

Electronic Supplementary Information

Cartesian Coordinates (in angstrom) of DFT-Optimized Structures:

C ₆₀				C	3.20328000	-0.07553700	-1.51277200
C	-0.61069800	2.23108800	2.68397900	C	2.70500900	1.22147300	-1.93520100
C	-1.54176800	1.15474900	2.97400300	C	1.65938200	1.30083900	-2.84715300
C	-1.06523900	-0.08664900	3.37825900	C	0.59739500	2.27233200	-2.65214600
C	0.36426400	-0.30710200	3.51059000	C	-0.65328400	1.65821300	-3.06224300
C	1.25515400	0.72264700	3.23336600	C	-1.82110600	1.92057700	-2.35584900
C	0.75712300	2.01998700	2.81069500	C	-2.75232500	0.84435500	-2.06583000
C	-1.12801100	2.97904500	1.55157200	C	-3.29713300	1.06740700	-0.73809700
C	-2.37859600	2.36484300	1.14140700	C	-3.54174500	-0.01170200	0.10288900
C	-2.63429900	1.23742300	2.02056700	C	-0.62623700	-3.12254500	1.55324000
C	-3.20310300	0.07539600	1.51286600	C	-2.70501400	-1.22144900	1.93511900
C	-1.65950100	-1.30089700	2.84727200	C	0.61062800	-2.23097100	-2.68374900
C	0.65330300	-1.65802200	3.06215200				
C	1.82094200	-1.92047700	2.35567200	C ₆₀ ²⁻			
C	2.75216600	-0.84425300	2.06565100	C	-1.70683700	2.73619400	-1.43493000
C	2.47553100	0.44823200	2.49500400	C	-2.56295700	1.63491500	-1.83852300
C	2.73118700	1.57583700	1.61597400	C	-3.32860300	0.95105800	-0.88800400
C	1.66920100	2.54729900	1.81105600	C	-3.27184200	1.34730400	0.50346200
C	1.17388700	3.26291300	0.72741700	C	-2.45031300	2.41374600	0.88935400
C	-0.25517700	3.48350400	0.59494500	C	-1.65270100	3.11697200	-0.09664000
C	-2.70268000	2.28171000	-0.20742100	C	-0.49836500	2.70787100	-2.24864800
C	-1.79058200	2.80888600	-1.20729000	C	-0.58415100	1.58395700	-3.12440600
C	-0.59384200	3.39651000	-0.81502700	C	-1.85063100	0.90460300	-2.86853400
C	0.62622300	3.12252600	-1.55315700	C	-1.93082100	-0.48462400	-2.91849800
C	1.71906700	3.03959400	-0.60008600	C	-3.41235600	-0.49510300	-0.93937600
C	2.73528400	2.11013100	-0.78676300	C	-3.32032900	0.14812700	1.31348800
C	3.25271500	1.36220500	0.34560400	C	-2.54672900	0.06119900	2.47606700
C	3.54186000	0.01154400	-0.10304100	C	-1.69058500	1.16568800	2.87041200
C	3.29723200	-1.06756000	0.73802500	C	-1.64428100	2.31874800	2.09126900
C	-0.59736700	-2.27218900	2.65204000	C	-0.37787400	3.00448800	1.85668800
C	1.12818800	-2.97913900	-1.55154900	C	-0.38294600	3.49363400	0.51599100
C	0.25536600	-3.48363300	-0.59485400	C	0.79213800	3.45354400	-0.27500800
C	-1.17394100	-3.26296500	-0.72749400	C	0.73627800	3.06424500	-1.64710000
C	-1.66912100	-2.54714100	-1.81099200	C	0.55948500	0.80078900	-3.41417800
C	-0.75707300	-2.01979900	-2.81065700	C	1.82938600	1.15889900	-2.78957500
C	1.54170100	-1.15463200	-2.97378400	C	1.91245700	2.25434100	-1.93392300
C	2.63441100	-1.23756600	-2.02051500	C	2.71924000	2.16881700	-0.72943500
C	2.37861200	-2.36486600	-1.14145100	C	2.00630000	2.89252400	0.30662700
C	2.70270800	-2.28171900	0.20745800	C	2.01111500	2.41561800	1.61427000
C	1.79072800	-2.80897300	1.20719700	C	0.80235600	2.46765700	2.42853800
C	0.59397100	-3.39664900	0.81487400	C	0.75457800	1.28608500	3.22793200
C	-1.71887200	-3.03944500	0.60002200	C	-0.47679000	0.62321700	3.46698000
C	-2.73540600	-2.11035200	0.78680600	C	-3.40689700	-0.99168600	0.42258300
C	-3.25265900	-1.36216500	-0.34553300	C	0.49832300	-2.70786500	2.24859600
C	-2.73134600	-1.57591500	-1.61602400	C	-0.73626700	-3.06425000	1.64713300
C	-2.47572400	-0.44829300	-2.49501700	C	-0.79214400	-3.45359600	0.27494500
C	-1.25530900	-0.72250000	-3.23332800	C	0.38290900	-3.49354800	-0.51598700
C	-0.36442600	0.30725000	-3.51056400	C	1.65269300	-3.11696000	0.09662100
C	1.06506700	0.08659200	-3.37813300				

C	-1.41313900	-0.00103300	-3.44101500	H	6.33806600	-0.00045700	-1.42231800
C	-2.09941000	-1.16131100	-2.94151200	H	4.70778000	-0.00068000	-2.20964200
C	-1.39191600	-2.30153700	-2.53479600	C	5.43265100	0.66981600	0.99562900
C	-2.89673700	-2.60888900	-0.59416500	C	5.43254200	-0.66923800	0.99608800
C	-3.50581700	-1.42691300	1.32949700	H	4.97849300	2.15766800	-0.61076500
C	-3.01250200	-0.72313200	2.42656200	H	4.97845500	-2.15808200	-0.60942200
C	-3.01248900	0.72463100	2.42613200	H	5.67890400	-1.32553700	1.83091100
C	-3.50578200	1.42776800	1.32864600	H	5.67909200	1.32664400	1.83001200
C	-2.82133000	2.60847800	0.83776500				
C	-2.89668200	2.60858900	-0.59572400				
C	-1.78745900	3.03186200	-1.36369300	Sm@C ₆₀			
C	-1.39187600	2.30000900	-2.53616400				
C	0.01390500	-0.00105600	-3.49557300	C	2.18033500	-2.72001100	-0.06613900
C	0.74366700	1.15941500	-3.06811500	C	2.17893000	-2.35319500	1.32969300
C	0.07011200	2.30360700	-2.60761700	C	1.04854400	-2.58842500	2.11687500
C	0.57439700	3.03351900	-1.49022300	C	-0.12388900	-3.21720600	1.52145700
C	-0.57191600	3.45755600	-0.69425800	C	-0.12524200	-3.56832400	0.17587300
C	-0.49934300	3.45798400	0.69557500	C	1.04689200	-3.31554700	-0.64562800
C	-1.64007700	3.03135900	1.48722000	C	2.91180300	-1.67647400	-0.77915900
C	-1.12604400	2.30116100	2.61381100	C	3.40131600	-0.70038300	0.18202600
C	-1.78883900	1.16173500	3.09206700	C	2.93023100	-1.09853100	1.46892600
C	-2.82138800	-2.60792200	0.83932300	C	2.47840300	-0.14572700	2.41958200
C	1.05222100	-1.15920300	2.92143300	C	0.60278000	-1.61778300	3.09290700
C	0.33518600	-2.30379800	2.53426100	C	-1.29105400	-2.59332300	2.11997300
C	0.72191300	-3.03654000	1.37182500	C	-2.41309100	-2.34182700	1.33928000
C	1.82081200	-2.58812000	0.60151400	C	-2.41571900	-2.70600200	-0.06630200
C	2.57623800	-1.44184300	1.01386400	C	-1.30123100	-3.30935800	-0.63891200
C	2.20457000	0.73586700	2.13762600	C	-0.84423100	-2.89649500	-1.95416700
C	1.05224300	1.16094200	2.92074500	C	0.60002100	-2.90807400	-1.95216000
C	0.37012500	0.00102300	3.42306900	C	1.30718700	-1.89779400	-2.63965800
C	-1.05437100	0.00105900	3.51595300	C	2.46545500	-1.28048700	-2.04621500
C	-1.78886100	-1.15986100	3.09276800	C	3.40145600	0.69910500	-0.18523400
C	-1.12608900	-2.29957900	2.61519300	C	2.92933200	1.09742500	-1.47170300
C	-0.49941100	-3.45756000	0.69764100	C	2.47626000	0.14479100	-2.42192200
C	-0.57198100	-3.45797800	-0.69219100	C	1.32158300	0.39806800	-3.21476200
C	0.57434500	-3.03444000	-1.48840500	C	0.58351900	-0.85404700	-3.34116300
C	1.74610300	-2.58674200	-0.83447800	C	-0.80892800	-0.84970200	-3.34189500
C	2.45313400	-1.43750400	-1.32205300	C	-1.53855900	-1.89271400	-2.63795300
C	3.25541800	-0.80017400	-0.19029100	C	-2.69997900	-1.27044600	-2.04342000
C	3.25543900	0.80001800	-0.19076600	C	-3.13838500	-1.66391500	-0.78201800
C	2.57628200	1.44241300	1.01301600	C	-0.82829300	-1.60756400	3.08729100
C	0.33523200	2.30532100	2.53289200	C	-3.13694200	1.66524200	0.78475700
C	0.72197400	3.03734700	1.37001300	C	-2.69755700	1.27159600	2.04576600
C	1.82086300	2.58844000	0.59996900	C	-1.53535800	1.89340900	2.63925900
C	1.74614900	2.58620300	-0.83602600	C	-0.84123300	2.89693900	1.95482100
C	2.45315500	1.43666800	-1.32291100	C	-1.29925800	3.30998100	0.63998700
C	1.96884900	0.73508400	-2.40568100	C	-2.41329600	2.34286800	-1.33718500
C	1.96884200	-0.73656400	-2.40524400	C	-3.14666400	1.09202100	-1.47791400
C	0.74365000	-1.16127500	-3.06741100	C	-3.59762300	0.68265100	-0.17513700
C	0.07007400	-2.30518600	-2.60623000	C	-3.59775700	-0.68113300	0.17831900
C	-1.64013800	-3.03042900	1.48902700	C	-3.14581500	-1.09070800	1.48068000
C	-1.78751900	-3.03265600	-1.36187500	C	-2.69737800	-0.14277000	2.41098200
C	2.20455000	-0.73462200	2.13805700	C	-0.80551800	0.85011900	3.34248200
C	4.79959900	1.11970900	-0.30505700	C	0.58692700	0.85386000	3.34051500
C	4.79956900	-1.11993100	-0.30436400	C	1.31038800	1.89733900	2.63832900
C	5.25102900	-0.00040400	-1.25362800	C	0.60299000	2.90789700	1.95150900

C	1.04886100	3.31515600	0.64451800
C	-0.12393600	3.56846900	-0.17590000
C	-0.12392900	3.21732600	-1.52147400
C	-1.29189900	2.59389900	-2.11893900
C	-2.69949800	0.14392300	-2.40861900
C	-1.54332700	0.39909200	-3.22014500
C	-0.83045700	1.60797500	-3.08668600
C	0.60061400	1.61756700	-3.09354100
C	1.04769400	2.58808300	-2.11792900
C	2.17870300	2.35236500	-1.33182200
C	2.18148500	2.71920400	0.06403500
C	2.91322000	1.67535600	0.77639900
C	2.46789200	1.27959200	2.04387800
C	-1.54056900	-0.39841800	3.22140600
C	1.32437600	-0.39852700	3.21348000
C	-2.41450800	2.70704400	0.06837900
Sm	0.66618600	-0.00033400	0.00003000

Sm@C₆₀-C₆H₅ [5,6] adduct

C	-0.58383600	1.88764400	3.01533700
C	0.49023100	2.52352900	2.28537800
C	0.21392200	3.30806000	1.16965600
C	-1.15729400	3.48290100	0.72704800
C	-2.19095600	2.85910800	1.42041100
C	-1.90007300	2.04709600	2.59382000
C	-0.10150000	0.58490200	3.47424700
C	1.25578800	0.43075600	3.06584400
C	1.62295400	1.61177000	2.28383000
C	2.44759600	1.50931900	1.17200200
C	1.05011300	3.19408900	0.00048600
C	-1.15729100	3.48312300	-0.72599700
C	-2.19094900	2.85954100	-1.41955400
C	-3.27240000	2.22161300	-0.69646700
C	-3.27240400	2.22140100	0.69712500
C	-3.65609000	1.02380800	1.42979700
C	-2.81737500	0.92030700	2.60405000
C	-2.35787600	-0.32844100	3.03057700
C	-1.00029600	-0.50349400	3.48778500
C	1.70389400	-0.81653400	2.56105800
C	0.77791900	-1.94543700	2.56813300
C	-0.53770000	-1.78710500	3.01412400
C	-1.62529100	-2.44364100	2.30242000
C	-2.75148400	-1.52767500	2.29978100
C	-3.56300900	-1.42434700	1.17568700
C	-4.02158200	-0.12234600	0.72467300
C	-4.02157900	-0.12212500	-0.72473200
C	-3.65608300	1.02424400	-1.42950600
C	0.21392800	3.30841900	-1.16865300
C	-1.00027900	-0.50242900	-3.48794600
C	-0.10148300	0.58596200	-3.47407300
C	1.25580300	0.43169200	-3.06570900
C	1.70390500	-0.81575100	-2.56129900
C	0.77793100	-1.94465200	-2.56872300
C	-1.62528000	-2.44293900	-2.30317500

C	-2.75147300	-1.52697300	-2.30026200
C	-2.35786100	-0.32751700	-3.03069100
C	-2.81736300	0.92110100	-2.60378600
C	-1.90006100	2.04788800	-2.59321000
C	-0.58382200	1.88856500	-3.01476900
C	1.62297000	1.61247200	-2.28334000
C	2.44761300	1.50968800	-1.17154300
C	3.27260700	0.25993100	-0.81568900
C	2.56814100	-0.93227100	-1.44001000
C	2.17223500	-2.10629400	-0.71112700
C	1.07428100	-2.75375300	-1.41033100
C	0.01870600	-3.38901500	-0.71769400
C	-1.34750500	-3.21080300	-1.17493000
C	-3.56300400	-1.42398900	-1.17614100
C	-3.28062500	-2.23465000	-0.00035000
C	-2.20314400	-3.11028200	-0.00048000
C	-1.34751100	-3.21116200	1.17394300
C	0.01870300	-3.38923400	0.71665900
C	1.07427500	-2.75418400	1.40949600
C	2.17223200	-2.10651200	0.71049400
C	2.56814000	-0.93271300	1.43973900
C	3.27260900	0.25968000	0.81578100
C	0.49024300	2.52422700	-2.28461300
C	2.11651200	2.27546500	0.00034700
C	-0.53768500	-1.78618600	-3.01467300
C	4.80767400	0.38998700	1.12518500
C	4.80766700	0.39028300	-1.12502900
C	5.27298400	1.32896500	0.00020700
H	6.36131300	1.46975200	0.00022700
H	4.77581400	2.30931800	0.00034800
C	5.42594100	-0.92088900	0.66909900
C	5.42579500	-0.92077900	-0.66928300
H	5.00183500	0.69358800	2.16088800
H	5.00184600	0.69414600	-2.16065200
H	5.70823000	-1.74090000	1.32849800
H	5.70798300	-1.74066500	-1.32888400
Sm	0.16284000	-0.33331800	0.00004900

Sm@C₆₀-C₆H₅ [6,6] adduct

C	3.22340600	-1.97742100	0.72143500
C	3.22341600	-1.97772900	-0.72053200
C	3.56828900	-0.81732000	-1.43049600
C	3.93082400	0.38709300	-0.69471600
C	3.93081500	0.38738900	0.69462400
C	3.56827100	-0.81671100	1.43091100
C	2.09396000	-2.80188800	1.15923100
C	1.42307200	-3.33157800	0.00072800
C	2.09397600	-2.80238700	-1.15799400
C	1.37322800	-2.40473500	-2.30245700
C	2.83588700	-0.42526400	-2.60670700
C	3.39383500	1.52266000	-1.42607500
C	2.86877900	2.60384400	-0.72715700
C	2.86877100	2.60415300	0.72610800
C	3.39381800	1.52326700	1.42549300

C	2.71386200	1.00914400	2.60350000	Sm	0.53261100	-0.64864500	0.00005400
C	2.83585600	-0.42415400	2.60694700				
C	1.73717100	-1.22068400	3.02499200				
C	1.37320100	-2.40374900	2.30351700				
C	-0.02483300	-3.42115600	0.00073800				
C	-0.76170700	-2.99298000	1.15882600	C	0.36184600	-1.09309400	-3.36465900
C	-0.09618600	-2.511139600	2.30827300	C	-0.30690400	0.19503200	-3.42186900
C	-0.62070400	-1.40131500	3.02428300	C	0.42596200	1.36596100	-3.26567700
C	0.50663200	-0.58143000	3.45431900	C	1.85998900	1.30140800	-3.04566300
C	0.40016700	0.80526800	3.45472400	C	2.49985800	0.06870500	-2.99066700
C	1.52285500	1.62313900	3.02429900	C	1.73442400	-1.15466900	-3.15356500
C	0.98095400	2.74412300	2.29820300	C	-0.51986800	-2.02676700	-2.68623600
C	1.63506000	3.23868900	1.16572100	C	-1.73358800	-1.31574900	-2.32475000
C	2.71389300	1.00803400	-2.60387100	C	-1.60205800	0.05747400	-2.77949700
C	-1.20008500	2.99470400	-1.16594000	C	-2.10750800	1.09677200	-2.00618800
C	-0.47336700	2.62878000	-2.30554700	C	-0.10294200	2.45190000	-2.45949600
C	-0.83367000	1.44997600	-3.03338000	C	2.21739200	2.34765800	-2.10372600
C	-1.91187500	0.66309600	-2.58485700	C	3.19930100	2.11607800	-1.14750100
C	-2.68585500	1.05929900	-1.43866800	C	3.86752700	0.82789500	-1.09009900
C	-2.33107700	2.18932700	0.73754500	C	3.52580000	-0.17322300	-1.99163000
C	-1.20010000	2.99520200	1.16467900	C	3.39415700	-1.54621700	-1.53656400
C	-0.52168800	3.50203200	-0.00073500	C	2.28682600	-2.15248900	-2.25459300
C	0.88435900	3.63127600	-0.00075500	C	1.44291600	-3.04574600	-1.60497900
C	1.63507200	3.23819400	-1.16705600	C	0.00899300	-2.98164000	-1.82530200
C	0.98098000	2.74314300	-2.29933300	C	-2.36405200	-1.58873700	-1.11637200
C	0.40020500	0.80379600	-3.45503400	C	-1.81246200	-2.58744900	-0.21730500
C	0.50667200	-0.58290300	-3.45404000	C	-0.65188400	-3.26861200	-0.56404300
C	-0.62067000	-1.40260800	-3.02367100	C	0.37396200	-3.51029300	0.43566200
C	-1.81391900	-0.77242900	-2.58231600	C	1.66852900	-3.37252000	-0.20788600
C	-2.50734700	-1.26589500	-1.43440700	C	2.72815000	-2.79208200	0.47937200
C	-3.34425800	-0.15736700	-0.80114100	C	3.60989800	-1.85877300	-0.19955800
C	-3.34427300	-0.15702300	0.80119900	C	3.96694800	-0.81263400	0.74250100
C	-2.68587700	1.05991600	1.43821700	C	4.09296400	0.50126100	0.30699600
C	-0.47339300	2.62976400	2.30445000	C	1.00433600	3.05906600	-1.74139800
C	-0.83370400	1.45126800	3.03277800	C	1.71787000	2.02440500	2.68184000
C	-1.91190400	0.66420200	2.58457900	C	1.18919800	2.97950100	1.82155900
C	-1.81394500	-0.77132600	2.58264500	C	-0.24502100	3.04549200	1.60192300
C	-2.50735700	-1.26527700	1.43493800	C	-1.08932100	2.15089000	2.25054200
C	-2.00026800	-2.34795500	0.73323600	C	-0.53663900	1.15262700	3.14963500
C	-2.00026400	-2.34827200	-0.73223700	C	1.50442000	-0.19716500	3.41797500
C	-0.76169500	-2.99348300	-1.15753800	C	2.79913400	-0.05995600	2.77456100
C	-0.09616000	-2.51238700	-2.30718700	C	2.93091800	1.31304500	2.31959200
C	1.52289000	1.62184800	-3.02494400	C	3.56390800	1.58740800	1.11292200
C	1.73720700	-1.22197300	-3.02443000	C	3.01174000	2.58547800	0.21399600
C	-2.33106600	2.18900900	-0.73847500	C	1.85051700	3.26635800	0.56063200
C	-4.88716100	-0.30968000	1.12120000	C	-0.47000400	3.37166700	0.20562800
C	-4.88713600	-0.31012400	-1.12108700	C	-1.52941700	2.78968200	-0.48142900
C	-5.31128800	-1.26912000	0.00024600	C	-2.41110700	1.85763600	0.19733000
H	-6.39218200	-1.45856100	0.00027600	C	-2.19781000	1.54640500	1.53443200
H	-4.75932200	-2.22051900	0.00044900	C	-2.32951000	0.17163400	1.98934300
C	-5.54613700	0.97722300	0.66903000	C	-1.30241500	-0.07073800	2.98713200
C	-5.54601100	0.97701600	-0.66943500	C	-0.66253400	-1.30398900	3.04344400
H	-5.06114300	-0.61839600	2.15826100	C	0.77166100	-1.36795000	3.26232100
H	-5.06111200	-0.61924100	-2.15802900	C	3.30597500	-1.09941200	2.00345600
H	-5.85115800	1.78767800	-1.33032800	C	2.54044800	-2.32286400	1.84092600
H	-5.85137700	1.78810600	1.32960800	C	1.30120200	-2.45423900	2.45652800

C₆₀-C₆H₅ [5,6] intermediate complex

C	0.19437400	-3.06137700	1.73880300
C	-1.01912000	-2.34996200	2.10153100
C	-2.00013600	-2.11748100	1.14446700
C	-2.66588400	-0.82885900	1.08628600
C	-2.89013100	-0.50309700	-0.31047700
C	-2.76795800	0.81025600	-0.74467200
C	0.82491000	3.50848200	-0.43853300
C	-1.34170100	2.32034100	-1.84343100
C	0.83582700	1.09080900	3.36034700
C	-5.96753300	-0.94027700	0.80196900
C	-5.83279400	0.48168500	1.14486300
C	-5.90491200	1.21634300	0.01583700
C	-6.11071600	0.30234500	-1.15658700
C	-6.11951800	-1.06176100	-0.53294600
H	-5.84059200	2.30161900	-0.05652500
H	-5.31699600	0.40977100	-1.91766900
H	-7.06199700	0.51736700	-1.67569700
H	-6.24340100	-1.98943700	-1.09043500
H	-5.69489800	0.86712600	2.15524100
H	-5.94071500	-1.75771100	1.52275900

C₆₀-C₆H₅ [6,6] intermediate complex

C	-1.96781500	1.37625000	-2.02181600
C	-2.40643100	0.06574800	-1.87130900
C	-2.87320900	-0.40260000	-0.57842400
C	-0.05297000	2.73112800	-2.15956100
C	-0.78182900	1.65712400	-2.81125700
C	-0.08907400	0.61691100	-3.42084300
C	-2.43653000	-1.77844500	-0.41529200
C	-2.02650200	-2.23548100	0.83068200
C	1.33704700	2.71939300	-2.14583200
C	-1.70217000	-2.16066500	-1.60761600
C	1.98420400	-3.11506400	0.96766900
C	1.29761700	-3.46979000	-0.18768300
C	1.76361800	-3.00143500	-1.48129100
C	2.89581000	-2.19915100	-1.56391100
C	3.61297300	-1.82883000	-0.35651400
C	1.24895000	-2.73191300	2.16020100
C	-0.14098100	-2.72042600	2.14667000
C	-0.85877100	-3.09130200	0.93954100
C	-0.15477500	-3.45900300	-0.20217100
C	0.59922400	-2.70028300	-2.29514500
C	0.61666000	-1.60950100	-3.15608700
C	1.79905000	-0.77111100	-3.24256800
C	2.91390500	-1.05952500	-2.46411500
C	3.64223900	0.01502500	-1.81317100
C	4.07441000	-0.46050000	-0.51068800
C	3.22498000	1.33158700	-1.96903600
C	2.06061500	1.63321800	-2.78286700
C	1.36297600	0.60480200	-3.40577200
C	-0.58608700	-2.98305700	-1.50395100
C	-0.55023100	-0.75130600	-3.26600400

C	3.16705400	-2.27682200	0.88151300
C	-5.96059900	-0.51266800	-1.09808700
C	-6.05348100	-1.22243500	0.04640200
C	-5.91211700	0.94964300	-0.76886200
H	-5.01006100	1.44640700	-1.17075700
H	-6.77174800	1.48959600	-1.20502200
H	-6.11390200	-2.30777800	0.12529100
H	-5.93946500	-0.91352600	-2.11099400
C	-1.68369800	-1.02094400	-2.50837500
C	-1.97165200	2.27746200	-0.88128000
C	-2.41378100	1.82613200	0.35713300
C	-2.87651400	0.45850100	0.51167100
C	-0.78803100	3.11441000	-0.96684400
C	-0.10092900	3.46899100	0.18893300
C	-2.44353500	-0.01705600	1.81421400
C	-2.03001200	-1.33371100	1.97209600
C	-1.71529400	1.05678000	2.46475700
C	1.97800800	-1.65807600	2.81176100
C	1.28579000	-0.61830100	3.42143000
C	1.74807100	0.75008200	3.26722000
C	2.88219000	1.01971900	2.51031800
C	3.60542600	-0.06697100	1.87372900
C	-0.86471700	-1.63431100	2.78417500
C	-0.16639300	-0.60619300	3.40839300
C	0.58158200	1.60775500	3.15746900
C	0.59901400	2.69859500	2.29658100
C	1.78378800	2.98035600	1.50546700
C	2.90068800	2.15941500	1.61015100
C	3.63508800	1.77691300	0.41704600
C	4.07075700	0.40109200	0.58010200
C	3.22139200	2.23198100	-0.82931400
C	2.05465600	3.08985100	-0.93878600
C	1.35132500	3.45615600	0.20293400
C	-0.60131100	0.76903200	3.24488800
C	-0.56579000	3.00004100	1.48226500
C	3.16319300	-1.37633700	2.02115200
C	-5.95810000	0.96735800	0.72992700
C	-6.05183000	-0.29967000	1.18619100
H	-6.11013700	-0.60276200	2.23145300
H	-5.93391800	1.87473600	1.33260400
C	-1.69726900	2.19699000	1.56469800

C₆₀-C₆H₅ [5,6] transition state

C	0.55707100	3.02521700	1.82531400
C	-0.53091100	2.29224400	2.44913500
C	-0.26101800	1.18006200	3.23820700
C	1.10923800	0.73596000	3.41993200
C	2.15053900	1.42891500	2.81346800
C	1.86864200	2.60056700	2.00141900
C	0.10660800	3.47715500	0.52111100
C	-1.25979200	3.02828200	0.34033500

C	-1.65704000	2.28638600	1.53805100
C	-2.46973100	1.17321500	1.43289200
C	-1.10262700	0.00856400	3.12302600
C	1.10931600	-0.71694100	3.42395200
C	2.15068800	-1.41312100	2.82130400
C	3.23993500	-0.69006700	2.19064700
C	3.23986100	0.70248900	2.18679700
C	3.63309100	1.42439200	0.99185300
C	2.78838500	2.60211500	0.87701400
C	2.35694100	3.02979700	-0.37212100
C	0.98871800	3.48327900	-0.55586300
C	-1.68596400	2.58567200	-0.89725700
C	-0.77642200	2.59870700	-2.02457000
C	0.53642000	3.03290800	-1.85809700
C	1.62068700	2.30159200	-2.48154100
C	2.74891500	2.29893700	-1.56592100
C	3.55319000	1.17187500	-1.45656300
C	4.00750000	0.72505900	-0.15029400
C	4.00758400	-0.72542200	-0.14627400
C	3.63319200	-1.41848200	0.99969400
C	-0.26092400	-1.16215900	3.24464900
C	0.98911600	-3.48624900	-0.53664600
C	0.10692100	-3.47427700	0.54025600
C	-1.25953200	-3.02667600	0.35698400
C	-1.68559300	-2.59078600	-0.88302700
C	-0.77603200	-2.61003600	-2.01026400
C	1.62100900	-2.31510300	-2.46878800
C	2.74924200	-2.30726900	-1.55320000
C	2.35727400	-3.03157600	-0.35538600
C	2.78866300	-2.59696400	0.89136500
C	1.86887800	-2.58926600	2.01570700
C	0.55734100	-3.01497800	1.84192100
C	-1.65687400	-2.27798100	1.55056100
C	-2.46988400	-1.16562800	1.43947100
C	-3.09297400	-0.75188000	0.15092500
C	-2.54201600	-1.41667600	-1.00151800
C	-2.17127200	-0.71742300	-2.16214400
C	-1.06353800	-1.43632600	-2.80507200
C	-0.02754300	-0.74218200	-3.40387600
C	1.34149500	-1.18589300	-3.23375000
C	3.55333100	-1.17949800	-1.45004300
C	3.26908500	-0.00605900	-2.25792900
C	2.18567700	-0.00853100	-3.12823400
C	1.34129300	1.16811800	-3.24023700
C	-0.02768600	0.72332800	-3.40794600
C	-1.06386500	1.42059900	-2.81295300
C	-2.17156500	0.70517200	-2.16623500
C	-2.54223400	1.41065400	-1.00916900
C	-3.09200200	0.75229300	0.14674300
C	-0.53073400	-2.27867500	2.46165400
C	-2.17955200	0.00599800	2.23333900
C	0.53684000	-3.04315300	-1.84134200
C	-5.15417800	1.15157300	0.30315400
C	-5.15071200	-1.14995100	0.30842600
C	-5.34881400	0.00283600	1.25422800
H	-6.41020300	0.00185100	1.56258300

H	-4.73296900	0.00592200	2.15995900
C	-5.58437400	0.69419200	-0.95845900
C	-5.58278200	-0.69917200	-0.95525300
H	-5.17372900	2.19665200	0.61467400
H	-5.17029600	-2.19359600	0.62481200
H	-5.74134100	1.32227700	-1.83475700
H	-5.73847400	-1.33162100	-1.82863800

C₆₀-C₆H₅ [6,6] transition state

C	-3.22438900	0.72716800	-2.19519500
C	-3.22437400	-0.72620500	-2.19553100
C	-3.61263400	-1.42134000	-1.05568700
C	-4.01512900	-0.69512500	0.13595900
C	-4.01514500	0.69495900	0.13628100
C	-3.61267800	1.42174700	-1.05502700
C	-2.07901900	1.17622600	-2.96445100
C	-1.36803700	0.00080400	-3.43691800
C	-2.07899100	-1.17485400	-2.96498900
C	-1.36920900	-2.30129000	-2.56428700
C	-2.87197100	-2.59725000	-0.63552900
C	-3.52215200	-1.42211900	1.29229900
C	-3.04631000	-0.72721700	2.39871000
C	-3.04632900	0.72602100	2.39904500
C	-3.52219200	1.42142400	1.29296300
C	-2.81599200	2.59733600	0.81721400
C	-2.87204800	2.59747200	-0.63430900
C	-1.77527200	3.02907100	-1.37209900
C	-1.36927400	2.30249300	-2.56319900
C	0.02137800	0.00083000	-3.48554700
C	0.76399200	1.17683500	-3.06733700
C	0.08105000	2.30557400	-2.61974500
C	0.57047600	3.02525000	-1.46437200
C	-0.57465600	3.47778700	-0.69080400
C	-0.52141000	3.47810100	0.69749000
C	-1.66598500	3.02880100	1.46882000
C	-1.16890100	2.30163500	2.62470000
C	-1.84539600	1.17494800	3.07830600
C	-2.81592100	-2.59778700	0.81599500
C	0.99751500	-1.17736300	2.96011900
C	0.28163400	-2.30769500	2.56839100
C	0.67975900	-3.02711500	1.37975400
C	1.77064600	-2.58129400	0.63835200
C	2.51821500	-1.41796400	1.05455800
C	2.14446300	0.73388600	2.19716800
C	0.99749000	1.17601100	2.96066100
C	0.28920300	-0.00079800	3.43387100
C	-1.09967200	-0.00083000	3.49302900
C	-1.84536300	-1.17643000	3.07775000
C	-1.16884100	-2.30289900	2.62362300
C	-0.52131900	-3.47844200	0.69585300
C	-0.57454900	-3.47743800	-0.69244200

C	0.57057400	-3.02451300	-1.46580000	C	-0.50539400	3.05014200	1.85153200
C	1.71532100	-2.58101000	-0.81062300	C	-1.57743400	2.31476300	2.48714700
C	2.43107500	-1.41606400	-1.28289900	C	-2.71866200	2.30692800	1.58844000
C	3.04136900	-0.72024100	-0.13552700	C	-3.51969500	1.17653500	1.49194700
C	3.04124600	0.72032200	-0.13521100	C	-3.99101600	0.72473900	0.19328800
C	2.51825900	1.41760000	1.05525200	C	-3.99103100	-0.72467500	0.19336300
C	0.28157600	2.30650200	2.56947800	C	-3.63141000	-1.42170200	-0.95544900
C	0.67968500	3.02649700	1.38118500	C	0.23167100	-1.16795200	-3.24680200
C	1.77062900	2.58111600	0.63958200	C	-0.97349300	-3.49372400	0.55518900
C	1.71524100	2.58148400	-0.80939200	C	-0.10069100	-3.47919700	-0.53098900
C	2.43091700	1.41673800	-1.28221000	C	1.26890000	-3.03643400	-0.36400600
C	1.96586700	0.73299200	-2.39260700	C	1.71454500	-2.60892800	0.86724200
C	1.96590700	-0.73178000	-2.39291700	C	0.81258700	-2.61856600	1.99928800
C	0.76403600	-1.17534500	-3.06787400	C	-1.57747100	-2.31449000	2.48738300
C	0.08111700	-2.30429800	-2.62082500	C	-2.71869600	-2.30673800	1.58867700
C	-1.66590400	-3.02953200	1.46740000	C	-2.34300400	-3.03610500	0.38780800
C	-1.77517500	-3.02844500	-1.37353100	C	-2.78732400	-2.60172900	-0.85369000
C	2.14447300	-0.73482300	2.19682200	C	-1.87997100	-2.59534600	-1.98819000
C	5.21232400	1.15449600	-0.29801100	C	-0.56637800	-3.01722700	-1.82533900
C	5.21195800	-1.15442600	-0.29828100	C	1.65214100	-2.27669600	-1.56981400
C	5.35159700	0.00007600	-1.24761300	C	2.46989600	-1.17120200	-1.47280900
H	6.39183900	-0.00014800	-1.62511700	C	3.26378500	-0.81442300	-0.21606800
H	4.68043000	0.00032500	-2.11580300	C	2.58478200	-1.43207600	0.97329000
C	5.59018000	0.70268500	0.96674500	C	2.21274300	-0.72530200	2.09197500
C	5.58997500	-0.70292500	0.96658100	C	1.10752700	-1.43564700	2.76849000
H	5.21215600	2.19883200	-0.61150800	C	0.08599400	-0.73723800	3.37576600
H	5.21196700	-2.19873400	-0.61188900	C	-1.28357300	-1.17889400	3.24048100
H	5.73674100	-1.33397100	1.84253000	C	-3.51971600	-1.17634900	1.49206900
H	5.73740300	1.33350800	1.84277600	C	-3.22398300	0.00013200	2.29203400

C₆₀-C₆H₅ [5,6] adduct

C	-0.56633200	3.01704700	-1.82564600	C	0.08600800	0.73757900	3.37569900
C	0.51378600	2.27798700	-2.45693300	C	1.10754300	1.43590900	2.76833600
C	0.23168500	1.16761600	-3.24692200	C	2.21273700	0.72546400	2.09188200
C	-1.14036500	0.72646400	-3.41407400	C	2.58481100	1.43213800	0.97314500
C	-2.17315800	1.42140400	-2.79510600	C	3.26378900	0.81436100	-0.21615100
C	-1.87993100	2.59516400	-1.98845200	C	0.51375700	-2.27825200	-2.45670900
C	-0.10063700	3.47914900	-0.53133900	C	2.15343700	-0.00013700	-2.24166900
C	1.26895500	3.03638300	-0.36430700	C	-0.50543800	-3.04994800	1.85183600
C	1.65216800	2.27650500	-1.57003600	C	4.81131000	1.12440300	-0.32080200
C	2.46990200	1.17100900	-1.47291600	C	4.81126700	-1.12446600	-0.32066300
C	1.06813500	-0.00017300	-3.13252300	C	5.28233700	-0.00009800	-1.25509200
C	-1.14037600	-0.72680000	-3.41400000	H	6.37275200	-0.00014500	-1.37635600
C	-2.17317100	-1.42165700	-2.79495700	H	4.79787600	-0.00014200	-2.24070400
C	-3.25233500	-0.69764900	-2.15225200	C	5.42260900	0.66923200	0.99154700
C	-3.25232100	0.69747100	-2.15232000	C	5.42252000	-0.66912300	0.99167200
C	-3.63138400	1.42164700	-0.95559200	H	5.00382400	2.15948800	-0.62598400
C	-2.78728000	2.60167400	-0.85395000	H	5.00381400	-2.15958400	-0.62571200
C	-2.34295300	3.03616500	0.38750400	H	5.70153100	1.32764500	1.81340900
C	-0.97343500	3.49378400	0.55483800	H	5.70136200	-1.32742400	1.81365000
C	1.71459000	2.60899800	0.86698700				
C	0.81262800	2.61875800	1.99902700				

C₆₀-C₆H₅ [6,6] adduct

C	-3.23843500	0.72709000	-2.15273900
C	-3.23844000	-0.72731800	-2.15265900
C	-3.61174400	-1.42245900	-1.00708600
C	-3.99489000	-0.69507200	0.18993000
C	-3.99488600	0.69511500	0.18985300
C	-3.61173300	1.42236400	-1.00724300
C	-2.10578500	1.17637800	-2.93707300
C	-1.39991600	-0.00019100	-3.41606200
C	-2.10579200	-1.17670500	-2.93694400
C	-1.39275900	-2.30601100	-2.54896300
C	-2.86771500	-2.59949900	-0.59838800
C	-3.48478400	-1.42259200	1.33861000
C	-2.98958400	-0.72706400	2.43663200
C	-2.98958100	0.72735100	2.43655200
C	-3.48477500	1.42276100	1.33845300
C	-2.78897200	2.59962000	0.85198100
C	-2.86769900	2.59945000	-0.59867800
C	-1.78285400	3.03331400	-1.35359000
C	-1.39274600	2.30572400	-2.54921700
C	-0.01166000	-0.00019700	-3.47326000
C	0.73562500	1.17596400	-3.06758800
C	0.05628700	2.30976000	-2.62366000
C	0.56038200	3.02937800	-1.48157300
C	-0.57249300	3.48310500	-0.69085800
C	-0.49754400	3.48339700	0.69584100
C	-1.62899400	3.03327800	1.48540400
C	-1.11183000	2.30581300	2.63186100
C	-1.77897900	1.17666400	3.09434700
C	-2.78899000	-2.59950900	0.85227000
C	1.06029200	-1.17595300	2.91665200
C	0.33696300	-2.31052700	2.54969800
C	0.71414000	-3.03127400	1.36057100
C	1.79432200	-2.58018000	0.60376500
C	2.56390100	-1.43545800	1.00782400
C	2.19499000	0.74123500	2.13524900
C	1.06029900	1.17627400	2.91652400
C	0.36089300	0.00018900	3.40076300
C	-1.02530000	0.00019600	3.49403000
C	-1.77898600	-1.17631200	3.09448100
C	-1.11184400	-2.30551500	2.63211900
C	-0.49756400	-3.48331800	0.69622800
C	-0.57251100	-3.48318300	-0.69047000
C	0.56036600	-3.02955100	-1.48123400
C	1.71585400	-2.57872900	-0.84505900
C	2.43598800	-1.43118900	-1.32852800
C	3.24308600	-0.80055000	-0.19785400
C	3.24309500	0.80051500	-0.19794200
C	2.56391500	1.43556000	1.00766800
C	0.33697700	2.31081200	2.54944300
C	0.71415700	3.03142100	1.36023500
C	1.79433600	2.58023600	0.60347900
C	1.71586800	2.57862400	-0.84534700
C	2.43599200	1.43102700	-1.32868600

C	1.94669200	0.74079800	-2.41137200
C	1.94669100	-0.74108000	-2.41129100
C	0.73562000	-1.17631400	-3.06745400
C	0.05627600	-2.31005800	-2.62340000
C	-1.62901300	-3.03310200	1.48574100
C	-1.78287100	-3.03345700	-1.35325100
C	2.19498400	-0.74100700	2.13533000
C	4.79007300	1.12105900	-0.31161900
C	4.79006200	-1.12110700	-0.31148000
C	5.23676600	-0.00008200	-1.26034700
H	6.32161200	-0.00009300	-1.42580100
H	4.70633400	-0.00013500	-2.22389700
C	5.41933500	0.66927100	0.99026400
C	5.41927700	-0.66916000	0.99037200
H	4.97439100	2.15731900	-0.61730700
H	4.97437500	-2.15740700	-0.61703500
H	5.70609900	-1.32930200	1.80837200
H	5.70619700	1.32951800	1.80816400

Ca@C₆₀

C	2.22807200	2.60494600	0.71755500
C	2.22603300	2.60573100	-0.72100200
C	1.09517700	3.04107900	-1.43043100
C	-0.07552000	3.49634100	-0.69235900
C	-0.07361000	3.49556900	0.69612500
C	1.09910500	3.03941400	1.43047100
C	2.98581000	1.42844900	1.15362300
C	3.49455600	0.73013000	-0.00439800
C	2.98241900	1.42967300	-1.16032000
C	2.51886200	0.74047400	-2.30020000
C	0.65018900	2.34073300	-2.60415700
C	-1.24891200	3.04578500	-1.42238200
C	-2.36464100	2.60495400	-0.72197400
C	-2.36263400	2.60414500	0.73112100
C	-1.24495800	3.04419000	1.42890500
C	-0.78199100	2.32248300	2.60440600
C	0.65733300	2.33791800	2.60474300
C	1.37201100	1.18153900	3.01077400
C	2.52536600	0.73798900	2.29415400
C	3.49378800	-0.73360100	-0.00522700
C	2.98431600	-1.43270600	1.15207600
C	2.52460300	-0.74304300	2.29331900
C	1.37081500	-1.18626000	3.00951700
C	0.64298200	-0.00223100	3.43856700
C	-0.74834000	-0.00153200	3.44574700
C	-1.48120800	1.18184200	3.02379900
C	-2.64350900	0.73032100	2.29987500
C	-3.08865200	1.42219400	1.17298200
C	-0.78919400	2.32533800	-2.59990700
C	-3.09325300	-1.41916000	-1.16466900
C	-2.65052600	-0.72772500	-2.29277800

C	-1.49065400	-1.18039700	-3.01989400	C	-1.06492000	3.00995400	0.70683100
C	-0.79145900	-2.32172800	-2.60241800	C	-0.44601800	3.31103900	-0.55723000
C	-1.25190100	-3.04298800	-1.42566900	C	0.95017600	3.46367900	-0.64898500
C	-2.36520500	-2.60265000	0.72829200	C	1.67061700	2.89920900	-1.75502100
C	-3.09004500	-1.42044600	1.17142900	C	2.92468200	2.38112700	-1.26257000
C	-3.54561500	-0.70072800	0.00439700	C	3.43789200	1.18009600	-1.76357700
C	-3.54492200	0.70420300	0.00518000	C	4.03136000	0.20969000	-0.87340100
C	-3.09183500	1.42346300	-1.16311800	C	3.68516700	-1.12478700	-1.35519400
C	-2.64981100	0.73282500	-2.29197000	C	3.42405500	-2.14269600	-0.43309500
C	-0.75777800	0.00224200	-3.44393000	C	0.28016000	-2.21879200	2.77678200
C	0.63354000	0.00156000	-3.44056700	C	0.09765100	-3.08144800	-1.72877600
C	1.36253800	-1.18293700	-3.01472500	C	-0.50102800	-3.37077700	-0.50838100
C	0.64787600	-2.33855300	-2.60669800	C	-1.73176300	-2.70182500	-0.11800900
C	1.09217100	-3.04056400	-1.43368200	C	-2.30682600	-1.75886900	-0.98844700
C	-0.07897500	-3.49552000	-0.69612300	C	-1.68541800	-1.45860000	-2.25208000
C	-0.07706700	-3.49630700	0.69235900	C	0.56114300	-1.37787400	-3.28636700
C	-1.24798600	-3.04457700	1.42561700	C	1.81275600	-1.86565800	-2.78376700
C	-2.64423800	-0.73024200	2.29905800	C	1.53863500	-2.92482900	-1.82232900
C	-1.48237800	-1.18371800	3.02250400	C	2.31856200	-3.05664000	-0.68028900
C	-0.78431700	-2.32459400	2.60189300	C	1.69447000	-3.35687400	0.59710500
C	0.65501500	-2.34146600	2.60220600	C	0.31697200	-3.51729100	0.68512600
C	1.09610000	-3.04217100	1.42720800	C	-1.67783700	-2.44570300	1.29554600
C	2.22549300	-2.60801000	0.71475500	C	-2.19824800	-1.22673700	1.78873900
C	2.22345900	-2.60716500	-0.72379900	C	-2.78806800	-0.26473800	0.90005100
C	2.98098200	-1.43134600	-1.16184200	C	-2.86838600	-0.50989200	-0.47891600
C	2.51814500	-0.74048900	-2.30105100	C	-2.64749200	0.55060000	-1.45085900
C	-1.48948200	1.18515600	-3.01860200	C	-1.88141300	-0.02706100	-2.51681600
C	1.36369200	1.18486700	-3.01344200	C	-0.82237500	0.67549800	-3.14529000
C	-2.36721300	-2.60183600	-0.72480400	C	0.38374400	0.01335500	-3.51283700
Ca	1.12421300	-0.00025900	-0.00015600	C	2.88032100	-0.98350500	-2.53958400
				C	2.70245100	0.43887000	-2.77744300
				C	1.48841800	0.92720600	-3.25127600
				C	0.95465600	2.17579700	-2.73871500
				C	-0.46931800	2.02261300	-2.64892500
				C	-1.19319300	2.58835900	-1.58538400
				C	-2.30956000	1.88733400	-0.96675700
				C	-2.19818200	2.11447800	0.44765100
				C	-2.44857500	1.08701600	1.39041600
				C	-0.41645700	-2.93569200	1.79729700
				C	-1.46935900	-0.48360500	2.80084500
				C	-0.49813900	-2.10038300	-2.62625000
				Ca	-0.40673300	0.40321300	-0.39536300
				C	-5.84386300	0.73856800	1.01331000
				C	-6.12274400	-1.08547900	-0.44711700
				C	-6.07334000	-0.74464900	1.01277700
				H	-7.01779200	-1.00775000	1.52235700
				H	-5.27793100	-1.29512200	1.54661600
				C	-5.79620800	1.18128500	-0.26032100
				C	-5.97070600	0.04257800	-1.17138400
				H	-5.74744700	1.34358900	1.91438500
				H	-6.27258900	-2.09166600	-0.83676200
				H	-5.64824000	2.21378300	-0.57751400
				H	-5.96803200	0.11298800	-2.25912500

Ca@C₆₀-C₆H₅ [5,6] intermediate complex

C	1.76000900	2.05450400	2.66910200				
C	0.68027400	1.31824500	3.31138900				
C	0.84303900	-0.05625300	3.55278500				
C	2.05768800	-0.72495600	3.16805100				
C	3.09578200	-0.01861100	2.55303900				
C	2.93051100	1.40448000	2.29813600				
C	1.16291500	3.02643900	1.76960900				
C	-0.28272200	2.86453300	1.86150100				
C	-0.56866500	1.83291200	2.82429900				
C	-1.64315300	0.94254000	2.55575200				
C	-0.25879500	-0.96786800	3.28642900				
C	1.71328300	-2.05995000	2.68689300				
C	2.41673500	-2.61671400	1.62147900				
C	3.48769000	-1.88030400	0.98350800				
C	3.81981100	-0.59660700	1.44764700				
C	4.09592200	0.45851100	0.49570800				
C	3.55648700	1.70406400	1.02140200				
C	2.99172700	2.64208500	0.16609400				
C	1.76145800	3.31565400	0.54964200				

Ca@C₆₀-C₆H₅ [6,6] intermediate complex

C	-3.18842200	-2.20987700	-0.71892700
C	-3.18803000	-2.21006000	0.71985900
C	-3.61621500	-1.07799100	1.43107600
C	-4.06513700	0.09653900	0.69524300
C	-4.06551700	0.09671200	-0.69325700
C	-3.61698800	-1.07763400	-1.42962800
C	-2.01624100	-2.97264700	-1.15670800
C	-1.32001700	-3.48754900	-0.00021600
C	-2.01560600	-2.97292500	1.15680000
C	-1.32307300	-2.51633400	2.29721600
C	-2.91248100	-0.63890700	2.60525700
C	-3.60680200	1.26596100	1.42672500
C	-3.15924800	2.37991500	0.72758900
C	-3.15964800	2.38009400	-0.72554200
C	-3.60758400	1.26631100	-1.42470500
C	-2.88995100	0.80081500	-2.60155700
C	-2.91390900	-0.63826200	-2.60410200
C	-1.76225200	-1.35900600	-3.01246400
C	-1.32434100	-2.51577700	-2.29740900
C	0.14353000	-3.49708600	-0.00061600
C	0.84539100	-2.99158800	-1.15845300
C	0.15631300	-2.52476800	-2.29851300
C	0.60526500	-1.37292500	-3.01333000
C	-0.57476900	-0.63664200	-3.44059800
C	-0.56719000	0.75460200	-3.44549800
C	-1.74529200	1.49379100	-3.02104900
C	-1.28563300	2.65219700	-2.29559400
C	-1.97382300	3.09958500	-1.16736400
C	-2.88851800	0.80017500	2.60305900
C	0.87014100	3.08377500	1.16847900
C	0.17613400	2.64434500	2.29749900
C	0.62164500	1.48124600	3.02202500
C	1.75763400	0.77538800	2.60052800
C	2.48010700	1.23324500	1.42446800
C	2.04837600	2.35387200	-0.72823500
C	0.86948600	3.08406000	-1.16850200
C	0.15304500	3.54120400	0.00024800
C	-1.25189600	3.54931100	0.00063600
C	-1.97317400	3.09929000	1.16892900
C	-1.28435600	2.65162300	2.29665800
C	-0.56528200	0.75374600	3.44569500
C	-0.57287400	-0.63749700	3.44046000
C	0.60692100	-1.37368200	3.01234800
C	1.76606400	-0.66453500	2.60312100
C	2.46287800	-1.11080900	1.42835900
C	2.92540200	0.05830600	0.69274100
C	2.92504400	0.05848900	-0.69465000
C	2.47932200	1.23361100	-1.42584900
C	0.17485500	2.64491800	-2.29724300
C	0.61997300	1.48199400	-3.02230100
C	1.75619900	0.77604700	-2.60161200
C	1.76462200	-0.66388700	-2.60455600
C	2.46208700	-1.11044100	-1.43029400

C	2.02585100	-2.24189500	-0.72099300
C	2.02625800	-2.24209300	0.71902500
C	0.84602900	-2.99188900	1.15694600
C	0.15758100	-2.52535000	2.29751800
C	-1.74362100	1.49303500	3.02208200
C	-1.76059800	-1.35974300	3.01281300
C	2.04878000	2.35368500	0.72737000
Ca	-0.56039000	-1.12241900	-0.00014600
C	5.96853900	-0.29086900	-1.17695400
C	5.96998200	-0.29748600	1.17525900
C	5.90011200	-1.22211700	-0.00341800
H	6.74641400	-1.93272200	-0.00591900
H	4.98663300	-1.84469500	-0.00463600
C	6.09803100	0.97692900	-0.73040200
C	6.09889100	0.97281300	0.73565000
H	5.93632200	-0.61295500	-2.21738000
H	5.93942400	-0.62546700	2.21388500
H	6.18437100	1.86223300	1.35972600
H	6.18263100	1.86984600	-1.34958700

Ca@C₆₀-C₆H₅ [5,6] transition state

C	-0.52859400	1.75387800	3.09173700
C	0.56017900	2.41169400	2.38676500
C	0.29669600	3.25380500	1.30947800
C	-1.06888600	3.46461500	0.87212800
C	-2.11390000	2.82610400	1.54417300
C	-1.83774500	1.96146500	2.67108000
C	-0.08122500	0.43057000	3.49778000
C	1.24977100	0.25773400	3.03805900
C	1.66775200	1.48004500	2.33764100
C	2.47901600	1.41007000	1.21874400
C	1.13755200	3.18067600	0.13108400
C	-1.07114500	3.52856600	-0.57513400
C	-2.12057900	2.95072500	-1.29514100
C	-3.21119900	2.29907600	-0.59595700
C	-3.20891400	2.23607200	0.79473200
C	-3.62919600	1.02096000	1.47103600
C	-2.77982800	0.84310900	2.62634900
C	-2.35728700	-0.42912900	3.00277800
C	-0.99923600	-0.65673300	3.45411000
C	1.67057500	-0.97832000	2.49887900
C	0.74662900	-2.10701200	2.46886000
C	-0.57272000	-1.91254500	2.92774000
C	-1.68086900	-2.50951300	2.17429200
C	-2.78883700	-1.58443200	2.22328800
C	-3.61269500	-1.41264700	1.10974700
C	-4.04237000	-0.08598400	0.72131300
C	-4.04383500	-0.01998300	-0.72544200
C	-3.63375500	1.14504500	-1.37467000
C	0.29198600	3.35465300	-1.03272400
C	-1.01602600	-0.35256400	-3.51003400

C	-0.10137200	0.73021100	-3.45712700	C	1.40371700	-3.45079200	-0.00026000
C	1.23447300	0.51481400	-3.00881500	C	2.08070200	-2.91000600	-1.15693400
C	1.65532800	-0.75707800	-2.59049000	C	1.37233200	-2.48164700	-2.29860600
C	0.72791600	-1.87830600	-2.65816700	C	2.89135200	-0.54455000	-2.60621500
C	-1.68814600	-2.30796200	-2.39868900	C	3.50614400	1.38696700	-1.42550800
C	-2.80232000	-1.38086100	-2.36318700	C	3.01250400	2.48201300	-0.72674200
C	-2.37522800	-0.16339200	-3.04083400	C	3.01249500	2.48190200	0.72715000
C	-2.79013700	1.07028600	-2.54819400	C	3.50612600	1.38675100	1.42575800
C	-1.84922600	2.18640400	-2.49475800	C	2.80917700	0.89261100	2.60317900
C	-0.54127100	2.01262100	-2.93464100	C	2.89131700	-0.54494700	2.60615900
C	1.65810600	1.67647700	-2.21319900	C	1.76713200	-1.30945800	3.01479700
C	2.47471200	1.50885600	-1.10700700	C	1.37229400	-2.48200100	2.29823200
C	3.06165400	0.20333600	-0.72976700	C	-0.05846400	-3.51321700	-0.00027200
C	2.51751400	-0.93867600	-1.45824300	C	-0.77969300	-3.03871400	1.15867900
C	2.13403900	-2.15751900	-0.81404500	C	-0.10473100	-2.55221100	2.30287500
C	1.02204200	-2.75868000	-1.56166600	C	-0.59567700	-1.42043300	3.01300700
C	-0.05420200	-3.38559300	-0.86561700	C	0.55413100	-0.63508700	3.44396200
C	-1.42728700	-3.13786600	-1.31461400	C	0.49020900	0.75396400	3.44954900
C	-3.61504200	-1.31036200	-1.23575100	C	1.63794800	1.53913400	3.02274100
C	-3.34494800	-2.17276700	-0.09830500	C	1.13054300	2.67851200	2.29831700
C	-2.27755400	-3.06777200	-0.14114600	C	1.79976100	3.15270500	1.16870300
C	-1.41499500	-3.24166300	1.01908500	C	2.80921300	0.89300700	-2.60301600
C	-0.04982400	-3.46853000	0.55789700	C	-1.04203000	3.01336100	-1.16931000
C	1.04591200	-2.90472500	1.30670800	C	-0.32741300	2.61293400	-2.30401200
C	2.14455100	-2.23635800	0.61310300	C	-0.72361300	1.43776800	-3.02670600
C	2.52527800	-1.06110200	1.35849000	C	-1.82537500	0.68360200	-2.58854300
C	3.07193800	0.13784000	0.72574100	C	-2.57049900	1.10587900	-1.42245200
C	0.55235200	2.60652800	-2.17972800	C	-2.19158700	2.24219900	0.73427200
C	2.19961400	2.27475000	0.09137600	C	-1.04204900	3.01318400	1.16973400
C	-0.58864600	-1.65483400	-3.10604300	C	-0.34446700	3.49613600	0.00025500
Ca	0.12927900	-0.90260300	0.08601500	C	1.05960200	3.56978600	0.00027100
C	5.26317800	0.27557600	1.15049400	C	1.79977800	3.15288300	-1.16821300
C	5.28437600	0.39227700	-1.15776600	C	1.13057600	2.67886200	-2.29791000
C	5.43710400	1.27642500	0.04475200	C	0.49026000	0.75448800	-3.44945000
H	6.48678900	1.62852100	0.07287200	C	0.55418100	-0.63456400	-3.44407800
H	4.79481300	2.16453400	0.08310100	C	-0.59563400	-1.41997200	-3.01325700
C	5.60946200	-0.97320400	0.63725400	C	-1.77529100	-0.75316500	-2.58949300
C	5.61870100	-0.90242400	-0.76993700	C	-2.46258300	-1.22403100	-1.42331400
H	5.26483600	0.53568900	2.20950700	C	-3.08531100	-0.08660900	-0.71905700
H	5.28503800	0.75775200	-2.18502000	C	-3.08534900	-0.08671400	0.71895800
H	5.72544900	-1.88451400	1.22310100	C	-2.57052200	1.10565800	1.42256000
H	5.74130900	-1.75027200	-1.44302100	C	-0.32744700	2.61258400	2.30438600
				C	-0.72365600	1.43730900	3.02689300
				C	-1.82540800	0.68320300	2.58859100
				C	-1.77533000	-0.75355400	2.58932400
				C	-2.46261800	-1.22424400	1.42306500
				C	-1.98727800	-2.33963200	0.72432700
				C	-1.98725600	-2.33951600	-0.72473100
				C	-0.77966400	-3.03851500	-1.15916200
				C	-0.10469000	-2.55184300	-2.30326900
				C	1.63799100	1.53959400	-3.02250100
				C	1.76717700	-1.30900200	-3.01499500
				C	-2.19157400	2.24231100	-0.73398200
				Ca	0.54750300	-1.11606500	0.00000000
				C	-5.25607000	-0.29316600	1.15489900
				C	-5.25612000	-0.29303100	-1.15492800

Ca@C₆₀-C₆H₅ [6,6] transition state

C	3.22159100	-2.10318700	0.71924700
C	3.22160100	-2.10307700	-0.71953200
C	3.60841700	-0.95542200	-1.43148400
C	4.00891300	0.23609700	-0.69424300
C	4.00890500	0.23599100	0.69432500
C	3.60839900	-0.95564100	1.43138000
C	2.08068500	-2.91018400	1.15650700

C	-5.37926200	-1.24418700	-0.00007100
H	-6.41387900	-1.63702000	-0.00007900
H	-4.69632200	-2.10300300	-0.00013700
C	-5.64856300	0.96637500	0.70326000
C	-5.64856900	0.96647200	-0.70311000
H	-5.24652200	-0.60536100	2.19959700
H	-5.24648700	-0.60505500	-2.19967700
H	-5.80755800	1.84018800	-1.33422900
H	-5.80754100	1.84001000	1.33449400

Ca@C₆₀-C₆H₅ [5,6] adduct

C	0.57283800	1.87532500	-3.01386100
C	-0.50039400	2.51636100	-2.28345400
C	-0.22146100	3.30385400	-1.17028200
C	1.14961300	3.47092300	-0.72695600
C	2.18136700	2.84256300	-1.41981500
C	1.88711400	2.03100300	-2.59125900
C	0.09007900	0.57326000	-3.47356600
C	-1.25991700	0.42097900	-3.05435000
C	-1.63352300	1.61056400	-2.28142700
C	-2.45143700	1.50524700	-1.16973100
C	-1.05770900	3.19220500	-0.00047900
C	1.14961300	3.47114300	0.72592200
C	2.18136300	2.84298300	1.41896700
C	3.26068900	2.20189300	0.69635700
C	3.26068700	2.20168500	-0.69701100
C	3.64438200	1.00314500	-1.42725300
C	2.80239900	0.89888900	-2.60042600
C	2.34724900	-0.34678400	-3.03012200
C	0.98522300	-0.52076900	-3.48568900
C	-1.69973500	-0.82159600	-2.54085400
C	-0.79446900	-1.95922500	-2.56123500
C	0.52369800	-1.79680800	-3.01120900
C	1.61209600	-2.45446500	-2.29751000
C	2.74241000	-1.54510800	-2.29949300
C	3.55561600	-1.44285700	-1.17570400
C	4.01687300	-0.14197900	-0.72503000
C	4.01687800	-0.14176300	0.72508700
C	3.64438600	1.00357400	1.42696500
C	-0.22145900	3.30420300	1.16929900
C	0.98522200	-0.51970700	3.48584800
C	0.09005900	0.57430700	3.47340300
C	-1.25995100	0.42191500	3.05428600
C	-1.69976500	-0.82081900	2.54111200
C	-0.79447400	-1.95843300	2.56182000
C	1.61209500	-2.45377700	2.29825000
C	2.74239800	-1.54441900	2.29995900
C	2.34723300	-0.34586700	3.03023000
C	2.80240800	0.89967800	2.60017000
C	1.88711600	2.03177700	2.59065800
C	0.57283400	1.87622400	3.01329800

C	-1.63353400	1.61123900	2.28096500
C	-2.45144900	1.50560300	1.16930500
C	-3.27438500	0.25678400	0.80964700
C	-2.56754500	-0.93936600	1.41854000
C	-2.21634000	-2.14126600	0.71782500
C	-1.11224000	-2.78626100	1.41978700
C	-0.04262900	-3.40452100	0.71618800
C	1.32937400	-3.22082400	1.17276700
C	3.55561900	-1.44250500	1.17614800
C	3.26809300	-2.24961600	0.00034400
C	2.18567400	-3.12210300	0.00046700
C	1.32938800	-3.22119000	-1.17181100
C	-0.04263100	-3.40471900	-0.71516400
C	-1.11223700	-2.78671500	-1.41896800
C	-2.21633000	-2.14146500	-0.71715400
C	-2.56751100	-0.93979500	-1.41820500
C	-3.27434000	0.25654100	-0.80971300
C	-0.50039300	2.51704100	2.28269700
C	-2.12271100	2.27500800	-0.00033100
C	0.52368800	-1.79588900	3.01172000
Ca	-0.28320000	-0.77974200	0.00007800
C	-4.80979400	0.38407200	-1.12520500
C	-4.80980700	0.38442400	1.12504800
C	-5.27676400	1.32298800	-0.00023100
H	-6.36535100	1.46258900	-0.00024500
H	-4.78056900	2.30377000	-0.00037100
C	-5.42862500	-0.92642700	-0.66908900
C	-5.42872500	-0.92618200	0.66931600
H	-5.00300200	0.68773500	-2.16100200
H	-5.00309400	0.68842600	2.16073100
H	-5.71238300	-1.74662700	-1.32771900
H	-5.71254800	-1.74615100	1.32820300

Ca@C₆₀-C₆H₅ [6,6] adduct

C	3.24418900	-2.05082800	0.71610200
C	3.24416800	-2.04839600	-0.72306500
C	3.60886300	-0.89132900	-1.43311400
C	3.98383500	0.30642100	-0.69424500
C	3.98381300	0.30412400	0.69497600
C	3.60877300	-0.89607000	1.42989100
C	2.12047500	-2.88153500	1.15247800
C	1.45215200	-3.42939300	-0.00566300
C	2.12042700	-2.87749900	-1.16210100
C	1.40299600	-2.45837800	-2.30268800
C	2.88598700	-0.49243700	-2.60865700
C	3.46014300	1.44887400	-1.42412900
C	2.94360400	2.53207800	-0.72317400
C	2.94360100	2.52966800	0.73137800
C	3.46014700	1.44412000	1.42868500
C	2.77562000	0.93452400	2.60644000
C	2.88608500	-0.50105200	2.60687700

C	1.77682100	-1.28723400	3.01463400
C	1.40308500	-2.46613500	2.29460100
C	-0.00970600	-3.50630500	-0.00582700
C	-0.73857500	-3.04529300	1.15197600
C	-0.06975500	-2.56089400	2.30094500
C	-0.58126700	-1.44679100	3.01653800
C	0.55263000	-0.63907800	3.44892700
C	0.46040300	0.74772800	3.45597900
C	1.59046000	1.55542700	3.02687100
C	1.05852700	2.68473300	2.30333500
C	1.71793300	3.17449100	1.17333800
C	2.77555600	0.94321800	-2.60351700
C	-1.11924600	2.96432400	-1.16266500
C	-0.39574600	2.59402100	-2.30187600
C	-0.76757800	1.41775200	-3.03043600
C	-1.85175600	0.64375500	-2.58400300
C	-2.62277100	1.04643700	-1.43696000
C	-2.25622400	2.16799500	0.74288600
C	-1.11922600	2.96044500	1.17236700
C	-0.43356900	3.45984100	0.00567000
C	0.96906200	3.57459200	0.00587300
C	1.71790900	3.17831100	-1.16295500
C	1.05847600	2.69237800	-2.29455100
C	0.46033900	0.75916600	-3.45366500
C	0.55260300	-0.62764200	-3.45119800
C	-0.58128500	-1.43676500	-3.02134000
C	-1.77075100	-0.79497800	-2.58345100
C	-2.46259500	-1.28016900	-1.43775900
C	-3.28898900	-0.16628900	-0.80070500
C	-3.28893900	-0.16892900	0.80006800
C	-2.62272100	1.04165700	1.44034100
C	-0.39570700	2.58638400	2.31033800
C	-0.76754700	1.40773000	3.03501500
C	-1.85173700	0.63520100	2.58605700
C	-1.77075200	-0.80352600	2.58074800
C	-2.46260800	-1.28492100	1.43351300
C	-1.96122800	-2.37188800	0.72640300
C	-1.96119100	-2.36941200	-0.73423800
C	-0.73851300	-3.04137300	-1.16200700
C	-0.06977700	-2.55318100	-2.30942000
C	1.59040900	1.56543900	-3.02185000
C	1.77679800	-1.27718900	-3.01907300
C	-2.25623100	2.17043700	-0.73578300
Ca	0.59095100	-1.10283400	-0.00081200
C	-4.83339600	-0.31143700	1.12051100
C	-4.83342100	-0.30782500	-1.12157600
C	-5.26440000	-1.26569500	-0.00209300
H	-6.34667500	-1.44772500	-0.00239100
H	-4.71972400	-2.22146700	-0.00365300
C	-5.48318300	0.98077000	0.67082200
C	-5.48347500	0.98279800	-0.66769200
H	-5.00925300	-0.62081600	2.15708100
H	-5.00936200	-0.61381500	-2.15914200
H	-5.78331100	1.79734700	-1.32631300
H	-5.78284000	1.79329300	1.33202500

Ca@C₆₀-C₆H₅ [5,6]-[5,6] intermediate complex

C	2.69218400	2.49959000	1.65245400
C	1.41969800	2.53745400	2.34254600
C	1.05867600	1.51026800	3.20928700
C	1.95258600	0.38555900	3.41091600
C	3.16968800	0.34043700	2.73603800
C	3.55015900	1.42325100	1.84120500
C	2.49898200	3.07033500	0.31960500
C	1.14039300	3.47225300	0.19537300
C	0.44478100	3.11578600	1.43693500
C	-0.85877000	2.65063200	1.41145300
C	-0.29254300	1.00641500	3.18161500
C	1.14006800	-0.81411800	3.51682600
C	1.58199400	-2.00371700	2.94302600
C	2.85458700	-2.05159200	2.25307400
C	3.63390300	-0.90104500	2.15168900
C	4.31355600	-0.58659700	0.90428600
C	4.26903400	0.84807400	0.71352700
C	4.08406300	1.38171200	-0.56097700
C	3.20427500	2.51105000	-0.77023700
C	0.44054100	3.21734600	-1.00700100
C	1.15760600	2.65679900	-2.14105800
C	2.50681400	2.29968800	-2.00968200
C	2.98335000	1.05996900	-2.61187400
C	3.95553600	0.48347000	-1.70246600
C	4.00453000	-0.89430300	-1.51745400
C	4.18445100	-1.44512200	-0.18599400
C	3.37340900	-2.64279900	-0.08072800
C	2.71665900	-2.94328000	1.11159400
C	-0.24971900	-0.42163700	3.38041400
C	-0.69692400	-3.24866700	-0.26513300
C	-1.38532600	-2.66510200	0.82388500
C	-2.26815000	-1.56786000	0.63843400
C	-2.39478000	-0.97557500	-0.63773500
C	-1.70616900	-1.57204500	-1.76883500
C	0.41209100	-2.73585000	-2.27807600
C	1.38284100	-3.31493800	-1.36840500
C	0.69342700	-3.62345900	-0.12097000
C	1.35931200	-3.44671400	1.09124900
C	0.65124200	-2.85639300	2.21863300
C	-0.67921100	-2.47783100	2.09191100
C	-2.10611200	-0.65087700	1.77003300
C	-2.16767700	0.71930800	1.58266800
C	-2.69606600	1.39954500	0.30825500
C	-2.49773600	0.42844700	-0.84051700
C	-1.86267600	0.73642700	-2.09089300
C	-1.36531900	-0.50239900	-2.68044900
C	-0.10960200	-0.55940300	-3.34471400
C	0.77806900	-1.69477800	-3.12517400
C	2.68878100	-2.83638000	-1.34628100
C	3.07702300	-1.75363600	-2.23716900
C	2.14682400	-1.20056600	-3.10967800

C	2.08992900	0.24160800	-3.29518100	C	1.66921500	1.07319300	-3.03411700
C	0.69127300	0.62233300	-3.44728600	C	0.57152700	0.24923900	-3.49137300
C	0.22364800	1.84033900	-2.88350100	C	-1.60138500	-1.35807800	-2.54993400
C	-1.05802000	1.91976600	-2.19246800	C	-0.25072800	-1.89473000	-2.58502300
C	-0.91051700	2.76909900	-1.04513300	C	0.80937200	-1.09297300	-3.03320000
C	-1.79072100	2.73758500	0.19000500	C	2.08544100	-1.13010600	-2.32938700
C	-1.13473800	-1.23343300	2.67678900	C	2.61344500	0.22264600	-2.31985100
C	-1.21064200	1.54757700	2.26484500	C	3.27143400	0.70370000	-1.19245700
C	-0.86319400	-2.67586300	-1.57286000	C	3.02754300	2.05674100	-0.72607700
Ca	0.17864900	0.31718200	-0.77045500	C	3.03598000	2.04134200	0.72423400
C	-2.88182400	3.86550100	0.29018800	C	2.14882700	2.84370600	1.44061900
C	-4.13884400	2.00579800	0.45747800	C	-2.35038400	2.91629300	1.21023600
C	-3.85960400	3.25589600	1.30898800	C	0.61419500	0.17618800	3.47862000
H	-4.75592400	3.87408600	1.44637700	C	-0.70666700	0.67932600	3.48023100
H	-3.40872100	3.03918100	2.28766300	C	-1.80468600	-0.12062600	3.05986700
C	-3.70161500	3.75260100	-0.98427400	C	-1.57046300	-1.41185000	2.53159100
C	-4.44930400	2.64699600	-0.88433600	C	-0.21963100	-1.94915100	2.53910300
H	-2.45216400	4.84885000	0.51551200	C	2.11364900	-1.17869100	2.27037700
H	-4.86077800	1.27285700	0.83634900	C	2.64234100	0.17508900	2.28324000
H	-3.60087800	4.40414400	-1.85162200	C	1.70668700	1.00991100	3.02589900
H	-5.08432800	2.21078300	-1.65503200	C	1.47844800	2.32254500	2.61221100
C	-5.64171900	-1.41204200	-0.46874700	C	0.12083400	2.84773600	2.61601700
C	-5.13571400	-2.56698400	-1.22391800	C	-0.93906800	2.05401600	3.03659800
C	-4.85785600	-3.56837300	-0.36496300	C	-2.72511200	0.73321700	2.30120200
C	-5.18003100	-3.12556900	1.03155500	C	-3.38884300	0.24674400	1.18824200
C	-5.66559100	-1.71809100	0.84452700	C	-3.48321400	-1.24205800	0.81324300
H	-4.46476100	-4.55197600	-0.61985900	C	-2.27103900	-1.93398400	1.40696700
H	-4.29961400	-3.17781900	1.69638300	C	-1.37338600	-2.79454000	0.69212400
H	-5.95336500	-3.76476300	1.49436100	C	-0.09048200	-2.81315900	1.38725100
H	-5.99756400	-1.07308300	1.65792800	C	1.14044200	-2.80856000	0.67591500
H	-5.00562900	-2.59251400	-2.30592300	C	2.24034400	-1.96994600	1.13432200
H	-5.94486100	-0.46466100	-0.91586400	C	3.28595100	0.67964800	1.15941400
				C	3.43253400	-0.15179600	-0.02636800
				C	2.92613400	-1.44533400	-0.03697200
				C	2.22575900	-1.94474000	-1.21009400
				C	1.13183200	-2.79399700	-0.75625200
				C	-0.10762700	-2.78267500	-1.45267400
				C	-1.38166000	-2.77909700	-0.74245200
				C	-2.28795400	-1.90356800	-1.42834600
				C	-3.49304400	-1.22508300	-0.80569100
				C	-2.19305000	2.08294100	2.31387700
				C	-3.49389700	1.08981800	0.02810500
				C	0.84642300	-1.15627900	2.98987200
				Ca	-0.36860100	-0.64591200	-0.00553000
				C	-4.88983100	-1.87544900	-1.11965800
				C	-4.87637800	-1.89884800	1.13047600
				C	-5.75534900	-1.30519800	0.01666100
				H	-6.76911900	-1.72553300	0.01840400
				H	-5.81199500	-0.20762800	0.02841400
				C	-4.77170600	-3.32484700	-0.67941500
				C	-4.76378500	-3.33879000	0.65881400
				H	-5.21516700	-1.69744300	-2.15155400
				H	-5.18923400	-1.74231500	2.16968800
				H	-4.61325100	-4.16995900	-1.34847900
				H	-4.59752000	-4.19760900	1.30824400
				C	5.78087400	-2.74163600	0.95090400

Ca@C₆₀-C₆H₅ [5,6]-[6,6] intermediate complex

C	6.33773500	-1.38675700	1.00956400
C	6.43923200	-0.89503400	-0.24400700
C	5.96697500	-1.93113600	-1.22001100
C	5.54559900	-3.06854400	-0.33811200
H	6.81968400	0.08567000	-0.52811300
H	6.77868900	-2.23527700	-1.90544100
H	5.14854100	-1.56656800	-1.86751600
H	5.13544400	-4.00896600	-0.70516700
H	6.61565000	-0.86806700	1.92697200
H	5.58659500	-3.37201100	1.81856300

Ca@C₆₀-C₆H₅ [6,6]-[6,6] intermediate complex

C	-2.59343300	2.19788500	0.72614600
C	-2.59299300	2.20263700	-0.71413700
C	-3.00069200	1.06137300	-1.42880500
C	-3.42599400	-0.12300300	-0.69580100
C	-3.42638800	-0.12750400	0.69227800
C	-3.00166600	1.05208800	1.43325400
C	-1.43632000	2.97838400	1.16691200
C	-0.74455900	3.50207800	0.01075200
C	-1.43564000	2.98612000	-1.14923500
C	-0.73420300	2.54186200	-2.29201900
C	-2.29633500	0.63948400	-2.60627100
C	-2.94960500	-1.28296800	-1.43119400
C	-2.48295700	-2.39200300	-0.73736600
C	-2.48342800	-2.39672000	0.71980000
C	-2.95055300	-1.29220300	1.42049700
C	-2.24633700	-0.81735700	2.60024700
C	-2.29799400	0.62263900	2.60839200
C	-1.15725500	1.36093100	3.02100200
C	-0.73567100	2.52680400	2.30718500
C	0.71937300	3.51521400	0.01129700
C	1.42780700	3.01868100	1.16639700
C	0.74002400	2.55968800	2.31392700
C	1.20489200	1.42145400	3.02380900
C	0.03854600	0.65960300	3.45261500
C	0.07354600	-0.72989200	3.45264100
C	-1.08940400	-1.48935400	3.01978200
C	-0.60539700	-2.63609700	2.29142900
C	-1.28508400	-3.09167600	1.15805300
C	-2.24460800	-0.80049600	-2.60739000
C	1.56031000	-2.98685600	-1.17690800
C	0.85327800	-2.58183200	-2.31422000
C	1.27427800	-1.41830500	-3.03744600
C	2.38959900	-0.69180000	-2.58701600
C	3.14264700	-1.13164900	-1.44179800
C	2.72853300	-2.24743600	0.73273300
C	1.55951700	-2.99442000	1.15820100
C	0.85368200	-3.45889400	-0.01111300
C	-0.55221900	-3.51549100	-0.01176800
C	-1.28432000	-3.08415500	-1.17929900

C	-0.60387000	-2.62125000	-2.30924100
C	0.07585200	-0.70761000	-3.45758800
C	0.04083400	0.68187300	-3.44862900
C	1.20688500	1.44096400	-3.01419300
C	2.36870700	0.74871700	-2.57992000
C	3.07969000	1.19936600	-1.43099100
C	3.85899800	0.04897100	-0.79940100
C	3.85846900	0.04373400	0.80185500
C	3.14166400	-1.14099300	1.43609700
C	0.85173200	-2.59668900	2.29763700
C	1.27225400	-1.43785200	3.02861400
C	2.38787600	-0.70852000	2.58361500
C	2.36695800	0.73204200	2.58582100
C	3.07878100	1.19007200	1.44034700
C	2.62302100	2.29947700	0.73870900
C	2.62353200	2.30429000	-0.72258200
C	1.42863700	3.02637100	-1.14652000
C	0.74156700	2.57475700	-2.29750500
C	-1.08738300	-1.46981200	-3.03046200
C	-1.15526700	1.38043700	-3.01335700
C	2.72903900	-2.24260500	-0.74587200
Ca	-0.00850400	1.13847300	0.00158900
C	5.40695400	0.11886100	1.12299200
C	5.40768100	0.12639800	-1.11901700
C	5.87893600	1.05950800	0.00529200
H	6.96792300	1.19515100	0.00609400
H	5.37493600	2.03723400	0.00844100
C	6.00154700	-1.19775900	0.66692700
C	6.00201700	-1.19324000	-0.67146000
H	5.59593900	0.41504300	2.16105900
H	5.59732500	0.42959400	-2.15493400
H	6.26602700	-2.01612000	-1.33496200
H	6.26510600	-2.02511300	1.32502400
C	-6.56752700	-1.15761300	-0.73491300
C	-6.56662000	-1.16183800	0.73132100
C	-6.48888800	0.10998800	1.17794300
C	-6.45678600	1.04334600	0.00449700
C	-6.49031100	0.11677300	-1.17427700
H	-6.46824200	0.43284300	2.21840000
H	-5.56745200	1.70015200	0.00589800
H	-7.32928600	1.72153600	0.00696400
H	-6.47109200	0.44563100	-2.21287800
H	-6.61362500	-2.05755000	1.35047600
H	-6.61524200	-2.04973100	-1.35918000

Ca@C₆₀-C₆H₅ [5,6]-[5,6] transition state

C	2.59747700	2.09343300	2.18332400
C	1.26201000	2.15914200	2.74107100
C	0.72270800	1.06366700	3.41064000
C	1.48992200	-0.16287200	3.53130200
C	2.76613700	-0.23373100	2.97710400

C	2.37022500	2.64537000	1.47701600	Ca@C ₆₀ -C ₆ H ₅ [6,6]-[6,6] transition state			
C	-2.11611000	2.98222000	1.32618500				
C	0.72395000	0.00477000	3.44280200				
C	-0.56560000	0.58177000	3.49024100	C	2.60890300	2.25129500	-0.72572900
C	-1.71789100	-0.13971900	3.07167500	C	2.60891800	2.25202200	0.72352600
C	-1.57040800	-1.42742800	2.50139700	C	3.02945600	1.11427400	1.42472100
C	-0.25466400	-2.04088400	2.46500300	C	3.59117800	-0.05504900	0.72014500
C	2.11870700	-1.40298200	2.17473100	C	3.59118200	-0.05572800	-0.72014100
C	2.73002900	-0.07135500	2.22041700	C	3.02944900	1.11287100	-1.42582800
C	1.85554400	0.78792300	3.00025500	C	1.44065500	3.01207300	-1.16065800
C	1.69649800	2.13141100	2.64186500	C	0.74177600	3.51949800	-0.00171000
C	0.37137300	2.72917400	2.68537100	C	1.44067600	3.01325300	1.15773200
C	-0.72623500	1.98259800	3.09780600	C	0.74223600	2.56309000	2.30334000
C	-2.59648400	0.78850900	2.35576700	C	2.32340000	0.68178300	2.59276200
C	-3.30722200	0.37744700	1.24050300	C	3.01289300	-1.21798100	1.42399900
C	-3.49840200	-1.09091000	0.82278000	C	2.57064900	-2.33198300	0.73587100
C	-2.32130800	-1.87362400	1.37502800	C	2.57065500	-2.33270700	-0.73365700
C	-1.48741100	-2.76007500	0.61537100	C	3.01290500	-1.21938000	-1.42287800
C	-0.19528300	-2.86908200	1.28657700	C	2.29510400	-0.75849700	-2.59074000
C	1.02306700	-2.89889300	0.55459000	C	2.32338700	0.67925900	-2.59344700
C	2.17780600	-2.15276200	1.01205700	C	1.17768400	1.40499700	-3.01793900
C	3.37110700	0.42448200	1.09955900	C	0.74222500	2.56081000	-2.30582000
C	3.56755800	-0.39952700	-0.11082800	C	-0.72232500	3.51579400	-0.00171100
C	2.96611800	-1.70638100	-0.15368100	C	-1.42552000	3.01319100	-1.15797100
C	2.13141300	-2.05299100	-1.31920200	C	-0.73282400	2.56872800	-2.30796400
C	0.99277000	-2.83639000	-0.87613700	C	-1.18311600	1.42603800	-3.02185500
C	-0.25412600	-2.74370500	-1.54902600	C	-0.00750100	0.68382500	-3.45334000
C	-1.51639300	-2.69503300	-0.81622900	C	-0.01989900	-0.70576600	-3.45745700
C	-2.38014800	-1.75000800	-1.46111300	C	1.15353700	-1.45161400	-3.02848200
C	-3.53266600	-1.02150100	-0.79593000	C	0.69102600	-2.60323300	-2.30563500
C	-1.98704300	2.10579300	2.40042000	C	1.38192400	-3.04013300	-1.16803800
C	-3.38110400	1.26152000	0.10918900	C	2.29510200	-0.75596900	2.59142700
C	0.86933600	-1.32494000	2.91095100	C	-1.46608600	-2.99671500	1.16912700
Ca	-0.40348900	-0.63253400	-0.01409200	C	-0.76649100	-2.58483700	2.30908800
C	-4.97111700	-1.57582000	-1.10448800	C	-1.20731100	-1.43016000	3.03492400
C	-4.92393700	-1.67135700	1.14341100	C	-2.33397800	-0.71972900	2.58682800
C	-5.78234100	-0.99052200	0.06392600	C	-3.07901800	-1.16813100	1.44000000
H	-6.81965400	-1.34887900	0.07055000	C	-2.64621600	-2.27054600	-0.73850300
H	-5.77169000	0.10746200	0.11037600	C	-1.46608900	-2.99784800	-1.16625200
C	-4.93549300	-3.04298600	-0.71110100	C	-0.75128500	-3.45064400	0.00165800
C	-4.90750500	-3.09985200	0.62574000	C	0.65691200	-3.47586600	0.00166900
H	-5.30123500	-1.34562700	-2.12449800	C	1.38192400	-3.03899600	1.17094500
H	-5.21039400	-1.52912900	2.19227600	C	0.69102900	-2.60099100	2.30812100
H	-4.83865600	-3.87448100	-1.40839100	C	-0.01989400	-0.70241000	3.45809400
H	-4.78296500	-3.98735100	1.24527700	C	-0.00749800	0.68718000	3.45262700
C	5.73129400	-0.91917400	-0.26185900	C	-1.18311100	1.42897300	3.02043100
C	4.76102200	-3.01476400	-0.32388500	C	-2.33632700	0.72124000	2.58445300
C	5.38170900	-2.00152500	-1.24108500	C	-3.05184900	1.16359300	1.43655400
H	6.32978900	-2.42950100	-1.61897300	C	-3.81335500	0.00315200	0.80077600
H	4.78309900	-1.69838200	-2.10938200	C	-3.81335800	0.00237200	-0.80081000
C	5.85981700	-1.51379900	0.99213800	C	-3.07901700	-1.16952900	-1.43889600
C	5.26920700	-2.79038400	0.95466300	C	-0.76649500	-2.58707600	-2.30661300
H	6.17125400	0.03697300	-0.54659800	C	-1.20731400	-1.43310300	-3.03356600
H	4.32178100	-3.95286100	-0.66468600	C	-2.33398000	-0.72224100	-2.58615900
H	6.24394600	-1.02271700	1.88563800	C	-2.33632500	0.71873500	-2.58518000
H	5.12336400	-3.44369600	1.81428200	C	-3.05185400	1.16219900	-1.43771300

C	-2.60913000	2.27527100	-0.73149400	C	0.49858700	3.45492500	-0.59522000
C	-2.60913600	2.27599200	0.72926900	C	1.30597300	3.01329400	-1.72433900
C	-1.42553300	3.01435100	1.15504000	C	2.62471400	2.60010100	-1.53115800
C	-0.73282500	2.57099800	2.30546600	C	3.10682800	1.41993900	-2.23302700
C	1.15354200	-1.44867300	3.02984900	C	3.98817600	0.69450200	-1.33232200
C	1.17768600	1.40794000	3.01654200	C	3.98809700	-0.69483000	-1.33231200
C	-2.64621400	-2.26982500	0.74067400	C	4.03549700	-1.42881900	-0.07536500
Ca	0.04090200	1.14899300	-0.00025700	C	3.19982600	-2.60788000	-0.20837500
C	-5.36283300	0.05422500	-1.12095100	C	2.41896900	-3.04325200	0.87350800
C	-5.36282900	0.05532900	1.12087300	C	-0.66992100	-0.71976100	3.16792700
C	-5.84911200	0.98418700	-0.00049600	C	-0.86490700	-3.03877500	-0.80605700
H	-6.94011400	1.10304300	-0.00055200	C	-1.84798500	-2.85838200	0.32761400
H	-5.35975300	1.96933400	-0.00098200	C	-2.78346600	-1.54160500	0.18860200
C	-5.93679900	-1.27272700	-0.66858400	C	-2.48921200	-0.70023800	-1.02893100
C	-5.93679800	-1.27206800	0.66981500	C	-1.75717500	-1.16187000	-2.17812900
H	-5.55661200	0.35040700	-2.15813700	C	0.42636800	-2.29742300	-2.61458000
H	-5.55660300	0.35253200	2.15776700	C	1.30562500	-3.01333500	-1.72429200
H	-6.18625400	-2.10142600	1.33090200	C	0.49821300	-3.45484200	-0.59515100
H	-6.18625600	-2.10273700	-1.32885300	C	1.07302000	-3.50650800	0.67493400
C	5.75966100	0.03289100	1.15447600	C	0.25991000	-3.01359100	1.79923800
C	5.75971500	0.03186600	-1.15450600	C	-1.04240900	-2.59196700	1.60152200
C	5.93826200	0.97564000	-0.00042700	C	-2.40338200	-0.68841000	1.39977400
H	6.99381000	1.30781400	-0.00055300	C	-2.40328500	0.68873500	1.39975100
H	5.30475200	1.87150600	-0.00083100	C	-2.78327300	1.54192500	0.18855900
C	6.08750500	-1.24608500	0.70333300	C	-2.48908000	0.70047100	-1.02891500
C	6.08753700	-1.24670900	-0.70220700	C	-1.75694300	1.16201100	-2.17805100
H	5.76767000	0.34536600	2.19909800	C	-1.28322600	0.00006500	-2.90234600
H	5.76776200	0.34339000	-2.19941100	C	0.03934700	-0.00000100	-3.47780200
H	6.19848000	-2.12809500	-1.33294300	C	0.88122700	-1.15909100	-3.29371300
H	6.19841200	-2.12690900	1.33485800	C	2.62441600	-2.60028300	-1.53110200

Ca@C₆₀-C₆H₅ [5,6]-[5,6] adduct

C	2.46839900	2.29839100	2.12501500	C	0.88136700	1.15903700	-3.29367300
C	1.13834400	2.28961700	2.69372800	C	0.42665600	2.29738400	-2.61455700
C	0.67882400	1.17207800	3.38897000	C	-0.90560400	2.30552400	-2.00093500
C	1.52445300	-0.00000500	3.52016300	C	-0.86459200	3.03898200	-0.80612300
C	2.79577900	-0.00007700	2.95185900	C	-1.84767100	2.85862900	0.32755400
C	3.28195600	1.17393200	2.24995400	C	-1.49241100	-1.39937200	2.26119700
C	2.41928500	3.04309100	0.87345000	C	-1.49226100	1.39963800	2.26116800
C	1.07337200	3.50649200	0.67485900	C	-0.90590500	-2.30544000	-2.00099600
C	0.26021400	3.01367700	1.79918000	Ca	0.12397000	-0.00063800	-0.92646200
C	-1.04214900	2.59218600	1.60148200	C	-2.92760900	3.99557700	0.46862600
C	-0.66984600	0.71996700	3.16791600	C	-4.22333200	2.17046000	0.24935600
C	0.67870400	-1.17200400	3.38899000	C	-4.01917400	3.28755400	1.28673400
C	1.13811200	-2.28960600	2.69377700	H	-4.91596600	3.90839600	1.40724600
C	2.46816600	-2.29853000	2.12506200	H	-3.68104300	2.92883600	2.26893800
C	3.28183200	-1.17414900	2.24997300	C	-3.60682400	4.07935900	-0.88792100
C	4.08477000	-0.72722500	1.12420400	C	-4.37604100	2.99226600	-1.01918400
C	4.08484900	0.72691100	1.12419600	H	-2.50786400	4.92565200	0.86967000
C	4.03565800	1.42849700	-0.07538200	H	-5.00059800	1.42302000	0.44980100
C	3.20010900	2.60763900	-0.20841000	H	-3.40187300	4.83662000	-1.64371400
				H	-4.92784700	2.67807600	-1.90454900
				C	-4.22354200	-2.17005100	0.24939900
				C	-2.92799000	-3.99527700	0.46878800
				C	-4.01948500	-3.28711900	1.28684800

H	-4.91632600	-3.90788200	1.40739700
H	-3.68130700	-2.92839600	2.26903500
C	-4.37613100	-2.99181600	-1.01918800
C	-3.60737500	-4.07920300	-0.88766000
H	-5.00077100	-1.42255500	0.44977500
H	-2.50829900	-4.92534300	0.86990900
H	-4.92775600	-2.67756400	-1.90464500
H	-3.40260200	-4.83663300	-1.64333100

C	-3.27180400	0.41784800	1.26870200
C	-3.50096800	-1.03982200	0.83147200
C	-2.33665400	-1.85694300	1.36138700
C	-1.52946400	-2.74617100	0.57902800
C	-0.23209600	-2.88777200	1.23433800
C	0.97995700	-2.92835100	0.49697300
C	2.16091300	-2.24064900	0.95288100
C	3.42302100	0.33873800	1.06926900
C	3.78035000	-0.48972100	-0.15878500
C	3.07775100	-1.92991200	-0.22227000
C	2.09331300	-2.10019100	-1.37528700
C	0.93915000	-2.84316900	-0.93548600
C	-0.31364500	-2.72147400	-1.59174900
C	-1.57045200	-2.66217300	-0.85034000
C	-2.41912200	-1.69072100	-1.47547200
C	-3.54828900	-0.94530400	-0.78749000
C	-1.90399700	2.10148600	2.44209100
C	-3.33518300	1.32037600	0.15137900
C	0.88447600	-1.39247700	2.85772600
Ca	-0.44839200	-0.60994000	-0.04215500
C	-5.00213700	-1.46124400	-1.08975200
C	-4.93651600	-1.59205100	1.15609200
C	-5.78838400	-0.87503000	0.09510700
H	-6.83366900	-1.20913700	0.10622600
H	-5.75175800	0.22155200	0.15793700
C	-4.99698500	-2.93467900	-0.71864900
C	-4.95805000	-3.01248100	0.61685900
H	-5.33627300	-1.20792100	-2.10290900
H	-5.21012500	-1.45914500	2.20955700
H	-4.92631500	-3.75760700	-1.42908300
H	-4.84899700	-3.91204200	1.22170400
C	5.31208400	-0.87880800	-0.25650600
C	4.32837000	-2.89237500	-0.34494200
C	5.23980200	-2.04885500	-1.24761800
H	6.21755200	-2.51995200	-1.40961600
H	4.78246500	-1.78290900	-2.21183900
C	5.65327300	-1.60537800	1.02817100
C	5.06606200	-2.80703000	0.97569800
H	5.93736200	-0.01834600	-0.52049900
H	4.04338000	-3.89271400	-0.69031100
H	6.18415000	-1.16662900	1.87241500
H	5.01768900	-3.55359400	1.76781100

Ca@C₆₀-C₆H₅ [5,6]-[6,6] adduct

C	-0.81617800	2.29244100	-2.88011500
C	-2.03761000	2.36776200	-2.11209900
C	-2.09354100	3.13366500	-0.95038200
C	-0.91593000	3.84999700	-0.49978900
C	0.26590800	3.76947600	-1.23324100
C	0.31719000	2.97665200	-2.45418200
C	-0.70726800	0.93531300	-3.41628800
C	-1.85615000	0.19658300	-3.01823300
C	-2.67472800	1.06282100	-2.16827700
C	-3.34042300	0.55423800	-1.06508300
C	-2.76710400	2.60577900	0.20996200
C	-0.87359700	3.76523000	0.95062300
C	0.34862900	3.60412800	1.59968100
C	1.57528300	3.53266400	0.83455500
C	1.53475600	3.61330600	-0.55446500
C	2.36837900	2.73560900	-1.36527800
C	1.62767100	2.35389200	-2.53530700
C	1.73771100	1.04600200	-3.02264900
C	0.56975800	0.33333400	-3.48263500
C	-1.71211000	-1.14528200	-2.58831900
C	-0.41133300	-1.78032400	-2.67513900
C	0.70930900	-1.04472800	-3.09445600
C	1.98761600	-1.22619100	-2.43442300
C	2.63178700	0.10260500	-2.37701000
C	3.35084900	0.47166300	-1.26448200
C	3.19766500	1.80180200	-0.73657200
C	3.24070700	1.71912200	0.70827400
C	2.45240000	2.57064200	1.48815400
C	-2.02538400	2.99736300	1.38284700
C	0.77235300	-0.06957600	3.41122300
C	-0.50416300	0.53149000	3.49039700
C	-1.67718800	-0.15975000	3.07705300
C	-1.56343900	-1.44206800	2.48704000
C	-0.26193500	-2.07847800	2.42313700
C	2.12240000	-1.49223900	2.10866700
C	2.76690000	-0.16374400	2.16888700
C	1.91403800	0.69546600	2.96980500
C	1.77970800	2.05109800	2.64602400
C	0.46876800	2.67465900	2.71483900
C	-0.64006700	1.94147200	3.12358300
C	-2.54101500	0.79664700	2.38280000

Ca@C₆₀-C₆H₅ [6,6]-[6,6] adduct

C	-2.60985800	-2.26227800	-0.73035300
C	-2.60986200	-2.26218800	0.73062300
C	-3.04481700	-1.14570500	1.43809000
C	-3.79628600	0.02047400	0.80094100
C	-3.79628000	0.02037600	-0.80093500
C	-3.04480000	-1.14586900	-1.43794100
C	-1.43322400	-3.01146800	-1.15715300

C	-0.73228300	-3.51499000	0.00020500	C	5.84017400	-0.94489100	0.00010100
C	-1.43322500	-3.01131500	1.15750200	H	6.93208100	-1.05469800	0.00011600
C	-0.73688900	-2.57015600	2.30755000	H	5.35890800	-1.93401800	0.00018300
C	-2.32844200	-0.70851500	2.58676500	C	5.90987500	1.31215000	-0.66933900
C	-3.05319100	1.18637500	1.43990200	C	5.90968400	1.31235700	0.66909900
C	-2.61046800	2.28363800	0.73971500	H	5.54281600	-0.31469800	-2.15794800
C	-2.61046700	2.28355000	-0.73997000	H	5.54281100	-0.31425600	2.15803500
C	-3.05318800	1.18620900	-1.44003200	H	6.15262300	2.14403500	1.32969900
C	-2.31368000	0.73209800	-2.58806800	H	6.15295200	2.14364000	-1.33012200
C	-2.32843200	-0.70880800	-2.58667100	C	-5.34649900	-0.01912600	1.12092900
C	-1.17934000	-1.42472000	-3.02247900	C	-5.34649300	-0.01930800	-1.12094100
C	-0.73688100	-2.57043300	-2.30725400	C	-5.83995200	-0.94469800	0.00006500
C	0.73226300	-3.51474800	0.00021000	H	-6.93185800	-1.05450600	0.00006900
C	1.43318900	-3.01120900	-1.15706300	H	-5.35869000	-1.93382700	0.00014500
C	0.73700800	-2.57044600	-2.30727600	C	-5.90954100	1.31251200	0.66909900
C	1.17953600	-1.42476100	-3.02251500	C	-5.90959500	1.31237900	-0.66933900
C	0.00009800	-0.69382900	-3.45816400	H	-5.54259000	-0.31410000	2.15801000
C	0.00014000	0.69548000	-3.46190300	H	-5.54256400	-0.31446000	-2.15797500
C	-1.17981400	1.43226100	-3.03508000	H	-6.15263100	2.14389500	-1.33010500
C	-0.72816800	2.58263900	-2.30886000	H	-6.15254100	2.14415600	1.32971800
C	-1.42402300	3.00004900	-1.16768400				
C	-2.31369100	0.73239500	2.58799300				
C	1.42431700	3.00005600	1.16735600				
C	0.72844600	2.58281300	2.30856500				
C	1.18004000	1.43250100	3.03495500				
C	2.31392400	0.73220700	2.58803600				
C	3.05340300	1.18615100	1.43992000				
C	2.61072600	2.28333000	-0.73994400				
C	1.42432500	2.99992500	-1.16767400				
C	0.70508500	3.44318900	-0.00018700				
C	-0.70475500	3.44324500	-0.00019000				
C	-1.42402600	3.00018100	1.16735400				
C	-0.72817700	2.58289700	2.30858200				
C	0.00012400	0.69587000	3.46185000				
C	0.00008200	-0.69343900	3.45827100				
C	1.17952200	-1.42442000	3.02271000				
C	2.32862500	-0.70864100	2.58687900				
C	3.04501200	-1.14589400	1.43810500				
C	3.79650200	0.02025800	0.80096700				
C	3.79651000	0.02016400	-0.80092900				
C	3.05342000	1.18598800	-1.44002700				
C	0.72845700	2.58255700	-2.30883800				
C	1.18005400	1.43216000	-3.03509300				
C	2.31393800	0.73191400	-2.58809100				
C	2.32863900	-0.70893100	-2.58676200				
C	3.04500500	-1.14605200	-1.43792500				
C	2.60999700	-2.26230700	-0.73036400				
C	2.60999600	-2.26221900	0.73065900				
C	1.43317800	-3.01105800	1.15742600				
C	0.73699500	-2.57017100	2.30758100				
C	-1.17982800	1.43260300	3.03493000				
C	-1.17935500	-1.42437600	3.02266200				
C	2.61071800	2.28341500	0.73971100				
Ca	-0.00213600	-1.14722900	-0.00007800				
C	5.34672400	-0.01952400	-1.12092300				
C	5.34670300	-0.01930500	1.12095000				