

Supporting Information for

**DFT Study on the Mechanism of Phosphine-Catalyzed Ring-Opening Reaction
of Cyclopropyl Ketone**

Xiaohan Yu and Yang Wang*

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* Corresponding Author: Wang Y. (wangyang@zzuli.edu.cn; 2017017@email.zzuli.edu.cn)

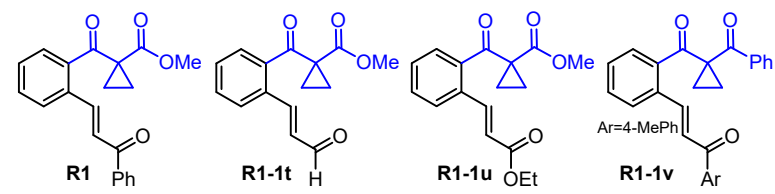
Part 1: Testing of different methods

Table S1. Benchmark studies associated with the rate-determining step using different methods

	B3LYP	Cam-B3LYP	B3PW91	ω B97X-D
R1	-1111.690091	-1111.119320	-1111.263038	-1111.329919
PPh₂Me	-844.411214	-844.090727	-844.170857	-844.217905
R1+PPh₂Me	-1956.101305	-1955.210047	-1955.433895	-844.217905
	(0.0 kcal/mol)	(0.0 kcal/mol)	(0.0 kcal/mol)	(0.0 kcal/mol)
TS1	-1956.054389	-1955.154803	-1955.385137	-1955.494369
	(29.4 kcal/mol)	(34.7 kcal/mol)	(30.6 kcal/mol)	(33.5 kcal/mol)

Part 2: Testing of substituent effects on the reaction

Table S2. Texting the substituent effects on the reaction

			
$\Delta G^\ddagger$ (kcal/mol)			
	TS1	TS2	
R1	28.9	15.8	
R1-1t	31.9	16.9	
R1-1u	31.3	18.4	
R1-1v	32.8	19.3	

Part 3: Direct and water-assisted proton transfer

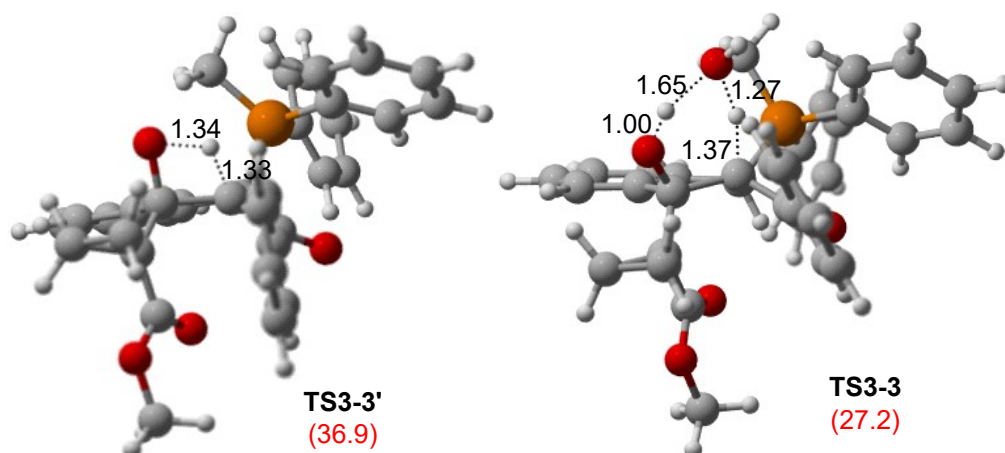


Fig. S1 Structures and energy barriers for the [1,3]-proton transfer

Part 4: Energies and Cartesian coordinates of all the stationary points

1. Energies of all the stationary points

	G (a.u.)	G-correct (a.u.)	Imaginary frequency (cm ⁻¹)
R1	-1111.230447	0.291639	–
PPh₂Me	-844.139915	0.181108	–
TS1	-1955.315027	0.489599	-548.47
TS1'	-1955.310078	0.495403	-536.21
M1	-1955.360169	0.496491	–
TS2	-1955.338035	0.499247	-282.23
M2	-1955.365935	0.503854	–
TS3	-1955.346042	0.493007	-1185.44
M3	-1955.36123	0.499673	–
TS4	-1955.345878	0.504417	-139.84
M4	-1955.381135	0.509331	–
TS5	-1955.351078	0.50388	-482.30
P	-1036.071456	0.293075	–
O=PPh₂Me	-919.368763	0.186276	–
TS2-1	-1955.306409	0.494953	-608.60
P1	-1111.230832	0.293783	–
TS3-2	-1955.317799	0.500182	-617.51
P2	-1111.280539	0.297985	–
TS1-3	-1955.333134	0.49691	-206.66
M1-3	-1955.335091	0.50169	–
TS2-3	-1955.332664	0.500348	-138.62
M2-3	-1955.338239	0.503436	–
TS3-3	-1955.303462	0.495507	-1646.80
M3-3	-1955.343517	0.50367	–
TS4-3	-1955.331983	0.501368	-167.35
P3	-1111.230818	0.29451	–
R1a	-883.473023	0.250828	–
TS1a	-1727.538646	0.454844	-553.50
R1b	-1153.626456	0.35379	–
TS1b	-1997.697447	0.558683	-550.94
R1-1t	-880.330481	0.215167	
R1-1u	-1034.079098	0.273058	
R1-1v	-1266.920981	0.360455	
TS1-1t	-1724.411843	0.416878	-545.04
TS1-1u	-1878.171547	0.472241	-541.09

TS1-1v	-2110.998236	0.565705	-525.67
M1-1t	-1724.458473	0.421129	
M1-1u	-1878.217676	0.476852	
M1-1v	-2111.047155	0.569245	
TS2-1t	-1724.43417	0.422453	-293.17
TS2-1u	-1878.190672	0.480155	-319.71
TS2-1v	-2111.022615	0.571117	-335.08

2. Cartesian coordinates of all the stationary points

R1

C	-3.10891800	3.29707200	0.11501700
C	-1.94856000	2.69741600	-0.36571600
C	-1.86075600	1.30916900	-0.50551000
C	-2.97215600	0.51960600	-0.14676000
C	-4.13844900	1.13187200	0.31344200
C	-4.21006900	2.51395200	0.45137000
H	-3.15482200	4.37636100	0.21581300
H	-1.10239200	3.30795500	-0.66525900
H	-4.98281200	0.50455200	0.57930300
H	-5.11944200	2.97594000	0.82030800
C	-2.98725300	-0.98125800	-0.20832500
O	-4.01143400	-1.56206800	-0.51794800
C	-1.73262900	-1.76239300	0.07453100
C	-1.83692400	-3.27688200	-0.00257100
C	-1.18934700	-2.54824700	-1.11525300
H	-2.84253400	-3.65179400	-0.15019200
H	-1.20638700	-3.82832900	0.68445000
H	-0.11063300	-2.56496900	-1.21579900
H	-1.75304900	-2.42953400	-2.03479200
C	-0.79592500	-1.22890600	1.10646400
O	-1.11630000	-0.45539000	1.98074800
O	0.43353300	-1.74670100	0.99398000
C	1.37652800	-1.29994700	1.97360900
H	2.31006300	-1.80824000	1.74019800
H	1.50617400	-0.21690700	1.89871600
H	1.03355000	-1.55638800	2.97733300
C	-0.63085600	0.70735500	-1.05076100
C	0.60483700	1.01199400	-0.63518400
H	-0.72701900	-0.06670000	-1.80932900
H	0.75580300	1.73602700	0.15880500
C	1.75780300	0.23366400	-1.16547500
O	1.59775700	-0.61239900	-2.03370900
C	3.10941700	0.44811200	-0.56216000
C	4.07054100	-0.55225900	-0.75100700

C	3.43861400	1.59070300	0.17494300
C	5.33801600	-0.42059000	-0.19884900
H	3.79877500	-1.42948100	-1.32862200
C	4.71433500	1.72724700	0.71585000
H	2.71779700	2.38898300	0.31457500
C	5.66067000	0.72114300	0.53604700
H	6.07576000	-1.20357400	-0.33880600
H	4.96837900	2.61877500	1.27904800
H	6.65083900	0.82685600	0.96747300

PPh2Me

P	-0.01546000	1.40771400	0.68896700
C	0.02095600	2.55076400	-0.76983800
H	-0.92810500	3.09113100	-0.79378000
H	0.82225200	3.28390200	-0.65339000
H	0.15236600	2.01392600	-1.71335300
C	-1.41669400	0.31306900	0.19255400
C	-2.56815900	0.30877200	0.98428600
C	-1.38084400	-0.48789600	-0.95642500
C	-3.66864400	-0.47442300	0.63472300
H	-2.60268700	0.92009800	1.88219600
C	-2.47582200	-1.27137700	-1.30573500
H	-0.48517000	-0.50406700	-1.57303600
C	-3.62254400	-1.26458800	-0.50961000
H	-4.55667000	-0.46974900	1.25861300
H	-2.43788600	-1.88906400	-2.19754800
H	-4.47577800	-1.87753300	-0.78219900
C	1.41506000	0.30640600	0.31585800
C	1.44331400	-0.97798700	0.87718700
C	2.51378700	0.73161400	-0.43747800
C	2.53324400	-1.81830800	0.67949400
H	0.59609600	-1.32592300	1.46374200
C	3.61047300	-0.10873800	-0.63023200
H	2.52329600	1.72157400	-0.88352900
C	3.62294900	-1.38464500	-0.07574100
H	2.53322200	-2.81301300	1.11426100
H	4.45374000	0.23616000	-1.22055900
H	4.47476300	-2.03913100	-0.23018300

TS1

C	4.61675100	-4.64509500	0.38295200
C	4.95646800	-3.30547800	0.54023200
C	4.06527400	-2.28701900	0.18653200
C	2.78958900	-2.63349200	-0.29505000

C	2.46502900	-3.97866600	-0.46804000
C	3.36692600	-4.98386300	-0.12782200
H	5.32561200	-5.41977500	0.65637600
H	5.93477700	-3.03537900	0.92813700
H	1.48519800	-4.23437000	-0.86056800
H	3.09158200	-6.02543900	-0.25721100
C	1.72345000	-1.63819500	-0.69633400
O	1.36311300	-1.64669500	-1.88192900
C	1.08508000	-0.76842800	0.26436000
C	-0.85786200	-0.89770400	0.04366600
C	0.06385600	0.19659100	-0.28296000
H	-1.14338600	-1.06963600	1.07339100
H	-0.92173100	-1.72686000	-0.65129800
H	0.18648800	0.35591100	-1.35254100
H	-0.04797100	1.11842600	0.28387800
C	1.40135900	-0.74037100	1.68219800
O	2.25695500	-1.37604600	2.27328000
O	0.57830900	0.11437400	2.35612200
C	0.79565100	0.18373800	3.76376500
H	0.06417400	0.89514900	4.14409700
H	0.64879800	-0.79478800	4.22534100
H	1.80865000	0.52952500	3.97885900
C	4.50195900	-0.89051100	0.32539700
C	4.15427700	0.09771600	-0.50909000
H	5.16814900	-0.65657900	1.15469300
H	3.53609600	-0.10857500	-1.37585000
C	4.59452000	1.49231000	-0.26214000
O	5.52246300	1.74904900	0.49188200
P	-3.05920700	-0.03587500	-0.50013700
C	-2.75275400	1.02974300	-1.96585400
H	-1.99098900	1.76418100	-1.69316900
H	-2.37072300	0.42841000	-2.79419600
H	-3.66126300	1.55246300	-2.27489100
C	-3.56939100	1.16126000	0.78832500
C	-2.68859400	1.45171100	1.83635500
C	-4.80726400	1.81471400	0.72970200
C	-3.04169100	2.38673600	2.80878500
H	-1.72406500	0.95341200	1.90687800
C	-5.15710600	2.74312700	1.70406200
H	-5.50160000	1.58939800	-0.07561900
C	-4.27374300	3.03024800	2.74484600
H	-2.35375700	2.60639800	3.61888500
H	-6.11889300	3.24308100	1.65192000
H	-4.54880400	3.75383800	3.50554700

C	-4.59822700	-0.93200700	-0.90384100
C	-5.38105900	-1.45137700	0.13631300
C	-4.96870000	-1.18464300	-2.22897400
C	-6.52180100	-2.19438000	-0.14622600
H	-5.10488100	-1.26022100	1.17014300
C	-6.10976200	-1.93468600	-2.50754400
H	-4.37605500	-0.79470100	-3.05083200
C	-6.88838900	-2.43841900	-1.46957900
H	-7.12589800	-2.58285300	0.66725000
H	-6.39047200	-2.12005800	-3.53929100
H	-7.77833400	-3.01866600	-1.68996400
C	3.84610200	2.59280200	-0.94838900
C	4.38584200	3.88283300	-0.92254200
C	2.61157000	2.37401800	-1.56829600
C	3.70699900	4.93795300	-1.51875200
H	5.34073500	4.03605800	-0.43074600
C	1.92494100	3.43429000	-2.15315700
H	2.17304300	1.38161400	-1.58501700
C	2.47387900	4.71422900	-2.13340900
H	4.13344800	5.93558000	-1.50404200
H	0.96259200	3.25980200	-2.62366900
H	1.94179300	5.53921100	-2.59620500

TS1'

C	-6.33386500	0.98077100	1.13891200
C	-5.26647700	1.27676000	0.29406000
C	-4.11025100	0.49311300	0.30482600
C	-4.01550700	-0.58343800	1.20568600
C	-5.07206300	-0.84530000	2.07457300
C	-6.23944700	-0.08669800	2.02692000
H	-7.23201700	1.58879100	1.10758000
H	-5.32732200	2.11541100	-0.39300600
H	-4.96877500	-1.64790200	2.79847700
H	-7.06346200	-0.31688000	2.69435900
C	-2.70829000	-1.31219400	1.42840900
O	-2.21103200	-1.21417100	2.55631900
C	-2.02235300	-2.00222500	0.36005900
C	-0.59604700	-2.42011700	0.62197100
C	-0.32199800	-1.09339600	0.05372300
H	-0.25516900	-3.26635100	0.03228900
H	-0.38557500	-2.51452700	1.68459300
H	-0.45963900	-0.22456600	0.68777200
H	-0.39066500	-0.94970800	-1.02037400
C	-2.66930300	-2.36300200	-0.88765700

O	-3.83969800	-2.18427800	-1.18838300
O	-1.79957600	-2.93115000	-1.76313900
C	-2.35580600	-3.27919400	-3.02935000
H	-1.53527800	-3.69599300	-3.61087400
H	-3.15045000	-4.01850100	-2.91071100
H	-2.76414800	-2.39615600	-3.52546600
C	-2.98299200	0.81769100	-0.59589500
C	-2.27003200	1.94935600	-0.54810800
H	-2.69385200	0.07558100	-1.33559800
H	-2.49951200	2.72985700	0.16942700
C	-1.09368400	2.08752400	-1.44502000
O	-0.88624200	1.28080000	-2.34465600
C	-0.12058200	3.19885000	-1.21020700
C	0.79194600	3.49352800	-2.23123500
C	-0.05560600	3.90151000	-0.00275900
C	1.75584000	4.47722500	-2.04965400
H	0.72748600	2.93899600	-3.16194600
C	0.91453300	4.88416400	0.17951300
H	-0.73544300	3.67144600	0.81025900
C	1.81758800	5.17342500	-0.84110200
H	2.45751300	4.70337500	-2.84551400
H	0.97011500	5.41793700	1.12244600
H	2.57161400	5.94046400	-0.69544500
P	2.06788600	-0.62876200	-0.16454700
C	2.25159700	0.08283500	-1.84656900
H	2.05461200	-0.70751400	-2.57551700
H	1.49570600	0.85980400	-1.98687800
H	3.24558500	0.50318900	-2.01648600
C	3.12932000	-2.11600300	-0.16576500
C	2.89507700	-3.10780700	0.79484300
C	4.15895600	-2.29427000	-1.09643800
C	3.69079900	-4.25073200	0.83521600
H	2.08996500	-2.98617000	1.51536300
C	4.94456600	-3.44264800	-1.06178600
H	4.35346600	-1.53734500	-1.84969300
C	4.71387000	-4.41959800	-0.09481500
H	3.50586500	-5.01093300	1.58686400
H	5.73908900	-3.57295400	-1.78914900
H	5.32876500	-5.31325200	-0.06941500
C	2.94572800	0.55867700	0.91718900
C	3.58887500	0.11760900	2.08014000
C	2.90753000	1.92979800	0.63376400
C	4.19728800	1.03001800	2.93600200
H	3.62734500	-0.94306700	2.31187400

C	3.51977200	2.83844500	1.49435000
H	2.41038800	2.29816500	-0.26119000
C	4.16533500	2.39272800	2.64487800
H	4.69974500	0.67506800	3.83011600
H	3.49087300	3.89755500	1.25849900
H	4.64135900	3.10357000	3.31238300
M1			
C	4.84942800	-4.40907300	0.34474600
C	5.16922300	-3.06118100	0.24459200
C	4.19908700	-2.09664900	-0.06921200
C	2.86399400	-2.51179700	-0.24654300
C	2.55439700	-3.86753300	-0.14592300
C	3.53153100	-4.81473100	0.14630500
H	5.62023300	-5.13577800	0.57941300
H	6.19433600	-2.73693300	0.40472400
H	1.52251600	-4.17860900	-0.28563700
H	3.26412600	-5.86390200	0.22529300
C	1.73778700	-1.57685200	-0.64009800
O	1.54482500	-1.45199400	-1.87486200
C	0.96524300	-0.92248500	0.33809400
C	-1.47169400	-0.87993500	-0.25504300
C	-0.16734300	-0.06422200	-0.15429900
H	-1.69966300	-1.38033300	0.69213500
H	-1.36866100	-1.65285300	-1.02490100
H	0.09227500	0.30171200	-1.15347900
H	-0.31965000	0.80123700	0.49980900
C	1.13024200	-1.15123600	1.74141400
O	2.01686300	-1.75704200	2.33417500
O	0.10107500	-0.58032100	2.46807400
C	0.20267800	-0.73576400	3.87687000
H	-0.66900100	-0.23666600	4.30146200
H	0.20118400	-1.79195500	4.15651800
H	1.11866900	-0.27713300	4.25718400
C	4.64362600	-0.69935900	-0.14152300
C	4.01168700	0.33545900	-0.71628600
H	5.60255500	-0.48775300	0.33293600
H	3.07716300	0.20727600	-1.24741000
C	4.57298000	1.70269200	-0.62211000
O	5.75643700	1.91728600	-0.39644300
C	3.61289500	2.83907200	-0.79901700
C	4.11098700	4.10351900	-1.12548200
C	2.23920400	2.66419700	-0.60106900
C	3.24259500	5.17781400	-1.27737700

H	5.18100200	4.22368400	-1.26209700
C	1.37240300	3.74486300	-0.73690500
H	1.85338600	1.69037000	-0.30984500
C	1.87205300	4.99873700	-1.08302500
H	3.62958800	6.15584800	-1.54422900
H	0.30859800	3.60758100	-0.56890000
H	1.19443800	5.83886000	-1.19735600
P	-2.92138700	0.10736300	-0.71139200
C	-2.52969500	1.06091500	-2.19894200
H	-1.78067600	1.81308800	-1.94322000
H	-2.12324300	0.39617800	-2.96414200
H	-3.42941400	1.54897500	-2.57716900
C	-3.34704400	1.24122500	0.62069200
C	-2.72209200	1.13827400	1.86773700
C	-4.32732700	2.21584500	0.39330600
C	-3.08204200	2.01911500	2.88486500
H	-1.95133400	0.39306700	2.04751900
C	-4.67833900	3.08791600	1.41646600
H	-4.81927400	2.29183900	-0.57247500
C	-4.05497300	2.98918500	2.66048200
H	-2.59810400	1.94597700	3.85286600
H	-5.43674200	3.84355100	1.24440600
H	-4.33040500	3.67215500	3.45721000
C	-4.33337100	-0.96494200	-1.04619400
C	-5.31068000	-1.16140200	-0.06548200
C	-4.41174200	-1.63917500	-2.27067300
C	-6.36635900	-2.03359100	-0.31378200
H	-5.25035600	-0.63555000	0.88255400
C	-5.47080000	-2.50789600	-2.50883900
H	-3.65733500	-1.49336100	-3.03813100
C	-6.44610200	-2.70402500	-1.53195900
H	-7.12669800	-2.18555800	0.44427400
H	-5.53545500	-3.02900700	-3.45765800
H	-7.27145200	-3.38174400	-1.72303300
TS2			
C	5.75459600	1.39663200	-1.90454700
C	4.87677200	1.57962800	-0.83657100
C	3.82820600	0.68211500	-0.64264800
C	3.67344000	-0.39276200	-1.52326900
C	4.52912000	-0.55992600	-2.60765500
C	5.58246500	0.33249200	-2.79099500
H	6.57033500	2.09702700	-2.05402300
H	4.99711000	2.42530200	-0.16580800

H	4.36952500	-1.38905400	-3.29081200
H	6.26698500	0.20540300	-3.62343900
C	2.48710300	-1.26003600	-1.23011800
O	1.81593100	-1.75133300	-2.14341300
C	2.13083800	-1.27670100	0.17932600
C	0.68349700	-1.41619700	0.59500800
C	-0.28468100	-0.72291900	-0.37553100
H	0.58796500	-0.94162200	1.57679800
H	0.38833800	-2.46802000	0.72454800
H	-0.25332700	-1.15811300	-1.37852000
H	-0.03810500	0.33903900	-0.48133200
C	3.14121200	-1.71653000	1.11436900
O	4.33954500	-1.87364100	0.90964800
O	2.62340900	-1.92452500	2.36058500
C	3.56969500	-2.32286400	3.34607800
H	3.00406400	-2.46386000	4.26628900
H	4.06257500	-3.25449800	3.05887400
H	4.33221900	-1.55340400	3.48714100
C	2.80737700	0.87150400	0.43698300
C	1.78480600	1.78512200	0.26062200
H	3.10058000	0.66855700	1.46661700
H	1.60830400	2.17921800	-0.73296300
C	0.89351200	2.10272700	1.33817200
O	0.95816900	1.56493700	2.45860700
C	-0.20838800	3.11171200	1.10055600
C	-1.07234200	3.39261800	2.16684300
C	-0.42091300	3.75734300	-0.12384800
C	-2.12786700	4.28602000	2.01476400
H	-0.89388600	2.89368300	3.11391100
C	-1.47409000	4.65486900	-0.27678300
H	0.22908200	3.57003800	-0.97070800
C	-2.33176300	4.92050800	0.78926600
H	-2.78921300	4.49169900	2.85038000
H	-1.62826700	5.14355600	-1.23361400
H	-3.15266400	5.62010800	0.66606700
P	-1.98805600	-0.77592000	0.22420500
C	-2.02817800	-0.19151800	1.93676500
H	-1.69761400	-1.00332400	2.58776600
H	-1.34151400	0.65364300	2.05161100
H	-3.04172400	0.10733100	2.20943000
C	-2.61148300	-2.46509800	0.15482800
C	-1.95626900	-3.43893900	-0.60565600
C	-3.78471100	-2.77883600	0.85133100
C	-2.47922900	-4.72817700	-0.66347100

H	-1.04358600	-3.20435600	-1.14593900
C	-4.29787400	-4.06882400	0.78765200
H	-4.29836000	-2.02210600	1.43791900
C	-3.64495000	-5.04112100	0.03089800
H	-1.97248000	-5.48706000	-1.24913700
H	-5.20460900	-4.31506300	1.32891400
H	-4.04719500	-6.04756100	-0.01653600
C	-3.04391700	0.27007900	-0.79738200
C	-3.66410500	-0.28074500	-1.92418800
C	-3.20409000	1.62464000	-0.48597800
C	-4.44534000	0.52859500	-2.74172600
H	-3.54381400	-1.33520500	-2.15601900
C	-3.99249400	2.42348600	-1.30940200
H	-2.72594300	2.06315500	0.38756700
C	-4.61054500	1.87748900	-2.43223900
H	-4.92893200	0.10404200	-3.61459300
H	-4.12150800	3.47313000	-1.06797600
H	-5.22639800	2.50528700	-3.06762300
M2			
C	-1.56952800	4.28985500	3.05116900
C	-0.56214800	3.84164100	2.19849300
C	-0.92203300	3.15850200	1.03836300
C	-2.27352800	2.93634300	0.76970100
C	-3.28944200	3.38752100	1.61161800
C	-2.92438900	4.07043000	2.76469400
H	-1.30125900	4.82386600	3.95766300
H	0.48240400	4.02734700	2.42939800
H	-4.32972900	3.19328100	1.36826000
H	-3.68308500	4.43211300	3.45044200
C	-2.40288800	2.14140200	-0.46569200
O	-3.42711900	1.81664000	-1.03210100
C	-0.98415800	1.70731000	-0.89755500
C	-0.83671700	0.20646300	-0.59359900
C	-1.06625300	-0.12361100	0.88423000
H	0.16656500	-0.09292000	-0.91060600
H	-1.56751400	-0.33102800	-1.20554200
H	-2.07078500	0.16448400	1.21933200
H	-0.34166400	0.39169500	1.52575500
C	-0.84422700	1.99789700	-2.38115900
O	-0.84026700	3.12128400	-2.83589400
O	-0.83627200	0.90377500	-3.14637900
C	-0.67483400	1.14611200	-4.54427300
H	-0.70031200	0.16872500	-5.02226800

H	-1.48243900	1.77750000	-4.91913700
H	0.28275300	1.63770100	-4.72767300
C	-0.02700100	2.63269700	-0.06186500
C	1.28267500	2.04475700	0.36683400
H	0.16713800	3.48212300	-0.73519400
H	1.53378300	2.00930500	1.42124000
C	2.12882100	1.61949300	-0.63322500
O	1.80663300	1.62304000	-1.87285400
C	3.50486900	1.08767000	-0.28721000
C	4.22516500	0.43578200	-1.29360700
C	4.10471600	1.22411000	0.97219100
C	5.49655200	-0.07866700	-1.05346500
H	3.75535000	0.34855400	-2.26719000
C	5.37609300	0.71145900	1.21803100
H	3.58319700	1.75018200	1.76597500
C	6.07827700	0.05409700	0.20654000
H	6.03526400	-0.58545200	-1.84896200
H	5.82400900	0.83057700	2.20017300
H	7.06981700	-0.34416600	0.39824600
P	-0.96119900	-1.89545700	1.26314600
C	-1.36007200	-2.10180100	3.01406700
H	-0.58870000	-1.58979800	3.59320300
H	-2.33222700	-1.65818700	3.23750400
H	-1.36209700	-3.16332100	3.26843500
C	0.69364300	-2.53271000	0.95900900
C	1.78798400	-1.66404900	0.89920800
C	0.87218500	-3.91900500	0.86175600
C	3.06821600	-2.19257600	0.74456600
H	1.65311800	-0.58414300	0.94780800
C	2.15359900	-4.43335700	0.70727400
H	0.01860100	-4.59036000	0.89883600
C	3.24777500	-3.57024000	0.65086600
H	3.91876100	-1.52077000	0.69277700
H	2.29760000	-5.50537500	0.62869300
H	4.24658800	-3.97637500	0.52818600
C	-2.13095700	-2.82336300	0.25574400
C	-1.79546100	-3.12645200	-1.07086400
C	-3.37205000	-3.20238700	0.77542000
C	-2.70797800	-3.80187900	-1.87248300
H	-0.82524900	-2.84533500	-1.47163100
C	-4.27712600	-3.88221400	-0.03455300
H	-3.63624600	-2.97853600	1.80387400
C	-3.94600600	-4.17899500	-1.35433200
H	-2.45050400	-4.03783400	-2.89905800

H	-5.23796200	-4.18262500	0.36841700
H	-4.65362000	-4.71069100	-1.98167900
TS3			
C	-5.14453400	-1.69864400	1.56649800
C	-4.31716800	-1.15496300	0.58942700
C	-3.03131800	-1.67295100	0.43871800
C	-2.60293600	-2.69984100	1.27391700
C	-3.42235900	-3.24845600	2.26360700
C	-4.70506200	-2.73912600	2.40144600
H	-6.15060900	-1.31005400	1.69095200
H	-4.66005500	-0.34112200	-0.04350200
H	-3.05337500	-4.04636400	2.90078800
H	-5.37385100	-3.13816100	3.15652200
C	-1.21689100	-3.06309500	0.93785200
O	-0.52954500	-3.92309300	1.44751500
C	-0.73830100	-2.12932000	-0.20414200
C	0.49972300	-1.35294000	0.28789300
C	0.91577000	-0.36137100	-0.79058000
H	1.26250200	-2.07720900	0.59230200
H	0.20676200	-0.79760000	1.19072800
H	-0.39258700	0.29036100	-0.78685400
H	1.09551800	-0.80716100	-1.77298000
C	-0.39850700	-3.05605400	-1.36551200
O	-1.21084200	-3.47855800	-2.15775800
O	0.89014100	-3.41146000	-1.38656500
C	1.25614700	-4.33590100	-2.41766600
H	2.32269200	-4.51024700	-2.29275100
H	0.69768700	-5.26660300	-2.30500500
H	1.04942200	-3.90573400	-3.39909500
C	-1.97086400	-1.22577600	-0.54229300
C	-1.72061800	0.27284100	-0.48189100
H	-2.30245000	-1.45153100	-1.56117800
H	-1.74512800	0.70723500	0.51800600
C	-2.27282200	1.07747100	-1.53855100
O	-2.57145600	0.64327900	-2.66237000
C	-2.32858700	2.56912800	-1.30929500
C	-2.05746200	3.41238700	-2.39119400
C	-2.64502100	3.13483000	-0.06985100
C	-2.06930600	4.79491900	-2.23325900
H	-1.83566500	2.96117100	-3.35323000
C	-2.67893100	4.51932900	0.08430600
H	-2.88493800	2.49352000	0.77365800
C	-2.38068100	5.35151400	-0.99346400

H	-1.84003500	5.43916200	-3.07629200
H	-2.94331400	4.94911000	1.04595800
H	-2.39821700	6.42947600	-0.86858000
P	2.15969900	0.78265100	-0.39801000
C	2.31665300	1.98688000	-1.74580900
H	2.61117100	1.45325900	-2.65204000
H	1.35459000	2.47592000	-1.91242200
H	3.07620000	2.73026800	-1.49745400
C	3.82776900	0.10248200	-0.13505200
C	4.03044200	-1.25449000	-0.39946600
C	4.89881200	0.90730600	0.27297700
C	5.30190400	-1.80657400	-0.25418700
H	3.19579800	-1.87267000	-0.72279000
C	6.16501500	0.35040400	0.41624100
H	4.74467500	1.96241500	0.48579800
C	6.36486800	-1.00558700	0.15328500
H	5.45984600	-2.86017700	-0.45859600
H	6.99624000	0.97179000	0.73203100
H	7.35415400	-1.43656300	0.26749100
C	1.68561900	1.67587900	1.10636100
C	2.30179400	1.42554900	2.33531000
C	0.61279700	2.57291900	1.03046700
C	1.85435800	2.08112100	3.48023100
H	3.12649600	0.72263800	2.40102100
C	0.17104200	3.22334700	2.17727600
H	0.10904900	2.75994400	0.08442600
C	0.79392300	2.97988900	3.40100600
H	2.33477600	1.88724400	4.43326200
H	-0.65983500	3.91828400	2.11105000
H	0.44899400	3.48965100	4.29471700

M3

C	-5.41338100	-1.31538400	1.19795800
C	-4.40153200	-0.60950600	0.54872100
C	-3.12916100	-1.17229200	0.49421300
C	-2.89882700	-2.41524000	1.08180200
C	-3.90003900	-3.12243500	1.74504300
C	-5.16892700	-2.55872600	1.79629300
H	-6.41239800	-0.89325600	1.24383500
H	-4.60555600	0.35706000	0.09724700
H	-3.68625900	-4.08784600	2.19335000
H	-5.97815900	-3.08099200	2.29530300
C	-1.49393800	-2.81443100	0.85036000
O	-0.90684100	-3.75957000	1.32933000

C	-0.89479600	-1.79941900	-0.15476700
C	0.60589300	-1.54847700	0.09849000
C	1.22972800	-0.69210700	-0.98218500
H	1.06272300	-2.53984800	0.21363500
H	0.69863000	-1.06561700	1.08011400
H	-0.31339400	0.80146600	0.54365600
H	1.26808300	-1.11457600	-1.98697700
C	-1.06999300	-2.45165900	-1.53092200
O	-1.87718600	-2.11645300	-2.36673800
O	-0.22304900	-3.46981300	-1.69973000
C	-0.30890000	-4.13711400	-2.96423800
H	0.44359200	-4.92204500	-2.93607700
H	-1.30434100	-4.56292800	-3.10040300
H	-0.10201400	-3.43489300	-3.77384100
C	-1.85277800	-0.58147100	-0.07195600
C	-1.32434600	0.53365300	0.85778300
H	-2.02255900	-0.17364800	-1.07038200
H	-1.29621400	0.18701000	1.89502200
C	-2.19427900	1.76942300	0.81203800
O	-2.91488900	2.06677500	1.74943500
C	-2.15900100	2.62120000	-0.42180300
C	-3.02563700	3.71709300	-0.49176000
C	-1.27799800	2.36742900	-1.48067500
C	-3.01143700	4.55435700	-1.60064900
H	-3.70024500	3.89904300	0.33849700
C	-1.26391800	3.21016700	-2.58922300
H	-0.59296300	1.52040800	-1.44551200
C	-2.12770100	4.30203400	-2.65019100
H	-3.68475000	5.40381500	-1.64864000
H	-0.57774100	3.01317800	-3.40680300
H	-2.11365800	4.95591900	-3.51630300
P	2.52942100	0.34073100	-0.65095700
C	2.98152100	1.27562900	-2.14332300
H	3.35024300	0.56813300	-2.88912900
H	2.10711200	1.79219900	-2.54153100
H	3.77139900	1.99255000	-1.91099000
C	4.14399300	-0.34186100	-0.07635300
C	4.36268200	-1.71173000	-0.22812100
C	5.14899000	0.46344400	0.47194000
C	5.57822900	-2.27601400	0.15657900
H	3.57228600	-2.33020200	-0.64796200
C	6.36244000	-0.09917600	0.85440100
H	4.97923400	1.52921800	0.60802300
C	6.57637000	-1.46942500	0.69653500

H	5.74356500	-3.34212100	0.03877400
H	7.14052300	0.52724000	1.27876700
H	7.52220100	-1.90683400	1.00023800
C	2.10024900	1.52787300	0.66176600
C	2.18592300	1.14283400	2.00429200
C	1.50426200	2.74918900	0.33154800
C	1.65256000	1.95680000	3.00094600
H	2.66533800	0.20447800	2.27148200
C	0.97876600	3.56465000	1.32957500
H	1.42567500	3.05827900	-0.70671900
C	1.04326000	3.16355800	2.66356000
H	1.71044100	1.64696700	4.03914700
H	0.51088500	4.50743100	1.06427600
H	0.62308000	3.79472600	3.43982400

TS4

C	5.32359400	-1.85439400	-2.25386200
C	4.37685400	-0.83858500	-2.13822800
C	3.61011300	-0.77037300	-0.97700500
C	3.80237200	-1.71660400	0.02652300
C	4.75128800	-2.73344100	-0.07550400
C	5.51480600	-2.79653800	-1.23363000
H	5.92871800	-1.91663400	-3.15293100
H	4.25164800	-0.11573300	-2.93835600
H	4.87388600	-3.45176600	0.72915100
H	6.26057200	-3.57463900	-1.35521200
C	2.86867900	-1.44928500	1.13533300
O	2.81019500	-2.01127400	2.20807800
C	1.90030900	-0.33121500	0.67497500
C	0.54718700	-1.01506300	0.39036900
C	-0.53329200	-0.01593500	0.00758000
H	0.29673800	-1.62150700	1.27238500
H	0.72474800	-1.73392100	-0.42449200
H	1.21594500	-0.32383300	-2.21260700
H	-0.85883700	0.58521200	0.85588900
C	1.84237500	0.68770400	1.80379000
O	2.69107100	1.53149800	1.98811100
O	0.80021900	0.51257500	2.61824300
C	0.70430000	1.45711300	3.69072800
H	-0.18902800	1.18376500	4.24786500
H	1.58868700	1.39970100	4.32722900
H	0.61279000	2.46696500	3.28356900
C	2.55963100	0.25734800	-0.59872300
C	1.62796600	0.58779900	-1.76856700

H	3.08912200	1.16478100	-0.29198100
H	2.23250000	1.05596900	-2.55901900
C	0.45465900	1.53816300	-1.53284900
O	-0.33402100	1.71671700	-2.47573500
C	0.63221400	2.67138600	-0.53898000
C	-0.42315400	3.12598500	0.25668600
C	1.83121600	3.39005200	-0.53578300
C	-0.26750500	4.23912500	1.07585700
H	-1.36968100	2.59633000	0.22977500
C	1.98861500	4.50975700	0.27959500
H	2.64918500	3.08753300	-1.18398600
C	0.94483400	4.93019600	1.09733400
H	-1.09409200	4.56995900	1.69723900
H	2.92880300	5.05203600	0.27315300
H	1.06822200	5.79586600	1.74037300
P	-1.91950100	-0.75316400	-0.73457800
C	-1.60238300	-1.16197600	-2.47632000
H	-2.51799300	-1.48660100	-2.97341000
H	-1.21609200	-0.25245100	-2.94473600
H	-0.85283900	-1.95554500	-2.53669200
C	-3.35005500	0.36627700	-0.69967200
C	-3.27255700	1.58438500	-1.38767900
C	-4.51588200	0.02832700	-0.00538400
C	-4.35826100	2.45606800	-1.36866900
H	-2.36165600	1.84965600	-1.92062000
C	-5.59567200	0.90771200	0.00799500
H	-4.58567700	-0.91634500	0.52399800
C	-5.51817800	2.12018800	-0.67257000
H	-4.29717400	3.40040800	-1.89993900
H	-6.49692300	0.64262600	0.55062500
H	-6.36170800	2.80286400	-0.66091800
C	-2.47935100	-2.30562700	0.05228300
C	-2.39584100	-2.38841300	1.44754800
C	-2.97718500	-3.38994900	-0.67550200
C	-2.81952800	-3.53761900	2.10780500
H	-1.99674300	-1.54782900	2.01218800
C	-3.39530500	-4.54135000	-0.01228400
H	-3.04369100	-3.34514500	-1.75803100
C	-3.31830300	-4.61456400	1.37680400
H	-2.75418000	-3.59575600	3.18919200
H	-3.78052800	-5.38110100	-0.58123800
H	-3.64327600	-5.51346600	1.89067000

M4

C	-0.52778300	5.17608500	-0.71808900
C	-0.88457900	3.89462900	-1.13514100
C	-1.18738400	2.94261500	-0.16594300
C	-1.11278800	3.28396300	1.18321800
C	-0.76530900	4.56467900	1.61031200
C	-0.47120100	5.51473700	0.64076900
H	-0.28992200	5.93037400	-1.46167200
H	-0.92716000	3.65101600	-2.19250600
H	-0.71791400	4.79584700	2.66991900
H	-0.18996800	6.52131200	0.93082900
C	-1.42117900	2.09865700	2.00595000
O	-1.55652500	2.03661900	3.20831000
C	-1.47936900	0.88428200	1.05319500
C	-0.12661400	0.15419200	1.17217100
C	-0.05330200	-0.99223500	0.16555500
H	0.01020700	-0.19582700	2.19767600
H	0.65614200	0.89786400	0.97691300
H	0.13793300	1.16078100	-1.53405500
H	-0.44007400	-1.91129300	0.61306700
C	-2.69013200	0.03743100	1.40842900
O	-3.82648800	0.43191200	1.27321400
O	-2.37932800	-1.17230700	1.87156800
C	-3.49203600	-2.05767300	2.05880300
H	-3.06766900	-2.99496900	2.41176800
H	-4.18520400	-1.64550400	2.79317900
H	-4.00437800	-2.20081600	1.10360900
C	-1.63967800	1.50912200	-0.36210000
C	-0.87583200	0.75351600	-1.46457400
H	-2.71122700	1.53537900	-0.58388000
H	-1.34321700	0.91953200	-2.44074100
C	-0.72191000	-0.75708000	-1.20995600
O	0.30573000	-1.30694900	-2.01211900
C	-2.00768700	-1.56434500	-1.39111600
C	-1.93450500	-2.95771500	-1.25179300
C	-3.24608000	-1.00128700	-1.69913000
C	-3.06119300	-3.75708100	-1.38892000
H	-0.97098200	-3.41837900	-1.05007000
C	-4.38439100	-1.80042300	-1.83713000
H	-3.34516000	0.06815700	-1.84828400
C	-4.29855800	-3.17806900	-1.67852200
H	-2.97645700	-4.83347600	-1.27610200
H	-5.33664700	-1.33614300	-2.07358000
H	-5.18247400	-3.79876400	-1.78485500
P	1.57172600	-1.38147300	-0.67409600

C	2.14603900	-2.96349400	-1.41862200
H	3.21018700	-3.10802000	-1.23001900
H	1.59876700	-3.77398800	-0.92669200
H	1.91839000	-2.97814500	-2.48357500
C	2.61178700	-1.66400800	0.90540900
C	4.01292500	-1.58294400	0.86562100
C	2.02946300	-2.11955400	2.09320000
C	4.79486200	-1.91193900	1.96810100
H	4.50642400	-1.24842300	-0.04480500
C	2.80587000	-2.45526400	3.20470700
H	0.95183800	-2.23256800	2.17223500
C	4.19047800	-2.34692400	3.14756300
H	5.87588900	-1.83053100	1.90749500
H	2.32293600	-2.80304700	4.11277300
H	4.79609800	-2.60465500	4.01056000
C	2.47679400	0.08268300	-1.30913100
C	2.59248900	0.25228300	-2.69315900
C	2.99820800	1.06070700	-0.45603100
C	3.23580900	1.37024200	-3.21378000
H	2.15133300	-0.48271600	-3.35778200
C	3.60874800	2.19856200	-0.97980400
H	2.93812600	0.93326400	0.62035100
C	3.73556800	2.35090600	-2.35779300
H	3.33297400	1.48475000	-4.28856500
H	3.99263600	2.95910200	-0.30793600
H	4.22039900	3.23225400	-2.76522000

TS5

C	-5.35608300	0.40076100	-2.14454600
C	-4.12636000	-0.24874900	-2.06218000
C	-3.46853200	-0.27824600	-0.83399700
C	-4.04904600	0.34312200	0.26984500
C	-5.28093500	0.99318100	0.19850700
C	-5.93416900	1.01805400	-1.02615400
H	-5.88085400	0.42932800	-3.09445100
H	-3.69667300	-0.72391300	-2.93897800
H	-5.70352600	1.46240900	1.08166100
H	-6.89420800	1.51344500	-1.12426600
C	-3.17463300	0.18359900	1.44866900
O	-3.39007400	0.55911000	2.58209400
C	-1.88428300	-0.52161200	0.98516000
C	-0.68619000	0.46129200	1.09425700
C	0.54305200	-0.15647300	0.46978100
H	-0.52198000	0.71294800	2.14404100

H	-0.99406800	1.39382600	0.59871400
H	-1.08043800	0.68129400	-1.52397500
H	1.20396900	-0.67447700	1.15954900
C	-1.69988800	-1.75743500	1.85079500
O	-2.17459000	-2.84379300	1.59962300
O	-0.99442800	-1.51580500	2.95803900
C	-0.83823100	-2.63358900	3.83905900
H	-0.24096500	-2.27282100	4.67348400
H	-1.81288200	-2.98153800	4.18517100
H	-0.32696400	-3.45041000	3.32562100
C	-2.13268400	-0.90653700	-0.49913300
C	-1.00545000	-0.40684300	-1.42312400
H	-2.20751800	-1.99623900	-0.58186000
H	-1.11007100	-0.84072900	-2.42144000
C	0.35052800	-0.74340600	-0.81470800
O	1.38613100	0.15409700	-1.92023100
C	0.81891100	-2.15184800	-1.10160000
C	0.90972700	-3.08385800	-0.06442700
C	1.08459000	-2.57925600	-2.40954700
C	1.26888200	-4.40700300	-0.32201200
H	0.70027600	-2.76850900	0.95283400
C	1.44188000	-3.89712900	-2.66843100
H	1.02918400	-1.85983900	-3.22033400
C	1.53543900	-4.81764600	-1.62357200
H	1.33588000	-5.11450700	0.49852600
H	1.65214600	-4.20807300	-3.68703400
H	1.81394000	-5.84687200	-1.82642500
P	2.05688900	1.26722800	-1.03367500
C	3.00691200	2.12369800	-2.34986300
H	3.70731600	1.41812600	-2.80099400
H	2.33290600	2.49886700	-3.12215400
H	3.56501800	2.96072400	-1.92250900
C	3.40928000	0.78062300	0.06892300
C	3.76250200	-0.56787100	0.16701700
C	4.18322800	1.75073000	0.71380500
C	4.86622400	-0.94376700	0.92606700
H	3.16906400	-1.32028600	-0.34529900
C	5.27697800	1.36682400	1.48660700
H	3.93730600	2.80532400	0.62053300
C	5.61887500	0.02119400	1.59401200
H	5.13580200	-1.99230900	0.99894100
H	5.86475100	2.12256900	1.99700800
H	6.47443700	-0.27474500	2.19208000
C	1.05447500	2.62779300	-0.38452000

C	1.10504500	3.03466900	0.95249500
C	0.18183800	3.26591500	-1.27020200
C	0.31002400	4.08805200	1.38799300
H	1.74317400	2.50644700	1.65534800
C	-0.63460100	4.30379200	-0.82151000
H	0.12425200	2.94838200	-2.30840000
C	-0.56314300	4.72289900	0.50317200
H	0.35846500	4.40441800	2.42479300
H	-1.32019400	4.78442800	-1.51155200
H	-1.19216100	5.53584200	0.85047100

P

C	3.44172900	-3.17027200	-0.66645800
C	2.17162200	-2.61816500	-0.81741200
C	1.95569100	-1.31459700	-0.37625000
C	3.00217300	-0.60365300	0.20645700
C	4.27793900	-1.14724500	0.36204500
C	4.49022200	-2.44472200	-0.08248100
H	3.62581500	-4.18396000	-1.00840300
H	1.37204000	-3.19349000	-1.27450600
H	5.06984000	-0.56338900	0.82085700
H	5.46735900	-2.90398800	0.02121200
C	2.53472100	0.73865400	0.59799900
O	3.17759100	1.63389200	1.10160400
C	1.02179700	0.82176500	0.28024800
C	0.23322900	0.98626600	1.59577100
C	-1.23131100	0.79602400	1.31286900
H	0.45331600	1.95567900	2.04136500
H	0.58408000	0.21518200	2.29668200
H	-0.17315700	-1.79036600	1.09430000
H	-1.94766900	1.52057300	1.68892200
C	0.83141100	2.00519800	-0.66026900
O	1.02201100	1.94922600	-1.85457800
O	0.48501900	3.12467200	-0.02667300
C	0.35275000	4.28346900	-0.85919200
H	0.06402000	5.09422500	-0.19440800
H	1.30305000	4.50487300	-1.34765200
H	-0.41327400	4.11508900	-1.61761500
C	0.67489000	-0.51125100	-0.43232700
C	-0.52504700	-1.24864200	0.20550100
H	0.43026300	-0.29597800	-1.47655200
H	-0.89506300	-1.99746600	-0.49879900
C	-1.61618600	-0.27892000	0.61000200
C	-3.03044300	-0.55455200	0.26816900

C	-3.50798100	-1.86962400	0.19399400
C	-3.92749400	0.49492600	0.02443600
C	-4.84489900	-2.12702800	-0.09728400
H	-2.83388700	-2.69925900	0.38654100
C	-5.26269000	0.23815400	-0.26702400
H	-3.56486500	1.51838800	0.04166900
C	-5.72765800	-1.07482100	-0.32806600
H	-5.19729500	-3.15270600	-0.14120900
H	-5.93982600	1.06440500	-0.45950100
H	-6.76849300	-1.27592300	-0.56008800

O=PPh2Me

O	0.03481400	2.09347300	-1.39234400
P	-0.02584600	1.24464000	-0.14955000
C	-0.08033800	2.21402500	1.38267000
H	0.82931800	2.81660600	1.43051300
H	-0.94336100	2.88300600	1.37516500
H	-0.13105200	1.56474400	2.25963700
C	1.43766600	0.18296200	0.01449300
C	2.45495200	0.32727000	-0.93017200
C	1.58205200	-0.73406300	1.06182500
C	3.61471300	-0.43867800	-0.82874800
H	2.32692300	1.04143400	-1.73798400
C	2.74080400	-1.49716500	1.16068000
H	0.78849900	-0.86171500	1.79438400
C	3.75708000	-1.34808600	0.21566700
H	4.40419100	-0.32533900	-1.56435600
H	2.85223700	-2.20974500	1.97122500
H	4.65995300	-1.94512800	0.29491400
C	-1.45363100	0.12229500	-0.08495100
C	-1.35788100	-1.17172200	-0.60841500
C	-2.68408700	0.57823600	0.40127900
C	-2.47637900	-2.00002000	-0.63916700
H	-0.40633200	-1.53481500	-0.98647000
C	-3.80098400	-0.25177500	0.37044100
H	-2.77905200	1.58202600	0.80507500
C	-3.69716200	-1.54079900	-0.14873000
H	-2.39378000	-3.00338800	-1.04354100
H	-4.75085500	0.10747300	0.75216300
H	-4.56833300	-2.18741400	-0.16996500

TS2-1

C	6.46400500	-1.43047700	-0.73737100
C	5.79295200	-0.33617600	-0.20522700

C	4.39719100	-0.22678900	-0.28174900
C	3.66923100	-1.28376500	-0.86492900
C	4.34961700	-2.37920800	-1.39311100
C	5.73888900	-2.45444900	-1.34141100
H	7.54581400	-1.48567200	-0.67709200
H	6.35382600	0.46418400	0.26961200
H	3.77691800	-3.18962100	-1.83465600
H	6.24993300	-3.31621300	-1.75836200
C	2.17136500	-1.29531300	-0.93517400
O	1.61939500	-0.78373200	-1.98500100
C	1.35453400	-1.81390600	0.03507000
C	-0.10893900	-1.71048100	-0.32963500
C	-0.26203600	-0.64422500	-1.40589700
H	-0.68196100	-1.44396800	0.56289900
H	-0.51329200	-2.66223100	-0.69640200
H	-0.54004000	-0.87419200	-2.42343500
H	-0.05799100	0.39389000	-1.16216100
C	1.80433900	-2.41733600	1.26716400
O	2.94926900	-2.50986200	1.68286200
O	0.75485600	-2.91124700	1.98169100
C	1.10094000	-3.51086000	3.22582500
H	0.16915000	-3.88137000	3.65056300
H	1.80354600	-4.33373600	3.07724600
H	1.55616800	-2.77825500	3.89651400
C	3.78072100	0.99263900	0.26020600
C	2.64153700	1.55622500	-0.17057600
H	4.33320700	1.50677100	1.04641600
H	2.09695100	1.11237600	-0.99277000
C	2.12956000	2.80168200	0.44272200
O	2.62167200	3.27538900	1.45754600
C	0.96207400	3.47990600	-0.21437700
C	0.30509800	4.49273900	0.49398000
C	0.53203300	3.15900300	-1.50707000
C	-0.77567400	5.16071900	-0.06928800
H	0.65696700	4.73818100	1.49086200
C	-0.54103000	3.84050500	-2.07825000
H	1.04246200	2.40077800	-2.09247200
C	-1.20150300	4.83457300	-1.35839400
H	-1.28571000	5.93770100	0.49088200
H	-0.85515800	3.59841700	-3.08856600
H	-2.04170900	5.35814500	-1.80303300
P	-2.52918100	-0.07509000	-0.89137400
C	-3.30361700	1.22866300	-1.92672500
H	-2.62627300	2.08141100	-2.01134200

H	-3.47029400	0.81693300	-2.92420100
H	-4.25470600	1.55482700	-1.49943700
C	-2.49721900	0.62683700	0.78952300
C	-2.69412600	-0.18297400	1.91580500
C	-2.13355700	1.96798100	0.96638000
C	-2.55419600	0.34762700	3.19552100
H	-2.96956500	-1.22699400	1.79369700
C	-1.99878600	2.49381800	2.24830400
H	-1.95257900	2.61210300	0.10872600
C	-2.21092900	1.68714700	3.36400300
H	-2.71689700	-0.28733700	4.06030300
H	-1.72588600	3.53728200	2.37085000
H	-2.10521900	2.10063400	4.36156100
C	-3.76985400	-1.41187500	-0.84886400
C	-5.00233100	-1.26311200	-0.19917200
C	-3.48908700	-2.59879500	-1.53146000
C	-5.93639800	-2.29261600	-0.23369800
H	-5.22642400	-0.34554000	0.33864900
C	-4.42810700	-3.62790300	-1.56689400
H	-2.53639500	-2.71999200	-2.04022600
C	-5.64930700	-3.47485000	-0.91707400
H	-6.88971400	-2.17356500	0.27064100
H	-4.20295500	-4.54621500	-2.09864700
H	-6.38034800	-4.27652200	-0.94172900
P1			
C	-4.49927800	2.06034700	0.14758300
C	-3.24671200	2.24758100	-0.42777200
C	-2.19029000	1.37284800	-0.15777800
C	-2.42873600	0.25685300	0.66626700
C	-3.68388100	0.08521700	1.25559000
C	-4.71644000	0.98251000	1.00167600
H	-5.30178500	2.75839100	-0.06626900
H	-3.06946600	3.09799000	-1.07961600
H	-3.85061800	-0.77257000	1.89963900
H	-5.68831600	0.83225800	1.45927400
C	-1.41961100	-0.79734000	0.92193000
O	-1.16675400	-1.01836300	2.23120500
C	-0.74968700	-1.62547100	0.09275700
C	0.10676800	-2.56582300	0.90870700
C	-0.27559600	-2.15973800	2.34540200
H	1.17385700	-2.42648500	0.70528900
H	-0.12834200	-3.61355700	0.70546000
H	-0.81998000	-2.94354800	2.87523300

H	0.57669000	-1.84506300	2.95055700
C	-0.82705900	-1.61950300	-1.36231100
O	-1.49935400	-0.87762100	-2.05399500
O	-0.02918000	-2.57183900	-1.88500300
C	-0.02327400	-2.64449000	-3.31136300
H	0.65464600	-3.45672800	-3.56576200
H	-1.02684300	-2.85249100	-3.68750400
H	0.32999900	-1.70412100	-3.73926300
C	-0.85737400	1.67704300	-0.70434500
C	0.26966800	1.54522600	0.00343200
H	-0.79951500	2.04539000	-1.72697100
H	0.22599800	1.21661100	1.03698900
C	1.59578100	1.79610600	-0.61242100
O	1.71371200	2.47130800	-1.62429400
C	2.79096300	1.16130100	0.02730000
C	4.06343900	1.55990400	-0.39471500
C	2.66914000	0.15616100	0.99279700
C	5.19786800	0.97135400	0.14967100
H	4.14163600	2.33376700	-1.15115800
C	3.80548800	-0.44270700	1.52850800
H	1.68880000	-0.17706700	1.31914000
C	5.06971300	-0.03226000	1.11107000
H	6.18288800	1.28991600	-0.17490000
H	3.70135600	-1.22701600	2.27130400
H	5.95625500	-0.49426300	1.53334000

TS3-2

C	5.61475000	0.46594600	-2.41312500
C	4.75110900	0.89580000	-1.40724200
C	3.92119200	-0.04067400	-0.79704000
C	3.96420400	-1.37161200	-1.21214500
C	4.82884300	-1.81291300	-2.21276400
C	5.65965800	-0.87655900	-2.81459900
H	6.26927100	1.18475100	-2.89641800
H	4.72832000	1.93762700	-1.10173300
H	4.83594400	-2.85716800	-2.50980400
H	6.34215800	-1.17881700	-3.60166600
C	2.96981000	-2.15892900	-0.45483100
O	2.79496000	-3.35839200	-0.47901800
C	2.11817100	-1.15331800	0.34500800
C	0.82180500	-0.90635600	-0.45056000
C	0.07053800	0.29903300	0.08028800
H	0.21768500	-1.81666700	-0.41976000
H	1.08505300	-0.72461400	-1.49764000

H	-0.17240700	1.14590500	-0.55155000
H	-0.03618300	0.41246600	1.15185400
C	1.90947300	-1.66208000	1.75415600
O	2.82255300	-1.95142500	2.49223900
O	0.62110700	-1.76663000	2.10523700
C	0.38708800	-2.16353400	3.46193600
H	-0.69463500	-2.21351800	3.57370700
H	0.84038200	-3.13680400	3.65431400
H	0.81029900	-1.42092500	4.14044500
C	2.95230300	0.16921900	0.34529300
C	2.06055100	1.37037000	0.26322100
H	3.51798800	0.20292800	1.28542900
H	2.03928300	1.92961400	-0.66516000
C	1.61691700	1.93708700	1.47754700
O	1.83131800	1.40119600	2.59199300
C	0.63609500	3.08821900	1.42509200
C	-0.00699300	3.44141300	2.61583000
C	0.25066000	3.73018700	0.24095300
C	-1.00869600	4.40714900	2.62979300
H	0.28993400	2.92428600	3.52178100
C	-0.75492600	4.69449500	0.25073000
H	0.72851700	3.48307300	-0.70181000
C	-1.39047800	5.03342000	1.44456600
H	-1.50031100	4.66507500	3.56275700
H	-1.04362400	5.17993400	-0.67657200
H	-2.17799100	5.78047500	1.44951900
P	-2.14801900	-0.15281200	-0.07426300
C	-2.74933500	1.12540100	1.09047600
H	-2.61463800	0.74365900	2.10571500
H	-2.14412500	2.03324000	0.98489300
H	-3.80274700	1.35916500	0.92288200
C	-3.10162300	-1.65813400	0.31014400
C	-2.44785300	-2.70489200	0.96776200
C	-4.46138400	-1.77361300	-0.00573900
C	-3.15170100	-3.85638800	1.31681000
H	-1.39036400	-2.61715900	1.20432000
C	-5.15747600	-2.92652100	0.34119700
H	-4.97001100	-0.96672600	-0.52636400
C	-4.50344300	-3.96652000	1.00339400
H	-2.64144600	-4.66635400	1.82743100
H	-6.21085300	-3.01466300	0.09629400
H	-5.05095500	-4.86418900	1.27148300
C	-2.70575400	0.39671900	-1.71303300
C	-2.92628500	-0.54127600	-2.73043500

C	-2.79129000	1.76318200	-2.00737600
C	-3.24821200	-0.11719300	-4.01503300
H	-2.85649800	-1.60371900	-2.51349900
C	-3.10821700	2.18188200	-3.29793500
H	-2.61795700	2.50781000	-1.23479400
C	-3.34007600	1.24454600	-4.30102200
H	-3.42616200	-0.85124500	-4.79397400
H	-3.17823700	3.24259800	-3.51550300
H	-3.59147300	1.57281300	-5.30413700
P2			
C	3.29633400	-3.22752100	-0.68262500
C	2.07583300	-2.55507800	-0.74896800
C	2.04119600	-1.20860300	-0.40207300
C	3.21369100	-0.56828800	0.00161100
C	4.43766300	-1.22866400	0.06081300
C	4.46971300	-2.57480100	-0.28588500
H	3.33839200	-4.27923500	-0.94784500
H	1.17914900	-3.07611000	-1.07142900
H	5.33105800	-0.69974600	0.37817600
H	5.40289900	-3.12627900	-0.24700700
C	2.91578000	0.84009100	0.35765000
O	3.70544100	1.71613800	0.63075700
C	1.38688300	0.95905900	0.39184500
C	0.87971400	0.61512600	1.81033500
C	-0.47079100	-0.09253500	1.61881900
H	0.81028400	1.50201500	2.44155300
H	1.59328200	-0.07245900	2.27509000
H	-0.62660900	-0.87170000	2.36751600
H	-1.28850200	0.62649100	1.72317500
C	0.88599900	2.26172800	-0.18545300
O	1.34546100	2.76822700	-1.18322800
O	-0.15649600	2.75583000	0.48623400
C	-0.79465700	3.88325500	-0.12421700
H	-1.59672600	4.17303900	0.55093600
H	-0.08253500	4.69966800	-0.25095400
H	-1.19563500	3.58940400	-1.09630700
C	0.87832100	-0.23711800	-0.45859900
C	-0.44980500	-0.68080200	0.16930800
H	0.72231200	0.06710600	-1.49843000
H	-0.53264100	-1.77150500	0.18255900
C	-1.63313700	-0.09318200	-0.59104300
O	-1.47547600	0.79337300	-1.41248900
C	-3.00854700	-0.58028000	-0.25560400

C	-4.09444500	0.02264700	-0.90084000
C	-3.23889400	-1.60164100	0.67200200
C	-5.39123700	-0.39094200	-0.62642600
H	-3.89865700	0.81500100	-1.61542000
C	-4.53938700	-2.01463500	0.94706300
H	-2.41287000	-2.08055800	1.18720700
C	-5.61458400	-1.41152300	0.29864500
H	-6.22888000	0.08023200	-1.12978400
H	-4.71187500	-2.80634000	1.66816000
H	-6.62773400	-1.73533400	0.51446700

TS1-3

C	-2.08456300	-2.21556800	3.37720000
C	-1.15606500	-1.45932700	2.66959400
C	-1.15158700	-1.42992300	1.27162600
C	-2.10204000	-2.21336300	0.58924600
C	-3.05396600	-2.94452000	1.30524900
C	-3.04766300	-2.95428400	2.69447700
H	-2.05834100	-2.22107600	4.46187700
H	-0.41844900	-0.87887800	3.21455400
H	-3.78755500	-3.52180000	0.75183000
H	-3.78255200	-3.53713000	3.23908400
C	-2.19171800	-2.33426400	-0.90696200
O	-3.28436600	-2.26237200	-1.44534100
C	-0.95881200	-2.50774200	-1.74138400
C	-1.16591300	-2.79913100	-3.22043400
C	-0.78761200	-1.43046300	-2.81392100
H	-2.19573100	-2.98399800	-3.50192400
H	-0.41236600	-3.42569200	-3.68233800
H	0.22871900	-1.07974100	-2.94882700
H	-1.56577900	-0.67319300	-2.81366600
C	0.25453700	-3.10661700	-1.10638100
O	0.23569500	-3.79278600	-0.10826000
O	1.36421600	-2.84010100	-1.79687900
C	2.57955300	-3.30513600	-1.20471200
H	3.38010500	-2.92838100	-1.83815000
H	2.66943600	-2.90119400	-0.19379900
H	2.59399600	-4.39615000	-1.16890700
C	-0.17273800	-0.56597200	0.53821500
C	1.18723700	-0.49197100	0.92820800
H	-0.27532900	-0.57387400	-0.54212600
H	1.48484700	-0.64313300	1.95836500
C	2.13440300	-0.13276800	-0.07294500
O	1.82522700	0.12648800	-1.25383600

C	3.59346500	-0.05542500	0.30956900
C	4.43913200	0.70685900	-0.50231400
C	4.13523100	-0.71670300	1.41649100
C	5.79313000	0.82464900	-0.20611900
H	4.00310200	1.20577100	-1.36168600
C	5.49286800	-0.60873200	1.70941100
H	3.50241500	-1.33876800	2.04238700
C	6.32414700	0.16598600	0.90246700
H	6.43655400	1.42828800	-0.83897800
H	5.90359600	-1.13373600	2.56628500
H	7.38130100	0.25192800	1.13363400
P	-0.98767800	1.45284000	0.76929900
C	-0.92890400	1.81398100	2.55886700
H	-1.77721600	1.33213600	3.04785300
H	-0.00026400	1.41432800	2.97480900
H	-0.96643100	2.89229300	2.72792700
C	-2.62426600	2.03405800	0.20822500
C	-3.55506700	1.10212800	-0.25890300
C	-2.96347400	3.39304500	0.25588700
C	-4.81769900	1.52490000	-0.67194800
H	-3.30518600	0.04597900	-0.30132200
C	-4.22466000	3.80916400	-0.15585900
H	-2.23849300	4.12312000	0.60596300
C	-5.15187000	2.87463700	-0.61922400
H	-5.53509900	0.79742500	-1.03695600
H	-4.48447700	4.86195500	-0.11815000
H	-6.13425200	3.20306000	-0.94254000
C	0.22816700	2.56494900	0.02480500
C	0.03522800	3.06000000	-1.27151100
C	1.42901400	2.82642600	0.69422500
C	1.03111000	3.80829000	-1.88588500
H	-0.89372500	2.85902500	-1.79809000
C	2.43008300	3.56493400	0.06645600
H	1.59410300	2.45207500	1.69911700
C	2.23325400	4.05511200	-1.22066700
H	0.87377100	4.19662600	-2.88681500
H	3.36382600	3.75405500	0.58607000
H	3.01280900	4.63298500	-1.70673300

M1-3

C	2.45184600	-2.03065000	-3.11190800
C	1.47520200	-1.23261400	-2.52169600
C	1.30523900	-1.19238200	-1.13569000
C	2.12473700	-2.01828300	-0.34546100

C	3.12919100	-2.78746400	-0.93618400
C	3.29799100	-2.79729900	-2.31619800
H	2.55495400	-2.04429600	-4.19191200
H	0.82480200	-0.63607000	-3.15449000
H	3.76073900	-3.39770900	-0.29822300
H	4.07303400	-3.40831600	-2.76621300
C	1.97140200	-2.17626500	1.14093500
O	2.95022900	-2.09811700	1.86475800
C	0.61602400	-2.42200900	1.73292800
C	0.57980700	-2.83347400	3.20136900
C	0.21924800	-1.44876000	2.84453100
H	1.55477900	-3.01260700	3.63894200
H	-0.21352000	-3.52031800	3.47095500
H	-0.81497100	-1.12883800	2.80987900
H	0.95451900	-0.67561300	3.04761500
C	-0.45123900	-3.01412200	0.86954100
O	-0.24459500	-3.61769400	-0.16035300
O	-1.66465200	-2.87478800	1.40797200
C	-2.73975700	-3.38267600	0.61508100
H	-3.65193900	-3.11186200	1.14330700
H	-2.71532100	-2.91342200	-0.37046300
H	-2.65914500	-4.46691500	0.51236200
C	0.30291900	-0.23303800	-0.52716500
C	-1.11830700	-0.31607600	-0.96237400
H	0.29412200	-0.28920300	0.56663100
H	-1.34657500	-0.48660300	-2.00720000
C	-2.09514900	-0.05115500	-0.00684400
O	-1.85808400	0.22942900	1.20529300
C	-3.54197900	-0.03516900	-0.45434500
C	-4.45119400	0.69052000	0.32089600
C	-4.01617200	-0.69456900	-1.59464400
C	-5.79415200	0.77278800	-0.03734100
H	-4.07082800	1.18669600	1.20766700
C	-5.36013700	-0.62255800	-1.95167000
H	-3.33493200	-1.28589200	-2.20018300
C	-6.25456600	0.11494500	-1.17645600
H	-6.48372000	1.34842000	0.57329600
H	-5.71179100	-1.14824100	-2.83450700
H	-7.30204100	0.17061900	-1.45625100
P	0.87804500	1.52844300	-0.80369800
C	0.69192700	2.00150500	-2.54219900
H	1.50708600	1.58285900	-3.13395600
H	-0.26392200	1.61354600	-2.90167600
H	0.69333000	3.08983500	-2.62574000

C	2.60668200	1.76425000	-0.33357100
C	3.09548700	1.09171400	0.79291300
C	3.46297000	2.57196200	-1.08890800
C	4.42851300	1.22938300	1.16297300
H	2.44350500	0.45813900	1.38723500
C	4.79623300	2.70706000	-0.71268800
H	3.09899100	3.09596900	-1.96700200
C	5.27857900	2.03675900	0.40936000
H	4.80038300	0.69891600	2.03291400
H	5.45780200	3.33405400	-1.30047400
H	6.31998200	2.14074600	0.69528600
C	-0.16279000	2.63871300	0.16676100
C	0.25757100	3.08103100	1.42384400
C	-1.41688800	3.01010300	-0.32939700
C	-0.58295500	3.88258000	2.18927800
H	1.23582500	2.80569300	1.80627000
C	-2.25298900	3.80771300	0.44467800
H	-1.75381400	2.65811500	-1.29902100
C	-1.83794000	4.24146100	1.70249700
H	-0.25573300	4.22713700	3.16428200
H	-3.22966100	4.08877400	0.06488500
H	-2.49191100	4.86556300	2.30282600

TS2-3

C	2.20777900	-3.85846700	-1.53250300
C	2.13995100	-2.53793800	-1.08620900
C	0.90449500	-1.94378200	-0.83381100
C	-0.26706600	-2.67936900	-1.03240700
C	-0.19579000	-3.99513800	-1.48238600
C	1.04101500	-4.59017800	-1.72761100
H	3.17539700	-4.30814800	-1.73056000
H	3.06396900	-1.98576500	-0.94151700
H	-1.11656000	-4.54657800	-1.65098100
H	1.09165800	-5.61540000	-2.08007700
C	-1.64765500	-2.06822200	-0.83244400
O	-2.42309500	-2.09238400	-1.80863200
C	-2.29325500	-2.16086500	0.55018700
C	-3.73218200	-1.71691200	0.61029700
C	-3.43582100	-3.17288200	0.64294100
H	-4.10618000	-1.31800900	-0.32404000
H	-4.05805600	-1.23043200	1.52023400
H	-3.54280900	-3.70564000	1.58096800
H	-3.61577600	-3.74271700	-0.26162400
C	-1.46858600	-2.05850200	1.78824300

O	-0.27258600	-2.24912600	1.85921900
O	-2.21437000	-1.80546000	2.87562600
C	-1.48032900	-1.66391000	4.09152200
H	-2.21896700	-1.45503100	4.86303700
H	-0.93551700	-2.58110100	4.32300500
H	-0.77400000	-0.83626300	4.00077900
C	0.66102000	-0.53843500	-0.31254700
C	-0.71244500	-0.08169800	-0.70165000
H	0.69829100	-0.52354300	0.78415700
H	-0.89165000	0.08832600	-1.75939700
C	-1.43415000	0.70258800	0.23976500
O	-1.12084700	0.79444700	1.44581700
C	-2.65790100	1.43840300	-0.24081800
C	-3.10511400	2.51940700	0.52310400
C	-3.34265700	1.09832300	-1.41299700
C	-4.20625000	3.26660100	0.11775000
H	-2.56310800	2.76234900	1.43127400
C	-4.45580900	1.83695200	-1.81005800
H	-3.03062900	0.22853200	-1.98655800
C	-4.88419800	2.92644200	-1.05230800
H	-4.53724700	4.11313000	0.71158200
H	-4.99269200	1.56077700	-2.71246500
H	-5.74585400	3.50516700	-1.37047200
P	1.89975900	0.71695600	-0.83167000
C	2.07033900	0.68206100	-2.63265900
H	2.54057100	-0.25832400	-2.92629700
H	1.07567500	0.73863200	-3.08032300
H	2.66811700	1.52753400	-2.97552500
C	3.51497900	0.46182800	-0.05942000
C	3.61406600	-0.31508200	1.10035700
C	4.64757000	1.09723200	-0.58055000
C	4.84562600	-0.45471100	1.73357000
H	2.74153200	-0.82046000	1.50530400
C	5.87483000	0.94961800	0.05729400
H	4.57880100	1.70908300	-1.47506700
C	5.97277300	0.17635400	1.21276400
H	4.92139200	-1.05828800	2.63127500
H	6.75358900	1.43910000	-0.34801000
H	6.93178800	0.06468200	1.70753400
C	1.31898900	2.34760400	-0.31877400
C	1.83330800	2.92828800	0.84411600
C	0.30700600	2.99126400	-1.04077000
C	1.32746300	4.14586100	1.28903000
H	2.62148800	2.43327600	1.40273400

C	-0.19597600	4.20581100	-0.58593800
H	-0.10471500	2.54429200	-1.94036700
C	0.31230000	4.78081600	0.57754500
H	1.72580000	4.59482300	2.19231000
H	-0.98978600	4.69798800	-1.13752700
H	-0.08369100	5.72769900	0.92969400

M2-3

C	1.67007200	-4.07538700	-1.81315900
C	1.85410300	-2.85893900	-1.15371900
C	0.74343000	-2.05917000	-0.89633600
C	-0.53341700	-2.45911100	-1.28267500
C	-0.71268700	-3.66729700	-1.94466200
C	0.39246400	-4.47780000	-2.20506100
H	2.52719300	-4.70541200	-2.02802300
H	2.85523100	-2.55293100	-0.85673000
H	-1.70929700	-3.95923700	-2.26428000
H	0.26321800	-5.42307300	-2.72362000
C	-1.65341100	-1.44793800	-0.97480900
O	-2.42640600	-1.16881700	-2.01049900
C	-2.49360800	-1.92273800	0.26054600
C	-3.85473100	-1.27701700	0.38286800
C	-3.75826800	-2.68626400	-0.08507300
H	-4.04465100	-0.53663200	-0.38484300
H	-4.23019400	-1.07863800	1.37887400
H	-4.06451100	-3.47992200	0.58603100
H	-3.88492700	-2.84536300	-1.14918400
C	-1.82979300	-2.34780400	1.52041500
O	-0.64033100	-2.53694900	1.67444600
O	-2.70495500	-2.55296200	2.52759100
C	-2.12566600	-2.98837900	3.75674500
H	-2.95185100	-3.08635000	4.45852300
H	-1.62233000	-3.94851700	3.62533800
H	-1.40258100	-2.25457800	4.11844900
C	0.67422900	-0.72083800	-0.18679900
C	-0.71596400	-0.16830300	-0.53846200
H	0.74333400	-0.82905100	0.90120600
H	-0.68253800	0.37954200	-1.48439800
C	-1.27686800	0.71036100	0.54501200
O	-0.97948600	0.54037200	1.72072600
C	-2.19532600	1.82178800	0.15136600
C	-2.40655000	2.85574500	1.06702000
C	-2.80414800	1.86090400	-1.10857700
C	-3.19900600	3.94386800	0.71949300

H	-1.92573400	2.79794700	2.03840700
C	-3.61062500	2.94556200	-1.44433300
H	-2.68108500	1.01208600	-1.78429200
C	-3.79599500	3.99130400	-0.53988200
H	-3.34920800	4.75483200	1.42507900
H	-4.09563500	2.97919500	-2.41496100
H	-4.41190100	4.84212000	-0.81469700
P	1.95657100	0.47581100	-0.69909500
C	2.25404700	0.30490600	-2.47578900
H	2.76538600	-0.64243700	-2.65098900
H	1.30057000	0.29543800	-3.00957400
H	2.87033100	1.13360800	-2.82878300
C	3.49961600	0.22373000	0.19680200
C	3.63040000	-0.79912800	1.14074800
C	4.57032200	1.08893900	-0.06368200
C	4.83787700	-0.95916500	1.81660700
H	2.80453600	-1.47244000	1.35002500
C	5.77065500	0.92041400	0.61470600
H	4.46638400	1.89493100	-0.78520400
C	5.90344400	-0.10326000	1.55312900
H	4.94175400	-1.75151700	2.54941600
H	6.60089100	1.58835400	0.41368900
H	6.84216600	-0.23087700	2.08177200
C	1.37240300	2.15001700	-0.36601100
C	1.49408200	2.67472500	0.92621200
C	0.72291600	2.88087900	-1.36670500
C	0.96637900	3.92918300	1.20917900
H	1.99750600	2.10803100	1.70459900
C	0.19989700	4.13654400	-1.07443700
H	0.61979900	2.48084400	-2.37075300
C	0.32051400	4.65776000	0.21072800
H	1.05890700	4.33792600	2.20948000
H	-0.30896400	4.69951000	-1.84913200
H	-0.09565500	5.63374500	0.43845100

TS3-3

C	1.45191200	-4.32398200	-0.19187200
C	1.71751800	-3.02597600	0.24249500
C	0.78829900	-2.02512800	-0.03089900
C	-0.38988800	-2.29611100	-0.72670100
C	-0.65167800	-3.59540600	-1.15348800
C	0.27345600	-4.60455300	-0.88454400
H	2.16058000	-5.11900800	0.01637500
H	2.62723500	-2.80582900	0.79532100

H	-1.56843100	-3.82786100	-1.68587900
H	0.07340300	-5.61946900	-1.21422400
C	-1.22461200	-1.03891000	-0.96609900
O	-1.06005000	-0.53081900	-2.27528400
C	-2.69717200	-1.26801600	-0.63037900
C	-3.75085300	-0.54044200	-1.43209700
C	-3.54231100	-1.98961400	-1.66976900
H	-3.33485700	0.13305800	-2.16932000
H	-4.63117400	-0.20593100	-0.89513600
H	-4.27626200	-2.70022900	-1.30810200
H	-3.00876700	-2.25721900	-2.57487500
C	-2.99872200	-1.53995300	0.79807800
O	-2.17145800	-1.57983900	1.68711100
O	-4.30942700	-1.73155600	1.03054300
C	-4.66543500	-1.93912300	2.39750600
H	-5.74005000	-2.11020500	2.40365900
H	-4.13686500	-2.80275400	2.80503300
H	-4.41802900	-1.05542000	2.99017500
C	0.85735200	-0.56439800	0.34412800
C	-0.44288300	0.05479100	-0.16592600
H	0.97965100	-0.38715900	1.41875800
H	-0.49396100	0.36449100	-1.45642300
C	-1.01604000	1.00304900	0.78523400
O	-0.40452800	1.39021700	1.78368300
C	-2.36665600	1.60422200	0.51692000
C	-3.32952300	1.56326600	1.52811100
C	-2.64808100	2.26297500	-0.68018800
C	-4.58010600	2.13951400	1.32878600
H	-3.08949600	1.06084000	2.46107700
C	-3.88775700	2.87180300	-0.86561300
H	-1.89748000	2.29511400	-1.46541600
C	-4.85819700	2.80006100	0.13173500
H	-5.33373400	2.08256300	2.10818700
H	-4.09965900	3.39455700	-1.79305200
H	-5.82874900	3.26167300	-0.02050800
P	2.25483200	0.25050600	-0.51158900
C	2.24408500	-0.32301200	-2.22596300
H	2.68526900	-1.32165700	-2.25860400
H	1.19699300	-0.38919000	-2.54888200
H	2.80967100	0.35958200	-2.86222800
C	3.83277700	-0.17016600	0.25553200
C	3.91697500	-0.31992500	1.64543600
C	4.97274300	-0.33183800	-0.53880000
C	5.13964100	-0.62886800	2.23321600

H	3.03648900	-0.20289200	2.27059600
C	6.19105000	-0.64178700	0.05719000
H	4.91516600	-0.21994400	-1.61716900
C	6.27380000	-0.79029700	1.43992300
H	5.20386800	-0.74729100	3.30924200
H	7.07396100	-0.77015600	-0.55944600
H	7.22485400	-1.03460400	1.90133700
C	2.04157700	2.04230800	-0.47962200
C	2.58681300	2.79867000	0.56111000
C	1.27285000	2.66000200	-1.47318300
C	2.35367800	4.16952000	0.61244300
H	3.19281500	2.32449000	1.32729400
C	1.04411700	4.03077000	-1.41366200
H	0.85347100	2.08004300	-2.29061200
C	1.58093300	4.78326500	-0.37076100
H	2.77734600	4.75648100	1.42006300
H	0.44932900	4.50977900	-2.18394800
H	1.40064900	5.85228000	-0.32755200

M3-3

C	1.44295600	-4.31079200	-0.36585600
C	1.70038900	-3.04720800	0.16610400
C	0.77804200	-2.02935200	-0.05620800
C	-0.38294000	-2.25162300	-0.79617700
C	-0.63654500	-3.51167500	-1.32750700
C	0.28336300	-4.53872000	-1.10736900
H	2.14586400	-5.12044900	-0.19840600
H	2.59967900	-2.86355400	0.74892500
H	-1.53730200	-3.70382300	-1.90101700
H	0.09351200	-5.52629000	-1.51602500
C	-1.22467200	-0.98325400	-0.92618500
O	-1.18309600	-0.62897100	-2.33381200
C	-2.69622600	-1.24029200	-0.55912600
C	-3.80489200	-0.51388000	-1.28152300
C	-3.59390200	-1.95766400	-1.56045800
H	-3.49253000	0.18223600	-2.04891700
H	-4.64918200	-0.19765000	-0.68105600
H	-4.29674700	-2.68062400	-1.16391300
H	-3.12884100	-2.20556900	-2.50729900
C	-2.94235600	-1.60041800	0.86810700
O	-2.08775900	-1.83877700	1.69365900
O	-4.25553900	-1.66823900	1.15922000
C	-4.56468700	-2.02248300	2.50666400
H	-5.65076100	-2.05969600	2.56385200

H	-4.13448000	-2.99435300	2.75592700
H	-4.17338100	-1.27177600	3.19719400
C	0.82780800	-0.59480000	0.39671100
C	-0.47963800	-0.00585400	-0.04499700
H	0.99785300	-0.45696200	1.47175400
H	-1.28802000	0.33183500	-2.35399000
C	-0.92358000	1.06760600	0.72399700
O	-0.22242600	1.60427500	1.62961800
C	-2.29955700	1.64832400	0.50771200
C	-3.26635000	1.50416900	1.50725500
C	-2.60967700	2.39215500	-0.63185300
C	-4.53520500	2.05373700	1.35064800
H	-3.01498200	0.94192400	2.40342800
C	-3.87389200	2.96152800	-0.78447600
H	-1.84959900	2.53602500	-1.39684900
C	-4.84196200	2.78459900	0.20158200
H	-5.28504400	1.91672600	2.12420300
H	-4.10377000	3.54198200	-1.67293700
H	-5.82869300	3.22045400	0.08015800
P	2.22396500	0.25360000	-0.46820400
C	2.21746000	-0.32466000	-2.18364600
H	2.62368100	-1.33742500	-2.22302800
H	1.17498200	-0.35381400	-2.51893600
H	2.80365200	0.34482400	-2.81482900
C	3.80462600	-0.16443000	0.29723500
C	3.89891500	-0.17400800	1.69539900
C	4.91649300	-0.50033300	-0.48200900
C	5.10303600	-0.51125000	2.30500400
H	3.03965900	0.08245900	2.30912400
C	6.11623700	-0.84043300	0.13582200
H	4.85217500	-0.49768900	-1.56546900
C	6.20922400	-0.84583500	1.52568700
H	5.17520700	-0.51723500	3.38702100
H	6.97710800	-1.10293000	-0.46927300
H	7.14553100	-1.11337000	2.00413800
C	2.02377000	2.04595500	-0.49077400
C	2.68442100	2.86224100	0.43016600
C	1.15683000	2.60708100	-1.43462900
C	2.46063800	4.23484100	0.41912500
H	3.37039000	2.43253300	1.15333400
C	0.93339500	3.98066300	-1.43574500
H	0.65492000	1.97772500	-2.16250000
C	1.58068100	4.79228700	-0.50703000
H	2.97321600	4.86868000	1.13466500

H	0.25768300	4.41497700	-2.16505900
H	1.40609500	5.86320000	-0.51050800
TS4-3			
C	1.03309200	-4.44330400	-0.30622800
C	1.27445000	-3.28355800	0.43162900
C	0.45570500	-2.18146900	0.21541300
C	-0.58572000	-2.22015700	-0.71524400
C	-0.81821300	-3.36863900	-1.45745500
C	-0.00060800	-4.48244700	-1.24277300
H	1.65355700	-5.32026900	-0.15220800
H	2.08663200	-3.23752700	1.15245200
H	-1.62094600	-3.41428800	-2.18575600
H	-0.17492700	-5.39138000	-1.80974700
C	-1.30921400	-0.87512500	-0.77061600
O	-1.05674900	-0.33348700	-2.08111700
C	-2.83080500	-1.04158900	-0.61188700
C	-3.78537500	-0.14790800	-1.36935400
C	-3.62785900	-1.56087800	-1.80064900
H	-3.34219400	0.61343000	-1.99817600
H	-4.68243900	0.15126600	-0.84218400
H	-4.42125100	-2.26799700	-1.59017100
H	-3.05693900	-1.73217000	-2.70579000
C	-3.28820000	-1.53423100	0.71996300
O	-2.56417300	-1.91679200	1.61309900
O	-4.62793900	-1.53007400	0.83238900
C	-5.13891400	-1.97793200	2.08881600
H	-6.22258900	-1.93718300	2.00060700
H	-4.80818200	-2.99720100	2.29593900
H	-4.79743900	-1.32073400	2.89196400
C	0.50302000	-0.82862800	0.81255300
C	-0.59411200	-0.09933400	0.33139200
H	0.89505700	-0.64824100	1.80778800
H	-1.19413200	0.62138000	-2.01009300
C	-0.92346000	1.12891100	0.98012900
O	-0.18072100	1.64814600	1.82955500
C	-2.24467800	1.79865700	0.69094800
C	-3.33160200	1.53807300	1.52994500
C	-2.38733000	2.70628200	-0.35836700
C	-4.55701400	2.15722200	1.30314000
H	-3.21293500	0.83577200	2.35182700
C	-3.61411900	3.33141200	-0.58248100
H	-1.53234400	2.93416600	-0.99075400
C	-4.70090800	3.05272100	0.24301400

H	-5.40056700	1.94023000	1.95147700
H	-3.71946000	4.03758600	-1.40016900
H	-5.65652800	3.53568900	0.06578300
P	2.41703200	-0.02209700	-0.25295100
C	2.33963300	-0.79182200	-1.90854600
H	2.68970100	-1.82418400	-1.83216600
H	1.29093000	-0.80636000	-2.22218400
H	2.93560700	-0.24341600	-2.64141000
C	4.12903500	-0.23208800	0.33703400
C	4.37172400	-0.08922000	1.70960400
C	5.18451200	-0.57560900	-0.51571600
C	5.65693100	-0.25809600	2.21731500
H	3.55282000	0.15112200	2.38363400
C	6.46570500	-0.75685700	-0.00200500
H	5.01136800	-0.69990000	-1.58016500
C	6.70377700	-0.59404200	1.36167600
H	5.83727500	-0.13874100	3.28048700
H	7.27988200	-1.02290500	-0.66816300
H	7.70390500	-0.73445900	1.75846500
C	2.18245500	1.75145600	-0.55963700
C	2.78834800	2.71544100	0.25632000
C	1.30111200	2.16209800	-1.56702000
C	2.51498200	4.06423200	0.06787000
H	3.47806200	2.41004200	1.03796700
C	1.03273100	3.51872100	-1.75361000
H	0.84759700	1.42867200	-2.22653500
C	1.63189400	4.46949300	-0.93409800
H	2.99395200	4.80342300	0.70173900
H	0.35974900	3.82867000	-2.54742300
H	1.42211100	5.52391100	-1.08064200

P3

C	-2.58894100	3.63971000	-0.89604000
C	-1.28922800	3.21306300	-1.18164300
C	-0.82019400	2.06810600	-0.54920300
C	-1.63052000	1.35538400	0.34438400
C	-2.91310000	1.78097300	0.63621600
C	-3.39006400	2.93481900	0.00150000
H	-2.97932800	4.53138200	-1.37567800
H	-0.66388000	3.76386500	-1.87739000
H	-3.54016200	1.23437000	1.33382000
H	-4.39597200	3.28470100	0.21006100
C	-0.85599500	0.16942500	0.91198600
O	-0.66196000	0.30275200	2.31408700

C	-1.58722600	-1.15883000	0.71878600
C	-1.39083800	-2.26510900	1.72367100
C	-2.67947300	-1.52070300	1.71384800
H	-0.68736400	-2.04612400	2.51605800
H	-1.36814500	-3.27223800	1.32732900
H	-3.56126300	-2.00570700	1.31310400
H	-2.84324900	-0.80358800	2.50940100
C	-1.81380700	-1.55555800	-0.69714700
O	-1.49564300	-0.89633700	-1.66309500
O	-2.43150100	-2.74286100	-0.80339300
C	-2.69122200	-3.17955600	-2.13975700
H	-3.18310400	-4.14536100	-2.04576600
H	-3.33975600	-2.46729600	-2.65314500
H	-1.75641600	-3.27842600	-2.69444100
C	0.48278600	1.39577600	-0.61911600
C	0.48408200	0.30431500	0.17003200
H	1.30482200	1.72720200	-1.24452900
H	-0.31928700	1.19121700	2.47759500
C	1.57583500	-0.68616900	0.27757300
O	1.33330400	-1.86332600	0.50499500
C	2.99088300	-0.24168400	0.06215600
C	3.90502300	-1.18626600	-0.41756600
C	3.43066500	1.04856600	0.37379400
C	5.23538400	-0.83727000	-0.61196200
H	3.55138000	-2.18806700	-0.63875600
C	4.76813700	1.39204500	0.19329100
H	2.73444600	1.77498300	0.77916200
C	5.66797800	0.45383200	-0.30659500
H	5.93741100	-1.56840200	-0.99904700
H	5.10693200	2.39109000	0.44651000
H	6.70835200	0.72535600	-0.45427800

R1a

C	-2.02587800	3.41286400	-0.14393400
C	-1.02342200	2.46227000	-0.30091600
C	-1.29740500	1.09333100	-0.19256600
C	-2.63015400	0.69059700	0.04309600
C	-3.63226100	1.65391000	0.18603600
C	-3.33471600	3.01019200	0.10734200
H	-1.78589700	4.46752100	-0.22893100
H	-0.01326500	2.78001800	-0.53864100
H	-4.65081900	1.34276600	0.39439800
H	-4.12059500	3.74653300	0.23492700
C	-2.97095600	-0.75677500	0.22316900

O	-2.15749000	-1.53560100	0.69838200
C	-4.32496700	-1.22085800	-0.17817700
C	-4.44081200	-2.68250400	-0.55572800
C	-4.98767600	-2.22794300	0.74515600
H	-3.51100300	-3.23933300	-0.54034100
H	-5.13070100	-2.91952600	-1.35630700
H	-6.06120800	-2.14612100	0.86450300
H	-4.42555300	-2.47742800	1.63816100
C	-0.21091700	0.11887000	-0.38512700
C	1.07029000	0.34133300	-0.05825900
H	-0.45647300	-0.84250000	-0.82721000
H	1.36884700	1.25512400	0.44387100
C	2.09099600	-0.70201100	-0.33149300
O	1.77032600	-1.80902100	-0.74165100
C	3.53349100	-0.38605800	-0.07905800
C	4.43266800	-1.45649300	-0.01332100
C	4.00917000	0.92098000	0.06693200
C	5.78356500	-1.22744500	0.21213300
H	4.04792300	-2.46306400	-0.13776300
C	5.36586500	1.15053200	0.28086600
H	3.33573900	1.76787000	-0.00731900
C	6.25168200	0.07880100	0.36013000
H	6.47353400	-2.06266300	0.27207300
H	5.73074400	2.16683900	0.38505200
H	7.30729900	0.26072500	0.53458000
H	-4.96263300	-0.52134400	-0.70259400

TS1a

C	5.73101900	-3.91062800	0.32208000
C	5.71375300	-2.53428900	0.51641600
C	4.54179900	-1.79023300	0.32520600
C	3.35101400	-2.46480100	-0.02115100
C	3.38068000	-3.84635300	-0.20951600
C	4.56062500	-4.56916800	-0.04850400
H	6.65183800	-4.46661200	0.46451500
H	6.62348400	-2.01575600	0.80711700
H	2.45975000	-4.36109200	-0.46918800
H	4.56210800	-5.64440300	-0.19613400
C	2.02830900	-1.73337600	-0.13616800
O	1.63772000	-1.34304300	-1.26926600
C	1.33092600	-1.51290800	1.05873300
C	-0.64110200	-1.74179300	0.61405300
C	0.16583200	-0.57401200	1.01717800
H	-0.98536600	-2.41793400	1.38758500

H	-0.44465900	-2.15645700	-0.36865100
H	0.27894800	0.19241800	0.24691100
H	-0.11855200	-0.14345700	1.97607100
C	4.59963800	-0.32864200	0.50122700
C	3.86706400	0.54213300	-0.20771700
H	5.29390500	0.05859100	1.24679400
H	3.21193900	0.17318500	-0.98479600
C	3.88719000	1.99211200	0.08386800
O	4.73269700	2.49646700	0.81070800
C	2.80219000	2.83775900	-0.51942100
C	2.86089500	4.22033800	-0.31121800
C	1.73962000	2.29829500	-1.25663600
C	1.88092000	5.05568300	-0.83198000
H	3.68870900	4.62047300	0.26484200
C	0.76313900	3.14040500	-1.78565800
H	1.65071200	1.22643800	-1.41640300
C	0.82974300	4.51590400	-1.57413300
H	1.93565700	6.12650400	-0.66580100
H	-0.04863500	2.71978900	-2.37212500
H	0.06662500	5.16696100	-1.98880500
P	-2.61219400	-0.79139400	-0.12093300
C	-2.04607800	-0.38702800	-1.81916800
H	-0.96734000	-0.19864500	-1.80403300
H	-2.22599100	-1.26457400	-2.44480800
H	-2.57663300	0.47147300	-2.23743100
C	-2.76603500	0.82363200	0.71058200
C	-3.59500800	0.94263300	1.83349300
C	-2.00587400	1.92520300	0.30362600
C	-3.66812100	2.14624400	2.52669000
H	-4.19293200	0.09493500	2.15820200
C	-2.07449500	3.12686700	1.00452800
H	-1.35227600	1.85483700	-0.56074900
C	-2.90702400	3.24013900	2.11480000
H	-4.31949700	2.22995000	3.39051400
H	-1.47620000	3.97168900	0.67670500
H	-2.96377700	4.17704000	2.65920000
C	-4.34441300	-1.34271700	-0.33631100
C	-5.34008500	-0.45788600	-0.77032300
C	-4.66854500	-2.67777700	-0.08249900
C	-6.64215400	-0.90980000	-0.95264100
H	-5.09715700	0.58466500	-0.95845100
C	-5.97504800	-3.12799500	-0.26705400
H	-3.90067200	-3.36422900	0.26376300
C	-6.95968300	-2.24543400	-0.70150500

H	-7.41034300	-0.22152000	-1.28985600
H	-6.22170200	-4.16526600	-0.06594000
H	-7.97723300	-2.59556900	-0.84168400
H	1.67071400	-1.92496300	1.99982500
R1b			
C	-0.25382000	3.76723300	0.44598900
C	-1.09649200	2.66316300	0.48929700
C	-0.68030100	1.41349300	0.01117400
C	0.63638200	1.28793800	-0.47760900
C	1.48056400	2.40147400	-0.50805500
C	1.03765300	3.64144700	-0.06183700
H	-0.60270900	4.72450500	0.81861400
H	-2.08670000	2.76132500	0.92251800
H	2.48535300	2.29373000	-0.90694200
H	1.69768300	4.50107700	-0.10159900
C	1.11847600	-0.00385900	-1.07063700
O	0.36217000	-0.68372600	-1.74205500
C	2.56025500	-0.38893100	-0.86401600
C	3.04323000	-1.51508500	-1.72738900
C	3.43332900	-0.11246200	-2.07492400
H	2.29793500	-2.00305500	-2.34363800
H	3.80972300	-2.15777800	-1.30979800
H	4.45406300	0.20167500	-1.88234300
H	2.95955800	0.35096800	-2.93429000
C	-1.59204900	0.26010300	0.07291700
C	-2.92903000	0.34514600	0.02263600
H	-1.15748200	-0.73155100	0.16616600
H	-3.42410400	1.29764800	-0.13125900
C	-3.75142400	-0.88779400	0.12018100
O	-3.23526800	-1.99668600	0.11098600
C	-5.23999500	-0.75381900	0.21276100
C	-6.01674100	-1.88590500	-0.05891800
C	-5.86887800	0.43931100	0.58210100
C	-7.40178900	-1.82256600	0.01890800
H	-5.51225600	-2.80606400	-0.33445600
C	-7.25701200	0.49805700	0.67324900
H	-5.28611300	1.32108200	0.82567400
C	-8.02379600	-0.62849100	0.38557500
H	-7.99840300	-2.70072500	-0.20494500
H	-7.73897500	1.42377700	0.96951300
H	-9.10601500	-0.57777800	0.44981800
C	3.09735300	-0.21931000	0.56273000
H	2.94409600	0.81302000	0.88968100

H	2.49434700	-0.85262700	1.22375300
C	4.55477800	-0.57297200	0.73012200
C	5.54682100	0.39219500	0.52935200
C	4.94404300	-1.86711600	1.08747100
C	6.89426200	0.07150900	0.67473300
H	5.25608100	1.40619800	0.26406200
C	6.29028600	-2.19247800	1.23514800
H	4.18148000	-2.62375100	1.25534500
C	7.26955100	-1.22313600	1.02780700
H	7.65059700	0.83407300	0.51825200
H	6.57377500	-3.20181800	1.51617300
H	8.31890500	-1.47351600	1.14566300

TS1b

C	6.15310500	-0.55101600	-1.14429700
C	5.54748900	0.55486900	-0.56056200
C	4.15155500	0.68488200	-0.53458900
C	3.35813800	-0.35300600	-1.06759900
C	3.97807300	-1.44774500	-1.66785600
C	5.36499000	-1.55254400	-1.70934000
H	7.23516300	-0.63206000	-1.15928400
H	6.15795700	1.34485500	-0.13078200
H	3.35789800	-2.24351100	-2.07065500
H	5.82998600	-2.42109700	-2.16512100
C	1.84738200	-0.31974900	-0.95534300
O	1.17567900	-0.04229400	-1.98543100
C	1.28489700	-0.53003000	0.31928000
C	-0.54258300	-1.41823800	-0.00005900
C	-0.13804900	-0.07545500	0.46431800
H	-0.52623300	-2.22860800	0.72075800
H	-0.32520000	-1.65864800	-1.03536600
H	-0.39278700	0.73921100	-0.21802100
H	-0.43945300	0.15220600	1.48733100
C	3.56710000	1.91109900	0.03231200
C	2.41908000	2.45551300	-0.40114500
H	4.11781800	2.41211000	0.82833100
H	1.90220600	1.99733500	-1.23292900
C	1.82762700	3.65433200	0.22904100
O	2.39557400	4.26126800	1.12761600
C	0.48156500	4.11162500	-0.26018800
C	-0.05271300	5.27877700	0.29839500
C	-0.24787800	3.42839400	-1.24214000
C	-1.28689200	5.76206400	-0.11785800
H	0.52151800	5.79595300	1.05978600

C	-1.48301800	3.91763800	-1.66237500
H	0.12337100	2.50825300	-1.68433600
C	-2.00433700	5.08248200	-1.10383900
H	-1.69007800	6.66968300	0.31918600
H	-2.03667000	3.38612300	-2.43065900
H	-2.96571700	5.46098900	-1.43633400
P	-2.78684400	-1.18068500	-0.39573500
C	-2.66643800	-0.40179300	-2.05242500
H	-1.73620800	0.17185900	-2.11605200
H	-2.61956500	-1.20591200	-2.79079900
H	-3.52603100	0.23713400	-2.26750300
C	-3.30742900	0.15572300	0.72416300
C	-3.81292700	-0.17087700	1.98942200
C	-3.09883400	1.49919600	0.39810300
C	-4.11228700	0.83255100	2.90475900
H	-3.98043800	-1.21177700	2.25485900
C	-3.38460700	2.50172300	1.32195100
H	-2.70184800	1.77543900	-0.57391500
C	-3.89344500	2.17020100	2.57486000
H	-4.51018200	0.57015900	3.87964200
H	-3.20346900	3.53930400	1.05607700
H	-4.11708800	2.95025800	3.29527300
C	-4.24580900	-2.28058800	-0.51359100
C	-5.55346900	-1.78829000	-0.41950400
C	-4.03521500	-3.64454400	-0.73701300
C	-6.63429200	-2.65419400	-0.55194200
H	-5.72466700	-0.73073200	-0.23919800
C	-5.12022000	-4.50750100	-0.87528800
H	-3.02197000	-4.03277000	-0.79940800
C	-6.41860400	-4.01292800	-0.78082200
H	-7.64573400	-2.26818700	-0.47741000
H	-4.95006000	-5.56492800	-1.04858600
H	-7.26373700	-4.68617300	-0.88143400
C	2.07275500	-0.89607200	1.55480500
H	1.35427900	-1.14602600	2.34749300
H	2.63076800	-0.02276700	1.93090100
C	3.04165200	-2.05375500	1.40803900
C	4.37790500	-1.91655500	1.78376100
C	2.61789300	-3.28263300	0.89206100
C	5.27480800	-2.97382400	1.64164700
H	4.72502500	-0.96007200	2.16716200
C	3.50654500	-4.34383500	0.75368800
H	1.58460400	-3.39524500	0.57449400
C	4.84255300	-4.19208000	1.12525900

H	6.31448600	-2.84042700	1.92587700
H	3.15845600	-5.29032300	0.35059000
H	5.53983400	-5.01601400	1.01002900

R1-1t

C	3.52965400	-1.63996500	0.33258000
C	2.23216300	-1.92917300	-0.07547500
C	1.31132200	-0.90822000	-0.33750700
C	1.72806200	0.43133800	-0.18923800
C	3.03900700	0.71062200	0.19999700
C	3.93736700	-0.31547000	0.46977500
H	4.22499000	-2.44908400	0.52960700
H	1.92866500	-2.96042500	-0.22630500
H	3.33778300	1.74867700	0.30051400
H	4.95039900	-0.08274200	0.77977400
C	0.84631200	1.62615400	-0.42403800
O	1.32702000	2.64080800	-0.89562000
C	-0.62435900	1.56448700	-0.12128800
C	-1.41878300	2.84346600	-0.33193500
C	-1.53000900	1.75997200	-1.33303000
H	-0.81811600	3.71045800	-0.57887700
H	-2.24749500	3.00022800	0.34814200
H	-2.42119800	1.14432100	-1.35833000
H	-1.00812000	1.88942000	-2.27527100
C	-1.06897200	0.70584700	1.01542900
O	-0.36613000	0.40461700	1.95409500
O	-2.35244800	0.34681000	0.90801800
C	-2.84605000	-0.47523200	1.96916400
H	-3.88761300	-0.67700900	1.72911000
H	-2.27396700	-1.40585200	2.01172900
H	-2.76212000	0.04317800	2.92570400
C	-0.04269300	-1.25546900	-0.79729400
C	-0.76452900	-2.29530100	-0.35434200
H	-0.51345800	-0.61286100	-1.53852900
H	-0.39541500	-2.97814900	0.40615400
C	-2.13808100	-2.50044000	-0.86435500
O	-2.68136600	-1.75775500	-1.65876500
H	-2.67340800	-3.38170300	-0.46590000

R1-1u

C	5.04734300	-4.04896400	0.72855400
C	5.26372000	-2.67566900	0.68105100
C	4.26506800	-1.79851900	0.24330200
C	3.01049600	-2.32333800	-0.11460500

C	2.80847400	-3.70226100	-0.08543400
C	3.81539400	-4.56612700	0.33863900
H	5.83801600	-4.71054500	1.06663100
H	6.22805800	-2.26935200	0.97346900
H	1.84220000	-4.09502000	-0.38757500
H	3.63531800	-5.63573800	0.36777700
C	1.84778900	-1.48590800	-0.59083100
O	1.43908300	-1.69193900	-1.74188100
C	1.19631800	-0.52734900	0.26973300
C	-0.74299700	-0.73026300	0.07397000
C	0.15067200	0.34208300	-0.38170700
H	-1.02605100	-0.77852900	1.11793400
H	-0.77820700	-1.64061900	-0.51234400
H	0.28118600	0.38733600	-1.46091300
H	0.01426000	1.31603700	0.08232500
C	1.53196200	-0.31709800	1.66685500
O	2.41116900	-0.85669400	2.31639500
O	0.69478100	0.59229200	2.24466200
C	0.92146900	0.83172500	3.63192800
H	0.16236600	1.55013800	3.93832900
H	0.82229600	-0.09304600	4.20387400
H	1.91994300	1.24330200	3.79278600
C	4.59366300	-0.36803200	0.16305600
C	4.12044500	0.49874400	-0.74031000
H	5.32955800	0.00327700	0.87520800
H	3.42540200	0.21737300	-1.52456800
C	4.56843000	1.90801000	-0.70978100
O	5.34663300	2.38512200	0.09113700
P	-2.97275800	-0.02727700	-0.57284500
C	-2.70800400	0.85495100	-2.16291800
H	-1.96424700	1.63640900	-1.99122300
H	-2.31621400	0.16590300	-2.91473600
H	-3.63199100	1.31308300	-2.52462400
C	-3.52435100	1.30998000	0.55092500
C	-2.66000500	1.76154200	1.55409300
C	-4.77911000	1.91410900	0.39936800
C	-3.04573200	2.80909100	2.39006900
H	-1.68311300	1.30328900	1.69171500
C	-5.16090700	2.95682100	1.23620800
H	-5.45984800	1.55981200	-0.37042600
C	-4.29314800	3.40581800	2.23210700
H	-2.37046300	3.15501600	3.16600900
H	-6.13464300	3.41955600	1.11250900
H	-4.59229100	4.21977100	2.88450500

C	-4.48413300	-1.01536200	-0.84725500
C	-5.22100700	-1.45364200	0.26202400
C	-4.87536600	-1.41711200	-2.12859000
C	-6.33517300	-2.26643700	0.08895900
H	-4.92740400	-1.14632600	1.26257600
C	-5.99024100	-2.23602900	-2.29737800
H	-4.31798800	-1.09227600	-3.00167400
C	-6.72189200	-2.66078600	-1.19200200
H	-6.90335500	-2.59184100	0.95436700
H	-6.28769300	-2.53749100	-3.29647200
H	-7.59100600	-3.29655300	-1.32601800
O	4.00425000	2.61629500	-1.69778600
C	4.38195500	4.00137400	-1.77052900
C	3.66489100	4.60200500	-2.95851900
H	5.46911200	4.06379300	-1.87242000
H	4.10414100	4.49104200	-0.83257100
H	3.92591900	5.65838700	-3.05146800
H	3.95221400	4.09084500	-3.88006200
H	2.58241700	4.52137400	-2.83635700

R1-1v

C	-2.85289300	1.90952700	2.75366300
C	-1.71778100	1.13733300	2.54202800
C	-1.72892700	0.05964500	1.64630200
C	-2.92585400	-0.23562000	0.96449500
C	-4.06899200	0.53252000	1.20359000
C	-4.03702600	1.60577100	2.08397800
H	-2.81676700	2.73998800	3.45086900
H	-0.80992600	1.34674900	3.09898100
H	-4.97891600	0.28172300	0.66852000
H	-4.92927600	2.19970000	2.25037000
C	-3.08925300	-1.33231500	-0.05210700
O	-4.15851500	-1.91500000	-0.11747300
C	-1.96784200	-1.74234100	-0.96711300
C	-1.57800600	-3.21120400	-0.81240400
C	-2.32744300	-2.79529900	-2.01424000
H	-2.11573700	-3.75079400	-0.04099500
H	-0.51483900	-3.40337500	-0.89859000
H	-1.78635000	-2.71613100	-2.94981600
H	-3.38190800	-3.03537100	-2.07324700
C	-0.85888000	-0.83157500	-1.41920600
O	0.22151700	-1.29753100	-1.73838000
C	-0.50912500	-0.74096400	1.45815700
C	0.72740100	-0.22660400	1.42707600

H	-0.61150000	-1.81065300	1.28671500
H	0.88445700	0.84022200	1.54343500
C	1.87853900	-1.12231600	1.13312300
O	1.75051000	-2.33740600	1.19031100
C	3.18485800	-0.51783500	0.73232100
C	4.26997300	-1.38168400	0.53419200
C	3.37132400	0.85366400	0.53038300
C	5.50543000	-0.88706600	0.14918300
H	4.11965700	-2.44422900	0.69246900
C	4.61356100	1.34353700	0.13777000
H	2.55884700	1.55848000	0.66967300
C	5.69697600	0.48553400	-0.05951000
H	6.33925400	-1.56887000	0.00555800
H	4.74298800	2.41091600	-0.01621100
C	7.03478600	1.01067400	-0.50686600
H	7.17779600	0.82991600	-1.57719400
H	7.11804100	2.08547600	-0.33455000
H	7.84973200	0.50823500	0.02000400
C	-1.11110500	0.63465600	-1.55163000
C	-0.01389800	1.49401500	-1.44670600
C	-2.38303700	1.15372300	-1.80364900
C	-0.19117700	2.86717700	-1.55846800
H	0.96722000	1.06323300	-1.26734500
C	-2.55642500	2.52854100	-1.93564400
H	-3.23519200	0.48824900	-1.91678200
C	-1.46454900	3.38395000	-1.80156100
H	0.65828900	3.53512100	-1.46024300
H	-3.54278600	2.93191100	-2.13860400
H	-1.60498100	4.45634000	-1.89161500

TS1-lt

C	-6.07469100	-2.46927800	-1.12081700
C	-6.01284500	-1.19816900	-0.56012900
C	-4.83324600	-0.71666700	0.02012700
C	-3.68392500	-1.52890700	-0.00744300
C	-3.75866400	-2.80829800	-0.55400800
C	-4.94356300	-3.28062700	-1.11442600
H	-7.00184100	-2.82412000	-1.55855800
H	-6.89635100	-0.56605400	-0.55436100
H	-2.86946400	-3.43139700	-0.55001300
H	-4.98037500	-4.27521200	-1.54680900
C	-2.35249300	-1.12175700	0.57592800
O	-1.92335500	-1.79213300	1.52488300
C	-1.59059700	-0.02519700	0.02966800

C	0.30482700	-0.53173500	-0.05543900
C	-0.38997900	0.41209400	0.82919400
H	0.51686200	-0.24591900	-1.07766700
H	0.22986700	-1.58771400	0.17699900
H	-0.45830100	0.08426300	1.86464900
H	-0.12761200	1.46162200	0.71983500
C	-1.96409600	0.71314600	-1.16375000
O	-2.95445900	0.56305500	-1.85860900
O	-1.02347700	1.64942100	-1.48048400
C	-1.28571300	2.39947700	-2.66456100
H	-0.45457600	3.09586300	-2.76607700
H	-1.33752500	1.74169800	-3.53466800
H	-2.22805000	2.94324600	-2.57429900
C	-4.87140400	0.61385400	0.63798100
C	-4.15499400	1.03550700	1.69279300
H	-5.59797600	1.31412200	0.22611600
H	-3.44847700	0.39536700	2.21287200
C	-4.33772900	2.40460700	2.21095900
O	-5.08869200	3.22834300	1.72280500
P	2.63741700	-0.36697200	0.57552400
C	2.58912700	-0.31972600	2.41170500
H	1.91514100	0.48660800	2.70956800
H	2.19191500	-1.26105800	2.79841100
H	3.57881100	-0.13513200	2.83667600
C	3.21630900	1.31249800	0.12548700
C	2.39547200	2.14712900	-0.63975900
C	4.47173900	1.77504700	0.54139900
C	2.82462400	3.42989000	-0.98046300
H	1.41867500	1.80731500	-0.97541000
C	4.89625400	3.05418000	0.20046400
H	5.12162900	1.12664500	1.12394800
C	4.07163300	3.88290300	-0.56181600
H	2.18373800	4.07137500	-1.57661100
H	5.86983600	3.40535900	0.52641300
H	4.40488300	4.88014300	-0.83036700
C	4.08150200	-1.41828200	0.18678500
C	4.71114400	-1.27009800	-1.05659500
C	4.52307100	-2.41603600	1.06208000
C	5.77227300	-2.09549000	-1.41006800
H	4.37671800	-0.49696900	-1.74365600
C	5.58576100	-3.24318300	0.70252500
H	4.04882900	-2.54934900	2.02967200
C	6.21244800	-3.08441900	-0.53050800
H	6.25747600	-1.96564200	-2.37198000

H	5.92657500	-4.00867900	1.39213400
H	7.04232500	-3.72678100	-0.80599500
H	-3.73759600	2.66072700	3.10367200
TS1-1u			
C	5.04734300	-4.04896400	0.72855400
C	5.26372000	-2.67566900	0.68105100
C	4.26506800	-1.79851900	0.24330200
C	3.01049600	-2.32333800	-0.11460500
C	2.80847400	-3.70226100	-0.08543400
C	3.81539400	-4.56612700	0.33863900
H	5.83801600	-4.71054500	1.06663100
H	6.22805800	-2.26935200	0.97346900
H	1.84220000	-4.09502000	-0.38757500
H	3.63531800	-5.63573800	0.36777700
C	1.84778900	-1.48590800	-0.59083100
O	1.43908300	-1.69193900	-1.74188100
C	1.19631800	-0.52734900	0.26973300
C	-0.74299700	-0.73026300	0.07397000
C	0.15067200	0.34208300	-0.38170700
H	-1.02605100	-0.77852900	1.11793400
H	-0.77820700	-1.64061900	-0.51234400
H	0.28118600	0.38733600	-1.46091300
H	0.01426000	1.31603700	0.08232500
C	1.53196200	-0.31709800	1.66685500
O	2.41116900	-0.85669400	2.31639500
O	0.69478100	0.59229200	2.24466200
C	0.92146900	0.83172500	3.63192800
H	0.16236600	1.55013800	3.93832900
H	0.82229600	-0.09304600	4.20387400
H	1.91994300	1.24330200	3.79278600
C	4.59366300	-0.36803200	0.16305600
C	4.12044500	0.49874400	-0.74031000
H	5.32955800	0.00327700	0.87520800
H	3.42540200	0.21737300	-1.52456800
C	4.56843000	1.90801000	-0.70978100
O	5.34663300	2.38512200	0.09113700
P	-2.97275800	-0.02727700	-0.57284500
C	-2.70800400	0.85495100	-2.16291800
H	-1.96424700	1.63640900	-1.99122300
H	-2.31621400	0.16590300	-2.91473600
H	-3.63199100	1.31308300	-2.52462400
C	-3.52435100	1.30998000	0.55092500
C	-2.66000500	1.76154200	1.55409300

C	-4.77911000	1.91410900	0.39936800
C	-3.04573200	2.80909100	2.39006900
H	-1.68311300	1.30328900	1.69171500
C	-5.16090700	2.95682100	1.23620800
H	-5.45984800	1.55981200	-0.37042600
C	-4.29314800	3.40581800	2.23210700
H	-2.37046300	3.15501600	3.16600900
H	-6.13464300	3.41955600	1.11250900
H	-4.59229100	4.21977100	2.88450500
C	-4.48413300	-1.01536200	-0.84725500
C	-5.22100700	-1.45364200	0.26202400
C	-4.87536600	-1.41711200	-2.12859000
C	-6.33517300	-2.26643700	0.08895900
H	-4.92740400	-1.14632600	1.26257600
C	-5.99024100	-2.23602900	-2.29737800
H	-4.31798800	-1.09227600	-3.00167400
C	-6.72189200	-2.66078600	-1.19200200
H	-6.90335500	-2.59184100	0.95436700
H	-6.28769300	-2.53749100	-3.29647200
H	-7.59100600	-3.29655300	-1.32601800
O	4.00425000	2.61629500	-1.69778600
C	4.38195500	4.00137400	-1.77052900
C	3.66489100	4.60200500	-2.95851900
H	5.46911200	4.06379300	-1.87242000
H	4.10414100	4.49104200	-0.83257100
H	3.92591900	5.65838700	-3.05146800
H	3.95221400	4.09084500	-3.88006200
H	2.58241700	4.52137400	-2.83635700

TS1-1v

C	5.39029200	-4.21150800	-1.20060600
C	5.47005700	-2.90874800	-0.71904000
C	4.35798800	-2.06081000	-0.73481400
C	3.12691400	-2.55605300	-1.20749300
C	3.06411400	-3.85622300	-1.70911300
C	4.18236100	-4.68636200	-1.70337100
H	6.26783000	-4.84936600	-1.18560200
H	6.41349600	-2.52828600	-0.33752000
H	2.11632700	-4.21951900	-2.09408800
H	4.10689200	-5.69914800	-2.08535300
C	1.83234700	-1.77221700	-1.26772700
O	1.27757200	-1.70694900	-2.37171700
C	1.23203400	-1.15487200	-0.09486300
C	-0.70349400	-1.58765400	-0.04654800

C	-0.01021300	-0.33623600	-0.36981700
H	-0.77480400	-1.91348400	0.98534700
H	-0.77859300	-2.34303700	-0.81996300
H	-0.09889300	-0.05965500	-1.41847600
H	-0.19502000	0.50396000	0.29310600
C	1.72328400	-1.33771000	1.26062100
O	2.60588700	-2.13454400	1.58339300
C	4.52069600	-0.67924300	-0.25890500
C	3.90081800	0.37698900	-0.79950200
H	5.18870700	-0.51420400	0.58528000
H	3.26791800	0.24878000	-1.67040400
C	4.01832500	1.72187000	-0.18476400
O	4.94485400	2.00198200	0.56331900
C	2.93308600	2.71447000	-0.45801700
C	3.04969400	3.99627000	0.09509300
C	1.78580200	2.39828500	-1.19297000
C	2.05097600	4.93770000	-0.09567300
H	3.93736500	4.23282000	0.67222000
C	0.78060100	3.34481000	-1.37277900
H	1.65613400	1.41235700	-1.62583400
C	0.90024300	4.62797000	-0.83477300
H	2.15740400	5.93181200	0.33028700
H	-0.10767100	3.08203800	-1.94171500
P	-2.97729100	-0.85465800	0.15659700
C	-2.92670100	-0.49331000	1.95764900
H	-3.02881300	-1.44104100	2.49234400
H	-1.95686800	-0.05607300	2.22288000
H	-3.73111300	0.18100500	2.26088600
C	-4.64937700	-1.55469600	-0.10229700
C	-4.77107400	-2.93360500	-0.29415100
C	-5.79824400	-0.75389200	-0.08109300
C	-6.02979300	-3.51072200	-0.45229300
H	-3.88056700	-3.55570700	-0.32251700
C	-7.05275400	-1.33254600	-0.24379600
H	-5.70908200	0.32038400	0.05782500
C	-7.16885600	-2.71042700	-0.42821200
H	-6.11835300	-4.58188000	-0.60068500
H	-7.94079700	-0.70919800	-0.22778500
H	-8.14880800	-3.15853700	-0.55685900
C	-3.06065800	0.79410700	-0.62282700
C	-3.38529000	0.87556800	-1.98419000
C	-2.74478600	1.96530300	0.07417500
C	-3.41378100	2.10710500	-2.62866200
H	-3.62884100	-0.02805400	-2.53755600

C	-2.77274500	3.19826900	-0.57522200
H	-2.48054800	1.92994300	1.12710500
C	-3.11154600	3.27265600	-1.92369600
H	-3.67554700	2.15862100	-3.68039400
H	-2.53484800	4.10088400	-0.02117500
H	-3.14447300	4.23430300	-2.42647600
C	1.06615200	-0.54112900	2.36748600
C	0.56669000	-1.23169900	3.47453100
C	1.00084300	0.85535300	2.34323900
C	-0.03241200	-0.53967900	4.52429700
H	0.64694000	-2.31476400	3.50080100
C	0.42055900	1.54942400	3.40225400
H	1.41283800	1.39923200	1.49566600
C	-0.10861900	0.85170200	4.48758300
H	-0.43622300	-1.08431400	5.37176400
H	0.38188700	2.63384000	3.37856500
H	-0.57379800	1.39179600	5.30588700
C	-0.17256800	5.66433300	-1.03702900
H	-0.65438800	5.91604800	-0.08665900
H	0.25147800	6.58882700	-1.43875600
H	-0.94008500	5.30852300	-1.72718700

M1-1t

C	5.90155000	-2.22399500	1.43894300
C	5.95805700	-1.10037700	0.62523600
C	4.81888400	-0.61564900	-0.03747800
C	3.58605200	-1.26300300	0.17354800
C	3.54082300	-2.39371100	0.98820900
C	4.68400700	-2.87844400	1.61682300
H	6.79812900	-2.58489200	1.93196100
H	6.90462600	-0.58540100	0.48299400
H	2.58474800	-2.88643100	1.14321300
H	4.62430300	-3.75749100	2.25104300
C	2.30139200	-0.84201900	-0.50786900
O	2.07174800	-1.38168000	-1.61920600
C	1.43757400	0.07784300	0.11309900
C	-0.98192700	-0.52928100	-0.11649000
C	0.15330300	0.39626900	-0.59963100
H	-1.07823300	-0.50061100	0.97438300
H	-0.76840400	-1.56450300	-0.40602500
H	0.30870600	0.22760500	-1.66914800
H	-0.13151400	1.44323000	-0.45353300
C	1.67895700	0.61728000	1.41644600
O	2.67504000	0.53357200	2.12777400

O	0.58162900	1.32378500	1.87734000
C	0.74415100	1.92175000	3.15585600
H	-0.19501900	2.43121600	3.37422900
H	0.94559100	1.16734600	3.92001600
H	1.56684900	2.64103200	3.15120200
C	5.00053300	0.56218600	-0.89140700
C	4.22959000	0.99952700	-1.90366400
H	5.90710500	1.13724000	-0.69773900
H	3.33865100	0.47401900	-2.22921800
C	4.62336500	2.20965000	-2.64497300
O	5.59222200	2.90053400	-2.38297500
P	-2.60735200	-0.13281700	-0.81164400
C	-2.45126800	0.03027700	-2.60719000
H	-1.83183800	0.90253900	-2.82426200
H	-1.97329100	-0.86156400	-3.01767200
H	-3.43768000	0.15762700	-3.05600500
C	-3.23009600	1.41516100	-0.13353200
C	-2.54878900	2.07277300	0.89546100
C	-4.42474400	1.93727000	-0.64613500
C	-3.07114900	3.25917700	1.40706500
H	-1.61511000	1.67801200	1.28878900
C	-4.93535000	3.12045300	-0.12712000
H	-4.96055600	1.42052000	-1.43779600
C	-4.25769500	3.78001100	0.89859500
H	-2.54731600	3.77659400	2.20345700
H	-5.86039600	3.52661500	-0.52095300
H	-4.65837300	4.70409300	1.30177100
C	-3.78803200	-1.44704000	-0.44236300
C	-4.68136300	-1.31285500	0.62498700
C	-3.76602100	-2.62143700	-1.20413000
C	-5.55420300	-2.35464800	0.92447600
H	-4.69988700	-0.40095500	1.21383500
C	-4.64293700	-3.65573800	-0.89770800
H	-3.07336800	-2.73594200	-2.03261500
C	-5.53616300	-3.52162300	0.16398800
H	-6.25087700	-2.25148400	1.74907000
H	-4.63053600	-4.56386400	-1.49008900
H	-6.22108800	-4.32981100	0.39786400
H	3.96893600	2.47898300	-3.49582300
M1-1u			
C	5.09868900	-3.95831200	0.34426300
C	5.32695000	-2.58834600	0.33938300
C	4.31501100	-1.67662800	0.00065300

C	3.02959000	-2.17014400	-0.29282400
C	2.81186300	-3.54727700	-0.29055000
C	3.83206700	-4.44095600	0.02139600
H	5.90050200	-4.64290900	0.60047700
H	6.31241300	-2.20521400	0.59178800
H	1.81636800	-3.91822100	-0.51956900
H	3.63685900	-5.50884600	0.02240900
C	1.87439600	-1.27794100	-0.69644100
O	1.76724100	-1.05241800	-1.92780300
C	0.99564500	-0.76968000	0.27810000
C	-1.44745500	-0.71396400	-0.30997800
C	-0.13833200	0.09429000	-0.19970400
H	-1.67534100	-1.22749200	0.63002600
H	-1.35896300	-1.47654300	-1.09200500
H	0.12619300	0.47430400	-1.19073500
H	-0.29024600	0.95043700	0.46629000
C	1.10455300	-1.09191500	1.66797900
O	1.97074600	-1.72592900	2.26193300
O	0.03584500	-0.58190400	2.38595100
C	0.07032800	-0.84264700	3.78217500
H	-0.83963000	-0.40595300	4.19547300
H	0.09233900	-1.91671900	3.98031300
H	0.94812300	-0.38564600	4.24581800
C	4.67687300	-0.25324800	0.00396200
C	4.07674100	0.76205600	-0.63402700
H	5.57314700	-0.00254500	0.57179300
H	3.21289800	0.63708400	-1.27608900
C	4.63809600	2.12215100	-0.49872800
O	5.60262600	2.43362800	0.17218700
P	-2.89477400	0.28808000	-0.74247200
C	-2.51020000	1.25779900	-2.22119100
H	-1.74993400	1.99762200	-1.96330900
H	-2.12041300	0.59949000	-3.00043600
H	-3.40857000	1.76106100	-2.58221000
C	-3.30847300	1.40776200	0.60535700
C	-2.68360200	1.27989100	1.84993600
C	-4.27931700	2.39512400	0.39342300
C	-3.03329400	2.14923600	2.88050900
H	-1.92025200	0.52400700	2.01578600
C	-4.62025700	3.25563100	1.42980500
H	-4.77181800	2.49020000	-0.57037800
C	-3.99637400	3.13251600	2.67146100
H	-2.54868600	2.05711300	3.84656700
H	-5.37128200	4.02116500	1.26964400

H	-4.26354000	3.80682800	3.47831000
C	-4.31590800	-0.77212200	-1.07943000
C	-5.29351900	-0.96515400	-0.09831300
C	-4.40254700	-1.43898400	-2.30738200
C	-6.35754900	-1.82629500	-0.34961600
H	-5.22691600	-0.44507300	0.85245700
C	-5.46995300	-2.29649200	-2.54871700
H	-3.64796300	-1.29583500	-3.07519800
C	-6.44552500	-2.48910100	-1.57136100
H	-7.11799500	-1.97551100	0.40890100
H	-5.54117600	-2.81145700	-3.50041600
H	-7.27762200	-3.15781800	-1.76494800
O	3.94143600	3.00892400	-1.22732500
C	4.40582600	4.36691900	-1.16958700
C	3.50150400	5.19082300	-2.05862200
H	5.44737400	4.39768400	-1.50239600
H	4.37751200	4.70510000	-0.12962200
H	3.82006700	6.23536500	-2.04329400
H	3.54254700	4.83053800	-3.08898600
H	2.46747700	5.13821700	-1.71050200

M1-1v

C	5.66776700	-3.97592400	-0.04309500
C	5.67887700	-2.58724100	-0.07837100
C	4.51665800	-1.84835200	-0.34800900
C	3.30518100	-2.54241800	-0.54308800
C	3.30874200	-3.93664000	-0.52260700
C	4.47382900	-4.65566100	-0.27254900
H	6.58259900	-4.52222100	0.16147200
H	6.60902600	-2.05217100	0.09476400
H	2.37299500	-4.46253300	-0.69105200
H	4.44810800	-5.74065200	-0.25110500
C	1.98855300	-1.87045900	-0.87518200
O	1.66499700	-1.88509400	-2.08398900
C	1.20129600	-1.25684300	0.13510600
C	-1.28697300	-1.47035400	-0.31384700
C	-0.04410300	-0.56390400	-0.35519200
H	-1.54771600	-1.75762400	0.71138200
H	-1.11675600	-2.38927800	-0.88606900
H	0.12937000	-0.25826900	-1.39351900
H	-0.26129600	0.33802600	0.22434500
C	1.50404800	-1.33985500	1.52512800
O	2.42240500	-1.98908600	2.05581500
C	4.65161500	-0.38503400	-0.38575100

C	3.83483100	0.49860000	-0.97807600
H	5.52779400	0.01841400	0.12290600
H	2.96301000	0.17882600	-1.53670900
C	4.08515600	1.95774200	-0.85236900
O	5.20308100	2.41665900	-0.66019500
P	-2.72460000	-0.65451700	-1.06144500
C	-2.35492000	-0.34160900	-2.80684200
H	-1.65943200	0.49706700	-2.87890900
H	-1.88728800	-1.22950000	-3.23758000
H	-3.27182700	-0.11143400	-3.35155000
C	-3.01699200	0.92322800	-0.24025100
C	-2.67803500	1.09788300	1.10773300
C	-3.58174600	1.97525800	-0.97139700
C	-2.91625800	2.32686800	1.71706000
H	-2.21737300	0.29620400	1.68392400
C	-3.80804600	3.20075600	-0.35337700
H	-3.84218600	1.84688800	-2.01750400
C	-3.47608600	3.37446600	0.98900100
H	-2.65317800	2.46359900	2.75966600
H	-4.24049900	4.01804900	-0.92029600
H	-3.65087700	4.33197800	1.46853900
C	-4.18512400	-1.70582200	-0.95074100
C	-5.13259500	-1.50080400	0.05655500
C	-4.32864400	-2.76201800	-1.85830100
C	-6.22448600	-2.35869900	0.15320500
H	-5.02203200	-0.67676700	0.75515600
C	-5.42382900	-3.61154100	-1.75389300
H	-3.59663300	-2.92695100	-2.64353700
C	-6.36931200	-3.40981000	-0.74942200
H	-6.96381400	-2.20204200	0.93084000
H	-5.53962500	-4.42777200	-2.45819000
H	-7.22386100	-4.07370700	-0.67259700
C	2.89257400	2.85582000	-0.93675400
C	3.05883300	4.22600700	-1.16072600
C	1.60638000	2.35185700	-0.73379100
C	1.95231000	5.06294700	-1.20113500
H	4.06091600	4.61865700	-1.30191100
C	0.50088400	3.19642400	-0.75566700
H	1.48005400	1.29646900	-0.52101900
C	0.65716900	4.56296500	-1.00123400
H	2.08655600	6.12564200	-1.38469800
H	-0.49495300	2.79000200	-0.57856700
C	-0.53556600	5.47950700	-1.06610300
H	-0.32705100	6.43373500	-0.57588200

H	-0.79727500	5.69697600	-2.10685200
H	-1.40729000	5.02454000	-0.59000000
C	0.59946200	-0.56680500	2.47184700
C	-0.28876100	-1.25476700	3.30183200
C	0.69582800	0.82335000	2.58081800
C	-1.08333200	-0.56281400	4.21560300
H	-0.35506200	-2.33741100	3.23018000
C	-0.08097700	1.51408600	3.50738500
H	1.38658600	1.36330100	1.93662700
C	-0.97597100	0.82267800	4.32402100
H	-1.77751400	-1.10609700	4.84920800
H	0.00743600	2.59344500	3.58915800
H	-1.58520200	1.36213300	5.04284700

TS2-1t

C	5.63307300	1.79603900	-1.54003900
C	4.86515200	1.74999300	-0.37616100
C	3.71201300	0.96732000	-0.33873300
C	3.34374200	0.23999100	-1.47554900
C	4.09024300	0.30857900	-2.64729900
C	5.24889600	1.08021000	-2.67491900
H	6.53124200	2.40515900	-1.56485000
H	5.15393700	2.33145700	0.49441000
H	3.76359800	-0.24798000	-3.52078800
H	5.85003600	1.13003400	-3.57699900
C	2.06321900	-0.51976600	-1.33011800
O	1.27450100	-0.63045600	-2.27514300
C	1.78792900	-0.90622700	0.04373600
C	0.35675800	-0.98589800	0.52085900
C	-0.51502500	0.13786900	-0.05851100
H	0.37636400	-0.88046200	1.60943500
H	-0.09834500	-1.96414300	0.30370100
H	-0.52729500	0.13803200	-1.15169100
H	-0.14410100	1.11721900	0.25951500
C	2.75998900	-1.75151400	0.70204400
O	3.91006700	-1.98924700	0.35220500
O	2.27257600	-2.27131700	1.86616000
C	3.18536000	-3.08843400	2.59099300
H	2.65361500	-3.41033800	3.48545900
H	3.48663300	-3.95567900	1.99896900
H	4.07905400	-2.52392900	2.86574500
C	2.80336600	0.93084400	0.85417800
C	1.95431400	1.99554800	1.11236600
H	3.12885400	0.36430400	1.72652800

H	1.79040400	2.76318300	0.36126600
C	1.19393500	2.06012300	2.31964400
O	1.11434600	1.17667300	3.18454100
P	-2.21566100	0.01912700	0.52715400
C	-2.18909400	-0.14373100	2.33087600
H	-1.92416000	-1.17206800	2.58431300
H	-1.42517800	0.52677300	2.73882500
H	-3.16764500	0.09832000	2.74833100
C	-3.00340200	-1.41718700	-0.22126000
C	-2.40817300	-2.04827700	-1.31917000
C	-4.22574800	-1.87511000	0.28500800
C	-3.04221700	-3.13903700	-1.90733500
H	-1.45427100	-1.70623200	-1.71194600
C	-4.84914100	-2.96632900	-0.30951800
H	-4.69209200	-1.38272200	1.13378500
C	-4.25774700	-3.59570200	-1.40435200
H	-2.58213600	-3.63183900	-2.75653300
H	-5.79500700	-3.32493500	0.08103700
H	-4.74704400	-4.44673800	-1.86612600
C	-3.13529700	1.50236900	0.07419000
C	-3.98071600	1.49187000	-1.03880800
C	-2.95914800	2.67166000	0.82303700
C	-4.65022200	2.65694700	-1.40124700
H	-4.11843100	0.58171900	-1.61467400
C	-3.63351800	3.82992300	0.45316500
H	-2.30463600	2.68310300	1.69012200
C	-4.47781700	3.82099900	-0.65665500
H	-5.30787400	2.65243400	-2.26339400
H	-3.50250500	4.73746900	1.03217500
H	-5.00482800	4.72595600	-0.94008100
H	0.62045500	3.00135100	2.46150600

TS2-1u

C	5.40705600	1.04718000	-2.40566000
C	4.65478100	1.34997700	-1.27089500
C	3.62152400	0.49888300	-0.87781200
C	3.35896500	-0.64354700	-1.63795000
C	4.08904100	-0.93530100	-2.78650800
C	5.12814800	-0.09172300	-3.16459900
H	6.21146800	1.71078300	-2.70742000
H	4.86228500	2.24990400	-0.69956200
H	3.83810000	-1.81862000	-3.36604700
H	5.71659900	-0.31150000	-4.04939000
C	2.18554400	-1.43254800	-1.16463800

O	1.46476700	-2.05039100	-1.94975200
C	1.90100100	-1.22061600	0.25634700
C	0.46088300	-1.15588200	0.70621400
C	-0.41962100	-0.46846100	-0.34623900
H	0.43904200	-0.56042900	1.62699300
H	0.05011400	-2.14281900	0.96265700
H	-0.43502700	-1.00980400	-1.29589800
H	-0.03344100	0.53392100	-0.55544600
C	2.88484500	-1.72048500	1.18903600
O	4.05576900	-1.99846200	0.95719700
O	2.38725500	-1.80263900	2.45560600
C	3.32234700	-2.21919800	3.44535200
H	2.77737700	-2.22734000	4.38830800
H	3.70640600	-3.21743400	3.22280900
H	4.16361900	-1.52452400	3.50121500
C	2.75166500	0.78295400	0.31418400
C	1.79864200	1.79147100	0.28290800
H	3.21162900	0.62303900	1.28979900
H	1.41583200	2.18280600	-0.65383900
C	1.19260500	2.23421900	1.50309700
O	1.50451300	1.93191500	2.65105100
P	-2.12541600	-0.23557100	0.18449300
C	-2.13481000	0.46666400	1.85049300
H	-1.76962700	-0.27173100	2.56637400
H	-1.47123900	1.33718900	1.84489200
H	-3.14581300	0.77937700	2.11760400
C	-3.00049100	-1.80640000	0.16836400
C	-2.42646100	-2.92350200	-0.44878800
C	-4.26250200	-1.89763400	0.76924900
C	-3.12127200	-4.12947000	-0.46396600
H	-1.44463800	-2.86530800	-0.90993100
C	-4.94941800	-3.10565000	0.74336900
H	-4.71179100	-1.03267700	1.24924500
C	-4.37843200	-4.21904100	0.12781600
H	-2.67712700	-4.99752300	-0.93818600
H	-5.92799200	-3.17908600	1.20463100
H	-4.91673600	-5.16080600	0.11188900
C	-2.91538100	0.94866000	-0.92173700
C	-4.01739200	0.59484400	-1.70269900
C	-2.38313100	2.24434600	-0.97847500
C	-4.59194100	1.54486800	-2.54371200
H	-4.42492800	-0.41018400	-1.65614400
C	-2.96795800	3.18429300	-1.81923500
H	-1.52099700	2.52384300	-0.37358100

C	-4.06979200	2.83418200	-2.60018500
H	-5.44779500	1.27493000	-3.15242500
H	-2.56225000	4.18923800	-1.86600100
H	-4.52085700	3.57101000	-3.25648600
O	0.13773700	3.09009900	1.27251500
C	-0.41534900	3.72512200	2.43028700
C	-1.65137100	4.47925200	1.98788900
H	0.33428100	4.39700500	2.86176500
H	-0.65082100	2.97013000	3.18712100
H	-2.08444000	5.01686700	2.83441000
H	-1.40332300	5.20177200	1.20629600
H	-2.40735800	3.79261700	1.59496600

TS2-1v

C	-4.26159400	-1.89655300	-4.00078600
C	-3.69304100	-2.19285500	-2.76251500
C	-3.06644700	-1.18490800	-2.03030100
C	-3.01878900	0.10739700	-2.55833500
C	-3.56131100	0.40277800	-3.80567800
C	-4.19787300	-0.60373200	-4.52514100
H	-4.75080100	-2.68333400	-4.56658700
H	-3.72579500	-3.20541600	-2.37147900
H	-3.48455500	1.41371200	-4.19472200
H	-4.63886200	-0.38971400	-5.49321300
C	-2.27256100	1.07993700	-1.71293100
O	-1.66911800	2.03352200	-2.20498900
C	-2.19176000	0.68212900	-0.29571600
C	-0.87794700	0.96935800	0.40563000
C	0.35946500	0.66440400	-0.46049600
H	-0.83062500	0.35030400	1.30721000
H	-0.82380600	2.01973400	0.72657000
H	0.29144700	1.10665500	-1.45880600
H	0.50642700	-0.41073000	-0.59049700
C	-3.44480800	0.67598000	0.43047200
O	-4.55142700	0.64471700	-0.12918500
C	-2.39634900	-1.44872800	-0.71570800
C	-1.18029000	-2.12136000	-0.66294100
H	-3.05066800	-1.61891700	0.13822000
H	-0.56490200	-2.18224600	-1.55413000
C	-0.64703200	-2.49566200	0.61022700
O	-1.24217800	-2.30943300	1.68803900
C	0.74764100	-3.07253500	0.65802700
C	1.43830300	-3.01159900	1.87508900
C	1.38961500	-3.64756700	-0.44226900

C	2.74266000	-3.47795100	1.98023400
H	0.92351300	-2.58716000	2.73172500
C	2.69114800	-4.13304600	-0.32814400
H	0.87237400	-3.73993700	-1.39196800
C	3.39314100	-4.04513100	0.87660600
H	3.26811800	-3.40649700	2.92935900
H	3.17127500	-4.58557100	-1.19202100
P	1.87581900	1.29718500	0.28828100
C	1.94631300	0.76518800	2.01525200
H	1.12651500	1.22915200	2.56734000
H	1.84629700	-0.32340200	2.05672500
H	2.90110100	1.05870900	2.45453300
C	1.89533600	3.09505200	0.21104300
C	0.95194900	3.78183300	-0.56196400
C	2.87936900	3.79366200	0.92220700
C	1.00266300	5.17264200	-0.61738500
H	0.17261800	3.25073000	-1.10525900
C	2.92045200	5.18108900	0.85553100
H	3.61609800	3.26221700	1.51832100
C	1.98222400	5.86843300	0.08627100
H	0.27177400	5.71119400	-1.21045900
H	3.68304300	5.72399000	1.40273400
H	2.01540600	6.95173000	0.03727600
C	3.30550100	0.62447200	-0.57914800
C	4.10975200	1.43979900	-1.38006100
C	3.57720100	-0.74419800	-0.45390000
C	5.19317900	0.88224000	-2.05381800
H	3.89549700	2.49961300	-1.47632100
C	4.66037000	-1.28949700	-1.13336000
H	2.95471000	-1.38777000	0.16472300
C	5.46778000	-0.47715500	-1.92939200
H	5.82101800	1.51169800	-2.67472000
H	4.87101700	-2.35009100	-1.04052800
H	6.31354000	-0.90820700	-2.45485400
C	4.81339400	-4.53401400	0.99416000
H	5.49044500	-3.70556600	1.22671100
H	4.91090100	-5.26764800	1.79952500
H	5.15140900	-4.99861300	0.06519800
C	-3.45084700	0.55176800	1.93826900
C	-4.28958400	-0.42631100	2.48457500
C	-2.75048600	1.39790600	2.80173000
C	-4.38535800	-0.59240200	3.86140900
H	-4.86701400	-1.05307800	1.81182600
C	-2.86642500	1.25040600	4.18302900

H	-2.13050600	2.19499500	2.40546000
C	-3.67160900	0.24720100	4.71578300
H	-5.02515100	-1.36832500	4.26994000
H	-2.32629000	1.92274600	4.84220700
H	-3.75113600	0.12600300	5.79148500