

Supporting Information

External Electric Field : A New Catalytic Strategy for the Anti-Markovnikov Hydrohydrazination of Parent Hydrazine

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Table S1. Relative energies (in kcal/mol) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine according to path M and path AM.

	path M	path AM
R	0.0	0.0
TS1/TS1'	28.1	27.8
IM/IM'	-37.5	-37.5
TS2/TS2'	11.6	12.8
P/P'	-47.8	-44.7

Table S2. Relative energies (in kcal/mol) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine at level of M06/6-311++G(d,p)//M062X/6-311G(d,p) at different field strengths (in $\times 10^{-4}$ au).

	0	-20	-40	-60
R	0.0	0.0	0.0	0.0
TS1	27.6	25.0	23.1	21.4
IM	-37.6	-39.0	-39.9	-40.8
TS2	15.7	13.3	11.4	9.6
P	-44.7	-45.9	-46.5	-46.8

Table S3. Relative energies (in kcal/mol) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine at level of M06/6-311++G(d,p)//M062X/6-311++G(d,p) at different field strengths (in $\times 10^{-4}$ au).

	0	-20	-40	-60
R	0.0	0.0	0.0	0.0
TS1	30.4	28.4	26.5	24.7
IM	-34.9	-35.7	-36.6	-37.9
TS2	18.4	16.5	14.6	12.7
P	-41.9	-42.6	-43.1	-43.7

Table S4. Natural bond orbital (NBO) charges (in e) on C1, C2, N4, H3, and H5 atoms in phenylacetylene under different directions of the external electric field (in $\times 10^{-4}$ au).

	0	Fx		Fy		Fz	
		20	-20	20	-20	20	-20
C1	-0.031	-0.018	-0.044	-0.031	-0.031	-0.031	-0.031
C2	-0.207	-0.226	-0.188	-0.207	-0.207	-0.207	-0.207
		Fx					
	20	0	-20	-40	-60	-150	-180
N4	-0.746	-0.750	-0.755	-0.759	-0.764	-0.787	-0.795
H3	0.374	0.375	0.376	0.378	0.379	0.387	0.390
H5	0.374	0.375	0.377	0.378	0.379	0.386	0.388

Table S5. Relative energies (in kcal/mol) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine under different directions of the external electric field (in $\times 10^{-4}$ au).

	Fx		Fy		Fz	
	-20	20	-20	20	-20	20
R	0.0	0.0	0.0	0.0	0.0	0.0
TS1	25.9	29.6	28.1	27.3	31.8	32.3
IM	-38.3	-36.6	-37.3	-37.5	-33.4	-32.7
TS2	11.2	14.8	13.2	12.8	17.1	17.6
P	-45.3	-43.8	-45.2	-43.9	-40.4	-40.2

Table S6. Relative energies (in kcal/mol) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine under Fx (in $\times 10^{-4}$ au) according to path AM.

	-60	-40	-20	20	40	60
R	0.0	0.0	0.0	0.0	0.0	0.0
TS1	22.1	24.0	25.9	29.6	31.4	33.4
IM	-40.9	-39.6	-38.3	-36.6	-35.8	-35.1
TS2	7.3	9.3	11.2	14.8	16.5	18.1
P	-46.7	-46.0	-45.3	-43.8	-42.9	-42.0

Table S7. Relative energies (in kcal/mol) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine under Fx (in $\times 10^{-4}$ au) according to path M.

	-60	-40	-20	20	40	60
R	0.0	0.0	0.0	0.0	0.0	0.0
TS1'	31.0	30.1	29.1	27.1	26.2	25.3
IM'	-38.0	-37.9	-37.8	-37.1	-36.8	-36.5
TS2'	14.8	13.7	12.7	10.7	9.8	9.0
P'	-47.0	-47.5	-47.8	-48.0	-47.9	-47.6

Table S8. Relative energies (in kcal/mol) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine in C₆H₆ and DMSO solvents, and the negative Fx (in $\times 10^{-4}$ au).

	C ₆ H ₆			DMSO		
	0	-20	-60	0	-20	-60
R	0.0	0.0	0.0	0.0	0.0	0.0
TS1	26.1	23.9	19.53	22.5	22.6	17.09
IM	-37.5	-38.8	-42.24	-39.5	-38.7	-43.50
TS2	12.9	10.9	5.93	10.8	10.8	4.29
P	-44.1	-44.9	-46.48	-45.6	-43.9	-45.59

Table S9. Relative energies (in kcal/mol) of the hydrohydrazination of trifluoromethyl phenylacetylene with parent hydrazine under the negative F_x (in $\times 10^{-4}$ au).

	-20	-40	-60
R	0.0	0.0	0.0
TS1	24.5	23.2	21.9
IM	-39.7	-40.7	-41.8
TS2	9.5	8.0	6.5
P	-45.3	-45.3	-45.1

Table S10. Relative energies (in kcal/mol) of the hydrohydrazination of 1-hexyne, 6-trifluoromethyl-1-hexyne with parent hydrazine in C₆H₆ solvents, and the negative Fx (in $\times 10^{-4}$ au).

	solvent				substituent	
	0	-60	0	-60	0	-60
R	0.0	0.0	0.0	0.0	0.0	0.0
TS1	30.3	24.8	29.5	22.8	29.3	24.7
IM	-34.9	-36.9	-34.0	-36.7	-35.5	-37.0
TS2	18.1	13.0	19.0	12.9	17.2	13.1
P	-45.5	-48.0	-44.7	-47.5	-46.1	-47.3

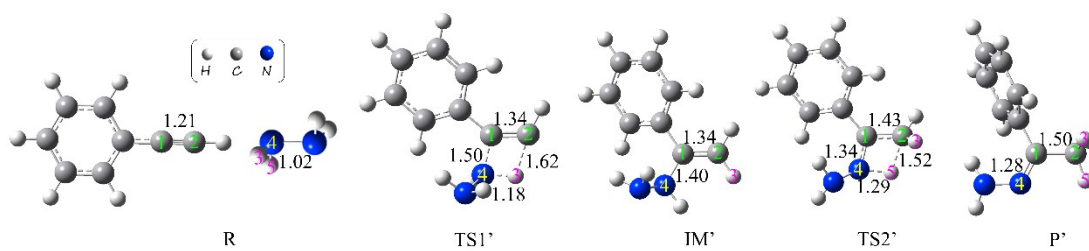


Fig. S1. Geometries (Bond lengths are given in Å) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine according to path M.

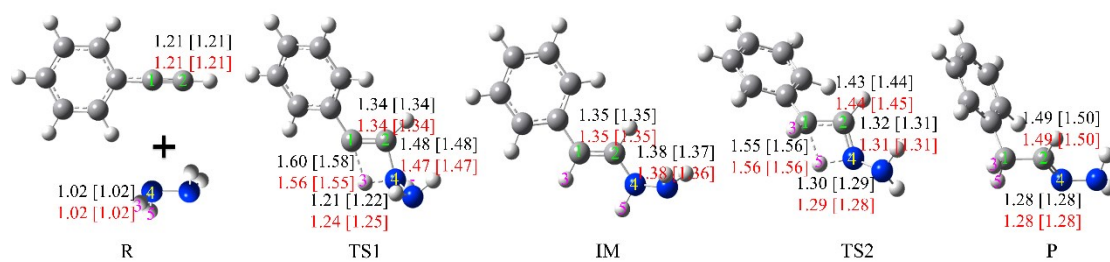


Fig. S2. Geometries (Bond lengths are given in Å) of the stationary points in hydrohydrazination of phenylacetylene with parent hydrazine in C_6H_6 and DMSO solvents (Red values were calculated in DMSO, values in square brackets were calculated in external electric field (in $\times 10^{-4}$ au)).

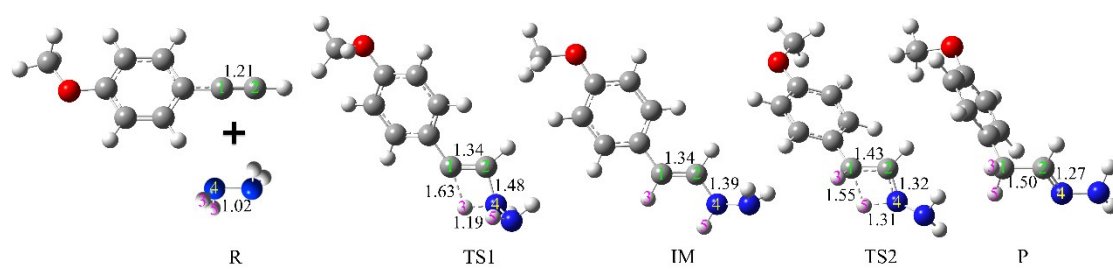


Fig. S3. Geometries (Bond lengths are given in Å) of the stationary points in hydrohydrazination of methoxyl phenylacetylene with parent hydrazine.

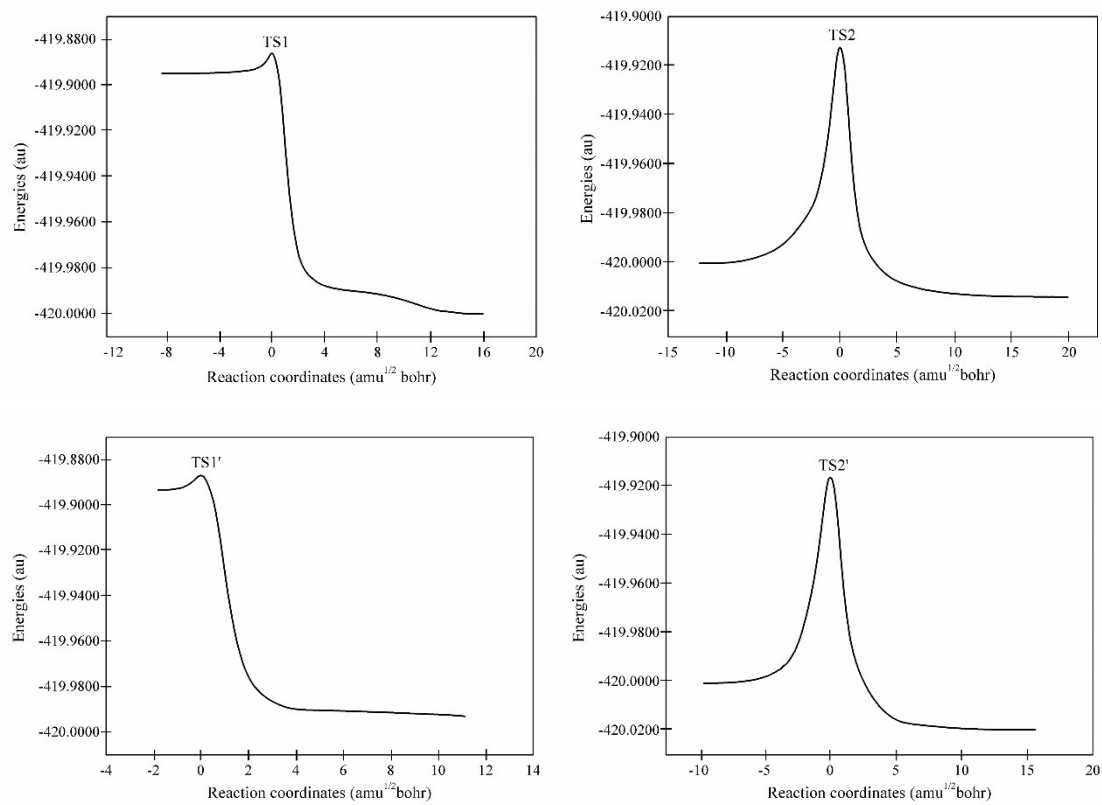


Fig. S4. IRC plots of transition states in anti-Markovnikov and Markovnikov hydrohydrazination of phenylacetylene with parent hydrazine.

Path AM:

R1:

N,0,1.5151689068,1.3191939982,2.1535869329
H,0,2.3152300172,1.5250116367,1.551514765
H,0,0.7485280624,1.7779136086,1.656703385
N,0,1.2671459537,-0.1139716924,1.9077878395
H,0,2.0343518063,-0.5728133519,2.4034433132
H,0,0.4674932536,-0.3199551991,2.5101837644

R2:

C,0,1.2361742827,-0.8501940569,0.0380913782
C,0,2.2722171151,-1.2316053089,0.5299538547
H,0,3.1884982112,-1.5715374928,0.9627643529
C,0,0.0127872596,-0.4009161325,-0.5443946352
C,0,-0.9800582314,0.1841267128,0.252905772
C,0,-0.2093707712,-0.5410585977,-1.9209386102
C,0,-2.1682195579,0.618339225,-0.3177601264
H,0,-0.8048399146,0.2910702619,1.3217918335
C,0,-1.39995636,-0.1045180184,-2.4846069189
H,0,0.5640760665,-0.995674001,-2.5372071955
C,0,-2.3815599511,0.4755934855,-1.6858100863
H,0,-2.9339342267,1.0709572862,0.3096970149
H,0,-1.5633906859,-0.2172480165,-3.554902163
H,0,-3.3145302364,0.8178336532,-2.130159471

TS1:

N,0,-2.8698594258,-5.0292505902,3.9086569347
H,0,-2.8609621072,-6.0502087256,3.9553935527
H,0,-2.5560608668,-4.8004232337,2.9617497793
N,0,-4.252420344,-4.6307999097,3.9114267681
H,0,-4.5623436931,-4.5798811411,4.8858885242
H,0,-4.4919229077,-3.6826926102,3.2358158519
C,0,-5.4565912571,-4.2772913208,2.0609557921
C,0,-5.1827739106,-5.2508013596,2.9394344774
H,0,-5.4603025169,-6.2948201158,3.1093501722
C,0,-6.2945997481,-4.4345043512,0.8798585459
C,0,-7.1264681664,-3.3798808447,0.47627446
C,0,-6.2800336381,-5.597010274,0.0922989
C,0,-7.9380564324,-3.4940879677,-0.6444476118
H,0,-7.1223223814,-2.465873664,1.0694603731
C,0,-7.0709912136,-5.7026556185,-1.0440781852
H,0,-5.6216429213,-6.4178025981,0.3788486234
C,0,-7.9101870083,-4.6545594263,-1.4132671686
H,0,-8.5848718403,-2.6657457601,-0.9311119244

Path M:

R1:

N,0,1.5151689068,1.3191939982,2.1535869329
H,0,2.3152300172,1.5250116367,1.551514765
H,0,0.7485280624,1.7779136086,1.656703385
N,0,1.2671459537,-0.1139716924,1.9077878395
H,0,2.0343518063,-0.5728133519,2.4034433132
H,0,0.4674932536,-0.3199551991,2.5101837644

R2:

C,0,1.2361742827,-0.8501940569,0.0380913782
C,0,2.2722171151,-1.2316053089,0.5299538547
H,0,3.1884982112,-1.5715374928,0.9627643529
C,0,0.0127872596,-0.4009161325,-0.5443946352
C,0,-0.9800582314,0.1841267128,0.252905772
C,0,-0.2093707712,-0.5410585977,-1.9209386102
C,0,-2.1682195579,0.618339225,-0.3177601264
H,0,-0.8048399146,0.2910702619,1.3217918335
C,0,-1.39995636,-0.1045180184,-2.4846069189
H,0,0.5640760665,-0.995674001,-2.5372071955
C,0,-2.3815599511,0.4755934855,-1.6858100863
H,0,-2.9339342267,1.0709572862,0.3096970149
H,0,-1.5633906859,-0.2172480165,-3.554902163
H,0,-3.3145302364,0.8178336532,-2.130159471

TS1':

N,0,-4.9381810915,-3.5768244564,4.1619467918
H,0,-4.0562356593,-3.3704001082,3.6868074647
H,0,-5.660085922,-3.1103117822,3.6075811271
N,0,-5.115258048,-4.9875330992,3.9572727394
H,0,-4.1178669982,-5.612416514,3.8962145008
H,0,-5.799732097,-5.3261542459,4.6400911572
C,0,-5.2394952377,-5.5133447636,2.5557030403
C,0,-4.0945225318,-6.1979179875,2.3895436397
H,0,-3.9153211434,-6.699660205,1.4280783254
C,0,-6.4355008305,-5.1617331092,1.7909955261
C,0,-7.5693550617,-4.5822937229,2.3774045199
C,0,-6.4692811603,-5.4163354932,0.4122045236
C,0,-8.6937410656,-4.2750749012,1.6171424971
H,0,-7.5937150085,-4.380251367,3.4498335403
C,0,-7.5900936245,-5.1129266466,-0.3437939263
H,0,-5.5917896932,-5.8590922015,-0.0575798914
C,0,-8.7105808216,-4.5378821606,0.2536500512
H,0,-9.5618534034,-3.8280578553,2.0993139117

H,0,-7.0382560049,-6.610952944,-1.6450128473
H,0,-8.5324979561,-4.7373721646,-2.3029682576

H,0,-7.5900389572,-5.3226746511,-1.4123145329
H,0,-9.5882826347,-4.2947917595,-0.3421708658

IM:

N,0,3.1162388197,-0.5229828046,2.8672696606
H,0,3.2022415738,-1.5249300673,3.019338923
H,0,3.6433141738,-0.2763756075,2.0290075694
N,0,1.7551873906,-0.2052939684,2.7110853149
H,0,1.5164258049,0.6395101798,3.2201387035
H,0,-0.1086827682,1.3317050411,1.5679331294
C,0,0.1844970519,0.4537252577,0.9848216923
C,0,1.1620326234,-0.3326209565,1.468717904
H,0,1.537579125,-1.189297708,0.9031225839
C,0,-0.5241034575,0.2538265655,-0.2727275148
C,0,-1.2882049209,1.3041077479,-0.8012704728
C,0,-0.4797409134,-0.9472421932,-0.9973406882
C,0,-1.9581220215,1.172143844,-2.0099202227
H,0,-1.3438422266,2.243061388,-0.2489217223
C,0,-1.1415688085,-1.0766213548,-2.2095930654
H,0,0.0649512815,-1.8004917586,-0.5931001859
C,0,-1.8847090003,-0.0180033547,-2.7263251551
H,0,-2.5418942458,2.0068551724,-2.3955400566
H,0,-1.0896449502,-2.0205456212,-2.7506877951
H,0,-2.4095075317,-0.1248998016,-3.6739216021

IM':

N,0,1.3564258726,1.4811688673,1.8745486742
H,0,1.7885129281,1.7898695941,1.001632931
H,0,0.4009786442,1.8303078549,1.8765607713
N,0,1.3110439531,0.0653252642,1.9228330193
H,0,2.8930957251,-1.8746806996,0.9926894674
H,0,2.0828113497,-0.2725846901,2.489482082
C,0,1.1894522378,-0.6377591523,0.7131914977
C,0,2.0248829826,-1.6343034974,0.3805820587
H,0,1.821154887,-2.2787617978,-0.4702044821
C,0,0.0286821585,-0.2641088472,-0.1229062248
C,0,-1.1907344921,0.0863931547,0.4680320898
C,0,0.1245273421,-0.2647215343,-1.5167848026
C,0,-2.2877889364,0.4141347324,-0.3176743016
H,0,-1.2720767668,0.0690708381,1.5547373781
C,0,-0.9741308392,0.0610375728,-2.302999871
H,0,1.0805124049,-0.5087491407,-1.9791073079
C,0,-2.1831181158,0.4031505719,-1.7061114156
H,0,-3.2332609925,0.6743229946,0.1557831872
H,0,-0.8821970636,0.0578406825,-3.38787158
H,0,-3.0426492794,0.664790232,-2.3209111711

TS2:

N,0,2.8177025682,-0.6626060824,3.0744882005
H,0,2.8024127706,-1.4848904041,3.6720117985
H,0,3.6363319697,-0.6721699818,2.4659686958
N,0,1.6295216508,-0.5974417827,2.3524920081
H,0,0.4967500966,0.0440262122,2.329703384
H,0,0.5370848065,1.4785657223,1.1828011366
C,0,0.4295692667,0.445044809,0.8327677234
C,0,1.6074205574,-0.333155077,1.0575908514
H,0,2.3902265372,-0.6736632147,0.3698932698
C,0,-0.4194287341,0.275532524,-0.3443892263
C,0,-1.2190433553,1.3240772218,-0.8207629468
C,0,-0.4684791056,-0.9477554874,-1.0285268307
C,0,-2.023471752,1.1612834077,-1.9395271481
H,0,-1.1977655164,2.2819744795,-0.2989714051
C,0,-1.2598575663,-1.1066738793,-2.1584898599
H,0,0.1163919741,-1.7883304063,-0.6512615465
C,0,-2.0443487428,-0.053752513,-2.6201893549
H,0,-2.6357099337,1.9919222058,-2.2886538562

TS2':

N,0,1.3796213761,1.2599209533,2.1336508045
H,0,0.9118508797,1.7666699546,1.3820539882
H,0,0.8935117996,1.4043384411,3.015137002
N,0,1.4650016587,-0.1106075471,1.8689207382
H,0,3.1359962293,-1.2158375604,0.1831390437
H,0,2.366085201,-1.0337086469,1.8326714456
C,0,1.1545852277,-0.6209971325,0.6664344394
C,0,2.1524783683,-1.6159483582,0.4480605746
H,0,1.9104446971,-2.5435721397,-0.0805444231
C,0,0.0162981726,-0.2263039139,-0.1642617875
C,0,-1.1602254991,0.2948483896,0.3945583834
C,0,0.0715182167,-0.43236977,-1.5471032298
C,0,-2.2424325186,0.6133518575,-0.411826809
H,0,-1.22647103,0.4197316066,1.4748921957
C,0,-1.0153238,-0.1189229618,-2.3537690532
H,0,0.9871118993,-0.8381008016,-1.9754609377
C,0,-2.1714227075,0.4091929123,-1.7887347013
H,0,-3.1532217298,1.0101031984,0.0334978969

H,0,-1.2757271264,-2.0654338641,-2.6755753821
H,0,-2.6737757655,-0.1808141796,-3.4992054013

H,0,-0.9585593694,-0.283622673,-3.4282291907
H,0,-3.0227819916,0.6587554819,-2.4196433198

P:

N,0,3.0067964657,-0.9966535212,2.3537835057
H,0,3.0868851948,-1.9484356341,2.6920258554
H,0,3.5422531838,-0.8631702819,1.4931938126
N,0,1.6863681396,-0.646945262,2.2593128537
H,0,-0.6278584728,0.2179098094,2.078976831
H,0,-0.1007974283,1.8032707866,1.4950276219
C,0,-0.0467860304,0.7220155132,1.2936069721
C,0,1.3664808383,0.2490582592,1.4110937033
H,0,2.1092874265,0.6864707669,0.7201637761
C,0,-0.6272758073,0.4378967545,-0.0704769893
C,0,-1.072256873,1.4651484718,-0.8999733292
C,0,-0.709957531,-0.8788052648,-0.5296765757
C,0,-1.5942341453,1.1872976002,-2.160200417
H,0,-1.0106756872,2.4969332597,-0.5514215515
C,0,-1.2320567953,-1.1610216871,-1.7854137262
H,0,-0.3586804661,-1.6857421181,0.1152202739
C,0,-1.6746992033,-0.1265210212,-2.6063005908
H,0,-1.9372684765,2.0023874349,-2.7956476588
H,0,-1.2937417534,-2.1930622231,-2.1275666354
H,0,-2.0825085788,-0.3457356429,-3.5917067318

P':

N,0,1.2290222428,1.4989326698,1.7962692128
H,0,0.2845096682,1.6861020102,1.457666642
H,0,1.3781672537,1.8516313041,2.7333940327
N,0,1.6531393097,0.202031997,1.7146833017
H,0,2.1452068611,-2.1021395074,-0.3209125879
H,0,2.5183613043,-2.0959402537,1.4228130392
C,0,1.148128593,-0.5741492015,0.8262231667
C,0,1.7239474486,-1.9479372191,0.6838954115
H,0,0.9531826936,-2.7198091097,0.8212437479
C,0,0.0240666697,-0.20722815,-0.080162097
C,0,-1.2652740767,-0.0234464298,0.4296745614
C,0,0.2322011406,-0.0608873617,-1.4536019171
C,0,-2.3218170613,0.3017632904,-0.4142651564
H,0,-1.4371581415,-0.156874089,1.4989684631
C,0,-0.8228613326,0.2649377589,-2.2978885126
H,0,1.2348247299,-0.198415038,-1.8586561892
C,0,-2.1015859323,0.4473304927,-1.780180857
H,0,-3.3215850872,0.4352590549,-0.0039709488
H,0,-0.6465467669,0.377873674,-3.3664018343
H,0,-2.9279145167,0.7006211079,-2.4420614787

Path AM:

Fx = 20 ($\times 10^{-4}$ au)

R1:

N,0,1.2625928302,-0.1947567085,5.2089029962
H,0,1.5953885988,-1.0838836893,4.8291427842
H,0,1.9206202669,0.4688522493,4.7944604521
N,0,0.0217851495,0.0481766003,4.4496126801
H,0,-0.6411084201,-0.6138744731,4.8576746745
H,0,-0.3100382452,0.9434895014,4.814122173

R2:

C,0,-0.0094225238,-0.0160553083,0.0056364637
C,0,0.0035487096,-0.0076947377,1.2145400087
H,0,0.0155781201,0.0004695592,2.2826517101
C,0,-0.022729366,-0.0262891957,-1.4221617564
C,0,-1.2375291135,-0.058597876,-2.11995053
C,0,1.179841985,-0.0040557136,-2.1409650769
C,0,-1.2452378368,-0.06855351,-3.507486394
H,0,-2.1698948564,-0.0757172405,-1.5584424277

Fx = -20 ($\times 10^{-4}$ au)

R1:

N,0,1.2612895619,-0.1926214053,5.2019883125
H,0,1.5929400564,-1.087514478,4.8362448879
H,0,1.9233078337,0.4705841802,4.7943216427
N,0,0.0204918509,0.0503011084,4.44252068
H,0,-0.6375344143,-0.6131777888,4.8575946338
H,0,-0.3112547085,0.9404318635,4.8212456031

R2:

C,0,-0.0093938029,-0.0160042543,0.005740279
C,0,0.0035703092,-0.0075827333,1.2140219456
H,0,0.0152032854,0.0001646803,2.2832038789
C,0,-0.0226594114,-0.026147685,-1.4213083585
C,0,-1.2368751345,-0.0584921768,-2.1203350023
C,0,1.1792672052,-0.0039476151,-2.1413863663
C,0,-1.2446758179,-0.068531745,-3.5079804998
H,0,-2.1684241233,-0.0756647889,-1.5577938629

C,0,1.1643740106,-0.0140746638,-3.528407531
H,0,2.1216678184,0.0212673809,-1.5957901731
C,0,-0.0464109908,-0.0463283477,-4.2147581733
H,0,-2.1927621019,-0.0941164938,-4.0423718566
H,0,2.1025449691,0.00356575,-4.0797863289
H,0,-0.0559191334,-0.0542145631,-5.3028212747

TS1:

N,0,2.2680386292,-1.6870263074,1.6451788199
H,0,2.9917849243,-0.9885768664,1.8274325454
H,0,1.4972997167,-1.4375058787,2.2713408667
N,0,1.7438527639,-1.3868269548,0.3365815235
H,0,2.3051962219,-1.8966154224,-0.3513404473
H,0,0.5736201051,-1.5113742893,0.2502180404
C,0,0.0416565258,0.0236712479,-0.0150667421
C,0,1.3816132091,0.0132655045,0.0139142125
H,0,2.207265049,0.7154537774,-0.1357703331
C,0,-0.7798727276,1.2056858092,-0.239405187
C,0,-2.0005329465,1.0740685216,-0.9168307544
C,0,-0.4216123949,2.4815302263,0.2261064701
C,0,-2.8130628881,2.1746574411,-1.1548285392
H,0,-2.2966080571,0.0815317912,-1.2545665241
C,0,-1.2451474137,3.578621917,0.0127692192
H,0,0.5115508484,2.5973960073,0.7791169542
C,0,-2.4406392505,3.4316035778,-0.6864567428
H,0,-3.7526456041,2.0496391073,-1.6908880868
H,0,-0.9541321264,4.5575365198,0.3926540199
H,0,-3.0868362248,4.2915683706,-0.854061625

IM:

N,0,3.3463368743,-1.2110834033,0.5702305368
H,0,4.0797216207,-0.7056141336,0.0786291023
H,0,3.223481721,-0.7792323122,1.4876643268
N,0,2.1590044773,-1.1094702118,-0.1847555854
H,0,1.652044729,-1.9890803015,-0.1675228459
H,0,-0.503509647,-0.9371318885,-0.0499919928
C,0,0.0185683405,0.0238730648,-0.0183186023
C,0,1.3614583762,0.0146118772,-0.0173562237
H,0,1.9394186505,0.9385316169,0.0713658
C,0,-0.8302525856,1.2088781512,0.0340913575
C,0,-2.186346439,1.058900355,0.354912242
C,0,-0.3574928204,2.5056453209,-0.2163214941
C,0,-3.0321080923,2.1561835774,0.4448817961
H,0,-2.5761206734,0.0577954201,0.5425960268

C,0,1.1638480465,-0.0140349468,-3.5289341638
H,0,2.1203181421,0.0213120754,-1.5951922443
C,0,-0.046411638,-0.0463443694,-4.2161064224
H,0,-2.1938470696,-0.0943039178,-4.040834996
H,0,2.1036946388,0.0035827367,-4.0783527429
H,0,-0.0559649396,-0.0544002202,-5.3048547841

TS1:

N,0,2.326101087,-1.6618547673,1.6345457384
H,0,3.1578369777,-1.0702259401,1.6863248271
H,0,1.6686784081,-1.2729758451,2.3146604986
N,0,1.703512437,-1.4011413431,0.3665253158
H,0,2.1976556248,-1.948656212,-0.34342111
H,0,0.5097195266,-1.4924684269,0.3598857991
C,0,0.0044747572,0.0123103685,0.0444936729
C,0,1.3426813106,-0.0106461738,0.0060103104
H,0,2.1569352716,0.681132619,-0.2237234035
C,0,-0.8083796144,1.1954800496,-0.2028314778
C,0,-1.9910735581,1.0821866951,-0.9486990401
C,0,-0.4727456552,2.461843688,0.3037451569
C,0,-2.781669706,2.1919589272,-1.2154552065
H,0,-2.2701796328,0.0979274255,-1.3242006922
C,0,-1.2768853121,3.5674441207,0.0600127629
H,0,0.4316832073,2.564335878,0.9039583023
C,0,-2.4308083307,3.440691457,-0.7088953109
H,0,-3.6856394937,2.0815678541,-1.8140023608
H,0,-0.9955110194,4.5390719346,0.4649425361
H,0,-3.0555979256,4.3103217912,-0.9077786288

IM:

N,0,3.4040742307,-1.1908703997,0.4737229845
H,0,4.0692571738,-0.7833105288,-0.1786042259
H,0,3.4444033192,-0.6755166229,1.352398108
N,0,2.1182908622,-1.1380816851,-0.0827311979
H,0,1.6305413865,-2.0220512517,0.0149391674
H,0,-0.5309997128,-0.9384594152,0.0742190508
C,0,-0.001755922,0.018990216,0.0595384733
C,0,1.3442936142,-0.0050367291,0.0336937819
H,0,1.9356510537,0.913396575,0.0627388258
C,0,-0.8412060007,1.207852645,0.076689882
C,0,-2.2181294061,1.0637336783,0.3043783377
C,0,-0.3514409325,2.5094956119,-0.119407463
C,0,-3.0644440557,2.1632115631,0.3504385335
H,0,-2.6225649141,0.0614379232,0.453058452

C,0,-1.2004275316,3.6036956561,-0.118504598
H,0,0.6796962648,2.6542590502,-0.5173083154
C,0,-2.542413255,3.4374462165,0.21410171
H,0,-4.0811678188,2.0092062346,0.6961196541
H,0,-0.809286374,4.6000924202,-0.3204527823
H,0,-3.203640127,4.2993388599,0.2787457376

TS2:

N,0,2.9333086348,-1.7586323319,0.5122482075
H,0,3.4808233304,-2.2972108083,-0.1539825181
H,0,3.49882646,-1.017885861,0.927732722
N,0,1.8050573327,-1.2495801566,-0.133988789
H,0,0.5126378584,-1.4312028175,-0.2087716797
H,0,-0.4085855333,-0.3720490117,0.9527208482
C,0,0.0107832718,0.015365068,0.0166798133
C,0,1.43704497,0.0140862277,0.0124912129
H,0,2.1602339152,0.8327033011,0.1095715082
C,0,-0.7842700363,1.0514135102,-0.6405249089
C,0,-2.0793722593,1.3598829947,-0.2023826564
C,0,-0.2749069786,1.7618846295,-1.7363087915
C,0,-2.8295549705,2.347085889,-0.8254574021
H,0,-2.4955948793,0.8127947637,0.6445176319
C,0,-1.0183104724,2.7614354413,-2.3505278858
H,0,0.7152236638,1.5055111985,-2.117612093
C,0,-2.300932477,3.0587719848,-1.8996029604
H,0,-3.8344664472,2.5672403854,-0.4685038096
H,0,-0.6002387319,3.3018762518,-3.199055124
H,0,-2.8899870313,3.832504391,-2.3884650953

P:

N,0,3.524509534,-0.7345122084,-0.7102734035
H,0,3.9110578548,-0.9631878948,-1.6192266188
H,0,3.9022889226,0.1538429557,-0.3717153911
N,0,2.1520651734,-0.7593277125,-0.7851830645
H,0,-0.332551472,-0.7845534887,-0.6675000062
H,0,-0.3613559424,-0.2914124692,1.0320080128
C,0,0.0092990365,-0.010567216,0.0342556871
C,0,1.5034611533,-0.0166713921,0.0216433889
H,0,2.0187215682,0.6751641416,0.7126339981
C,0,-0.5461769426,1.3407012975,-0.3468291574
C,0,-1.3582698678,2.0661624591,0.5223213445
C,0,-0.239791912,1.8884255702,-1.5947277877
C,0,-1.8627841121,3.3096469362,0.1523547827
H,0,-1.6057773549,1.6463840237,1.4981507155

C,0,-1.195442051,3.6087906415,-0.0654531904
H,0,0.7059292083,2.6646115086,-0.3326563162
C,0,-2.5587957646,3.4462633888,0.1703301043
H,0,-4.1289502458,2.0152383192,0.5305033039
H,0,-0.7835162216,4.6053368628,-0.2196836129
H,0,-3.2182299316,4.3118132692,0.2046928514

TS2:

N,0,2.9359378995,-1.7656776617,0.4851226651
H,0,3.4402649945,-2.3382096182,-0.1865562118
H,0,3.5416651502,-1.0436253326,0.8749769408
N,0,1.8024523886,-1.2355328475,-0.1149967497
H,0,0.5224250268,-1.425002191,-0.1871036711
H,0,-0.4013009034,-0.3281522629,0.9904811355
C,0,0.0087145909,0.0262199481,0.0371347214
C,0,1.441955352,0.0255425488,0.0273067324
H,0,2.1672082759,0.8397557114,0.1361485433
C,0,-0.7841431995,1.0560432088,-0.629386791
C,0,-2.0884116822,1.3558537014,-0.2093553423
C,0,-0.2712083572,1.770531903,-1.7222914135
C,0,-2.8404944079,2.3341563616,-0.8442654669
H,0,-2.5070976878,0.8092880574,0.6372233806
C,0,-1.0162837114,2.761484974,-2.3473758897
H,0,0.7275240661,1.5287195693,-2.0891291873
C,0,-2.307639679,3.0490823258,-1.9141725201
H,0,-3.8505895368,2.5483814162,-0.4954364995
H,0,-0.5883841745,3.3064988613,-3.1879454456
H,0,-2.8948747848,3.8206363769,-2.4096007005

P:

N,0,3.5065009757,-0.7921815391,-0.7620200289
H,0,3.8809121593,-1.0803917016,-1.6578124919
H,0,3.9515068171,0.06135003,-0.4194800629
N,0,2.1438202235,-0.7625033421,-0.7987674189
H,0,-0.3184105908,-0.7601322066,-0.6048092569
H,0,-0.303835038,-0.2293564716,1.0831675318
C,0,0.0425224846,0.0296800402,0.070242898
C,0,1.5366030566,0.007554485,0.0169399342
H,0,2.0844745473,0.6888074391,0.6911372354
C,0,-0.5352385217,1.3665632897,-0.3270600679
C,0,-1.4056543271,2.0614580044,0.5105027057
C,0,-0.2004295201,1.9300356612,-1.5605786288
C,0,-1.9374641748,3.2886601301,0.1247424163
H,0,-1.6681081536,1.6334048117,1.4790832791

C,0,-0.7425186451,3.1279264929,-1.9685762926
H,0,0.3963004565,1.3218285976,-2.2767835199
C,0,-1.5564189019,3.8436450539,-1.0939096045
H,0,-2.501551355,3.8611173408,0.8402820248
H,0,-0.5037178053,3.537758504,-2.948933993
H,0,-1.9549740381,4.8134038384,-1.3866334453

Fy = 20 ($\times 10^{-4}$ au)

R1:

N,0,1.2664746498,-0.1787716366,5.206167151
H,0,1.5772997138,-1.0891957551,4.860415845
H,0,1.9338644326,0.4583413472,4.7659288286
N,0,0.0252358879,0.0642762604,4.4473435276
H,0,-0.6265780267,-0.6242193954,4.8288410268
H,0,-0.3270564775,0.9375726596,4.845219381

R2:

C,0,-0.0041007218,-0.0160434548,0.0056130035
C,0,0.0044630096,-0.0076725784,1.2142001356
H,0,-0.0023582365,0.0001999324,2.2828851476
C,0,-0.0183254093,-0.0263134059,-1.4218660022
C,0,-1.234277118,-0.0585496638,-2.1178282636
C,0,1.1824826853,-0.0041423605,-2.1434815883
C,0,-1.2446570172,-0.0685216806,-3.5054672711
H,0,-2.1654189396,-0.0754689325,-1.554831858
C,0,1.1644145719,-0.0141657023,-3.5309166452
H,0,2.1247470722,0.0212911371,-1.5987610674
C,0,-0.0474750125,-0.0463859184,-4.2153402191
H,0,-2.1940403559,-0.0939820542,-4.036938891
H,0,2.1023558672,0.003577824,-4.0837039274
H,0,-0.0601607054,-0.0542181022,-5.3036758935

TS1:

N,0,2.3285057508,-1.6621905171,1.6333359797
H,0,3.1366722554,-1.0400465684,1.6940243801
H,0,1.6560233134,-1.3101832095,2.3186604812
N,0,1.6995910102,-1.4077946675,0.3675392779
H,0,2.1762089731,-1.9731275497,-0.3404038743
H,0,0.5048752152,-1.4819104008,0.3717652245
C,0,0.0184218445,0.0272783529,0.0448946647
C,0,1.3551674833,-0.0162183149,-0.0053317042
H,0,2.1793035741,0.6586595677,-0.2525984862
C,0,-0.7942994768,1.2077983774,-0.2073348479
C,0,-1.9769052984,1.0858525466,-0.9526294164

C,0,-0.7295597551,3.1535293772,-1.9505119631
H,0,0.4873104843,1.3918177553,-2.2141149915
C,0,-1.6013467052,3.8380201543,-1.1070791316
H,0,-2.6127454857,3.8202333275,0.7940661506
H,0,-0.4570971678,3.578954586,-2.9152438713
H,0,-2.0119459584,4.8002709994,-1.4090465674

Fy = -20 ($\times 10^{-4}$ au)

R1:

N,0,1.2578624899,-0.20820382,5.2040051214
H,0,1.6100636968,-1.0815812183,4.8061964757
H,0,1.9097105321,0.4801693835,4.8223099629
N,0,0.0166201751,0.0348358258,4.4451523967
H,0,-0.6507297705,-0.6024047644,4.8852504562
H,0,-0.2942869435,0.9451880734,4.7910013471

R2:

C,0,-0.0144408753,-0.0161204152,0.0057508394
C,0,0.0029624878,-0.0073164328,1.2142234268
H,0,0.0330585632,0.000293922,2.2824486034
C,0,-0.0268220303,-0.0261825185,-1.4217076019
C,0,-1.2400308373,-0.0584017353,-2.1222152165
C,0,1.1767292326,-0.0040384544,-2.1390037342
C,0,-1.2453907294,-0.0684069148,-3.5097890169
H,0,-2.1727607309,-0.0756706963,-1.5610118443
C,0,1.1636979074,-0.0140927836,-3.526582718
H,0,2.1174675733,0.021027681,-1.5924973607
C,0,-0.0455677262,-0.046288487,-4.2154079512
H,0,-2.1928463247,-0.0941791318,-4.0458391815
H,0,2.1037327974,0.0033414521,-4.0746841744
H,0,-0.0521396176,-0.0543604455,-5.30379741

TS1:

N,0,2.2780981067,-1.6797825205,1.6443560607
H,0,3.0430957733,-1.0179583012,1.7934754013
H,0,1.536195995,-1.3700144954,2.2785412267
N,0,1.7395400815,-1.3848575155,0.3403880749
H,0,2.3026031378,-1.8876029067,-0.351348425
H,0,0.5685677496,-1.5201416844,0.262986501
C,0,0.0215473545,0.0073316608,-0.0039583661
C,0,1.3619646551,0.0110228596,0.0186530265
H,0,2.176362048,0.7239912709,-0.1356979735
C,0,-0.7977246331,1.1922254344,-0.2280531205
C,0,-2.0109175619,1.0726859456,-0.9204904298

C,0,-0.4672757655,2.4760428722,0.2999045001
C,0,-2.7773031358,2.1888381544,-1.2159039904
H,0,-2.2518399211,0.0994838784,-1.3245168935
C,0,-1.2830121211,3.5746048698,0.0609759917
H,0,0.4360318205,2.5834012128,0.9015327918
C,0,-2.4372207032,3.4393906859,-0.705901331
H,0,-3.6835584079,2.0695550258,-1.8085344931
H,0,-1.0135666413,4.5472961981,0.4727473042
H,0,-3.0750314094,4.301573586,-0.8961278688

IM:

N,0,3.3904394443,-1.1900240225,0.5019943701
H,0,4.0764673308,-0.7395352714,-0.0981999551
H,0,3.3806641109,-0.7197018335,1.4067121146
N,0,2.1304851416,-1.1269563446,-0.1115137287
H,0,1.6455335809,-2.0167963556,-0.0603865596
H,0,-0.5287646333,-0.9410768819,0.0167685321
C,0,-0.000657667,0.0163937817,0.0300989522
C,0,1.3448643649,-0.0024340394,0.0267218437
H,0,1.9297786825,0.9188324539,0.0935563599
C,0,-0.8394669054,1.2060586208,0.0615549111
C,0,-2.2102740615,1.063635708,0.3239617831
C,0,-0.353392274,2.5053177989,-0.1560981479
C,0,-3.0541277088,2.1638762637,0.3854122209
H,0,-2.6122706707,0.0631948589,0.4872953863
C,0,-1.195161282,3.6060501123,-0.0862340713
H,0,0.6973292404,2.6547391066,-0.4049717057
C,0,-2.5516447883,3.4456477716,0.1857971278
H,0,-4.1135658919,2.0171085701,0.5914500655
H,0,-0.7880333557,4.6017585073,-0.2607614211
H,0,-3.2112369676,4.3107567651,0.229647772

TS2:

N,0,2.926068638,-1.7769438302,0.4849495655
H,0,3.4051249129,-2.3838350289,-0.174634182
H,0,3.5535155924,-1.0616983121,0.8515830991
N,0,1.7987053176,-1.2350452759,-0.1148810033
H,0,0.5135071654,-1.4064675251,-0.1773747044
H,0,-0.3881875313,-0.3110047058,0.9991376396
C,0,0.0223075792,0.048215628,0.0480765248
C,0,1.4541083279,0.0311947568,0.0265778425
H,0,2.1911189627,0.8366934229,0.1266320378
C,0,-0.7732608426,1.0736225639,-0.6206173971
C,0,-2.0838845453,1.3567996173,-0.2084876148

C,0,-0.4355019569,2.4638245245,0.2460391652
C,0,-2.8097414072,2.1816840826,-1.1673812604
H,0,-2.3087298201,0.0839847053,-1.2691512395
C,0,-1.2448810525,3.5692501226,0.0229361004
H,0,0.4922851387,2.5715595908,0.8089180373
C,0,-2.4317155081,3.4347161507,-0.6931906863
H,0,-3.7409069562,2.0682897578,-1.7211426903
H,0,-0.9464569091,4.5450110957,0.4039395322
H,0,-3.0628958753,4.3030843222,-0.8737212447

IM:

N,0,3.37369016,-1.2036397575,0.5225512131
H,0,4.0765278218,-0.7553504969,-0.060802009
H,0,3.3302363981,-0.6989377832,1.4091328748
N,0,2.1343655622,-1.136098505,-0.1451991636
H,0,1.6254616279,-2.0083407819,-0.042823168
H,0,-0.5134781024,-0.93550893,0.0488769411
C,0,0.0131448532,0.0240277857,0.0311653451
C,0,1.3559396062,0.00338442,-0.0086408616
H,0,1.9461051208,0.9227462381,0.0148732068
C,0,-0.8336663085,1.2106138757,0.0603729375
C,0,-2.2022089916,1.0596028421,0.3224148462
C,0,-0.3507943983,2.5106897837,-0.1531576359
C,0,-3.0512149107,2.1565652259,0.3864399663
H,0,-2.599432282,0.0562945157,0.4839706149
C,0,-1.196668621,3.60778447,-0.0812997409
H,0,0.7002224304,2.6670448514,-0.3954714166
C,0,-2.5525624761,3.4395986709,0.1897681945
H,0,-4.1103044689,2.0080599858,0.5925271499
H,0,-0.7947308838,4.605719847,-0.2493584968
H,0,-3.2136664473,4.3025893126,0.2374650524

TS2:

N,0,2.9420267578,-1.7482376466,0.5128316806
H,0,3.5106327181,-2.2533111706,-0.1622681782
H,0,3.4865284313,-1.0033132992,0.9488959078
N,0,1.8080561285,-1.2502905606,-0.1328974958
H,0,0.5211839245,-1.4490211824,-0.2154109991
H,0,-0.4190654485,-0.3854812064,0.9456517111
C,0,-0.0013407494,-0.004549154,0.0059931647
C,0,1.4260297977,0.0087810573,0.0115297776
H,0,2.1383843639,0.835279217,0.1150035923
C,0,-0.7943396092,1.0349177638,-0.6496043853
C,0,-2.0832425734,1.3578904757,-0.2040230471

C,0,-0.2625092044,1.7940699279,-1.7105026709
C,0,-2.8459319553,2.3221277352,-0.850597289
H,0,-2.5032584049,0.8007857637,0.6311199547
C,0,-1.0181467302,2.7727116636,-2.3426918751
H,0,0.7396743015,1.5607210076,-2.0739888417
C,0,-2.3163549495,3.0423565929,-1.9187709019
H,0,-3.8636432913,2.5163954217,-0.5134695424
H,0,-0.5956495833,3.3174976106,-3.1866041731
H,0,-2.9155841396,3.797798016,-2.4246782384

P:

N,0,3.5077041357,-0.8033698742,-0.7613569651
H,0,3.8746583393,-1.118825996,-1.6510107061
H,0,3.952058468,0.0619112758,-0.4486801897
N,0,2.143987561,-0.7748353747,-0.7918711355
H,0,-0.3218033496,-0.7548184981,-0.594186901
H,0,-0.2918487421,-0.2206611953,1.0902898222
C,0,0.0475679956,0.0358609551,0.0747555306
C,0,1.5407211581,0.010485604,0.0111003038
H,0,2.094265177,0.7030746899,0.67042565
C,0,-0.5286572336,1.3734279009,-0.3217949785
C,0,-1.4103870735,2.0610752986,0.5101282621
C,0,-0.1871188773,1.9423063604,-1.5510485419
C,0,-1.9476650786,3.2850919599,0.1222503677
H,0,-1.6841510311,1.6258916321,1.4720834154
C,0,-0.7213192898,3.1631108587,-1.9428134307
H,0,0.5035643761,1.4061215758,-2.2031568811
C,0,-1.6048272272,3.8397534833,-1.1054106709
H,0,-2.6388118118,3.8057311908,0.7838186162
H,0,-0.4497173357,3.5884589884,-2.9080971663
H,0,-2.0264041607,4.7959851645,-1.4120664013

Fz = 20 ($\times 10^{-4}$ au)

R1:

N,0,1.3394906893,0.0202804043,5.0759929188
H,0,1.4229663668,-0.9267356854,5.4464776149
H,0,1.9898470911,0.0985487082,4.2992059304
N,0,0.0385889014,0.2857403919,4.5661403344
H,0,-0.4243909011,-0.5595970929,4.231144672
H,0,-0.5172619675,0.6497667539,5.3349542896

R2:

C,0,-0.0090990852,-0.0088796589,0.0056250862
C,0,0.0033711617,-0.0042631221,1.2142061148

C,0,-0.2834735023,1.7407700441,-1.7477734738
C,0,-2.8240668471,2.3570270783,-0.81978751
H,0,-2.4980801191,0.8188368401,0.6491259749
C,0,-1.0170357158,2.7517776399,-2.3547653509
H,0,0.7035009635,1.4777092658,-2.1321133094
C,0,-2.2927465042,3.0649445543,-1.8949670504
H,0,-3.8211214442,2.5951076858,-0.4516749859
H,0,-0.5938287301,3.2935583189,-3.1994575652
H,0,-2.8702822219,3.853599329,-2.3735102277

P:

N,0,3.5247566882,-0.7303762103,-0.7047847311
H,0,3.9194900004,-0.9390697437,-1.6149895012
H,0,3.9044866644,0.1472905866,-0.341598667
N,0,2.1540196553,-0.7522840938,-0.7872123648
H,0,-0.3266568794,-0.7882816661,-0.6795877062
H,0,-0.3692322549,-0.297801048,1.0223460023
C,0,0.0066443942,-0.0143174185,0.0268292639
C,0,1.5013150888,-0.0164397061,0.0234146649
H,0,2.01055714,0.670606971,0.7223351758
C,0,-0.5527706379,1.3354316587,-0.3541972597
C,0,-1.3532583546,2.0656270499,0.5215765299
C,0,-0.255446566,1.8800329792,-1.6055718277
C,0,-1.8537766399,3.3119982646,0.1556935988
H,0,-1.5875880228,1.650942431,1.5031050963
C,0,-0.7546262731,3.1220745966,-1.9756424591
H,0,0.3776405131,1.3133380024,-2.2903534978
C,0,-1.556160855,3.8431332287,-1.0938592785
H,0,-2.4763433589,3.8717710149,0.8517675849
H,0,-0.5164741366,3.5336183875,-2.9552019267
H,0,-1.9447601653,4.8184807154,-1.3807106969

Fz = -20 ($\times 10^{-4}$ au)

R1:

N,0,1.2465984033,-0.4273712958,5.0834791718
H,0,1.7971334264,-0.7980194948,4.314027525
H,0,1.7114098013,0.4209121695,5.4083730391
N,0,-0.0583191022,-0.1666646077,4.5816672788
H,0,-0.7030176805,-0.2375455668,5.3637835579
H,0,-0.1445646682,0.7766922756,4.2025851874

R2:

C,0,-0.0090390638,-0.0232902699,0.0057299836
C,0,0.0035387455,-0.0106656128,1.214247481

H,0,0.0151305578,-0.0212780774,2.2827724922
C,0,-0.0226045101,-0.0156582,-1.4218458925
C,0,-1.2371504781,-0.0505531334,-2.1199988393
C,0,1.1795474801,0.0039893453,-2.1414361967
C,0,-1.2450377852,-0.0662404919,-3.5075343855
H,0,-2.1689072893,-0.0726291997,-1.5578143682
C,0,1.1639988671,-0.0117195085,-3.5288809213
H,0,2.1211730345,0.024309971,-1.5958522851
C,0,-0.0465602348,-0.0467974872,-4.2153919034
H,0,-2.1932783162,-0.1012046674,-4.0410290237
H,0,2.1031022267,-0.0032627479,-4.0793177591
H,0,-0.056035939,-0.066207982,-5.3036154584

TS1:

N,0,2.3388736625,-1.653025541,1.6276515647
H,0,3.1422430962,-1.0224877948,1.6738631274
H,0,1.6672120463,-1.2809886924,2.3044236975
N,0,1.7016149754,-1.406097378,0.3608842693
H,0,2.1877016598,-1.9588670446,-0.3507719441
H,0,0.5164353042,-1.5042649596,0.3757457032
C,0,-0.0014754662,0.0120855731,0.0663653971
C,0,1.3357835014,-0.0167576446,0.0003751572
H,0,2.1490031104,0.6654510493,-0.2609356285
C,0,-0.8128040065,1.195283257,-0.1836098419
C,0,-1.9879095687,1.0807894584,-0.9407364304
C,0,-0.4784755347,2.4614962429,0.3230196351
C,0,-2.7717051223,2.1918187263,-1.2211431533
H,0,-2.2648772516,0.0973320771,-1.3190915882
C,0,-1.2787904382,3.5677348784,0.0685356495
H,0,0.4220718557,2.5634532614,0.9299573886
C,0,-2.4235182798,3.4408861641,-0.7136684207
H,0,-3.6664386776,2.0828188665,-1.8324617796
H,0,-1.0009338288,4.540861267,0.4727569883
H,0,-3.0432226775,4.3107823334,-0.9250621012

IM:

N,0,3.3943498446,-1.1925446683,0.4862027611
H,0,4.0705260494,-0.7842841916,-0.1550227126
H,0,3.4082379036,-0.65798096,1.3549889669
N,0,2.1217663876,-1.1413587263,-0.106804566
H,0,1.629110473,-2.0222922941,-0.0052594815
H,0,-0.5266930151,-0.937431612,0.0863041578
C,0,0.0030943516,0.0196324317,0.0665824259
C,0,1.3469084813,-0.0050315656,0.0197773379

H,0,0.0150997524,0.0217314882,2.2824608516
C,0,-0.0223705958,-0.0368476948,-1.4216881732
C,0,-1.2369669658,-0.0665615417,-2.1200053833
C,0,1.1797305663,-0.0120497998,-2.1412025892
C,0,-1.244964029,-0.0708217508,-3.5076211263
H,0,-2.1689646939,-0.078805344,-1.5579079374
C,0,1.1640718796,-0.0163947969,-3.5287236217
H,0,2.1211077207,0.018179849,-1.5956663569
C,0,-0.046536796,-0.0458452248,-4.2153999708
H,0,-2.1935296552,-0.0871788518,-4.0414531472
H,0,2.1028627896,0.0104269401,-4.0790938563
H,0,-0.0563899646,-0.04227235,-5.303789494

TS1:

N,0,2.2611782449,-1.6902401107,1.6500002011
H,0,3.0244639122,-1.0334627436,1.824159943
H,0,1.5107763037,-1.4083233538,2.2858652517
N,0,1.7410077609,-1.3843457195,0.3446141816
H,0,2.303358423,-1.8943033525,-0.3421171128
H,0,0.5622362134,-1.5001517277,0.2478546501
C,0,0.0432643011,0.021496988,-0.0304535648
C,0,1.3823600946,0.0150284084,0.016007367
H,0,2.2049545712,0.7241167729,-0.1132024006
C,0,-0.7783213598,1.2043440974,-0.2549349438
C,0,-2.0012086526,1.0761202939,-0.9293153042
C,0,-0.421043779,2.478819837,0.2157091466
C,0,-2.8171457201,2.1766785246,-1.1562041272
H,0,-2.2978364377,0.0837995741,-1.2681185318
C,0,-1.2458626249,3.5764374422,0.010592
H,0,0.51205317,2.5932349766,0.7681979857
C,0,-2.4447307665,3.4320567815,-0.6833605657
H,0,-3.7614493709,2.0520526357,-1.6852816331
H,0,-0.9534445427,4.5526218892,0.3959315262
H,0,-3.0938213807,4.2923228861,-0.839846379

IM:

N,0,3.3643220432,-1.2037816317,0.5485957184
H,0,4.0822006118,-0.7055203309,0.0285836772
H,0,3.2807028578,-0.7796090974,1.4731189901
N,0,2.1496573563,-1.1119028448,-0.1564784888
H,0,1.6501188087,-1.9952019443,-0.1272629575
H,0,-0.512180492,-0.9396694234,-0.0500250193
C,0,0.0103868083,0.0210249596,-0.0175417367
C,0,1.3545254418,0.0101963265,0.0004101709

H,0,1.9386582769,0.9137745874,0.0315988049
C,0,-0.837732456,1.209196434,0.0851849953
C,0,-2.2134877971,1.0626006677,0.3136783601
C,0,-0.3476981532,2.5099240661,-0.1116380841
C,0,-3.0614345425,2.1610860197,0.3563388492
H,0,-2.6184218018,0.0598072289,0.4563919124
C,0,-1.1930908674,3.6084512919,-0.0610529282
H,0,0.7087986807,2.6645675575,-0.3304346403
C,0,-2.5561941793,3.4438120657,0.1739819945
H,0,-4.1267927868,2.0124607039,0.5277361481
H,0,-0.7846587858,4.6050674226,-0.2236922926
H,0,-3.2182803736,4.3073891109,0.1979438412

TS2:

N,0,2.9373679011,-1.7658039833,0.4927186023
H,0,3.4363577834,-2.3350052156,-0.1868055759
H,0,3.5440291421,-1.0250039502,0.8460112989
N,0,1.7938273079,-1.2452149523,-0.1129412548
H,0,0.50817526,-1.4248410833,-0.1693155643
H,0,-0.4003053126,-0.3301018292,0.9973191871
C,0,0.0097666762,0.0314700202,0.0468031604
C,0,1.4389405123,0.0201019285,0.0244471131
H,0,2.1701162275,0.8333701821,0.1019852751
C,0,-0.783504147,1.0606128033,-0.6219754746
C,0,-2.089733731,1.3558248349,-0.2074925326
C,0,-0.264861607,1.7760950431,-1.7107483345
C,0,-2.8410990144,2.3320491654,-0.8467509464
H,0,-2.5147665229,0.8026621955,0.6317005438
C,0,-1.0084840721,2.7662156335,-2.3390249687
H,0,0.7336096503,1.5322142335,-2.0771567869
C,0,-2.3027667219,3.0491796275,-1.9122254582
H,0,-3.8565138798,2.5386369667,-0.5103503725
H,0,-0.5807374675,3.309415265,-3.180485981
H,0,-2.8916983647,3.8141181648,-2.4149337005

P:

N,0,3.5153158404,-0.8471494016,-0.741406871
H,0,3.8527677595,-1.2334592246,-1.6157636708
H,0,3.9421638773,0.0627156955,-0.5530004822
N,0,2.1467246905,-0.839393072,-0.7377874778
H,0,-0.3212526994,-0.7550366227,-0.5513098632
H,0,-0.2472268359,-0.1813941483,1.1181552466
C,0,0.064539699,0.0530096068,0.0874497612
C,0,1.5554700979,0.0277886445,-0.0148246489

H,0,1.9323779987,0.9326586273,0.100604104
C,0,-0.8359112488,1.206732516,0.0301806749
C,0,-2.1954410417,1.0603237083,0.3404345351
C,0,-0.3600167264,2.5042280791,-0.2133301921
C,0,-3.0387610035,2.1594529558,0.4292308451
H,0,-2.5868269993,0.0600105384,0.5297138136
C,0,-1.2006553278,3.6040322501,-0.1163879324
H,0,0.681194376,2.6531248475,-0.4994050553
C,0,-2.5453922892,3.4408571938,0.2065590691
H,0,-4.0881904212,2.0140442486,0.68141208
H,0,-0.8024700085,4.6004420969,-0.3042572576
H,0,-3.2026750541,4.3054024946,0.2786508113

TS2:

N,0,2.9316124819,-1.7577742366,0.5066436757
H,0,3.4871576268,-2.2990976276,-0.1494349645
H,0,3.491752353,-1.0376723575,0.961963477
N,0,1.8148472805,-1.2395628243,-0.1368167464
H,0,0.5287852613,-1.4319639032,-0.2296801827
H,0,-0.4095141692,-0.3731449229,0.9421621896
C,0,0.0102495825,0.0090080346,0.0040458384
C,0,1.4400607586,0.0195186533,0.0143566936
H,0,2.1559423988,0.8391220553,0.1445224108
C,0,-0.784755824,1.0466050999,-0.6495768941
C,0,-2.0767423207,1.3603372914,-0.2038189939
C,0,-0.2823390675,1.7558945768,-1.7499608227
C,0,-2.8278440508,2.3501552017,-0.8212648208
H,0,-2.4853825388,0.819776879,0.6508506244
C,0,-1.0274590641,2.7568409338,-2.3598426159
H,0,0.7073405375,1.500999001,-2.1331709783
C,0,-2.3060139689,3.0594288673,-1.9005167472
H,0,-3.826294705,2.578427095,-0.4504509425
H,0,-0.61022485,3.2990283895,-3.2080746865
H,0,-2.893458102,3.8400688435,-2.381157284

P:

N,0,3.5209524938,-0.6991951671,-0.7125648586
H,0,3.9437132107,-0.8372440231,-1.622668289
H,0,3.9124543871,0.1187249896,-0.2404879428
N,0,2.1559664992,-0.6908002312,-0.8275425403
H,0,-0.3250049697,-0.7824146152,-0.7164537393
H,0,-0.3995286918,-0.3243107718,0.9927892044
C,0,-0.0033558252,-0.0238328397,0.0111176552
C,0,1.4915291811,-0.0329747947,0.039244353

H,0,2.117465401,0.7993138772,0.5424178745
C,0,-0.5234695311,1.3831171644,-0.3161094571
C,0,-1.4396346131,2.0452090172,0.4994647766
C,0,-0.1596514243,1.9723012003,-1.5289597686
C,0,-1.9881684852,3.2638619563,0.1115928044
H,0,-1.7303460273,1.5941982908,1.4495831643
C,0,-0.7030828225,3.1898338023,-1.9196196123
H,0,0.5561404446,1.4586414655,-2.171799816
C,0,-1.6205420945,3.8403497606,-1.0988074368
H,0,-2.7060843138,3.7652117993,0.7593650629
H,0,-0.4114004223,3.6330278244,-2.8703292539
H,0,-2.0479125409,4.7936283642,-1.404952332

Fx = -60 ($\times 10^{-4}$ au)

R1:

N,0,1.2605711906,-0.1888214326,5.1951760268
H,0,1.5892240667,-1.0909560954,4.8465304711
H,0,1.9278494011,0.4703175347,4.7908170613
N,0,0.0195003401,0.0542367676,4.4360447468
H,0,-0.6330881484,-0.6134876464,4.8539699076
H,0,-0.31481585,0.9367148722,4.8313787863

R2:

C,0,-0.0091240299,-0.0161007872,0.0059876357
C,0,0.0034389081,-0.0072328022,1.2140442945
H,0,0.014462851,-0.0000961774,2.284627023
C,0,-0.0224500865,-0.0261047397,-1.4198576179
C,0,-1.2362281292,-0.0584024231,-2.1207080305
C,0,1.1788893073,-0.0039308477,-2.1419741303
C,0,-1.2441543228,-0.0684565838,-3.5084657215
H,0,-2.1670156421,-0.0756306802,-1.5571373592
C,0,1.1633576173,-0.0140183646,-3.5296161132
H,0,2.1192831715,0.0211958814,-1.5948728907
C,0,-0.0464766398,-0.0463068166,-4.2178998461
H,0,-2.1950691918,-0.0943774885,-4.0393299372
H,0,2.1048849785,0.0035649111,-4.0772768385
H,0,-0.0561497917,-0.0544980813,-5.3076324681

TS1:

N,0,2.3625916879,-1.647924097,1.6301698239
H,0,3.2702699775,-1.1815777816,1.5739121645
H,0,1.8216360901,-1.1356502803,2.3292058112
N,0,1.6701134973,-1.4111955504,0.3984123271
H,0,2.1096974165,-1.9911733976,-0.3215202024

H,0,1.9910931185,0.5703456446,0.8173102903
C,0,-0.5537529764,1.3315074802,-0.3627497562
C,0,-1.3199500799,2.0800745216,0.5280618164
C,0,-0.2853063772,1.8609785427,-1.6272231562
C,0,-1.8158037546,3.328985258,0.1640717858
H,0,-1.5321948076,1.6774448534,1.5191471904
C,0,-0.7819739428,3.1040951234,-1.996250072
H,0,0.3229960957,1.2788484392,-2.3215723981
C,0,-1.5500857842,3.8433251947,-1.0995814741
H,0,-2.4119471267,3.9016065341,0.8727295644
H,0,-0.5692556244,3.501322774,-2.9881333584
H,0,-1.9387290256,4.8192890873,-1.3858862749

Fx = -180 ($\times 10^{-4}$ au)

R1:

N,0,1.259063778,-0.1761852088,5.1728399006
H,0,1.5759454615,-1.1007042212,4.8813768391
H,0,1.9433213472,0.4686757674,4.7778098819
N,0,0.0161357418,0.0680107894,4.4171177263
H,0,-0.6187507228,-0.6155227384,4.839909704
H,0,-0.3264746058,0.9237296116,4.8648629482

R2:

C,0,-0.0091305576,-0.0007371399,0.0076805815
C,0,0.0017849554,0.0149727349,1.217438081
H,0,0.0111038244,0.028159017,2.2938977027
C,0,-0.021918339,-0.020088466,-1.4117340783
C,0,-1.2349002738,-0.0571863501,-2.1223940114
C,0,1.178431473,-0.0033787655,-2.1439968002
C,0,-1.2423786968,-0.0770879193,-3.5102873407
H,0,-2.1643249542,-0.0710006382,-1.5565892106
C,0,1.1624695261,-0.0233145403,-3.5317927707
H,0,2.1175767674,0.0246698857,-1.5950075215
C,0,-0.0460859853,-0.0601440614,-4.2260986666
H,0,-2.1987217543,-0.1076424008,-4.0358946896
H,0,2.1095608201,-0.0103789795,-4.074731718
H,0,-0.0558178152,-0.0772373866,-5.3206015576

TS1:

N,0,2.3521721167,-1.6825615744,1.6479119182
H,0,3.3528487873,-1.5257385876,1.5058491761
H,0,2.0336300634,-0.9972802041,2.3318103471
N,0,1.6448757161,-1.4028749368,0.4397997372
H,0,2.076932328,-1.9616551529,-0.3019174095

H,0,0.4576607991,-1.4637271121,0.4451412587
C,0,-0.0150204524,0.0132781968,0.0852293241
C,0,1.3198495981,-0.0272804178,0.0034350247
H,0,2.1281732887,0.6498764294,-0.2797588869
C,0,-0.824178929,1.1937001775,-0.1815810051
C,0,-1.9772738715,1.0903430393,-0.9754159939
C,0,-0.5135411701,2.4542827333,0.355771637
C,0,-2.7587197204,2.2028659891,-1.2574323773
H,0,-2.235060548,0.1124221873,-1.3825595413
C,0,-1.3087450231,3.5622054068,0.093753858
H,0,0.3703481185,2.5516257228,0.9858870583
C,0,-2.4318699478,3.4461378537,-0.7213079837
H,0,-3.6337067822,2.0999426864,-1.900614743
H,0,-1.0375669336,4.5294530852,0.5157735511
H,0,-3.0438700957,4.3207001292,-0.9404021052

IM:

N,0,3.4455629325,-1.1849410672,0.3763229118
H,0,4.0176527632,-0.8309397734,-0.3859872506
H,0,3.6351169163,-0.6548324123,1.2244589051
N,0,2.0958362254,-1.1429744895,0.0333162857
H,0,1.6281524538,-2.0346534513,0.1467537801
H,0,-0.5457896783,-0.9361634447,0.1693126175
C,0,-0.015263035,0.0198685154,0.1276226086
C,0,1.3356206529,-0.0108188993,0.09399383
H,0,1.9320395328,0.9041641206,0.0853260337
C,0,-0.8491555909,1.2074010746,0.1146530597
C,0,-2.2390832977,1.0677793863,0.2681528571
C,0,-0.3517527658,2.5138149121,-0.0430682297
C,0,-3.0853334747,2.1681883354,0.2743688037
H,0,-2.6515993404,0.064515923,0.3894241611
C,0,-1.1965927938,3.6125301115,-0.0310720447
H,0,0.7163631698,2.6733322592,-0.1859597167
C,0,-2.5724060809,3.4528116948,0.1276354903
H,0,-4.1591058816,2.0187439064,0.3977797903
H,0,-0.7725356061,4.6084428489,-0.153332927
H,0,-3.2307621016,4.3205774493,0.1331068538

TS2:

N,0,2.9398409563,-1.7725163631,0.4496610174
H,0,3.3961372976,-2.3763060516,-0.2288220832
H,0,3.5862374961,-1.0724413883,0.8129133801
N,0,1.8004488015,-1.2190459828,-0.0965071115
H,0,0.5313114563,-1.4150870011,-0.1669492175

H,0,0.37824755,-1.3982924299,0.4381379198
C,0,-0.0075602769,0.0328186189,0.0854184031
C,0,1.3306130822,-0.0073388798,0.0599442486
H,0,2.144373034,0.678032472,-0.1809876677
C,0,-0.8256580736,1.2008151721,-0.1926105543
C,0,-1.9778884208,1.0964000169,-0.995313666
C,0,-0.5409963923,2.4670849461,0.3560756343
C,0,-2.7764627204,2.2006180626,-1.2674940715
H,0,-2.2060317597,0.1222766598,-1.4316809497
C,0,-1.3449689392,3.567148955,0.0934167334
H,0,0.3472083453,2.5778576069,0.9769630657
C,0,-2.4712383244,3.4462060179,-0.7211423288
H,0,-3.6382467631,2.0933958135,-1.9349824435
H,0,-1.0643702069,4.5371177011,0.5031708831
H,0,-3.0766921455,4.3242747228,-0.9562699756

IM:

N,0,3.5000402756,-1.2364787412,0.0492010642
H,0,3.9235895821,-0.9109767224,-0.8152959623
H,0,3.9408239512,-0.8240032434,0.8668105995
N,0,2.1201596475,-1.12524414,0.0571257416
H,0,1.6388302011,-2.0170524671,0.1170335626
H,0,-0.5025111922,-0.9352326981,0.0720426939
C,0,0.0166870502,0.0265727071,0.0020879151
C,0,1.3873512405,-0.0032784382,-0.0074765829
H,0,1.9907190091,0.9045936195,-0.0670270177
C,0,-0.820037435,1.1908839546,-0.0658715233
C,0,-2.2276312937,1.0485909229,-0.0240180326
C,0,-0.3347458405,2.5164701238,-0.1771161507
C,0,-3.0816854921,2.1421785701,-0.0862083335
H,0,-2.64007578,0.0395438889,0.0623858845
C,0,-1.1892286056,3.6015928426,-0.2384425175
H,0,0.7383159241,2.6956709172,-0.2166679489
C,0,-2.5782721819,3.4360793066,-0.194440714
H,0,-4.1662754774,1.977484214,-0.0482149605
H,0,-0.7571190744,4.5981274298,-0.3230093476
H,0,-3.2410155485,4.3025795231,-0.24163992

TS2:

N,0,2.9783577588,-1.8604549098,0.1490034968
H,0,3.2876272096,-2.5286726906,-0.5516009271
H,0,3.7310033613,-1.2410260564,0.4524741953
N,0,1.8272224073,-1.2387411415,-0.2021791131
H,0,0.5733688353,-1.4379493139,-0.2921155605

H,0,-0.3967406767,-0.2820711369,1.0323573011
C,0,0.0054499477,0.0386597021,0.0634713729
C,0,1.4467595948,0.0384299028,0.0488643115
H,0,2.173696813,0.8479581192,0.1731269727
C,0,-0.7841628586,1.0609322823,-0.6142364918
C,0,-2.0985738434,1.3524428367,-0.2152527875
C,0,-0.2661631353,1.7784898704,-1.7047960336
C,0,-2.8516623225,2.3204725128,-0.8650573728
H,0,-2.5213579075,0.8080533581,0.6313680858
C,0,-1.0122382029,2.7588392514,-2.3438428286
H,0,0.7415520029,1.551291076,-2.054948135
C,0,-2.313315545,3.0367746692,-1.9314536148
H,0,-3.8677558672,2.5292284664,-0.5263668615
H,0,-0.5735536537,3.3068530684,-3.1768207617
H,0,-2.8981923532,3.8050378081,-2.4359291419

P:

N,0,3.4845821919,-0.8489285773,-0.8151308795
H,0,3.8442322947,-1.194976477,-1.6952061292
H,0,3.9988361468,-0.0435757911,-0.4565395435
N,0,2.1352414541,-0.7642168556,-0.812509939
H,0,-0.3019756569,-0.733103197,-0.5374930818
H,0,-0.2427071471,-0.1604127735,1.1350807296
C,0,0.0792074023,0.0732631848,0.1072520525
C,0,1.5717553812,0.032123864,0.0128224974
H,0,2.1530659519,0.6989220088,0.6710919639
C,0,-0.5213339768,1.394473483,-0.3083080206
C,0,-1.4482308962,2.055515892,0.4963067642
C,0,-0.162042996,1.9751899292,-1.5269072078
C,0,-2.0095706642,3.2641668688,0.0942759595
H,0,-1.7234551888,1.6182828469,1.4576106934
C,0,-0.719768396,3.1807048575,-1.9332772455
H,0,0.5746000956,1.4687839187,-2.1511648003
C,0,-1.6477999069,3.8302546084,-1.1227342837
H,0,-2.7212797078,3.7732223625,0.7443398052
H,0,-0.4182969982,3.6226487686,-2.8817648334
H,0,-2.0732440335,4.7834359083,-1.4343868313

Solvent = C₆H₆

R1:

N,0,1.5151024348,1.3191834461,2.1516369748
H,0,2.316072233,1.5268696083,1.5512062211
H,0,0.7482344941,1.7799852322,1.6568089709
N,0,1.267323905,-0.1140277586,1.9094518745

H,0,-0.391273653,-0.2464779672,1.0172267338
C,0,0.013581827,-0.0079485206,0.0235484978
C,0,1.48317513,-0.0013601529,0.0174503502
H,0,2.2059486821,0.7898165843,0.2340803666
C,0,-0.7615440577,0.9852460977,-0.6969446412
C,0,-2.1045640743,1.2656047723,-0.3649242677
C,0,-0.2228285818,1.6982594819,-1.7897792845
C,0,-2.8525077453,2.2002123941,-1.0709699692
H,0,-2.5450485224,0.7454528942,0.4907017062
C,0,-0.9647636335,2.6397802881,-2.4831618089
H,0,0.8088054074,1.5055613677,-2.0848947691
C,0,-2.2935088213,2.9013303151,-2.1380250538
H,0,-3.8856955911,2.4065669385,-0.7640584235
H,0,-0.4916752668,3.1821075701,-3.3010210285
H,0,-2.8650766713,3.6582692488,-2.6786644997

P:

N,0,3.3993365933,-0.9061156511,-0.7129247771
H,0,3.8505900702,-1.6598954121,-1.211545249
H,0,3.968494612,-0.3293048088,-0.0957484894
N,0,2.085032926,-0.8837059927,-0.7006337902
H,0,-0.3313209152,-0.8937345883,-0.649114638
H,0,-0.4817190406,-0.2051594374,0.9718297718
C,0,-0.0464197829,-0.0271214615,-0.0296596212
C,0,1.4487553729,-0.0210822913,0.0136660559
H,0,1.961990028,0.7155962162,0.648782723
C,0,-0.6961984407,1.2159914988,-0.5993044042
C,0,-2.0099169278,1.5538686967,-0.2595586938
C,0,-0.0138442075,2.047441876,-1.4908765342
C,0,-2.6284408769,2.6795031282,-0.7960553544
H,0,-2.5433266378,0.9215864836,0.4569137614
C,0,-0.6224299959,3.179151328,-2.0234939547
H,0,1.0155339674,1.8023128256,-1.7518143237
C,0,-1.933752622,3.5001173955,-1.6813384515
H,0,-3.6521240855,2.9345279043,-0.4997627287
H,0,-0.0551533561,3.8197776165,-2.6964332342
H,0,-2.3968189108,4.4018578937,-2.0856569278

Solvent = C₆H₆; Fx = -60 (×10⁻⁴ au)

R1:

N,1.264850310085,-0.175940268369,5.189207268799
H,1.577231964183,-1.095563529205,4.872608613901
H,1.944617211845,0.460659443640,4.769632931972
N,0.020469091139,0.068061022167,4.437185819670

H,0,2.0344882038,-0.5748091053,2.4038249433
H,0,0.4666967292,-0.3218214229,2.5102910154

R2:

C,0,1.2358519588,-0.8511618819,0.0382519624
C,0,2.2731124595,-1.230964222,0.5303501597
H,0,3.1919846807,-1.5688404465,0.963959791
C,0,0.0116487956,-0.4024847473,-0.5446136235
C,0,-0.9806877478,0.1832882678,0.2537025143
C,0,-0.2096447893,-0.5429862588,-1.9217395791
C,0,-2.1683668449,0.6185816727,-0.3173582454
H,0,-0.8069539827,0.2902039035,1.3230135335
C,0,-1.3999878646,-0.1045224451,-2.4850466556
H,0,0.5627370397,-0.9978511119,-2.5394800499
C,0,-2.3809983828,0.476416725,-1.6858563327
H,0,-2.9339949647,1.0713931029,0.3101696091
H,0,-1.563415599,-0.2161232933,-3.5555098411
H,0,-3.3133927584,0.820219735,-2.1304182428

TS1:

N,0,-2.8689945989,-5.031954028,3.9278185617
H,0,-2.8615521233,-6.048540338,4.0348572382
H,0,-2.5340033707,-4.8532426716,2.9777457911
N,0,-4.2442107405,-4.6221911642,3.9013629595
H,0,-4.5738273556,-4.5555404551,4.8685626395
H,0,-4.4957415826,-3.6777622973,3.1924668283
C,0,-5.4486218223,-4.278315007,2.0549373383
C,0,-5.166076875,-5.2494734633,2.9332845861
H,0,-5.4418740813,-6.2946040769,3.0966974333
C,0,-6.2947393025,-4.435116935,0.8774809027
C,0,-7.1340881016,-3.3828043496,0.4802209409
C,0,-6.2775010336,-5.5935662554,0.0825706045
C,0,-7.9488095719,-3.4951941833,-0.638880478
H,0,-7.1351844235,-2.4702913441,1.0763974654
C,0,-7.073534175,-5.6979373016,-1.0509459367
H,0,-5.6136677984,-6.4131212213,0.3601673446
C,0,-7.9187295927,-4.6519987836,-1.4137256136
H,0,-8.5999301051,-2.6677822046,-0.9188305894
H,0,-7.0383747952,-6.6035797574,-1.6559165228
H,0,-8.5437025504,-4.7335991626,-2.3017434936

IM:

N,0,3.0956343586,-0.5828869037,2.8998928747
H,0,3.0780654576,-1.5796461039,3.1059658672

H,-0.624303398109,-0.622342593358,4.830572924054
H,-0.333624179174,0.933129924831,4.854709441604

R2:

C,-0.009257054407,-0.015936343575,0.006027167336
C, 0.003765632462,-0.007532563326,1.215496345366
H, 0.015146675446,-0.000031001050,2.291409862412
C,-0.022664307049,-0.026103263509,-1.420792361638
C,-1.238410585398,-0.058391044616,-2.120612355620
C, 1.180742323554,-0.003884018311,-2.141712315872
C,-1.245771133791,-0.068614627326,-3.509450205239
H,-2.170612579883,-0.075490626073,-1.558497225780
C, 1.164887128278,-0.013940874955,-3.530427049412
H, 2.122388747844,0.021264672883,-1.595865474772
C,-0.046463622015,-0.046355640177,-4.219190415738
H,-2.197166125319,-0.094623999791,-4.039761794712
H, 2.107076636053,0.003722633089,-4.077270898758
H,-0.056012735774,-0.054478303263,-5.309465277574

TS1:

N,2.369552692412,-1.673051360862,1.632563300384
H,3.333208047089,-1.357179925082,1.491258236138
H,1.968200059781,-1.049142291825,2.334750952749
N,1.643022828009,-1.415780346385,0.428466131646
H,2.083162692760,-1.958838019056,-0.321242702775
H,0.370208959843,-1.412550923802,0.433027463000
C,-0.018001151120,0.013432756252,0.093080530147
C,1.320005426314,-0.027079436173,0.066964053504
H,2.129669905792,0.668456973079,-0.158848578470
C,-0.827388194144,1.192856959034,-0.188298461740
C,-1.977879857099,1.090842884702,-0.990643127682
C,-0.524201273608,2.456817586170,0.352693410984
C,-2.764710236366,2.202208191724,-1.272209919706
H,-2.231074972141,0.116342574275,-1.411857466481
C,-1.320046484043,3.563823487403,0.085257248825
H,0.357428967954,2.560411336632,0.985169027382
C,-2.443653192889,3.446874925635,-0.732743500901
H,-3.634627237117,2.096752060152,-1.922558967269
H,-1.047751629874,4.531243489722,0.506352938119
H,-3.054338352855,4.321864078057,-0.955081565244

IM:

N,3.473039500324,-1.187595595441,0.251664324694
H,3.867124047055,-0.772534281661,-0.592703499399

H,0,3.6519559428,-0.4434042616,2.055468384
N,0,1.775072696,-0.1414755205,2.7002490638
H,0,1.6079070568,0.7507607157,3.1548997249
H,0,-0.0552404456,1.3915548495,1.5153683728
C,0,0.212605109,0.4876704483,0.960658108
C,0,1.1684405244,-0.3100531553,1.4733773667
H,0,1.51239046,-1.204831246,0.9487840386
C,0,-0.5063835562,0.2695206808,-0.2873344681
C,0,-1.324117137,1.2936672737,-0.7892395029
C,0,-0.4255395067,-0.9186207829,-1.0323924214
C,0,-2.0135649444,1.1484781625,-1.9859285693
H,0,-1.4087801333,2.2230555202,-0.2242088598
C,0,-1.1087422726,-1.0609432057,-2.2313591162
H,0,0.1720656257,-1.7508906897,-0.6603923506
C,0,-1.9080967415,-0.0291346909,-2.7191095764
H,0,-2.638609542,1.9638035827,-2.348360452
H,0,-1.0254759925,-1.994627904,-2.786617678
H,0,-2.4471399591,-0.1463677691,-3.6576328061

TS2:

N,0,2.8157239149,-0.6709747284,3.0809071397
H,0,2.768040162,-1.4840261935,3.6909227202
H,0,3.6339227396,-0.7287368532,2.4732400665
N,0,1.6364496939,-0.578900216,2.3505489711
H,0,0.5110090933,0.0630907078,2.3284055869
H,0,0.5552048465,1.4934776039,1.1582401036
C,0,0.4355822889,0.4545196816,0.828087835
C,0,1.614780369,-0.3274863036,1.05677129
H,0,2.4022878211,-0.666311468,0.3745880116
C,0,-0.4147072232,0.2792128356,-0.3475490497
C,0,-1.2265827719,1.3224829192,-0.818624579
C,0,-0.4594045649,-0.9432750062,-1.0356302488
C,0,-2.036235553,1.1556573921,-1.9335376451
H,0,-1.2099165801,2.2799144112,-0.2955012447
C,0,-1.2561237405,-1.1055586892,-2.1617950173
H,0,0.1354120606,-1.7807593469,-0.6669612266
C,0,-2.0522068717,-0.0581201112,-2.6174439965
H,0,-2.6565237013,1.9829297718,-2.2771121058
H,0,-1.2661939757,-2.0633132185,-2.6813648726
H,0,-2.6847130077,-0.1880831885,-3.4940267384

P:

N,0,3.0109665293,-0.994728226,2.3379771585
H,0,3.0939695032,-1.9601412303,2.6386030214

H,3.808718075950,-0.652789385774,1.052710261431
N,2.078203132843,-1.141660571559,0.197277886104
H,1.623369399767,-2.045724895327,0.270730152531
H,-0.553956421261,-0.945563892938,0.265468573980
C,-0.026905934443,0.011167918321,0.199622670469
C,1.337537960501,-0.019150283586,0.171404539165
H,1.937466502851,0.892215589195,0.122514383081
C,-0.849295104516,1.196125241203,0.156068722381
C,-2.253364741555,1.065446795808,0.231375399082
C,-0.343851076272,2.511121712048,0.039015978671
C,-3.095843383408,2.169965955152,0.194927919946
H,-2.676077055905,0.062600070324,0.323673696283
C,-1.187921558509,3.609541984711,0.003267975168
H,0.731284198164,2.673857439789,-0.025369634641
C,-2.575239652593,3.457312220027,0.079962859000
H,-4.175990859558,2.020191599752,0.257588681614
H,-0.751684559142,4.604033703097,-0.088071887484
H,-3.229649469880,4.328283677024,0.051675997122

TS2:

N,2.950752597676,-1.786684886308,0.328979442660
H,3.273663111290,-2.414205330161,-0.406082863774
H,3.677727016930,-1.106848942987,0.564894894560
N,1.782243488406,-1.180855051627,-0.046954528298
H,0.524175960157,-1.371519692747,-0.114950400667
H,-0.408024862694,-0.166113737939,1.160607501143
C,-0.012060934887,0.069402893368,0.163394367857
C,1.451426627993,0.063231425676,0.146479559991
H,2.187083589910,0.852087195270,0.324836847802
C,-0.781340019172,1.075683279664,-0.553041139936
C,-2.123604961772,1.348384302677,-0.219269437688
C,-0.236151943538,1.793265336190,-1.637650455978
C,-2.872563155108,2.283964391877,-0.923139135612
H,-2.570852098348,0.814043503354,0.622280858045
C,-0.980843484923,2.737271963685,-2.330445581364
H,0.796428181015,1.601050854799,-1.932561859891
C,-2.309419254976,2.991897249489,-1.984884901308
H,-3.906973505384,2.474955427400,-0.628862803911
H,-0.514960627709,3.280912559356,-3.152012224092
H,-2.888987724676,3.736072259275,-2.530838139177

P:

N,3.463299535027,-0.928948319651,-0.853086251131
H,3.785843887434,-1.281196834514,-1.748527026530

H,0,3.5463349624,-0.8358732999,1.4810900098
N,0,1.6850634121,-0.6544395724,2.243211123
H,0,-0.6342945847,0.2049502007,2.0851428182
H,0,-0.1218544904,1.7989185144,1.5096446368
C,0,-0.0569988162,0.7195454241,1.3035386908
C,0,1.3614924448,0.2613338694,1.4167804595
H,0,2.1046456934,0.723447178,0.7440691562
C,0,-0.6343690445,0.4349309449,-0.0622088714
C,0,-1.0604072301,1.4635248022,-0.9011724253
C,0,-0.727637402,-0.8833974411,-0.5162911272
C,0,-1.5732676023,1.1849408522,-2.165288882
H,0,-0.9904759889,2.4964520524,-0.5576041031
C,0,-1.241139687,-1.1659216061,-1.7758520179
H,0,-0.3918160721,-1.6926927778,0.1342971529
C,0,-1.6641785211,-0.1303240335,-2.6062051812
H,0,-1.9010200503,2.0010054255,-2.8078084792
H,0,-1.3110270797,-2.1991059647,-2.1132872266
H,0,-2.064712976,-0.350129112,-3.5946149133

Substituent = -CF₃:

R1:

N,0,1.515169,1.319194,2.153587
H,0,2.31523,1.525012,1.551515
H,0,0.748528,1.777914,1.656703
N,0,1.267146,-0.113972,1.907788
H,0,2.034352,-0.572813,2.403443
H,0,0.467493,-0.319955,2.510184

R2:

C,0,1.2374829054,-0.8375224089,0.0341319378
C,0,2.2771020531,-1.209780553,0.5244378854
H,0,3.1971420879,-1.5420801137,0.9558382139
C,0,0.0099149957,-0.3991183032,-0.545780529
C,0,-0.9910688257,0.1653969581,0.2560433943
C,0,-0.2099834573,-0.532854566,-1.9234112299
C,0,-2.1847856647,0.5857517159,-0.3083189642
H,0,-0.8205764376,0.2653995994,1.3257673148
C,0,-1.4045339468,-0.1117866985,-2.4849446269
H,0,0.5669513453,-0.9735331431,-2.5443819688
C,0,-2.3939049319,0.4449104859,-1.6777681349
H,0,-2.9635820047,1.0180699241,0.3155858514
H,0,-1.5747478437,-0.2215776403,-3.5536695545
C,0,-3.6586207751,0.9541677827,-2.2979644308
F,0,-4.019104991,0.2275917798,-3.3614353365

H,4.006820750727,-0.124180180564,-0.533165333812
N,2.114802172219,-0.797299287361,-0.812302151162
H,-0.307484296209,-0.707625692971,-0.433549930151
H,-0.160581987440,-0.067839214798,1.207383502910
C,0.118813981226,0.118500395686,0.157899246488
C,1.605285759287,0.048401115964,0.003170149488
H,2.230627267804,0.718254804436,0.612982834141
C,-0.498422340073,1.423680747311,-0.283860945765
C,-1.492922756381,2.040638479507,0.477954308583
C,-0.104384419618,2.028991528993,-1.480535269781
C,-2.085431810338,3.227899012234,0.054714378099
H,-1.792755034070,1.586468973341,1.424122146210
C,-0.691422489172,3.215535953631,-1.906578787962
H,0.683329351479,1.564920216267,-2.074910813013
C,-1.686821853254,3.819596939356,-1.140576733745
H,-2.847544795862,3.703006106591,0.673384126046
H,-0.356916535955,3.678051194780,-2.834069492619
H,-2.132319036124,4.758918891465,-1.467090286828

Substituent = -CF₃: Fx = -60 (×10⁻⁴ au)

R1:

N,1.266961228041,-0.512964308030,6.522548277528
H,1.433659333606,-1.447192186786,6.144604277313
H,2.012219079743,0.041966423096,6.098230909871
N,0.049094178999,-0.060889770179,5.823882044741
H,-0.683091559962,-0.625347027380,6.261579938075
H,-0.123593820064,0.854766729430,6.246137922440

R2:

C,-0.017124000000,-0.000404000000,1.419696000000
C,-0.018108000000,-0.043241000000,2.626951000000
H,-0.018741000000,-0.080438000000,3.697420000000
C,-0.015458000000,0.048452000000,-0.003636000000
C,-1.222906000000,0.139175000000,-0.714117000000
C,1.191064000000,0.002540000000,-0.715477000000
C,-1.219069000000,0.179531000000,-2.097409000000
H,-2.158412000000,0.173581000000,-0.160297000000
C,1.192336000000,0.043890000000,-2.101208000000
H,2.125852000000,-0.068558000000,-0.164024000000
C,-0.011928000000,0.127637000000,-2.794714000000
H,-2.158164000000,0.244039000000,-2.644901000000
H,2.132570000000,0.004329000000,-2.646024000000
C,-0.039834000000,0.214326000000,-4.282541000000
F,-0.297961000000,1.462145000000,-4.713318000000

F,0,-3.5187499793,2.2183592277,-2.7195699037
F,0,-4.6792106697,0.9393962033,-1.4337311882

TS1:

N,0,-2.8814851301,-5.1040616164,3.9181824484
H,0,-2.9443268556,-6.1159729361,4.0460166675
H,0,-2.5424138612,-4.9681545429,2.9627842406
N,0,-4.2269886859,-4.6031012197,3.8833286135
H,0,-4.5375514347,-4.4658267241,4.8490291635
H,0,-4.411647112,-3.6782707702,3.1409650816
C,0,-5.4197756654,-4.2671543138,2.0263107421
C,0,-5.2023276237,-5.2106993332,2.9486341113
H,0,-5.553350194,-6.2223929605,3.166895094
C,0,-6.2767433164,-4.4172578633,0.8628434675
C,0,-7.1954760122,-3.4097538528,0.5343102655
C,0,-6.1920847987,-5.5349622152,0.0140054545
C,0,-8.024938409,-3.5264512495,-0.5706530068
H,0,-7.2488113026,-2.527779444,1.1707736573
C,0,-7.0009373845,-5.6432063903,-1.1043029857
H,0,-5.4698364263,-6.3179297914,0.2436740105
C,0,-7.9293535196,-4.6439279541,-1.3946847214
H,0,-8.7428388761,-2.743219368,-0.8019492589
H,0,-6.9301372579,-6.5133977542,-1.755886748
C,0,-8.7660992194,-4.7821790383,-2.623508705
F,0,-8.0350492388,-4.6307800942,-3.7397497204
F,0,-9.3261764755,-5.9993557709,-2.704407944
F,0,-9.7550734704,-3.8827957069,-2.6743486475

IM:

N,0,3.0868471984,-0.5789494598,2.9051061171
H,0,3.0971015921,-1.579879938,3.0850770659
H,0,3.6653839558,-0.3852807998,2.0879851557
N,0,1.7647278804,-0.1648286081,2.6917877655
H,0,1.5450979216,0.6825408166,3.2038603664
H,0,-0.1073753258,1.3569120565,1.5443500189
C,0,0.1923921971,0.4782998404,0.9667218633
C,0,1.1715004079,-0.3049132248,1.4583989043
H,0,1.5491270209,-1.1647628661,0.8997534461
C,0,-0.5066153242,0.2693890188,-0.2905652362
C,0,-1.3207196795,1.2950763424,-0.7973788537
C,0,-0.410343336,-0.9133369054,-1.0416693008
C,0,-1.988054352,1.1589057583,-2.0027701465
H,0,-1.4158537186,2.2208076803,-0.2297955691
C,0,-1.069787002,-1.0514481096,-2.2511306627

F,1.120061000000,-0.153497000000,-4.847093000000
F,-0.998179000000,-0.563416000000,-4.815157000000

TS1:

N,2.349573953501,-2.044517487001,1.116456228287
H,3.270968089670,-1.607953972268,1.186742482595
H,1.820274960784,-1.738659942934,1.934622665036
N,1.665408436382,-1.467593587559,0.000890245955
H,2.095994347260,-1.833264082356,-0.852905957275
H,0.438968687516,-1.499010702006,0.023515413605
C,0.006753360812,0.013052612777,0.074228991600
C,1.339872012578,-0.022126974337,-0.000507485715
H,2.155665908681,0.698672629508,-0.076911304683
C,-0.812662807710,1.207095545811,0.143187390967
C,-1.862278010882,1.404082642593,-0.769560100665
C,-0.624191611579,2.178346259848,1.144002824167
C,-2.667889595491,2.529540722275,-0.707959643181
H,-2.023695368517,0.654224848352,-1.543109644836
C,-1.438471622077,3.294891297162,1.218981466497
H,0.182214584319,2.041892245851,1.863237659168
C,-2.462982383258,3.480488097732,0.289394900482
H,-3.460188365310,2.675002476938,-1.439504268614
H,-1.269785423091,4.045892268334,1.990105704384
C,-3.347269889859,4.669503117111,0.424578798854
F,-4.191681367988,4.554900583056,1.472985232127
F,-2.656325893547,5.797024545200,0.632235053507
F,-4.120507431072,4.868986718900,-0.656591303466

IM:

N,3.493172014087,-1.152674672524,0.286587491610
H,3.954859335300,-0.807576602157,-0.551324225963
H,3.803723216335,-0.626783739608,1.100307687724
N,2.112360453573,-1.114515870016,0.148906699997
H,1.658433386131,-2.013304934791,0.255972847067
H,-0.526307673363,-0.909311563458,0.213179778852
C,0.003263698368,0.044063205011,0.132338923256
C,1.358335578447,0.012529078948,0.111838353236
H,1.954932923994,0.925207942748,0.052898502292
C,-0.825371918909,1.225357330613,0.058431518117
C,-2.224434174895,1.080575943793,0.151506258826
C,-0.329090005082,2.533598463072,-0.101932828643
C,-3.072626583767,2.169460638889,0.091850323992
H,-2.637675629088,0.079252464891,0.277856470630
C,-1.175790939999,3.626734282088,-0.160582879064

H,0,0.1794858847,-1.7480405048,-0.664790447
C,0,-1.8596859896,-0.0142161248,-2.7423395359
H,0,-2.6080120024,1.9703282462,-2.3796635274
H,0,-0.9786367562,-1.9746937503,-2.8190873179
C,0,-2.6322478577,-0.177849684,-4.0097371274
F,0,-3.8967910173,-0.562805087,-3.7748494056
F,0,-2.0901251728,-1.0987885415,-4.8166000824
F,0,-2.7051752248,0.9685095446,-4.6999477506

TS2:

N,0,2.8123524501,-0.6694400504,3.0733560546
H,0,2.7854859269,-1.4959967723,3.6643017314
H,0,3.6427166232,-0.6710682626,2.4812091377
N,0,1.6407822005,-0.5939808087,2.3326102244
H,0,0.4918993822,0.0061218756,2.3213432406
H,0,0.4947863721,1.4782183484,1.1950951041
C,0,0.418276307,0.4463184079,0.8331199178
C,0,1.6230222462,-0.3005081747,1.0476670575
H,0,2.4276120863,-0.5882547896,0.3615110745
C,0,-0.4226333153,0.2658349847,-0.3438759958
C,0,-1.283943702,1.2853293936,-0.7827680047
C,0,-0.4097994737,-0.935749012,-1.0668762091
C,0,-2.080319687,1.116364663,-1.9000584362
H,0,-1.3140035937,2.2251588965,-0.2310649225
C,0,-1.1943559498,-1.1045332002,-2.1983310675
H,0,0.2205973181,-1.7561372864,-0.7217780018
C,0,-2.0328481615,-0.0783873722,-2.6199891702
H,0,-2.7406317089,1.9169633588,-2.2317523112
H,0,-1.1654504163,-2.0394955511,-2.7534593678
C,0,-2.905502738,-0.2190947697,-3.8225860171
F,0,-2.6934814257,0.7726439601,-4.7020507021
F,0,-2.7072607743,-1.3737931223,-4.4685119069
F,0,-4.2074923664,-0.1615586265,-3.5007737495

P:

N,0,2.9862384117,-1.0256202232,2.3503241293
H,0,3.0518909176,-1.9748368267,2.6979156271
H,0,3.5381084063,-0.8971989569,1.4997872159
N,0,1.6763023039,-0.6526821351,2.2454010864
H,0,-0.6159261386,0.2619057596,2.0731213002
H,0,-0.0677120479,1.8306491797,1.4632962907
C,0,-0.0296568933,0.7460048936,1.2793076246
C,0,1.3766825406,0.2512319465,1.3977632103
H,0,2.1296294817,0.6802974212,0.7133407783

H,0.743193937066,2.701653433515,-0.187129501959
C,-2.556307673341,3.455996282823,-0.061612447507
H,-4.151142439176,2.031527336493,0.171580204053
H,-0.759669417497,4.624334093122,-0.283432685484
C,-3.499298247064,4.598652142923,-0.169922284919
F,-4.178052319393,4.592183232707,-1.336969584663
F,-2.896370833042,5.786954151038,-0.081741798328
F,-4.448559889344,4.562491549533,0.790320401420

TS2:

N,2.909134329700,-1.695402864741,0.692081859480
H,3.313957036997,-2.434392548926,0.123867839000
H,3.590826876113,-0.963697763772,0.890780980649
N,1.760918019699,-1.216413597156,0.106300131381
H,0.495070152795,-1.416742232396,0.078718639646
H,-0.424558950425,-0.066825260844,1.073459705047
C,-0.027142168411,0.056250226985,0.058690353268
C,1.419638343302,0.046632547754,0.033934107939
H,2.150018255309,0.861870884002,0.022502993408
C,-0.821415223241,0.914984662711,-0.803020549263
C,-2.155008185499,1.231503737528,-0.480492799751
C,-0.306098976990,1.437292356346,-2.001968244175
C,-2.924426400601,2.029281758124,-1.304991261292
H,-2.575432676089,0.840755539980,0.447194460435
C,-1.069117833684,2.250322512907,-2.825143071278
H,0.715151629234,1.189402023496,-2.291920173619
C,-2.385578519664,2.551272393821,-2.483539283536
H,-3.953050991442,2.270586450091,-1.034772472530
H,-0.640267776083,2.650157541542,-3.741458018521
C,-3.257155823291,3.384144913002,-3.352562449560
F,-3.869654392183,4.365070193272,-2.660228709362
F,-2.599891867109,3.963192897085,-4.359600856783
F,-4.259676628481,2.663791119080,-3.905100750656

P:

N,3.453960150990,-1.101234996093,0.070436719821
H,3.873082305969,-1.964246731874,-0.249754100975
H,3.937072433644,-0.261315380673,-0.249083362479
N,2.109306889937,-1.115359824345,-0.007823894193
H,-0.329066672477,-1.051976205446,0.139694888830
H,-0.381758563670,0.557492154150,0.867217313936
C,-0.018024950370,-0.006402716577,-0.006918326777
C,1.477671241777,-0.004131642901,-0.038957214062
H,1.998998408661,0.966602913234,-0.069845692709

C,0,-0.6231793918,0.4465557396,-0.0750628533
C,0,-1.0623714873,1.4668148495,-0.9186995689
C,0,-0.7265800485,-0.8760870745,-0.5100059869
C,0,-1.5957746297,1.1754529977,-2.1666112664
H,0,-0.9879545008,2.5032734319,-0.5895029989
C,0,-1.2603791888,-1.177136786,-1.7552189282
H,0,-0.3822618711,-1.6766903814,0.1453312534
C,0,-1.6956211293,-0.1481254416,-2.5850716822
H,0,-1.9404976045,1.9744064548,-2.8211262135
H,0,-1.3430781136,-2.2100516895,-2.084933237
C,0,-2.2278338798,-0.4261454469,-3.9552657419
F,0,-1.3387518114,-0.0865631721,-4.9006871788
F,0,-3.3380831507,0.2816533286,-4.204088015
F,0,-2.523188385,-1.717257049,-4.1359059252
C,-0.672288722713,0.542870259799,-1.250174917018
C,-1.728252214804,1.453063138516,-1.164949036391
C,-0.250936178090,0.126196807043,-2.514023144940
C,-2.358754226384,1.921407526617,-2.307366421994
H,-2.053131203251,1.799831419193,-0.183427345616
C,-0.876634577633,0.588554082070,-3.664723451046
H,0.583168723926,-0.571170865832,-2.587105311220
C,-1.935091935545,1.485737133212,-3.560683109735
H,-3.176679362956,2.637884575670,-2.235527664104
H,-0.538107829946,0.258318378376,-4.643990467075
C,-2.668554395430,1.981731868938,-4.761562211016
F,-2.756019624347,3.320537968100,-4.777118308967
F,-3.943562496954,1.533361744899,-4.775208133258
F,-2.111028862388,1.600376982530,-5.911381637618