

Electronic Supporting Information (ESI) for the paper:

**A DFT Study on the *Endo*-selectivity
Mechanism of Diels-Alder Reaction in
Lindenane Dimeric Sesquiterpenes
Synthesis Promoted by Pyridines**

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This file contains:

S1. Geometry Structure

S2. Energy profiles

S3. XYZ coordinates of optimized geometries

S1. Geometry Structure

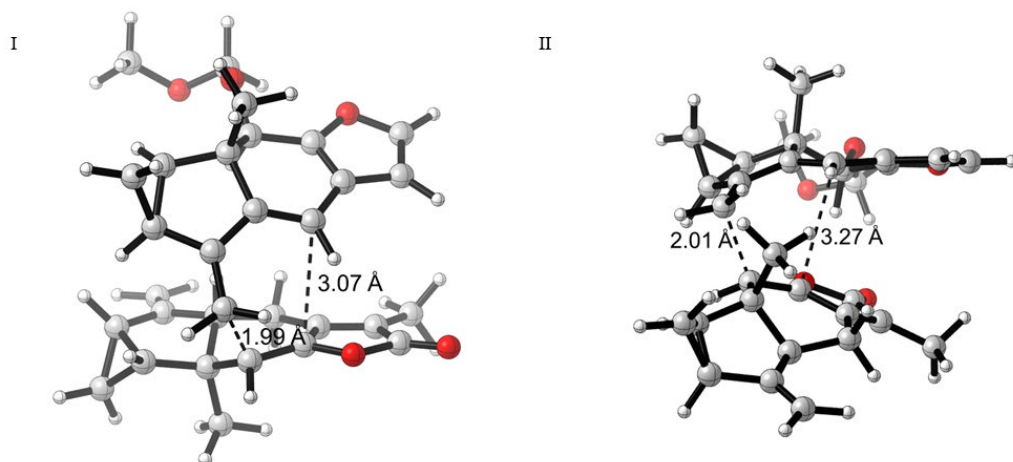


Figure S1. Structures of the transition states in the none-promoted D-A cycloaddition. (The roman numerals of I and II represent the *endo*- or *exo*- process, respectively.)

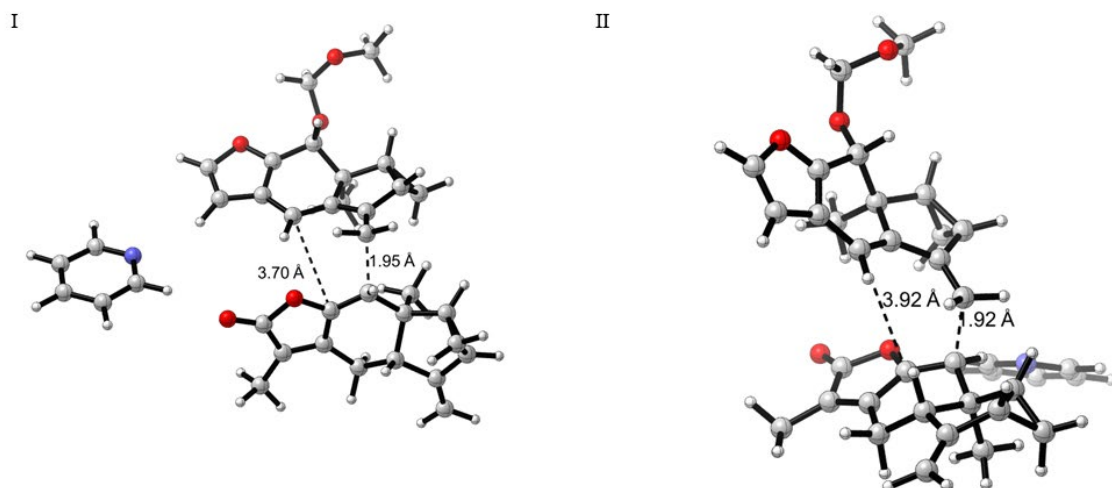


Figure S2. Structures of the transition states in the py promoted D-A cycloaddition. (The roman numerals of I and II represent the *endo*- or *exo*- process, respectively.)

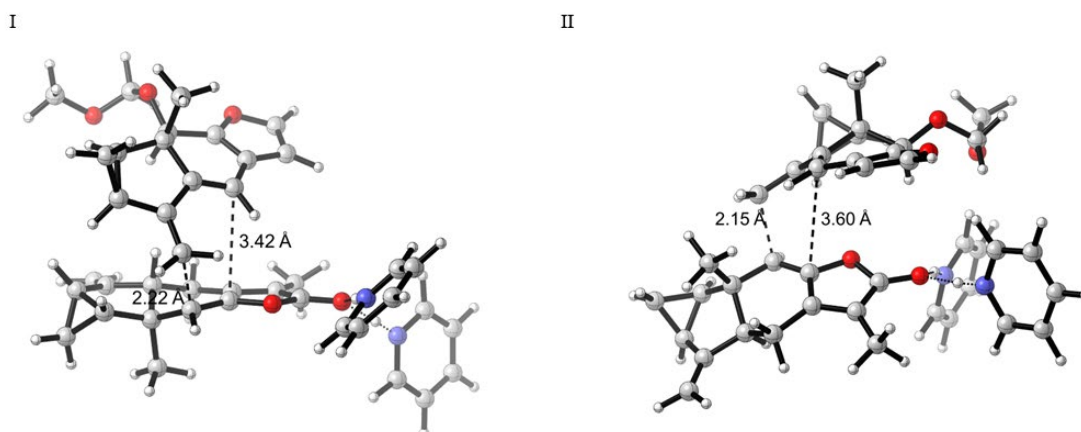


Figure S3. Structures of the transition states in the double py-H^+ promoted D-A cycloaddition.

(The roman numerals of I and II represent the *endo*- or *exo*- process, respectively.)

S2. Energy profiles

Table S1. Single point energies (Hartree) of reactants(RC), intermediates(INT), transition states(TS1/TS2), and products(P) calculated at M06-2X/6-311+G(d,p), M06-2X-D3/6-311+G(d,p), and M06-2X-D3/def2-TZVP. All structures are optimized at B3LYP/6-31+G(d) level.

		M06-2X/ 6-311+G(d,p)	M06-2X-D3/ 6-311+G(d,p)	M06-2X-D3/ def2-TZVP
none	<i>endo</i> -RC	-1577.499663	-1577.505942	-1577.673307
	<i>endo</i> -TS	-1577.474311	-1577.482515	-1577.646121
	<i>endo</i> -P	-1577.558614	-1577.566728	-1577.728017
	<i>exo</i> -RC	-1577.500478	-1577.507384	-1577.674323
	<i>exo</i> -TS	-1577.464007	-1577.471536	-1577.635311
	<i>exo</i> -P	-1577.565101	-1577.572596	-1577.734502
py	<i>endo</i> -RC	-1825.753250	-1825.749502	-1825.943792
	<i>endo</i> -TS	-1825.703932	-1825.727125	-1825.917458
	<i>exo</i> -RC	-1825.746023	-1825.757588	-1825.950860
	<i>exo</i> -TS	-1825.706031	-1825.720029	-1825.910344
py- H^+	<i>endo</i> -RC	-1826.154017	-1826.163494	-1826.359851

	<i>endo</i> -TS	-1826.131975	-1826.141434	-1826.333467
	<i>endo</i> -P	-1826.207604	-1826.217097	-1826.416719
	<i>exo</i> -RC	-1826.157618	-1826.165679	-1826.358301
	<i>exo</i> -TS	-1826.119503	-1826.128850	-1826.320719
	<i>exo</i> -P	-1826.226493	-1826.236454	-1826.424961
2py-H⁺	<i>endo</i> -RC	-2074.708387	-2074.719579	-2074.719579
	<i>endo</i> -TS1	-2074.698260	-2074.709427	-2074.709427
	<i>endo</i> -INT	-2074.727143	-2074.738397	-2074.738397
	<i>endo</i> -TS2	-2074.725886	-2074.737367	-2074.737367
	<i>endo</i> -P	-2074.764418	-2074.775760	-2074.775760
	<i>exo</i> -RC	-2074.715953	-2074.726090	-2074.947548
	<i>exo</i> -TS1	-2074.692603	-2074.704582	-2074.923787
	<i>exo</i> -INT	-2074.723378	-2074.735746	-2074.952601
	<i>exo</i> -TS2	-2074.723056	-2074.734076	-2074.934076
	<i>exo</i> -P	-2074.785702	-2074.797441	-2075.013531

Table S2. Relative single point energies (kcal/mol) profiles (calculated at M06-2X/6-311+G(d,p), M06-2X-D3/6-311+G(d,p), and M06-2X-D3/def2-TZVP) of py-H⁺ model which is optimized using B3LYP/6-31+G(d) and B3LYP-D3/6-31+G(d). Obviously, it indicates that London dispersion effects is already well treated by M06-2X/6-311+G(d,p)//B3LYP/6-31+G(d) for this case, since it shows little impact on the reaction energetic features if considering more notable dispersion with D3 or using bigger basis set.

optimized using B3LYP/6-31+G(d)			
ΔE_{sp} (kcal/mol)	M06-2X/ 6-311+G(d,p)	M06-2X-D3/ 6-311+G(d,p)	M06-2X-D3/ def2-TZVP
$\Delta E_{sp(endo-TS)}$	13.8	13.8	16.5
$\Delta E_{sp(endo-P)}$	-33.6	-33.6	-35.7
$\Delta E_{sp(exo-TS)}$	23.9	23.1	23.7
$\Delta E_{sp(exo-P)}$	-43.2	-44.4	-41.8
optimized using B3LYP-D3/6-31+G(d)			
ΔE_{sp} (kcal/mol)	M06-2X/ 6-311+G(d,p)	M06-2X-D3/ 6-311+G(d,p)	M06-2X-D3/ def2-TZVP
$\Delta E_{sp(endo-TS)}$	12.7	12.7	12.7
$\Delta E_{sp(endo-P)}$	-25.3	-24.5	-23.1

$\Delta E_{sp(exo-TS)}$	22.2	21.8	23.4
$\Delta E_{sp(exo-P)}$	-41.9	-42.6	-39.4

Table S3. Relative Gibbs free energies (kcal/mol) profiles of py-H⁺ model calculated at M06-2X/6-311+G(d,p)//B3LYP/6-31+G(d) with SMD solvation model. It indicates that solvent effect is not notable and would not affect the relative energy characteristics.

$\Delta G(\text{kcal/mol})$	gas phase	SMD-toluene	SMD-pyridine
$\Delta G_{endo-TS}$	15.8	17.6	17.3
ΔG_{exo-TS}	24.4	27.3	25.5
ΔG_{endo-P}	-26.6	-27.9	-27.9
ΔG_{exo-P}	-36.9	-34.3	-35.7

S3. XYZ coordinates of optimized geometries

endo-reactant of non-promoted model

C	3.50847100	-0.23363900	-0.89046300
C	2.20732800	0.06445600	-1.67463400
C	1.47204100	1.17392200	-1.43637500
C	1.84379300	2.02159700	-0.31111300
C	2.72641000	1.54576700	0.62095800
C	3.33616800	0.16903500	0.59935900
C	3.67243900	-1.76070500	-1.04663000
C	2.64668300	-2.26953100	-2.04698000
C	1.85500800	-1.08689400	-2.53177300
C	1.40181300	3.30213400	0.17682900
C	2.05399900	3.49652000	1.35733400
O	2.86459500	2.42178300	1.65029500
C	0.95114900	-1.11917300	-3.52790100

C	4.12699900	-2.31457900	-2.37275500
C	4.69039600	0.56372300	-1.49908500
O	4.59957900	0.10277500	1.26632200
C	4.53044200	-0.14486700	2.65646400
O	4.28971600	-1.49298800	2.97414400
C	5.39078500	-2.35768600	2.71139300
H	0.55482900	1.38407400	-1.97990400
H	2.64505800	-0.54358200	1.08119300
H	3.90338900	-2.33111700	-0.15111100
H	2.12409200	-3.21295100	-1.90679400
H	0.69364200	3.97483200	-0.28990300
H	2.07724400	4.30159800	2.07579400
H	0.40429000	-0.23146500	-3.83642200
H	0.74419300	-2.03725300	-4.07189400
H	4.59733300	-3.29562000	-2.36458600
H	4.51290900	-1.64765900	-3.13800900
H	4.73722700	0.42160900	-2.58195100
H	4.57626700	1.63605900	-1.31221300
H	5.63836600	0.23781300	-1.06110400
H	5.50211800	0.17987200	3.05118900
H	3.71708400	0.41923800	3.12114200
H	5.08871800	-3.35597500	3.03660900
H	5.64188500	-2.37868200	1.64394200
H	6.27752100	-2.04360700	3.28254900
C	-3.50217000	-1.45531200	-0.45732300
C	-3.87846100	-0.92680800	0.96988200
C	-4.59243900	0.42751400	0.94783400
C	-3.70212100	1.37061300	0.17297300
C	-2.72792300	0.83334000	-0.77755900
C	-2.55344500	-0.46092300	-1.09304400
C	-3.56145900	2.71892600	0.19237400
C	-2.47310900	3.06191200	-0.74841000
O	-2.00400600	1.87844200	-1.32027700
C	-4.74099300	-1.58376700	-1.38529000
O	-1.99100900	4.13479800	-1.03105700
H	-2.90227600	-0.74264400	1.44781000
H	-4.76081000	0.80792200	1.96288700
H	-5.58010300	0.35161400	0.47163300
H	-1.81294000	-0.77199800	-1.82633800
H	-5.56058500	-2.12577900	-0.90183600

H	-5.11800700	-0.59886200	-1.67746000
H	-4.47067600	-2.12033300	-2.30184100
C	-2.88487200	-2.83439800	-0.10326000
H	-1.82859300	-2.98298600	-0.31387500
C	-3.48011200	-3.26602700	1.23576800
H	-2.86863500	-3.74653600	1.99682300
C	-3.77801800	-4.04906500	-0.02484600
H	-3.28980400	-5.01750500	-0.11104700
H	-4.77809700	-4.02744000	-0.44510700
C	-4.40503900	-2.15481500	1.67836400
C	-5.42313800	-2.24259900	2.53918200
H	-5.69704700	-3.18751400	3.00245800
H	-6.01450100	-1.37354700	2.81942400
C	-4.28152600	3.76815700	0.97517400
H	-3.57405400	4.39187300	1.53473900
H	-4.83457000	4.44235300	0.30877800
H	-4.99108400	3.32474900	1.68032200

endo-TS of non-promoted model

C	-2.19449000	-0.03513500	1.38304800
C	-0.72839700	0.30991700	1.73559000
C	-0.19567900	1.54681700	1.44342000
C	-0.94732300	2.40100500	0.55414300
C	-2.01907600	1.88489100	-0.13828300
C	-2.51064200	0.46057100	-0.05487100
C	-2.22541500	-1.57245900	1.50435300
C	-0.86600400	-2.04849200	1.99857500
C	-0.01464400	-0.83346300	2.18610800
C	-0.78973800	3.75475200	0.08511600
C	-1.77051200	3.94867500	-0.83790700
O	-2.52776400	2.80530600	-0.99100900
C	1.34653100	-0.83060700	2.55579100
C	-2.09975500	-2.18367000	2.87654600
C	-3.16932900	0.65108000	2.37502300
O	-3.90936200	0.33693500	-0.31260100
C	-4.26101900	0.19347800	-1.67771700
O	-4.02141400	-1.09272200	-2.18435700
C	-4.91768700	-2.08911500	-1.70037100
H	0.77258900	1.86006700	1.81464100

H	-1.95967900	-0.16212800	-0.77951200
H	-2.76877500	-2.12988000	0.74640500
H	-0.40425100	-2.95929700	1.63080400
H	-0.04867200	4.47722200	0.40096800
H	-2.07495400	4.78750600	-1.44468100
H	1.70713400	0.06461700	3.05817600
H	1.72346900	-1.74338700	3.01303200
H	-2.49370600	-3.18921300	3.00874400
H	-2.17816900	-1.55814200	3.76086300
H	-2.88182400	0.44046200	3.40788100
H	-3.16966000	1.73773100	2.24716800
H	-4.18870600	0.28880900	2.21436400
H	-5.33004500	0.43929700	-1.71862900
H	-3.68401500	0.87500500	-2.30870100
H	-4.64256100	-3.02293100	-2.19570000
H	-4.83677100	-2.21156100	-0.61339900
H	-5.95709700	-1.83506300	-1.95675000
C	2.62037900	-1.72033900	0.00153700
C	1.50511400	-1.32069600	-1.02345500
C	1.82269400	-0.04833600	-1.81056500
C	2.28134900	1.00334400	-0.83009200
C	2.59371900	0.65879500	0.51979100
C	2.67110000	-0.63036200	1.08937400
C	2.57844100	2.33466600	-1.01030200
C	3.04665400	2.85292900	0.26715000
O	3.05493700	1.77095200	1.18636000
C	4.03234100	-1.76602600	-0.64370200
O	3.38618000	3.96589600	0.61922900
H	0.63442900	-1.08664400	-0.39083000
H	0.93880500	0.29882100	-2.36168300
H	2.60393300	-0.23031500	-2.56232900
H	3.48070800	-0.74689000	1.81147600
H	4.03405600	-2.32683600	-1.58388000
H	4.41018000	-0.76270500	-0.85950900
H	4.74128300	-2.25143100	0.03738700
C	2.16363900	-3.13912600	0.43159900
H	1.95155100	-3.31835200	1.48062600
C	1.23845400	-3.68465000	-0.65215200
H	0.34306600	-4.25474500	-0.41214300
C	2.58025500	-4.33424200	-0.39435400

H	2.55785500	-5.29959400	0.10733700
H	3.36258900	-4.24960700	-1.14093500
C	1.13603800	-2.61667100	-1.71297700
C	0.75429700	-2.78640000	-2.98268100
H	0.48851300	-3.76676800	-3.37133000
H	0.68194600	-1.95195000	-3.67642800
C	2.49124000	3.18192100	-2.24004300
H	1.83137400	4.04467800	-2.08338300
H	3.47441700	3.58450100	-2.51727500
H	2.10516900	2.60947300	-3.08990100

endo-product of non-promoted model

C	2.13057800	-1.02455400	1.09697600
C	0.64648600	-0.71584800	1.32082900
C	-0.43579700	-1.39711900	0.51850000
C	0.11014800	-1.60816700	-0.88165900
C	1.38320700	-1.24520200	-1.22910700
C	2.45150000	-0.61528600	-0.37024000
C	2.81770100	-0.09795600	2.11828100
C	1.74307800	0.71967200	2.81904400
C	0.45137500	0.23777600	2.24412900
C	-0.42493900	-2.29874800	-2.02818200
C	0.54846500	-2.27324900	-2.97942300
O	1.66166700	-1.63109800	-2.50834500
C	-0.92082400	0.68921000	2.64084800
C	2.55508600	-0.30619800	3.58967900
C	2.49032900	-2.51013500	1.32380000
O	3.76031500	-1.05787300	-0.73801800
C	4.40244800	-0.27631800	-1.72750300
O	4.94247700	0.92183600	-1.23117300
C	6.09271700	0.74624200	-0.40926200
H	-0.61655300	-2.39696300	0.93950700
H	2.41923400	0.48152800	-0.43805100
H	3.76456600	0.35243600	1.83458200
H	1.86788100	1.77510300	3.05395600
H	-1.40134700	-2.75328800	-2.12609200
H	0.61674700	-2.64786900	-3.98961200
H	-1.32134100	0.00934600	3.40714500
H	-0.90422300	1.68021400	3.10796800

H	3.31053600	0.06682000	4.27799800
H	2.04642600	-1.20559200	3.92745600
H	2.18451600	-2.82831800	2.32488700
H	1.99879600	-3.16415200	0.59600400
H	3.57019500	-2.65593800	1.22858400
H	5.19272900	-0.92259400	-2.13114100
H	3.70370400	0.01684500	-2.51582900
H	6.43279700	1.74606600	-0.12982400
H	5.85929000	0.17115600	0.49512000
H	6.89291800	0.23330000	-0.96383200
C	-1.82740300	1.91601500	0.44924000
C	-1.33695000	1.45406200	-0.96192900
C	-2.28867300	0.46815900	-1.63677400
C	-2.67039000	-0.56693000	-0.60873100
C	-1.86400300	-0.69476000	0.67711700
C	-1.89183800	0.68365400	1.44363200
C	-3.75066500	-1.36568200	-0.54555600
C	-3.74279100	-2.05363000	0.76679300
O	-2.64621700	-1.62838400	1.47486800
C	-3.26500000	2.48755100	0.36515200
O	-4.54003000	-2.84535900	1.21893100
H	-0.39990100	0.91213100	-0.77212100
H	-1.79918600	-0.00313300	-2.49851600
H	-3.18902900	0.96678900	-2.01779200
H	-2.89611600	0.69976800	1.87849800
H	-3.38595300	3.20078000	-0.45602900
H	-3.99858700	1.68959000	0.20992700
H	-3.52490900	2.99841100	1.30011200
C	-0.78874600	3.03482200	0.75996500
H	-0.12353600	2.91204600	1.60657900
C	-0.22182500	3.53557200	-0.56375100
H	0.83557300	3.76749700	-0.67517000
C	-1.05755200	4.45081200	0.30491300
H	-0.51970100	5.24075000	0.82524300
H	-2.04646900	4.74482300	-0.02977700
C	-0.88319500	2.72381100	-1.64829700
C	-0.99298600	3.04085300	-2.94216700
H	-0.60718700	3.97965700	-3.33277900
H	-1.46260000	2.37086900	-3.65905500
C	-4.86533600	-1.57175800	-1.52189900

H	-4.90348100	-2.61710400	-1.85353000
H	-5.83532400	-1.35878600	-1.05641600
H	-4.75138600	-0.93518900	-2.40462800

exo-reactant of non-promoted model

C	-3.04398700	-1.33070300	-0.22384700
C	-2.01323300	-2.10900800	0.63079200
C	-1.78582600	-1.79404900	1.92630600
C	-2.41788400	-0.60069800	2.47340800
C	-2.97611100	0.30733300	1.61221000
C	-2.97341100	0.18648700	0.11234100
C	-2.58629300	-1.61040400	-1.67112200
C	-1.48620400	-2.65986900	-1.64882200
C	-1.25551100	-3.05378100	-0.21717800
C	-2.52577300	-0.01640000	3.78399600
C	-3.13956500	1.18874400	3.60726200
O	-3.41371300	1.40267000	2.27873000
C	-0.44399400	-4.04798000	0.18784600
C	-2.83679600	-2.97377700	-2.26293700
C	-4.47514200	-1.84924800	0.06480600
O	-4.06251300	0.90077500	-0.47286700
C	-3.72104000	2.06060100	-1.20855900
O	-3.38138600	1.78802600	-2.54721400
C	-4.48064700	1.37197200	-3.34976400
H	-1.05809900	-2.34026000	2.52354400
H	-2.02554600	0.59299000	-0.27198900
H	-2.52612900	-0.76121100	-2.34601800
H	-0.62410700	-2.60267200	-2.30931700
H	-2.20143100	-0.43716200	4.72692900
H	-3.45677900	1.97228900	4.27826700
H	0.09697500	-4.66125200	-0.52821800
H	-0.30402400	-4.28622500	1.23957400
H	-2.87172900	-3.04450000	-3.34804700
H	-3.48793500	-3.67848400	-1.75413100
H	-4.52543300	-2.93664200	-0.03699000
H	-4.78547200	-1.59713400	1.08386000
H	-5.18957300	-1.39912500	-0.63087200
H	-4.61344000	2.69915300	-1.16522600
H	-2.85301200	2.56592000	-0.77724800

H	-4.10225300	1.26508000	-4.36947900
H	-4.89002100	0.41306400	-3.00811700
H	-5.28062900	2.12803700	-3.33885700
C	3.52370300	-0.74241400	0.32230400
C	4.34403800	0.29264900	-0.52246700
C	4.16992800	1.73715300	-0.04661100
C	1.74030700	0.89531200	0.05255800
C	2.05351000	-0.40478200	0.18508100
C	3.96895700	-2.07497900	-0.33737800
C	5.33883800	-1.83285600	-0.96812100
C	0.53470200	2.78029600	-0.10561800
O	0.45145600	1.39189200	0.00001200
C	5.18689000	-2.79094800	0.19394500
C	3.87895400	-0.68551400	1.83344300
O	-0.45750000	3.46955900	-0.16771100
H	3.87744900	0.24680800	-1.52028500
H	4.68490800	2.44288400	-0.71010300
H	4.59464500	1.88010800	0.95703000
H	1.28514000	-1.16919600	0.27493200
H	3.21260800	-2.65813300	-0.85688000
H	5.59623100	-2.25144500	-1.93900400
H	5.27298900	-3.84905800	-0.04377600
H	5.60084900	-2.52552400	1.16074300
H	4.96074200	-0.71150400	2.00194700
H	3.49014400	0.22743100	2.29457300
H	3.43150700	-1.53785300	2.35710400
C	2.39954400	4.58081200	-0.24314500
H	1.96192600	5.05131000	-1.13198900
H	2.05761000	5.16514800	0.62050600
H	3.48898900	4.66343400	-0.30427700
C	1.96469500	3.15617000	-0.12740800
C	2.68404900	2.01071400	-0.03513200
C	5.68371100	-0.38266100	-0.71491000
C	6.89877100	0.17324400	-0.70909400
H	7.79623500	-0.41700100	-0.87854300
H	7.04085800	1.23885700	-0.54234500
<i>exo</i> -TS of non-promoted model			
C	-2.56134000	-1.16717800	0.73277900

C	-1.08120000	-1.11463700	1.18209100
C	-0.58787700	-0.04678800	1.89702000
C	-1.39728200	1.14395800	1.96682000
C	-2.50951600	1.25335300	1.15901300
C	-2.98824100	0.22284000	0.17389100
C	-2.55387200	-2.26066900	-0.35686300
C	-1.15470900	-2.85299300	-0.44049200
C	-0.31972900	-2.15305000	0.57401500
C	-1.27001300	2.41799900	2.62986200
C	-2.30404100	3.17970300	2.17929100
O	-3.06567100	2.47839500	1.27229700
C	1.07153800	-2.29926500	0.71159000
C	-2.32461300	-3.69078500	0.05632600
C	-3.47718600	-1.53012000	1.92882300
O	-4.40291600	0.31616900	-0.00674000
C	-4.84710500	0.64082800	-1.31003900
O	-4.97461000	-0.47599100	-2.15432900
C	-6.04578900	-1.34702900	-1.80782500
H	0.41988300	-0.04253000	2.30096300
H	-2.49074700	0.40575500	-0.79051100
H	-3.12659700	-2.07166100	-1.26034800
H	-0.69449900	-3.12311500	-1.38890200
H	-0.51793300	2.71807500	3.34763700
H	-2.64496700	4.18131800	2.39201400
H	1.51059400	-3.22553500	0.34574100
H	1.49040100	-1.97115000	1.65493300
H	-2.68559100	-4.46502900	-0.61742900
H	-2.34999700	-3.96983700	1.10587800
H	-3.13628900	-2.44700000	2.41663600
H	-3.48247900	-0.73497300	2.68114200
H	-4.50521700	-1.67852500	1.58609900
H	-5.82350000	1.12253900	-1.16609500
H	-4.14384600	1.31290800	-1.80966800
H	-6.08646600	-2.11684200	-2.58223900
H	-5.88195300	-1.81835200	-0.83066300
H	-7.00218900	-0.80262200	-1.78857100
C	3.51640400	-0.83486800	0.07291800
C	4.10779700	0.46213200	-0.59563800
C	3.36778100	1.73352500	-0.15731900
C	1.41138100	0.19019500	-0.68269700

C	2.08297400	-1.03275400	-0.48063300
C	4.53269600	-1.90525800	-0.40414600
C	5.83933600	-1.18959200	-0.73811400
C	-0.11284800	1.58602300	-1.57073900
O	0.19858300	0.23210600	-1.32753300
C	5.77479500	-2.17050600	0.41270200
C	3.53559200	-0.66473600	1.61197900
O	-1.15337700	1.88454200	-2.13507600
H	3.90365200	0.34307400	-1.67241500
H	3.76039900	2.61664600	-0.67599900
H	3.49581400	1.91720100	0.91753100
H	1.99336700	-1.73947300	-1.30563500
H	4.16308800	-2.70366600	-1.04400300
H	6.43157300	-1.46629000	-1.60801300
H	6.26806000	-3.12770400	0.25724400
H	5.85057900	-1.79954200	1.42965400
H	4.45634300	-0.17021700	1.93886000
H	2.69913300	-0.04885100	1.95554200
H	3.48762100	-1.63010200	2.12416500
C	1.04324400	3.87222100	-1.23662500
H	0.84312700	4.16606900	-2.27459500
H	0.27944700	4.36377600	-0.61856900
H	2.01906800	4.27506200	-0.94504300
C	0.99440900	2.38626500	-1.07506600
C	1.92177800	1.51499800	-0.54053000
C	5.60624400	0.28014300	-0.47857800
C	6.53327300	1.21332300	-0.24237200
H	7.59197500	0.96758400	-0.20182000
H	6.26879700	2.25757100	-0.09114700

exo-product of non-promoted model

C	-2.26466400	-1.18012600	0.56840400
C	-0.85193200	-0.87315000	0.06439800
C	-0.08301100	0.33501600	0.54270100
C	-1.07681100	1.45991500	0.74851100
C	-2.41813500	1.27826000	0.56115400
C	-3.15655200	0.03074300	0.16041300
C	-2.64033500	-2.43767200	-0.23691000
C	-1.50593700	-2.73496200	-1.20374900

C	-0.46056300	-1.70627300	-0.91119800
C	-0.92581100	2.81796300	1.20566700
C	-2.17838200	3.35072000	1.23704300
O	-3.10367500	2.42322200	0.84537500
C	0.83650800	-1.60754900	-1.65285700
C	-1.82381600	-3.69511500	-0.06997800
C	-2.33504600	-1.40955800	2.09350300
O	-4.43510300	-0.05463200	0.79952600
C	-5.51535100	0.48247800	0.06207100
O	-6.00504800	-0.38841800	-0.92612900
C	-6.71179500	-1.51271200	-0.41257400
H	0.37941000	0.13025500	1.51941800
H	-3.30374600	-0.00340700	-0.92827700
H	-3.67636000	-2.54537600	-0.54501100
H	-1.67739200	-3.05065900	-2.23090900
H	-0.01250300	3.32981200	1.47259400
H	-2.56974700	4.32235700	1.49773500
H	0.61846800	-1.34167700	-2.69783300
H	1.32020900	-2.59411300	-1.69691600
H	-2.31276000	-4.63243100	-0.32722300
H	-1.11089200	-3.77171900	0.74753100
H	-1.66271400	-2.22228500	2.38645100
H	-2.04905300	-0.51179400	2.65228000
H	-3.35269500	-1.67746000	2.39153500
H	-6.29189900	0.69881600	0.80763900
H	-5.22129300	1.39452600	-0.46462400
H	-7.07812700	-2.07290400	-1.27603000
H	-6.06259100	-2.15611900	0.19423600
H	-7.56784300	-1.18908500	0.19888900
C	2.90816900	-1.15310400	-0.10378000
C	3.84127000	0.02573400	0.32803100
C	3.12273400	1.13241800	1.11881100
C	1.08753400	0.67487700	-0.45332800
C	1.82345200	-0.57266900	-1.06335100
C	3.94545500	-2.05137800	-0.84752900
C	5.32385700	-1.73945200	-0.26644200
C	1.02724200	2.67764700	-1.59982100
O	0.51197000	1.40703300	-1.56167600
C	4.71138500	-3.11186300	-0.09228200
C	2.31400600	-1.90193900	1.10790600

O	0.69745700	3.48961400	-2.43478000
H	4.13371400	0.49985200	-0.62420200
H	3.81647000	1.92931100	1.40828700
H	2.66972000	0.73994500	2.03851000
H	2.38537600	-0.15050400	-1.90680700
H	3.82103900	-2.18314700	-1.92011800
H	6.20010500	-1.65493000	-0.90645300
H	5.15323600	-3.90792800	-0.68811700
H	4.38789000	-3.43512200	0.89129000
H	3.08929900	-2.13871200	1.84255200
H	1.55260300	-1.32868700	1.63484600
H	1.85436300	-2.84311800	0.78954800
C	2.81310900	4.08035800	-0.35541500
H	3.36731600	4.31580900	-1.27221900
H	2.13701100	4.92578700	-0.17704400
H	3.52247500	4.02265200	0.47558100
C	2.03536600	2.81308100	-0.51691000
C	2.09451000	1.64350700	0.14468700
C	5.11464700	-0.66161200	0.77349100
C	5.90378900	-0.36166400	1.80858600
H	6.81138500	-0.92407800	2.01490300
H	5.67534700	0.46007200	2.48391900

endo-reactant of py model

C	-3.64618500	-0.23100400	-1.23372700
C	-2.41052200	0.57087100	-0.75536100
C	-1.84911100	0.34972400	0.45496300
C	-2.52183300	-0.55857100	1.37634500
C	-3.81541500	-0.92635900	1.12001100
C	-4.62906600	-0.44252200	-0.05074800
C	-4.25919900	0.67667900	-2.32061100
C	-3.30825600	1.82928300	-2.59812900
C	-2.10379600	1.65275200	-1.71538400
C	-2.18720100	-1.14298900	2.64978700
C	-3.30196700	-1.81359500	3.05521100
O	-4.31541800	-1.68309000	2.13115000
C	-0.99368000	2.40965500	-1.76792600
C	-3.57408900	0.78013900	-3.65958400
C	-3.20528200	-1.61216400	-1.78231900

O	-5.65745500	-1.35930000	-0.43481300
C	-6.88464400	-1.20389200	0.24983800
O	-7.66826300	-0.14423000	-0.23883200
C	-8.23388700	-0.38411100	-1.52367800
H	-0.98240600	0.91352800	0.79223800
H	-5.09406400	0.52603900	0.20013300
H	-5.33278400	0.83989800	-2.28474800
H	-3.66775500	2.84022600	-2.77500100
H	-1.24376800	-1.08333800	3.17811800
H	-3.53802900	-2.41901200	3.91695900
H	-0.89868600	3.21486100	-2.49217000
H	-0.15614600	2.26116500	-1.09113100
H	-4.18566800	1.08676300	-4.50560100
H	-2.77888100	0.08759600	-3.91900200
H	-2.40802800	-1.49875700	-2.52184200
H	-2.82244000	-2.24796900	-0.97778900
H	-4.04939800	-2.12459000	-2.25335100
H	-7.40484700	-2.16238100	0.12216700
H	-6.72395700	-0.99030900	1.31009700
H	-8.83839900	0.49259400	-1.76771500
H	-7.45855600	-0.52040000	-2.28739100
H	-8.87964400	-1.27523700	-1.50460700
C	4.19324200	-0.42430700	-1.28081000
C	4.98166000	-1.65817600	-0.73077600
C	4.06887700	-2.73861900	-0.14278200
C	3.19324100	-2.06224900	0.88499900
C	2.96675300	-0.62088600	0.80771000
C	3.42147900	0.21166600	-0.14415000
C	5.29988200	0.38828800	-1.97066600
C	6.39604600	-0.60969900	-2.36132100
C	2.53089700	-2.53222100	1.97135200
C	1.86763500	-1.37905800	2.61248100
O	2.16777000	-0.23649200	1.87341200
C	6.66608200	0.51013200	-1.36206400
C	3.18625500	-0.82001600	-2.39577200
O	1.16893200	-1.32574200	3.60092800
H	5.55301300	-1.27801300	0.12927400
H	4.65318600	-3.54213000	0.32185800
H	3.45193500	-3.20796200	-0.92127200
H	3.17015300	1.27164400	-0.13991400

H	4.98597400	1.15511100	-2.67554000
H	6.89300500	-0.56682100	-3.32668400
H	6.83680300	0.27097000	-0.31576700
H	7.28174700	1.32862300	-1.72641800
H	3.69633900	-1.34006200	-3.21491100
H	2.38592200	-1.46195400	-2.01550000
H	2.71228100	0.07994800	-2.80465800
C	2.41135500	-3.91556500	2.52365400
H	3.04068800	-4.62165000	1.97316900
H	2.69934200	-3.94043400	3.58153400
H	1.37351200	-4.26881700	2.47238300
C	5.99980900	-1.94433800	-1.81384100
C	6.41504000	-3.13935200	-2.24813500
H	7.15671600	-3.23283100	-3.03803300
H	6.03045200	-4.06618200	-1.82959600
C	2.33407400	4.76228700	0.21085300
C	1.94486000	5.85995300	0.98224900
C	1.48054900	5.63007400	2.27876000
C	1.42739600	4.31600500	2.74518700
C	1.84017300	3.28630600	1.89478200
N	2.28794200	3.49486000	0.64639500
H	1.16657600	6.45716000	2.91061700
H	2.70011600	4.90535900	-0.80465100
H	2.00415600	6.86470900	0.57299500
H	1.07242500	4.08460300	3.74547700
H	1.81197400	2.25013300	2.22436300

endo-TS of py model

C	0.17751700	2.96254500	0.40324500
C	-0.07206500	1.61807900	-0.32413000
C	0.90129500	0.64524200	-0.35374700
C	2.23315200	1.00951600	0.06867900
C	2.54091500	2.34182600	0.24057200
C	1.58722300	3.48813500	0.02735300
C	-0.95000900	3.86952400	-0.13289300
C	-1.90196200	3.00946500	-0.96442400
C	-1.30788400	1.64381900	-1.04072700
C	3.47113800	0.29005200	0.25619000
C	4.40916600	1.23564500	0.52713200

O	3.85475900	2.50286200	0.51117100
C	-1.79973100	0.61846200	-1.89056100
C	-2.34361600	3.62737600	0.36024500
C	0.10464100	2.78495300	1.94254100
O	1.90364800	4.63450400	0.81767800
C	2.82847000	5.53179500	0.22933600
O	2.25835800	6.35518400	-0.75451900
C	1.39352500	7.36495300	-0.24246500
H	0.72220000	-0.32593000	-0.80545000
H	1.59004100	3.77685400	-1.03744400
H	-0.68150900	4.86933600	-0.46287900
H	-2.37515100	3.39720900	-1.86432300
H	3.65228900	-0.77761100	0.20700700
H	5.46260900	1.19940500	0.75746000
H	-2.56912300	0.95393000	-2.58589800
H	-1.03504600	0.02072500	-2.38308100
H	-3.05033600	4.45104400	0.28314300
H	-2.50884400	2.98393500	1.21669400
H	-0.81646900	2.27482500	2.23450400
H	0.94224900	2.18698600	2.31305200
H	0.13631800	3.76002700	2.43734000
H	3.21224000	6.13004700	1.06577100
H	3.64123600	4.99361500	-0.26562300
H	1.05881900	7.95336500	-1.09980700
H	0.52448300	6.93247800	0.26849200
H	1.93248300	8.01983700	0.45849200
C	-3.94212900	-0.71628300	-0.32058900
C	-4.31452400	-2.06509400	0.39421200
C	-3.22637000	-2.50193000	1.38497000
C	-1.94353200	-2.58610800	0.59172500
C	-1.80323300	-1.86857400	-0.62407000
C	-2.71586000	-0.96371700	-1.22201600
C	-5.25625600	-0.33698300	-1.01564200
C	-6.38778700	-1.02072500	-0.24365400
C	-0.87425400	-3.45901300	0.69693300
C	-0.03927300	-3.25760300	-0.46968000
O	-0.66444700	-2.27852800	-1.27754700
C	-6.09382700	-1.38388900	-1.69415900
C	-3.66912100	0.37199800	0.73905200
O	1.01376500	-3.76516800	-0.82298100

H	-4.32669200	-2.84212800	-0.38452000
H	-3.46220900	-3.48104300	1.81927600
H	-3.14756100	-1.79602800	2.22183100
H	-2.96566100	-1.20125000	-2.25759300
H	-5.37140300	0.69501300	-1.34068700
H	-7.32103000	-0.51005100	-0.02211500
H	-5.68293400	-2.36228800	-1.92911500
H	-6.81366100	-1.02678900	-2.42647000
H	-4.40467800	0.31383900	1.54962400
H	-2.66727300	0.27807900	1.17057800
H	-3.74803900	1.36232500	0.28829500
C	-0.56051600	-4.47842400	1.74500100
H	-1.39729000	-4.60838600	2.43966900
H	-0.32910000	-5.45231100	1.29607500
H	0.32034500	-4.18810800	2.33487900
C	-5.75559900	-1.86205900	0.81788900
C	-6.34073800	-2.28810300	1.94289300
H	-7.39047700	-2.09091000	2.14871800
H	-5.79388500	-2.84971000	2.69616800
C	4.33670600	-3.91714100	-0.43324000
C	4.90339400	-5.14441700	-0.79349700
C	6.26257100	-5.35235700	-0.55797900
C	7.00280600	-4.32451900	0.03051400
C	6.34545500	-3.13512000	0.35350300
N	5.04034000	-2.92158400	0.13145700
H	6.73614000	-6.29396300	-0.82560900
H	3.27843000	-3.73167500	-0.60055700
H	4.28279800	-5.91179000	-1.24740900
H	8.06396900	-4.43719000	0.23590500
H	6.89254900	-2.31339400	0.81391200

exo-reactant of py model

C	4.32367400	-1.43113500	0.05038400
C	4.53212100	-1.70677300	-1.45925700
C	5.47205100	-1.05246000	-2.17750600
C	6.20162100	0.03531600	-1.53601800
C	5.72999700	0.54866200	-0.35805900
C	4.47455100	0.08812300	0.33554100
C	2.87947500	-1.91149100	0.30174800

C	2.36882800	-2.62130200	-0.94217600
C	3.47418200	-2.61169000	-1.95941800
C	7.33585500	0.84662700	-1.89235100
C	7.45871100	1.77888600	-0.90527000
O	6.47432900	1.61476900	0.04030000
C	3.45319200	-3.26237900	-3.13584200
C	2.59581600	-3.39000000	0.34491600
C	5.37247100	-2.21223100	0.88297600
O	4.50066400	0.31190800	1.74770300
C	4.07189900	1.59131100	2.16335400
O	2.67592500	1.76017100	2.12267400
C	1.96676100	1.00200000	3.10435900
H	5.60844800	-1.24084100	-3.24027900
H	3.60523200	0.61579200	-0.09154400
H	2.21783800	-1.26369700	0.86796400
H	1.34689200	-2.49583600	-1.29026800
H	7.97732000	0.74367400	-2.75785400
H	8.15702200	2.57932800	-0.71417500
H	2.60207000	-3.87188700	-3.42775600
H	4.27889800	-3.20607300	-3.84116200
H	1.70360300	-3.69061400	0.88785700
H	3.41422900	-4.10323900	0.38593800
H	5.39243400	-3.26492400	0.58910200
H	6.37808100	-1.80663100	0.73167400
H	5.13362600	-2.15217200	1.94874000
H	4.44401500	1.69356200	3.19114000
H	4.48390300	2.37712600	1.52362900
H	0.90869000	1.24089100	2.97998800
H	2.11401500	-0.07392400	2.96449900
H	2.29015500	1.28760300	4.11647200
C	-5.47568500	0.44632900	-0.18387300
C	-5.81824400	-1.04660900	-0.51684300
C	-5.36530400	-2.02948300	0.56590200
C	-3.89114200	-1.78003200	0.78294600
C	-3.31230200	-0.48911800	0.41505300
C	-3.97093800	0.57744600	-0.06937700
C	-6.11819600	1.16926200	-1.39748800
C	-7.22981700	0.26486700	-1.92744200
C	-2.89026900	-2.56701700	1.25164200
C	-1.64274100	-1.77934600	1.18004400

O	-1.94896200	-0.52255500	0.66550400
C	-7.55960800	1.61088500	-1.31815600
C	-6.08682800	0.90738200	1.16747200
O	-0.50818000	-2.08040900	1.48181200
H	-5.19836900	-1.26747800	-1.40144800
H	-5.53762400	-3.06941600	0.26180100
H	-5.92329000	-1.87735600	1.50065100
H	-3.46223500	1.51629400	-0.28868100
H	-5.45439300	1.69316300	-2.08069700
H	-7.39504700	0.13864500	-2.99558200
H	-7.86999400	2.38689700	-2.01470300
H	-8.07079700	1.65391400	-0.36214400
H	-7.14945200	0.65448500	1.24534400
H	-5.56957300	0.44185800	2.01183500
H	-5.98427100	1.99303300	1.27438000
C	-2.90485800	-3.97226300	1.75990500
H	-2.59571500	-4.01170100	2.81221000
H	-3.90150200	-4.41688400	1.67907200
H	-2.19722200	-4.59775000	1.20221700
C	-7.22568400	-0.97789700	-1.06599900
C	-8.23140100	-1.83618100	-0.87244700
H	-9.20394100	-1.68927100	-1.33628900
H	-8.11720600	-2.72030600	-0.24886200
C	-1.90478200	4.67122300	-0.78322700
C	-0.81679700	5.52327000	-0.57938300
C	0.34590800	4.99362600	-0.01562700
C	0.37457100	3.63817100	0.31670200
C	-0.76798100	2.87137500	0.06831700
N	-1.89403300	3.36748600	-0.46919900
H	1.21311000	5.62523700	0.16143000
H	-2.82834400	5.05064800	-1.21802200
H	-0.88464800	6.57221500	-0.85504000
H	1.25117700	3.17691800	0.76385900
H	-0.78375700	1.81111300	0.31212400
<i>exo</i> -TS of py model			
C	2.72515100	0.53834000	0.00281500
C	1.60802200	-0.43690100	-0.44811800
C	1.74122500	-1.79075300	-0.26573200

C	3.04253400	-2.29582900	0.11093600
C	4.13563000	-1.46515600	0.01948900
C	4.09834300	-0.03075900	-0.44489900
C	2.35343200	1.84893700	-0.72130800
C	1.01447300	1.65389800	-1.42727600
C	0.59042000	0.25169400	-1.18184600
C	3.56362400	-3.58792300	0.48058600
C	4.91199900	-3.43490900	0.58706000
O	5.27815000	-2.13910300	0.29748600
C	-0.60817200	-0.31376600	-1.66885400
C	1.14643300	2.60136900	-0.23866600
C	2.73248300	0.71074000	1.54422200
O	5.15727000	0.75663900	0.09937900
C	6.36209800	0.73894900	-0.64319000
O	6.32571100	1.54886500	-1.78964800
C	6.33992600	2.94731700	-1.51619200
H	0.95093200	-2.48464600	-0.54044100
H	4.15988400	0.00059400	-1.54609300
H	3.15148100	2.40746900	-1.20264100
H	0.79991500	2.09381100	-2.39890400
H	3.00708200	-4.49896200	0.65661400
H	5.72192400	-4.09443300	0.85845200
H	-1.04612100	0.22518200	-2.50629800
H	-0.59959600	-1.39027300	-1.82779200
H	1.09512200	3.66244300	-0.47247800
H	0.66823800	2.32058700	0.69289100
H	1.74104500	0.96336600	1.92238400
H	3.05173800	-0.20691000	2.04741900
H	3.42759400	1.50810900	1.82314300
H	7.13046100	1.08858700	0.05851900
H	6.59421700	-0.26881900	-0.99891900
H	6.34619500	3.45443800	-2.48371700
H	5.45642600	3.25615400	-0.94453800
H	7.24521800	3.22467400	-0.95551700
C	-3.22541100	-1.17017800	-0.95846600
C	-2.86850100	-2.60341700	-0.42978300
C	-2.90427300	-2.72573700	1.09404300
C	-2.09618400	-1.58361400	1.65912000
C	-1.77358300	-0.45891600	0.85628100
C	-2.11801700	-0.19147400	-0.48933500

C	-3.35478400	-1.42548100	-2.48615200
C	-3.60331200	-2.91610600	-2.69900900
C	-1.61702200	-1.35104900	2.93561600
C	-0.94853800	-0.06565000	2.91615100
O	-1.07120900	0.45477400	1.59725000
C	-4.67129600	-1.90429100	-3.05209700
C	-4.55884300	-0.63849500	-0.36928800
O	-0.35734600	0.57260000	3.76960300
H	-1.81462600	-2.74910700	-0.72151100
H	-2.49284600	-3.69087900	1.41737000
H	-3.93702200	-2.68769400	1.46946200
H	-2.32383400	0.85972600	-0.69956700
H	-2.70756700	-0.88120400	-3.16454200
H	-3.12955200	-3.46655900	-3.50950700
H	-4.83497200	-1.72586300	-4.11294000
H	-5.57732600	-1.86525700	-2.45726300
H	-5.36505700	-1.37439900	-0.45239800
H	-4.45467100	-0.38033000	0.68813200
H	-4.86708100	0.26711300	-0.90306200
C	-1.70578800	-2.19612500	4.16648700
H	-2.26387500	-1.68807600	4.96459500
H	-2.20441500	-3.14918900	3.96004200
H	-0.70894900	-2.41235400	4.57341400
C	-3.63513600	-3.54838500	-1.33002600
C	-4.19386900	-4.71743100	-1.00085500
H	-4.71003000	-5.32875700	-1.73753900
H	-4.15234400	-5.10796600	0.01346400
C	-3.75556900	4.30044600	-1.10585900
C	-4.05937200	5.53470600	-0.52577500
C	-3.63108100	5.77829300	0.78073300
C	-2.91950000	4.77954400	1.44668700
C	-2.66577300	3.57850600	0.77767200
N	-3.07319600	3.33216500	-0.47762600
H	-3.84792800	6.72552800	1.26831500
H	-4.07512200	4.07675500	-2.12265700
H	-4.61669400	6.28038000	-1.08618600
H	-2.56412600	4.91936500	2.46370700
H	-2.11257900	2.77968900	1.26638800

endo-reactant of py-H⁺ model

C	-1.63649000	-2.37657200	1.32848500
C	-2.80902100	-1.37612900	1.45987600
C	-3.78528900	-1.29861600	0.52629800
C	-3.63463500	-2.06717100	-0.70192100
C	-2.41473800	-2.61601500	-0.99659800
C	-1.17575900	-2.48335200	-0.15136600
C	-0.53921200	-1.75261200	2.21784500
C	-1.13724100	-0.58845800	2.99535800
C	-2.59040200	-0.49056500	2.62309300
C	-4.47831500	-2.34931900	-1.83377200
C	-3.70396500	-3.04152200	-2.71572300
O	-2.43127800	-3.20273700	-2.21929500
C	-3.49624200	0.29785200	3.23397700
C	-0.67795600	-1.84298700	3.71414200
C	-2.09137000	-3.77576300	1.81935600
O	-0.28748800	-3.58978400	-0.29628900
C	0.66880300	-3.47948500	-1.33202900
O	1.80914300	-2.74402000	-0.95953000
C	2.65863200	-3.43346800	-0.03785200
H	-4.62369400	-0.61232700	0.63283400
H	-0.63967800	-1.55778600	-0.42653200
H	0.46244600	-1.68805800	1.80100600
H	-0.58908000	0.33328300	3.17622800
H	-5.52101700	-2.09188000	-1.96522700
H	-3.88705100	-3.49209400	-3.67913300
H	-4.54554100	0.29355300	2.94564700
H	-3.22239800	0.91684200	4.08455900
H	0.23223600	-1.75553500	4.30280000
H	-1.42524900	-2.49576900	4.15421100
H	-2.56884300	-3.70824400	2.80011800
H	-2.81755400	-4.21589500	1.12931700
H	-1.23527900	-4.45167400	1.89277000
H	0.94032800	-4.51195400	-1.58339100
H	0.25177000	-2.96876700	-2.20458700
H	3.54357900	-2.80956400	0.10399800
H	2.15759300	-3.59254900	0.92411700
H	2.96615000	-4.40506200	-0.44939600
C	4.13258300	1.79625300	0.48189600
C	4.11428600	0.39362900	-0.21879400

C	3.52179500	0.41819400	-1.63133000
C	2.16460400	1.06425500	-1.51853900
C	1.86008400	1.91179800	-0.37440900
C	2.70482400	2.27840800	0.60312900
C	1.04960100	1.00022800	-2.30025600
C	0.02703300	1.79544300	-1.62838400
O	0.53451300	2.33407200	-0.47253900
C	4.90716600	2.86490800	-0.33901900
O	-1.14436200	2.00475700	-1.95057900
H	3.40764000	-0.19686700	0.38737100
H	3.41896100	-0.59451700	-2.03745500
H	4.15667700	0.98422600	-2.32749500
H	2.39775400	2.95677500	1.39611000
H	5.88575700	2.49241700	-0.65626300
H	4.35509700	3.15729100	-1.23765000
H	5.06567700	3.76521900	0.26451800
C	4.84089500	1.44909900	1.81821400
H	4.26950600	1.55310300	2.73777700
C	5.69371600	0.20664300	1.56429200
H	5.76270600	-0.58946400	2.30255500
C	6.34654800	1.53025600	1.89617800
H	6.77649500	1.61447400	2.89146000
H	6.91091500	2.05483900	1.13269400
C	5.46831000	-0.18831300	0.12207900
C	6.27020300	-0.92093500	-0.65558400
H	7.22216700	-1.30115100	-0.29359400
H	6.00388600	-1.17160800	-1.67999600
C	0.80266000	0.28602000	-3.59029500
H	-0.14915000	-0.25578000	-3.56372000
H	0.74362500	0.99279000	-4.42803800
H	1.60390700	-0.42667400	-3.80356200
C	-3.52388200	2.85150700	0.61047300
C	-4.55438400	3.53425500	1.24208100
C	-5.09103000	4.67121200	0.63120600
C	-4.58676800	5.10314800	-0.60052200
C	-3.55578000	4.38624500	-1.18864800
N	-3.05849700	3.29408300	-0.57418400
H	-5.89769300	5.21816800	1.11050400
H	-3.06112200	1.95997900	1.02358900
H	-4.92287700	3.17483400	2.19642000

H	-4.98426500	5.98067400	-1.09840600
H	-3.10465000	4.64649800	-2.13964200
H	-2.27006300	2.77294600	-1.04897300

endo-TS of py-H⁺ model

C	2.38605200	-1.39974400	1.64342100
C	0.95715700	-0.81465000	1.55612900
C	-0.01886300	-1.42723000	0.80712700
C	0.38158100	-2.48153700	-0.09004600
C	1.72280200	-2.65904700	-0.35621100
C	2.84781500	-1.83505000	0.22560100
C	3.20782500	-0.21872800	2.19798300
C	2.25971500	0.93937300	2.48934700
C	0.88325700	0.49012400	2.13859900
C	-0.31645900	-3.41629500	-0.93708300
C	0.64511100	-4.08036500	-1.63213500
O	1.89920500	-3.61430600	-1.28947100
C	-0.26933100	1.28530500	2.22688600
C	2.96303100	0.19754900	3.62000100
C	2.42505100	-2.63178300	2.58434300
O	4.07447300	-2.54563000	0.31342600
C	4.88570100	-2.49356100	-0.85752600
O	5.50536700	-1.25497900	-1.04398700
C	6.61792800	-1.01287400	-0.18181800
H	-1.04816600	-1.08477900	0.82238700
H	2.99393400	-0.93701800	-0.39833100
H	4.18935300	-0.03650200	1.77021800
H	2.53048700	1.97543600	2.31950500
H	-1.38393500	-3.57762300	-1.00478300
H	0.63302200	-4.87806500	-2.35864400
H	-1.22018800	0.76618800	2.31454600
H	-0.20190700	2.17752800	2.84432700
H	3.75539600	0.74498200	4.12440400
H	2.36985800	-0.42926000	4.27858300
H	1.98008900	-2.39799100	3.55436500
H	1.87348000	-3.47743100	2.16265400
H	3.45965300	-2.94733100	2.74243600
H	5.62038400	-3.29537000	-0.71762800
H	4.28488300	-2.67178300	-1.75354000

H	7.02084900	-0.03744100	-0.46130700
H	6.31562900	-0.99929000	0.87250900
H	7.39205600	-1.77960300	-0.32521500
C	0.15687600	3.09144900	-0.19271500
C	1.11251400	2.17148900	-1.02427800
C	0.42327800	1.46298500	-2.19320600
C	-0.85433200	0.85101200	-1.67619500
C	-1.36825700	1.21325500	-0.41028800
C	-0.89315200	2.19187700	0.47853800
C	-1.76685700	-0.00367500	-2.28832900
C	-2.83806200	-0.17610500	-1.36605700
O	-2.58864500	0.56779100	-0.21807200
C	-0.63771100	4.08828700	-1.08364500
O	-3.89178700	-0.85022000	-1.43966500
H	1.40673800	1.38145100	-0.31551700
H	1.07558500	0.69132200	-2.62189600
H	0.19743100	2.16250900	-3.01066600
H	-1.65129400	2.70864500	1.06666400
H	0.02089400	4.60470700	-1.78792700
H	-1.41287100	3.58449000	-1.66787500
H	-1.12221700	4.84850700	-0.46047700
C	1.15351500	3.84433200	0.72574300
H	1.04097100	3.74389700	1.80059900
C	2.53101300	3.77878200	0.07023400
H	3.43742200	3.62003600	0.65100000
C	1.81887300	5.10369000	0.21999200
H	2.21179700	5.77790900	0.97760300
H	1.45067900	5.61000100	-0.66539700
C	2.36468000	3.00152300	-1.21336600
C	3.17658900	3.02022700	-2.27403200
H	4.06635600	3.64434400	-2.29993700
H	2.98899100	2.40628400	-3.15186700
C	-1.72677400	-0.62854600	-3.64959200
H	-1.75448100	-1.72347500	-3.59093000
H	-2.58497800	-0.31840300	-4.25890400
H	-0.81540700	-0.34486100	-4.18458300
C	-5.99793200	0.08357400	1.21578400
C	-7.15304400	0.15818400	1.98185300
C	-8.27983400	-0.56341000	1.57503400
C	-8.22515600	-1.34028200	0.41359900

C	-7.04236800	-1.37566900	-0.31251500
N	-5.97206200	-0.67267500	0.10287300
H	-9.19466000	-0.51979400	2.15870300
H	-5.07919000	0.60934000	1.45249200
H	-7.16771700	0.76971300	2.87740000
H	-9.08346800	-1.90921900	0.07339700
H	-6.91192200	-1.94817400	-1.22435200
H	-5.06140000	-0.71319800	-0.48902800

endo-product of the py-H⁺ model

C	-1.62756600	-2.26254500	-0.10044800
C	-0.58665100	-1.19410100	-0.45103800
C	0.15948400	-0.43672500	0.62218100
C	-0.79705200	-0.23101300	1.78216300
C	-2.07127800	-0.73229300	1.76543400
C	-2.75775900	-1.53704000	0.68892100
C	-2.10699500	-2.72319500	-1.48989500
C	-1.40043900	-1.88047400	-2.54242700
C	-0.48914000	-0.98314800	-1.77270600
C	-0.60645900	0.31124700	3.10456600
C	-1.78179400	0.12318900	3.76587900
O	-2.68538800	-0.51179900	2.96030300
C	0.46137700	0.01703900	-2.35656000
C	-1.12201000	-3.36999600	-2.42943800
C	-1.05760400	-3.42685900	0.73907200
O	-3.67139000	-2.48386300	1.23296000
C	-5.00585300	-2.01405100	1.37994000
O	-5.70551900	-1.94706400	0.16935700
C	-6.11912900	-3.21287300	-0.34387700
H	0.97868500	-1.06495300	1.00323200
H	-3.29668200	-0.88064400	-0.00909000
H	-3.15497500	-2.98534500	-1.59894600
H	-1.90391400	-1.50360700	-3.43016600
H	0.28259700	0.77350700	3.51204500
H	-2.12625900	0.36109100	4.76093100
H	1.44729500	-0.45243600	-2.49860900
H	0.15049400	0.33602600	-3.35680300
H	-1.53416800	-4.01494300	-3.20185500
H	-0.14624700	-3.67903600	-2.06230700

H	-0.21586000	-3.89710100	0.22102200
H	-0.70897400	-3.08864300	1.72083500
H	-1.82766000	-4.18537600	0.90350800
H	-5.47565300	-2.72164000	2.07386800
H	-5.01850300	-1.00152600	1.79286400
H	-6.67611900	-3.01000700	-1.26090500
H	-5.26030300	-3.85707300	-0.56926900
H	-6.77609300	-3.72563100	0.37298800
C	-0.47602600	2.37983800	-1.52921100
C	-1.25184800	2.48208800	-0.17599100
C	-0.36179400	2.89934000	0.99393000
C	0.89390300	2.07492000	0.92321500
C	0.93148500	0.83819200	0.04486200
C	0.63465900	1.24977700	-1.44755800
C	2.12146800	2.32349100	1.43319800
C	3.02096600	1.29730400	0.91332600
O	2.36002900	0.45356700	0.09503600
C	0.26771600	3.70421300	-1.83333700
O	4.23132900	1.15911400	1.12452300
H	-1.59799800	1.46059100	0.03430200
H	-0.87699100	2.72672700	1.94744700
H	-0.10829000	3.96624000	0.95973700
H	1.56765500	1.72690400	-1.76575300
H	-0.37045300	4.58102600	-1.69281900
H	1.13836600	3.83280100	-1.18048200
H	0.62660200	3.70918600	-2.86919800
C	-1.65857800	2.14936300	-2.51610800
H	-1.71041200	1.21599700	-3.06427500
C	-2.92485100	2.70412000	-1.87099200
H	-3.87455200	2.17915700	-1.94934600
C	-2.36476700	3.34003500	-3.12364800
H	-2.91934900	3.15958200	-4.04170400
H	-1.92671300	4.33056100	-3.06819900
C	-2.52113000	3.23226100	-0.51786600
C	-3.17071800	4.12751900	0.23124500
H	-4.09291800	4.59123400	-0.10981800
H	-2.81356100	4.42442200	1.21496200
C	2.60028800	3.42886500	2.32234300
H	3.41304500	3.99220000	1.84890000
H	1.79138300	4.12381100	2.56254500

H	2.99666800	3.02969700	3.26390100
C	5.22135400	-1.76385700	-0.64482700
C	6.03130400	-2.78419600	-1.12216600
C	7.38292000	-2.79801900	-0.76244400
C	7.89385900	-1.79293600	0.06520200
C	7.03896500	-0.79635700	0.51408800
N	5.74161000	-0.80920900	0.15070000
H	8.03440500	-3.58778800	-1.12474600
H	4.16433900	-1.67036100	-0.86910200
H	5.60958500	-3.55144400	-1.76208600
H	8.93738600	-1.77953800	0.35995000
H	7.34806700	0.01960600	1.15795600
H	5.10045600	-0.03718300	0.50798200

exo-reactant of py-H⁺ model

C	-4.11934700	-1.38122200	-0.09534700
C	-4.73483800	-1.73787000	1.28205000
C	-4.41867700	-1.05380000	2.40393200
C	-3.36261200	-0.04946700	2.32846800
C	-2.55153600	-0.01608600	1.22814700
C	-2.62943100	-0.97658400	0.07548400
C	-4.26310500	-2.69289900	-0.89672200
C	-5.12708300	-3.66271900	-0.10636000
C	-5.54103800	-2.97188000	1.16343300
C	-2.83596900	0.93661400	3.23570900
C	-1.75452400	1.48562700	2.61491200
O	-1.55855500	0.90810100	1.37874900
C	-6.43794400	-3.43986600	2.04692600
C	-5.62094300	-3.09309700	-1.41936400
C	-4.90477700	-0.20112600	-0.72226800
O	-2.10882900	-0.40053800	-1.13820500
C	-0.77033100	-0.77681800	-1.44818900
O	-0.65122900	-2.07021400	-1.95808900
C	-1.12903600	-2.22958000	-3.29606700
H	-4.84741200	-1.31389000	3.36859800
H	-2.04408800	-1.88106100	0.30459400
H	-3.38604300	-3.04640500	-1.43117400
H	-4.89828100	-4.72435700	-0.05995400
H	-3.21183000	1.20055700	4.21547400

H	-1.04950300	2.25751800	2.88391700
H	-6.94945600	-4.38465500	1.88583700
H	-6.68908400	-2.89791000	2.95512900
H	-5.64145400	-3.77291100	-2.26800200
H	-6.44523300	-2.38650400	-1.40236500
H	-5.97859000	-0.40120600	-0.71414600
H	-4.74254400	0.72134900	-0.15341400
H	-4.59383600	-0.04350600	-1.76045000
H	-0.43139900	-0.03257700	-2.18176800
H	-0.14614600	-0.74187900	-0.55194600
H	-0.93095400	-3.26634700	-3.57406900
H	-2.20449900	-2.02985500	-3.36453200
H	-0.58876900	-1.55989400	-3.98066600
C	4.73511200	-1.55455200	-0.07768600
C	5.80173900	-0.40718300	-0.00833800
C	5.44934300	0.69175400	0.99976300
C	3.17508500	0.31028800	-0.11915000
C	3.42032300	-0.94958200	-0.51619500
C	5.40629800	-2.51834100	-1.09147400
C	6.91145100	-2.25943000	-1.02776300
C	2.09470900	2.22261000	0.24939000
O	1.98286500	0.99458500	-0.35208700
C	6.34241800	-3.58830000	-0.58257900
C	4.48850700	-2.22389400	1.30353500
O	1.17100000	3.03351800	0.19999600
H	5.74835000	0.06693800	-1.00240300
H	6.16461000	1.52194600	0.95819600
H	5.46766900	0.31146100	2.03074400
H	2.67622900	-1.53376500	-1.05363000
H	4.90999000	-2.67670100	-2.04606900
H	7.51849200	-2.24517700	-1.93034600
H	6.52106600	-4.43102300	-1.24625600
H	6.35980200	-3.85171900	0.46949400
H	5.43028800	-2.49654800	1.78905500
H	3.94604700	-1.55637700	1.98034700
H	3.89145100	-3.13413000	1.18202700
C	3.84056500	3.57258500	1.61633300
H	3.76748200	4.46086100	0.97748600
H	3.20422700	3.75433900	2.49135900
H	4.87388500	3.48272700	1.96238100

C	3.40798500	2.34364400	0.88247400
C	4.06370800	1.17255200	0.64741600
C	7.11968000	-1.14916400	-0.02263500
C	8.23083600	-0.86861600	0.66288400
H	9.13108300	-1.46865500	0.55796300
H	8.28653500	-0.02486700	1.34717200
C	-2.33853800	2.84006900	-1.27589000
C	-3.44690100	3.52034800	-1.76458400
C	-3.43893800	4.91727900	-1.78651400
C	-2.31872600	5.61460400	-1.31981900
C	-1.23567400	4.89343200	-0.84357500
N	-1.27697400	3.54459200	-0.83508300
H	-4.29958500	5.46148000	-2.16436300
H	-2.27168000	1.75510400	-1.22305000
H	-4.30176400	2.95431400	-2.11747000
H	-2.28390200	6.69842100	-1.32419000
H	-0.32438300	5.33955300	-0.46244700
H	-0.42670600	3.06361400	-0.46642200

exo-TS of py-H⁺ model

C	-1.13600500	-2.85730500	0.40106200
C	0.21573000	-2.34894000	0.95484500
C	0.27545400	-1.49151100	2.02013200
C	-0.94922000	-0.85270200	2.43862200
C	-2.05565800	-0.93147400	1.62357800
C	-2.13342800	-1.66095400	0.30758800
C	-0.75026000	-3.42232000	-0.98278800
C	0.76329600	-3.31114900	-1.15212400
C	1.30269200	-2.69600900	0.08360200
C	-1.30735700	0.03764800	3.51356200
C	-2.58739400	0.42307100	3.26943500
O	-3.05529200	-0.15374300	2.10166500
C	2.62921700	-2.29619400	0.25938000
C	0.08195400	-4.67028600	-1.02850400
C	-1.73857700	-3.94051700	1.33109200
O	-3.47644900	-2.07667100	0.06056200
C	-4.05328700	-1.68525300	-1.17225700
O	-3.71413900	-2.49988600	-2.25703800
C	-4.33291600	-3.78853000	-2.24735400

H	1.22104200	-1.18603100	2.46020600
H	-1.81287600	-0.97320700	-0.49022400
H	-1.41229500	-3.21161500	-1.81713400
H	1.23267900	-3.06351200	-2.10151500
H	-0.70037900	0.33150400	4.35952000
H	-3.29989900	1.03263200	3.80408700
H	3.39313700	-2.79774700	-0.32968100
H	2.93514200	-2.04178300	1.26604700
H	0.04436200	-5.26125600	-1.94017300
H	0.25338300	-5.25450800	-0.12952500
H	-1.01648700	-4.73728800	1.52351200
H	-2.03410000	-3.52227300	2.29819600
H	-2.62628400	-4.38189200	0.86986200
H	-5.13631100	-1.71201200	-0.99287600
H	-3.72222800	-0.67764100	-1.44852900
H	-4.06460400	-4.26800700	-3.19066800
H	-3.97524800	-4.39823200	-1.40944500
H	-5.42609500	-3.69256800	-2.18679100
C	4.32674100	0.05106800	-0.16361400
C	4.38383600	1.60131300	-0.44486900
C	3.40460400	2.38683800	0.44041900
C	1.91651800	0.48488900	-0.34490800
C	2.93776700	-0.44113000	-0.62342800
C	5.50078800	-0.45626400	-1.03934200
C	6.46038500	0.71389800	-1.24784800
C	-0.07703200	1.45909000	-0.54985400
O	0.61867000	0.29829900	-0.79536400
C	6.89434500	-0.50174500	-0.45995400
C	4.56859800	-0.20129400	1.34542800
O	-1.28594800	1.50628700	-0.88913200
H	4.02639100	1.71776100	-1.48090500
H	3.41128800	3.45324000	0.18489300
H	3.68169500	2.31531200	1.50002200
H	2.88736000	-0.93106000	-1.59408900
H	5.26495900	-1.12945100	-1.86081600
H	6.93455400	0.89159500	-2.21054400
H	7.60479900	-1.16363300	-0.94959600
H	7.04592800	-0.41283300	0.61071100
H	5.35340500	0.45886900	1.72725100
H	3.66691000	-0.00794400	1.93548800

H	4.89093200	-1.22946600	1.53111400
C	0.39913500	3.82169900	0.38614700
H	0.02193100	4.36411400	-0.49192500
H	-0.38935500	3.84771500	1.15108600
H	1.24837900	4.38831600	0.77972400
C	0.79643600	2.41718800	0.04763500
C	2.04116600	1.79942300	0.16238000
C	5.86643900	1.89716000	-0.52089300
C	6.51000800	2.98254300	-0.08232000
H	7.58307300	3.09912000	-0.21205600
H	5.98911900	3.79921600	0.41260900
C	-4.35208300	2.51338900	0.16979700
C	-5.58559600	3.14562200	0.25305000
C	-5.82877800	4.26419300	-0.54979600
C	-4.83493000	4.72400100	-1.41992100
C	-3.62118000	4.05250200	-1.46274800
N	-3.41203300	2.98133600	-0.67435300
H	-6.78700500	4.77301900	-0.50032800
H	-4.07903000	1.63825400	0.75141300
H	-6.33970600	2.76397000	0.93270000
H	-4.99644800	5.58620300	-2.05758300
H	-2.80057000	4.33650300	-2.11224900
H	-2.47050500	2.46125100	-0.72823800

exo-product of the py-H⁺ model

C	-1.05902000	-2.52110800	0.48678600
C	0.08733000	-1.60702300	0.03843300
C	0.64268700	-0.53130900	0.94072500
C	-0.50079500	0.01435700	1.77060300
C	-1.77434100	-0.47179500	1.64847400
C	-2.27285200	-1.57711700	0.74719400
C	-1.29284400	-3.39277700	-0.75955300
C	-0.38099000	-2.88936600	-1.86965200
C	0.41771900	-1.78883800	-1.24974100
C	-0.54459900	0.97579800	2.84301200
C	-1.83596500	1.00977000	3.27260400
O	-2.60248000	0.13481300	2.55098400
C	1.43067600	-0.98176900	-1.99983600
C	-0.17325600	-4.26625600	-1.26274500

C	-0.74820700	-3.36042900	1.74336800
O	-3.36164000	-2.31696700	1.29786500
C	-4.63566700	-1.70864200	1.18962600
O	-5.08137400	-1.55340300	-0.14063900
C	-5.51289900	-2.76804800	-0.76426900
H	1.37537900	-0.95694400	1.64036300
H	-2.59040700	-1.17589500	-0.22620900
H	-2.30949300	-3.71206000	-0.96843200
H	-0.69762100	-2.80855800	-2.90738100
H	0.27342300	1.55120100	3.25282000
H	-2.35252900	1.55766600	4.04623300
H	0.91139600	-0.42483300	-2.79419500
H	2.12689400	-1.64934600	-2.52599000
H	-0.45864300	-5.12608900	-1.86384700
H	0.70906700	-4.42186700	-0.64727600
H	0.13888200	-3.97873500	1.57739100
H	-0.56605400	-2.73228000	2.62192100
H	-1.58862800	-4.02088600	1.97420400
H	-5.30730000	-2.36654500	1.75234000
H	-4.63128800	-0.70414000	1.61883400
H	-5.84262300	-2.50499300	-1.77153400
H	-4.69791400	-3.49753600	-0.82348800
H	-6.35336600	-3.20543600	-0.20927700
C	3.64734200	-0.49610100	-0.68190700
C	4.33007500	0.65024200	0.13116800
C	3.59072700	1.00904100	1.43459600
C	1.40404400	0.55397100	0.09381900
C	2.23568400	0.00503700	-1.12176100
C	4.64194200	-0.59644800	-1.88015100
C	5.99993900	-0.09052300	-1.39164400
C	0.54760300	2.68564900	0.05619800
O	0.37773500	1.44732000	-0.45341100
C	5.82391000	-1.53415600	-1.80404200
C	3.60105600	-1.82436900	0.10315400
O	-0.22636900	3.60249400	-0.22746200
H	4.22990900	1.54019600	-0.51341400
H	4.10765300	1.80090900	1.98576700
H	3.50732200	0.14066600	2.09985300
H	2.42727700	0.89915100	-1.72950200
H	4.27522800	-0.31879700	-2.86601000

H	6.62374500	0.54243400	-2.01933700
H	6.27875500	-1.81646200	-2.75076200
H	5.86334900	-2.31590100	-1.05374900
H	4.57276800	-2.04690100	0.55256000
H	2.87724600	-1.81957800	0.91749400
H	3.34336800	-2.65562500	-0.56075100
C	2.19083800	4.00235400	1.55793600
H	2.43966900	4.75608700	0.80129600
H	1.39592700	4.42998800	2.18051300
H	3.07098700	3.84395500	2.18639400
C	1.73375200	2.72920800	0.91694800
C	2.25321300	1.48162400	0.94109900
C	5.80801900	0.32708100	0.04872900
C	6.73433600	0.42898900	1.00434600
H	7.77551100	0.18040000	0.81533300
H	6.49099100	0.76908800	2.00859200
C	-3.17043300	1.88202400	-0.92548700
C	-4.46976700	1.54150900	-1.27678400
C	-5.25305600	2.49548800	-1.93472600
C	-4.72474500	3.75872000	-2.22554800
C	-3.42082100	4.04398200	-1.84863400
N	-2.68783000	3.10610000	-1.21681600
H	-6.27373800	2.25679000	-2.21933800
H	-2.48492700	1.21652800	-0.41228900
H	-4.84801200	0.55164800	-1.03134700
H	-5.31388900	4.51411900	-2.73388700
H	-2.93459500	4.99621300	-2.02865700
H	-1.69969200	3.32298400	-0.91027100

endo-reactant of double py-H⁺ model

C	3.61033100	1.94786100	0.82041700
C	2.10014400	2.10620100	0.51769400
C	1.16002800	1.56235700	1.32570300
C	1.59192700	0.68503100	2.40508000
C	2.87271100	0.19677500	2.37993200
C	3.88583100	0.49690300	1.30153300
C	4.27618600	2.23082900	-0.54172500
C	3.21451800	2.70686400	-1.52659400
C	1.90110000	2.73753800	-0.80414000

C	0.96128500	0.07570700	3.54758800
C	1.90737200	-0.72382100	4.11771500
O	3.07973800	-0.66502100	3.40369900
C	0.74745600	3.20075400	-1.32419000
C	4.30475700	3.64702600	-1.04428300
C	4.05714400	2.94422700	1.92033300
O	5.23250900	0.38013800	1.73755100
C	5.77028600	-0.93476100	1.67367900
O	6.05348700	-1.35233500	0.36461300
C	7.24578500	-0.78566300	-0.18830800
H	0.09740800	1.67582400	1.11449500
H	3.72102800	-0.19137500	0.45491400
H	5.07021300	1.56106000	-0.85882700
H	3.21844500	2.41833000	-2.57499800
H	-0.04279400	0.23498300	3.91898300
H	1.93026600	-1.34891000	4.99725200
H	-0.17787500	3.19466700	-0.75134400
H	0.71078300	3.62880600	-2.32255500
H	5.07374100	3.90142800	-1.76928200
H	4.03332300	4.46519500	-0.38445400
H	3.74949000	3.96349600	1.67428800
H	3.61637500	2.69092300	2.88923700
H	5.14516100	2.92555000	2.02573900
H	6.67912300	-0.89465900	2.28435700
H	5.06464200	-1.66487100	2.07962800
H	7.36138100	-1.21272100	-1.18649000
H	7.17542900	0.30621300	-0.25857600
H	8.11817300	-1.05447700	0.42203500
C	1.05813700	-2.00603300	-2.14461500
C	0.95734400	-2.87982000	-0.84575100
C	-0.45667300	-3.40905900	-0.57650900
C	-1.37619900	-2.21690200	-0.58782500
C	-0.97219500	-1.00662200	-1.26643400
C	0.15412200	-0.81089700	-1.97818400
C	-2.60736400	-1.99210900	-0.02126200
C	-2.96184200	-0.63116600	-0.35139500
O	-1.98013500	-0.04763800	-1.09030500
C	0.56076200	-2.75608900	-3.41646100
O	-3.97773900	0.05335800	-0.06899300
H	1.17535600	-2.17338700	-0.02820000

H	-0.51762000	-3.93238900	0.38522800
H	-0.76997700	-4.12897000	-1.34648100
H	0.36569700	0.14336600	-2.45658800
H	1.01028200	-3.75086700	-3.48096100
H	-0.52688000	-2.88159400	-3.41791000
H	0.83757400	-2.20010600	-4.31808100
C	2.58002200	-1.71210600	-2.18800400
H	2.90184300	-0.68002700	-2.07187300
C	3.27472700	-2.83982600	-1.42183900
H	4.11771700	-2.63151300	-0.76643800
C	3.49117900	-2.67577500	-2.90952100
H	4.46191200	-2.28882600	-3.20885000
H	3.08589400	-3.41178100	-3.59516000
C	2.18549200	-3.76041900	-0.92032700
C	2.29238700	-5.04820400	-0.58412500
H	3.23716500	-5.57921100	-0.66338000
H	1.44602100	-5.61878600	-0.20801900
C	-3.45492100	-2.91148600	0.80361800
H	-3.74634000	-2.44534600	1.75296800
H	-4.37140500	-3.20640200	0.27590400
H	-2.91217600	-3.82963200	1.04295600
C	-3.18455000	3.09895700	-2.03384800
C	-2.94230800	4.41294300	-2.40393400
C	-3.00135900	5.41432500	-1.42890100
C	-3.30506800	5.07950900	-0.10401500
C	-3.54591400	3.75249400	0.21408400
N	-3.48304900	2.80737300	-0.74954700
H	-2.80866900	6.44875400	-1.69793000
H	-3.14205000	2.26071600	-2.71910700
H	-2.70477200	4.64400900	-3.43659200
H	-3.35159300	5.83483200	0.67288300
H	-3.78338300	3.40895400	1.21431700
H	-3.65774100	1.81334800	-0.49603100
C	-7.39955400	-1.11165800	-0.26570500
C	-8.69828900	-1.49023400	0.03745500
C	-9.09060100	-1.55194700	1.37956400
C	-8.17432000	-1.23224200	2.38823400
C	-6.88714500	-0.85970300	2.03275200
N	-6.53608100	-0.80914300	0.72882600
H	-10.10326500	-1.84779800	1.63774400

H	-7.01500500	-1.04094100	-1.27685600
H	-9.38736600	-1.73326400	-0.76412400
H	-8.45113600	-1.27238800	3.43618200
H	-6.11803000	-0.60028000	2.75138100
H	-5.56172300	-0.53413400	0.47622300

endo-TS1 of double py-H⁺ model

C	3.42793000	-0.02387700	-1.91240800
C	2.04305300	-0.60175900	-1.53890300
C	0.90694900	0.15854000	-1.63533000
C	1.05385800	1.57316400	-1.87185800
C	2.30019000	2.14587900	-1.72053300
C	3.56335000	1.41166800	-1.33394500
C	4.40701100	-1.01524700	-1.25274100
C	3.60083500	-2.15071300	-0.62939900
C	2.16245300	-1.89092200	-0.90439600
C	0.15225100	2.66281000	-2.15284500
C	0.91559200	3.78867700	-2.15728000
O	2.23085000	3.47930200	-1.88057300
C	1.12046100	-2.72984500	-0.51753100
C	4.50239800	-2.39049300	-1.83932000
C	3.60278600	0.03734500	-3.45257900
O	4.73772300	2.02391200	-1.83448300
C	5.31701800	3.01241500	-0.97706700
O	5.93540600	2.46519000	0.14592400
C	7.22561500	1.89703100	-0.10053500
H	-0.07561200	-0.26337500	-1.44195800
H	3.62136200	1.35498200	-0.23316000
H	5.27457800	-0.60819500	-0.74196400
H	3.87684300	-2.62893800	0.30336800
H	-0.90900000	2.61051700	-2.35530900
H	0.71770300	4.83246700	-2.34680300
H	0.16409000	-2.63129400	-1.02156300
H	1.37436600	-3.73938300	-0.20736600
H	5.40555100	-2.96103700	-1.63955700
H	4.04305300	-2.61155600	-2.79741800
H	3.37635900	-0.92684600	-3.91358400
H	2.94151300	0.78330600	-3.90358700
H	4.63268700	0.30738600	-3.69852800

H	6.02862500	3.54370600	-1.61881900
H	4.54715900	3.69440900	-0.60492300
H	7.59628000	1.54167000	0.86255300
H	7.16810200	1.06024000	-0.80729200
H	7.91227800	2.65782300	-0.49461500
C	1.00439900	-1.96192600	2.55609900
C	1.57640900	-0.50986000	2.43443500
C	0.50850500	0.58377500	2.53298000
C	-0.62418000	0.20543800	1.61477400
C	-0.72903300	-1.09530300	1.09334600
C	0.07756900	-2.20353700	1.36747300
C	-1.75420500	0.92908000	1.19984500
C	-2.52496800	0.04047200	0.42345000
O	-1.90135200	-1.18400200	0.33951400
C	0.11605000	-2.15778000	3.82148200
O	-3.65193500	0.16579600	-0.17748000
H	1.96833800	-0.46304900	1.40645600
H	0.92052900	1.56285900	2.25611200
H	0.13221900	0.69002200	3.56097100
H	-0.36553400	-3.19139500	1.26564200
H	0.62015000	-1.77701200	4.71391700
H	-0.84241000	-1.63709100	3.73771400
H	-0.08687500	-3.22229900	3.98112900
C	2.29603400	-2.81163200	2.65003700
H	2.46984000	-3.56356100	1.88679500
C	3.41809800	-1.89078100	3.12752000
H	4.42293900	-1.94910600	2.71484700
C	2.94325800	-3.03021400	3.99840200
H	3.60960100	-3.88592200	4.07579500
H	2.41070500	-2.81048300	4.91697600
C	2.80755400	-0.52225400	3.31625200
C	3.27812200	0.47222800	4.07323200
H	4.18767000	0.36129000	4.65763900
H	2.78055200	1.43757200	4.13182600
C	-2.10629300	2.35421100	1.51141300
H	-2.60136000	2.83871600	0.66163500
H	-2.76971800	2.44241100	2.38305700
H	-1.20805800	2.93776800	1.73517700
C	-4.13578400	-3.12217400	-1.51396900
C	-4.45844900	-4.16726500	-2.36731100

C	-4.86056100	-3.87418400	-3.67494200
C	-4.92958700	-2.54240200	-4.09910100
C	-4.59788800	-1.53612000	-3.20419400
N	-4.21579000	-1.84741700	-1.94808300
H	-5.11720300	-4.67747600	-4.35937500
H	-3.80598800	-3.25635600	-0.49021800
H	-4.39468600	-5.19031600	-2.01280000
H	-5.23471900	-2.28636600	-5.10790100
H	-4.62218800	-0.48121900	-3.45320100
H	-3.97174800	-1.07008100	-1.27285300
C	-6.34445900	1.24575900	1.86189400
C	-7.41482500	1.95666200	2.38406200
C	-7.77115000	3.17397800	1.79334000
C	-7.04838000	3.65114600	0.69416500
C	-5.98643600	2.90040000	0.21252900
N	-5.66458400	1.72879800	0.80054400
H	-8.60540400	3.74718700	2.18708000
H	-6.00209100	0.29762200	2.26098100
H	-7.95616800	1.56340600	3.23767200
H	-7.30142400	4.59200700	0.21759900
H	-5.37457400	3.20056300	-0.63055500
H	-4.85055000	1.16883100	0.42470900

endo-intermediate of double py-H⁺ model

C	-3.45276300	1.83336600	-0.26966000
C	-2.05320500	1.56350200	0.32488200
C	-0.91790800	1.52865600	-0.49552900
C	-1.12404900	1.40302600	-1.89361200
C	-2.40457100	1.11465100	-2.36536300
C	-3.64724800	0.93656400	-1.52416700
C	-4.38922900	1.44759600	0.89339200
C	-3.51864800	0.99721000	2.06981800
C	-2.11354800	1.12650000	1.64711600
C	-0.26522300	1.38931700	-3.05625500
C	-1.07074500	1.11381400	-4.11003400
O	-2.38235200	0.93306400	-3.68375200
C	-0.96176700	0.77419600	2.52545900
C	-4.34318600	2.29558100	2.12005100
C	-3.62700600	3.31680200	-0.68358000

O	-4.82706500	1.29668700	-2.21025200
C	-5.48504800	0.22037800	-2.89831100
O	-6.09447100	-0.68044300	-2.03290600
C	-7.36297000	-0.25701000	-1.51850200
H	0.08594500	1.54902300	-0.08548200
H	-3.70570400	-0.11980700	-1.20953300
H	-5.30862400	0.91870300	0.66026600
H	-3.79810000	0.20265600	2.75161400
H	0.79857000	1.57741500	-3.09231300
H	-0.92192300	1.02229000	-5.17483300
H	-0.20456500	1.56390600	2.44557900
H	-1.30429300	0.77014400	3.56397300
H	-5.19946000	2.26468000	2.78826800
H	-3.81231500	3.24212000	2.11772900
H	-3.37552000	3.98802000	0.14068500
H	-2.99019800	3.58141500	-1.53360200
H	-4.66397900	3.49868500	-0.97553200
H	-6.20640200	0.72301200	-3.55142500
H	-4.76051000	-0.35041900	-3.48639300
H	-7.72634800	-1.06974300	-0.88758800
H	-7.26967600	0.66080900	-0.92526400
H	-8.07275300	-0.08936700	-2.33864200
C	-0.91172500	-1.94616200	2.34422800
C	-1.54444000	-2.19605600	0.93129100
C	-0.51047200	-2.46991600	-0.16525000
C	0.58140400	-1.43974400	-0.03746800
C	0.66049300	-0.59865200	1.04702000
C	-0.14199900	-0.58345200	2.30024000
C	1.73352700	-1.20600800	-0.85755300
C	2.47954000	-0.23894900	-0.20221300
O	1.82815500	0.15327100	0.96327100
C	0.12126700	-3.03498300	2.72971900
O	3.62769100	0.33115600	-0.44554100
H	-2.02542500	-1.23942200	0.67029400
H	-0.97716600	-2.43167800	-1.15907800
H	-0.08635000	-3.47985100	-0.06902900
H	0.55467000	-0.56077200	3.15075400
H	-0.24750100	-4.03970700	2.50514500
H	1.06809400	-2.91035600	2.19486100
H	0.33003700	-2.99166600	3.80457000

C	-2.15187000	-2.01176700	3.27206000
H	-2.37411500	-1.15892100	3.90669700
C	-3.26332700	-2.75231600	2.53011000
H	-4.30478000	-2.44198600	2.58534300
C	-2.63633200	-3.35601200	3.76499500
H	-3.24207400	-3.34769300	4.66794700
H	-2.01754300	-4.24068400	3.66283100
C	-2.70154500	-3.14125600	1.18516000
C	-3.15744400	-4.10067000	0.37483300
H	-4.01098000	-4.71668100	0.64566700
H	-2.69968200	-4.30561400	-0.59019700
C	2.07421200	-1.87964300	-2.15561200
H	2.82870900	-1.31082200	-2.71071400
H	2.46061100	-2.89881000	-2.01460700
H	1.19398800	-1.96373800	-2.80372900
C	4.06065700	2.47321400	2.30533700
C	4.43333400	3.56133500	3.08211500
C	4.98060300	4.68499900	2.45376500
C	5.14011300	4.69410800	1.06376200
C	4.75121000	3.57724600	0.33801500
N	4.22874700	2.50609900	0.96833900
H	5.28034500	5.54730400	3.04212300
H	3.62253000	1.56551100	2.70487700
H	4.29811800	3.52702500	4.15774800
H	5.55936900	5.55206300	0.54942900
H	4.84011800	3.50421700	-0.74026700
H	3.94591000	1.64061900	0.39578200
C	6.02877500	-2.22872300	-0.40863900
C	7.07681300	-3.06459800	-0.76645300
C	7.68405200	-2.89063300	-2.01465700
C	7.22770200	-1.88557600	-2.87435400
C	6.17514500	-1.08009000	-2.46439500
N	5.60806900	-1.26674500	-1.25505000
H	8.50571100	-3.53385500	-2.31576300
H	5.50295100	-2.29880000	0.53699700
H	7.40788100	-3.83658000	-0.08031600
H	7.67791400	-1.72886000	-3.84858200
H	5.75964200	-0.28398000	-3.07204100
H	4.79602500	-0.63421700	-0.95439100

endo-TS2 of double py-H⁺ model

C	-3.28103500	1.58020300	-0.98710400
C	-1.96447000	1.53546100	-0.18049800
C	-0.73063900	1.07499200	-0.77892000
C	-0.92085200	0.26191900	-1.95466000
C	-2.19038900	-0.16655600	-2.31033500
C	-3.50033400	0.18464800	-1.64202000
C	-4.32434200	1.90200200	0.10377700
C	-3.60050200	2.00814200	1.44223900
C	-2.16306300	1.77994800	1.14501400
C	-0.03386600	-0.25942800	-2.96817900
C	-0.81812400	-0.95011800	-3.83541900
O	-2.13734900	-0.89677000	-3.43640600
C	-1.08175400	1.69113200	2.16932400
C	-4.24189200	3.23176900	0.79674700
C	-3.25857900	2.66298300	-2.09343900
O	-4.57122500	0.23182300	-2.56544000
C	-5.31566700	-0.98442600	-2.69586000
O	-6.12816000	-1.24626600	-1.59595100
C	-7.34251000	-0.48890100	-1.55593900
H	0.18473300	1.65013500	-0.68891900
H	-3.72844800	-0.54823400	-0.85275700
H	-5.29584400	1.42210200	0.03372700
H	-4.01627300	1.63418100	2.37325200
H	1.03532200	-0.11981800	-3.04634800
H	-0.63457600	-1.49773000	-4.74712700
H	-0.31888200	2.45376200	1.95698100
H	-1.46805700	1.92127100	3.16544900
H	-5.15024200	3.60269600	1.26407400
H	-3.58778400	4.00939500	0.41342200
H	-3.00273700	3.63939900	-1.67460000
H	-2.53168800	2.43314600	-2.87912000
H	-4.24336700	2.73477500	-2.56158600
H	-5.89770700	-0.84846300	-3.61418900
H	-4.63709800	-1.83767500	-2.79021100
H	-7.88559700	-0.82266300	-0.67013400
H	-7.14261800	0.58711200	-1.48477100
H	-7.94910700	-0.68755500	-2.44928900
C	-1.08721600	-0.96217900	2.70191800

C	-1.70127600	-1.68482400	1.45346400
C	-0.64581800	-2.30759400	0.53614700
C	0.47579600	-1.32527100	0.37801500
C	0.38308700	-0.01918300	0.92201400
C	-0.31391500	0.32151300	2.22308700
C	1.72357700	-1.48150500	-0.22830700
C	2.43149600	-0.28404500	0.02412500
O	1.65361800	0.58602800	0.73770400
C	-0.05493200	-1.85521100	3.43379500
O	3.61016100	0.09862000	-0.29473300
H	-2.18787700	-0.88280900	0.88138400
H	-1.07705100	-2.55324800	-0.44583300
H	-0.25683500	-3.25128700	0.94190500
H	0.48475700	0.50225400	2.95626500
H	-0.41278800	-2.88173100	3.55432900
H	0.89780700	-1.90814800	2.89387600
H	0.14893200	-1.45405700	4.43291800
C	-2.34690200	-0.72805700	3.57791300
H	-2.60366200	0.28545000	3.86651400
C	-3.43519600	-1.69709700	3.12198300
H	-4.47804700	-1.39689100	3.04938900
C	-2.82440800	-1.82878900	4.49752800
H	-3.44654100	-1.52229300	5.33487600
H	-2.19273600	-2.68359900	4.71349500
C	-2.84583400	-2.51236300	1.99981000
C	-3.27233800	-3.69846000	1.55693300
H	-4.12332900	-4.20155100	2.00834100
H	-2.79685000	-4.20885800	0.72224200
C	2.24748900	-2.66708100	-0.98461000
H	2.80215800	-2.36099800	-1.88037800
H	2.91455900	-3.29234000	-0.37519100
H	1.42648900	-3.30770700	-1.31914800
C	3.78607600	3.27882900	1.37320700
C	4.04986000	4.61166300	1.65300200
C	4.60937100	5.41557900	0.65389700
C	4.89135100	4.86791400	-0.60271500
C	4.61008900	3.52884900	-0.82853700
N	4.07275400	2.77620500	0.15439000
H	4.82322200	6.46181400	0.85205800
H	3.34533700	2.58714900	2.08176600

H	3.81991200	5.01060900	2.63501300
H	5.32176000	5.46862000	-1.39659700
H	4.79518600	3.02893100	-1.77257700
H	3.86942300	1.75618400	-0.02748900
C	6.30218700	-2.09015000	0.48747300
C	7.41484900	-2.91367000	0.40226700
C	7.92605900	-3.23199900	-0.86078300
C	7.31239200	-2.71850300	-2.00890900
C	6.20192600	-1.90005400	-1.86709500
N	5.72988400	-1.60830700	-0.63635900
H	8.79582800	-3.87631600	-0.94997500
H	5.84244800	-1.79765300	1.42476900
H	7.86932700	-3.29847600	1.30876700
H	7.68632500	-2.94996200	-3.00036400
H	5.66715800	-1.46583900	-2.70421900
H	4.88172800	-0.98835300	-0.54371300

endo-product of double py-H⁺ model

C	-3.09500200	1.73028600	-0.33233000
C	-1.84627900	1.12317900	0.31568800
C	-0.72402900	0.55021800	-0.51805800
C	-1.33979700	-0.07506200	-1.75422600
C	-2.68965100	-0.03684700	-1.98518000
C	-3.77808800	0.58747600	-1.14432800
C	-3.93454300	2.13940700	0.89320700
C	-3.18994000	1.70769900	2.14984900
C	-1.92028200	1.09999000	1.65594000
C	-0.75273500	-0.63614300	-2.94612900
C	-1.78984300	-0.91850100	-3.78317200
O	-2.97438700	-0.55843800	-3.20764700
C	-0.82387100	0.53829300	2.50884600
C	-3.39384700	3.18112400	1.83621700
C	-2.79225700	2.92834700	-1.25926500
O	-4.83206200	1.10718900	-1.93928800
C	-5.91036300	0.20005400	-2.17580500
O	-6.71600800	0.00209100	-1.05368000
C	-7.63120900	1.06660000	-0.78204700
H	-0.07638900	1.36819500	-0.86961600
H	-4.18853300	-0.14228500	-0.43170100

H	-5.01240400	2.03251200	0.82178900
H	-3.69116200	1.27798900	3.01421200
H	0.29466400	-0.80161500	-3.16178300
H	-1.85857800	-1.34593400	-4.77217700
H	-0.06806300	1.31686900	2.70326500
H	-1.18771800	0.24807100	3.49931700
H	-4.12029400	3.72162600	2.43766700
H	-2.52331800	3.76801300	1.55265200
H	-2.25887100	3.71213600	-0.71217700
H	-2.18344400	2.63586600	-2.12181900
H	-3.72507500	3.35072800	-1.64123500
H	-6.47007100	0.64947200	-3.00403700
H	-5.52739300	-0.78508700	-2.45696100
H	-8.21236800	0.76102000	0.08992800
H	-7.10498800	2.00448700	-0.56549400
H	-8.30849300	1.21948600	-1.63310100
C	-0.84530200	-2.07728800	1.95473300
C	-1.32256800	-2.55946100	0.54653600
C	-0.16643000	-2.79194200	-0.42713500
C	0.75823000	-1.61593400	-0.31703900
C	0.27828800	-0.34854100	0.35076600
C	-0.12977900	-0.66565700	1.84256300
C	2.07970200	-1.52006700	-0.61876800
C	2.52754100	-0.21997600	-0.15521700
O	1.53040400	0.45754900	0.42098900
C	0.20398400	-3.05385500	2.54310000
O	3.66653600	0.30715200	-0.21665300
H	-1.91627100	-1.72863900	0.14154000
H	-0.54242000	-2.87603600	-1.45524500
H	0.38037800	-3.71856000	-0.21263600
H	0.83351000	-0.77934000	2.35211600
H	-0.10626600	-4.09828700	2.45397100
H	1.17113300	-2.96238700	2.03350700
H	0.36851600	-2.84033500	3.60553100
C	-2.18670300	-2.13918300	2.74332400
H	-2.60593500	-1.22211200	3.13980600
C	-3.10398300	-3.13209400	2.03416700
H	-4.16651400	-2.93220200	1.91527700
C	-2.59147600	-3.42678800	3.42485400
H	-3.31601700	-3.34024000	4.23089200

H	-1.87494900	-4.22752900	3.57026000
C	-2.34389900	-3.63856700	0.83491400
C	-2.55902600	-4.76413300	0.14903400
H	-3.34092000	-5.46263400	0.43502500
H	-1.97379500	-5.02694100	-0.72956800
C	2.97536800	-2.53095800	-1.26986900
H	3.44304800	-2.12467500	-2.17572500
H	3.77587500	-2.86261400	-0.59608400
H	2.41088800	-3.41809300	-1.56710800
C	2.51067800	3.49675700	1.33471400
C	2.38087000	4.83988300	1.65467900
C	3.18428700	5.77612000	0.99525700
C	4.10112000	5.34813300	0.02773200
C	4.19542200	3.99466600	-0.25420300
N	3.40791500	3.11367100	0.40097300
H	3.09578900	6.83263900	1.23094900
H	1.92268600	2.70470800	1.78240500
H	1.66039300	5.14427800	2.40602300
H	4.73285300	6.05270700	-0.50215000
H	4.87564100	3.58220100	-0.99029800
H	3.49170600	2.09915800	0.18154000
C	6.83667900	-1.25081500	0.54487100
C	8.11525900	-1.78153400	0.46862200
C	8.72024200	-1.91458700	-0.78645500
C	8.03250300	-1.51215200	-1.93726900
C	6.75583900	-0.98753500	-1.80770600
N	6.19643200	-0.87077700	-0.58302200
H	9.72056100	-2.32990600	-0.86743500
H	6.29633200	-1.11645200	1.47511600
H	8.62475300	-2.08631700	1.37634300
H	8.47690500	-1.60522200	-2.92231100
H	6.15564700	-0.65631100	-2.64758100
H	5.23201500	-0.48068100	-0.50075800

exo-reactant of double py-H⁺ model

C	4.20235400	-2.06490000	0.09233500
C	3.66751800	-3.51310200	-0.04064400
C	2.65613800	-3.82701400	-0.87909300
C	1.96864900	-2.73713700	-1.56355500

C	2.16466700	-1.45022100	-1.14950200
C	3.03015700	-1.04854300	0.01158000
C	4.86323200	-2.06243300	1.48908000
C	4.93305200	-3.49197600	2.00498600
C	4.33703600	-4.38247300	0.95007800
C	0.98461600	-2.67321600	-2.61243300
C	0.65824000	-1.36012500	-2.75192500
O	1.36624500	-0.58252000	-1.85245400
C	4.36875900	-5.72487800	0.95193400
C	6.20099500	-2.73669300	1.67045100
C	5.20495200	-1.78063900	-1.05645600
O	3.54654200	0.29045300	-0.13622400
C	2.81104100	1.30302900	0.48581000
O	3.00118100	1.39673100	1.88270600
C	4.32729800	1.80419500	2.26134200
H	2.28593800	-4.84431000	-0.97514300
H	2.45130100	-1.09501800	0.94883100
H	4.60766500	-1.24769400	2.16146300
H	4.74066700	-3.73467100	3.04697200
H	0.58845400	-3.49481500	-3.19472500
H	0.00706000	-0.82350000	-3.42541500
H	4.85981300	-6.27750500	1.74783900
H	3.91442900	-6.31359600	0.15923400
H	6.80806100	-2.41047200	2.51156700
H	6.77952600	-3.04279000	0.80454700
H	5.94735300	-2.57860600	-1.12504300
H	4.69378500	-1.72846900	-2.02336100
H	5.72935100	-0.83570100	-0.88688800
H	3.14066000	2.23549100	0.00473400
H	1.73142800	1.15561300	0.35514800
H	4.35342600	1.81016500	3.35244700
H	5.07549500	1.10342300	1.88127200
H	4.54107700	2.81252200	1.88064000
C	-4.77765300	-1.76926000	0.66616300
C	-5.48956800	-1.01780400	-0.51211300
C	-4.53089600	-0.59027600	-1.62986900
C	-3.16565000	0.03467300	0.43653800
C	-3.75725300	-0.83896500	1.27186500
C	-5.99104100	-2.12580800	1.56487900
C	-7.21855500	-2.17768100	0.65361500

C	-1.76912800	1.58778000	-0.32298600
O	-2.13807100	0.91277500	0.80136100
C	-6.71674400	-3.42981700	1.33610200
C	-3.99584200	-3.02976800	0.19232300
O	-0.85883500	2.44243800	-0.23617200
H	-5.85319500	-0.08272400	-0.05417900
H	-5.04046300	0.00820600	-2.39448600
H	-4.10135700	-1.46081600	-2.14617900
H	-3.45727600	-0.92243200	2.31457700
H	-6.04760200	-1.66622700	2.54896600
H	-8.17452500	-1.77212400	0.97676700
H	-7.31925200	-3.79771700	2.16275600
H	-6.26526700	-4.21764300	0.74302500
H	-4.61971600	-3.65490100	-0.45258500
H	-3.09597400	-2.76203000	-0.37051800
H	-3.68802300	-3.63150700	1.05364800
C	-2.44861000	1.73083300	-2.83225700
H	-2.50785700	2.82607900	-2.82298700
H	-1.49656500	1.45242600	-3.30237400
H	-3.24913900	1.36243800	-3.47905000
C	-2.57357200	1.16387500	-1.45194100
C	-3.43364600	0.20820700	-0.97616500
C	-6.74320000	-1.83350900	-0.73972000
C	-7.32149500	-2.14625300	-1.90161000
H	-8.23799200	-2.72870400	-1.94154500
H	-6.91021300	-1.82555900	-2.85619000
C	1.79997200	2.52339900	-2.82919300
C	2.68089700	2.98851000	-3.79553100
C	2.58764300	4.31695200	-4.22222200
C	1.61185300	5.15833600	-3.67311200
C	0.75417400	4.65078300	-2.71087700
N	0.86943400	3.36169400	-2.31887600
H	3.26901700	4.69608900	-4.97836000
H	1.80264300	1.50554100	-2.44867200
H	3.42687000	2.31441100	-4.20245500
H	1.51590800	6.19222800	-3.98650600
H	-0.02878900	5.23204700	-2.23723200
H	0.21264700	3.00224300	-1.59741100
C	0.51370300	2.80139100	3.35578700
C	0.51801500	3.19379900	4.68772200

C	-0.54925700	3.94748000	5.18488300
C	-1.60788900	4.29812400	4.33797000
C	-1.57243000	3.88339300	3.01714100
N	-0.52453600	3.15763700	2.56709800
H	-0.55831600	4.26075700	6.22482800
H	1.31304200	2.22503900	2.89119800
H	1.34932400	2.90871800	5.32318100
H	-2.44876300	4.88220900	4.69570800
H	-2.35076100	4.10483200	2.29615600
H	-0.53987400	2.85112600	1.57622400

exo-TS1 of double py-H⁺ model

C	0.88049500	-3.11432000	-0.92934000
C	-0.48478100	-2.52677900	-1.35334400
C	-0.59853400	-1.68381800	-2.42339700
C	0.61725600	-1.15762500	-2.99947800
C	1.79564700	-1.29599300	-2.30344400
C	1.95258000	-1.99090500	-0.97344000
C	0.60928900	-3.62116100	0.50328700
C	-0.87384700	-3.42691600	0.81687900
C	-1.50534200	-2.81914400	-0.37972700
C	0.93291700	-0.37679100	-4.16892000
C	2.26349100	-0.11115000	-4.09316900
O	2.80410800	-0.65479200	-2.93799700
C	-2.83920000	-2.43991900	-0.46986600
C	-0.27393900	-4.82188200	0.66507500
C	1.30926400	-4.25797000	-1.88613700
O	3.25948700	-2.53896700	-0.81473700
C	4.15114000	-1.80774100	-0.01003000
O	3.96129500	-2.02436800	1.37214600
C	4.42602200	-3.31000100	1.81980800
H	-1.56282600	-1.32278300	-2.77113700
H	1.75550900	-1.27005600	-0.16246300
H	1.36393500	-3.43133800	1.26158400
H	-1.24484600	-3.14361700	1.79912500
H	0.26758600	-0.08608500	-4.97098000
H	2.96813000	0.37400500	-4.75142300
H	-3.55445300	-2.90100200	0.20567300
H	-3.22423700	-2.19953400	-1.45131300

H	-0.18190800	-5.39307700	1.58509700
H	-0.55560800	-5.41731100	-0.19715300
H	0.50975600	-4.99289600	-1.99970600
H	1.55041500	-3.88039200	-2.88395500
H	2.19370000	-4.76636400	-1.49367100
H	5.15347200	-2.12799300	-0.31466600
H	4.02849500	-0.72856600	-0.15859100
H	4.22332800	-3.36399200	2.89133500
H	3.89940600	-4.11962700	1.30487100
H	5.50559000	-3.40394700	1.64971000
C	-4.52525800	-0.04713200	-0.04892800
C	-4.59658200	1.51484000	0.17402500
C	-3.64577400	2.27112600	-0.76755400
C	-2.11456500	0.42905800	0.06479300
C	-3.12093500	-0.49381000	0.39810900
C	-5.67070400	-0.53364900	0.87480700
C	-6.64220000	0.63298500	1.05557800
C	-0.14890200	1.46130800	0.21307100
O	-0.80007200	0.29238800	0.50969800
C	-7.07640400	-0.61976900	0.33000800
C	-4.80157000	-0.35232600	-1.54324200
O	1.07504900	1.57512200	0.58400100
H	-4.21854500	1.67988000	1.19637100
H	-3.66007500	3.34824800	-0.56330800
H	-3.94267300	2.14764900	-1.81664800
H	-3.03106800	-0.98842500	1.36209700
H	-5.40687400	-1.16838800	1.71838700
H	-7.09683400	0.84440300	2.02066700
H	-7.76555500	-1.26956800	0.86358400
H	-7.25453700	-0.57895800	-0.73932900
H	-5.59371000	0.29763400	-1.92581000
H	-3.91574000	-0.18342500	-2.16428000
H	-5.13576500	-1.38321800	-1.68443400
C	-0.68726000	3.76837700	-0.82374000
H	-0.13636200	4.29625500	-0.03460000
H	-0.07602700	3.79761900	-1.73603500
H	-1.59043900	4.34957000	-1.03093100
C	-1.03034400	2.36550900	-0.41805300
C	-2.27100400	1.71341000	-0.49317000
C	-6.08173800	1.79171900	0.26526000

C	-6.74798800	2.84587800	-0.21244200
H	-7.81987500	2.95332300	-0.06863100
H	-6.24975100	3.64548700	-0.75597500
C	3.70670800	2.53870000	-1.61097200
C	4.74382300	3.25046300	-2.19700500
C	5.00623900	4.55308000	-1.76032300
C	4.22443800	5.11540800	-0.74497100
C	3.20125300	4.36050200	-0.19208600
N	2.96979200	3.10567000	-0.63254800
H	5.81277000	5.12653200	-2.20785300
H	3.43584700	1.52779200	-1.89665200
H	5.33403700	2.79012300	-2.98191900
H	4.40295200	6.12368800	-0.38738400
H	2.54944300	4.72249400	0.59468600
H	2.18611700	2.54490800	-0.19435800
C	2.51285000	-0.13436200	3.53100600
C	2.76529600	-0.34956100	4.88009100
C	2.06580700	0.39306600	5.83575900
C	1.12230300	1.34172800	5.42379600
C	0.90803800	1.52382600	4.06700100
N	1.59981200	0.79149700	3.16734800
H	2.25292000	0.23542000	6.89400000
H	3.01004600	-0.68141900	2.73142800
H	3.50207200	-1.08944800	5.17324100
H	0.56283100	1.93155400	6.14171500
H	0.19920700	2.23676200	3.66122800
H	1.41607700	0.97329200	2.14650100

exo-intermediate of double py-H⁺ model

C	1.35650800	-3.43705000	-0.39573300
C	0.17872600	-2.81240000	-1.17635600
C	0.38060900	-2.21917100	-2.41874800
C	1.71414500	-1.95207600	-2.82285200
C	2.71981900	-2.03130600	-1.86283900
C	2.51921700	-2.40858700	-0.41318500
C	0.75170200	-3.64369300	1.00642900
C	-0.70460300	-3.14955100	0.97525500
C	-0.97074900	-2.67595500	-0.38358700
C	2.34858600	-1.44668600	-4.01933800

C	3.65445000	-1.27822500	-3.70108900
O	3.87962400	-1.61839500	-2.36749500
C	-2.26950700	-2.08530100	-0.79716300
C	-0.34356000	-4.64173900	1.13008100
C	1.84649200	-4.77189200	-1.01075200
O	3.68396100	-2.95306600	0.17758800
C	4.53228700	-2.01857200	0.83129800
O	4.03235700	-1.61170700	2.07998900
C	4.19267900	-2.59693300	3.11437800
H	-0.45266300	-1.87433200	-3.02582000
H	2.20279400	-1.50414900	0.13425700
H	1.37049200	-3.43777800	1.87479900
H	-1.19532000	-2.67414600	1.81736200
H	1.89643300	-1.27480000	-4.98671000
H	4.53385500	-0.97527900	-4.24818200
H	-3.00381500	-2.90638000	-0.77504900
H	-2.22583200	-1.72092800	-1.82525600
H	-0.55278800	-5.05008700	2.11492300
H	-0.57779700	-5.31201500	0.30956200
H	1.02187200	-5.47717700	-1.13218800
H	2.30361200	-4.62802300	-1.99431400
H	2.59623100	-5.22651700	-0.35821800
H	5.49227900	-2.53429600	0.93526800
H	4.64470000	-1.10853000	0.23425600
H	3.72801700	-2.18861700	4.01395700
H	3.70185400	-3.53798000	2.84469000
H	5.25745900	-2.78073400	3.30368400
C	-4.34489900	-0.65415900	-0.18699600
C	-4.76311100	0.57123200	0.69949000
C	-4.08531700	1.87907000	0.28282900
C	-2.10609900	0.32328900	0.11455100
C	-2.85269300	-0.97560000	0.14199700
C	-5.32673700	-1.74569200	0.31230600
C	-6.52983600	-1.04069200	0.93470200
C	-0.35413100	1.69324000	0.22702300
O	-0.71998400	0.35913800	0.13138900
C	-6.69272300	-1.86357600	-0.32259300
C	-4.52193900	-0.34607100	-1.69127700
O	0.93680900	1.96479500	0.25847200
H	-4.38128700	0.33300600	1.70782200

H	-4.28146400	2.66686400	1.02194500
H	-4.48292100	2.24928000	-0.67306800
H	-2.83580200	-1.39144500	1.16188800
H	-4.90810600	-2.63184800	0.78722000
H	-6.99258600	-1.41130200	1.84652800
H	-7.20372700	-2.81696600	-0.21168100
H	-6.90430200	-1.36041700	-1.26032900
H	-5.46523300	0.17571300	-1.87671100
H	-3.71871900	0.29456300	-2.07131200
H	-4.54140400	-1.26576900	-2.28611500
C	-1.52606900	3.98304000	0.41291800
H	-0.51901100	4.40179700	0.52750700
H	-1.99006600	4.47736300	-0.45199800
H	-2.11257300	4.28905000	1.28956200
C	-1.48170400	2.48928000	0.26772300
C	-2.60715600	1.59382200	0.19313800
C	-6.26806200	0.44047300	0.81873100
C	-7.17130100	1.42379600	0.85136500
H	-8.23319300	1.21805500	0.95839600
H	-6.88505200	2.47077200	0.78184200
C	0.65168700	3.83641800	-2.64981500
C	0.94658000	4.67066400	-3.71976400
C	2.24747700	5.16599600	-3.85278500
C	3.22225400	4.81166500	-2.91382400
C	2.86887100	3.97263900	-1.86655100
N	1.60805900	3.50928600	-1.75725500
H	2.49953500	5.82457500	-4.67880600
H	-0.33178000	3.41775300	-2.46826100
H	0.16872700	4.93007300	-4.42981300
H	4.23897300	5.18200600	-2.98902900
H	3.56564500	3.65437900	-1.09879900
H	1.34857400	2.86178600	-0.91915500
C	2.80622700	1.29494000	3.21513100
C	3.30042600	1.48838800	4.49890300
C	2.81938800	2.55665100	5.26200400
C	1.85141800	3.41096400	4.72331800
C	1.39747800	3.17637300	3.43374100
N	1.87910100	2.13921600	2.71831400
H	3.19423200	2.72248100	6.26781200
H	3.12793800	0.47693300	2.57608000

H	4.05190700	0.81134700	4.89010700
H	1.45529000	4.24594100	5.29103200
H	0.65148200	3.78992800	2.94113500
H	1.51032100	2.00813000	1.70984500

exo-TS2 of double py-H⁺ model

C	0.45573700	-2.83591100	-1.54384400
C	-0.93169300	-2.17158600	-1.44719600
C	-1.24878600	-1.00386200	-2.18739000
C	-0.14536600	-0.28462100	-2.73355300
C	1.14085400	-0.61086800	-2.33290500
C	1.53381800	-1.72430200	-1.39175300
C	0.42994700	-3.82163700	-0.35404200
C	-0.91825700	-3.67838700	0.35913100
C	-1.67366900	-2.65617600	-0.39609300
C	-0.00928600	0.83120700	-3.64042800
C	1.31911200	1.08142100	-3.72749400
O	2.03604700	0.20868200	-2.91414000
C	-2.98806800	-2.08937000	0.00083400
C	-0.55142700	-4.95353800	-0.39866700
C	0.66351700	-3.56516700	-2.89399800
O	2.83263900	-2.22877600	-1.68697600
C	3.87814500	-1.76065100	-0.86555100
O	3.92324000	-2.38738800	0.39538200
C	4.43967300	-3.72996900	0.35618000
H	-2.26435800	-0.74890100	-2.45807900
H	1.51199200	-1.34265100	-0.36113000
H	1.34510500	-3.96296900	0.21413800
H	-1.04091900	-3.73816700	1.43774300
H	-0.79516400	1.34775600	-4.17475600
H	1.91696600	1.76755800	-4.30779800
H	-3.44572900	-2.68779100	0.79304300
H	-3.64935100	-2.16164300	-0.86708500
H	-0.33487100	-5.82495200	0.21359700
H	-1.09325400	-5.17489500	-1.31294100
H	-0.14740300	-4.27249700	-3.08036400
H	0.69314200	-2.86666900	-3.73619600
H	1.60683700	-4.11713700	-2.88331000
H	4.79833800	-1.95332800	-1.42788500

H	3.76602600	-0.69028000	-0.65775600
H	4.42044400	-4.10502300	1.38113900
H	3.82336900	-4.37038400	-0.28273100
H	5.47360200	-3.72793000	-0.00988900
C	-4.37627700	0.12782900	0.16745800
C	-4.23005000	1.65963700	0.44934900
C	-3.30403200	2.35304200	-0.56139000
C	-1.88705400	0.30826400	-0.03821800
C	-2.99933600	-0.56533200	0.46714800
C	-5.48127600	-0.26312000	1.18748000
C	-6.26842000	1.00247200	1.52620700
C	0.11912100	1.23820200	0.32267700
O	-0.59752400	0.07770200	0.46092800
C	-6.93531900	-0.14114100	0.79722700
C	-4.84248700	-0.09237700	-1.29130600
O	1.33733100	1.24312400	0.74589500
H	-3.72276200	1.72757900	1.42811200
H	-3.20183900	3.42083500	-0.33835000
H	-3.69702200	2.28385800	-1.58308300
H	-2.88178700	-0.60202400	1.56102400
H	-5.22372100	-0.97795800	1.96624400
H	-6.59139400	1.21492900	2.54282200
H	-7.64397400	-0.73103300	1.37332500
H	-7.21794500	-0.01406500	-0.24244800
H	-5.60479100	0.64317200	-1.56431200
H	-4.02911400	0.02308300	-2.01397300
H	-5.29142400	-1.07942600	-1.43577200
C	-0.27478800	3.65864600	-0.48692300
H	0.26195100	4.08853000	0.36880200
H	0.37904600	3.73946900	-1.36625500
H	-1.14027300	4.29943200	-0.67814600
C	-0.69747000	2.24360100	-0.22551900
C	-1.97215900	1.66388400	-0.38985800
C	-5.64640900	2.12244600	0.72824200
C	-6.21249800	3.28043600	0.37919400
H	-7.23858600	3.51569400	0.64937000
H	-5.67425000	4.03980800	-0.18367200
C	3.97138400	2.68525400	-1.15335800
C	5.02819700	3.49703800	-1.53964800
C	5.34877400	4.61145800	-0.75696000

C	4.60429000	4.88772700	0.39513300
C	3.55867600	4.04252800	0.73577600
N	3.27086500	2.97416700	-0.03661700
H	6.17133800	5.26048700	-1.04291900
H	3.65109700	1.80816500	-1.70521800
H	5.58798600	3.25973000	-2.43790400
H	4.82803100	5.74579600	1.01967800
H	2.93222000	4.18856400	1.60841000
H	2.46755300	2.33774100	0.24161200
C	2.71791300	-1.14729900	3.14508600
C	2.99638500	-1.70885800	4.38479000
C	2.35772800	-1.20730300	5.52281300
C	1.44833200	-0.15016300	5.39986700
C	1.20601100	0.37868600	4.14195700
N	1.83921300	-0.12562200	3.06121800
H	2.56555200	-1.63578900	6.49900900
H	3.16574400	-1.48896100	2.21353900
H	3.70518100	-2.52688900	4.45347000
H	0.93610200	0.25839800	6.26418400
H	0.51905500	1.19683500	3.95670600
H	1.63794300	0.31453700	2.12235600

exo-product of double py-H⁺ model

C	-3.46701200	-0.39954900	-0.74156700
C	-2.37753800	0.53051700	-0.19689300
C	-1.15650000	0.87519700	-1.01321700
C	-0.77580700	-0.34851200	-1.82056000
C	-1.51343100	-1.50136400	-1.76200900
C	-2.77205100	-1.77752300	-0.96941000
C	-4.45802100	-0.46629900	0.43455300
C	-3.86588300	0.31408300	1.60200500
C	-2.58608600	0.88128400	1.08185100
C	0.22258800	-0.56743800	-2.83741900
C	0.02631400	-1.83462000	-3.29799600
O	-1.02373600	-2.41985300	-2.64697600
C	-1.66005900	1.72602800	1.90138200
C	-5.12369500	0.80028100	0.90165900
C	-4.12799000	0.09385000	-2.04552800
O	-3.65835100	-2.67910600	-1.62110700

C	-3.35599000	-4.05615600	-1.46696600
O	-3.47514300	-4.51309100	-0.13854700
C	-4.82846200	-4.71803600	0.29504900
H	-1.38772400	1.67489800	-1.73042800
H	-2.53035700	-2.18563000	0.02259100
H	-4.98879500	-1.39994900	0.59434400
H	-3.92961400	-0.01986100	2.63536400
H	0.95789800	0.13243700	-3.20966400
H	0.49513000	-2.43388500	-4.06424100
H	-1.26324000	1.11595800	2.72676700
H	-2.22483100	2.53167900	2.38936700
H	-6.06462100	0.68852100	1.43406600
H	-5.05449800	1.70267300	0.29991300
H	-4.56327800	1.08655000	-1.89992400
H	-3.41340800	0.15322100	-2.87370200
H	-4.92717800	-0.58901200	-2.34550600
H	-4.06070300	-4.57270000	-2.12670200
H	-2.32579800	-4.26804700	-1.76501500
H	-4.77899700	-5.06422100	1.32924800
H	-5.40611400	-3.78906800	0.24444900
H	-5.31272400	-5.48539500	-0.32151500
C	-0.69890100	3.82471500	0.64757200
C	0.60299400	4.28700300	-0.07921800
C	0.89975200	3.49812600	-1.37374300
C	-0.01502600	1.43512400	-0.08670100
C	-0.48802900	2.34618700	1.10497600
C	-0.69395100	4.82109100	1.84872500
C	0.08546100	6.06367700	1.41063600
C	1.92720100	0.22653100	0.08280200
O	0.66369600	0.26394500	0.50713000
C	-1.38949200	6.15585500	1.72357300
C	-1.96015900	4.01838700	-0.22089000
O	2.67397300	-0.70929200	0.45769700
H	1.41709800	4.02343600	0.61826600
H	1.79797900	3.86890400	-1.87664600
H	0.06633800	3.56890600	-2.08275800
H	0.38245300	2.37751700	1.77419000
H	-0.55716300	4.40997000	2.84657200
H	0.77824700	6.56108400	2.08596000
H	-1.64642000	6.65426900	2.65510700

H	-2.09800000	6.34070100	0.92398000
H	-1.97394000	5.01466500	-0.67016200
H	-2.03773900	3.30841700	-1.04419900
H	-2.86463000	3.91664100	0.38647000
C	3.58968100	1.61745000	-1.35436100
H	4.34734500	1.75332900	-0.57210900
H	3.90998300	0.78380000	-1.99222000
H	3.59512600	2.51855900	-1.97195500
C	2.23206500	1.36636300	-0.77122800
C	1.09562500	2.10309300	-0.86308200
C	0.55395600	5.80026900	-0.00226800
C	0.88468700	6.68891000	-0.94104700
H	0.81719300	7.75814900	-0.75906000
H	1.23578300	6.38686700	-1.92542000
C	5.66978300	-2.14195100	-1.04132800
C	6.98677200	-2.51833800	-1.25638600
C	7.98297500	-2.01064300	-0.41448300
C	7.63858100	-1.13867100	0.62478400
C	6.30701700	-0.79323300	0.79778400
N	5.36652900	-1.29820600	-0.03057200
H	9.02078800	-2.29197100	-0.56769900
H	4.83963600	-2.48652200	-1.64763800
H	7.22574800	-3.19498400	-2.06968300
H	8.39015400	-0.72974900	1.29139100
H	5.95696600	-0.12331800	1.57509500
H	4.36889900	-1.02111100	0.11074800
C	0.05406600	-3.15535000	1.15212600
C	-0.72610300	-4.18868000	1.65244300
C	-0.34664300	-4.78975200	2.85755500
C	0.79447800	-4.34442400	3.53696700
C	1.53612900	-3.30731600	2.99509400
N	1.15135800	-2.74875700	1.82632800
H	-0.93973800	-5.60097500	3.26981500
H	-0.16340200	-2.62135300	0.23371500
H	-1.61770400	-4.49780500	1.10919200
H	1.10368400	-4.79176000	4.47540900
H	2.42621700	-2.89891300	3.45970700
H	1.70945200	-1.97400400	1.41721200

endo-reactant of model 1a

C	-0.18959700	3.20899300	1.33068300
C	1.30921500	2.88291000	1.12351200
C	1.97566600	3.27759400	0.01498100
C	1.21902600	3.89191200	-1.06759000
C	-0.14719200	3.79645500	-1.05999500
C	-0.95859600	3.07909300	-0.01263400
C	-0.64475400	2.14052300	2.34809500
C	0.57787100	1.39358300	2.86133400
C	1.78791500	1.99116500	2.20017900
C	1.56186000	4.55345900	-2.29931300
C	0.38174400	4.80400300	-2.93256500
O	-0.67587400	4.33452400	-2.18811300
C	3.06493400	1.71544000	2.52881100
C	-0.22886600	2.28360400	3.78790100
C	-0.34361200	4.65618300	1.86604700
O	-2.27305300	3.61315800	0.13705400
C	-3.24761200	3.09304000	-0.74607800
O	-3.76695500	1.85151100	-0.33506600
C	-4.62579300	1.93609100	0.80494100
H	3.03200500	3.05596800	-0.12439800
H	-1.03623800	2.00983300	-0.27677100
H	-1.57012600	1.61201100	2.13540100
H	0.56868200	0.32173300	3.04518600
H	2.54732200	4.82182900	-2.65644700
H	0.11699400	5.29714100	-3.85529300
H	3.90208000	2.20568800	2.03638500
H	3.30079100	1.03709700	3.34518900
H	-0.83908400	1.77811200	4.53276900
H	0.21439400	3.21070700	4.13789700
H	0.31169800	4.82511500	2.72426100
H	-0.07669300	5.38914700	1.09866900
H	-1.37652500	4.84198600	2.17257100
H	-4.03879400	3.85205700	-0.77691300
H	-2.83220700	2.93000400	-1.74426600
H	-5.03183300	0.93566100	0.96800200
H	-4.07686700	2.26638700	1.69452300
H	-5.45379800	2.63315600	0.61320900
C	-3.46013900	-3.49844200	0.33941400
C	-4.05756300	-2.10229700	-0.05060400

C	-3.60379000	-1.60026100	-1.42484200
C	-2.09617100	-1.64673900	-1.42498900
C	-1.39636900	-2.50271700	-0.47508200
C	-1.95421500	-3.36603600	0.38926200
C	-1.15826700	-0.98654700	-2.15950200
C	0.14643400	-1.41058900	-1.65171800
O	-0.02470700	-2.32185000	-0.63579300
C	-3.78674300	-4.59980200	-0.70755700
O	1.27294000	-1.06235200	-1.99678300
H	-3.61048200	-1.40853800	0.68053100
H	-3.94567700	-0.57447500	-1.60449300
H	-4.00399100	-2.22517300	-2.23572000
H	-1.34720200	-4.00133600	1.03040500
H	-4.85103100	-4.60983800	-0.96147000
H	-3.22537800	-4.44704900	-1.63441700
H	-3.52170300	-5.58744900	-0.31445200
C	-4.15936700	-3.75040700	1.70124600
H	-3.53594500	-3.79615500	2.59125200
C	-5.45590800	-2.94153700	1.69688600
H	-5.79274700	-2.41165000	2.58540900
C	-5.49528300	-4.45350700	1.72427600
H	-5.78889400	-4.90687800	2.66815200
H	-5.84830500	-4.99461400	0.85302600
C	-5.50505500	-2.20575200	0.37681700
C	-6.58480000	-1.72329100	-0.24454100
H	-7.58250500	-1.84760900	0.16916700
H	-6.51126300	-1.18228100	-1.18528200
C	-1.30685300	-0.00256500	-3.27503500
H	-2.34978700	0.30440100	-3.39174600
H	-0.69650700	0.89014500	-3.09770600
H	-0.96973800	-0.43297300	-4.22676100
C	4.17981000	-0.93739400	0.19202100
C	5.44805600	-1.14391000	0.67580100
C	6.33534600	-2.04918000	0.01547700
C	5.82254200	-2.70187300	-1.14901300
C	4.54322100	-2.44673100	-1.57495200
N	3.73905200	-1.58108800	-0.91455900
H	3.48402200	-0.25356100	0.66985800
H	5.74916900	-0.60349200	1.56306400
H	6.42261100	-3.40164800	-1.71471700

H	4.11674800	-2.91843700	-2.45307600
H	2.77345300	-1.40872300	-1.26940100
N	7.58805100	-2.27493900	0.46432700
C	8.47341900	-3.20732800	-0.24118300
H	9.42995800	-3.24870900	0.27811300
H	8.05011800	-4.21846900	-0.25835700
H	8.65723000	-2.87675700	-1.27023400
C	8.08304400	-1.58600900	1.66066400
H	9.10560600	-1.90632800	1.85596800
H	8.08625900	-0.49890700	1.51855800
H	7.47428100	-1.83166900	2.53864200

endo-TS of model 1a

C	2.97557700	-1.46355000	1.73992700
C	1.58917100	-0.80950500	1.53852300
C	0.64976600	-1.37157800	0.70667800
C	1.07532000	-2.43596500	-0.16757900
C	2.42360100	-2.67937000	-0.32057800
C	3.53519400	-1.92011700	0.36464800
C	3.80488300	-0.32509500	2.36814100
C	2.89257800	0.87595500	2.58957100
C	1.52873500	0.49215300	2.12528600
C	0.40689900	-3.32163200	-1.08804900
C	1.39026200	-4.02563700	-1.70988000
O	2.63198400	-3.63101000	-1.25219800
C	0.40797000	1.33809100	2.12246600
C	3.46687000	0.10071100	3.76894300
C	2.87231700	-2.69748800	2.67365700
O	4.70868400	-2.69919200	0.55532800
C	5.62639300	-2.68461500	-0.53392300
O	6.33744100	-1.48558500	-0.64079700
C	7.36740900	-1.31945100	0.33391100
H	-0.36174100	-0.98549800	0.64356800
H	3.78739000	-1.02987400	-0.23621600
H	4.82549200	-0.18963500	2.02219100
H	3.22546700	1.89808400	2.44557000
H	-0.65744800	-3.42250400	-1.25249700
H	1.40042500	-4.81126400	-2.44946000
H	-0.56774800	0.85936200	2.14129100

H	0.46543800	2.22595300	2.74742800
H	4.24284600	0.60700300	4.33785400
H	2.79383200	-0.49827900	4.37461300
H	2.35554200	-2.44301600	3.60204200
H	2.31891700	-3.51385800	2.19984900
H	3.87212900	-3.06434000	2.92020900
H	6.29459200	-3.53254000	-0.34125200
H	5.10290800	-2.81326200	-1.48526600
H	7.85527100	-0.36845000	0.11112400
H	6.95921400	-1.29536900	1.35171000
H	8.10457700	-2.13137900	0.26013200
C	1.08963200	3.12105200	-0.24143200
C	2.07553400	2.17198100	-1.00260600
C	1.45457300	1.48989700	-2.22380400
C	0.12050900	0.92400800	-1.81043100
C	-0.47966800	1.29796200	-0.58554300
C	-0.03958700	2.25698400	0.34354000
C	-0.76857900	0.10750400	-2.49933400
C	-1.92064800	-0.03554100	-1.66578800
O	-1.73135600	0.69878400	-0.49418200
C	0.40151900	4.14843600	-1.18392700
O	-2.98221200	-0.66991700	-1.82095800
H	2.28822200	1.37123000	-0.27686600
H	2.10867800	0.69527900	-2.60608300
H	1.31716200	2.19769200	-3.05427900
H	-0.82619900	2.80330800	0.86407100
H	1.12812000	4.64616900	-1.83282300
H	-0.34361000	3.67439500	-1.82905300
H	-0.10451000	4.92160700	-0.59445200
C	2.03816500	3.83508000	0.75585500
H	1.84158700	3.73205200	1.81823300
C	3.45898700	3.72554500	0.20778500
H	4.31232900	3.53291300	0.85493700
C	2.78297300	5.07365700	0.31314300
H	3.13946900	5.72911800	1.10460600
H	2.50221900	5.59856600	-0.59328100
C	3.36535300	2.96036800	-1.09015800
C	4.25699300	2.95712500	-2.08507600
H	5.16577600	3.55191300	-2.03714200
H	4.11809200	2.35410900	-2.97938100

C	-0.63013200	-0.50938600	-3.85811400
H	-0.49799600	0.25148100	-4.63849000
H	0.23337400	-1.18472300	-3.91213700
H	-1.52495400	-1.08857900	-4.10426400
C	-5.52807300	0.24442400	0.57483600
C	-6.77443700	0.32588300	1.14667100
C	-7.88508600	-0.34380600	0.54591600
C	-7.61063200	-1.07666400	-0.64986000
C	-6.33631800	-1.11035300	-1.16118900
N	-5.31466600	-0.46213300	-0.55734200
H	-4.65932800	0.73870700	0.99567200
H	-6.88850900	0.90565900	2.05264300
H	-8.38965600	-1.61355500	-1.17403100
H	-6.08513300	-1.65162100	-2.06653700
H	-4.34747300	-0.50516000	-0.98706600
N	-9.12529500	-0.28649100	1.07796800
C	-10.24234500	-0.98359300	0.43280900
H	-11.14856200	-0.81253200	1.01244900
H	-10.41045400	-0.60698200	-0.58305800
H	-10.06300400	-2.06438500	0.39011200
C	-9.37140900	0.47560700	2.30577500
H	-10.42549200	0.39405100	2.56796300
H	-8.78041700	0.08207000	3.14128900
H	-9.13504400	1.53734800	2.16731500

endo-product of model 1a

C	-1.96988700	2.40030700	-0.04044600
C	-1.11224300	1.19318300	0.35263600
C	-0.54988200	0.25008800	-0.68466200
C	-1.56775200	0.14722800	-1.80512600
C	-2.73632900	0.86049000	-1.78985600
C	-3.23576100	1.83513000	-0.75134700
C	-2.31002100	3.02167100	1.32786400
C	-1.70769000	2.14262200	2.41471000
C	-0.99153600	1.05661600	1.68208100
C	-1.51953500	-0.49830500	-3.09339400
C	-2.66789800	-0.15029600	-3.73698800
O	-3.42147500	0.67826500	-2.95279000
C	-0.19497700	-0.05133600	2.30082900

C	-1.19312200	3.55408900	2.18923100
C	-1.24199200	3.39663400	-0.97001700
O	-3.99237100	2.89244000	-1.33382500
C	-5.39037900	2.65216000	-1.42335800
O	-6.05482700	2.78221200	-0.19749400
C	-6.21887700	4.12917200	0.24349400
H	0.35456600	0.69648200	-1.12453800
H	-3.85509100	1.32620200	0.00102600
H	-3.29524000	3.46135600	1.45055200
H	-2.22909200	1.91316000	3.34170500
H	-0.73706300	-1.13131500	-3.48975500
H	-3.08262100	-0.38448400	-4.70577400
H	0.86393700	0.24446200	2.35685300
H	-0.49634400	-0.23923000	3.33658300
H	-1.46092800	4.30735700	2.92649200
H	-0.19610400	3.67139700	1.77160400
H	-0.31384200	3.74457000	-0.50618600
H	-0.99228900	2.94519700	-1.93615200
H	-1.87809200	4.26470800	-1.16281800
H	-5.75375200	3.38639700	-2.15282400
H	-5.58995700	1.63379900	-1.76821800
H	-6.78031500	4.08442400	1.17903600
H	-5.25203300	4.61756900	0.41700000
H	-6.78959600	4.71180000	-0.49380800
C	-1.58402400	-2.25063900	1.69137200
C	-2.43652700	-2.29129400	0.38106900
C	-1.70370600	-2.94244600	-0.79096100
C	-0.31305100	-2.36980000	-0.82808000
C	0.00237800	-1.10725900	-0.04539200
C	-0.29215600	-1.35489900	1.48356700
C	0.81866100	-2.88060700	-1.36030200
C	1.92434700	-2.01270900	-0.95101700
O	1.46890400	-1.00460000	-0.17587400
C	-1.08047300	-3.66883700	2.05941300
O	3.12321800	-2.12612800	-1.21187300
H	-2.59656900	-1.23821900	0.11113300
H	-2.22678500	-2.73394900	-1.73282900
H	-1.65427800	-4.03388200	-0.69137100
H	0.55353000	-1.97215600	1.80436300
H	-1.87450100	-4.41917100	2.00717600

H	-0.28264500	-3.99764600	1.38419400
H	-0.67525200	-3.67537100	3.07819200
C	-2.65017300	-1.74361900	2.70733800
H	-2.49934700	-0.78648000	3.19240000
C	-4.02969800	-2.08760900	2.15471000
H	-4.86047000	-1.38972100	2.23513700
C	-3.53118300	-2.74110900	3.42427300
H	-3.99291000	-2.40449400	4.34979400
H	-3.28855500	-3.79804100	3.41906900
C	-3.80333400	-2.76382400	0.82646200
C	-4.64784600	-3.56265300	0.16800900
H	-5.62153200	-3.82090300	0.57678200
H	-4.40415600	-3.98009000	-0.80651100
C	1.03712200	-4.11566200	-2.17769700
H	0.10465500	-4.66853400	-2.31988900
H	1.43840200	-3.86462100	-3.16730500
H	1.76625800	-4.78050600	-1.69967000
C	5.10503300	0.57485800	0.26771000
C	6.20576500	1.32810200	0.59185100
C	7.50517800	0.93406200	0.14252500
C	7.56876400	-0.26055500	-0.64098500
C	6.42365700	-0.96181900	-0.92482500
N	5.21460000	-0.54948600	-0.47712600
H	4.10244600	0.83736000	0.58676000
H	6.06178700	2.21791500	1.18961700
H	8.50847100	-0.63484800	-1.02390900
H	6.42746600	-1.87117800	-1.51522600
H	4.36062500	-1.10780200	-0.71429700
N	8.60943500	1.64928700	0.44089800
C	9.92692000	1.21587100	-0.03731000
H	10.67927800	1.92300200	0.30931800
H	10.18317300	0.22465800	0.35456500
H	9.96094100	1.19004800	-1.13272600
C	8.50830900	2.87056900	1.24688900
H	9.50349900	3.29477600	1.37288600
H	7.87778300	3.61918600	0.75302000
H	8.10021700	2.65525700	2.24137200

exo-reactant of model 1a

C	-3.15047900	-2.67686100	-0.02131300
C	-3.43360400	-3.41645700	1.31125200
C	-3.12917200	-2.87056400	2.50948300
C	-2.38803200	-1.61380800	2.52977000
C	-1.79167600	-1.17458100	1.38037400
C	-1.80290600	-1.91004100	0.07006700
C	-3.08228700	-3.82311400	-1.05346200
C	-3.53962100	-5.11276300	-0.39077000
C	-3.90953400	-4.78792700	1.02999400
C	-2.00136900	-0.67972100	3.55494600
C	-1.20802400	0.24615500	2.94647400
O	-1.06138900	-0.04586200	1.60766600
C	-4.50810000	-5.62962300	1.88887100
C	-4.36028000	-4.48933900	-1.50030500
C	-4.29464000	-1.67145000	-0.30945500
O	-1.64506900	-1.01749300	-1.04768300
C	-0.31723300	-0.92012800	-1.54769300
O	0.07620300	-2.01413300	-2.32295500
C	-0.54356200	-2.08343500	-3.60844300
H	-3.32247600	-3.39844400	3.44018200
H	-0.97973200	-2.64186900	0.04685000
H	-2.23927000	-3.82523800	-1.73855700
H	-3.04747500	-6.06199200	-0.58675300
H	-2.27932100	-0.69362100	4.60063400
H	-0.69888300	1.13603500	3.28404900
H	-4.78177200	-6.63846900	1.59281200
H	-4.74184100	-5.34074400	2.91042500
H	-4.34216100	-4.99581400	-2.46262500
H	-5.32208300	-4.05022200	-1.25268800
H	-5.26875200	-2.15994200	-0.23045100
H	-4.28274600	-0.84815600	0.41331000
H	-4.19593200	-1.26045500	-1.31954600
H	-0.30656100	0.00426500	-2.14142200
H	0.40062100	-0.85511000	-0.72621300
H	-0.11332100	-2.95003700	-4.11400600
H	-1.62921300	-2.20854300	-3.52391100
H	-0.32543300	-1.17690500	-4.19171200
C	5.24466300	-0.68240400	-0.66003800
C	6.08452500	0.52090800	-0.10777200

C	5.55182700	1.07823100	1.21602500
C	3.36828000	0.75713500	-0.08995900
C	3.83448100	-0.19735300	-0.91235800
C	6.06460800	-1.05672100	-1.92310700
C	7.49765000	-0.58157200	-1.68559700
C	1.96247900	2.17396300	0.90354200
O	2.06906900	1.25834400	-0.11753300
C	7.18850700	-2.05767100	-1.80267000
C	5.14722800	-1.85710200	0.35329000
O	0.90797800	2.76715500	1.10846200
H	5.92936300	1.31805000	-0.85366200
H	6.10451900	1.97237100	1.52855300
H	5.65190000	0.34566100	2.02923100
H	3.20120200	-0.66048800	-1.66597800
H	5.58986000	-0.92619700	-2.89277400
H	8.07732100	-0.12077400	-2.48249700
H	7.50770500	-2.54124400	-2.72296400
H	7.27025700	-2.69203100	-0.92664200
H	6.13003200	-2.12596500	0.75220100
H	4.50269500	-1.60116700	1.19995100
H	4.72328000	-2.74217200	-0.13341900
C	3.45745800	3.19532500	2.76417300
H	3.18580100	4.22533100	2.50446300
H	2.83226400	2.90647900	3.61833400
H	4.50113200	3.18561400	3.09052300
C	3.24470500	2.27479300	1.60536800
C	4.09732900	1.40977300	0.99013900
C	7.51591500	0.08389900	-0.32805300
C	8.56901400	0.27564200	0.47051000
H	9.56192300	-0.07141900	0.19611300
H	8.48153400	0.79321700	1.42324100
C	-2.53490000	2.16387600	-0.51604000
C	-3.75775200	2.62351200	-0.94017900
C	-4.09730700	4.00577800	-0.81833800
C	-3.10074700	4.85501100	-0.24337900
C	-1.89825800	4.33018600	0.15771500
N	-1.62506900	3.01085300	0.02275500
H	-2.24700600	1.11911900	-0.59093900
H	-4.44974700	1.90696000	-1.36144700
H	-3.26895500	5.91522100	-0.11115400

H	-1.11298400	4.93228300	0.60031800
H	-0.70049200	2.67598000	0.34828300
N	-5.29315100	4.48505700	-1.22258000
C	-5.60903000	5.90975800	-1.08056000
H	-6.61189800	6.09021800	-1.46545700
H	-5.58630600	6.21776900	-0.02851100
H	-4.90765400	6.52954400	-1.65149700
C	-6.29483500	3.58510500	-1.80300500
H	-7.18210800	4.16207100	-2.06064400
H	-5.91803900	3.11053800	-2.71665800
H	-6.58797500	2.80635700	-1.08921200

exo-TS of model 1a

C	-0.31941200	3.20357900	0.34252000
C	-1.54231500	2.39076500	0.83002700
C	-1.46229800	1.56155500	1.91838300
C	-0.14959900	1.24619000	2.42789700
C	0.95708200	1.58214800	1.68129700
C	0.94475900	2.28880200	0.35193100
C	-0.73686600	3.63141400	-1.08090100
C	-2.16042100	3.14786800	-1.33907000
C	-2.61796400	2.44723400	-0.11462000
C	0.34210100	0.48430500	3.54812100
C	1.69098600	0.42081300	3.39482300
O	2.08178100	1.07972900	2.24346400
C	-3.81983200	1.74149300	0.00030500
C	-1.84554400	4.63509300	-1.22242000
C	-0.06644200	4.41802500	1.27136200
O	2.16153100	3.01793800	0.18105400
C	2.89295500	2.77991200	-1.00682000
O	2.44736400	3.50226100	-2.11925900
C	2.72921000	4.90191300	-2.06696900
H	-2.33271800	1.04760000	2.31661200
H	0.86117800	1.53147200	-0.44310300
H	0.01149500	3.57752500	-1.86555800
H	-2.48685000	2.76961400	-2.30517300
H	-0.23044800	0.05936200	4.36180300
H	2.49227200	0.00454900	3.98610400
H	-4.63390900	2.02035600	-0.66463500

H	-4.13567400	1.48032700	1.00196300
H	-1.88902200	5.20189800	-2.14919300
H	-2.21636100	5.17449700	-0.35603900
H	-0.97458700	5.01307500	1.39230800
H	0.25701900	4.10167600	2.26789600
H	0.71364200	5.05891300	0.85135600
H	3.92590300	3.05801400	-0.75728300
H	2.82555400	1.72546500	-1.29668600
H	2.42790100	5.31550200	-3.03135800
H	2.16801500	5.39392000	-1.26397800
H	3.80447800	5.07502300	-1.91709000
C	-4.82889200	-0.98971100	-0.23964500
C	-4.46332700	-2.51332700	-0.41074100
C	-3.32829500	-2.94603500	0.52945100
C	-2.38608800	-0.77086400	-0.38501200
C	-3.61233000	-0.17241700	-0.72963700
C	-6.07727600	-0.87748200	-1.15202900
C	-6.68375000	-2.27373200	-1.27974200
C	-0.19949700	-1.19455000	-0.53540900
O	-1.18090900	-0.27704800	-0.85520700
C	-7.44410400	-1.16880900	-0.58066200
C	-5.16452700	-0.71276200	1.24728500
O	0.97825600	-0.94924000	-0.87306700
H	-4.06562500	-2.59826000	-1.43515700
H	-3.04586500	-3.99052600	0.35090900
H	-3.63468700	-2.87852100	1.58133000
H	-3.67291500	0.23065000	-1.73931700
H	-6.01289100	-0.22291200	-2.01855500
H	-7.07311900	-2.63688500	-2.22831300
H	-8.29537400	-0.75689800	-1.11765400
H	-7.58928900	-1.22272600	0.49322100
H	-5.74431700	-1.53705500	1.67399900
H	-4.25812300	-0.60859800	1.85231400
H	-5.76328100	0.19525100	1.35941400
C	-0.04862100	-3.53167300	0.55902200
H	0.51021700	-3.97810600	-0.27451400
H	0.67762200	-3.30255700	1.35118300
H	-0.72513800	-4.29754700	0.95073600
C	-0.80213400	-2.30983000	0.13117400
C	-2.16448000	-2.03735300	0.21047400

C	-5.80984800	-3.20200400	-0.47011900
C	-6.14804500	-4.38935000	0.04044800
H	-7.14740900	-4.79873700	-0.08465300
H	-5.43793500	-5.00084100	0.59268500
C	4.25508400	-1.00339400	0.35422300
C	5.60761700	-1.21013800	0.47761700
C	6.27058600	-2.16081800	-0.35851900
C	5.45054900	-2.85381700	-1.30224800
C	4.10403700	-2.59277200	-1.36833100
N	3.51824800	-1.68821400	-0.55130300
H	3.71411500	-0.28695600	0.96406700
H	6.14942800	-0.63309600	1.21490700
H	5.86658700	-3.58677100	-1.98002500
H	3.44954100	-3.09098500	-2.07482600
H	2.48708300	-1.49146600	-0.63505800
N	7.59813800	-2.39016400	-0.26503800
C	8.24788000	-3.36306900	-1.14912800
H	9.31082400	-3.39987300	-0.91413400
H	7.83188600	-4.36729500	-1.00624100
H	8.14026900	-3.07582600	-2.20181500
C	8.41037100	-1.65671600	0.71071800
H	9.44232100	-1.99832100	0.64087900
H	8.39211700	-0.57849500	0.51170400
H	8.05934600	-1.83882500	1.73313800

exo-product of model 1a

C	0.17190000	2.73822200	0.45951500
C	-0.81914000	1.66525300	-0.00611700
C	-1.34571200	0.60887300	0.93583400
C	-0.23681800	0.26305700	1.90779600
C	0.98247300	0.88125600	1.85820600
C	1.44672900	1.96646000	0.91804600
C	0.43672100	3.52711500	-0.83520300
C	-0.30027500	2.83463000	-1.97279100
C	-1.03750800	1.70473900	-1.32984000
C	-0.19220900	-0.60674600	3.05587800
C	1.04872900	-0.46165300	3.59646900
O	1.78181100	0.44125900	2.87486600
C	-1.88644300	0.73373800	-2.08993600

C	-0.71165200	4.22406100	-1.51791700
C	-0.35665300	3.63379600	1.59939900
O	2.38136800	2.86590100	1.51733200
C	3.72245900	2.42151900	1.54551900
O	4.33165300	2.37166300	0.27120100
C	4.62997200	3.65812000	-0.28009600
H	-2.18239900	1.00474500	1.52797000
H	1.91328500	1.53785700	0.01908600
H	1.43041700	3.94040900	-0.98019800
H	0.12744700	2.70535100	-2.96483700
H	-0.97827700	-1.24222500	3.43837700
H	1.54561600	-0.89117500	4.45321700
H	-1.23964300	0.17391500	-2.78198800
H	-2.59193000	1.27792000	-2.73299100
H	-0.45860600	5.05886100	-2.16707000
H	-1.66354800	4.32873100	-1.00360800
H	-1.28353900	4.12854300	1.29455900
H	-0.56017800	3.06021900	2.50989600
H	0.37807900	4.40467300	1.84805100
H	4.24180900	3.13515700	2.19554500
H	3.79754300	1.40828300	1.94732700
H	5.08837700	3.48539200	-1.25626400
H	3.72308000	4.25968400	-0.40382000
H	5.33731200	4.19787800	0.36437800
C	-4.15975200	0.11641200	-0.93216300
C	-4.79719900	-1.03166700	-0.08501900
C	-4.15431600	-1.20602900	1.30410900
C	-1.90446700	-0.61815000	0.12601000
C	-2.66859000	-0.26070500	-1.19975400
C	-5.03864500	0.01475500	-2.21725400
C	-6.37825700	-0.59887600	-1.80879400
C	-0.83337100	-2.64160700	0.34827500
O	-0.74592800	-1.43072300	-0.25029600
C	-6.31244600	0.81919100	-2.32833000
C	-4.32572400	1.49845700	-0.26491700
O	0.04766900	-3.48682800	0.20961700
H	-4.54375800	-1.95212000	-0.63827900
H	-4.63816200	-2.00681200	1.87233900
H	-4.22779600	-0.28672700	1.89845700
H	-2.70915600	-1.21570500	-1.73996100

H	-4.55201700	-0.29663300	-3.13900000
H	-6.86972000	-1.34316300	-2.43196300
H	-6.69969900	0.97528200	-3.33265300
H	-6.50607400	1.64753300	-1.65572100
H	-5.35587900	1.65108500	0.06823800
H	-3.69534700	1.63264700	0.61360000
H	-4.08176800	2.29895300	-0.97058200
C	-2.47249800	-4.00625200	1.81143500
H	-2.56206100	-4.83928200	1.10389300
H	-1.70379100	-4.29226500	2.53932300
H	-3.42359900	-3.90025800	2.33971500
C	-2.08812600	-2.74359100	1.10578900
C	-2.73218600	-1.56382100	0.97548300
C	-6.28537800	-0.88147900	-0.32634800
C	-7.28566500	-1.01404000	0.54757800
H	-8.32346700	-0.89804900	0.24564700
H	-7.10756100	-1.24824200	1.59487200
C	2.87322700	-1.46347900	-0.52135700
C	4.13818400	-0.98683900	-0.75730200
C	5.19284800	-1.89668600	-1.08212300
C	4.84293400	-3.28229600	-1.14927200
C	3.55438300	-3.68280900	-0.89743500
N	2.58873900	-2.78616300	-0.59070900
H	2.03959600	-0.81954200	-0.26567400
H	4.30812000	0.08056700	-0.67706700
H	5.57685000	-4.03883000	-1.39192200
H	3.25079100	-4.72313100	-0.93054500
H	1.61792500	-3.09714100	-0.37126900
N	6.45243200	-1.47038700	-1.31155300
C	7.50489700	-2.42353100	-1.67583400
H	8.43889000	-1.88168700	-1.81914900
H	7.65866200	-3.16405000	-0.88229400
H	7.26440500	-2.94407100	-2.61071000
C	6.77209400	-0.03909800	-1.25922800
H	7.84722500	0.08600800	-1.38329700
H	6.26256800	0.50889900	-2.06136000
H	6.48206700	0.39639300	-0.29806500

endo-reactant of model 1b

C	2.88617400	-2.57796000	-0.64751800
C	4.02251400	-1.56308200	-0.37813900
C	4.31412500	-1.13966900	0.87379800
C	3.43324100	-1.54020900	1.96349300
C	2.21007800	-2.08202200	1.66824500
C	1.67056700	-2.28918400	0.27625600
C	2.54232200	-2.33503100	-2.13365700
C	3.59186800	-1.41188000	-2.73828700
C	4.58803100	-1.08716700	-1.65985800
C	3.48313700	-1.43184400	3.39799400
C	2.29355300	-1.91484100	3.85264900
O	1.49605800	-2.30679600	2.80090900
C	5.75673900	-0.44524100	-1.84805300
C	3.47965400	-2.85500200	-3.19061800
C	3.39924000	-4.01618200	-0.37386000
O	0.74424200	-3.36980800	0.18374200
C	-0.59743200	-3.05538700	0.50125900
O	-1.26494300	-2.35523500	-0.52013200
C	-1.55266900	-3.15130500	-1.67178600
H	5.13376800	-0.44974400	1.06735800
H	1.17158100	-1.36512200	-0.06598500
H	1.49246100	-2.22642800	-2.39205500
H	3.33742400	-0.63459400	-3.45543200
H	4.29876700	-1.06600800	4.00758700
H	1.87705800	-2.07277200	4.83570900
H	6.44999200	-0.26106600	-1.03039000
H	6.07707500	-0.13842700	-2.84066200
H	3.06586300	-3.01740500	-4.18300100
H	4.27048900	-3.54926100	-2.92496500
H	4.35095600	-4.19371900	-0.88079200
H	3.56194900	-4.17906300	0.69582200
H	2.67261800	-4.75308500	-0.72607700
H	-1.07604200	-4.02443000	0.68861700
H	-0.65681600	-2.41769200	1.38751400
H	-2.08128700	-2.50468200	-2.37552500
H	-0.63545400	-3.52912400	-2.13774600
H	-2.19670200	-4.00095300	-1.40398600
C	-4.84226500	0.77871200	-0.90232800
C	-4.74073900	-0.42288200	0.10011900
C	-4.20435700	-0.02083900	1.47752900

C	-2.88652900	0.67183300	1.23776300
C	-2.61357700	1.26697600	-0.06212200
C	-3.45137900	1.33488600	-1.10903700
C	-1.78721500	0.85721400	2.02216400
C	-0.80924100	1.56226200	1.20034700
O	-1.32501100	1.80096200	-0.04525000
C	-5.72141900	1.93987400	-0.35893900
O	0.33498300	1.92660800	1.48553200
H	-3.96868700	-1.07504100	-0.33894400
H	-4.06407100	-0.89359500	2.12617600
H	-4.89747300	0.65323600	2.00036900
H	-3.16871500	1.83494500	-2.03273300
H	-6.68009100	1.57215800	0.01910000
H	-5.22331200	2.47143900	0.45798400
H	-5.92587400	2.66496100	-1.15427200
C	-5.47959600	0.08209400	-2.13370200
H	-4.88990000	0.02399100	-3.04574300
C	-6.24071300	-1.13771400	-1.61554600
H	-6.22424000	-2.08296100	-2.15380900
C	-6.98387100	0.01838200	-2.24734900
H	-7.38785100	-0.15850800	-3.24139000
H	-7.61065100	0.65203900	-1.62917800
C	-6.03411500	-1.17636500	-0.11798600
C	-6.80299100	-1.77853300	0.79297000
H	-7.70847500	-2.31013600	0.51174100
H	-6.55403000	-1.76939000	1.85178300
C	-1.51518000	0.45600500	3.43675800
H	-2.35942600	-0.09653700	3.85839000
H	-0.62004500	-0.17363500	3.50254700
H	-1.33415600	1.33523200	4.06722600
C	3.10950400	2.36841700	-0.47910300
C	4.16164500	2.88165400	-1.21789500
C	3.21293200	5.09496200	-0.93499600
C	2.17891400	4.52140700	-0.20157500
N	2.15143600	3.18972300	0.00581200
H	2.99736400	1.31412400	-0.24751200
H	4.91653600	2.20386400	-1.60156200
H	3.22519900	6.16690100	-1.09443500
H	1.35709600	2.74803300	0.56379700
C	4.20947100	4.26198200	-1.44521400

H	5.02361300	4.69361900	-2.02021600
Cl	0.90342700	5.45464800	0.47370200

endo-TS of model 1b

C	2.66563600	-1.39838300	1.69077200
C	1.28400400	-0.71031400	1.60357700
C	0.24285100	-1.28758800	0.91760400
C	0.53382600	-2.41924500	0.07455800
C	1.84930000	-2.71939100	-0.21104500
C	3.05229700	-1.95801200	0.29425600
C	3.59238400	-0.25266900	2.14541000
C	2.74404900	0.99055000	2.39030200
C	1.32635900	0.62769800	2.11060900
C	-0.25957800	-3.33590600	-0.70595000
C	0.62688200	-4.11138700	-1.38516900
O	1.92335200	-3.73256400	-1.09502300
C	0.23938800	1.50924000	2.19331100
C	3.42940500	0.26746400	3.54445800
C	2.63591500	-2.56801800	2.70881600
O	4.21774200	-2.76242600	0.40280800
C	5.00668900	-2.84512700	-0.78181800
O	5.72337800	-1.67565600	-1.04909000
C	6.86753200	-1.47842600	-0.21725200
H	-0.75591300	-0.86424600	0.93554000
H	3.25699600	-1.11575000	-0.38847900
H	4.56901400	-0.17306400	1.67695100
H	3.08494200	1.99077100	2.14687000
H	-1.33798300	-3.41114700	-0.74366000
H	0.53158800	-4.94212700	-2.06712700
H	-0.74382300	1.06881900	2.33571500
H	0.39281200	2.42722800	2.75478400
H	4.27719700	0.78339700	3.98822800
H	2.81531200	-0.27051000	4.25994200
H	2.23359200	-2.24034400	3.67026300
H	2.01224200	-3.39378300	2.35343800
H	3.64735100	-2.95139000	2.86630600
H	5.67472900	-3.69671600	-0.60667300
H	4.37523200	-3.02238200	-1.65672700
H	7.34308900	-0.55638400	-0.55722300

H	6.58632900	-1.38142500	0.83852100
H	7.57402000	-2.31293300	-0.32735600
C	0.70024700	3.16168600	-0.33942700
C	1.56695200	2.13858100	-1.14841100
C	0.79441800	1.41311900	-2.25290600
C	-0.50080200	0.91766600	-1.66396100
C	-0.95389900	1.38474300	-0.41126100
C	-0.38581600	2.37342300	0.40781300
C	-1.48095100	0.08608200	-2.20172300
C	-2.53192800	0.03481400	-1.24556700
O	-2.20682500	0.83031000	-0.15104200
C	-0.05489500	4.16359500	-1.25861800
O	-3.62619100	-0.58000600	-1.24915800
H	1.83617400	1.37077400	-0.40602200
H	1.37828500	0.57649800	-2.65820700
H	0.58436000	2.07835000	-3.10316400
H	-1.08363100	2.96875800	0.99598900
H	0.61370400	4.59986200	-2.00627500
H	-0.87849100	3.68432200	-1.79529100
H	-0.47045600	4.98422500	-0.66281200
C	1.77343000	3.89049400	0.50963000
H	1.69216200	3.84706100	1.59109200
C	3.12075600	3.70299000	-0.18438000
H	4.03434100	3.51236300	0.37514800
C	2.50177200	5.07781600	-0.07727100
H	2.96345600	5.75801500	0.63485800
H	2.13815400	5.56766000	-0.97375000
C	2.86058900	2.87704100	-1.42119400
C	3.63341300	2.79372700	-2.50763400
H	4.55771700	3.35951700	-2.59339600
H	3.37786900	2.15165600	-3.34733300
C	-1.50288000	-0.61921100	-3.52413900
H	-1.39500800	0.08423800	-4.35954500
H	-0.69000800	-1.35189800	-3.60704000
H	-2.44901900	-1.15216400	-3.65484200
C	-5.39105300	0.82408900	1.30029600
C	-6.40735300	1.16259500	2.17706500
C	-7.80900200	-0.49353800	1.10046900
C	-6.74584100	-0.78653300	0.24821400
N	-5.57646100	-0.13189500	0.36506100

H	-4.40819700	1.28350600	1.29774500
H	-6.24652700	1.93248100	2.92321800
H	-4.73036200	-0.34314100	-0.31577800
C	-7.63182900	0.49110200	2.07128800
Cl	-6.86688900	-1.98215600	-0.98111900
H	-8.44943300	0.73386300	2.74368200
H	-8.74473000	-1.02989600	0.99373700

endo-product of model 1b

C	-2.02652500	-2.24763500	-0.32512100
C	-0.95720000	-1.17371800	-0.54920800
C	-0.21275200	-0.54714500	0.60598500
C	-1.18086400	-0.44340800	1.76938900
C	-2.46534300	-0.90993100	1.68491100
C	-3.15278900	-1.58541400	0.52360500
C	-2.49430900	-2.54966400	-1.76195400
C	-1.74678200	-1.62461600	-2.71241400
C	-0.82856500	-0.83397400	-1.84089100
C	-0.99855500	-0.04322500	3.14246800
C	-2.18767900	-0.27009400	3.76615800
O	-3.09267400	-0.79802100	2.88843800
C	0.15683100	0.19674700	-2.30101300
C	-1.50890000	-3.12465300	-2.74715800
C	-1.49510100	-3.50831800	0.39259300
O	-4.08990800	-2.56475800	0.96072900
C	-5.41878600	-2.08997800	1.13351200
O	-6.10294500	-1.90672100	-0.07420300
C	-6.52178000	-3.11713300	-0.70343500
H	0.59178500	-1.22602700	0.92671500
H	-3.67256900	-0.85097100	-0.10798600
H	-3.54676700	-2.76967800	-1.91362200
H	-2.22504000	-1.14614900	-3.56451400
H	-0.10575300	0.35493600	3.60579000
H	-2.54192900	-0.12655500	4.77578300
H	1.13803100	-0.27716200	-2.45583700
H	-0.11989700	0.61646000	-3.27394800
H	-1.92324500	-3.67616900	-3.58781900
H	-0.54808300	-3.49564400	-2.39896400
H	-0.65363900	-3.93705100	-0.16020200
H	-1.15804000	-3.28756600	1.41117100

H	-2.28382700	-4.26239600	0.45985500
H	-5.90746800	-2.84849200	1.75717800
H	-5.42327700	-1.11739600	1.63358300
H	-7.06486300	-2.82738400	-1.60535600
H	-5.66609900	-3.74748100	-0.97505000
H	-7.19290400	-3.68495300	-0.04329800
C	-0.78054200	2.47283800	-1.26151100
C	-1.57410800	2.45597800	0.08558600
C	-0.69729900	2.74730100	1.30277100
C	0.54728500	1.91368800	1.17200300
C	0.58513600	0.76958500	0.17604000
C	0.32076600	1.33217100	-1.27208800
C	1.77037000	2.09235200	1.72127100
C	2.66211800	1.10900400	1.11175300
O	2.00627100	0.36280300	0.21004600
C	-0.02481600	3.81441100	-1.43212100
O	3.87085800	0.94129400	1.32884300
H	-1.93398200	1.42350700	0.19468800
H	-1.23024400	2.49187200	2.22759500
H	-0.42815200	3.80837100	1.37530400
H	1.26283100	1.83056300	-1.52356800
H	-0.65999700	4.67918300	-1.22046100
H	0.83827600	3.87764600	-0.75953800
H	0.34816600	3.91230500	-2.45848600
C	-1.95167600	2.34534900	-2.28007800
H	-2.00484200	1.46534800	-2.91030700
C	-3.22109600	2.85227400	-1.60240200
H	-4.17438400	2.34611000	-1.73932700
C	-2.63961500	3.59284300	-2.78591300
H	-3.18450000	3.50084000	-3.72272200
H	-2.19380500	4.57009800	-2.63691700
C	-2.83014800	3.24969300	-0.20136200
C	-3.48031500	4.08003200	0.61873200
H	-4.39235700	4.58460600	0.30991800
H	-3.13361800	4.28027000	1.63024600
C	2.24895700	3.10224200	2.71786500
H	3.10383900	3.66682900	2.32786800
H	1.45604700	3.80882600	2.97721700
H	2.58424700	2.61520100	3.64194500
C	6.15928200	-0.90389200	-0.82097400

C	7.21238000	-1.78411900	-1.05570800
C	7.25251200	-2.27766600	1.31751300
C	6.20415300	-1.39082200	1.48740100
N	5.68465300	-0.73253000	0.42760900
H	7.58628400	-1.91428300	-2.06461800
H	7.66362000	-2.80045700	2.17358200
H	5.74466200	-1.16642900	2.44354900
H	4.87762200	-0.05548500	0.63187800
C	7.75895700	-2.47374600	0.02641800
H	8.58188900	-3.16286100	-0.13918100
Cl	5.42161100	0.00202300	-2.08011600

exo-reactant of model 1b

C	5.44195400	-0.64518800	0.20722300
C	6.01990700	-1.35414500	-1.04470900
C	5.29702200	-1.51396000	-2.17487400
C	3.88863100	-1.13337300	-2.15477400
C	3.28150900	-0.88795200	-0.95524600
C	3.93992500	-1.00898700	0.38801700
C	6.30656900	-1.20405700	1.35841000
C	7.46825600	-1.98721700	0.76772000
C	7.35198100	-1.91310100	-0.72945900
C	2.85124900	-1.04082900	-3.14927200
C	1.70264400	-0.74879100	-2.47812800
O	1.94459700	-0.66099400	-1.12207200
C	8.27689800	-2.34142900	-1.60425300
C	7.72009800	-0.70250900	1.52819900
C	5.58186900	0.88895000	0.03615600
O	3.29197400	-0.16026900	1.35609300
C	2.58207500	-0.84215100	2.38158500
O	3.39458200	-1.37732400	3.38101200
C	3.97107700	-0.41414300	4.26314400
H	5.70701200	-2.01787100	-3.04663100
H	3.87129800	-2.05064900	0.74084600
H	5.78459300	-1.57294000	2.23629800
H	7.80931800	-2.92058700	1.20828700
H	2.94966600	-1.16927700	-4.21920500
H	0.68398500	-0.55383900	-2.77777600
H	9.21271400	-2.77866900	-1.26760800

H	8.13041200	-2.27077200	-2.67904900
H	8.16264800	-0.80142400	2.51677200
H	8.06249000	0.16929500	0.97870400
H	6.59997600	1.15595400	-0.25666300
H	4.91009200	1.26105300	-0.74521200
H	5.35277500	1.40069500	0.97688800
H	1.89548600	-0.09027300	2.79601600
H	2.02336600	-1.68675700	1.96496400
H	4.50367400	-0.97753100	5.03148800
H	4.67456200	0.24189100	3.73683700
H	3.18679400	0.19272100	4.73892700
C	-6.15488400	-0.91719900	1.18183700
C	-6.69223200	-1.01949800	-0.28780600
C	-5.66440500	-1.58398700	-1.27417800
C	-4.20155600	0.02489800	0.08128100
C	-4.96619400	0.01679600	1.18548100
C	-7.41837100	-0.40363300	1.92128700
C	-8.62886200	-0.84245400	1.09793200
C	-2.51651100	0.47152900	-1.30128500
O	-3.02158500	0.75522600	-0.05863600
C	-8.39963600	-1.40381900	2.48376400
C	-5.65875100	-2.28399500	1.73182100
O	-1.46609100	0.99296800	-1.68228100
H	-6.85089600	0.02981100	-0.58742400
H	-6.03806100	-1.55960400	-2.30481700
H	-5.42622400	-2.63346400	-1.05028400
H	-4.69692400	0.59244600	2.06828100
H	-7.37845800	0.58864600	2.36457000
H	-9.48061300	-0.18138200	0.95380500
H	-9.06732800	-1.04247100	3.26230100
H	-8.11992100	-2.44547700	2.59914700
H	-6.39624000	-3.07415800	1.56232300
H	-4.72456400	-2.59165200	1.25197400
H	-5.47547900	-2.21538500	2.80959400
C	-3.12052500	-0.96716100	-3.37622200
H	-2.89131300	-0.13886500	-4.05613100
H	-2.25580700	-1.64289800	-3.38818300
H	-3.97861400	-1.51510500	-3.77538500
C	-3.39596900	-0.46683300	-1.99412100
C	-4.42670700	-0.73207900	-1.14207300

C	-8.09072400	-1.56984600	-0.11349100
C	-8.72592800	-2.46327400	-0.87604500
H	-9.74551100	-2.77232600	-0.66059800
H	-8.25648600	-2.91282800	-1.74824800
C	1.19542800	2.22524000	0.12874800
C	2.11904500	3.00165400	0.80828500
C	0.68137100	4.92429200	0.46574400
C	-0.21136200	4.09663500	-0.20552700
N	0.06360800	2.78451700	-0.35576500
H	3.01843000	2.52991900	1.18692700
H	-0.61618700	2.14810500	-0.85949300
C	1.85549800	4.36511900	0.97538200
Cl	-1.68466500	4.67845700	-0.87444000
H	2.56311700	4.99975300	1.50106100
H	1.32745800	1.16508200	-0.06273700
H	0.45262900	5.97757800	0.57903800

exo-TS of model 1b

C	0.67400200	3.24086400	0.21568200
C	-0.64556700	2.64930500	0.76375800
C	-0.67123600	1.89939400	1.90920300
C	0.58878100	1.43478500	2.43719100
C	1.72005900	1.54767800	1.66059800
C	1.78907100	2.15278600	0.28220800
C	0.30350200	3.62562100	-1.23274900
C	-1.17906300	3.33317800	-1.45206700
C	-1.71538300	2.78703800	-0.18300200
C	0.98110600	0.69380200	3.60929300
C	2.30316200	0.42030600	3.45360100
O	2.76677400	0.92647400	2.25172500
C	-3.00171700	2.27032800	-0.01745800
C	-0.65206800	4.76479000	-1.43409000
C	1.11709400	4.46601500	1.05482900
O	3.09153200	2.68636900	0.04660200
C	3.78166800	2.20995300	-1.09453200
O	3.42062500	2.83670700	-2.29130800
C	3.89640300	4.17847000	-2.42178700
H	-1.60170800	1.54152300	2.34189100
H	1.57813400	1.36302800	-0.45524800

H	1.02605000	3.40984900	-2.01394700
H	-1.57098200	2.94794000	-2.39054700
H	0.36643100	0.42217000	4.45714500
H	3.04620100	-0.05811400	4.07334300
H	-3.77885000	2.61271600	-0.69643600
H	-3.33495700	2.10432900	0.99877000
H	-0.63213200	5.27103700	-2.39588700
H	-0.92889700	5.40474600	-0.60187900
H	0.30935300	5.19681700	1.13657400
H	1.40461200	4.17543200	2.06993300
H	1.97764000	4.95216200	0.58731500
H	4.84258400	2.38401200	-0.87101000
H	3.57974100	1.14391100	-1.24821800
H	3.62613200	4.50692300	-3.42717400
H	3.43412200	4.84090800	-1.68058100
H	4.98914800	4.21407600	-2.30953300
C	-4.41609000	-0.29155200	-0.18106000
C	-4.29310100	-1.86265100	-0.24711700
C	-3.27319200	-2.40632000	0.76471600
C	-1.96723900	-0.47251000	-0.23657600
C	-3.06979200	0.28990100	-0.66317100
C	-5.60050300	-0.04425300	-1.15065000
C	-6.41787300	-1.33300700	-1.22035500
C	0.12301200	-1.23994800	-0.25815400
O	-0.67884700	-0.20719200	-0.67726100
C	-7.01386600	-0.07930600	-0.62028200
C	-4.75142200	0.12845100	1.27190500
O	1.34590100	-1.19069800	-0.55626800
H	-3.88169000	-2.07641600	-1.24696100
H	-3.15493100	-3.49161900	0.66108800
H	-3.59981600	-2.22223000	1.79632500
H	-3.03008400	0.65772400	-1.68654800
H	-5.40557900	0.53304800	-2.05196400
H	-6.82867200	-1.69123000	-2.16167300
H	-7.77123600	0.42599200	-1.21492400
H	-7.19813600	-0.03995100	0.44810900
H	-5.47235900	-0.56338500	1.71806700
H	-3.86083900	0.12352900	1.90869200
H	-5.19648600	1.12657300	1.30611000
C	-0.13282800	-3.48797800	0.99642400

H	0.32274300	-4.11371300	0.21753300
H	0.63157000	-3.31260300	1.76616200
H	-0.93009200	-4.07429000	1.46308700
C	-0.66341600	-2.19950000	0.44451500
C	-1.97080900	-1.71326700	0.44208100
C	-5.73025600	-2.33176100	-0.32028500
C	-6.26896300	-3.41311500	0.24961600
H	-7.31644700	-3.66816100	0.10990300
H	-5.68208000	-4.08884400	0.86774400
C	4.32061300	-1.86392900	0.63747700
C	5.60721000	-2.32137100	0.86849800
C	5.18721800	-4.12861600	-0.68871000
C	3.90589500	-3.61664300	-0.87898600
N	3.50364200	-2.51639000	-0.21844800
H	6.25498800	-1.78908900	1.55589500
H	2.50408200	-2.08733600	-0.36673000
C	6.04096000	-3.47003800	0.19567100
Cl	2.78359200	-4.34882800	-1.95854400
H	7.04460700	-3.85284300	0.35614200
H	3.89564300	-0.98139800	1.10589800
H	5.49552900	-5.01710400	-1.22742700

exo-product of model 1b

C	-0.51194300	-2.96148100	0.19441600
C	0.47959300	-1.83968000	-0.13463000
C	0.92482100	-0.84324400	0.90892600
C	-0.24384800	-0.59379600	1.83964500
C	-1.44499400	-1.22815700	1.67277400
C	-1.82933500	-2.24571500	0.62466000
C	-0.68160900	-3.66143800	-1.16556400
C	0.10236000	-2.87396600	-2.20634000
C	0.77273900	-1.77804400	-1.44307100
C	-0.36848600	0.17844000	3.05006800
C	-1.63270600	-0.03232500	3.50894400
O	-2.30634600	-0.88573900	2.67724500
C	1.63707300	-0.73623900	-2.08250100
C	0.52177600	-4.28316100	-1.82493700
C	-0.03503800	-3.92682300	1.29933000
O	-2.78303900	-3.20370900	1.08148800

C	-4.13041700	-2.76951900	1.09851000
O	-4.65228400	-2.48481400	-0.18201300
C	-4.94611200	-3.64368500	-0.97032800
H	1.73923600	-1.26015000	1.51737500
H	-2.24059200	-1.75305500	-0.26848000
H	-1.65404400	-4.08598500	-1.39647000
H	-0.26925000	-2.68370000	-3.21101800
H	0.38239600	0.79270200	3.52651200
H	-2.18342900	0.31553300	4.36988000
H	1.01723600	-0.14763400	-2.77536300
H	2.39560400	-1.21726300	-2.71525300
H	0.32805900	-5.07477200	-2.54461800
H	1.44470500	-4.40361300	-1.26344800
H	0.91876300	-4.38329800	1.01889300
H	0.10061200	-3.41712400	2.25917700
H	-0.76744700	-4.72542100	1.44635600
H	-4.68206700	-3.58946100	1.57160300
H	-4.24156700	-1.84784100	1.67423000
H	-5.34491700	-3.28487900	-1.92147400
H	-4.04612800	-4.24119000	-1.15150000
H	-5.70126200	-4.26457600	-0.47045700
C	3.82170400	-0.13709600	-0.75688700
C	4.37372600	0.96479100	0.20365400
C	3.65137700	1.01836400	1.56383100
C	1.49160500	0.45268900	0.22114900
C	2.33589400	0.21482300	-1.08224800
C	4.76576900	0.08243200	-1.97948300
C	6.06020300	0.70351200	-1.45302200
C	0.34353200	2.41818300	0.53151200
O	0.32682700	1.25991700	-0.15973500
C	6.06941600	-0.67492700	-2.07318500
C	3.99494400	-1.55862000	-0.18051100
O	-0.56361000	3.24511700	0.41178600
H	4.12055900	1.91541200	-0.29623100
H	4.07673200	1.78877200	2.21463300
H	3.72185500	0.06006700	2.09332900
H	2.37445700	1.20713000	-1.55069300
H	4.32043500	0.44477600	-2.90347100
H	6.56041300	1.50442000	-1.99347600
H	6.51616300	-0.74769100	-3.06211800

H	6.25252400	-1.54329100	-1.44996200
H	5.00910700	-1.70524100	0.20071200
H	3.32081300	-1.77507600	0.64780800
H	3.81799400	-2.31239100	-0.95427100
C	1.85102800	3.72279300	2.17861000
H	1.95539000	4.60849300	1.54056700
H	1.03353200	3.93226300	2.87870000
H	2.77305200	3.60322200	2.75323900
C	1.54880200	2.50582100	1.36117800
C	2.23913900	1.35781000	1.18073400
C	5.87717500	0.87579200	0.03786000
C	6.82272100	0.97394100	0.97485200
H	7.87875800	0.91010700	0.72533700
H	6.58005600	1.12693900	2.02417600
C	-3.21978400	1.28315200	-0.49137200
C	-4.45137300	0.77665400	-0.87031200
C	-5.09089300	3.01920700	-1.55011800
C	-3.83572700	3.46729000	-1.14948300
N	-2.94207100	2.59837800	-0.63720800
H	-4.66194800	-0.28298000	-0.74422000
H	-1.98527100	2.92629100	-0.30611300
C	-5.39384900	1.66448800	-1.40490600
Cl	-3.35649700	5.11223000	-1.27686700
H	-6.37114500	1.30182800	-1.71020600
H	-2.41858500	0.68788600	-0.06617000
H	-5.80395100	3.72446800	-1.96103300

endo-reactant of model 1c

C	-0.95261200	3.49581100	1.16371200
C	0.59256500	3.48010300	1.07477000
C	1.24440700	3.89257400	-0.03619500
C	0.46071000	4.21339900	-1.22108200
C	-0.85195800	3.82532000	-1.27379400
C	-1.57203500	3.06090800	-0.19263200
C	-1.25164400	2.46960900	2.27787600
C	0.05757900	2.06212800	2.93915800
C	1.16366800	2.83044600	2.27273500
C	0.74942100	4.80694300	-2.50049300
C	-0.40583700	4.73182800	-3.21864700

O	-1.39473700	4.12091800	-2.48170100
C	2.44203400	2.87208100	2.69802900
C	-0.98366600	2.85352700	3.70827700
C	-1.44582200	4.92416500	1.51210500
O	-2.97700000	3.30525400	-0.17330200
C	-3.74637700	2.51145300	-1.05606200
O	-3.99737600	1.21594400	-0.56668000
C	-4.93610300	1.17941700	0.51154300
H	2.33130900	3.89447000	-0.09279100
H	-1.40089900	1.97888300	-0.33170700
H	-2.02920600	1.73549500	2.08459100
H	0.25694100	1.04042500	3.25437300
H	1.68053400	5.24602800	-2.83344400
H	-0.69806400	5.06171900	-4.20376800
H	3.19325500	3.48001600	2.19804800
H	2.74663200	2.35920800	3.60737200
H	-1.52885900	2.31211600	4.47779900
H	-0.76961500	3.88630800	3.96491600
H	-0.90748400	5.32221300	2.37587100
H	-1.28122400	5.61133000	0.67670400
H	-2.51485700	4.91312600	1.74080700
H	-4.68443000	3.06332800	-1.19046700
H	-3.23823300	2.37803500	-2.01481400
H	-5.11139600	0.12627900	0.74062900
H	-4.54697600	1.69497000	1.39725100
H	-5.88571500	1.64452100	0.21197500
C	-2.63751600	-3.93026200	0.45780100
C	-3.45539700	-2.69672400	-0.05946900
C	-2.94583500	-2.13297200	-1.38992400
C	-1.47356000	-1.86326800	-1.20812400
C	-0.73983500	-2.53770600	-0.14670400
C	-1.20973600	-3.48576900	0.68032700
C	-0.60471900	-1.03403200	-1.85478700
C	0.67785100	-1.17021100	-1.17515300
O	0.57703400	-2.07517100	-0.15173400
C	-2.59393500	-5.09303400	-0.57340200
O	1.74822500	-0.59666200	-1.39857000
H	-3.25656200	-1.91267600	0.68999200
H	-3.46581900	-1.20444500	-1.65219200
H	-3.10288500	-2.84080800	-2.21611200

H	-0.56940500	-3.96964700	1.41458900
H	-3.59301100	-5.32876300	-0.95185300
H	-1.96396900	-4.84217000	-1.43238100
H	-2.18419300	-5.99681700	-0.10946100
C	-3.43497600	-4.30137300	1.73573000
H	-2.93261000	-4.20129600	2.69513200
C	-4.85929600	-3.78230300	1.54167100
H	-5.40677700	-3.32043900	2.36052900
C	-4.58951800	-5.26816200	1.62746400
H	-4.89950600	-5.75794800	2.54751600
H	-4.71090900	-5.88512700	0.74368700
C	-4.89256500	-3.09474000	0.19536800
C	-5.96082100	-2.85949800	-0.57132000
H	-6.95559700	-3.18339000	-0.27568500
H	-5.88220100	-2.32978400	-1.51800900
C	-0.80870800	-0.12672300	-3.02552100
H	-1.86858900	-0.05184000	-3.28289900
H	-0.42690500	0.87923600	-2.81841400
H	-0.26956800	-0.49599500	-3.90720500
C	4.11052700	0.19741400	0.93045300
C	5.27895100	0.30683500	1.66671900
C	6.22957700	-1.49747900	0.35501700
C	5.02593200	-1.56921800	-0.36106200
N	4.02094000	-0.72558300	-0.04833000
H	3.23635800	0.82198300	1.09309200
H	5.35324600	1.04805700	2.45416600
H	3.10146300	-0.77345200	-0.59630200
C	6.34368900	-0.54673900	1.37524400
Cl	4.74807500	-2.67924500	-1.63388500
H	7.27269000	-0.48508200	1.93378100
Cl	7.54431600	-2.55274000	-0.00604900

endo-TS of model 1c

C	2.98452000	-1.48816700	1.72524900
C	1.64032400	-0.73238200	1.61942200
C	0.58480600	-1.25324800	0.91108100
C	0.83395200	-2.39283700	0.06586600
C	2.13807300	-2.75514500	-0.20024700
C	3.36772300	-2.05435500	0.33007700

C	3.95711600	-0.39237400	2.20701800
C	3.16647300	0.88991600	2.44583600
C	1.73899600	0.59993900	2.13466800
C	0.00960000	-3.26306700	-0.73532600
C	0.86794000	-4.07601500	-1.40650800
O	2.17648800	-3.76349800	-1.09204000
C	0.69594000	1.53387600	2.19646300
C	3.79116800	0.12398400	3.60682300
C	2.88017200	-2.66318800	2.73200800
O	4.49546500	-2.90833000	0.45299500
C	5.27670200	-3.05250700	-0.73195500
O	6.01817000	-1.91091000	-1.04688200
C	7.17293000	-1.70853900	-0.23112900
H	-0.39275100	-0.78273100	0.91545700
H	3.62133300	-1.21747600	-0.34304500
H	4.94641100	-0.35794100	1.76010800
H	3.56133200	1.87400800	2.21865200
H	-1.07040600	-3.28512100	-0.79132100
H	0.74346900	-4.89600300	-2.09672900
H	-0.31197800	1.14331400	2.30753200
H	0.87898700	2.44180100	2.76498500
H	4.65395800	0.59369700	4.07246300
H	3.13670900	-0.38869900	4.30486800
H	2.47778100	-2.32431400	3.68957000
H	2.22314600	-3.45422900	2.35842600
H	3.86863500	-3.09733700	2.90301800
H	5.92553400	-3.91208800	-0.52670700
H	4.63657500	-3.24810300	-1.59622900
H	7.66608900	-0.81083900	-0.60892300
H	6.90229500	-1.56552300	0.82214600
H	7.85961900	-2.56241400	-0.31450600
C	1.31152600	3.17232100	-0.31750600
C	2.15646200	2.11124800	-1.09943200
C	1.38822100	1.42615600	-2.23247200
C	0.05282500	0.98911500	-1.68838400
C	-0.41990000	1.47480800	-0.45057300
C	0.16472800	2.43550300	0.38901700
C	-0.94644600	0.20357400	-2.26104600
C	-2.02816200	0.20145800	-1.34076900
O	-1.70609100	0.97835900	-0.23491400

C	0.63533200	4.20925700	-1.25958000
O	-3.15071400	-0.36432800	-1.38386200
H	2.36195800	1.32900300	-0.35169100
H	1.94599600	0.56538800	-2.62322000
H	1.23635200	2.10345700	-3.08559700
H	-0.52221200	3.05962100	0.95967900
H	1.35005300	4.62087600	-1.97802900
H	-0.18530100	3.76643900	-1.83090700
H	0.23077100	5.04367400	-0.67552700
C	2.38675500	3.84860600	0.57143500
H	2.26681500	3.80398800	1.64920400
C	3.74685200	3.60105600	-0.07758600
H	4.63122200	3.36831600	0.51221000
C	3.18784900	5.00254600	0.01392800
H	3.65601500	5.65969700	0.74317300
H	2.87550000	5.50914900	-0.89217700
C	3.49228600	2.78873100	-1.32434700
C	4.30015900	2.66766200	-2.38133400
H	5.25209500	3.19018100	-2.43245600
H	4.04647300	2.03712000	-3.23022600
C	-0.95529500	-0.50024600	-3.58440000
H	-0.75629200	0.19264900	-4.41159400
H	-0.19426000	-1.28985300	-3.62870400
H	-1.92964200	-0.96428900	-3.76201400
C	-4.88374100	1.08864700	1.13136700
C	-5.90493900	1.45885200	1.99112000
C	-7.36527600	-0.09770400	0.84541400
C	-6.29287900	-0.43254200	0.00238300
N	-5.10033800	0.16643300	0.17397600
H	-3.87861500	1.49511500	1.16188100
H	-5.73015900	2.20187000	2.76107700
H	-4.23715700	-0.07944700	-0.49907200
C	-7.15626800	0.85760400	1.84421000
Cl	-6.41763100	-1.58410200	-1.25964500
H	-7.97990500	1.12303400	2.49966700
Cl	-8.91117900	-0.84158200	0.66256600

endo-product of model 1c

C	-2.06009500	-2.30971500	-0.18195100
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C	-1.14679800	-1.12600900	-0.51644300
C	-0.46331800	-0.32315500	0.56539100
C	-1.40011900	-0.27311300	1.75749700
C	-2.61427400	-0.90600200	1.75102800
C	-3.24114200	-1.73657700	0.65728100
C	-2.51873900	-2.77441200	-1.57769000
C	-1.92129100	-1.83404600	-2.61530000
C	-1.09318300	-0.87006600	-1.83242600
C	-1.22872800	0.23305100	3.09663700
C	-2.35726000	-0.10631500	3.77903200
O	-3.21237300	-0.80106000	2.96974700
C	-0.25864000	0.24052500	-2.39316800
C	-1.49071600	-3.28943300	-2.55260400
C	-1.35038900	-3.43505000	0.60351600
O	-4.03793900	-2.79349700	1.18190500
C	-5.40821000	-2.47061300	1.38252400
O	-6.14619700	-2.42326600	0.19391100
C	-6.43908100	-3.70140500	-0.36952100
H	0.43898400	-0.85887900	0.89615600
H	-3.86230200	-1.11427600	-0.00283400
H	-3.53657100	-3.13891100	-1.67792100
H	-2.47695600	-1.48474200	-3.48306200
H	-0.38168600	0.77115200	3.50070500
H	-2.69486200	0.05227500	4.79209200
H	0.77462200	-0.11165700	-2.53320700
H	-0.59831900	0.54246700	-3.38918500
H	-1.84970200	-3.95023800	-3.33805100
H	-0.48117200	-3.50649000	-2.21251300
H	-0.48205900	-3.80039400	0.04681700
H	-1.00815200	-3.09384400	1.58644700
H	-2.03525200	-4.27225600	0.76248300
H	-5.78317100	-3.25278700	2.05385500
H	-5.51261100	-1.48392100	1.84247100
H	-7.04504400	-3.51801300	-1.25919900
H	-5.52441400	-4.23765800	-0.65074600
H	-7.01303200	-4.31494900	0.33947800
C	-1.47523600	2.44900000	-1.50455000
C	-2.26023000	2.40106100	-0.15242600
C	-1.43445800	2.89509100	1.03497600
C	-0.07768400	2.25551400	0.93599600

C	0.12633500	1.06153300	0.02284400
C	-0.23168300	1.46652000	-1.45868300
C	1.10833300	2.65563500	1.44917600
C	2.13363100	1.77712800	0.89332900
O	1.59281500	0.87645700	0.06031300
C	-0.90557400	3.86813200	-1.75368800
O	3.35633000	1.81222000	1.09812500
H	-2.46449100	1.33582800	0.02342800
H	-1.91691900	2.61655700	1.98039100
H	-1.33136600	3.98731300	1.04235900
H	0.63170000	2.06255300	-1.77286000
H	-1.64856900	4.65120800	-1.57782600
H	-0.05552900	4.07878600	-1.09511700
H	-0.55413200	3.96068800	-2.78802900
C	-2.61638200	2.10984200	-2.50816500
H	-2.54368800	1.20420100	-3.09829100
C	-3.94575500	2.46503000	-1.85034400
H	-4.81860900	1.82464800	-1.95825500
C	-3.47053500	3.22342200	-3.06958500
H	-3.99354000	3.01269600	-3.99963700
H	-3.16749900	4.25947100	-2.96626100
C	-3.61869900	2.98549900	-0.47390400
C	-4.38517000	3.75156900	0.30743700
H	-5.36180300	4.09903800	-0.01994100
H	-4.07304900	4.05130300	1.30548600
C	1.43490300	3.79128800	2.36873200
H	0.54170100	4.37226100	2.61318900
H	1.86859700	3.42467200	3.30723200
H	2.17325700	4.46531400	1.91844700
C	6.45435100	1.41767400	0.20222500
C	7.73623900	1.02252000	-0.14116300
C	6.93719400	-1.26160800	-0.31193900
C	5.65680200	-0.80817700	0.04129400
N	5.46564200	0.50421300	0.28023200
H	6.16520800	2.43822300	0.42546500
H	8.53424100	1.75358100	-0.20438000
H	4.49594700	0.87877100	0.55759100
C	7.97547300	-0.32837200	-0.40057000
Cl	4.29849300	-1.83684600	0.19448300
H	8.96873800	-0.67221300	-0.67232600

Cl	7.23337100	-2.92926500	-0.62959300
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exo-reactant of model 1c

C	5.42191200	-0.96259300	0.25818700
C	6.04510300	-1.71290000	-0.94695800
C	5.35992200	-1.92201500	-2.09246400
C	3.94862300	-1.55385000	-2.13151400
C	3.30148300	-1.26741800	-0.96230300
C	3.91753000	-1.33243600	0.40465300
C	6.25429900	-1.46900400	1.45656600
C	7.44121600	-2.26192300	0.93271300
C	7.37164000	-2.24577600	-0.56914500
C	2.94229500	-1.51289600	-3.16080100
C	1.77023200	-1.20771600	-2.53794600
O	1.96787800	-1.06300100	-1.17972400
C	8.32740900	-2.69665700	-1.39820500
C	7.65718900	-0.94687300	1.65101800
C	5.55540000	0.56496600	0.03201200
O	3.23236800	-0.45412900	1.31922800
C	2.50067800	-1.10224700	2.35148400
O	3.28909800	-1.58025500	3.39760000
C	3.82251400	-0.56967700	4.25356200
H	5.80171800	-2.45493200	-2.93074000
H	3.84507800	-2.36087000	0.79372700
H	5.70861800	-1.80974800	2.33140500
H	7.77651300	-3.17437100	1.41912400
H	3.07555600	-1.68381400	-4.22095800
H	0.75924400	-1.04041300	-2.87755300
H	9.25638200	-3.11115700	-1.01680800
H	8.21382000	-2.66722900	-2.47889500
H	8.06926000	-1.00352500	2.65596000
H	8.00853900	-0.09288700	1.07964000
H	6.58008900	0.82988800	-0.23884400
H	4.90617600	0.90003600	-0.78443400
H	5.29312300	1.11095700	0.94454900
H	1.79103100	-0.34392200	2.71194500
H	1.96743300	-1.97251700	1.95487300
H	4.33791300	-1.08952600	5.06316900
H	4.53304500	0.07331900	3.72066400

H	3.01419500	0.04525400	4.67583700
C	-6.15733600	-1.12716700	1.22128000
C	-6.71896000	-1.30454500	-0.23232900
C	-5.70834200	-1.92207500	-1.20481100
C	-4.21893000	-0.25182500	0.04276900
C	-4.96666700	-0.19863400	1.15730700
C	-7.40710100	-0.57114800	1.95301000
C	-8.63179700	-1.04895500	1.17368200
C	-2.55272800	0.11245900	-1.38524400
O	-3.03757300	0.46388200	-0.15236700
C	-8.38222700	-1.53607900	2.58370600
C	-5.65503200	-2.46448200	1.83470100
O	-1.50424000	0.60723000	-1.80732200
H	-6.88136700	-0.27193200	-0.58339300
H	-6.09798500	-1.94876000	-2.22945400
H	-5.47011400	-2.95980400	-0.93148900
H	-4.68193200	0.42178600	2.00423600
H	-7.35750400	0.44318800	2.34208900
H	-9.48369500	-0.39323900	1.00765900
H	-9.03586900	-1.13023900	3.35214900
H	-8.10443300	-2.57121000	2.75102200
H	-6.39810800	-3.25955300	1.72244600
H	-4.73112800	-2.80192100	1.35486900
H	-5.45095700	-2.33835500	2.90352100
C	-3.19377300	-1.42766900	-3.37397100
H	-2.97919900	-0.63643400	-4.10118700
H	-2.32703200	-2.10076700	-3.36514200
H	-4.05712600	-1.99793400	-3.72779000
C	-3.44634100	-0.85494100	-2.01585000
C	-4.46553600	-1.07020600	-1.13567700
C	-8.11495100	-1.84204000	-0.00549500
C	-8.76390000	-2.77519800	-0.70622900
H	-9.77974100	-3.06993900	-0.45589500
H	-8.31051700	-3.27370200	-1.56009900
C	1.15455900	1.85702200	-0.04793800
C	2.08296400	2.64629300	0.61227600
C	0.67543100	4.57763000	0.19616000
C	-0.23418200	3.73828100	-0.45937000
N	0.03889600	2.41961400	-0.55556100
H	1.27306000	0.78964600	-0.20391000

H	2.97492200	2.18127000	1.01620300
H	-0.65040300	1.77362300	-1.04168800
C	1.83983000	4.01410400	0.73275200
Cl	-1.69540500	4.28787600	-1.16378700
H	2.54817300	4.66140800	1.24086900
Cl	0.37635500	6.27038100	0.34510500

exo-TS of model 1c

C	-0.53169800	3.51077600	0.09427700
C	-1.67418600	2.61510700	0.62636100
C	-1.55928700	1.93550900	1.80910200
C	-0.25134500	1.85070700	2.41292700
C	0.84905000	2.23209000	1.67854600
C	0.82947100	2.77136400	0.27179900
C	-0.90964700	3.70719600	-1.38955400
C	-2.25104100	3.02429700	-1.64581300
C	-2.69497100	2.42370700	-0.36536500
C	0.26048600	1.29541800	3.64037400
C	1.61394800	1.38427700	3.55510600
O	1.98984900	1.94406100	2.34649800
C	-3.81352800	1.60305200	-0.21564200
C	-2.11557800	4.54296700	-1.70348700
C	-0.47821500	4.85080800	0.87131900
O	1.94625200	3.63293600	0.05710000
C	2.82907800	3.28240300	-0.99356300
O	2.39415000	3.66967300	-2.26475800
C	2.48522800	5.07379100	-2.51829800
H	-2.38261900	1.36039200	2.22422900
H	0.88283800	1.92273400	-0.42732800
H	-0.11453200	3.64522200	-2.12649100
H	-2.47787100	2.49957800	-2.57100600
H	-0.30424600	0.90532300	4.47665600
H	2.42286100	1.15448300	4.23183400
H	-4.61307600	1.69281300	-0.94678300
H	-4.14712900	1.40546800	0.79458100
H	-2.17549200	4.98250400	-2.69591800
H	-2.59344900	5.13349400	-0.92785900
H	-1.45370500	5.34245400	0.87223000
H	-0.18330400	4.69896100	1.91425700

H	0.24922100	5.52408600	0.41004000
H	3.77535800	3.77731500	-0.73876900
H	2.95307200	2.19478700	-1.04394400
H	2.21036100	5.21816800	-3.56488200
H	1.80230100	5.64195600	-1.87584400
H	3.51306400	5.42923000	-2.36031200
C	-4.49638400	-1.25735600	-0.23972800
C	-3.95913000	-2.73952300	-0.19284200
C	-2.87278300	-2.92895200	0.87693800
C	-2.08643800	-0.78149500	-0.22477400
C	-3.33226200	-0.36951900	-0.72914700
C	-5.66046700	-1.39414800	-1.25403500
C	-6.10509300	-2.85576300	-1.25180500
C	0.12949200	-0.96232900	-0.14707200
O	-0.89769300	-0.20807500	-0.65261000
C	-7.03683900	-1.77060400	-0.75999400
C	-4.99248500	-0.85449000	1.17151500
O	1.30778300	-0.60193500	-0.42203900
H	-3.46566600	-2.89674900	-1.16569800
H	-2.46799900	-3.94779300	0.85109700
H	-3.27658700	-2.77672900	1.88618500
H	-3.35065700	-0.06045600	-1.77217600
H	-5.58398200	-0.84323800	-2.18903300
H	-6.36518100	-3.36819900	-2.17535400
H	-7.87242800	-1.52386900	-1.41072300
H	-7.27496000	-1.71435200	0.29707800
H	-5.52390900	-1.68519500	1.64570500
H	-4.16069100	-0.58431400	1.82989100
H	-5.68651300	-0.01093000	1.12471100
C	0.42996300	-3.11803300	1.25332200
H	1.08057200	-3.63255500	0.53403000
H	1.07310800	-2.70383200	2.04227400
H	-0.20342600	-3.87694300	1.72227900
C	-0.39927100	-2.05321300	0.60095200
C	-1.78842800	-1.93480100	0.53646600
C	-5.21720800	-3.57781900	-0.26632500
C	-5.47477200	-4.72634000	0.36514700
H	-6.41112800	-5.25894400	0.21895800
H	-4.75683300	-5.18261200	1.04300000
C	4.25953800	-0.50289200	0.95658500

C	5.60344400	-0.63953800	1.26669300
C	5.71494200	-2.52242700	-0.25378800
C	4.35169400	-2.33518800	-0.53111300
N	3.67678400	-1.34622400	0.08175200
H	3.61203700	0.26181100	1.37389200
H	6.07326000	0.03983800	1.96903000
H	2.59883800	-1.16560900	-0.13544800
C	6.33406900	-1.66004500	0.65622600
Cl	3.47781100	-3.31210100	-1.63688100
Cl	6.61711100	-3.78119600	-1.01394900
H	7.38848700	-1.79590900	0.87606500

exo-product of model 1c

C	-0.40052900	3.15602700	0.05302000
C	-1.14048800	1.84443100	-0.23421100
C	-1.46119000	0.85782000	0.86306600
C	-0.33361300	0.90550600	1.87333300
C	0.73707400	1.74364800	1.71755200
C	0.99528900	2.73641900	0.60860800
C	-0.27358200	3.77717900	-1.34919900
C	-0.82358800	2.78165700	-2.36145700
C	-1.32687200	1.63449500	-1.54686300
C	-0.15123000	0.26303200	3.15040600
C	1.01672500	0.74523700	3.65707400
O	1.57550000	1.64774500	2.79265600
C	-1.93493600	0.40324100	-2.14310600
C	-1.52473900	4.10736900	-2.12040700
C	-1.12144100	4.08824900	1.04851900
O	1.72431400	3.88782500	1.03078900
C	3.12420700	3.71726000	1.15382900
O	3.77334800	3.44172100	-0.06957800
C	3.90116100	4.57352500	-0.93804700
H	-2.37963600	1.15140100	1.38971700
H	1.54759100	2.26651600	-0.21829000
H	0.61518100	4.36346000	-1.56263000
H	-0.35590500	2.59550200	-3.32595800
H	-0.80582300	-0.44632500	3.63667900
H	1.56175600	0.57387000	4.57309400
H	-1.17076000	-0.10171200	-2.75283100

H	-2.72669500	0.68335900	-2.85147300
H	-1.43463600	4.86830500	-2.89172600
H	-2.48979500	4.08764900	-1.62055000
H	-2.12145400	4.33606800	0.68074600
H	-1.22637100	3.63000200	2.03770200
H	-0.56031400	5.01896800	1.16989700
H	3.48392900	4.65889700	1.58301000
H	3.36399200	2.87795900	1.81065600
H	4.42479800	4.22749500	-1.83163400
H	2.92066400	4.97306500	-1.21854800
H	4.49136800	5.36226400	-0.45327500
C	-4.05150600	-0.51388400	-0.89116700
C	-4.44879700	-1.63107100	0.12630300
C	-3.82446000	-1.44659000	1.52312800
C	-1.72476300	-0.56879400	0.25552000
C	-2.50723700	-0.59240500	-1.10643700
C	-4.84997400	-1.00007200	-2.14041900
C	-6.03583900	-1.82253800	-1.63455900
C	-0.24911300	-2.24595000	0.78932300
O	-0.40436600	-1.15997900	0.00576600
C	-6.26423700	-0.52053000	-2.36750300
C	-4.53064200	0.88428700	-0.44558500
O	0.80525400	-2.88743900	0.78781500
H	-3.98601400	-2.54722700	-0.27887900
H	-4.13946700	-2.23689200	2.21170900
H	-4.11142900	-0.48521700	1.96701500
H	-2.32494400	-1.60387300	-1.49279600
H	-4.28099300	-1.33369600	-3.00547500
H	-6.33573400	-2.74233700	-2.13232800
H	-6.64697400	-0.60746600	-3.38180300
H	-6.65212900	0.33777100	-1.83015600
H	-5.57832100	0.85780800	-0.13411300
H	-3.96942400	1.28669900	0.39746100
H	-4.44616400	1.60078800	-1.26878200
C	-1.59014000	-3.69840900	2.45634500
H	-1.47890700	-4.63078900	1.89003200
H	-0.79896200	-3.69321900	3.21548700
H	-2.55602800	-3.72052000	2.96737400
C	-1.46903600	-2.50751600	1.55760600
C	-2.35073000	-1.53134100	1.24546700

C	-5.92678100	-1.84858600	-0.12677000
C	-6.89862500	-2.06132100	0.76308000
H	-7.92789100	-2.22227100	0.45286600
H	-6.70400000	-2.08842500	1.83301100
C	3.07891200	-0.52295500	-0.13966300
C	4.21825200	0.17885500	-0.49940100
C	5.30789500	-1.94234200	-0.96468500
C	4.12932800	-2.60196500	-0.58771200
N	3.06733600	-1.87045600	-0.19320700
H	2.15529600	-0.06436500	0.19644500
H	4.22582900	1.26581400	-0.45141400
H	2.16746200	-2.35365900	0.11947700
C	5.33900100	-0.54403900	-0.91331000
Cl	3.94743600	-4.30369000	-0.59431200
Cl	6.69569600	-2.82858600	-1.47899200
H	6.25135800	-0.03034300	-1.20075000