

Supporting Information

Supporting Information for

The roles of benzoic acid and water on the Michael reactions of pentanal and nitrostyrene catalyzed by diarylprolinol silyl ether

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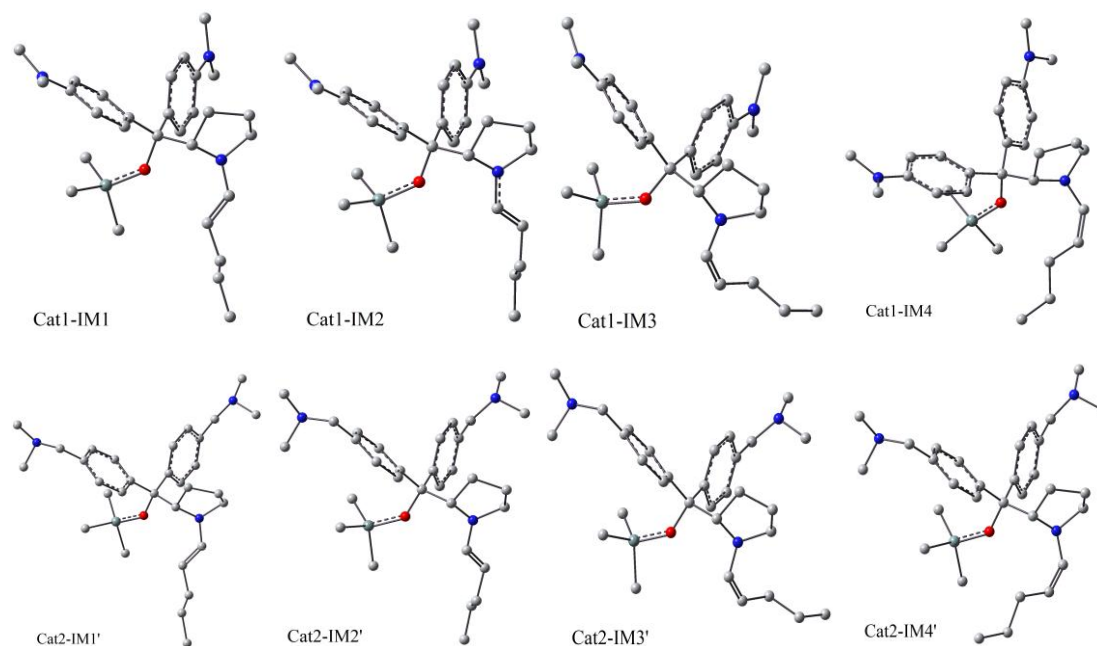
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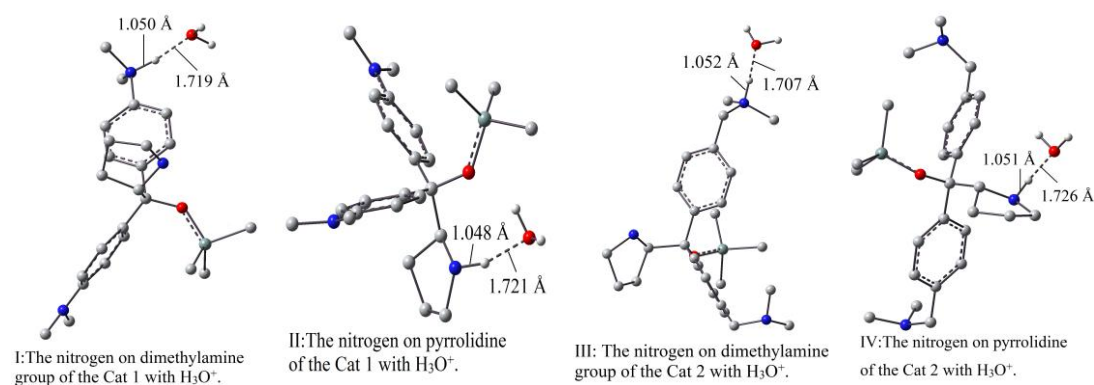
S1.The optimized structures of intermediates for the Michael reactions of pentanal and catalysts at the B3LYP/6-31G(d,p) level of theory -----	2
S2.The optimized complex structures and the key bond lengths of catalysts and a hydronium at the CPCM(water)/B3LYP/6-31G(d,p) level of theory-----	2
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S1.The optimized structures of intermediates for the Michael reactions of pentanal and catalysts at the B3LYP/6-31G(d,p) level of theory



S2.The optimized complex structures and the key bond lengths of catalysts and a hydronium at the CPCM_(water)/B3LYP/6-31G(d,p)level of theory

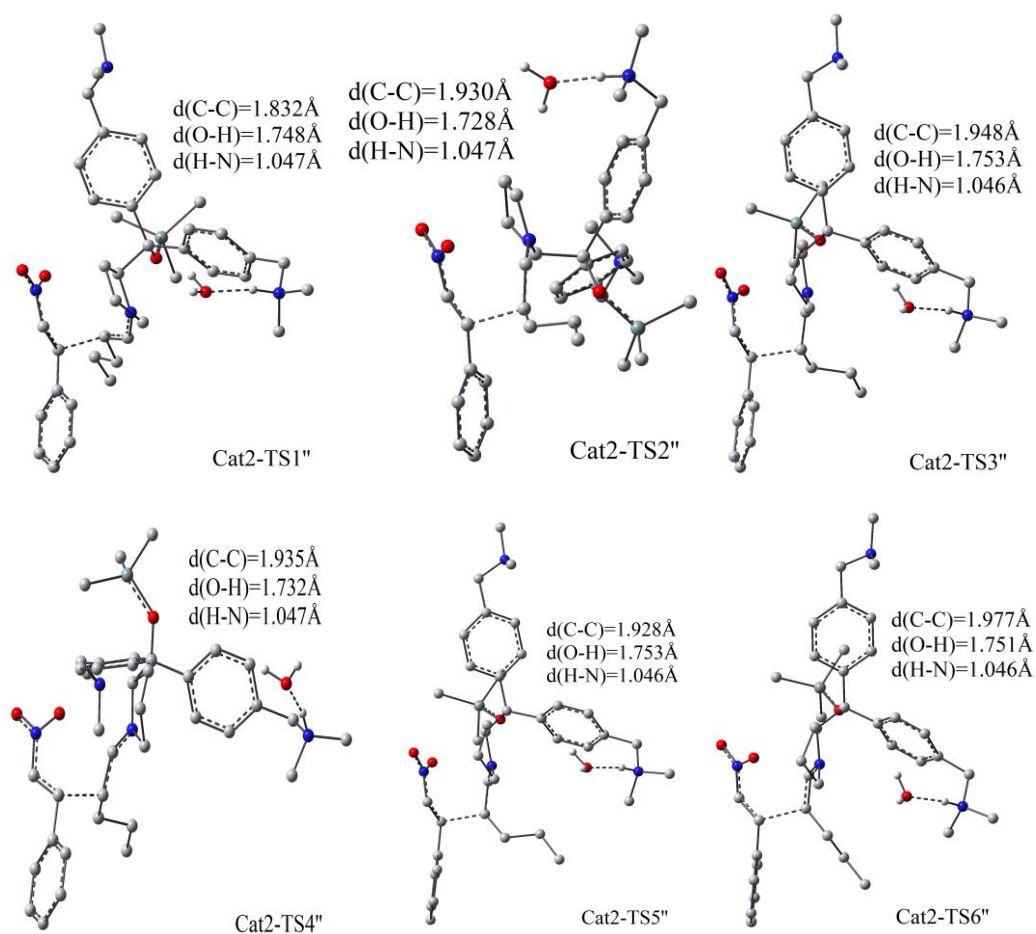


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S3. The corresponding complexation energies (ΔE , in kcal/mol) of the formed various complexes in gas-phase at the B3LYP/6-31G(d,p) level and solvent-phase at the CPCM_(water)/B3LYP/6-31G(d,p)

		Benzoic Acid		H ₃ O ⁺		Nitrostyrene	
		Gas phase	Solvent phase	Gas phase	Solvent phase	Gas phase	Solvent phase
Nitrostyrene		-8.07	-7.17	-61.65	-22.10		
Cat1	N of N(CH ₃) ₂	-10.69	-8.97	-84.63	-43.08		
	N of pyrrolidine	-18.32	-15.98	-102.55	-54.68	-3.97	-4.50
Cat2	N of N(CH ₃) ₂	-13.70	-11.33	-83.26	-48.57		
	N of pyrrolidine	-14.19	-13.12	-90.10	-49.16	-5.57	-4.61

S4. The optimized structures of transition states for the Michael reactions of pentanal and nitrostyrene catalyzed by Cat 2 with a hydronium at the B3LYP/6-31G(d,p) level of theory



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S5.Cartesian Coordinates of enamine intermediates

Cat1-IM1

N	-2.10357600	-0.79378900	-1.36150400
C	-2.82522800	-1.92138200	-0.97540700
C	-2.43564800	-2.95563900	-0.20972700
C	-0.63325000	-0.80995200	-1.41518500
C	-0.27129000	-0.22743400	-2.81367600
C	-1.60065500	-0.17170800	-3.58591000
C	-2.62317200	0.02604300	-2.46106100
C	0.04791300	-0.05182900	-0.20628000
C	1.58051800	-0.03609800	-0.35589400
C	-0.58252200	1.34272600	-0.06987800
O	-0.30292100	-0.84789700	0.93950800
Si	0.28736700	-1.00532800	2.50569900
C	1.88216800	-2.01466300	2.56041500
C	0.55398500	0.64195500	3.39409700
C	-1.08023000	-1.96064600	3.38347100
C	2.37691100	0.95659700	0.23426000
C	3.76778900	0.91898900	0.20020700
C	4.45512900	-0.14165100	-0.42927200
C	3.66006800	-1.14463300	-1.02684000
C	2.27157800	-1.08900200	-0.97571900
C	-1.75731600	1.50330300	0.67817400
C	-2.42184300	2.72203700	0.76083000
C	-1.95116600	3.86241500	0.07209000
C	-0.76917900	3.70558300	-0.68155200
C	-0.11688100	2.47583300	-0.75102000
H	-3.84691400	-1.91107900	-1.35442600
H	-1.44431200	-2.95788700	0.23197000
H	-0.32027200	-1.85619600	-1.33829400
H	0.48328000	-0.83673300	-3.31653000
H	0.14466800	0.77773900	-2.71496600
H	-1.62199700	0.62524000	-4.33592400
H	-1.79257200	-1.12286400	-4.09573500
H	-3.63594500	-0.28929800	-2.72656000
H	-2.66786300	1.08074700	-2.16071000
H	1.75478800	-2.97678100	2.05296100
H	2.71881000	-1.49441200	2.08597600
H	2.15960900	-2.22268300	3.60104800
H	0.75886800	0.45213800	4.45486700
H	-0.33088300	1.28218900	3.33150700
H	1.40276700	1.20096300	2.99066000
H	-0.80913300	-2.16862500	4.42500500
H	-2.01874900	-1.39696300	3.38623700

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H	-1.27485200	-2.91722600	2.88853600
H	1.90395300	1.79392200	0.73447700
H	4.12323300	-1.98250900	-1.53319900
H	1.72514000	-1.90589600	-1.43323200
H	-2.16369500	0.64605700	1.20014900
H	-3.31875400	2.77858800	1.36545400
H	-0.34285900	4.54402600	-1.21839500
H	0.79195100	2.41839300	-1.34083300
C	-3.33061400	-4.12626400	0.09649800
H	-4.33717800	-3.94188400	-0.30465300
H	-3.45539100	-4.23486000	1.18608800
C	-2.80932100	-5.46595300	-0.45892200
H	-1.79159200	-5.63741300	-0.08284600
H	-2.71862100	-5.38508500	-1.54973400
C	-3.69770800	-6.65896300	-0.09435800
H	-3.30161800	-7.59595300	-0.50020900
H	-3.77800600	-6.77559400	0.99273000
H	-4.71378200	-6.53132600	-0.48580800
H	4.31596600	1.72741500	0.66818000
N	5.84257700	-0.20245500	-0.44931300
N	-2.62907500	5.07849300	0.12521600
C	-3.68016200	5.25759100	1.11224200
H	-3.32334200	5.15049300	2.14916800
H	-4.10858000	6.25504000	0.99991000
H	-4.48948300	4.53560100	0.95904100
C	-1.98048800	6.27009900	-0.39280100
H	-1.74953900	6.15826100	-1.45779600
H	-2.66031700	7.11826100	-0.29479100
H	-1.04340100	6.51727100	0.13197500
C	6.50052700	-1.18985400	-1.28725700
H	6.27444000	-1.06543900	-2.35800700
H	7.58051900	-1.10763800	-1.15562700
H	6.21178700	-2.20661600	-0.99819200
C	6.61187600	0.94745900	-0.00716100
H	6.38864600	1.19197800	1.03744800
H	7.67515300	0.71030600	-0.06708600
H	6.42608000	1.84860600	-0.61268800
Cat1-IM2			
N	1.62552200	-0.77970500	1.92272100
C	2.39991800	-1.77184900	1.35453300
C	3.74476600	-1.86626200	1.36178100
C	0.16691800	-0.76188700	1.82201800
C	-0.28366300	0.11235200	3.01809700

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C	0.94316300	0.19752700	3.94147200
C	2.12462400	0.10518300	2.96732100
C	-0.36363500	-0.26262800	0.41433900
C	-1.90188900	-0.22957800	0.37337600
C	0.29640700	1.08135100	0.07252800
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Si	-0.28392600	-1.78893800	-2.04268000
C	-1.91141400	-2.74411900	-2.09056200
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C	-2.59802100	0.58861100	-0.52938500
C	-3.98347300	0.55725400	-0.65411100
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C	-2.68814100	-1.10327600	1.13991700
C	1.56186000	1.10734600	-0.53023300
C	2.23913100	2.29634800	-0.77875100
C	1.68752000	3.54491000	-0.41514100
C	0.41413700	3.52356100	0.19155400
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H	-1.16124000	-0.30537800	3.51664200
H	-0.55487500	1.11251500	2.67253900
H	0.95492700	1.10966800	4.54588700
H	0.96826300	-0.65871200	4.62490100
H	3.01629000	-0.33439300	3.42651900
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H	-0.41753300	-0.80157300	-4.31731200
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H	1.00079600	-3.39074200	-3.46815000
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H	-0.07422800	4.44625200	0.47972200

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H	-1.22810500	2.36849100	0.89718400
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H	4.81107700	-2.16629100	-1.19998700
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H	-4.45113300	1.22747300	-1.36482400
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C	1.66552800	5.99627200	-0.47609000
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H	0.81145700	6.10238700	-1.16451800
H	1.28842900	6.10908000	0.54629200
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H	4.32683200	4.07112900	-1.06727700
H	3.34567000	4.40065000	-2.51048400
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C	-6.83127300	0.64050200	-0.78720700
H	-6.48619400	0.63324300	-1.82712700
H	-7.90095700	0.42590400	-0.79706100
H	-6.68832700	1.65803000	-0.39041400
Cat1-IM3			
N	-1.64911800	-1.56280500	-1.06443100
C	-2.10112700	-2.52483400	-0.17291000
C	-3.35158400	-2.75428700	0.27770400
C	-0.21375200	-1.34832400	-1.26384900
C	-0.10424900	-0.77820200	-2.69679800
C	-1.42365700	-1.17476500	-3.37502200
C	-2.43010500	-1.11792500	-2.21905000
C	0.43985500	-0.44760400	-0.13768400
C	1.93931200	-0.21622600	-0.39628700
C	-0.37015700	0.84866000	0.00497300
O	0.27843400	-1.24702400	1.04719000
Si	1.01327400	-1.35784400	2.55221000

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C	2.74368100	-2.10563400	2.44937500
C	1.08922500	0.29060000	3.47346400
C	-0.11618500	-2.54408100	3.48505100
C	2.61625100	0.88810400	0.14366800
C	3.99029400	1.06203100	0.01179900
C	4.78402800	0.11606000	-0.67342900
C	4.10973900	-0.99752100	-1.22113600
C	2.73564600	-1.15385600	-1.07116500
C	-1.50066800	0.88333900	0.83300700
C	-2.31660100	2.00616800	0.92468400
C	-2.05481800	3.16736300	0.16409800
C	-0.91686700	3.13734800	-0.66899200
C	-0.11025400	2.00384400	-0.74550000
H	-1.29883600	-3.15493900	0.20491200
H	-3.45721400	-3.62286500	0.92523300
H	0.29329100	-2.32024900	-1.18985200
H	0.77653800	-1.15712400	-3.21987500
H	-0.02044100	0.31097200	-2.66419800
H	-1.68917700	-0.51653900	-4.20811200
H	-1.36501500	-2.19956600	-3.75963200
H	-3.28199900	-1.78643700	-2.36812200
H	-2.81695800	-0.09721300	-2.08447400
H	2.72613200	-3.06326200	1.91827500
H	3.44947100	-1.45016300	1.93195700
H	3.13263800	-2.29324600	3.45774900
H	1.41531800	0.11947700	4.50657100
H	0.11044000	0.77895500	3.50641400
H	1.79645900	0.98890500	3.01680600
H	0.24011700	-2.70623500	4.50883200
H	-1.13957800	-2.15972400	3.53977800
H	-0.15787200	-3.51899400	2.98818000
H	2.05616300	1.64608500	0.67942600
H	4.65745500	-1.75618800	-1.76635900
H	2.28922100	-2.04554800	-1.49634500
H	-1.75109900	0.00531900	1.41555300
H	-3.16821300	1.96878800	1.59290000
H	-0.64590400	4.00143200	-1.26305900
H	0.75554200	2.04164500	-1.39861700
C	-4.61211100	-1.96182000	0.04757100
H	-4.38921400	-1.00246100	-0.43184200
H	-5.04721100	-1.70699600	1.02704200
C	-5.69328300	-2.70354000	-0.76307000
H	-5.89326400	-3.67334200	-0.28801200
H	-5.30061700	-2.93666200	-1.76161000

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C	-6.99966900	-1.91415500	-0.89054200
H	-7.74940800	-2.46531000	-1.46812300
H	-7.43064400	-1.70042400	0.09455000
H	-6.83500200	-0.95310000	-1.39159100
H	4.44104500	1.94574800	0.44635800
N	6.15957200	0.26715400	-0.79284300
N	-2.88770000	4.28275100	0.22396600
C	-2.44962100	5.52345100	-0.39003600
H	-3.23472200	6.27354500	-0.28004600
H	-1.52442400	5.92581700	0.05393100
H	-2.27540600	5.38809200	-1.46308400
C	-3.87974800	4.36618700	1.28216500
H	-4.44625100	5.29200700	1.16805200
H	-4.59261900	3.53698200	1.21813100
H	-3.43790700	4.35469200	2.29145500
C	6.77350800	1.52575600	-0.40663800
H	7.85318800	1.45431100	-0.54648600
H	6.40676000	2.38184900	-0.99461500
H	6.59388900	1.74300800	0.65227200
C	6.89851000	-0.61467900	-1.67961600
H	6.57960200	-0.53452400	-2.73082700
H	7.95987000	-0.36766000	-1.62599000
H	6.78972400	-1.66131100	-1.37382700
Cat1-IM4			
N	1.11113800	2.11942000	-1.46470600
C	0.83803200	3.47818600	-1.29850000
C	-0.26378600	4.18899700	-0.98288100
C	0.07139200	1.07969100	-1.52559100
C	0.32972100	0.31132100	-2.85729100
C	1.42752700	1.11279900	-3.58034300
C	2.17902700	1.76754300	-2.41500800
C	0.06036800	0.15786700	-0.23870400
C	-1.02893100	-0.92647300	-0.34914700
C	1.47044800	-0.40233400	0.00577900
O	-0.27713400	1.06420200	0.82502300
Si	-0.84787100	0.89618700	2.39763600
C	-2.70721800	0.57000600	2.42192600
C	0.03365100	-0.43763500	3.40653900
C	-0.49094900	2.57896600	3.16768500
C	-0.94550500	-2.13777200	0.35414700
C	-1.96792100	-3.08182200	0.34418900
C	-3.16074000	-2.85952300	-0.37805000
C	-3.25185600	-1.64310800	-1.08987300

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C	-2.21930500	-0.71196400	-1.06105500
C	2.39914900	0.35088100	0.73784300
C	3.71699500	-0.06019600	0.90767400
C	4.18576100	-1.26958600	0.34723100
C	3.25985200	-2.02035200	-0.40760400
C	1.94333300	-1.59197900	-0.56531200
H	1.74338000	4.06400300	-1.44631300
H	-0.07937800	5.26098400	-0.93015400
H	-0.89726900	1.57402400	-1.55235700
H	-0.58399800	0.22327200	-3.45053200
H	0.67709300	-0.70382100	-2.65509600
H	2.06672600	0.48510800	-4.20947100
H	0.98490400	1.88987400	-4.21372100
H	2.74273900	2.65796100	-2.70330600
H	2.87778700	1.05665100	-1.95839800
H	-3.25063600	1.34635400	1.87273900
H	-2.95954300	-0.39494000	1.97298700
H	-3.08001100	0.57110500	3.45336600
H	-0.23091700	-0.32160900	4.46485000
H	1.12139100	-0.35836800	3.32185300
H	-0.25535900	-1.44825000	3.10582900
H	-0.91324400	2.64657900	4.17687500
H	0.58620500	2.76118900	3.24223200
H	-0.91965600	3.38668300	2.56663500
H	-0.05210000	-2.36227700	0.92520200
H	-4.13549300	-1.41269500	-1.67210100
H	-2.36786800	0.20687500	-1.61671100
H	2.08226400	1.29464600	1.16363200
H	4.38399900	0.57424400	1.47853100
H	3.55739600	-2.95044100	-0.87593000
H	1.27307700	-2.21874700	-1.14415000
C	-1.69288500	3.78783200	-0.70182400
H	-1.72873800	2.85920500	-0.12257700
H	-2.23721600	3.58775200	-1.64029300
C	-2.45838100	4.88366000	0.05818700
H	-2.40282400	5.82099000	-0.51235900
H	-1.94940000	5.08116200	1.01095600
C	-3.92511000	4.53212900	0.31778200
H	-4.44258200	5.33517900	0.85323100
H	-4.46322800	4.35874200	-0.62155000
H	-4.01540000	3.62095200	0.92034700
H	-1.82699400	-3.99931100	0.90232200
N	-4.19644400	-3.78473500	-0.38176200
N	5.49406700	-1.70658100	0.54176700

Supporting Information

C	-5.30286200	-3.60984000	-1.30653800
H	-5.82509200	-2.66421300	-1.12212400
H	-4.98739600	-3.62171700	-2.36167800
H	-6.02393200	-4.41498500	-1.15779200
C	-3.97621900	-5.10272400	0.18758100
H	-3.71411900	-5.03426600	1.24944600
H	-4.89823300	-5.68158500	0.11554000
H	-3.17736200	-5.66391100	-0.32239500
C	5.99663000	-2.80475500	-0.26545500
H	5.98274500	-2.58983600	-1.34620400
H	7.02588000	-3.02052100	0.02615200
H	5.41161700	-3.71541800	-0.09650300
C	6.46643500	-0.78830500	1.10954200
H	6.15957500	-0.46292700	2.10926500
H	7.42375100	-1.30193800	1.21376600
H	6.62347200	0.11221500	0.49420600
Cat2-IM1'			
N	1.79689900	1.84547100	-1.07626900
C	1.86427800	3.18801500	-0.70330300
C	0.91568700	3.96638900	-0.15461900
C	0.50650500	1.20303900	-1.36972600
C	0.70920100	0.48526700	-2.73667200
C	2.04144600	1.02732300	-3.28128900
C	2.81819600	1.32799800	-1.99468300
C	-0.00061400	0.26013600	-0.20611600
C	-1.32555000	-0.43543100	-0.58750300
C	1.12890800	-0.71405700	0.17363000
O	-0.24662800	1.15486900	0.88578000
Si	-1.13774400	1.11578900	2.31317200
C	-2.98304900	1.34319900	1.98636500
C	-0.86499100	-0.45016000	3.33444700
C	-0.48348100	2.60056600	3.26957900
C	-1.70920400	-1.65166400	0.00270000
C	-2.94903500	-2.23183900	-0.25743300
C	-3.86378200	-1.61672500	-1.12008600
C	-3.49841800	-0.39799300	-1.69738600
C	-2.25703200	0.18228000	-1.43510300
C	2.08993000	-0.31190300	1.11118900
C	3.18039400	-1.12519600	1.41868300
C	3.35246900	-2.36954400	0.80362500
C	2.40322300	-2.77126300	-0.14219600
C	1.31540700	-1.95619600	-0.45462700
H	2.84888100	3.61859600	-0.88285500

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H	-0.05664300	3.54963700	0.08818200
H	-0.23777300	2.00059200	-1.46014200
H	-0.12908100	0.66870600	-3.41262200
H	0.77821100	-0.59636400	-2.59971100
H	2.55029700	0.31680100	-3.94003900
H	1.88191900	1.95612500	-3.84074700
H	3.62017900	2.05932600	-2.12479900
H	3.26376800	0.40982000	-1.58977900
H	-3.17376900	2.24793000	1.39960800
H	-3.41101200	0.49542300	1.44391100
H	-3.52250200	1.44389600	2.93588000
H	-1.31387800	-0.31969400	4.32659900
H	0.19972100	-0.66036100	3.47354400
H	-1.32543900	-1.33126700	2.87915400
H	-1.02527000	2.72711200	4.21393500
H	0.57939700	2.48525500	3.50509800
H	-0.59281600	3.52311600	2.69129700
H	-1.02559200	-2.15890300	0.67331300
H	-4.19437700	0.11168400	-2.35955900
H	-2.03305200	1.13856200	-1.89300000
H	1.98596400	0.65681500	1.58296900
H	3.91217100	-0.78255300	2.14686600
H	2.53034700	-3.72757100	-0.64024000
H	0.59467700	-2.30891800	-1.18457900
C	4.50347200	-3.27971600	1.18717200
H	4.12449900	-4.06610900	1.85375800
H	5.24134600	-2.70377700	1.78084300
N	5.12236900	-3.94925000	0.04312300
C	5.83798300	-3.01604000	-0.81896600
H	6.69850100	-2.53467600	-0.31442200
H	6.21509400	-3.54494400	-1.69998700
H	5.16084800	-2.22835900	-1.15838000
C	5.98551000	-5.04399400	0.46470700
H	6.37864100	-5.56187800	-0.41593100
H	6.84836000	-4.71347000	1.07515800
H	5.41113700	-5.76560200	1.05438300
C	1.13940800	5.41910900	0.16969900
H	2.19224800	5.68280500	-0.00338800
H	0.95535100	5.60220600	1.24057900
C	0.24398900	6.37830100	-0.63842700
H	-0.80749300	6.09636500	-0.49127600
H	0.44808400	6.23662100	-1.70742800
C	0.43768400	7.84907400	-0.25819400
H	-0.21239700	8.50639200	-0.84523200

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H	0.21106600	8.01722000	0.80106700
H	1.47253000	8.16930600	-0.42662600
C	-5.18569500	-2.28054000	-1.45531000
H	-4.99532400	-3.10089300	-2.16030600
H	-5.83268700	-1.55817400	-1.99202500
N	-5.85516700	-2.85894100	-0.29122200
C	-6.91505800	-3.77881700	-0.68143000
H	-7.34992800	-4.23687800	0.21250400
H	-7.73526900	-3.29241300	-1.24445300
H	-6.50422800	-4.57839300	-1.30615800
C	-6.35406000	-1.83440800	0.61913400
H	-7.14195200	-1.20224100	0.16551400
H	-6.77240100	-2.30860700	1.51237700
H	-5.53506100	-1.18220100	0.93214200
H	-3.22486700	-3.16827300	0.21776100
Cat2-IM2'			
N	1.84238900	-1.08910800	1.81956800
C	2.32413800	-2.26874500	1.28281900
C	3.61310700	-2.63127300	1.13084500
C	0.41424900	-0.79211500	1.91236000
C	0.31991900	0.26602800	3.03934900
C	1.65871300	0.17159000	3.78893600
C	2.64657700	-0.24062000	2.69058400
C	-0.22625200	-0.34461400	0.53198200
C	-1.72495200	-0.00761600	0.68073500
C	0.60790200	0.80303100	-0.06130200
O	-0.09387100	-1.51255200	-0.28985200
Si	-0.81425000	-2.13163600	-1.67857300
C	-2.54086500	-2.80705800	-1.32672300
C	-0.89019000	-0.89377300	-3.10361900
C	0.32830200	-3.55378500	-2.14905900
C	-2.37457100	0.81676000	-0.25465100
C	-3.74633500	1.05054100	-0.19578600
C	-4.53255400	0.46564200	0.80410200
C	-3.89897900	-0.36908500	1.72780000
C	-2.52456700	-0.60413300	1.66630200
C	1.74379500	0.50833700	-0.82745200
C	2.57079700	1.52397800	-1.30774000
C	2.29624000	2.86908000	-1.04258800
C	1.17198500	3.16872700	-0.26558300
C	0.34734300	2.15462000	0.21955300
H	1.53565900	-2.94058900	0.95557800
H	4.41174100	-1.93919500	1.39231800

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H	-0.11543800	-1.71316100	2.18817500
H	-0.54239100	0.09261100	3.68661200
H	0.20735600	1.26496400	2.61162000
H	1.93244000	1.10774700	4.28469600
H	1.61543000	-0.61338700	4.55215600
H	3.49582500	-0.81234900	3.07857400
H	3.04570100	0.63405300	2.15550600
H	-2.52291700	-3.53152100	-0.50579700
H	-3.24428800	-2.01380800	-1.05869700
H	-2.93180100	-3.31987400	-2.21378100
H	-1.14130100	-1.42090900	-4.03198300
H	0.07126100	-0.39281500	-3.25236600
H	-1.65115000	-0.12375000	-2.94846300
H	-0.04143700	-4.07517700	-3.03936400
H	1.34040400	-3.19693200	-2.36556600
H	0.40171100	-4.28809400	-1.34014600
H	-1.79634300	1.28900900	-1.04027000
H	-4.48617400	-0.85012000	2.50649600
H	-2.08942400	-1.27790100	2.39477500
H	1.99195300	-0.52623900	-1.02898600
H	3.44787800	1.26217300	-1.89516200
H	0.95352200	4.20718900	-0.03616600
H	-0.52191700	2.42816900	0.80823900
C	3.15871000	3.97365300	-1.62229400
H	2.63409000	4.41650800	-2.47964700
H	4.09195200	3.53373000	-2.02728000
N	3.42796600	5.05769800	-0.67766300
C	4.29796900	4.63246000	0.41261500
H	5.31129000	4.34641800	0.06932200
H	4.40346200	5.44584400	1.13749600
H	3.85851400	3.77322900	0.92510700
C	3.96124600	6.23527600	-1.34837100
H	4.08590800	7.04591400	-0.62328700
H	4.94267500	6.06054700	-1.83104000
H	3.26179000	6.57451000	-2.11917300
C	4.03206300	-3.96954500	0.58441300
H	3.14209100	-4.58635800	0.39817500
H	4.62658300	-4.52014500	1.33166900
C	4.86209300	-3.87861900	-0.71028300
H	5.73430900	-3.23480800	-0.53260900
H	4.26439000	-3.37224000	-1.47905900
C	5.32909900	-5.24292200	-1.22603000
H	5.91852300	-5.14671300	-2.14399500
H	5.95200700	-5.75524500	-0.48349400

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H	4.47689400	-5.89634000	-1.44603400
C	-6.01482200	0.77025700	0.90649900
H	-6.13621400	1.77825500	1.32536100
H	-6.48177200	0.07691300	1.63433700
N	-6.69957400	0.75503600	-0.38547900
C	-8.01330900	1.37952400	-0.30535800
H	-8.46704300	1.40733100	-1.30104700
H	-8.71222200	0.84810900	0.36945700
H	-7.91591400	2.40972800	0.05170400
C	-6.78860900	-0.58940400	-0.94369100
H	-7.40467900	-1.27219300	-0.32678900
H	-7.23204000	-0.54320800	-1.94317400
H	-5.78987600	-1.02335500	-1.03448000
H	-4.22548300	1.68424100	-0.93584500
Cat2-IM3'			
N	-1.72529300	-1.71498600	-1.18302300
C	-1.98498900	-2.86966100	-0.45548600
C	-3.14573700	-3.29018900	0.08593600
C	-0.34791500	-1.32363300	-1.48429000
C	-0.45459500	-0.49799400	-2.78759400
C	-1.80892800	-0.89959100	-3.39032900
C	-2.67191500	-1.15405800	-2.14804500
C	0.36073700	-0.58145000	-0.27679700
C	1.80230900	-0.15878600	-0.63067800
C	-0.52997200	0.58488900	0.18241800
O	0.40967200	-1.58646500	0.74360900
Si	1.28452300	-1.87940900	2.14893300
C	3.05954400	-2.40059500	1.77480100
C	1.28933900	-0.41523400	3.34214900
C	0.36165100	-3.32768300	2.92261200
C	2.44611300	0.87650400	0.06918100
C	3.77900000	1.20241700	-0.17059900
C	4.53015100	0.50317000	-1.12317900
C	3.90418600	-0.53932900	-1.81035000
C	2.56939100	-0.86626400	-1.56740900
C	-1.56335500	0.34591100	1.09830600
C	-2.44642400	1.36096700	1.46736500
C	-2.33172400	2.64989900	0.93767800
C	-1.30923400	2.89142100	0.01363100
C	-0.42948400	1.87637300	-0.36069700
H	-1.09943200	-3.48583400	-0.31302100
H	-3.11051900	-4.27279400	0.55290100
H	0.24226000	-2.23612000	-1.64570400

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H	0.38540300	-0.68708500	-3.45919500
H	-0.45546400	0.57117000	-2.56128800
H	-2.22390000	-0.13306700	-4.05190200
H	-1.71290900	-1.82696500	-3.96652700
H	-3.47850900	-1.86860400	-2.33124700
H	-3.12210100	-0.21849600	-1.78442300
H	3.08426900	-3.24108100	1.07339600
H	3.64295300	-1.58389100	1.34067100
H	3.55958100	-2.72176300	2.69647300
H	1.68961700	-0.73270000	4.31261800
H	0.27942900	-0.02754100	3.50585600
H	1.91201000	0.41061100	2.98595900
H	0.80754700	-3.61175200	3.88260100
H	-0.69077000	-3.08269000	3.09643200
H	0.39071300	-4.20549500	2.26864300
H	1.89415900	1.44329900	0.81021600
H	4.46647300	-1.11132800	-2.54471400
H	2.13987200	-1.69708600	-2.11452600
H	-1.68649500	-0.64989900	1.50546100
H	-3.24168900	1.14238400	2.17637100
H	-1.21632000	3.88237800	-0.42016900
H	0.35595200	2.10501400	-1.07337800
C	-3.25660000	3.76647300	1.38264800
H	-2.71422400	4.41876500	2.08025000
H	-4.09994800	3.33522500	1.95826500
N	-3.71983400	4.60860400	0.27960700
C	-4.62405400	3.89409300	-0.61381400
H	-5.56817500	3.59143000	-0.12023500
H	-4.87764200	4.53135900	-1.46692100
H	-4.13623300	2.99311800	-0.99377100
C	-4.32304900	5.84313600	0.76221200
H	-4.59606100	6.47562600	-0.08854100
H	-5.23581800	5.68009900	1.36811000
H	-3.60393200	6.39382000	1.37709200
C	-4.47158700	-2.57988000	0.16890100
H	-4.37581500	-1.53543400	-0.14736600
H	-4.77959100	-2.54093000	1.22575800
C	-5.60773400	-3.25599000	-0.62357900
H	-5.68028400	-4.30792800	-0.31665100
H	-5.34499100	-3.27422700	-1.68956300
C	-6.96423100	-2.57032100	-0.43492200
H	-7.75222400	-3.07158200	-1.00679500
H	-7.26582700	-2.57284100	0.61893700
H	-6.92930600	-1.52497000	-0.76320900

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C	5.96143200	0.90068500	-1.42927500
H	5.94835900	1.82489000	-2.02245600
H	6.42633100	0.12825300	-2.07403800
N	6.75595400	1.16829100	-0.23116900
C	7.99063100	1.87251300	-0.55021000
H	8.52614800	2.11018500	0.37432900
H	8.67522200	1.28941900	-1.19642100
H	7.76229800	2.81327000	-1.06126000
C	7.02375900	-0.04582400	0.53126500
H	7.64833900	-0.77324000	-0.02296800
H	7.54482300	0.21047700	1.45893700
H	6.08386600	-0.53757600	0.79360900
H	4.25576800	2.00039700	0.39043800
Cat2-IM4'			
N	1.45950000	2.33487400	-1.15776900
C	1.29460000	3.70529300	-0.94186400
C	0.23056300	4.50417000	-0.72560600
C	0.34868600	1.41423100	-1.44018500
C	0.72002200	0.71013100	-2.78152800
C	1.99559900	1.41952800	-3.27314000
C	2.61974200	1.92581800	-1.96695000
C	0.06484600	0.41548700	-0.24254000
C	-1.07183000	-0.56778400	-0.60228800
C	1.37900900	-0.27379100	0.16532000
O	-0.37907000	1.26337300	0.82463200
Si	-1.19954800	1.04355700	2.27993600
C	-3.05572400	0.85914300	1.99230500
C	-0.57977100	-0.41781200	3.30445000
C	-0.85066800	2.64389700	3.20949700
C	-1.17339100	-1.82685200	0.01351600
C	-2.25324100	-2.67431600	-0.22586400
C	-3.28501800	-2.29654100	-1.09270800
C	-3.20152800	-1.03948400	-1.69707500
C	-2.11971500	-0.19216100	-1.45636600
C	2.21557500	0.35052200	1.10058900
C	3.45655700	-0.19271100	1.43286400
C	3.90803200	-1.37996000	0.84773400
C	3.08204600	-2.00273800	-0.09451300
C	1.84402600	-1.45704600	-0.43228000
H	2.26219700	4.20311500	-0.93419400
H	0.50276400	5.54867500	-0.58210000
H	-0.55784500	2.00400000	-1.55555300
H	-0.09806100	0.77525400	-3.50312000

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H	0.91646900	-0.35188500	-2.62170000
H	2.65727500	0.75621600	-3.83892600
H	1.74184400	2.27177400	-3.91331700
H	3.30359300	2.76621300	-2.10550900
H	3.16959500	1.12086000	-1.46517600
H	-3.45981500	1.71077500	1.43492900
H	-3.28815700	-0.04903700	1.42899100
H	-3.58535100	0.80732200	2.95104600
H	-1.02130400	-0.36425800	4.30715100
H	0.50823500	-0.40522500	3.41659300
H	-0.86380800	-1.38169900	2.87345800
H	-1.40662900	2.68139200	4.15330800
H	0.21422600	2.74136100	3.44480800
H	-1.13655400	3.51630600	2.61399900
H	-0.39244900	-2.15529000	0.68913600
H	-3.99558800	-0.71098100	-2.36356000
H	-2.11797300	0.77935600	-1.93631300
H	1.89515900	1.28291600	1.54720800
H	4.08561000	0.31933400	2.15760200
H	3.42377800	-2.91717100	-0.56969100
H	1.22819700	-1.97714500	-1.15807300
C	5.22797900	-2.00385100	1.25847700
H	5.02403900	-2.85230800	1.92544300
H	5.80584700	-1.27306000	1.85896000
N	6.00200900	-2.52114000	0.13010700
C	6.50819200	-1.45313100	-0.72380600
H	7.23337900	-0.79485900	-0.20691100
H	7.00649000	-1.88566000	-1.59716500
H	5.67921400	-0.83419500	-1.07571500
C	7.07836100	-3.39681900	0.57258500
H	7.59346200	-3.81411600	-0.29854100
H	7.83485700	-2.88366800	1.19789400
H	6.66755100	-4.22830500	1.15428400
C	-1.25270400	4.22821800	-0.65508300
H	-1.44431200	3.27687500	-0.14755800
H	-1.68302700	4.13199500	-1.66621900
C	-2.01309600	5.34924300	0.07226300
H	-1.80133400	6.30619900	-0.42412300
H	-1.61907300	5.44637400	1.09265200
C	-3.52610700	5.12410300	0.12035200
H	-4.03851300	5.94306100	0.63599500
H	-3.94808700	5.05144000	-0.88887600
H	-3.77383100	4.19510200	0.64696300
C	-4.42919700	-3.24256100	-1.40326600

Supporting Information

H	-4.07206600	-4.00316300	-2.11046300
H	-5.23078600	-2.68648000	-1.92913100
N	-4.93129100	-3.95061300	-0.22684900
C	-5.76329700	-5.08788000	-0.59636500
H	-6.06349700	-5.63048900	0.30558900
H	-6.68476200	-4.80151300	-1.13978300
H	-5.19534000	-5.77461200	-1.23202300
C	-5.63246300	-3.06131700	0.69233500
H	-6.55044000	-2.62453600	0.25329300
H	-5.91793100	-3.61447500	1.59252500
H	-4.97693900	-2.24009800	0.99232600
H	-2.31213000	-3.63848100	0.26983200

S6.Cartesian Coordinates of transition states

Cat1-TS1

N	-1.12063000	0.92609200	-0.79424600
C	-2.16338400	0.85681200	0.02038600
C	-2.63530700	-0.27671900	0.71864800
C	-0.03142100	-0.07164300	-0.95179000
C	0.33882500	0.03658700	-2.45538900
C	-0.47151500	1.22436400	-3.03389900
C	-0.97523400	1.99166400	-1.80491900
C	1.16862300	0.14441300	0.05737700
C	2.24883900	-0.91463800	-0.23213700
C	1.68142700	1.59365000	-0.00677000
O	0.57640400	-0.07507900	1.34870300
Si	1.16797300	-0.66908400	2.81433800
C	1.31976500	-2.54578500	2.79909200
C	2.79954100	0.12010800	3.35057400
C	-0.16216700	-0.15467200	4.05006300
C	3.60321200	-0.67675400	0.04380700
C	4.58313900	-1.64956700	-0.12931700
C	4.25149500	-2.94152700	-0.59307200
C	2.88859100	-3.18376200	-0.87676800
C	1.92011000	-2.20417200	-0.69084800
C	1.18669800	2.55746400	0.88214600
C	1.54602800	3.89976400	0.79997300
C	2.42815000	4.36150900	-0.20195600
C	2.94231700	3.39039100	-1.08956800
C	2.57128400	2.05223800	-0.99019800
H	-2.79682800	1.74298000	0.00454100
H	-1.90196600	-1.06240800	0.87699100
H	-0.43787000	-1.04600400	-0.69895300
H	0.08026000	-0.89697600	-2.95717700

Supporting Information

H	1.41067900	0.19026600	-2.57828900
H	0.12718900	1.86432600	-3.68744900
H	-1.32182600	0.85372400	-3.61332200
H	-1.93392300	2.49333700	-1.95506400
H	-0.24131300	2.72576700	-1.46197200
H	0.39991200	-3.00981200	2.42810700
H	2.13985800	-2.88466300	2.16056500
H	1.50130800	-2.91979300	3.81403900
H	2.97625500	-0.10441600	4.40963100
H	2.77740900	1.20906300	3.24086600
H	3.65294300	-0.26087500	2.78440200
H	0.09911500	-0.49368600	5.05914500
H	-0.27698300	0.93410700	4.08649100
H	-1.13482400	-0.58664300	3.79746800
H	3.91396500	0.29773700	0.40304600
H	2.56635200	-4.14924400	-1.24572000
H	0.89599100	-2.48851200	-0.91101300
H	0.49599000	2.24599200	1.65625800
H	1.13579600	4.58799400	1.52887500
H	3.64745400	3.67113400	-1.86207000
H	3.01442800	1.35122500	-1.68895500
C	-3.69614200	-1.25396300	-0.61575900
C	-2.97155000	-1.59722500	-1.79211200
N	-1.94320200	-2.49998700	-1.74787500
O	-1.34028600	-2.80937500	-2.81047800
O	-1.57720900	-2.96548900	-0.62012200
C	-4.97487100	-0.51056300	-0.83661500
C	-5.03954200	0.61778900	-1.67163700
C	-6.24248800	1.28835200	-1.88444100
C	-7.41330800	0.84616300	-1.26442300
C	-7.36747900	-0.27408900	-0.43498500
C	-6.16089300	-0.94277300	-0.22388400
H	-3.78461300	-2.08792300	0.07695500
H	-3.17295800	-1.19204100	-2.77183600
H	-4.13811000	0.96678300	-2.16768400
H	-6.26707700	2.15684200	-2.53672800
H	-8.35085900	1.36886300	-1.42893600
H	-8.27219600	-0.63268400	0.04753600
H	-6.14087900	-1.82353400	0.41137200
C	-3.52195500	0.00481100	1.93293000
H	-4.42523800	0.54793400	1.62458400
H	-2.98052200	0.67738000	2.61228600
C	-3.92196400	-1.23957700	2.73923900
H	-3.01843000	-1.80088000	3.00983100

Supporting Information

H	-4.52241400	-1.91847700	2.12445200
C	-4.70635500	-0.88470200	4.00585600
H	-4.98067200	-1.78222500	4.56913200
H	-4.11691500	-0.24205900	4.66964800
H	-5.63057800	-0.34851800	3.76189900
N	2.76821500	5.70557400	-0.31398400
C	2.41602300	6.61629300	0.76240500
H	2.88282000	6.35005600	1.72393100
H	2.73582400	7.62481000	0.49549600
H	1.33116500	6.64645300	0.91152500
C	3.85678700	6.08927100	-1.19692400
H	3.96284400	7.17511800	-1.18126100
H	4.82312200	5.64473600	-0.91045000
H	3.64439200	5.79640900	-2.23086500
H	5.61088000	-1.39122300	0.09483100
N	5.21363500	-3.92833400	-0.75362600
C	6.61851900	-3.57903600	-0.64324800
H	6.84595400	-3.16897900	0.34742300
H	7.22206500	-4.47900300	-0.77054800
H	6.93910700	-2.84143700	-1.39591700
C	4.86052700	-5.16513500	-1.43147100
H	4.05764700	-5.68914700	-0.90153300
H	4.53181500	-5.00583000	-2.46984200
H	5.72950600	-5.82480500	-1.44538000
Cat1-TS2			
N	0.62158100	-1.51944200	-1.23384800
C	1.67794000	-2.01502900	-0.60115500
C	2.63077800	-1.33206100	0.19192300
C	0.09122400	-0.13417100	-1.20387400
C	-0.43493600	0.03645000	-2.64729300
C	-0.84371800	-1.36709500	-3.13875900
C	-0.01428400	-2.34451900	-2.29522800
C	-0.95243700	0.14178200	-0.04203700
C	-1.57977800	1.53895500	-0.22310800
C	-1.98264900	-0.99427100	0.03886800
O	-0.14689600	0.14016200	1.15730100
Si	-0.36127200	0.85879900	2.67452900
C	-0.02099700	2.71397700	2.65251200
C	-2.05403000	0.51959200	3.44157800
C	0.94743200	0.03227200	3.74817900
C	-2.86378700	1.84643900	0.24945300
C	-3.39750000	3.13007600	0.18481200
C	-2.65987100	4.20276400	-0.36245800

Supporting Information

C	-1.36605500	3.89971000	-0.84490500
C	-0.85102200	2.61175000	-0.76329900
C	-1.75714900	-2.09751700	0.87216200
C	-2.63010400	-3.17980600	0.92245800
C	-3.78920900	-3.22302600	0.11560100
C	-4.02123700	-2.11024400	-0.72347300
C	-3.13471300	-1.03764600	-0.75896900
H	1.87172400	-3.05605800	-0.83847900
H	2.25995700	-0.45193500	0.70828800
H	0.92918800	0.53098800	-1.00719100
H	0.38755600	0.39643600	-3.26990200
H	-1.25284700	0.75522000	-2.70663900
H	-1.91036600	-1.54581900	-2.99723100
H	-0.61036200	-1.48412100	-4.19840800
H	0.79923400	-2.79354200	-2.87302300
H	-0.62425500	-3.12874100	-1.83692000
H	0.96198000	2.92787100	2.21923000
H	-0.76888200	3.27582700	2.08793300
H	-0.01684400	3.09465000	3.68129600
H	-2.03013700	0.80734800	4.49974100
H	-2.31567300	-0.54153600	3.38892500
H	-2.85507900	1.08868600	2.96385900
H	0.94083900	0.46750400	4.75428000
H	0.76379500	-1.04169900	3.85121800
H	1.95269800	0.16612400	3.33675600
H	-3.47824500	1.06310100	0.67715200
H	-0.75088200	4.67272000	-1.28825400
H	0.15236700	2.45698700	-1.14444900
H	-0.87421600	-2.10864400	1.50008000
H	-2.40176900	-3.99461800	1.59848100
H	-4.90084600	-2.07147800	-1.35402600
H	-3.36303800	-0.21035000	-1.42290000
C	3.86183000	-0.46408900	-1.11748500
N	2.86886900	-1.11900300	-3.21168600
O	3.09215000	-2.32703900	-2.86978600
O	2.28340900	-0.83597800	-4.29243400
C	4.48094300	0.64784700	-0.33501000
C	3.80020200	1.85006800	-0.08011400
C	4.40634900	2.88037500	0.63576700
C	5.70801200	2.72981900	1.12019200
C	6.39518800	1.54013100	0.88052200
C	5.78544800	0.50974000	0.16351800
H	4.48194500	-1.35466100	-1.18651700
H	2.78386500	1.97787800	-0.44209700

Supporting Information

H	3.86096300	3.80201400	0.81870200
H	6.17953800	3.53202700	1.68009000
H	7.40871300	1.41172900	1.24965800
H	6.33140800	-0.40965000	-0.02898100
C	3.56125800	-2.22380200	1.00452800
H	4.39010500	-1.61600900	1.38704200
H	4.01133900	-2.96537700	0.32892900
C	2.90685500	-2.96620700	2.18142900
H	2.07668300	-3.57940300	1.80603000
H	2.46246300	-2.23938800	2.86970100
C	3.89841700	-3.85324900	2.94136800
H	3.41339000	-4.37423900	3.77332400
H	4.33765200	-4.61218100	2.28388400
H	4.72177000	-3.26032200	3.35573700
C	3.24789100	-0.12440400	-2.34982800
H	2.99271500	0.87733100	-2.66141100
N	-4.65333300	-4.30947300	0.14071700
C	-5.93047100	-4.22083300	-0.54573000
H	-6.57679600	-3.42119500	-0.15081400
C	-4.49490300	-5.32080100	1.17172300
H	-4.60871100	-4.91722400	2.19003200
H	-5.24622800	-6.09853100	1.02770600
H	-3.51113200	-5.79930400	1.10709100
H	-6.45922100	-5.16921600	-0.43998300
H	-5.78974100	-4.04182700	-1.61763400
H	-4.40110800	3.28875700	0.55949900
N	-3.17487100	5.48792200	-0.41863500
C	-2.46350400	6.51402700	-1.16233600
H	-2.36128400	6.27394700	-2.23167200
H	-3.00433700	7.45737300	-1.07582200
H	-1.45872600	6.67291900	-0.75437400
C	-4.56999000	5.71419600	-0.08205200
H	-4.78243700	5.40622900	0.94815000
H	-4.78735600	6.78049300	-0.15653500
H	-5.26312200	5.17533500	-0.74634000
Cat1-TS3			
N	-0.99156300	-0.14485300	-0.90433200
C	-1.71578200	-0.07717000	0.20345400
C	-3.11782000	0.12971100	0.25326100
C	0.40790100	-0.67343200	-0.96377900
C	0.74039100	-0.61282000	-2.47028500
C	-0.62228700	-0.64712500	-3.17141500
C	-1.48609300	0.20877600	-2.25043700

Supporting Information

C	1.42568500	0.04226800	0.01062100
C	2.85701700	-0.47136000	-0.23139400
C	1.32548500	1.57213400	-0.13602500
O	0.99994300	-0.28179800	1.34168700
Si	1.44568200	-1.37406000	2.55661400
C	1.57040200	-3.16496600	1.99451700
C	3.04270900	-0.82349300	3.40137700
C	0.01049300	-1.21262500	3.76986000
C	3.96610600	0.30552900	0.13584200
C	5.27181600	-0.15513300	0.01154000
C	5.54491500	-1.44967200	-0.48569500
C	4.43152300	-2.23871300	-0.85055000
C	3.13237400	-1.75983100	-0.71421500
C	0.59563700	2.33947800	0.77968100
C	0.44286000	3.71595400	0.63894700
C	1.01278200	4.40921600	-0.45056000
C	1.77966600	3.64442500	-1.35645900
C	1.92491900	2.26935800	-1.19570900
H	-1.17462100	-0.31187600	1.10826600
H	-3.55878900	0.64652600	-0.59673900
H	0.33689900	-1.71823400	-0.64260500
H	1.38287400	-1.44031900	-2.76927100
H	1.25817300	0.31745900	-2.71386400
H	-0.58901600	-0.25749200	-4.19248500
H	-1.00401000	-1.67216200	-3.18874400
H	-2.55069600	0.00454600	-2.33930300
H	-1.31785000	1.28172600	-2.41823800
H	0.69330300	-3.44070200	1.39988600
H	2.47554900	-3.36763300	1.41655300
H	1.59176900	-3.81040900	2.88183500
H	3.21672500	-1.43115700	4.29771100
H	2.98373400	0.22395500	3.71642900
H	3.91418100	-0.93045500	2.74945100
H	0.19936800	-1.80108000	4.67505000
H	-0.15077400	-0.17369900	4.07719700
H	-0.91369200	-1.58904900	3.31875500
H	3.80882900	1.30317500	0.53057300
H	4.57107200	-3.23887700	-1.24116600
H	2.32542100	-2.43115300	-0.98553800
H	0.15529300	1.84766400	1.63795600
H	-0.12091000	4.24949800	1.39421000
H	2.28574700	4.12011800	-2.18735400
H	2.56278600	1.74247600	-1.89735500
C	-3.86848700	-1.71014600	-0.09726400

Supporting Information

C	-3.06144300	-2.47215900	-0.98003300
N	-1.85915500	-2.95638800	-0.54318400
O	-1.08421800	-3.56078200	-1.33655100
O	-1.52752200	-2.74007300	0.66809300
C	-5.27600300	-1.43527800	-0.51011900
C	-6.31925300	-1.60868000	0.41298300
C	-7.64688700	-1.37704800	0.05108000
C	-7.95805200	-0.96097200	-1.24310000
C	-6.93069600	-0.77983900	-2.17235800
C	-5.60620900	-1.01162800	-1.80850400
H	-3.75986000	-2.00369500	0.94342000
H	-3.27836800	-2.65465600	-2.02156400
H	-6.08528700	-1.94525400	1.41912700
H	-8.43708800	-1.52472300	0.78158200
H	-8.99025500	-0.77818900	-1.52673300
H	-7.16248100	-0.45498600	-3.18272200
H	-4.81818700	-0.86332600	-2.54177200
C	-3.69704600	0.56339700	1.58869900
H	-3.20430400	0.00384000	2.39549700
H	-4.75989300	0.29459300	1.62783100
C	-3.56502000	2.07261600	1.85920000
H	-4.05896300	2.62530700	1.04867100
H	-2.50608300	2.35731700	1.81620700
C	-4.16351700	2.49199100	3.20525400
H	-4.06155600	3.56968100	3.36979900
H	-5.23053800	2.24761000	3.25845900
H	-3.66637500	1.98017200	4.03701800
N	0.82908900	5.77860200	-0.62311800
C	1.63529500	6.48137500	-1.60622000
H	2.71533200	6.44170700	-1.39102200
C	0.26480500	6.55763200	0.46590500
H	0.87941600	6.53310800	1.37995800
H	0.16770500	7.59701500	0.14782900
H	-0.73757600	6.19977700	0.72434000
H	1.33143400	7.52920200	-1.63357100
H	1.47656300	6.06931600	-2.60856500
H	6.08108000	0.50224600	0.30450300
N	6.84184600	-1.92655600	-0.59941400
C	7.08501300	-3.18307500	-1.28704700
H	8.15288400	-3.40437600	-1.26037000
H	6.56490800	-4.01160400	-0.79281200
H	6.76482400	-3.16300200	-2.34022000
C	7.95841000	-1.02274200	-0.38589500
H	7.97567000	-0.18603800	-1.10159800

Supporting Information

H	7.93706300	-0.59994700	0.62519600
H	8.89221800	-1.57723100	-0.48872700
Cat1-TS4			
N	0.58959400	-1.09069000	-1.01816700
C	1.40976800	-0.42452100	-0.21641900
C	2.66866700	-0.84359600	0.29865200
C	-0.53286000	-0.42470500	-1.74759200
C	-0.92363300	-1.45427900	-2.82830000
C	0.31377500	-2.34849400	-2.98751400
C	0.86029300	-2.43393100	-1.56131900
C	-1.76022300	0.05077100	-0.86813200
C	-2.35871400	-1.14940400	-0.11531100
C	-1.40148500	1.22674800	0.05925200
O	-2.67785100	0.47644900	-1.88680000
Si	-3.83991600	1.68559300	-2.04949700
C	-4.84260500	1.08680800	-3.53117800
C	-4.96973300	1.84164900	-0.54490600
C	-3.07714600	3.35847400	-2.46092100
C	-3.54151600	-1.76166400	-0.54443200
C	-4.06989300	-2.88390600	0.08886000
C	-3.42007700	-3.47319000	1.19375800
C	-2.23016000	-2.85194300	1.63603200
C	-1.72089800	-1.72789600	0.99300400
C	-0.52975500	2.24920400	-0.35849300
C	-0.21854400	3.33557700	0.44948100
C	-0.79376200	3.48228700	1.73250500
C	-1.70922300	2.48418700	2.13694900
C	-1.98857700	1.38941200	1.32276100
H	1.06340400	0.56301900	0.05620600
H	2.88190300	-1.90848900	0.21647800
H	-0.10531300	0.45975600	-2.22197700
H	-1.21189600	-0.95585400	-3.75388500
H	-1.77585500	-2.05077100	-2.49313600
H	0.07998400	-3.33319300	-3.40133800
H	1.05625000	-1.87166100	-3.63633800
H	1.92545300	-2.66217400	-1.51800600
H	0.31828300	-3.17915200	-0.96507400
H	-4.20236400	0.94755100	-4.40847800
H	-5.33735800	0.13150100	-3.32598700
H	-5.61927800	1.81271800	-3.79764700
H	-5.82546400	2.48113200	-0.79323300
H	-4.45358600	2.28883900	0.30906200
H	-5.36125800	0.86864200	-0.23082300

Supporting Information

H	-3.86604900	4.07461000	-2.72141400
H	-2.50910400	3.77132100	-1.62321300
H	-2.40074600	3.28474900	-3.31911300
H	-4.06183600	-1.35181400	-1.40161800
H	-1.69733100	-3.23784200	2.49637600
H	-0.81241900	-1.28457400	1.38544200
H	-0.02136100	2.20498000	-1.31485200
H	0.50152700	4.04849300	0.06838700
H	-2.20352900	2.54930000	3.09860500
H	-2.68883600	0.64674600	1.68838700
C	3.97975700	-0.12315800	-1.00061100
C	4.03172900	1.29646800	-0.94281700
N	2.99396300	2.02431900	-1.45747100
O	2.96219600	3.27322200	-1.33122100
O	2.05275800	1.38833800	-2.04887700
C	5.22007100	-0.90249700	-0.70344100
C	5.40970600	-2.14529700	-1.32985700
C	6.55168400	-2.90841600	-1.09458300
C	7.53403900	-2.44416200	-0.21835500
C	7.36205100	-1.21154900	0.41337700
C	6.21875500	-0.44955600	0.17481400
H	3.45473300	-0.48761900	-1.87979600
H	4.76225600	1.87853600	-0.40319100
H	4.65423900	-2.50863600	-2.02278100
H	6.67697900	-3.86215100	-1.59925700
H	8.42601900	-3.03505800	-0.03254300
H	8.12248300	-0.83820900	1.09329800
H	6.10741800	0.50816400	0.67212000
C	3.06070300	-0.25212700	1.64491500
H	2.97947000	0.84140600	1.59084900
H	4.11716500	-0.47660000	1.83239400
C	2.22892300	-0.76600100	2.83235100
H	2.25871400	-1.86392900	2.85037200
H	1.17629300	-0.48934800	2.68633200
C	2.71713100	-0.21755800	4.17703700
H	2.10690700	-0.58999800	5.00626200
H	3.75556400	-0.50984400	4.37015900
H	2.67270900	0.87703300	4.19627100
N	-0.45938600	4.54532400	2.55663100
C	-1.23047100	4.78382200	3.76381800
H	-2.29257400	4.99397300	3.56136200
C	0.33950500	5.63733200	2.02137100
H	-0.16448000	6.17614600	1.20441900
H	0.55115800	6.34849800	2.82142100

Supporting Information

H	1.29827000	5.27115900	1.64100300
H	-1.18159700	3.92256300	4.44005100
H	-0.80942800	5.63973800	4.29346500
H	-4.99616300	-3.29855200	-0.28914900
N	-3.91991800	-4.61586700	1.81155400
C	-3.36394900	-5.03174300	3.08794800
H	-3.49047300	-4.27791500	3.88134800
H	-3.85677200	-5.95081500	3.40916600
H	-2.29410200	-5.24933600	2.99769200
C	-5.26012000	-5.06767100	1.47801200
H	-5.33931200	-5.30478900	0.41151800
H	-5.47681600	-5.98253600	2.03182400
H	-6.03891800	-4.32652400	1.71859400
Cat1-TS5			
N	-0.90206400	-0.08458400	-0.73533600
C	-1.59392000	-0.30936500	0.36650200
C	0.50139800	-0.57984300	-0.91194300
C	0.77813900	-0.35649800	-2.41447000
C	-0.60696600	-0.24491300	-3.06446600
C	-1.41899100	0.48654400	-1.99931400
C	1.53223600	0.07832500	0.08744000
C	2.96659500	-0.37316700	-0.23332600
C	1.37828400	1.61039500	0.06079100
O	1.15341200	-0.35714100	1.40303000
Si	1.65969300	-1.53870100	2.50290900
C	1.75445400	-3.27378200	1.77919100
C	3.29058200	-1.06305900	3.32512100
C	0.28241200	-1.48285700	3.79179700
C	4.06467300	0.38579600	0.19940000
C	5.37747300	-0.02962300	0.01010200
C	5.67113000	-1.25003300	-0.63987600
C	4.56873500	-2.03199500	-1.04971500
C	3.26179900	-1.59907700	-0.84779000
C	0.56712500	2.26496700	0.99624900
C	0.34789600	3.63866700	0.95416900
C	0.93108700	4.44366800	-0.04871200
C	1.77256100	3.79127200	-0.97582100
C	1.98078000	2.41596100	-0.91668000
H	-1.02180300	-0.78793500	1.14494400
H	0.45237000	-1.65045600	-0.68729800
H	1.36156400	-1.17610100	-2.83306400
H	1.33936600	0.56740900	-2.56887100
H	-0.58857400	0.29875700	-4.01311700

Supporting Information

H	-1.02052400	-1.24411200	-3.22681000
H	-2.48976300	0.32278200	-2.07882800
H	-1.21467300	1.56478400	-2.01133400
H	0.86914900	-3.49970200	1.17471100
H	2.64622100	-3.42370500	1.16492800
H	1.79421400	-3.99928300	2.60152600
H	3.49398700	-1.73989800	4.16384700
H	3.24917400	-0.04357400	3.72348400
H	4.13566400	-1.12035600	2.63388800
H	0.52131600	-2.13410800	4.64036800
H	0.13225100	-0.47062000	4.18181400
H	-0.66682200	-1.83170600	3.37107700
H	3.89212300	1.32814000	0.70791500
H	4.72201200	-2.99126100	-1.52779000
H	2.46578600	-2.26087100	-1.17002400
H	0.11062400	1.68425900	1.78820700
H	-0.27743700	4.08277400	1.71892500
H	2.28409000	4.35507600	-1.74590000
H	2.66335700	1.97444300	-1.63522100
C	-3.72017400	-1.87044900	-0.03264700
C	-3.04387100	-2.40252500	-1.17099600
N	-1.79905900	-2.93891900	-1.01410100
O	-1.29871600	-2.97898200	0.16394800
O	-1.14436700	-3.35425300	-2.01119300
C	-5.19593900	-1.66476500	-0.11838600
C	-5.84537500	-1.27765600	-1.30265900
C	-7.23009900	-1.11704600	-1.34211000
C	-7.99833300	-1.33893500	-0.19793000
C	-7.36891700	-1.72477600	0.98686600
C	-5.98408100	-1.88129200	1.02417600
H	-3.41982100	-2.37762800	0.87972100
H	-3.40281300	-2.37810300	-2.18828800
H	-5.26617900	-1.11016300	-2.20551300
H	-7.71011800	-0.82231700	-2.27094800
H	-9.07687500	-1.21645000	-0.23058900
H	-7.95633500	-1.90820800	1.88197800
H	-5.50130600	-2.18887800	1.94824900
C	-3.74967800	1.07749800	-0.01848000
H	-4.30716300	0.79935700	-0.92136400
H	-3.03719100	1.85330900	-0.32246800
C	-5.50134200	2.88836000	0.40697500
H	-6.18390200	3.31895700	1.14671200
H	-4.81947300	3.68283700	0.08170200
H	-6.09947300	2.58837600	-0.46059500

Supporting Information

H	6.17576000	0.60468300	0.37511100
C	-2.99692000	-0.12341500	0.56995200
H	-3.22618500	-0.25015600	1.62778300
N	6.97802600	-1.65663900	-0.86978000
N	0.68652300	5.81240500	-0.12207400
C	8.06804500	-0.94170800	-0.22740300
H	8.01644600	-0.97648700	0.87211700
H	9.01628300	-1.38257000	-0.53842900
H	8.08058300	0.11083100	-0.53119800
C	7.23024600	-3.01026100	-1.33587900
H	6.73513600	-3.19318600	-2.29571300
H	8.30230800	-3.13996100	-1.49150300
H	6.88951400	-3.78034700	-0.62639100
C	0.02948900	6.47234600	0.99349900
H	0.59957800	6.40496900	1.93390400
H	-0.10821100	7.52780100	0.75270300
H	-0.96341300	6.04529200	1.17040400
C	1.50538200	6.63052900	-1.00023900
H	1.15439300	7.66287300	-0.95570700
H	2.57420400	6.61839300	-0.73269500
H	1.41486200	6.29977200	-2.04045700
C	-4.73468500	1.69630800	0.98527300
H	-4.18024500	2.01125100	1.87968200
H	-5.44371600	0.92841400	1.31448400
Cat1-TS6			
N	-0.79896800	0.09282400	-0.91285200
C	0.58481000	-0.43303000	-1.10861100
C	0.91009200	-0.06978800	-2.57419100
C	-0.45652400	0.16817600	-3.23076200
C	-1.25342100	0.82995500	-2.10643100
C	1.59133100	0.09722400	-0.01445900
C	3.02407700	-0.37951700	-0.30132800
C	1.48979200	1.63045300	0.07643800
O	1.12292500	-0.42818900	1.23709600
Si	1.50099100	-1.73388100	2.24662500
C	1.48728800	-3.40465300	1.38042200
C	3.14133200	-1.46860600	3.14191500
C	0.10178100	-1.66588400	3.51035300
C	4.12117700	0.28604700	0.26662600
C	5.42732800	-0.15979100	0.10471700
C	5.71601600	-1.31840300	-0.65246300
C	4.61309000	-2.00832400	-1.20189900
C	3.31264600	-1.54472000	-1.02617200

Supporting Information

C	0.62673100	2.23544800	0.99892300
C	0.44890000	3.61453300	1.05089000
C	1.12909100	4.47578900	0.16158500
C	2.02123400	3.87103000	-0.75015500
C	2.18663100	2.48875000	-0.78625100
H	0.50327500	-1.51737900	-0.99051600
H	1.47896300	-0.86020600	-3.06497800
H	1.50516000	0.84486900	-2.62206700
H	-0.39922300	0.79268100	-4.12662500
H	-0.92575100	-0.78461400	-3.49611100
H	-2.33076700	0.73840500	-2.22638300
H	-0.99535800	1.89124200	-2.00841000
H	0.55220800	-3.60482800	0.84485800
H	2.32055700	-3.51550400	0.68068000
H	1.59568000	-4.18901600	2.14040500
H	3.27061100	-2.24080300	3.90995100
H	3.16588500	-0.49497000	3.64318800
H	3.99835200	-1.52034800	2.46538700
H	0.25385700	-2.41748400	4.29330800
H	0.04721700	-0.68526300	3.99481100
H	-0.87034300	-1.87114100	3.04985200
H	3.95134100	1.17747400	0.86078600
H	4.76079500	-2.91941100	-1.76799700
H	2.51366400	-2.13584300	-1.45928000
H	0.09382800	1.60852500	1.70307600
H	-0.22208600	4.01843200	1.79897700
H	2.60533000	4.47654500	-1.43193800
H	2.90812900	2.08132500	-1.48698000
C	-3.88188000	-1.73333600	-0.58071800
C	-3.47245500	-2.96873300	-0.00714000
N	-2.21694400	-3.45421100	-0.23107400
O	-1.83026300	-4.51004900	0.32887400
O	-1.44178600	-2.78265500	-0.99812000
C	-5.33606900	-1.41299800	-0.47822600
C	-6.02307100	-0.91079300	-1.59405800
C	-7.39011200	-0.63569200	-1.53514000
C	-8.09741300	-0.85329800	-0.35308300
C	-7.42658400	-1.34783100	0.76857400
C	-6.06187600	-1.62140300	0.70754600
H	-3.46173300	-1.54285100	-1.56537700
H	-4.05329500	-3.53375000	0.70576000
H	-5.48163300	-0.75359200	-2.52323700
H	-7.90141300	-0.25532100	-2.41482700
H	-9.16114000	-0.64022200	-0.30405700

Supporting Information

H	-7.96851100	-1.51955500	1.69421200
H	-5.55088200	-1.99867000	1.58847400
C	-3.62042800	1.15545300	-0.06899800
H	-4.23406300	1.06458200	-0.97565700
H	-2.85128700	1.90470300	-0.29155600
C	-5.16995300	3.03522900	0.69908200
H	-5.78070600	3.41266700	1.52554100
H	-4.42594700	3.80344200	0.45762300
H	-5.82468500	2.92226200	-0.17219700
H	6.22473800	0.40086200	0.57651400
C	-2.96184100	-0.17995100	0.29459900
H	-3.19854100	-0.49275900	1.30915700
C	-1.57986500	-0.41944500	0.02935100
H	-1.05903300	-1.10107500	0.68232400
C	-4.50264600	1.70627700	1.06240800
H	-3.88552900	1.83542800	1.96166900
H	-5.26982100	0.96697700	1.31630000
N	7.01934700	-1.75168700	-0.85140300
N	0.92708700	5.85310000	0.18046100
C	7.25130800	-3.05941300	-1.44236400
H	8.32543200	-3.21555800	-1.55285600
H	6.84371200	-3.88384500	-0.83686600
H	6.80649100	-3.12221600	-2.44140100
C	8.09336900	-1.15244500	-0.07693700
H	9.04233200	-1.59804100	-0.37883000
H	8.16165500	-0.07567800	-0.26713900
H	7.97422300	-1.29841100	1.00801600
C	0.20268200	6.44598000	1.29192500
H	0.11807300	7.52167500	1.12906800
H	-0.81422800	6.04386700	1.35538000
H	0.69247900	6.28243400	2.26505900
C	1.82693600	6.70950700	-0.57278100
H	1.50187800	7.74627600	-0.47118200
H	2.87348100	6.64197000	-0.23488600
H	1.80107000	6.46226200	-1.63962400
Cat2-TS1'			
N	-1.37985400	0.82583300	-0.58140200
C	-2.47259900	0.61404800	0.13842400
C	-2.95220100	-0.62377700	0.62563500
C	-0.24078000	-0.10402600	-0.78593400
C	0.22441700	0.21336900	-2.23184600
C	-0.54947100	1.47659300	-2.68999500
C	-1.20473900	2.03065200	-1.41731400

Supporting Information

C	0.87710100	0.01313600	0.32869600
C	2.01888400	-0.97230400	-0.01166500
C	1.34009200	1.47506300	0.48013300
O	0.21863100	-0.39306500	1.53442800
Si	0.74490400	-1.11924600	2.97024900
C	1.13992700	-2.94490600	2.73808400
C	2.20932700	-0.22516900	3.76011200
C	-0.74935400	-0.93592200	4.10528400
C	3.33838100	-0.71972400	0.40022100
C	4.36030200	-1.64054300	0.17833100
C	4.10305500	-2.85136400	-0.47479500
C	2.79251000	-3.10782200	-0.88628100
C	1.76166500	-2.19659000	-0.65263400
C	0.74984500	2.29353800	1.45236200
C	1.08098800	3.64543000	1.55813800
C	2.01867200	4.22909700	0.70141600
C	2.60984900	3.41764200	-0.27466500
C	2.27612500	2.06900400	-0.38426600
H	-3.13594500	1.47586200	0.19927800
H	-2.20060100	-1.40168800	0.73143500
H	-0.61971500	-1.11649400	-0.68986100
H	-0.00258300	-0.63969300	-2.87314600
H	1.30191500	0.37063900	-2.26879100
H	0.10124300	2.22065000	-3.15656200
H	-1.31956000	1.20374500	-3.41666100
H	-2.17377900	2.50465400	-1.58839300
H	-0.55056200	2.74178800	-0.90565800
H	0.34093100	-3.45391900	2.18951700
H	2.07129300	-3.09863300	2.18675600
H	1.24124900	-3.43192700	3.71556200
H	2.35637200	-0.60449600	4.77863800
H	2.03758600	0.85357800	3.82790300
H	3.14100200	-0.38550700	3.21191100
H	-0.53342100	-1.35679800	5.09394300
H	-1.02379800	0.11508500	4.24587900
H	-1.62195300	-1.46094500	3.70575600
H	3.57657500	0.21149700	0.90103200
H	2.56151500	-4.03789500	-1.39923400
H	0.76596200	-2.47669000	-0.98061900
H	0.01307200	1.86384100	2.11957900
H	0.60253200	4.25352900	2.32261100
H	3.33513000	3.85810500	-0.95175900
H	2.77388900	1.46936200	-1.13789400
C	-3.85775100	-1.41760300	-0.90215500

Supporting Information

C	-3.02438400	-1.58248900	-2.04751300
N	-1.97234300	-2.45639800	-2.03176800
O	-1.27281400	-2.61029800	-3.06898100
O	-1.68049700	-3.05309100	-0.94361800
C	-5.13541100	-0.67511300	-1.14064900
C	-5.15668400	0.55481600	-1.81957100
C	-6.35418100	1.22844800	-2.05203100
C	-7.56267500	0.68675200	-1.60826600
C	-7.55971700	-0.53505300	-0.93572400
C	-6.35820700	-1.20642100	-0.70431800
H	-3.98605600	-2.34392300	-0.34600100
H	-3.16471400	-1.06106800	-2.98188600
H	-4.22389800	0.98123900	-2.17830700
H	-6.34530500	2.17678100	-2.58200000
H	-8.49626600	1.21141800	-1.78807300
H	-8.49354700	-0.97053600	-0.59201700
H	-6.36975400	-2.16440300	-0.19262500
C	2.43669600	5.67792300	0.86727000
H	3.39825600	5.70417800	1.39705700
H	1.71038300	6.19557000	1.52536800
N	2.62575600	6.37849800	-0.40193700
C	1.36514500	6.60223500	-1.09932700
H	0.67771700	7.27039800	-0.54487200
H	1.56042500	7.05342900	-2.07709700
H	0.85492300	5.64917700	-1.26053300
C	3.35914100	7.62502600	-0.22540600
H	3.53847300	8.08604000	-1.20173700
H	2.82589000	8.36341200	0.40414400
H	4.33008500	7.42363200	0.23799000
C	-3.93567000	-0.54877200	1.79506800
H	-4.83021600	0.01684600	1.50236200
H	-3.46609400	0.02216700	2.60759200
C	-4.35445300	-1.90978300	2.37042800
H	-3.45590600	-2.49535600	2.60352600
H	-4.90314800	-2.49050700	1.62154600
C	-5.21979400	-1.77003800	3.62638800
H	-5.50899500	-2.74904900	4.02115700
H	-4.68417600	-1.23609800	4.41946900
H	-6.13860300	-1.21162900	3.41421700
C	5.20588200	-3.87078700	-0.68687800
H	5.40730300	-4.37418000	0.26824800
H	4.84698800	-4.65719100	-1.37970700
N	6.46545600	-3.27617400	-1.13481900
C	6.36736600	-2.74401300	-2.48952900

Supporting Information

H	7.30295700	-2.24195500	-2.75531000
H	6.17086800	-3.52697800	-3.24729900
H	5.55922000	-2.01057100	-2.54332900
C	7.57189200	-4.21649200	-1.01781800
H	7.45584700	-5.11334400	-1.65675100
H	8.50577400	-3.72172200	-1.30296700
H	7.66866400	-4.55144000	0.01992700
H	5.37508700	-1.41758900	0.49357400
Cat2-TS2'			
N	0.93759100	-1.52329300	-1.07319100
C	2.08805400	-1.89007200	-0.52015300
C	3.04839400	-1.08068100	0.13538600
C	0.30389300	-0.18242700	-1.07935700
C	-0.36438600	-0.14917900	-2.47334100
C	-0.69553700	-1.60983100	-2.84150700
C	0.28740500	-2.46108500	-2.02760100
C	-0.64433500	0.10330800	0.16042100
C	-1.39363100	1.44020800	-0.04761900
C	-1.57362600	-1.09551700	0.41237100
O	0.25829700	0.25252700	1.27122300
Si	0.15326600	1.07813700	2.74919800
C	0.31761700	2.94562100	2.54348000
C	-1.40901400	0.66779200	3.72721300
C	1.64753900	0.45430300	3.70857900
C	-2.64184300	1.68313300	0.54795400
C	-3.26602200	2.92631800	0.45459200
C	-2.67031500	3.97990500	-0.24696600
C	-1.43030300	3.74553600	-0.84832600
C	-0.80049100	2.50647700	-0.74224800
C	-1.17763300	-2.11001600	1.29277200
C	-1.96880300	-3.24293000	1.48871900
C	-3.18506900	-3.40033700	0.81815000
C	-3.58029600	-2.39356100	-0.07115500
C	-2.78662300	-1.26620100	-0.27438900
H	2.34446400	-2.92708100	-0.70957200
H	2.64890400	-0.20289000	0.63457400
H	1.10109600	0.55327900	-1.00240800
H	0.36509300	0.23301200	-3.19128100
H	-1.24292400	0.49630000	-2.49858900
H	-1.72646500	-1.86199900	-2.58976300
H	-0.55015100	-1.77646100	-3.91003500
H	1.08512900	-2.87271800	-2.65345900
H	-0.20567300	-3.26665500	-1.47510500

Supporting Information

H	1.20205900	3.20002300	1.95000100
H	-0.55348900	3.40033000	2.06560900
H	0.44027300	3.40770700	3.53066800
H	-1.29912300	1.04411500	4.75147900
H	-1.57874400	-0.41165200	3.78439200
H	-2.30424700	1.12869300	3.30235700
H	1.72401800	0.97707000	4.66890700
H	1.57405200	-0.61687300	3.91985700
H	2.57906200	0.62942900	3.16145200
H	-3.13943900	0.89030600	1.09333900
H	-0.94552700	4.54178400	-1.40780000
H	0.16282200	2.38389700	-1.22349300
H	-0.23578000	-2.01182600	1.81884600
H	-1.63189000	-4.01585100	2.17570400
H	-4.51414100	-2.51043300	-0.61219900
H	-3.12482300	-0.50636200	-0.97103500
C	4.07593400	-0.20784500	-1.31737300
N	2.95688600	-1.07289200	-3.26518600
O	3.30558100	-2.23464500	-2.86814700
O	2.25434200	-0.91287900	-4.30063700
C	4.66888300	0.99923800	-0.66474100
C	3.91842000	2.16314900	-0.42893000
C	4.49835200	3.28368300	0.16227200
C	5.84375500	3.26358500	0.53810100
C	6.60085300	2.11362600	0.31598500
C	6.01736100	0.99289100	-0.27654000
H	4.76205900	-1.04783300	-1.39517100
H	2.86917500	2.19020000	-0.70940500
H	3.89954300	4.17418400	0.33159400
H	6.29536700	4.13614800	1.00065700
H	7.64852800	2.08685200	0.60148900
H	6.61641900	0.10466000	-0.45687500
C	-4.07615800	-4.59927200	1.08232500
H	-4.88309400	-4.29257900	1.76129100
H	-3.49598000	-5.37216900	1.62483300
N	-4.70649000	-5.12996200	-0.12502600
C	-3.74076700	-5.76482400	-1.01490800
H	-3.26474100	-6.65874900	-0.56743700
H	-4.23945500	-6.07336700	-1.93880100
H	-2.95184100	-5.05500500	-1.27554400
C	-5.80401700	-6.03393600	0.19293000
H	-6.29199300	-6.35731200	-0.73184000
H	-5.48214900	-6.94130100	0.73981200
H	-6.54843200	-5.51568000	0.80571900

Supporting Information

C	4.11572100	-1.84318100	0.91187700
H	4.91675100	-1.14691500	1.18714100
H	4.57096000	-2.58532800	0.24038400
C	3.62587200	-2.56369500	2.17900400
H	2.82314100	-3.26386600	1.91118500
H	3.17933400	-1.83478500	2.86375700
C	4.74809200	-3.32132600	2.89618000
H	4.37724300	-3.83131800	3.79115200
H	5.19643900	-4.07850800	2.24296500
H	5.54813000	-2.64097700	3.20933200
C	3.33146300	0.00348100	-2.50803700
H	2.97351600	0.96079500	-2.85611200
C	-3.32648900	5.34629900	-0.31012100
H	-3.14750500	5.86274100	0.64249600
H	-2.82590700	5.95614100	-1.08844600
N	-4.77386600	5.28501100	-0.50334900
C	-5.40891500	6.56424300	-0.21413500
H	-5.08533800	7.37821000	-0.89120300
H	-6.49462200	6.46335500	-0.30810600
H	-5.18427500	6.86889500	0.81295500
C	-5.12953800	4.80860500	-1.83583300
H	-6.21609100	4.70118700	-1.90923900
H	-4.79753800	5.49258400	-2.64046800
H	-4.67849900	3.82951700	-2.01517800
H	-4.23681700	3.08618200	0.91340700
Cat2-TS3'			
N	-1.17801500	-0.13901400	-0.77997200
C	-1.94580600	-0.30862800	0.28772400
C	-3.35251300	-0.12275200	0.32142400
C	0.22053400	-0.65942300	-0.90341900
C	0.60099200	-0.29747300	-2.35540600
C	-0.73919500	-0.19199900	-3.09142100
C	-1.63421500	0.46838800	-2.04749000
C	1.21169000	-0.17348400	0.22647500
C	2.64509200	-0.67442300	-0.05636900
C	1.15155700	1.36218500	0.36188800
O	0.73851000	-0.72655100	1.45672400
Si	1.09509200	-2.04194800	2.46805200
C	1.25016700	-3.69380700	1.58319800
C	2.63671800	-1.67878400	3.49533100
C	-0.41447100	-2.08551400	3.59587600
C	3.74677200	-0.00948900	0.50810600
C	5.04541100	-0.48240200	0.33967600

Supporting Information

C	5.29670600	-1.64333600	-0.40237500
C	4.20530200	-2.31492300	-0.95757800
C	2.90143300	-1.84762700	-0.78009200
C	0.37700500	1.95673600	1.36449600
C	0.26236900	3.34500200	1.45987000
C	0.92372200	4.18944300	0.56521800
C	1.71240300	3.60096800	-0.43089200
C	1.82606400	2.21600000	-0.52825200
H	-1.43777300	-0.72015300	1.14681000
H	-3.76334200	0.56420300	-0.41573300
H	0.13362800	-1.74721000	-0.80660200
H	1.25878900	-1.04755700	-2.79300900
H	1.11650100	0.66459000	-2.39253200
H	-0.67561000	0.39086200	-4.01417200
H	-1.11453000	-1.19323500	-3.32178700
H	-2.69439000	0.28368400	-2.20495500
H	-1.46730000	1.55353100	-1.99866400
H	0.41370600	-3.83798600	0.89151100
H	2.19142300	-3.79980400	1.03844300
H	1.20892700	-4.49491900	2.33209500
H	2.77605800	-2.46328000	4.24888100
H	2.54572700	-0.72345600	4.02348700
H	3.54178200	-1.63898800	2.88286500
H	-0.27696300	-2.81820000	4.39928300
H	-0.60310500	-1.11302000	4.06313400
H	-1.30476500	-2.37997100	3.03040100
H	3.58577200	0.89146100	1.08950000
H	4.36878000	-3.22051400	-1.53658600
H	2.08978100	-2.42447700	-1.20817900
H	-0.13031500	1.32344900	2.08094400
H	-0.35015500	3.77479700	2.24924700
H	2.23742500	4.24254700	-1.13184900
H	2.48271800	1.79968000	-1.28452600
C	-4.07369500	-1.83659100	-0.43545600
C	-3.22217100	-2.40523900	-1.41888300
N	-2.03553200	-2.96316200	-1.03623500
O	-1.21829500	-3.39504000	-1.89788400
O	-1.75690300	-2.98817600	0.20818200
C	-5.46317800	-1.48214000	-0.85020600
C	-5.73463900	-0.79610400	-2.04580100
C	-7.04241900	-0.49306400	-2.41783100
C	-8.11118200	-0.86568900	-1.59888100
C	-7.85845400	-1.54467300	-0.40727200
C	-6.54746400	-1.84655800	-0.03670300

Supporting Information

H	-4.01347400	-2.34179300	0.52503400
H	-3.39616500	-2.37796800	-2.48386600
H	-4.91370600	-0.49880200	-2.69277200
H	-7.22874700	0.03635600	-3.34785900
H	-9.13038400	-0.62773400	-1.88836400
H	-8.68136500	-1.84316600	0.23574400
H	-6.35885000	-2.38716600	0.88657600
C	0.84848700	5.69785600	0.70455000
H	1.78435700	6.05763700	1.15250600
H	0.04431600	5.95958300	1.42091100
N	0.69105700	6.38966800	-0.57474900
C	-0.61680000	6.14703400	-1.17199100
H	-1.45027200	6.55164800	-0.56519700
H	-0.66154000	6.61283600	-2.16144000
H	-0.77664100	5.07270400	-1.29323500
C	0.95732400	7.81639300	-0.45078700
H	0.89636800	8.28835500	-1.43657300
H	0.24740800	8.33995600	0.21866200
H	1.96815100	7.97437100	-0.06159900
C	-3.99044300	0.01932200	1.69302600
H	-3.52888800	-0.69897900	2.38413700
H	-5.05159800	-0.25054100	1.62705300
C	-3.88403900	1.43667000	2.28277300
H	-4.33381600	2.15120000	1.58030300
H	-2.82640400	1.71875800	2.36433900
C	-4.56271200	1.56525700	3.64985700
H	-4.47517300	2.58244700	4.04507100
H	-5.62979100	1.32403200	3.58646400
H	-4.11342500	0.88424500	4.38142100
C	6.70735600	-2.18059100	-0.55052000
H	6.99824200	-2.66385400	0.39174800
H	6.71662300	-2.97733300	-1.32061300
N	7.69599000	-1.13838900	-0.82437700
C	9.05590200	-1.62151000	-0.62576400
H	9.33796000	-2.43895600	-1.31743700
H	9.76237900	-0.79897200	-0.77551600
H	9.17522700	-1.98893800	0.39844700
C	7.52964100	-0.56019800	-2.15291800
H	8.23398100	0.26718800	-2.28405000
H	7.70439200	-1.29085300	-2.96642800
H	6.51660700	-0.16551300	-2.26323200
H	5.88366300	0.05588800	0.77111400

Cat2-TS4'

Supporting Information

N	0.52265100	-1.22068500	-0.87968400
C	1.42360700	-0.58956900	-0.13758600
C	2.60470500	-1.12072100	0.45537700
C	-0.46122900	-0.49404700	-1.74235100
C	-0.96338200	-1.58737900	-2.71257100
C	0.12548100	-2.66791300	-2.69166100
C	0.59455100	-2.64914700	-1.23741600
C	-1.64681800	0.24997600	-1.00689700
C	-2.38620300	-0.73422200	-0.08184500
C	-1.22769800	1.53392100	-0.25795100
O	-2.54961500	0.59948800	-2.06016500
Si	-2.73050800	1.87944400	-3.14705100
C	-4.15738100	1.28375300	-4.22438500
C	-3.21869200	3.49213300	-2.30467100
C	-1.19673900	2.13545000	-4.21608100
C	-3.62086200	-1.28415700	-0.45161000
C	-4.27422900	-2.20448200	0.36812400
C	-3.71434000	-2.61056800	1.58395300
C	-2.48096100	-2.06438100	1.95469100
C	-1.83088500	-1.13631400	1.14164700
C	-0.11792200	2.30708200	-0.63317100
C	0.16977800	3.51313600	0.01270000
C	-0.65400100	4.00616700	1.02678200
C	-1.77457800	3.24686600	1.39114800
C	-2.05242500	2.03582300	0.76414300
H	1.22216700	0.46172000	0.01575800
H	2.65608900	-2.20685900	0.51398200
H	0.11543700	0.24964900	-2.29445300
H	-1.13175600	-1.17948700	-3.70957800
H	-1.91119900	-2.00140900	-2.35996800
H	-0.24321500	-3.65095800	-2.99662500
H	0.95702900	-2.39418000	-3.34970900
H	1.60558800	-3.03245800	-1.10219200
H	-0.08390100	-3.21566400	-0.58679200
H	-3.91350600	0.34429700	-4.73106400
H	-5.05935900	1.11593000	-3.62651000
H	-4.40187600	2.02422900	-4.99439700
H	-3.49677900	4.23215600	-3.06498100
H	-2.40690800	3.91356800	-1.70639600
H	-4.08256100	3.35008500	-1.64742200
H	-1.39346400	2.92477600	-4.95171700
H	-0.31599300	2.43850900	-3.64251800
H	-0.93698700	1.22975200	-4.77486400
H	-4.07153200	-0.97255200	-1.38587700

Supporting Information

H	-2.02582900	-2.35808500	2.89774600
H	-0.89177900	-0.71083500	1.47653900
H	0.57642200	1.98635600	-1.40361400
H	1.06176500	4.05696700	-0.28763300
H	-2.41858300	3.61063200	2.18605900
H	-2.92721700	1.47270800	1.07049400
C	4.00768200	-0.79088200	-0.89061300
C	4.27790200	0.60062100	-1.01696600
N	3.35949000	1.40271400	-1.63273700
O	3.50488000	2.64796100	-1.66354300
O	2.33007700	0.83878300	-2.15392700
C	5.11582400	-1.70359500	-0.47361700
C	5.11429600	-3.02978300	-0.93604500
C	6.12888200	-3.91915300	-0.58775900
C	7.17163700	-3.49989200	0.24006100
C	7.18856100	-2.18581500	0.70987100
C	6.17246700	-1.29759500	0.35833200
H	3.43535400	-1.18262900	-1.72773100
H	5.09110100	1.12998400	-0.54558200
H	4.31181900	-3.36059700	-1.59147500
H	6.10840400	-4.93689600	-0.96677700
H	7.96491800	-4.18925800	0.51331700
H	7.99791200	-1.84756600	1.35040100
H	6.20829400	-0.27852200	0.72877500
C	-0.37426700	5.34400900	1.68370000
H	-1.06854800	6.08804400	1.27065000
H	0.64246900	5.68280100	1.40402700
N	-0.57080800	5.33059800	3.13372000
C	0.43397800	4.52160000	3.81444800
H	1.46024500	4.92086000	3.69878000
H	0.20609900	4.47690900	4.88411500
H	0.42046100	3.50230900	3.42036300
C	-0.61658900	6.68044500	3.67971800
H	-0.82738300	6.63513100	4.75294300
H	0.32821900	7.24171000	3.54420400
H	-1.41926200	7.24960100	3.20005100
C	3.07359100	-0.42887500	1.72737200
H	3.12130600	0.65346800	1.54928300
H	4.09762500	-0.75254700	1.94621200
C	2.19737600	-0.70745200	2.96023200
H	2.10821500	-1.79261200	3.10475500
H	1.17897700	-0.33971600	2.77636200
C	2.74941600	-0.06331300	4.23585600
H	2.10937800	-0.27315200	5.09876300

Supporting Information

H	3.75283300	-0.43884300	4.46592400
H	2.82039700	1.02507000	4.13055800
C	-4.45493200	-3.56316000	2.50395400
H	-5.24845600	-3.00615800	3.01984700
H	-3.76531600	-3.91826200	3.29595400
N	-5.09657700	-4.67129800	1.79792500
C	-4.12434400	-5.60766200	1.24761200
H	-4.64069800	-6.36935600	0.65501400
H	-3.43003100	-5.07807700	0.59048900
H	-3.53277700	-6.12449700	2.02854800
C	-6.07081100	-5.35420800	2.63821600
H	-6.57814700	-6.12996900	2.05596400
H	-5.62273000	-5.83871600	3.52758700
H	-6.82655000	-4.64277600	2.98577100
H	-5.22778600	-2.62616300	0.06543100
Cat2-TS5'			
N	-1.18993900	-0.20626800	-0.65962200
C	0.22320400	-0.68944700	-0.83259700
C	0.56258100	-0.26668700	-2.27521700
C	-0.79268200	-0.22554400	-2.98626300
C	-1.70462500	0.37516700	-1.92096500
C	1.22977700	-0.22552800	0.29330900
C	2.66538300	-0.68935000	-0.03908700
C	1.14650700	1.30316700	0.48539500
O	0.79766700	-0.82981000	1.51332900
Si	1.20746900	-2.15949300	2.48570300
C	1.40576300	-3.78085500	1.55419700
C	2.74776800	-1.77246200	3.50593400
C	-0.28961900	-2.28085000	3.62414900
C	3.76684200	-0.02563400	0.52721200
C	5.07011900	-0.46517000	0.31088200
C	5.32640100	-1.58974800	-0.48358200
C	4.23536600	-2.26186700	-1.03888300
C	2.92726600	-1.82896800	-0.81239100
C	0.38169300	1.84658700	1.52368300
C	0.25088300	3.22870200	1.67566500
C	0.88381400	4.11679200	0.80290100
C	1.66023200	3.57883900	-0.23072400
C	1.79073800	2.20043800	-0.38423900
H	0.15448600	-1.78152100	-0.77303200
H	1.25787600	-0.96369900	-2.74148200
H	1.01864600	0.72596700	-2.29137900
H	-0.77849900	0.37124100	-3.90216900

Supporting Information

H	-1.12022400	-1.24280300	-3.21992100
H	-2.74808900	0.10997200	-2.05718500
H	-1.61106900	1.46851800	-1.87536300
H	0.55824400	-3.93869500	0.87886000
H	2.33580600	-3.83384000	0.98293800
H	1.41549300	-4.60265300	2.28136500
H	2.91968300	-2.56955500	4.23925700
H	2.63326000	-0.83296900	4.05735600
H	3.64438900	-1.69079200	2.88513000
H	-0.12280800	-3.03280700	4.40378800
H	-0.50295200	-1.32881800	4.12181700
H	-1.17626200	-2.58496400	3.05794600
H	3.60211400	0.84833100	1.14740700
H	4.40258400	-3.14052900	-1.65697000
H	2.11669500	-2.40536400	-1.24296700
H	-0.10723500	1.17941600	2.22191400
H	-0.35186700	3.61863500	2.49264200
H	2.16199000	4.25427400	-0.91686400
H	2.43655100	1.82306600	-1.16975700
C	-4.02148800	-2.02111200	-0.13799700
C	-3.25795300	-2.51840300	-1.23592100
N	-2.02275600	-3.04250400	-1.00057700
O	-1.28035200	-3.41239400	-1.95566000
O	-1.61316600	-3.10853000	0.21015400
C	-5.48115600	-1.78316500	-0.33835700
C	-6.02295400	-1.35306800	-1.56105500
C	-7.39525700	-1.15961600	-1.70788800
C	-8.25791500	-1.38444700	-0.63304400
C	-7.73475800	-1.80528000	0.59028800
C	-6.36153900	-1.99998700	0.73370800
H	-3.80446500	-2.56367400	0.77746200
H	-3.53759800	-2.46242000	-2.27660200
H	-5.36819100	-1.17029000	-2.40770200
H	-7.79238200	-0.83273800	-2.66465800
H	-9.32710700	-1.23386500	-0.74891500
H	-8.39587000	-1.98767900	1.43261500
H	-5.96129600	-2.33580900	1.68686900
C	0.78907500	5.61694100	1.00317700
H	1.73338800	5.97593000	1.43372500
H	0.00487800	5.83641700	1.75510600
N	0.57705000	6.35438900	-0.24223300
C	-0.74257900	6.10428900	-0.80977700
H	-1.56626700	6.46481800	-0.16293000
H	-0.82813000	6.60752400	-1.77796100

Supporting Information

H	-0.88184200	5.03206900	-0.96911400
C	0.81398700	7.78107000	-0.06785200
H	0.71048200	8.29102800	-1.03084700
H	0.11381800	8.25905300	0.64457000
H	1.83274400	7.94795400	0.29611700
C	-4.12536000	0.88865500	0.12017100
H	-5.16825000	0.72644700	0.41130200
H	-4.14061800	0.97151400	-0.97034200
C	-4.52100300	3.40795600	0.29231200
H	-4.16474100	4.34482900	0.73267300
H	-4.51620600	3.53080200	-0.79689400
H	-5.56267700	3.26846700	0.60236100
C	6.74366800	-2.08959600	-0.68851400
H	7.06806500	-2.60682300	0.22432800
H	6.75045400	-2.85170200	-1.49289900
N	7.70325600	-1.01501800	-0.94024300
C	9.07739500	-1.47755000	-0.79814100
H	9.35725700	-2.25688200	-1.53327200
H	9.76308600	-0.63433100	-0.92818800
H	9.23087300	-1.88807200	0.20493400
C	7.49055100	-0.38327700	-2.23749000
H	8.17466600	0.46357100	-2.34997100
H	7.65835100	-1.07418800	-3.08638600
H	6.46730500	-0.00556500	-2.30465900
H	5.90763000	0.07254300	0.74442100
C	-3.64966300	2.22378400	0.72238600
H	-2.60591000	2.40848400	0.43999300
H	-3.65341400	2.14348100	1.81757900
C	-1.90485900	-0.45509900	0.42457400
H	-1.33711200	-0.93127000	1.20826000
C	-3.31883700	-0.31428000	0.60773400
H	-3.55135100	-0.50781500	1.65584000
Cat2-TS6'			
N	-0.98213000	-0.02142000	-0.90407400
C	0.40110200	-0.56509100	-1.07436700
C	0.81399600	-0.05972300	-2.47318400
C	-0.51401600	0.19150700	-3.19692500
C	-1.39216000	0.76247700	-2.08517300
C	1.35680200	-0.20710100	0.13274900
C	2.81078900	-0.63736900	-0.15193900
C	1.24882900	1.29930300	0.44641000
O	0.84469100	-0.91656600	1.26255400
Si	1.19369200	-2.33191800	2.13790700

Supporting Information

C	1.37174300	-3.87610000	1.08046500
C	2.71438300	-2.06621100	3.22375900
C	-0.33830100	-2.52211900	3.21842800
C	3.87316800	-0.02868500	0.53762600
C	5.18870300	-0.45002500	0.36351500
C	5.49712600	-1.50090300	-0.50955400
C	4.44538100	-2.11651600	-1.19173300
C	3.12522000	-1.70067500	-1.00875700
C	0.40127900	1.74963100	1.46477700
C	0.24063800	3.11313700	1.71720600
C	0.92305800	4.07413200	0.96698800
C	1.77656000	3.62876400	-0.04968700
C	1.93795300	2.26809800	-0.30305800
H	0.28643000	-1.65361100	-1.07569700
H	1.44465200	-0.78173400	-2.99203600
H	1.37450900	0.87486600	-2.39940500
H	-0.41781300	0.87426100	-4.04541700
H	-0.94048800	-0.75154200	-3.55403300
H	-2.45779600	0.64426000	-2.27062200
H	-1.17740700	1.82549600	-1.92095500
H	0.47387500	-4.04496100	0.47537100
H	2.25328800	-3.86265900	0.43466500
H	1.46969000	-4.73818100	1.75265000
H	2.83812100	-2.91722600	3.90401300
H	2.61035800	-1.16388700	3.83600800
H	3.63206800	-1.97029400	2.63708300
H	-0.14789600	-3.24337100	4.02153900
H	-0.63682000	-1.57742000	3.68468000
H	-1.17806600	-2.91153200	2.63286200
H	3.66644200	0.78492400	1.22383900
H	4.65415700	-2.93701300	-1.87382600
H	2.34292200	-2.23085200	-1.53862000
H	-0.13033900	1.02130500	2.06385700
H	-0.42520000	3.43157100	2.51608700
H	2.31378200	4.36197800	-0.64353600
H	2.64156700	1.96109200	-1.06975600
C	-4.07467700	-1.83964600	-0.66703500
C	-3.68404200	-3.06497100	-0.05621200
N	-2.42066600	-3.54654900	-0.22495000
O	-2.03743300	-4.56948000	0.40021600
O	-1.63174000	-2.90862300	-1.00665900
C	-5.53270000	-1.52029400	-0.62976600
C	-6.16792900	-1.02315700	-1.77810500
C	-7.53621400	-0.74852100	-1.78332600

Supporting Information

C	-8.29685100	-0.96189100	-0.63407400
C	-7.67807100	-1.45148200	0.51924200
C	-6.31187000	-1.72446800	0.52227000
H	-3.61873800	-1.66901500	-1.63935300
H	-4.28066100	-3.60759200	0.66091500
H	-5.58446900	-0.87015200	-2.68226500
H	-8.00674000	-0.37235000	-2.68719800
H	-9.36181400	-0.74955300	-0.63490700
H	-8.26196700	-1.62011500	1.41950900
H	-5.84264600	-2.09828500	1.42749700
C	0.79541300	5.55283000	1.27864800
H	1.71145800	5.88728700	1.78343300
H	-0.02859900	5.70367600	2.00438500
N	0.63511500	6.38304300	0.08460900
C	-0.65153400	6.16602400	-0.56561000
H	-1.51070200	6.46702600	0.06517700
H	-0.69560200	6.74278100	-1.49479500
H	-0.76841000	5.10823400	-0.81443900
C	0.84448600	7.79435800	0.37931500
H	0.77967500	8.37562800	-0.54591900
H	0.10495200	8.20940800	1.09135700
H	1.84245400	7.94254800	0.80400500
C	-3.83945000	1.04639100	-0.15998600
H	-4.42071700	0.95426500	-1.08732000
H	-3.06672900	1.79917800	-0.35454900
C	-5.42139600	2.91957900	0.55586800
H	-6.05923500	3.29507600	1.36235800
H	-4.67362500	3.69103500	0.33760800
H	-6.04808700	2.80274800	-0.33527100
C	6.92374600	-1.99296600	-0.66238700
H	7.17717800	-2.60491800	0.21356900
H	6.98499000	-2.66987200	-1.53781600
N	7.90536500	-0.91192500	-0.73193400
C	9.26216800	-1.40516000	-0.53591700
H	9.59079200	-2.11156400	-1.32262900
H	9.96113300	-0.56293400	-0.52972900
H	9.33757600	-1.91527800	0.42957300
C	7.79430100	-0.14880200	-1.96988300
H	8.49085900	0.69497300	-1.94517500
H	8.01947600	-0.75271900	-2.87037000
H	6.78158900	0.24903500	-2.07256100
H	5.99652700	0.04270000	0.89559000
C	-3.19000700	-0.28825800	0.22491200
H	-3.45761100	-0.59621300	1.23334000

Supporting Information

C	-1.79931800	-0.53304300	0.00813100
H	-1.30345800	-1.21751600	0.67809200
C	-4.76050400	1.59382000	0.94176800
H	-4.17300000	1.72633300	1.86012000
H	-5.53232000	0.85158500	1.17149000
Cat2-TS1"			
N	-1.39700900	0.69652000	-0.43950000
C	-2.49450700	0.38542200	0.23706100
C	-2.94989300	-0.91788000	0.58703700
C	-0.22536100	-0.17509000	-0.71828000
C	0.21117900	0.25405600	-2.14445700
C	-0.64069900	1.49341900	-2.52069700
C	-1.28434900	1.95249400	-1.20457300
C	0.90109000	-0.11284800	0.39829600
C	2.05476200	-1.06030200	-0.00167000
C	1.37536000	1.34228400	0.59975900
O	0.25579700	-0.52720300	1.59657900
Si	0.65518100	-1.58543100	2.87457900
C	0.73468100	-3.37216200	2.30318300
C	2.24161400	-1.07401100	3.76085800
C	-0.78235900	-1.33399700	4.06446400
C	3.35297300	-0.84870000	0.49721900
C	4.39752200	-1.72214600	0.20599200
C	4.18491200	-2.84561100	-0.60226300
C	2.89656300	-3.06240700	-1.09685800
C	1.84177100	-2.19723100	-0.79961600
C	0.80748400	2.12149100	1.61708700
C	1.15992600	3.46087900	1.78870600
C	2.09656100	4.06698000	0.94292600
C	2.69886600	3.28303500	-0.05465300
C	2.33892100	1.94824900	-0.22770900
H	-3.19107800	1.21404800	0.35652000
H	-2.15885500	-1.66155700	0.66749800
H	-0.56334900	-1.20659100	-0.68124100
H	0.02813800	-0.57140500	-2.83466300
H	1.27828700	0.47436400	-2.17848400
H	-0.05264600	2.29586500	-2.97917000
H	-1.41825200	1.21402600	-3.23559300
H	-2.27135500	2.40223900	-1.32772900
H	-0.64351700	2.66047300	-0.66857600
H	-0.10128700	-3.61643500	1.63961900
H	1.65861300	-3.59216900	1.76217500
H	0.68524100	-4.04127900	3.17033200

Supporting Information

H	2.29884500	-1.60633100	4.71779200
H	2.25762300	-0.00168300	3.98504400
H	3.14245100	-1.31966300	3.19413500
H	-0.62254600	-1.92146400	4.97554300
H	-0.88405100	-0.28535200	4.36473700
H	-1.73286400	-1.65455900	3.63005500
H	3.55733900	0.00771100	1.13120000
H	2.69903100	-3.92525800	-1.72711900
H	0.86595400	-2.45254100	-1.19874900
H	0.08640400	1.65820900	2.27833900
H	0.71277100	4.02855500	2.60138600
H	3.48197900	3.70843300	-0.67928300
H	2.85340100	1.35800800	-0.97626000
C	-3.76107900	-1.58304900	-0.91530900
C	-2.90398900	-1.66080700	-2.07229300
N	-1.81353700	-2.47309100	-2.08137800
O	-1.07841500	-2.53602600	-3.10712300
O	-1.50032600	-3.10233300	-1.01125200
C	-5.06530800	-0.87735600	-1.16598200
C	-5.11122200	0.39516000	-1.75760900
C	-6.32637200	1.03259700	-2.00305500
C	-7.52729400	0.40785200	-1.66044400
C	-7.49948700	-0.85886900	-1.07769200
C	-6.28026400	-1.49294300	-0.83313100
H	-3.90123800	-2.56591100	-0.46396000
H	-3.08524200	-1.12812700	-2.99327400
H	-4.18408100	0.88218900	-2.04965600
H	-6.33810800	2.01452400	-2.46765700
H	-8.47484300	0.90193000	-1.85177900
H	-8.42712800	-1.35903300	-0.81632700
H	-6.27274600	-2.48659100	-0.39453100
C	2.47469900	5.51501200	1.08827000
H	3.51729100	5.67891900	0.80646200
H	2.32791700	5.88948900	2.10462800
N	1.65232100	6.43319100	0.17253500
C	0.23687700	6.58325500	0.63831100
H	0.23065700	7.10807900	1.59519200
H	-0.31811000	7.15410200	-0.10615700
H	-0.20281300	5.59332300	0.74639600
C	2.31274200	7.76491700	-0.00377200
H	1.70315300	8.38072000	-0.66584400
H	2.40672000	8.25030700	0.96898700
H	3.30073100	7.61798000	-0.44107800
C	-3.94014500	-0.95682800	1.76080300

Supporting Information

H	-4.85486500	-0.41087700	1.49682200
H	-3.49466000	-0.41705400	2.60635100
C	-4.30497200	-2.36720600	2.24759800
H	-3.38498600	-2.92811700	2.45720800
H	-4.82085700	-2.92449500	1.45854600
C	-5.18961900	-2.33825300	3.49780000
H	-5.43860400	-3.35070600	3.82886400
H	-4.68774900	-1.83047600	4.32913900
H	-6.13007300	-1.81010500	3.30594800
C	5.31078500	-3.82270000	-0.88444900
H	5.43533400	-4.46732100	-0.00443900
H	5.01478000	-4.49143200	-1.71565700
N	6.59365100	-3.16599500	-1.12907700
C	6.61250600	-2.47082700	-2.41218700
H	7.55715700	-1.92953300	-2.52272700
H	6.50717300	-3.15512500	-3.27520100
H	5.79603300	-1.74480100	-2.45516000
C	7.70675700	-4.10392900	-1.02415000
H	7.67170000	-4.91037400	-1.78015200
H	8.65104500	-3.56591900	-1.15156800
H	7.71155700	-4.56707200	-0.03273300
H	5.39556700	-1.53438300	0.58930700
H	1.59426900	5.96501100	-0.76191400
H	1.37525300	4.10245800	-2.04911100
O	1.10827100	5.02754400	-2.15492600
H	1.18056400	5.22687800	-3.09792600
Cat2-TS2"			
N	-0.91342300	1.36131600	-0.88200200
C	-2.09512900	1.69070200	-0.35744600
C	-3.09204900	0.82472500	0.16583700
C	-0.28104900	0.02413300	-0.95845500
C	0.39778500	0.05691700	-2.34637900
C	0.69482000	1.53847900	-2.66783500
C	-0.23803900	2.35218400	-1.75475900
C	0.65639700	-0.32278500	0.28183500
C	1.43589900	-1.62753400	0.01415000
C	1.56589900	0.88449000	0.57403900
O	-0.24486400	-0.50364500	1.37624800
Si	-0.19505400	-1.46329100	2.78849600
C	-0.35505600	-3.30284900	2.42971200
C	1.34371900	-1.12400100	3.82866700
C	-1.71158200	-0.89680300	3.74208300
C	2.68347300	-1.87230100	0.61089900

Supporting Information

C	3.34087200	-3.09117900	0.45251000
C	2.77858100	-4.11703100	-0.31502300
C	1.53825700	-3.88004100	-0.91579000
C	0.87549800	-2.66533400	-0.74748400
C	1.16780100	1.84054200	1.51823400
C	1.91492300	2.99779900	1.73304600
C	3.07929500	3.24319200	0.99326800
C	3.49855200	2.27681200	0.06739300
C	2.75368900	1.11768600	-0.13737500
H	-2.33096700	2.74491100	-0.44559700
H	-2.71173600	-0.09141400	0.61005100
H	-1.07278200	-0.72006100	-0.92046300
H	-0.31516800	-0.30931200	-3.08732600
H	1.28983000	-0.56805500	-2.39084100
H	1.75071900	1.76300300	-2.47723100
H	0.47328200	1.74456600	-3.71538400
H	-1.02353600	2.85052600	-2.33119200
H	0.29672700	3.08753400	-1.14143400
H	-1.21492000	-3.51040300	1.78450700
H	0.53435900	-3.72928000	1.96056800
H	-0.52152000	-3.83235000	3.37553600
H	1.21567700	-1.59332100	4.81126100
H	1.49825200	-0.05318800	3.99683500
H	2.25497100	-1.53630000	3.38818100
H	-1.80503200	-1.47377400	4.66904300
H	-1.65431700	0.16074700	4.01731500
H	-2.62962600	-1.04974300	3.16654000
H	3.15430100	-1.10637600	1.21690700
H	1.07899300	-4.65533300	-1.52340300
H	-0.08790100	-2.54190900	-1.22876000
H	0.26029600	1.66809900	2.08252200
H	1.58922000	3.70741900	2.48984000
H	4.41973300	2.42340300	-0.49159200
H	3.10859700	0.38212700	-0.85007000
C	-4.03475800	0.10173600	-1.35498900
N	-2.80182300	1.12032600	-3.15091400
O	-3.14891700	2.24517500	-2.64388000
O	-2.04120200	1.06349000	-4.15874200
C	-4.66915200	-1.15825500	-0.85289100
C	-3.93592700	-2.34434400	-0.68674900
C	-4.55186000	-3.51047300	-0.23689800
C	-5.91652300	-3.51264100	0.06223100
C	-6.65701800	-2.34123900	-0.09378400
C	-6.03734000	-1.17456600	-0.54378800

Supporting Information

H	-4.72404500	0.94199700	-1.41057100
H	-2.87329200	-2.35617200	-0.91572500
H	-3.96868200	-4.41940200	-0.12073400
H	-6.39695900	-4.42081100	0.41291500
H	-7.71923400	-2.33371100	0.13119800
H	-6.62340000	-0.26930400	-0.67540300
C	3.87650200	4.50606200	1.16826400
H	4.93375200	4.33350300	0.95599400
H	3.78934900	4.92597900	2.17389200
N	3.43917100	5.61773500	0.20456000
C	2.12498300	6.22355300	0.58922600
H	2.23456900	6.73715900	1.54588300
H	1.82650400	6.93220600	-0.18349200
H	1.38283500	5.43113300	0.66782200
C	4.49963700	6.66425100	0.05975000
H	4.15231200	7.42972700	-0.63482000
H	4.69694800	7.11278800	1.03474200
H	5.40713300	6.19981900	-0.32681700
C	-4.18256700	1.52553900	0.97319900
H	-5.00471800	0.82039400	1.13852100
H	-4.59444100	2.33951800	0.36020200
C	-3.74126400	2.10109300	2.32812600
H	-2.90704400	2.80010300	2.17291000
H	-3.35070700	1.29462800	2.95752100
C	-4.88140500	2.81691800	3.05961900
H	-4.54912200	3.21709000	4.02263500
H	-5.27178200	3.65195700	2.46737700
H	-5.71484700	2.13357800	3.25497900
C	-3.23056600	-0.01239600	-2.52888500
H	-2.89399400	-0.94176800	-2.96329000
C	3.47068200	-5.46174700	-0.44299400
H	3.26059800	-6.04176900	0.46525300
H	3.01735800	-6.02858900	-1.27961100
N	4.92134600	-5.35060700	-0.56535800
C	5.58564200	-6.62069600	-0.28860800
H	5.31783600	-7.41945900	-1.00483900
H	6.66986900	-6.48159200	-0.33164500
H	5.32773400	-6.96487500	0.71756700
C	5.31958900	-4.82040900	-1.86604500
H	6.40425300	-4.67939700	-1.88842900
H	5.04322800	-5.48631700	-2.70505300
H	4.84734500	-3.84873100	-2.03516500
H	4.30998200	-3.25702900	0.91224200
H	3.28330300	5.18016300	-0.73331600

Supporting Information

O	2.73895200	4.54249600	-2.24402900
H	2.37067500	3.64893400	-2.29146900
H	2.59407800	4.94015200	-3.11226900
Cat2-TS3"			
N	-1.04539700	-0.30469800	-0.75467900
C	-1.80303400	-0.56449000	0.30758200
C	-3.22671900	-0.50812800	0.32709300
C	0.38599600	-0.73132600	-0.88594200
C	0.73776600	-0.33367400	-2.33461200
C	-0.60696900	-0.35034600	-3.06902300
C	-1.55680800	0.23922200	-2.03058700
C	1.34679600	-0.21017300	0.25738300
C	2.81316800	-0.58297800	-0.04325700
C	1.16638000	1.31581100	0.41443200
O	0.91427700	-0.79712200	1.47664300
Si	1.36340500	-2.13021500	2.45700200
C	1.64085800	-3.72863400	1.51340800
C	2.87148500	-1.66948300	3.48973300
C	-0.14839300	-2.30023500	3.56517300
C	3.86079700	0.15368000	0.53535400
C	5.19241800	-0.20495600	0.34465000
C	5.53064200	-1.32199800	-0.42967500
C	4.49265300	-2.06772500	-0.99414200
C	3.15651700	-1.71383700	-0.79819200
C	0.36803900	1.82583900	1.44563900
C	0.12482600	3.19403700	1.56585300
C	0.67259200	4.10105800	0.65207100
C	1.52248700	3.60502600	-0.34979000
C	1.76408300	2.23677600	-0.46520500
H	-1.26277000	-0.91607400	1.17303600
H	-3.67939100	0.15668200	-0.40703100
H	0.37109600	-1.82414500	-0.80237100
H	1.46116100	-1.01998300	-2.77169100
H	1.17163200	0.66988500	-2.37511400
H	-0.59668100	0.21878700	-4.00271000
H	-0.89216100	-1.38434100	-3.28183400
H	-2.59461300	-0.04293200	-2.18712400
H	-1.49991500	1.33983900	-2.00150000
H	0.81646800	-3.91672700	0.81835400
H	2.58701100	-3.74629200	0.96730900
H	1.66280300	-4.55346500	2.23652500
H	3.06817100	-2.45685700	4.22691100
H	2.71250900	-0.73600900	4.04045500

Supporting Information

H	3.77246900	-1.55358100	2.88087200
H	0.03113200	-3.04965100	4.34401300
H	-0.40154900	-1.36000800	4.06711300
H	-1.01395900	-2.63332300	2.98322200
H	3.63595800	1.01511300	1.15588600
H	4.72476500	-2.94353700	-1.59443300
H	2.39099500	-2.34707300	-1.23150800
H	-0.04789400	1.13553100	2.16730300
H	-0.48773000	3.55227700	2.38968500
H	2.02597000	4.29370600	-1.02526500
H	2.46854000	1.88967000	-1.21194700
C	-3.82237500	-2.21248200	-0.40354100
C	-2.93901600	-2.71561200	-1.40513800
N	-1.70152300	-3.14434700	-1.03701300
O	-0.84562900	-3.50006600	-1.89764700
O	-1.40693000	-3.11086100	0.20820900
C	-5.24305700	-1.97934400	-0.80991300
C	-5.57825900	-1.31432000	-2.00081200
C	-6.90957500	-1.12876800	-2.36710000
C	-7.93639700	-1.59999100	-1.54537600
C	-7.61961600	-2.25882800	-0.35766900
C	-6.28535600	-2.44332300	0.00700300
H	-3.72123800	-2.73592200	0.54485200
H	-3.14283200	-2.73066500	-2.46510900
H	-4.79049900	-0.94645300	-2.65371100
H	-7.14777600	-0.61877300	-3.29597100
H	-8.97381200	-1.45673700	-1.83146600
H	-8.40987700	-2.63532300	0.28476300
H	-6.04596400	-2.97188100	0.92551200
C	0.36952300	5.57143300	0.72245400
H	1.19984100	6.16465700	0.33273900
H	0.14809700	5.91000200	1.73798500
N	-0.84924600	5.95956800	-0.12929700
C	-2.14006100	5.48591500	0.46621200
H	-2.30345200	5.99742200	1.41638000
H	-2.94877000	5.71615700	-0.22743800
H	-2.08288300	4.40972600	0.61868100
C	-0.88056900	7.43113800	-0.39929900
H	-1.75089200	7.66301600	-1.01399500
H	-0.94496300	7.96759500	0.54874700
H	0.03062400	7.71744700	-0.92532600
C	-3.87182200	-0.39211800	1.70108000
H	-3.37337000	-1.08209800	2.39473100
H	-4.91614200	-0.71786900	1.63430300

Supporting Information

C	-3.84204700	1.03035100	2.28553700
H	-4.32910100	1.71646400	1.57799000
H	-2.79861200	1.36633400	2.36889500
C	-4.52852400	1.12917900	3.65135300
H	-4.49620300	2.15022900	4.04540200
H	-5.58075800	0.83299900	3.58615200
H	-4.04639700	0.47441700	4.38511000
C	6.98004700	-1.73897300	-0.59558900
H	7.29633100	-2.25358800	0.32113800
H	7.05530300	-2.48675000	-1.40894100
N	7.88226600	-0.60712800	-0.79501400
C	9.27478200	-0.98045200	-0.56779000
H	9.64445100	-1.74491100	-1.27633600
H	9.91045100	-0.09557000	-0.66778200
H	9.39478600	-1.37124900	0.44722400
C	7.70797800	0.00294600	-2.10901300
H	8.34502300	0.88886500	-2.18976700
H	7.96597600	-0.68104200	-2.93966900
H	6.66883500	0.31755600	-2.23964800
H	5.98966000	0.38463800	0.78600400
H	-0.76073400	5.45148800	-1.03966000
O	-0.87344900	4.23549200	-2.29735900
H	-0.94244800	4.32243100	-3.25730100
H	-0.21059800	3.54828000	-2.12948500
Cat2-TS4"			
N	0.35219500	-1.17845800	-0.96472200
C	1.39002100	-0.76315700	-0.23401700
C	2.45463000	-1.54433300	0.31057400
C	-0.47238400	-0.22675200	-1.77688000
C	-1.20822600	-1.15115800	-2.76936700
C	-0.30432700	-2.38354200	-2.88433700
C	0.20700000	-2.56244300	-1.45535400
C	-1.45398400	0.74453600	-1.00454800
C	-2.39377600	-0.07321400	-0.09756600
C	-0.75684000	1.86641700	-0.20453500
O	-2.27043100	1.31459000	-2.02485300
Si	-2.13481300	2.63960000	-3.08895600
C	-3.67933300	2.42684800	-4.14594500
C	-2.20496400	4.29130600	-2.19361200
C	-0.59829100	2.51712200	-4.17140500
C	-3.75565500	-0.19510500	-0.40872200
C	-4.61945500	-0.91568800	0.41563400
C	-4.14168200	-1.55905500	1.56694700

Supporting Information

C	-2.78255600	-1.43342500	1.88485900
C	-1.92524800	-0.69744600	1.06862400
C	0.49013900	2.38975200	-0.58021700
C	1.05162600	3.46949800	0.10612100
C	0.37780100	4.08487600	1.16395200
C	-0.87738700	3.57866000	1.52816600
C	-1.43205600	2.49181800	0.85846100
H	1.36757500	0.28841600	0.01636400
H	2.28797300	-2.62123100	0.30877000
H	0.23641000	0.39901600	-2.32087600
H	-1.37244600	-0.65486200	-3.72527000
H	-2.18951700	-1.43530800	-2.37442000
H	-0.82566200	-3.26929100	-3.25729000
H	0.53871800	-2.17721100	-3.55115500
H	1.15550000	-3.09550000	-1.40222400
H	-0.52185800	-3.09789100	-0.83064000
H	-3.68570100	1.46299100	-4.66555100
H	-4.59056200	2.49137500	-3.54156500
H	-3.73522000	3.21246700	-4.90748000
H	-2.31808200	5.09646700	-2.92931600
H	-1.30153400	4.49352200	-1.61326100
H	-3.06163300	4.34166900	-1.51401700
H	-0.59641100	3.34883700	-4.88617000
H	0.33921800	2.57355400	-3.61069100
H	-0.58462900	1.59177000	-4.75756000
H	-4.12886900	0.31720400	-1.28660400
H	-2.39269600	-1.88315800	2.79480000
H	-0.89054000	-0.58351400	1.36560400
H	1.07971100	1.95714400	-1.38197700
H	2.03715400	3.81232200	-0.19749500
H	-1.40574700	4.04153300	2.35578700
H	-2.41018800	2.13559400	1.16507300
C	3.90422600	-1.44439300	-0.96718700
C	4.38941500	-0.10538100	-1.06920600
N	3.59131800	0.83229500	-1.64663400
O	3.90050700	2.04638300	-1.66758900
O	2.46970800	0.42220400	-2.13856900
C	4.85539500	-2.52347900	-0.55568200
C	4.65590300	-3.82451000	-1.04482200
C	5.51861900	-4.86477100	-0.70526800
C	6.60300500	-4.62364700	0.13989300
C	6.81522800	-3.33669400	0.63653100
C	5.95061700	-2.29742700	0.29438400
H	3.30351400	-1.72935000	-1.82766400

Supporting Information

H	5.28576000	0.28043000	-0.60948900
H	3.82252100	-4.01663300	-1.71709000
H	5.35037600	-5.85978000	-1.10659700
H	7.28013800	-5.42994300	0.40455900
H	7.66038700	-3.13825400	1.28876300
H	6.13789300	-1.30302600	0.68605200
C	0.96085400	5.29460600	1.86972100
H	0.46744000	6.19324400	1.47668200
H	2.03116600	5.39083700	1.60424800
N	0.74436200	5.27641100	3.31543200
C	1.55325800	4.25624900	3.97453000
H	2.64024600	4.44149000	3.88234300
H	1.30469500	4.22207400	5.03972900
H	1.33915300	3.27430900	3.54335900
C	0.96898100	6.58984100	3.91007900
H	0.73839100	6.55108600	4.97907400
H	2.00974100	6.94793400	3.80099400
H	0.30583900	7.32676100	3.44672000
C	3.01182200	-1.03323100	1.63551800
H	3.27734000	0.02614400	1.52575200
H	3.94341600	-1.56610500	1.85384900
C	2.05911000	-1.19981400	2.83078900
H	1.75789500	-2.25372100	2.91031700
H	1.13768900	-0.62909300	2.64536400
C	2.68094600	-0.74145900	4.15352100
H	1.98487000	-0.86753600	4.98887300
H	3.58491700	-1.31502600	4.38487500
H	2.96262200	0.31625100	4.11186800
C	-5.08445900	-2.32717600	2.45129600
H	-6.07176300	-1.85965800	2.47505000
H	-4.71769700	-2.41217000	3.47764400
N	-5.32616000	-3.76182000	1.96619300
C	-4.10861200	-4.62349400	2.09542100
H	-4.31201800	-5.58789200	1.62992400
H	-3.27843900	-4.13469100	1.58834900
H	-3.87755100	-4.75794100	3.15354400
C	-6.50589300	-4.37776300	2.65055100
H	-6.65534000	-5.38672900	2.26483400
H	-6.31759700	-4.41716400	3.72466000
H	-7.39012000	-3.77131900	2.45218400
H	-5.68057900	-0.95042700	0.17663400
H	-5.53453500	-3.71012800	0.94164600
H	-5.06786300	-2.99855400	-1.17484800
O	-5.52944900	-3.75698800	-0.78965700

Supporting Information

H	-6.22156900	-4.00208600	-1.41763900
Cat2-TS5"			
N	-1.11016200	-0.29509200	-0.60804200
C	0.32405400	-0.70671000	-0.81044500
C	0.62896000	-0.23519600	-2.24506700
C	-0.73463700	-0.23628600	-2.94160000
C	-1.66559900	0.28782800	-1.85209600
C	1.32883500	-0.24625200	0.31992100
C	2.77195600	-0.66578000	-0.03136500
C	1.20953300	1.28080100	0.51650200
O	0.91192200	-0.84678300	1.53833600
Si	1.37282300	-2.18285900	2.50817700
C	1.66903700	-3.76790000	1.54903300
C	2.86720600	-1.71534100	3.55690400
C	-0.14342700	-2.38336600	3.60650600
C	3.85900300	-0.00467100	0.56626900
C	5.17110900	-0.40875500	0.33550900
C	5.44954700	-1.49599100	-0.50252400
C	4.37235500	-2.16493300	-1.08900200
C	3.05538000	-1.76764100	-0.85076100
C	0.41869100	1.79589800	1.55101900
C	0.24361100	3.17063100	1.71328400
C	0.85394400	4.07771700	0.83990200
C	1.68566000	3.57160900	-0.17189200
C	1.85751600	2.19761900	-0.33097700
H	0.30264300	-1.80178000	-0.77737000
H	1.34761700	-0.89032200	-2.73494800
H	1.04875800	0.77563400	-2.24707200
H	-0.75940600	0.38072800	-3.84414000
H	-1.01202900	-1.26264700	-3.19752600
H	-2.69458500	-0.02442800	-1.99221500
H	-1.63407800	1.38653500	-1.78138500
H	0.84590400	-3.95850700	0.85267600
H	2.61256300	-3.76686200	0.99809800
H	1.70398500	-4.60033600	2.26278900
H	3.06146400	-2.50296200	4.29441400
H	2.69702000	-0.78396900	4.10781700
H	3.77298900	-1.59352400	2.95655400
H	0.04675100	-3.13157100	4.38400400
H	-0.41835100	-1.45010700	4.10976500
H	-1.00161800	-2.73244100	3.02260400
H	3.67996700	0.83245700	1.23334400
H	4.55752100	-3.01627000	-1.73874800

Supporting Information

H	2.25832900	-2.34621500	-1.30310100
H	-0.04468100	1.10472300	2.24256200
H	-0.36189600	3.53353300	2.54024700
H	2.23028400	4.25501300	-0.82020000
H	2.54714500	1.83803700	-1.08574100
C	-3.81586000	-2.35105000	-0.17715700
C	-3.03417600	-2.72885800	-1.31938800
N	-1.75365500	-3.13210900	-1.12502700
O	-0.98405900	-3.39255100	-2.09562200
O	-1.31811200	-3.18270600	0.08349300
C	-5.29869300	-2.24677300	-0.34584400
C	-5.90281700	-1.81977900	-1.53967600
C	-7.29036800	-1.75886300	-1.65664200
C	-8.10415900	-2.11533500	-0.57929300
C	-7.51871700	-2.53490100	0.61595700
C	-6.13029400	-2.59728300	0.72951700
H	-3.54174000	-2.94226300	0.69278700
H	-3.35267900	-2.68215900	-2.34937500
H	-5.28753400	-1.53890900	-2.38925400
H	-7.73771100	-1.43660700	-2.59232500
H	-9.18487500	-2.07083600	-0.67288100
H	-8.14208400	-2.82220000	1.45738300
H	-5.68109600	-2.93807100	1.65887500
C	0.64109300	5.56067600	0.96439300
H	1.52096300	6.11382900	0.62821900
H	0.40683200	5.87005400	1.98627000
N	-0.51907000	6.06198900	0.09197200
C	-1.85675200	5.66040700	0.63411000
H	-2.01487800	6.15422500	1.59450800
H	-2.62643600	5.96338400	-0.07552300
H	-1.87741200	4.57891200	0.75392200
C	-0.44020300	7.54013700	-0.12733600
H	-1.27381200	7.85258100	-0.75706700
H	-0.49552500	8.04831700	0.83675200
H	0.50380800	7.77915800	-0.61793800
C	-4.14322200	0.47126800	0.19793100
H	-5.16787300	0.20411800	0.47308400
H	-4.16693800	0.61791800	-0.88551800
C	-4.77212600	2.92240000	0.54122900
H	-4.52235700	3.85518600	1.06040100
H	-4.78578400	3.12819700	-0.53530700
H	-5.79190000	2.65349900	0.83485800
C	6.87601700	-1.96880300	-0.71212200
H	7.17295100	-2.56031400	0.16387700

Supporting Information

H	6.90876500	-2.66207200	-1.57511600
N	7.83153700	-0.87153700	-0.84292800
C	9.20520000	-1.32690000	-0.65367900
H	9.53284500	-2.05790400	-1.41610600
H	9.88335100	-0.46945400	-0.69786200
H	9.31093300	-1.79202300	0.33107900
C	7.68019600	-0.16641400	-2.11149000
H	8.35846700	0.69179900	-2.13826200
H	7.90048500	-0.80428500	-2.98843000
H	6.65668200	0.20544500	-2.21202100
H	5.99951600	0.12127400	0.79467300
C	-3.78591800	1.80098700	0.88486100
H	-2.76478000	2.09583100	0.60335400
H	-3.76745400	1.64858800	1.97194200
C	-1.81220000	-0.68345600	0.44910400
H	-1.20660200	-1.12164700	1.22502400
C	-3.24174200	-0.69149400	0.61969500
H	-3.45097700	-0.93738100	1.66216800
H	-0.43952400	5.57943400	-0.83303100
O	-0.63184700	4.43406500	-2.14572000
H	-0.04025500	3.67975300	-2.00477900
H	-0.67293400	4.57552300	-3.10073300
Cat2-TS6"			
N	-0.87296000	-0.17947400	-0.82232400
C	0.53742300	-0.63922500	-1.02010100
C	0.90129700	-0.10898700	-2.42247600
C	-0.45135500	0.02138200	-3.13212300
C	-1.35798900	0.54137500	-2.01722800
C	1.48332400	-0.24031800	0.18134900
C	2.95722900	-0.58776600	-0.10171600
C	1.29433300	1.26236000	0.47793400
O	1.00808700	-0.93977600	1.32650400
Si	1.39497300	-2.39616400	2.14036900
C	1.42523100	-3.89394500	1.00892400
C	3.01335000	-2.22690800	3.08831900
C	-0.03392800	-2.52694300	3.36047400
C	3.98153900	0.05890800	0.61108700
C	5.31785600	-0.29276500	0.44301800
C	5.68551600	-1.31327800	-0.44317200
C	4.67139500	-1.96736200	-1.14736700
C	3.33073400	-1.61882700	-0.97464700
C	0.40620600	1.66816600	1.48174400
C	0.16147100	3.01855800	1.72785200

Supporting Information

C	0.79454800	4.01059100	0.96949100
C	1.71849700	3.61321300	-0.01012400
C	1.96026700	2.26111100	-0.25340500
H	0.49604700	-1.73241300	-1.03647000
H	1.58680600	-0.77735600	-2.94278600
H	1.38767600	0.86975100	-2.36171100
H	-0.42225200	0.68606600	-4.00048800
H	-0.80510200	-0.96145600	-3.45673400
H	-2.41182400	0.33268100	-2.18806000
H	-1.24082900	1.62653000	-1.88423500
H	0.50246600	-4.02927700	0.43266800
H	2.27173900	-3.87625200	0.31672100
H	1.54227000	-4.78857000	1.63346300
H	3.13325300	-3.08883600	3.75527100
H	3.02258000	-1.32600700	3.71095300
H	3.88550100	-2.19225000	2.43046800
H	0.11154200	-3.38968400	4.01989500
H	-0.11088000	-1.63700700	3.99419000
H	-0.99372500	-2.66970100	2.85298900
H	3.73265000	0.84047600	1.32169400
H	4.92619800	-2.76583600	-1.83934600
H	2.58313200	-2.17738200	-1.52509400
H	-0.07980800	0.90799700	2.07888700
H	-0.51885500	3.29661900	2.52912400
H	2.27790200	4.36304500	-0.56591400
H	2.71445300	1.98389500	-0.98116000
C	-3.98612900	-2.11680300	-0.80713000
C	-3.50140900	-3.40576700	-0.44524200
N	-2.21238700	-3.74291800	-0.71428200
O	-1.72641100	-4.83615200	-0.34341700
O	-1.49277100	-2.86045500	-1.31871300
C	-5.44617200	-1.88353900	-0.59964300
C	-6.20833300	-1.26847900	-1.60440400
C	-7.58044800	-1.06883300	-1.44460900
C	-8.21398300	-1.47559200	-0.27047600
C	-7.46688200	-2.08435900	0.74161000
C	-6.09745800	-2.28395200	0.57983900
H	-3.61919700	-1.75967500	-1.76685000
H	-4.04729000	-4.12203400	0.14976400
H	-5.72504800	-0.96867000	-2.53074200
H	-8.15401700	-0.60344200	-2.24070500
H	-9.28158500	-1.32391800	-0.14440800
H	-7.95334700	-2.40642200	1.65749100
H	-5.52707500	-2.75598500	1.37477400

Supporting Information

C	0.50458600	5.47026400	1.18177800
H	1.37325800	6.08457400	0.93478200
H	0.20089400	5.69627400	2.20730400
N	-0.63089700	5.98088100	0.28113700
C	-1.97524700	5.48414400	0.71857300
H	-2.20303900	5.89449500	1.70372200
H	-2.72100500	5.81115400	-0.00598900
H	-1.95226700	4.39664600	0.75483300
C	-0.61075500	7.47285900	0.16773100
H	-1.42314700	7.79230700	-0.48577900
H	-0.74198500	7.90922600	1.15926100
H	0.34579100	7.78667000	-0.25118900
C	-3.74653500	0.64896700	-0.00705000
H	-4.35464600	0.63484800	-0.92141400
H	-2.98345600	1.42357400	-0.15978600
C	-5.31756400	2.43713200	0.92168100
H	-5.93475900	2.73303700	1.77535200
H	-4.57840900	3.23250100	0.75469600
H	-5.96615800	2.40218500	0.03988900
C	7.13605900	-1.73773600	-0.58189800
H	7.37872900	-2.40391200	0.25629200
H	7.25365500	-2.34596400	-1.49996400
N	8.07050500	-0.61642800	-0.53338800
C	9.43468300	-1.06020300	-0.26463600
H	9.84731300	-1.71209900	-1.05694100
H	10.08996100	-0.18891200	-0.17257100
H	9.46781200	-1.61040600	0.68057000
C	8.00921000	0.19773900	-1.74280100
H	8.66394200	1.06753200	-1.63344400
H	8.32111900	-0.35355700	-2.65007000
H	6.98853500	0.55791300	-1.89931600
H	6.09754000	0.22458800	0.99290300
C	-3.07314700	-0.70802500	0.23705300
H	-3.32929600	-1.11967200	1.21057900
C	-1.67277900	-0.87264900	0.00089200
H	-1.13428300	-1.55759000	0.63590700
C	-4.64088400	1.08578200	1.16382700
H	-4.03506000	1.13098300	2.07908300
H	-5.40563600	0.32232600	1.33895100
H	-0.47777900	5.56857000	-0.66791500
O	-0.50761400	4.49235100	-2.04942600
H	0.14086100	3.78475400	-1.91402700
H	-0.53417700	4.66545500	-2.99967700

Supporting Information

Cat2-TS1'''

N	0.50817500	1.22142700	-0.07288400
C	0.69160600	2.46103400	0.35442100
C	-0.22054900	3.54700900	0.36431400
C	-0.75476900	0.57286000	-0.53509600
C	-0.27168000	-0.32391700	-1.71289700
C	1.26541200	-0.17881800	-1.79413000
C	1.66042100	0.35979200	-0.41785400
C	-1.57294700	-0.16331700	0.61073600
C	-2.68719700	-1.01747700	-0.03580500
C	-0.61945800	-0.97871100	1.50224500
O	-2.13530000	0.89475100	1.39243200
Si	-3.67977600	1.19621700	2.03233300
C	-4.98912600	1.50823200	0.71920900
C	-4.21851000	-0.16052600	3.23259000
C	-3.43136000	2.78239700	3.01890900
C	-3.15483100	-2.18718200	0.58588400
C	-4.20561200	-2.92683200	0.04697100
C	-4.82678100	-2.52592600	-1.14141000
C	-4.36677100	-1.36140500	-1.76237400
C	-3.32554800	-0.60820900	-1.21876700
C	-0.15296500	-0.43866500	2.70614200
C	0.80427900	-1.10740100	3.47221000
C	1.33572100	-2.33196300	3.05683600
C	0.84994900	-2.88786800	1.86609200
C	-0.10878000	-2.22624400	1.10411500
H	1.73048300	2.68423400	0.59456300
H	-1.27129000	3.26599700	0.38901100
H	-1.42928300	1.35319100	-0.86386800
H	-0.75641100	0.00838600	-2.63219100
H	-0.55680400	-1.36327700	-1.54950200
H	1.77206800	-1.12034800	-2.02078500
H	1.54083700	0.54461000	-2.56750500
H	2.57961700	0.94829200	-0.41239700
H	1.75096100	-0.44842800	0.31188900
H	-4.57973600	2.10901000	-0.10011900
H	-5.39033900	0.58491900	0.29473600
H	-5.82244700	2.06350100	1.16730900
H	-5.09981000	0.17712800	3.79130200
H	-3.43253800	-0.38825500	3.96078700
H	-4.48587700	-1.08829700	2.72102200
H	-4.36506700	3.05695600	3.52344000
H	-2.66061400	2.67186300	3.78826800
H	-3.15263800	3.61723100	2.36865600

Supporting Information

H	-2.69451000	-2.52740900	1.50649300
H	-4.82997700	-1.02363700	-2.68595500
H	-3.03698500	0.29986600	-1.73869800
H	-0.54032100	0.51836900	3.03252000
H	1.14616400	-0.66318500	4.40412700
H	1.23647500	-3.84265500	1.52119400
H	-0.46894700	-2.69673900	0.19633500
N	-1.88405100	2.85185700	-2.42469400
O	-2.19105800	1.98334100	-3.29281700
O	-2.70523100	3.19296300	-1.51362200
C	1.07522200	4.99211800	-1.63827700
C	1.15730200	6.38786600	-1.52788100
C	2.35469600	7.06040900	-1.77550000
C	3.49835200	6.34745900	-2.13495000
C	3.43344300	4.95687000	-2.24816000
C	2.23541500	4.28869200	-2.00161800
H	0.26938700	6.95175700	-1.25582100
H	2.39156900	8.14249900	-1.68866200
H	4.43139000	6.86881000	-2.32693300
H	4.31745900	4.39211200	-2.53056700
H	2.19641100	3.20719400	-2.10097300
C	2.41829500	-3.04119800	3.84109100
H	2.21060700	-4.11627300	3.85742500
H	2.42194400	-2.69653800	4.88855600
N	3.76287300	-2.87113100	3.23838800
C	4.27489200	-1.50176000	3.40302300
H	4.44526300	-1.25439800	4.46353100
H	5.21412200	-1.41431800	2.85312400
H	3.55744300	-0.78855700	2.99142200
C	4.72478700	-3.84084400	3.78303200
H	5.66985000	-3.73060500	3.24670400
H	4.89909400	-3.69382800	4.86100000
H	4.35022300	-4.85648000	3.62646700
C	0.15827800	4.69068200	1.30318500
H	-0.50342300	5.54262000	1.10041200
H	1.17271100	5.03687800	1.06624900
C	0.09047600	4.35400700	2.80178500
H	0.76447400	3.51300700	3.01480500
H	-0.91613900	4.00764700	3.05477600
C	0.46473800	5.54659900	3.68764300
H	0.41846300	5.28483600	4.74962200
H	1.48084400	5.89805400	3.47467200
H	-0.21617500	6.38953400	3.52424200
C	-0.62373900	3.37444300	-2.41250500

Supporting Information

H	0.03304400	2.99405800	-3.17952300
C	-6.00206000	-3.30280400	-1.70383200
H	-6.89616400	-3.05679800	-1.11545700
H	-6.20878800	-2.95753100	-2.73590100
N	-5.82464500	-4.75303900	-1.63324300
C	-7.08025900	-5.45998300	-1.84670400
H	-7.51137100	-5.29779000	-2.85365100
H	-6.92130000	-6.53578100	-1.72123700
H	-7.81971400	-5.13799700	-1.10657400
C	-4.79224500	-5.22265500	-2.55019100
H	-4.63334600	-6.29609000	-2.40649200
H	-5.05060100	-5.05375400	-3.61355400
H	-3.85029900	-4.70800500	-2.34493100
H	-4.54444800	-3.83484500	0.53614500
C	4.07933300	-3.43952700	-2.19002800
C	4.23366200	-3.52899000	-3.57277000
C	5.47890600	-3.28111000	-4.15519300
C	6.57271800	-2.94642300	-3.35278300
C	6.42161700	-2.85768500	-1.97100900
C	5.17414800	-3.10117700	-1.38271600
H	3.11985400	-3.63549600	-1.72498400
H	3.38482200	-3.79375900	-4.19638000
H	5.59694600	-3.35043700	-5.23279400
H	7.54126300	-2.75592200	-3.80559100
H	7.25498200	-2.60091900	-1.32599500
C	5.05292500	-2.98619100	0.10313700
O	6.00664300	-2.72582000	0.82735700
O	3.81416000	-3.18389000	0.55449200
H	3.79530000	-3.08458700	1.57316500
C	-0.22672100	4.29195000	-1.39049500
H	-1.03012200	4.97310800	-1.10901600
Cat2-TS2'''			
N	1.08963000	-1.65898300	-0.82758100
C	2.05564400	-2.52478100	-0.53921800
C	3.42694900	-2.26862100	-0.29361900
C	1.16223600	-0.17769300	-0.89002100
C	0.16554600	0.14324600	-2.02794200
C	-0.89174900	-0.97773100	-2.01467000
C	-0.16902100	-2.19030700	-1.41872900
C	0.91434500	0.55586900	0.49679400
C	0.79660200	2.08156600	0.27573100
C	-0.29359000	-0.06225300	1.22111000
O	2.11085400	0.29576400	1.25323900

Supporting Information

Si	2.87577700	1.11158400	2.53016200
C	3.72720400	2.69940300	1.97430800
C	1.72126800	1.46163900	3.98263600
C	4.20440200	-0.09644000	3.09489000
C	0.06263200	2.89785400	1.15123700
C	0.04712800	4.28533400	1.01596800
C	0.76298400	4.91683600	-0.00670100
C	1.49661500	4.11197300	-0.88327900
C	1.52211800	2.72569200	-0.73904800
C	-0.10130700	-1.12562800	2.11088300
C	-1.18423100	-1.74829000	2.73283700
C	-2.49698200	-1.33191200	2.49153600
C	-2.69508800	-0.27185000	1.59602200
C	-1.61373800	0.34357200	0.96801100
H	1.73994800	-3.56014800	-0.61445100
H	3.64452700	-1.29749200	0.13976500
H	2.17938200	0.08729000	-1.16886500
H	0.70856700	0.09728300	-2.97538800
H	-0.27572400	1.13528400	-1.92973600
H	-1.75761100	-0.70427200	-1.41006500
H	-1.23642900	-1.19544200	-3.02704400
H	0.12732100	-2.90864000	-2.18989700
H	-0.75347600	-2.69768100	-0.64518600
H	4.40302800	2.50979500	1.13363400
H	3.02597600	3.48249500	1.67689400
H	4.33428900	3.08688300	2.80165800
H	2.31990700	1.77030300	4.84822900
H	1.15542500	0.57031200	4.26995400
H	1.00706000	2.26284800	3.77637000
H	4.82282700	0.36463000	3.87374300
H	3.77291700	-1.01008600	3.51474200
H	4.86810300	-0.38104700	2.27242400
H	-0.50959400	2.44758900	1.95337400
H	2.05918200	4.57219200	-1.69181100
H	2.11423800	2.15242100	-1.44274300
H	0.90624500	-1.46901900	2.31082600
H	-1.00174200	-2.57145700	3.41934200
H	-3.70051600	0.07443900	1.37745700
H	-1.80653000	1.16084900	0.28145200
C	4.24971800	-2.02452700	-2.07842400
N	2.32596500	-2.26269400	-3.50475800
O	2.20717000	-3.44366100	-3.03588700
O	1.49345000	-1.79319700	-4.32786900
C	5.49386300	-1.24531400	-1.79596100

Supporting Information

C	5.46566800	0.13612900	-1.54194700
C	6.64019400	0.84507500	-1.29764200
C	7.87204000	0.18606400	-1.29584300
C	7.91613500	-1.18610300	-1.54136800
C	6.73821900	-1.89374000	-1.78549000
H	4.41660300	-3.09247700	-2.19820400
H	4.51422400	0.66068000	-1.53207800
H	6.59460600	1.91363200	-1.10684600
H	8.78723800	0.73801200	-1.10347800
H	8.86816000	-1.70903600	-1.54540800
H	6.78160500	-2.96050600	-1.98688800
C	-3.65905600	-1.98579600	3.21007900
H	-4.18329600	-1.23597700	3.81522200
H	-3.27156800	-2.74478800	3.91123400
N	-4.66783100	-2.58817900	2.31291900
C	-4.11158300	-3.67229200	1.48800100
H	-3.76574700	-4.51919300	2.10283200
H	-4.88756900	-4.01458800	0.80056700
H	-3.26707900	-3.29577800	0.90746900
C	-5.81779000	-3.07987500	3.08831200
H	-6.57633600	-3.44645600	2.39380200
H	-5.53308600	-3.88951800	3.77937900
H	-6.24359600	-2.25859100	3.67236400
C	4.20616600	-3.43739400	0.29849200
H	5.27853900	-3.21848100	0.23177400
H	4.03432300	-4.32355800	-0.32928300
C	3.86086700	-3.79078200	1.75436900
H	2.78736500	-4.01045100	1.82959700
H	4.03997300	-2.91863800	2.39273400
C	4.66657600	-4.98369500	2.27910200
H	4.40381300	-5.21876400	3.31560500
H	4.48463600	-5.88147600	1.67754100
H	5.74264900	-4.77867800	2.24776300
C	3.36410600	-1.49443000	-3.05307400
H	3.39620900	-0.48703800	-3.44024700
C	0.78080400	6.42920000	-0.12675100
H	1.46967500	6.83052700	0.62848400
H	1.20424600	6.71331400	-1.11053400
N	-0.52505800	7.04133500	0.10965800
C	-0.41367300	8.47562400	0.34254300
H	-0.01369100	9.03229500	-0.52670600
H	-1.40105700	8.88582800	0.57604700
H	0.24304300	8.66500800	1.19751800
C	-1.46792500	6.75312500	-0.96595600

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H	-2.45138800	7.15940400	-0.71045900
H	-1.15953700	7.18688000	-1.93666000
H	-1.56934100	5.67260600	-1.09429300
H	-0.53958400	4.89380400	1.69712000
C	-7.32984200	0.67071300	-1.19696200
C	-8.05578000	1.42445600	-2.11781700
C	-8.98706000	0.80278900	-2.95266400
C	-9.19383500	-0.57640900	-2.86606600
C	-8.47072700	-1.33174200	-1.94658500
C	-7.53499000	-0.71246500	-1.10787400
H	-6.60447100	1.14221200	-0.54401200
H	-7.89554900	2.49653400	-2.18542000
H	-9.55078300	1.39224400	-3.67021400
H	-9.91752700	-1.06008800	-3.51543900
H	-8.61209900	-2.40351700	-1.85934300
C	-6.78251400	-1.56356500	-0.13779100
O	-6.96123100	-2.77171100	-0.03924400
O	-5.90606200	-0.88722500	0.60809400
H	-5.42147800	-1.53214600	1.23470200
Cat2-TS3'''			
N	-0.50174400	-0.89441900	-0.44404500
C	-0.95586600	-1.83485300	0.37292200
C	-2.32194800	-2.18326500	0.53547500
C	0.93131300	-0.76191300	-0.85453000
C	0.89380200	0.37404200	-1.90301300
C	-0.55490200	0.40083300	-2.40604200
C	-1.35073500	0.09429900	-1.14192500
C	1.93959600	-0.59192800	0.35524900
C	3.36020700	-0.25269700	-0.13991000
C	1.39726400	0.47639300	1.32559400
O	1.95499600	-1.83392100	1.06001800
Si	2.88502700	-3.25510700	1.07292700
C	3.25245200	-3.97130400	-0.62678600
C	4.47895500	-2.97247300	2.04336800
C	1.76950600	-4.44440400	2.01756900
C	4.26172400	0.40166400	0.71613800
C	5.57807000	0.64711500	0.33488400
C	6.04716300	0.24696400	-0.92270800
C	5.15811800	-0.41160600	-1.77548600
C	3.84087000	-0.66758900	-1.38964900
C	0.75266600	0.10224200	2.50987800
C	0.14493700	1.05398300	3.33104800
C	0.15022000	2.40968000	2.99120200

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C	0.84760800	2.79274900	1.83911800
C	1.46864200	1.84728000	1.02814400
H	-0.18986100	-2.42941200	0.84846800
H	-3.04505000	-1.40021300	0.31685200
H	1.18445700	-1.70652900	-1.34815100
H	1.60474500	0.19159700	-2.70816800
H	1.14538300	1.33383300	-1.44875700
H	-0.83805800	1.35981300	-2.84738800
H	-0.70309100	-0.39442200	-3.14198900
H	-2.33743100	-0.31751800	-1.34013100
H	-1.45823100	0.98554900	-0.50833900
H	2.34002200	-4.01952100	-1.23006900
H	4.01773700	-3.41190000	-1.17051900
H	3.62249900	-4.99634400	-0.49758600
H	5.01549600	-3.92111500	2.16461600
H	4.27098400	-2.57840400	3.04402400
H	5.14933800	-2.27068300	1.53922600
H	2.29046500	-5.38795600	2.21634300
H	1.45306500	-4.03140200	2.98142200
H	0.87700600	-4.67805100	1.42786100
H	3.92867000	0.72143400	1.69741600
H	5.49486300	-0.73477400	-2.75740100
H	3.19928400	-1.20410400	-2.07880000
H	0.73133600	-0.94437200	2.78443600
H	-0.34996400	0.73103000	4.24386400
H	0.89806000	3.84297700	1.56521400
H	2.03424300	2.18856800	0.16876500
C	-2.69373300	-3.37475500	-1.03685900
C	-1.92747200	-3.03197300	-2.18168900
N	-0.58393300	-3.27919300	-2.18859500
O	0.13541300	-2.90662000	-3.15803500
O	-0.07232600	-3.84989300	-1.16881400
C	-4.18033500	-3.33396000	-1.16750700
C	-4.84790200	-2.25865600	-1.77758300
C	-6.23520000	-2.25439300	-1.90335700
C	-6.98914000	-3.32501000	-1.41648100
C	-6.34201200	-4.39845500	-0.80511000
C	-4.95219600	-4.40029400	-0.68005200
H	-2.31787000	-4.25352200	-0.51932000
H	-2.30480700	-2.51555000	-3.05116500
H	-4.27647000	-1.41715200	-2.15983400
H	-6.72966100	-1.41277800	-2.37981100
H	-8.07076200	-3.32022800	-1.51282400
H	-6.91725000	-5.23828600	-0.42620200

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H	-4.45367900	-5.24630700	-0.21510800
C	-0.59259700	3.44335800	3.80783900
H	-0.01087300	4.37044600	3.83897200
H	-0.71240000	3.10033700	4.84914000
N	-1.91397000	3.78156600	3.22264700
C	-2.88917500	2.69257400	3.38970900
H	-3.11474900	2.50623100	4.45251000
H	-3.80739100	2.96641700	2.86611500
H	-2.49527800	1.77355300	2.95073700
C	-2.44839600	5.03131400	3.78276700
H	-3.37354700	5.27872700	3.25768400
H	-2.65298200	4.95020000	4.86250100
H	-1.72989900	5.84085400	3.62504200
C	-2.67845000	-3.00609100	1.76171200
H	-1.91174600	-3.77779400	1.91548800
H	-3.62054100	-3.53684500	1.57721600
C	-2.83234500	-2.17523300	3.04768900
H	-3.59331100	-1.40021900	2.88389500
H	-1.89472400	-1.64142700	3.24930000
C	-3.21809700	-3.02494000	4.26230900
H	-3.32619800	-2.41088500	5.16225700
H	-4.16973800	-3.54246800	4.09703700
H	-2.45919400	-3.78792000	4.46908200
C	7.49308000	0.47333200	-1.32134000
H	8.11546300	-0.27837000	-0.81766100
H	7.60608800	0.28769700	-2.40798900
N	8.00201700	1.78722700	-0.93116800
C	9.45539700	1.84656300	-1.01476000
H	9.84271500	1.70645300	-2.04251200
H	9.80361300	2.82031600	-0.65626200
H	9.89718400	1.07320500	-0.37844900
C	7.38455300	2.86389800	-1.69731000
H	7.73476200	3.83004900	-1.32089800
H	7.61771700	2.81247700	-2.77849500
H	6.29833000	2.82748300	-1.58266700
H	6.25497500	1.16678700	1.00585800
H	-1.89158100	3.97412300	1.54882400
O	-1.89746700	4.04799900	0.52816700
C	-3.12391700	4.34910100	0.10169700
O	-4.08463100	4.50525100	0.84598500
C	-3.22636500	4.47164300	-1.38552300
C	-4.48355400	4.72525100	-1.94812700
C	-2.10633600	4.34053100	-2.21815100
C	-4.62192900	4.84071100	-3.32936900

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H	-5.33475400	4.82755800	-1.28370200
C	-2.24723900	4.45888500	-3.60035100
H	-1.13560600	4.15399200	-1.77325400
C	-3.50436000	4.70666000	-4.15708000
H	-5.59871900	5.03607100	-3.76197900
H	-1.37743700	4.36219600	-4.24364900
H	-3.61211900	4.79755600	-5.23417500
Cat2-TS4'''			
N	-0.53732800	-0.71199200	-0.51524300
C	-1.03022100	-1.76247100	0.12987500
C	-2.40037300	-2.09409900	0.32019300
C	0.89001400	-0.64051400	-0.94645100
C	0.89360900	0.52358200	-1.96577100
C	-0.56857000	0.67261700	-2.41206800
C	-1.34660400	0.34967600	-1.13827200
C	1.90827200	-0.54612500	0.26573700
C	3.34216000	-0.25492000	-0.21991700
C	1.40898100	0.52006600	1.26165900
O	1.85413700	-1.80784800	0.92955100
Si	2.75426700	-3.25179100	0.99085500
C	3.13755300	-3.99755200	-0.69041400
C	4.32989100	-2.97935000	1.99492800
C	1.59849000	-4.41760700	1.91388100
C	4.27024800	0.34583400	0.64682900
C	5.59344700	0.55155000	0.26536400
C	6.04369400	0.16391400	-1.00303100
C	5.12824300	-0.44111800	-1.86729300
C	3.80426600	-0.65647300	-1.48055200
C	0.73725600	0.14153200	2.42902200
C	0.16802800	1.09567700	3.27414300
C	0.23859700	2.45932200	2.97473800
C	0.96055300	2.84333000	1.83824800
C	1.54408500	1.89407400	1.00384500
H	-0.27551700	-2.43291000	0.51502600
H	-3.11171400	-1.28660600	0.15375600
H	1.09604900	-1.59227300	-1.44393100
H	1.56430900	0.32139300	-2.80128600
H	1.22934000	1.44989000	-1.49730800
H	-0.80009600	1.66943800	-2.79566200
H	-0.80936700	-0.06068100	-3.18900300
H	-2.36151000	0.00251800	-1.32986900
H	-1.39560500	1.21882700	-0.46927800
H	2.21014500	-4.16339400	-1.24855700

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H	3.82755300	-3.39746900	-1.28894700
H	3.60383200	-4.97822500	-0.53250400
H	4.83619500	-3.93840200	2.15691800
H	4.10518400	-2.55347300	2.97890600
H	5.03347700	-2.31003000	1.49215000
H	2.15706600	-5.28251100	2.29040300
H	1.11999000	-3.93539700	2.77293300
H	0.82580400	-4.80465100	1.24069400
H	3.95267500	0.65437500	1.63671400
H	5.44992300	-0.75428100	-2.85745100
H	3.14012400	-1.15254500	-2.17831100
H	0.66320100	-0.91107200	2.66998000
H	-0.34862000	0.76899000	4.17338900
H	1.06037900	3.89765200	1.59530200
H	2.13120100	2.23432200	0.15830800
C	-2.81817200	-3.23259300	-1.25648000
C	-2.17635500	-4.49510500	-1.14852400
N	-0.82251200	-4.57307000	-1.31658600
O	-0.21439400	-5.65358600	-1.11310100
O	-0.19577000	-3.51008100	-1.66002400
C	-4.30931700	-3.18440500	-1.33020700
C	-4.92231500	-2.13779600	-2.03867700
C	-6.30873900	-2.04969800	-2.14508100
C	-7.11845400	-3.01050600	-1.53698300
C	-6.52665800	-4.05703000	-0.82828800
C	-5.13851400	-4.14359300	-0.72503000
H	-2.33711300	-2.57496200	-1.97612200
H	-2.63521200	-5.40582300	-0.79707700
H	-4.29846200	-1.39082000	-2.52413500
H	-6.75618600	-1.23393900	-2.70557300
H	-8.19949100	-2.94595900	-1.61712800
H	-7.14705000	-4.81296100	-0.35552500
H	-4.69906300	-4.96976100	-0.17592700
C	-0.46174300	3.50202300	3.81731000
H	0.15790400	4.40308300	3.87111800
H	-0.59686500	3.13864800	4.84959800
N	-1.76804600	3.90861300	3.24115800
C	-2.78944200	2.85962300	3.39004300
H	-3.02134600	2.66413900	4.44972300
H	-3.69534600	3.18189800	2.87281600
H	-2.43615400	1.93242900	2.93415300
C	-2.24782300	5.16920400	3.82653500
H	-3.16271300	5.46563500	3.30884800
H	-2.45412000	5.07621400	4.90489400

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H	-1.49581200	5.95030600	3.68251500
C	-2.72521100	-2.93608100	1.54340000
H	-2.00438000	-3.76049800	1.61600900
H	-3.71061500	-3.39710400	1.40712000
C	-2.73655500	-2.14532000	2.86281700
H	-3.44986200	-1.31411700	2.77777300
H	-1.75316600	-1.68439500	3.02101500
C	-3.10225400	-3.01362200	4.07061800
H	-3.10586400	-2.43026000	4.99717800
H	-4.09780800	-3.45613600	3.95290600
H	-2.38909700	-3.83583300	4.19715800
C	7.49572400	0.34534900	-1.40194700
H	8.09171800	-0.43691100	-0.91327700
H	7.59941700	0.17476900	-2.49203600
N	8.05228300	1.63309900	-0.99051300
C	9.50670300	1.64206400	-1.07807000
H	9.88574600	1.50764400	-2.10961300
H	9.89044400	2.59581600	-0.70255200
H	9.92234800	0.84161700	-0.45792400
C	7.47125700	2.74458800	-1.73492700
H	7.85782900	3.69068000	-1.34349800
H	7.69799600	2.70380200	-2.81799300
H	6.38486700	2.74556100	-1.61568400
H	6.29138900	1.02984400	0.94548100
H	-1.73389600	4.13769100	1.57744100
O	-1.73143500	4.23979800	0.55794100
C	-2.94612800	4.58673400	0.13287700
O	-3.90785800	4.74695700	0.87468300
C	-3.03453100	4.75606700	-1.35090100
C	-4.28367000	5.04236400	-1.91553300
C	-1.90887100	4.63861500	-2.17799200
C	-4.40892300	5.20274200	-3.29361700
H	-5.13923000	5.13410900	-1.25518900
C	-2.03638800	4.80293700	-3.55687400
H	-0.94410400	4.42801600	-1.73066700
C	-3.28587700	5.08244400	-4.11592800
H	-5.37971500	5.42293200	-3.72773000
H	-1.16189000	4.71856200	-4.19561400
H	-3.38325100	5.20950900	-5.19034500
Cat2-TS5'''			
N	-0.45244200	-0.93460500	-0.33342000
C	-0.90275900	-1.86752000	0.48653400
C	0.98923000	-0.85794100	-0.74352800

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C	0.98638200	0.20406200	-1.86452000
C	-0.45493300	0.21804100	-2.38768600
C	-1.27133200	0.02325800	-1.11450300
C	1.98603700	-0.62828500	0.46455400
C	3.42191700	-0.37261800	-0.03609400
C	1.46178100	0.52301500	1.34519200
O	1.95335100	-1.81466800	1.25859600
Si	2.85400900	-3.24065000	1.44603500
C	3.30748800	-4.09970400	-0.16369600
C	4.38675600	-2.89798700	2.49188200
C	1.65655100	-4.33527000	2.40533200
C	4.33730100	0.31412900	0.77901400
C	5.66466000	0.48527600	0.39534800
C	6.13153800	-0.02535800	-0.82245700
C	5.22831000	-0.71640800	-1.63361200
C	3.89940000	-0.89709100	-1.24492500
C	0.76170100	0.25139300	2.52643200
C	0.18405900	1.27950600	3.27330600
C	0.27185300	2.61147300	2.85823100
C	1.01055800	2.88947100	1.70171600
C	1.60332100	1.86762400	0.96532000
H	-0.12359300	-2.47932200	0.91295200
H	1.21632600	-1.84397200	-1.16327400
H	1.70449900	-0.04583700	-2.64487800
H	1.24858300	1.18863300	-1.47224500
H	-0.71504400	1.14850600	-2.89915200
H	-0.61062100	-0.62641700	-3.06489500
H	-2.26199000	-0.38427100	-1.29160000
H	-1.35998100	0.96252700	-0.55363400
H	2.43119600	-4.18236400	-0.81581000
H	4.11262400	-3.59760000	-0.70571000
H	3.64957700	-5.11614000	0.06885600
H	4.90020600	-3.83728400	2.72967500
H	4.11928700	-2.41641800	3.43864500
H	5.09875800	-2.24830900	1.97489900
H	2.14643000	-5.26533600	2.71526700
H	1.28092000	-3.84132200	3.30775800
H	0.80213000	-4.60773000	1.77670500
H	4.00682800	0.71809200	1.72962700
H	5.56263600	-1.12518200	-2.58387700
H	3.24551200	-1.46278000	-1.89818400
H	0.67424100	-0.77485000	2.85872300
H	-0.34836600	1.03658000	4.18983200
H	1.11979400	3.91763800	1.36777100

Supporting Information

H	2.20306100	2.12784100	0.10060000
C	-2.58497100	-3.56879900	-0.68366800
C	-1.96698300	-3.23510700	-1.92722000
N	-0.61826200	-3.38062900	-2.05627500
O	-0.02405400	-3.02135500	-3.11198400
O	0.04086300	-3.85657300	-1.06503100
C	-4.05889600	-3.80653800	-0.66538200
C	-4.95629100	-3.11244000	-1.49386500
C	-6.32348800	-3.38538600	-1.45680700
C	-6.82488900	-4.35779600	-0.58990100
C	-5.94645400	-5.05721500	0.23944600
C	-4.58072900	-4.78031800	0.20239500
H	-2.03213700	-4.34703600	-0.16532000
H	-2.46265300	-2.81067200	-2.78651000
H	-4.58459700	-2.36007600	-2.18258700
H	-6.99767900	-2.83964500	-2.11063000
H	-7.88934800	-4.57115000	-0.56415900
H	-6.32359900	-5.82203500	0.91223500
H	-3.90097900	-5.33342400	0.84551600
C	-0.42155800	3.72999200	3.60393800
H	0.20484400	4.62746800	3.57558200
H	-0.55564700	3.46197800	4.66532000
N	-1.72617700	4.09380100	2.99724700
C	-2.75659100	3.07443700	3.24805600
H	-2.98600900	2.98073100	4.32210000
H	-3.66173800	3.35566200	2.70580700
H	-2.41315800	2.10528100	2.87989000
C	-2.19026200	5.40888000	3.46266200
H	-3.10505800	5.66438900	2.92359900
H	-2.39063000	5.42069900	4.54617800
H	-1.43163700	6.16502600	3.24117100
C	-3.38043600	-1.18090700	0.83187300
H	-3.96576100	-1.12913300	-0.09406300
H	-2.94675400	-0.18431300	0.97564300
C	-4.34354800	-1.45724800	1.99704700
H	-3.77148500	-1.47704900	2.93479300
H	-4.77671700	-2.45670900	1.87812800
C	-5.46419000	-0.41956000	2.09642400
H	-6.12543900	-0.62894800	2.94326200
H	-5.06317000	0.59204900	2.22890200
H	-6.07822400	-0.41474200	1.18926300
C	7.58876300	0.11979100	-1.21752100
H	8.18009900	-0.60322600	-0.63993600
H	7.71013200	-0.16444000	-2.28164300

Supporting Information

N	8.13449600	1.44685700	-0.93616900
C	9.59003000	1.45381100	-0.99774900
H	9.98894300	1.21172400	-2.00184300
H	9.96377200	2.44431700	-0.71981500
H	9.99667200	0.72653100	-0.28789600
C	7.56372700	2.46946500	-1.80558100
H	7.93520900	3.45473200	-1.50717800
H	7.81533700	2.31733500	-2.87312600
H	6.47497700	2.47315000	-1.71096300
H	6.35287700	1.03169400	1.03278600
H	-1.69978800	4.15310800	1.31157500
O	-1.70794800	4.14734100	0.28894800
C	-2.92068600	4.47809700	-0.15490600
O	-3.86621500	4.73939500	0.57943700
C	-3.02820700	4.49364700	-1.64637300
C	-4.27509200	4.76907400	-2.22157300
C	-1.92269200	4.24314900	-2.47095200
C	-4.41783800	4.78838100	-3.60697100
H	-5.11496900	4.96396600	-1.56347600
C	-2.06791600	4.26521200	-3.85751300
H	-0.95940600	4.04005300	-2.01711000
C	-3.31483900	4.53565700	-4.42646000
H	-5.38667600	5.00084800	-4.04927700
H	-1.20930200	4.07544000	-4.49505900
H	-3.42596800	4.55145000	-5.50691800
C	-2.26449100	-2.23047000	0.73366200
H	-2.30251300	-2.92296900	1.57443000
Cat2-TS6'''			
N	-0.45468200	-0.74439000	-0.49517400
C	-0.96652900	-1.78913600	0.14239000
C	0.98896100	-0.73277500	-0.88785900
C	1.05890000	0.37195300	-1.96459500
C	-0.37451500	0.48260500	-2.49866700
C	-1.21575400	0.27973700	-1.24040800
C	1.96572000	-0.60563100	0.35241100
C	3.42311800	-0.37489200	-0.09448700
C	1.45790000	0.51768400	1.27812700
O	1.85507000	-1.83404200	1.07035300
Si	2.73057900	-3.28052100	1.26324200
C	3.19952600	-4.12407100	-0.34859300
C	4.24638200	-2.97171100	2.34573700
C	1.49966700	-4.37709400	2.17472600
C	4.33602800	0.25098300	0.77079900

Supporting Information

C	5.67636400	0.40292800	0.42613700
C	6.16061500	-0.06796700	-0.80089100
C	5.26049800	-0.69962400	-1.66223400
C	3.91822800	-0.85924700	-1.31272100
C	0.71720200	0.21131500	2.42505900
C	0.15646800	1.22011100	3.20996000
C	0.30108700	2.56769300	2.86636200
C	1.07748400	2.87748800	1.74320700
C	1.65342400	1.87366400	0.96951000
H	-0.21239900	-2.48554600	0.47537700
H	1.17647200	-1.71516800	-1.33267300
H	1.77836900	0.12410700	-2.74522300
H	1.36331300	1.32601300	-1.52967000
H	-0.58193500	1.44090500	-2.98191500
H	-0.57984700	-0.32108500	-3.21339700
H	-2.22384200	-0.07212900	-1.44864800
H	-1.27650700	1.20490100	-0.65440700
H	2.30938600	-4.31351400	-0.95847300
H	3.93917200	-3.57246900	-0.93404400
H	3.63410100	-5.10212200	-0.10569900
H	4.72239400	-3.92551700	2.60272600
H	3.96820400	-2.47713000	3.28275900
H	4.99348800	-2.34857300	1.84629300
H	2.01430300	-5.24027100	2.61249000
H	0.99261300	-3.84668300	2.98752500
H	0.75030200	-4.77005400	1.47923900
H	3.99314400	0.62211500	1.73021700
H	5.60849800	-1.07801900	-2.62016000
H	3.26551100	-1.37861900	-2.00447800
H	0.58347400	-0.82751900	2.69816100
H	-0.40831000	0.95003200	4.09908300
H	1.22969600	3.91683300	1.46510700
H	2.28346600	2.15589000	0.13350800
C	-1.99589800	-4.58135200	-0.89349300
N	-0.68344100	-4.53605500	-1.25460800
O	0.06135900	-5.53670900	-1.07947300
O	-0.22680000	-3.44399300	-1.74306600
C	-4.27897400	-3.62721300	-0.81831800
C	-5.17582200	-2.98256000	-1.68386100
C	-6.55199100	-3.19161000	-1.58219500
C	-7.05921100	-4.04846200	-0.60577200
C	-6.17943000	-4.69378800	0.26726000
C	-4.80612000	-4.48316700	0.16413500
H	-2.30494800	-5.50986400	-0.43832900

Supporting Information

H	-4.78698500	-2.32582800	-2.45766300
H	-7.22543600	-2.68738500	-2.26924500
H	-8.12942200	-4.21344200	-0.52416700
H	-6.56486500	-5.36267000	1.03141300
H	-4.13424300	-4.98632500	0.85306500
C	-0.37255700	3.67212300	3.65023300
H	0.28215800	4.54915300	3.67619200
H	-0.53857800	3.36009900	4.69474200
N	-1.65238500	4.10504700	3.03504800
C	-2.72132500	3.11308300	3.22963600
H	-2.97023000	2.98493600	4.29568600
H	-3.60752100	3.44666500	2.68599900
H	-2.40560900	2.14794100	2.82782000
C	-2.08023500	5.41691500	3.54271300
H	-2.97546000	5.72427300	2.99774600
H	-2.30146900	5.39462200	4.62192600
H	-1.29215500	6.15410100	3.36447000
C	-3.39267400	-1.01294000	0.60695200
H	-4.02573700	-0.93857700	-0.28719500
H	-2.91559800	-0.03314800	0.72602400
C	-4.29711700	-1.24678300	1.82767900
H	-3.67199900	-1.27477200	2.73062100
H	-4.76878300	-2.23195900	1.74759900
C	-5.37707100	-0.17243700	1.97796100
H	-5.99415000	-0.35106800	2.86431600
H	-4.93857900	0.82773300	2.07343300
H	-6.04246400	-0.15888000	1.10779700
C	7.63019600	0.05660600	-1.15430500
H	8.19228800	-0.69021300	-0.57801600
H	7.77405100	-0.20626600	-2.22117100
N	8.19286100	1.36641200	-0.82861000
C	9.64944500	1.34742900	-0.85578400
H	10.06757800	1.12026900	-1.85551500
H	10.03428400	2.32433900	-0.54675300
H	10.02584700	0.59708500	-0.15335500
C	7.66201100	2.41958700	-1.68651200
H	8.04482600	3.39032900	-1.35649600
H	7.93586000	2.28759000	-2.75134000
H	6.57155400	2.44209600	-1.61696200
H	6.36191100	0.90312400	1.10318600
H	-1.58964300	4.23050900	1.35750900
O	-1.57523300	4.26894100	0.33446100
C	-2.77236600	4.63643500	-0.12207800
O	-3.73158600	4.88033000	0.60003000

Supporting Information

C	-2.84468000	4.71664000	-1.61398200
C	-4.07898600	5.01218300	-2.20589600
C	-1.71864700	4.50832600	-2.42242200
C	-4.18947800	5.09174000	-3.59216900
H	-4.93493000	5.17481700	-1.55985900
C	-1.83124100	4.59211900	-3.80977400
H	-0.76501100	4.29118200	-1.95477300
C	-3.06615300	4.88108700	-4.39573100
H	-5.14889900	5.31908600	-4.04736100
H	-0.95624300	4.43757900	-4.43456600
H	-3.15190900	4.94510500	-5.47672400
C	-2.32734500	-2.10331000	0.44379500
H	-2.35848500	-2.82849300	1.25415000
C	-2.80954100	-3.41517300	-0.97835700
H	-2.55450700	-2.76307800	-1.81041700