(optimized at BP86/AE1 level):

H,0,1.8924409789,2.2118733703,-3.5124642126
H,0,3.1789997676,-0.1426792856,-3.0778243546
C,0,1.6794752406,1.5111423624,-2.7019946561
H,0,-5.8066298214,-0.5185906557,1.7721866056
H,0,-3.7274597499,0.5436201066,3.1748807181
C,0,2.3703569423,0.2604441714,-2.4651538446
H,0,-4.6217846492,0.7413009238,-0.8690666858
H,0,2.0516911842,-2.9534175796,-2.3135633008
H,0,-2.439176372,1.7211375453,0.3985925381
H,0,4.9971117987,2.5590809669,-2.0090457101
C,0,-4.8669193372,-1.021378383,2.0063809171
C,0,-3.765092833,-0.4579919586,2.7437827522
H,0,0.3600639007,-2.4984741904,-1.9965363225
C,0,-3.669421317,0.2229716461,-0.7440541095
C,0,0.6967677844,1.7016562316,-1.6600501735
H,0,0.0328237113,2.5623900159,-1.5611366355
C,0,-2.5087035357,0.7384231061,-0.0700444858
C,0,1.3129034163,-2.7726974535,-1.5111580601
H,0,3.0939020377,4.3222078127,-1.181186217
C,0,4.4212527904,2.494805014,-1.0843454942
C,0,1.7857665498,-0.3273738767,-1.2900443676
H,0,3.9239747561,-2.1832575813,-0.8190320121
H,0,1.1671005311,-3.7235641532,-0.9644916522
Fe,0,2.6041612333,1.5541192812,-0.8896217798
C,0,3.4156380604,3.4272039941,-0.6462015549
C,0,0.7679332043,0.553550628,-0.7998534327
Fe,0,-3.1751023021,-0.976674841,0.8451249641
C,0,1.8054317252,-1.6569082306,-0.5513550489
C,0,-4.4992008875,-2.3545222171,1.6041097565
H,0,5.1768994472,0.5814972406,-0.151348774
C,0,-2.720226894,-1.4466819067,2.80225911
C,0,4.5121552324,1.445111216,-0.1031146749
C,0,-3.361808588,-1.1090863227,-1.1911901784
H,0,-5.1110620397,-3.0393938758,1.014791795
C,0,3.1900779906,-2.059488187,-0.0014472986
H,0,-4.0388687437,-1.7852811715,-1.7159683058
H,0,-1.7508815299,-1.3313366849,3.2894143783
C,0,-1.4626778558,-0.2624561045,-0.0962352972
H,0,3.1299307038,-3.0215373675,0.5424534629
H,0,3.5773823022,-1.2924473534,0.6902114669

C,0,-3.1709349069,-2.616440312,2.0947655662
C,0,-0.0174358161,-0.043942214,0.3714901398
C,0,2.8878105936,2.9548974171,0.6065058761
C,0,-2.0119822598,-1.406573252,-0.7903741865
C,0,0.7777542841,-1.3904934125,0.6232230482
C,0,3.5648669548,1.7314205583,0.941082193
H,0,0.085970138,-2.2415815389,0.7552757377
H,0,2.1005180633,3.4331015855,1.1909641628
H,0,-2.604134421,-3.5379522673,1.9517181823
H,0,-0.430781017,1.8498722169,1.4268495423
H,0,1.3350431744,-1.2955370506,1.5736114342
H,0,3.3941766756,1.1266621904,1.8331982065
H,0,-1.5029436952,-2.3555539827,-0.9633208369
C,0,0.0120819932,0.8579394922,1.6262131197
H,0,1.0548000807,1.0184810799,1.9431537163
H,0,-0.5498506126,0.3946321994,2.4554265888

Redundant internal coordinates for **4b**
(optimized at B3YLP/AE1 level):

H,0,3.4247419543,-0.6170125455,2.9504836689
H,0,3.5819265993,1.8231364113,1.8121857404
C,0,2.7630525077,-0.23361339,2.1833716059
H,0,-5.8418290894,-1.7293822763,-0.0028520764
H,0,-3.9360267241,-2.2355337445,-1.8483006082
C,0,2.8493201569,1.062198882,1.5741182953
H,0,-3.6453054721,-1.8791218891,2.4266278249
H,0,1.379832989,3.8856024864,1.0928406845
H,0,-1.677182997,-2.4186318119,0.6843695364
H,0,5.948042627,-0.4599209662,0.5464447939
C,0,-5.2546319155,-0.9892655598,-0.5308516938
C,0,-4.2458177331,-1.2567357597,-1.5057182067
H,0,-0.0427627974,2.8980671724,1.4333217474
C,0,-3.0079338997,-1.1474360499,1.9467947718
C,0,1.6848211638,-0.955206763,1.5732266167
H,0,1.3834515148,-1.9663010504,1.8154028056
C,0,-1.9635675038,-1.429897306,1.0167975092
C,0,0.5733607088,3.3068587841,0.626890719
H,0,4.6308788654,-2.8156540488,0.5853018075
C,0,5.1707205715,-0.765199641,-0.1421666354
C,0,1.8089159121,1.1391129945,0.6008298194
H,0,2.916274552,3.3647053044,-0.8120140429
H,0,-0.0401540779,4.0007066656,0.0381890117
Fe,0,3.140756674,-0.4453244049,0.1722858397
C,0,4.4746899038,-2.011334588,-0.12190302
C,0,1.0992218496,-0.0905139961,0.60299256
Fe,0,-3.4253681086,-0.2488348559,0.1225612418
C,0,1.1524841795,2.1897506019,-0.2717164092
C,0,-5.3331350845,0.4259050651,-0.3539349161
H,0,4.945666616,1.0239066913,-1.4733555305
C,0,-3.7029707984,-0.0067113038,-1.932099187

C,0,4.6374503729,0.0214596081,-1.207478352
C,0,-3.0837006499,0.2677035638,2.0995668239
H,0,-5.9904553732,0.945851362,0.330958399
C,0,2.092229698,2.835140276,-1.3054293396
H,0,-3.7899776872,0.8074391806,2.7173168557
H,0,-2.9132242453,0.1300023495,-2.6589788891
C,0,-1.3746626515,-0.1940148457,0.5849146139
H,0,1.5494409897,3.5649817402,-1.9199270256
H,0,2.5252604715,2.0813127593,-1.9694258765
C,0,-4.3731913555,1.0329451316,-1.2193582382
C,0,-0.1319254772,-0.0653753044,-0.2986344561
C,0,3.5107121961,-1.9960902193,-1.1748354663
C,0,-2.0863805409,0.8516729333,1.2621479153
C,0,0.0169243966,1.352194938,-0.9788453607
C,0,3.6139414302,-0.7406253539,-1.8463378128
H,0,-0.9343511209,1.8930646812,-0.9803911874
H,0,2.81421296,-2.7897131586,-1.4108570091
H,0,-4.1786116092,2.0939692989,-1.3082784534
H,0,-0.086272173,-2.1767180743,-0.9018376322
H,0,0.2864539761,1.2041768143,-2.0305477883
H,0,3.0158197478,-0.4187301185,-2.688813011
H,0,-1.9170368349,1.9124542108,1.1464372065
C,0,-0.1163262368,-1.1830818386,-1.3613190807
H,0,0.7705382293,-1.0868650486,-1.992089885
H,0,-1.0079766569,-1.1308359937,-1.9940232246

Redundant internal coordinates for **4c**
(optimized at BP86/AE1 level):

H,0,1.7826522467,-3.0155611881,1.0723299133
H,0,1.5751832008,-1.1012019788,2.9920792865
C,0,1.4498449784,-1.9870472751,0.9123127512
H,0,-5.5695089469,-0.7590218021,0.0084225805
H,0,-3.763145222,-0.0042503949,1.8940769259
C,0,1.3422108334,-0.9659643676,1.9333888453
H,0,-4.5820808953,1.5496658575,-1.9136379974
H,0,-0.8400744616,1.0112206672,3.3370718199
H,0,-2.6039592471,2.3913870526,-0.268204364
H,0,4.8235428716,-1.6440356548,1.9218936942
C,0,-4.5579008425,-1.1540860377,0.121392647
C,0,-3.5973513932,-0.7493306733,1.113868255
H,0,-1.6852756243,1.0657541199,1.7586304323
C,0,-3.5552734285,1.1779790953,-1.9088099461
C,0,1.0951721353,-1.4029783242,-0.3635949542
H,0,1.1088601899,-1.9219127347,-1.3244109079
C,0,-2.5012678324,1.6193304391,-1.0328397621
C,0,-0.9290121091,1.566539502,2.3851429841
H,0,4.5445136584,-2.2190100618,-0.7257649328
C,0,4.5962361679,-0.9277819335,1.1296950516
C,0,0.9033980453,0.2396670279,1.2824860155

H,0,1.5682589267,1.9454371201,3.5118517043
H,0,-1.2917356611,2.5852701912,2.6203324745
Fe,0,2.7043136734,-0.441778276,0.4825812489
C,0,4.4500280038,-1.2314768094,-0.2694832726
C,0,0.7464627094,-0.0311902669,-0.1188986911
Fe,0,-2.8779997481,-0.3974266102,-0.7883669447
C,0,0.4355218783,1.6401797753,1.6531694715
C,0,-3.940553807,-2.1522930108,-0.7130950204
H,0,4.3861115042,1.0200748616,2.2548633134
C,0,-2.3852891399,-1.495477607,0.8926663724
C,0,4.3592679196,0.481350741,1.3060572465
C,0,-3.0218984946,0.141957828,-2.7525727848
H,0,-4.4014848809,-2.6434037035,-1.5724924073
C,0,1.4277132027,2.4327588947,2.5292038329
H,0,-3.5713514395,-0.4178695042,-3.5123855964
H,0,-1.4568214832,-1.4062509351,1.4585492077
C,0,-1.2978059557,0.8735703089,-1.3286626278
H,0,1.0507611171,3.4561909362,2.7153785141
H,0,2.4138514872,2.5094626875,2.0410907868
C,0,-2.5974021982,-2.3604440397,-0.237204855
C,0,0.1469487782,1.1551809697,-0.8664811565
C,0,4.122154679,-0.0104533763,-0.9581139215
C,0,-1.6449249924,-0.0556447986,-2.3845188117
C,0,0.2799575352,2.2870248733,0.2267072921
C,0,4.0677441252,1.0477424966,0.0156093177
H,0,-0.5524380017,3.0116008059,0.1893262731
H,0,3.9340936703,0.0899229428,-2.0286498679
H,0,-1.8601955747,-3.0412713428,-0.6660682147
H,0,0.9492730128,0.748130337,-2.8849383065
H,0,1.201232174,2.8547278298,0.0015661507
H,0,3.8429668291,2.0971296016,-0.1886994798
H,0,-0.9684581609,-0.7853605861,-2.8347208354
C,0,0.9412509504,1.5605128531,-2.1376715229
H,0,1.9857924853,1.7964587407,-1.8740534938
H,0,0.4838836758,2.4482854668,-2.6115251187

Redundant internal coordinates for **4c**
(optimized at B3LYP/AE1 level):

H,0,-1.7145289723,-2.6706788267,-1.7203216903
H,0,-2.0617723247,-0.2450266811,-2.8480440033
C,0,-1.435867079,-1.7224912574,-1.2769763224
H,0,5.4880124637,-0.1130862716,-1.2841939609
H,0,3.3215253459,0.982565831,-2.4596205131
C,0,-1.6237883069,-0.4313110499,-1.8754044091
H,0,4.7543507486,1.4604378844,1.4616038777
H,0,0.0218009517,2.1626751465,-2.8882513209
H,0,2.4455220863,2.4862750143,0.5666600646
H,0,-5.0213325357,-1.6006164677,-1.4253980067
C,0,4.5007282567,-0.5540336024,-1.3350587681

C,0,3.3524171775,0.02709456,-1.9523297331
H,0,1.1932441245,1.8068319609,-1.6048946371
C,0,3.7844483396,0.984657833,1.5292813173
C,0,-0.8614124402,-1.543543526,0.0258405312
H,0,-0.6234360596,-2.3367118489,0.7230982965
C,0,2.5524970756,1.5244955025,1.0492138221
C,0,0.2932126232,2.3772366029,-1.8475111278
H,0,-4.1450197819,-2.8844726979,0.7810216403
C,0,-4.6868293829,-1.1332912187,-0.5081137539
C,0,-1.1473410837,0.536773261,-0.941871458
H,0,-2.3994414491,2.7509191416,-2.2749146165
H,0,0.5343532339,3.4457818845,-1.7776820837
Fe,0,-2.7124490163,-0.6074721348,-0.1141542366
C,0,-4.2230887348,-1.8118627435,0.6580399172
C,0,-0.6753253515,-0.1429248916,0.2141832064
Fe,0,3.0066736446,-0.2746084109,0.084619871
C,0,-0.8690155259,2.026737665,-0.8914561639
C,0,4.1116339847,-1.8081483864,-0.7744531422
H,0,-4.8651779171,1.053107821,-0.9645486576
C,0,2.2535251168,-0.8665140053,-1.7729722183
C,0,-4.6005524276,0.2706022524,-0.2655903882
C,0,3.5109423715,-0.2992894406,2.0857496225
H,0,4.7517473966,-2.4832291201,-0.2210067714
C,0,-2.0763757454,2.9135641185,-1.2392603017
H,0,4.2359837165,-0.9782632643,2.5159734451
H,0,1.2382941846,-0.7100803221,-2.1091129516
C,0,1.4988570759,0.5886334619,1.3100004251
H,0,-1.817871363,3.9750902231,-1.1365663548
H,0,-2.9261545462,2.7027364492,-0.5834799087
C,0,2.7226896998,-1.9991887649,-1.0441406445
C,0,-0.0217091264,0.8025986722,1.2110109605
C,0,-3.8490316084,-0.8279728212,1.6219892825
C,0,2.1138086704,-0.547452786,1.9362296232
C,0,-0.4424210467,2.1968137021,0.6092102682
C,0,-4.0842881397,0.4590304184,1.0514132142
H,0,0.3367250226,2.9552715315,0.7274054225
H,0,-3.4428394575,-1.0249122061,2.6053083568
H,0,2.1231101643,-2.8443290834,-0.733081887
H,0,-0.3955172769,-0.3285613667,3.0599567862
H,0,-1.3080027698,2.5549475555,1.1776210927
H,0,-3.8946099203,1.4116190386,1.5292301233
H,0,1.5989348299,-1.4454114255,2.2533697897
C,0,-0.5780556841,0.6698917533,2.6494525894
H,0,-1.6566897085,0.8488688309,2.6581922173
H,0,-0.0958195235,1.3961865056,3.3141212683

Redundant internal coordinates for **4e**
(optimized at BP86/AE1 level):

Fe,0,2.5744571539,1.0227248203,0.5839140953

Fe, 0, -2.7756184227, -1.5450828221, 0.3032869943
C, 0, 0.9514382896, 1.8633360066, -0.4317832938
C, 0, 0.6192972603, 0.5441858492, 0.0339120736
C, 0, 0.7903694371, 0.5082493235, 1.4621393444
C, 0, 1.2231177967, 1.8266638554, 1.8738034795
C, 0, 1.3371062345, 2.6630687601, 0.6981685717
C, 0, 4.2454448456, 0.8751079167, -0.6317303948
C, 0, 3.9237934437, -0.4084530778, -0.0661737788
C, 0, 3.9585026046, -0.2852900193, 1.3672077621
C, 0, 4.3058582806, 1.0747382895, 1.6871164982
C, 0, 4.4792588503, 1.7933650879, 0.4516693245
C, 0, -1.5199766316, -0.3875660385, -0.8933440584
C, 0, -2.4215515453, -1.1919410031, -1.6906225337
C, 0, -3.7769705011, -0.8537185864, -1.3451220727
C, 0, -3.7315472194, 0.155072361, -0.3198532133
C, 0, -2.3477796483, 0.4354958721, -0.0383556733
C, 0, -2.3752399594, -3.5291859561, 0.6873006433
C, 0, -3.7774001608, -3.2510532199, 0.8624184417
C, 0, -3.9068865484, -2.2353260444, 1.875048367
C, 0, -2.5855448043, -1.8844771338, 2.3259905236
C, 0, -1.6400256972, -2.6870721988, 1.594773541
C, 0, 0.0036106622, -0.3088138379, -1.0709906712
C, 0, 0.3576693371, 0.5710785914, -2.3467228338
C, 0, 0.6079975804, 2.058134725, -1.902271053
C, 0, -0.684816522, 2.9102251411, -2.024936843
C, 0, 1.7158625182, 2.727523517, -2.7412031493
C, 0, 0.6047055297, -1.7229632749, -1.2205348006
H, 0, 0.6316358229, -0.344244452, 2.1250666347
H, 0, 1.4636715229, 2.1275995592, 2.8965503177
H, 0, 1.6663146085, 3.7045709433, 0.6896062541
H, 0, 4.3161076948, 1.1068824668, -1.6956278304
H, 0, 3.7060262773, -1.3204316135, -0.6244424569
H, 0, 3.7461028911, -1.0793270633, 2.0857114609
H, 0, 4.395106804, 1.4946768109, 2.6909442615
H, 0, 4.7309284081, 2.8511693187, 0.3542157603
H, 0, -2.1265569739, -1.9383447594, -2.4310790924
H, 0, -4.6779090243, -1.3041353013, -1.7671709839
H, 0, -4.5922510355, 0.6085818151, 0.1760803434
H, 0, -1.9745889301, 1.1356828203, 0.7109463412
H, 0, -1.9454479947, -4.2446122071, -0.0164467947
H, 0, -4.5974605813, -3.7139369941, 0.3098705101
H, 0, -4.8418031258, -1.7913490702, 2.2227052143
H, 0, -2.3423979662, -1.131434949, 3.0781809774
H, 0, -0.5551268979, -2.6628708043, 1.7126870812
H, 0, 1.2887186303, 0.1687158301, -2.7879887203
H, 0, -0.4293468514, 0.498537085, -3.1188675101
H, 0, -1.5263640536, 2.4569346966, -1.4753722251
H, 0, -0.9806233296, 3.0015589895, -3.0869163928
H, 0, -0.5226603379, 3.9292423951, -1.6281295888
H, 0, 1.9156662663, 3.7563565529, -2.388518826
H, 0, 1.4142942684, 2.7923871823, -3.8036668267
H, 0, 2.6580740079, 2.1578873901, -2.6824428572

H,0,1.6942720749,-1.6566581628,-1.3724958535
H,0,0.1702470524,-2.2485416708,-2.090274104
H,0,0.4078031628,-2.3358981948,-0.3257786273

Redundant internal coordinates for **4ts**
(NImag = 1 (-45 cm⁻¹); optimized at BP86/AE1 level):

Fe,0,-2.7892172773,-0.6857974169,-0.243204048
Fe,0,3.227288595,-0.1757926547,-0.0537801364
C,0,-1.7639084885,1.0856409934,-0.6657124418
C,0,-0.8440896627,0.0669245845,-0.2376638017
C,0,-0.9708668994,-1.0634185933,-1.1181774112
C,0,-1.97330145,-0.7240698663,-2.1057849779
C,0,-2.4747250724,0.6027619874,-1.8177834389
C,0,-4.2412153264,-0.3969710598,1.2055259838
C,0,-3.3236584474,-1.4265073133,1.6165057977
C,0,-3.3490481986,-2.4682481926,0.6238710243
C,0,-4.2863739633,-2.0835398763,-0.3989353084
C,0,-4.8348965935,-0.8012013427,-0.0418890253
C,0,1.4672319387,0.9123142078,0.2766397888
C,0,2.5835901508,1.4618650063,1.0154174018
C,0,3.6194390455,1.8308765951,0.0869051415
C,0,3.1635773513,1.4953410398,-1.2361327439
C,0,1.8483519134,0.9225478205,-1.117088387
C,0,3.3265943393,-1.9241567886,1.0541680817
C,0,4.6097606901,-1.2770904771,1.0134181269
C,0,5.005961717,-1.1603009189,-0.3655952346
C,0,3.9655767175,-1.7359992007,-1.1773949119
C,0,2.9268730399,-2.206022519,-0.2990848943
C,0,0.0873993257,0.5669022798,0.8613985901
C,0,-0.6672412052,1.8983222046,1.2863030259
C,0,-1.5582629334,2.3918810722,0.0893663365
C,0,-0.7895297471,3.3937789835,-0.8150935374
C,0,-2.8541593717,3.0675521801,0.5807383101
C,0,0.2255795257,-0.3907251475,2.063519336
H,0,-0.4262789816,-2.0081438346,-1.0634326523
H,0,-2.3225018092,-1.3769217545,-2.9096509286
H,0,-3.257348157,1.1203027519,-2.3771368268
H,0,-4.4606968682,0.5215243809,1.7519138722
H,0,-2.7235111236,-1.4257891603,2.5279041873
H,0,-2.752990236,-3.3828188247,0.6367192471
H,0,-4.5202257563,-2.6522324681,-1.3010907762
H,0,-5.5629261223,-0.2304617154,-0.6215145369
H,0,2.6346049233,1.5794444446,2.1002759403
H,0,4.5904719492,2.2585428523,0.3457806907
H,0,3.7261291621,1.6237843508,-2.1633539735
H,0,1.2352974862,0.5456733312,-1.9374855516
H,0,2.756635042,-2.1523217873,1.9561079806
H,0,5.1755320256,-0.920000848,1.8762679563
H,0,5.9225181669,-0.6947180625,-0.733278155
H,0,3.955384988,-1.7862468793,-2.268044523

H,0,1.9946421682,-2.6817052816,-0.6094321505
H,0,-1.3278897016,1.6528690688,2.1387750409
H,0,0.0377568264,2.6779279697,1.6262959305
H,0,0.1651308165,2.9724630263,-1.1714391365
H,0,-0.5665322054,4.3206211907,-0.2539843253
H,0,-1.3953360867,3.6685329579,-1.6980985162
H,0,-3.4987438189,3.3566496494,-0.2699202976
H,0,-2.6224294247,3.9869313702,1.1507670236
H,0,-3.4327842425,2.3925327689,1.2331119499
H,0,-0.7536722824,-0.5336437716,2.5488877593
H,0,0.9308794543,0.0072451094,2.8151758343
H,0,0.6000216563,-1.3746883367,1.7360327553

Redundant internal coordinates for **4ts**

(NImag = 1 (-29 cm⁻¹); optimized at B3YLP/AE1 level):

Fe,0,-2.7748509267,-0.7094481517,-0.2286441099
Fe,0,3.2325539259,-0.1861389112,-0.0696537485
C,0,-1.7390396423,1.0844255966,-0.6577145708
C,0,-0.8185668583,0.0863661435,-0.2304086124
C,0,-0.9225287237,-1.0330178424,-1.1090115342
C,0,-1.9140586399,-0.7064405889,-2.0931987433
C,0,-2.4293055932,0.601945259,-1.8074624871
C,0,-4.2222845861,-0.4783640196,1.2701842299
C,0,-3.3208780004,-1.5267242555,1.6229950594
C,0,-3.3791431407,-2.5212775043,0.6019279548
C,0,-4.319490746,-2.0886813295,-0.3811705923
C,0,-4.8385018334,-0.824301483,0.0307249143
C,0,1.4753595116,0.9409087621,0.3138414146
C,0,2.5878876204,1.4329870856,1.0740951766
C,0,3.6211416697,1.8326656935,0.1742461124
C,0,3.166683317,1.5754810918,-1.1527608955
C,0,1.8545693091,1.0207850633,-1.0653901414
C,0,3.2527611235,-2.0671414211,0.8506132203
C,0,4.5156362398,-1.4239547828,1.0124419583
C,0,5.0501254469,-1.1702372355,-0.2862912329
C,0,4.1157979907,-1.6548473116,-1.2508743716
C,0,3.0039420546,-2.2076846313,-0.5477007422
C,0,0.0942923578,0.5879461675,0.8770756672
C,0,-0.6700340851,1.9101967395,1.2951347455
C,0,-1.5703428026,2.3861703952,0.103873572
C,0,-0.8354023511,3.4162088002,-0.7871894884
C,0,-2.8803834151,3.0200298879,0.5984350451
C,0,0.2202319804,-0.3638791361,2.079686836
H,0,-0.3691115619,-1.9614903044,-1.0536433566
H,0,-2.245451021,-1.3548741554,-2.8950798246
H,0,-3.2057692218,1.1090921174,-2.3663791922
H,0,-4.4108089596,0.4176615149,1.8457448562
H,0,-2.7035201217,-1.5643035002,2.5102162257
H,0,-2.8008613191,-3.4356564935,0.5702427262
H,0,-4.5767591398,-2.6157385557,-1.2908265921

H,0,-5.5612770186,-0.2266360798,-0.5094822717
 H,0,2.6390574741,1.4959001388,2.153653987
 H,0,4.5886314749,2.2301748777,0.4537708009
 H,0,3.7264474138,1.7435787758,-2.0640631788
 H,0,1.2446520575,0.7022984899,-1.8997942809
 H,0,2.5986051627,-2.385520652,1.6506462228
 H,0,4.9789151705,-1.1597232887,1.9543324588
 H,0,5.9880436597,-0.674909572,-0.5023167851
 H,0,4.2216092263,-1.593210359,-2.3262936786
 H,0,2.1227370744,-2.6450941756,-0.9986794367
 H,0,-1.3163694987,1.6699392478,2.1474085738
 H,0,0.022845121,2.6923691277,1.6221977134
 H,0,0.1211197353,3.0318543857,-1.1507899856
 H,0,-0.6384581491,4.3353821011,-0.2213005489
 H,0,-1.4478040818,3.6821047233,-1.6572732725
 H,0,-3.5263053253,3.2967675436,-0.2438935989
 H,0,-2.6752357879,3.9333609274,1.1709670475
 H,0,-3.4382764933,2.3324023147,1.2398414972
 H,0,-0.7567251442,-0.5187012384,2.544210256
 H,0,0.8970005821,0.0425497881,2.8396297638
 H,0,0.6115674886,-1.3358657799,1.7681042381

Cartesian coordinates for **TS_{4b4c}**
 (NImag = 1 (-122 cm⁻¹); optimized at BP86/AE1 level):

H	2.77179921	2.62153718	2.52890738
H	2.24721030	3.96987522	0.22785169
C	2.16095245	2.25349640	1.70147098
H	-5.85551900	-1.67740600	0.16043200
H	-3.98333400	-2.34705600	-1.70109500
C	1.88805421	2.96821277	0.47168847
H	-3.64695200	-1.89075600	2.40634300
H	-0.41968228	4.29186545	-1.36562772
H	-1.67587800	-2.42239800	0.62784700
H	5.37908058	2.57759319	0.24418474
C	-5.25493700	-0.97988000	-0.42562100
C	-4.26106000	-1.33386300	-1.40648400
H	-1.42327824	3.12767973	-0.46754729
C	-3.01177400	-1.15043000	1.91669300
C	1.53310601	0.95408547	1.63077795
H	1.57721704	0.18316631	2.40227383
C	-1.96552600	-1.42791600	0.97032600
C	-0.86755435	3.28198278	-1.40885233
H	5.05491802	0.29379791	1.69172529
C	4.89912698	1.66077306	-0.10208260
C	1.06593554	2.11137794	-0.33955403
H	1.51451779	3.53935150	-2.78858621
H	-1.58833514	3.26670694	-2.24819223
Fe	2.90273400	1.22129308	0.11216139
C	4.72836364	0.45311874	0.66277802

C	0.85290373	0.88385781	0.36763029
Fe	-3.41670500	-0.24746300	0.11956300
C	0.22938412	2.20199651	-1.60670896
C	-5.29549900	0.45662000	-0.33005400
H	4.25241466	2.19126355	-2.20031325
C	-3.69345100	-0.11495900	-1.92103600
C	4.29761198	1.45755214	-1.39429573
C	-3.09396400	0.27695800	2.07399200
H	-5.93284200	1.03817900	0.33800600
C	1.03386576	2.54767188	-2.87754844
H	-3.80365500	0.81620600	2.70374800
H	-2.91227800	-0.03782600	-2.67871200
C	-1.37889100	-0.17831400	0.53332400
H	0.37155261	2.57533791	-3.76386712
H	1.82538746	1.80087280	-3.05791493
C	-4.32841400	0.99104700	-1.25350900
C	-0.12934300	-0.04820600	-0.34811800
C	4.02416707	-0.49641097	-0.15786184
C	-2.09656000	0.87107700	1.22346800
C	-0.38379666	0.74498484	-1.69533793
C	3.75844199	0.12418037	-1.42731093
H	-1.46024636	0.77422883	-1.94182432
H	3.72950955	-1.50429824	0.13784013
H	-4.11197400	2.04830100	-1.41561100
H	0.77313439	-1.95592119	0.29789071
H	0.10718512	0.19816827	-2.52162666
H	3.24187586	-0.33609160	-2.27114023
H	-1.93379600	1.94300300	1.10482300
C	0.47618534	-1.44129632	-0.63312255
H	1.37950702	-1.33307193	-1.25423763
H	-0.24963082	-2.08385381	-1.16068940

Cartesian coordinates for **TS_{4a4b}**
(NImag = 1 (-130 cm⁻¹); optimized at BP86/AE1 level):

H	2.20969737	-4.19511735	0.72586814
H	3.72955825	-2.05765208	1.43954275
C	1.93713057	-3.14645651	0.58710013
H	-5.85551900	-1.67740600	0.16043200
H	-3.98333400	-2.34705600	-1.70109500
C	2.75031610	-2.00732579	0.95961649
H	-3.64695200	-1.89075600	2.40634300
H	2.92906434	0.61728527	2.83921771
H	-1.67587800	-2.42239800	0.62784700
H	4.80235439	-3.51271035	-1.47237094
C	-5.25493700	-0.97988000	-0.42562100
C	-4.26106000	-1.33386300	-1.40648400
H	1.15868251	0.43588514	2.79535587
C	-3.01177400	-1.15043000	1.91669300
C	0.72902914	-2.66636596	-0.04350389
H	-0.07027481	-3.29126736	-0.44609482

C	-1.96552600	-1.42791600	0.97032600
C	2.01051254	0.96037144	2.32845825
H	2.50327785	-4.41402298	-2.62043823
C	4.05266996	-2.89954037	-1.97517458
C	2.02085120	-0.82740751	0.58036294
H	4.27074459	0.94792221	0.73617436
H	1.90180809	2.04484069	2.51914006
Fe	2.41434001	-2.05670981	-1.06405455
C	2.83759734	-3.37596328	-2.58280983
C	0.79072237	-1.23136518	-0.03274322
Fe	-3.41670500	-0.24746300	0.11956300
C	2.08946780	0.67545943	0.80484977
C	-5.29549900	0.45662000	-0.33005400
H	4.87963687	-0.80921574	-1.75404689
C	-3.69345100	-0.11495900	-1.92103600
C	4.09041673	-1.46755019	-2.11978829
C	-3.09396400	0.27695800	2.07399200
H	-5.93284200	1.03817900	0.33800600
C	3.36269962	1.34530683	0.24636939
H	-3.80365500	0.81620600	2.70374800
H	-2.91227800	-0.03782600	-2.67871200
C	-1.37889100	-0.17831400	0.53332400
H	3.33875696	2.43778046	0.42219043
H	3.45669690	1.16952705	-0.83853314
C	-4.32841400	0.99104700	-1.25350900
C	-0.12934300	-0.04820600	-0.34811800
C	2.12671843	-2.23886052	-3.10491879
C	-2.09656000	0.87107700	1.22346800
C	0.79626370	1.17675500	0.04126960
C	2.90039262	-1.06126173	-2.81867801
H	0.23919670	1.92202142	0.63676019
H	1.16217781	-2.26487035	-3.61392205
H	-4.11197400	2.04830100	-1.41561100
H	-1.06814826	-0.89735136	-2.15609111
H	1.10440371	1.69183706	-0.88747404
H	2.63473473	-0.03766691	-3.08778448
H	-1.93379600	1.94300300	1.10482300
C	-0.52679187	0.01209551	-1.84042861
H	0.37885187	0.09107861	-2.46256814
H	-1.17733495	0.88142142	-2.03812072

Cartesian coordinates for **TS_{4a4c}**
(NImag = 1 (-141 cm⁻¹); optimized at BP86/AE1 level):

H	-0.62591265	-4.04659115	-0.44148776
H	-2.12540659	-2.38368413	-1.98237508
C	-0.66584149	-2.95818523	-0.35110220
H	5.21508400	-0.98690100	-1.83492400
H	2.74023900	-2.09915000	-2.06483900
C	-1.46713964	-2.07278714	-1.16800457

H	3.82213200	1.84222900	-1.91157000
H	-1.17031361	0.44396141	-3.23376258
H	1.28705600	0.84692500	-1.86302500
H	-3.97237934	-3.96698881	0.44760230
C	4.58266200	-1.32051300	-1.00977600
C	3.27324600	-1.90619100	-1.13178000
H	0.26348573	0.93517706	-2.28460877
C	3.23218000	1.63049200	-1.01740100
C	0.03056587	-2.16831214	0.64106518
H	0.69326175	-2.55989679	1.41506134
C	1.89130200	1.10688400	-0.99200100
C	-0.82599961	1.06888786	-2.38928723
H	-2.22376723	-4.20863740	2.52161783
C	-3.65258365	-3.16398009	1.11477152
C	-1.24829682	-0.73650420	-0.68669279
H	-3.48636815	0.37829327	-2.13152920
H	-1.01618184	2.12702595	-2.64966319
Fe	-2.00927961	-1.96305920	0.81668538
C	-2.72921475	-3.29186309	2.21135864
C	-0.33262671	-0.79515522	0.41951185
Fe	3.18972900	-0.16508200	-0.03530700
C	-1.57919778	0.69525194	-1.08399763
C	4.89929000	-1.22409600	0.39169800
H	-4.74239680	-1.36287771	0.29502593
C	2.78311600	-2.17583700	0.19475500
C	-4.05661557	-1.78467081	1.03171484
C	3.66856700	1.79025500	0.34463900
H	5.81426200	-0.80510100	0.81524700
C	-3.08407060	0.96883203	-1.28748042
H	4.64879900	2.14507500	0.67008700
H	1.82036600	-2.62738800	0.44100700
C	1.47731200	0.94719000	0.38517800
H	-3.25779891	2.03734022	-1.51577554
H	-3.65937526	0.70881570	-0.38282163
C	3.78565800	-1.75122700	1.13712000
C	0.07480700	0.59338500	0.89715500
C	-2.56288282	-1.99177942	2.80677010
C	2.59593300	1.36348800	1.20416600
C	-1.01432379	1.48221868	0.15519781
C	-3.38440160	-1.06114148	2.07813978
H	-0.60633801	2.46809606	-0.13165646
H	-1.91679249	-1.75369162	3.65385907
H	3.71160500	-1.80989700	2.22478900
H	0.71663087	0.18571459	2.95941898
H	-1.84132096	1.66134598	0.86729557
H	-3.48239353	0.00687287	2.28402910
H	2.62760200	1.35247400	2.29566100
C	-0.02159411	0.80509586	2.42372353
H	-1.03138184	0.53813608	2.77732900
H	0.16847377	1.86072692	2.69071079