

Table S1. Cartesian coordinates of the optimized stationary points involved in the C-H activation process

Names	Cartesian coordinates			
CAT	C	1.233964000	-2.003038000	-0.205530000
	C	2.584541000	-1.761153000	-0.557241000
	C	2.844454000	-0.947374000	-1.712193000
	C	1.781178000	-0.356727000	-2.425639000
	C	0.408715000	-0.585432000	-2.058637000
	C	0.159364000	-1.423537000	-0.947708000
	H	0.991809000	-2.536764000	0.709289000
	H	3.874049000	-0.684155000	-1.960568000
	H	2.001588000	0.359604000	-3.219824000
	H	-0.857408000	-1.570300000	-0.584917000
	C	-0.695502000	0.115022000	-2.800995000
	H	-1.677277000	-0.241962000	-2.472268000
	H	-0.660652000	1.201139000	-2.626372000
	H	-0.591056000	-0.067269000	-3.882227000
	C	3.730029000	-2.292186000	0.281673000
	H	4.623288000	-1.711873000	-0.003624000
	C	3.981707000	-3.766238000	-0.073995000
	H	4.166042000	-3.898086000	-1.151675000
	H	4.857276000	-4.150279000	0.472059000
	H	3.112849000	-4.387021000	0.198158000
	C	3.508811000	-2.093299000	1.785263000
	H	4.396174000	-2.431213000	2.342058000
	H	3.332644000	-1.033501000	2.017669000
	H	2.646946000	-2.670412000	2.153557000
	Ru	1.579248000	0.149348000	-0.318410000
	C	2.679835000	2.380975000	0.210531000
	O	1.696089000	2.302121000	-0.600653000
	O	3.174954000	1.292430000	0.610891000
	C	3.180520000	3.707687000	0.691286000
	C	-0.078640000	0.122188000	2.208309000
	O	-0.300740000	-1.088271000	2.119157000
	O	0.634006000	0.813781000	1.381291000
	C	-0.674970000	0.940616000	3.339443000
	H	4.222494000	3.628142000	1.026523000
	H	3.080174000	4.466571000	-0.096477000
	H	2.560622000	4.018106000	1.548235000
	H	-1.581005000	1.443909000	2.966727000
	H	0.027305000	1.715711000	3.675884000
	H	-0.955880000	0.284895000	4.173464000
	C	-4.098578000	-1.765855000	-0.181108000

	C	-3.373426000	-1.727094000	1.151518000
	H	-4.115096000	-2.040025000	1.913612000
	H	-3.121254000	-0.671448000	1.342092000
	O	-2.256579000	-2.557490000	1.112413000
	H	-1.531381000	-2.102084000	1.593092000
	C	-1.352011000	3.172338000	0.014586000
	H	-1.813445000	4.137931000	0.296077000
	H	-0.656613000	2.863924000	0.812449000
	C	-2.477173000	2.152582000	0.012549000
	O	-0.731608000	3.242572000	-1.232192000
	H	0.213223000	3.030592000	-1.097514000
	F	-4.605394000	-2.977677000	-0.449370000
	F	-5.117128000	-0.887325000	-0.180778000
	F	-3.288431000	-1.441084000	-1.210553000
	F	-3.392711000	2.392996000	-0.928496000
	F	-3.109174000	2.152507000	1.210259000
	F	-2.022517000	0.895760000	-0.180548000
1	C	3.844712000	-0.975882000	0.001109000
	C	2.464519000	-1.176149000	0.000611000
	C	1.584129000	-0.083652000	-0.000316000
	C	2.113785000	1.215939000	-0.000888000
	C	3.494848000	1.417893000	-0.000476000
	C	4.364107000	0.322560000	0.000568000
	H	4.520463000	-1.834869000	0.001901000
	H	2.029880000	-2.176908000	0.000907000
	H	1.449462000	2.081356000	-0.001852000
	H	3.895060000	2.434671000	-0.001015000
	H	5.445298000	0.481851000	0.000917000
	C	0.108576000	-0.381421000	-0.000733000
	O	-0.274047000	-1.572883000	-0.002427000
	C	-0.808228000	0.701936000	0.000945000
	H	-0.616590000	1.771027000	0.003178000
	S	-2.454926000	0.341836000	0.000620000
	C	-2.846326000	-0.729412000	1.399895000
	H	-3.889043000	-1.059210000	1.300562000
	H	-2.127345000	-1.558958000	1.375643000
	H	-2.713117000	-0.096172000	2.286212000
	O	-3.329155000	1.530931000	0.002677000
	C	-2.846627000	-0.724864000	-1.402025000
	H	-2.127702000	-1.554535000	-1.380650000
	H	-3.889338000	-1.054934000	-1.303541000
	H	-2.713564000	-0.088769000	-2.286318000
TS-1C	C	-0.058178000	0.874403000	-2.105502000
	C	0.609259000	-0.373671000	-2.363377000

	C	1.856936000	-0.587603000	-1.736535000
	C	2.376832000	0.368474000	-0.817890000
	C	1.730964000	1.626080000	-0.597861000
	C	0.516823000	1.877273000	-1.288876000
	H	-1.063170000	1.008884000	-2.506506000
	H	2.349341000	-1.556708000	-1.806136000
	H	3.245200000	0.104676000	-0.217121000
	H	-0.060191000	2.778443000	-1.086975000
	C	2.330941000	2.634505000	0.358559000
	H	1.578451000	3.421109000	0.508428000
	Ru	0.389136000	-0.063762000	-0.198320000
	C	1.097605000	-2.890244000	0.540992000
	O	0.278570000	-1.885909000	0.622946000
	O	2.322382000	-2.786253000	0.426043000
	C	0.432897000	-4.245046000	0.605589000
	C	-1.297521000	1.192886000	2.074957000
	O	-2.231517000	1.607051000	1.356539000
	O	-0.286847000	0.533029000	1.664489000
	C	-1.331018000	1.480041000	3.562209000
	H	-0.289961000	-4.335896000	-0.218656000
	H	1.186591000	-5.039558000	0.546638000
	H	-0.142564000	-4.332093000	1.538255000
	H	-1.022480000	2.527951000	3.707153000
	H	-0.646761000	0.825574000	4.116207000
	H	-2.359345000	1.381043000	3.937221000
	C	-2.821082000	-2.273074000	-0.522258000
	O	-2.804207000	-2.936140000	-1.575654000
	C	-2.731880000	-2.981327000	0.799441000
	C	-3.016501000	-4.354600000	0.817395000
	C	-2.387910000	-2.339253000	1.996658000
	C	-2.969594000	-5.073281000	2.011920000
	H	-3.263615000	-4.838924000	-0.128713000
	C	-2.321946000	-3.060097000	3.188969000
	H	-2.121584000	-1.285198000	1.993409000
	C	-2.617284000	-4.427544000	3.201674000
	H	-3.198703000	-6.141792000	2.015788000
	H	-2.029361000	-2.553475000	4.111645000
	H	-2.568713000	-4.989541000	4.137723000
	C	-3.029074000	-0.857334000	-0.514024000
	H	-3.009503000	-0.187291000	0.343367000
	S	-3.684278000	-0.173702000	-1.907758000
	O	-2.869966000	0.164435000	-3.110243000
	C	-4.507428000	1.320348000	-1.350251000
	H	-5.048905000	1.705028000	-2.224015000

	H	-5.178817000	1.091325000	-0.514241000
	H	-3.721662000	2.031330000	-1.055127000
	C	-5.033445000	-1.212639000	-2.507820000
	H	-5.817667000	-1.261262000	-1.741930000
	H	-5.381698000	-0.755862000	-3.442558000
	H	-4.578547000	-2.195738000	-2.679251000
	C	-0.048462000	-1.444657000	-3.185277000
	H	-1.090615000	-1.606721000	-2.880267000
	H	-0.062753000	-1.142661000	-4.245192000
	H	0.498120000	-2.393655000	-3.098728000
	C	2.686351000	2.040464000	1.727320000
	H	3.428995000	1.231869000	1.649856000
	H	3.108757000	2.828592000	2.369927000
	H	1.792736000	1.630630000	2.216917000
	C	3.560154000	3.265230000	-0.319513000
	H	3.303022000	3.709187000	-1.293974000
	H	3.977026000	4.060307000	0.317903000
	H	4.348048000	2.511973000	-0.481244000
	C	-1.031955000	5.058870000	0.796447000
	C	-2.332990000	4.540380000	0.200154000
	H	-3.048605000	4.435912000	1.036414000
	H	-2.703808000	5.326712000	-0.477376000
	O	-2.149042000	3.358095000	-0.509069000
	H	-2.091616000	2.612197000	0.156545000
	F	-0.092117000	5.252828000	-0.146624000
	F	-0.508767000	4.195381000	1.693738000
	F	-1.228877000	6.226590000	1.426797000
	C	5.759939000	-1.228734000	-0.524079000
	C	5.329789000	-1.718845000	0.851995000
	H	6.162812000	-1.482924000	1.536339000
	H	5.244328000	-2.818196000	0.783933000
	O	4.161710000	-1.111976000	1.295534000
	H	3.393143000	-1.676927000	1.024070000
	F	4.870815000	-1.564604000	-1.482677000
	F	6.943292000	-1.760592000	-0.869426000
	F	5.885491000	0.111702000	-0.562951000
INT-1C	C	0.939391000	-0.586164000	-2.363959000
	C	-0.235844000	0.194454000	-2.612299000
	C	-1.447361000	-0.215423000	-2.009335000
	C	-1.503367000	-1.387384000	-1.201942000
	C	-0.361887000	-2.181939000	-0.963073000
	C	0.865384000	-1.743110000	-1.560644000
	H	1.900692000	-0.262284000	-2.759652000
	H	-2.345832000	0.386235000	-2.120659000

	H	-2.447649000	-1.621288000	-0.718292000
	H	1.779897000	-2.290169000	-1.349392000
	C	-0.417549000	-3.424799000	-0.097483000
	H	0.624431000	-3.688507000	0.131467000
	Ru	0.063170000	-0.055243000	-0.383983000
	C	-2.418782000	0.556658000	1.275101000
	O	-1.148428000	0.373856000	1.263614000
	O	-3.127441000	0.767991000	0.281403000
	C	-3.056849000	0.470931000	2.650733000
	C	1.942115000	-1.357277000	1.758768000
	O	2.335954000	-2.326527000	1.079662000
	O	1.316733000	-0.335838000	1.317620000
	C	2.230962000	-1.355147000	3.249715000
	H	-3.877514000	1.196684000	2.723396000
	H	-3.484258000	-0.538284000	2.760866000
	H	-2.323109000	0.633747000	3.449772000
	H	1.680889000	-2.191514000	3.709301000
	H	1.922522000	-0.415814000	3.725191000
	H	3.303151000	-1.540160000	3.410417000
	C	-0.122132000	3.043350000	-0.475583000
	O	0.043817000	3.603367000	-1.557872000
	C	-1.256470000	3.439005000	0.408866000
	C	-2.380251000	4.021839000	-0.197086000
	C	-1.213119000	3.316855000	1.805312000
	C	-3.453834000	4.453065000	0.576534000
	H	-2.392750000	4.117384000	-1.283537000
	C	-2.278634000	3.773805000	2.581858000
	H	-0.355696000	2.854839000	2.293658000
	C	-3.402576000	4.334019000	1.969615000
	H	-4.335006000	4.883568000	0.095549000
	H	-2.236969000	3.678931000	3.669064000
	H	-4.242340000	4.676452000	2.579225000
	C	0.809115000	1.982109000	-0.021418000
	H	0.978521000	1.896796000	1.056753000
	S	2.413190000	2.253722000	-0.739026000
	O	2.631838000	1.971341000	-2.170317000
	C	3.574885000	1.312602000	0.233450000
	H	4.568200000	1.713177000	-0.001548000
	H	3.332804000	1.376913000	1.298948000
	H	3.503868000	0.278759000	-0.130187000
	C	2.876745000	3.971203000	-0.432384000
	H	2.811378000	4.181322000	0.643412000
	H	3.898954000	4.092046000	-0.813522000
	H	2.164430000	4.574076000	-1.007735000

	C	-0.202256000	1.380922000	-3.527480000
	H	0.729066000	1.946799000	-3.420940000
	H	-0.275831000	1.013504000	-4.565705000
	H	-1.047079000	2.054714000	-3.340014000
	C	-1.135065000	-3.180516000	1.235637000
	H	-2.209390000	-2.996451000	1.091728000
	H	-1.035645000	-4.064784000	1.884136000
	H	-0.715961000	-2.309491000	1.758538000
	C	-1.069003000	-4.574762000	-0.882108000
	H	-0.546979000	-4.763210000	-1.833616000
	H	-1.046259000	-5.504775000	-0.292051000
	H	-2.122379000	-4.344765000	-1.109053000
	C	5.960123000	-1.303693000	0.581163000
	C	5.194089000	-2.263494000	-0.317777000
	H	5.042690000	-3.189207000	0.265780000
	H	5.861482000	-2.497127000	-1.164667000
	O	4.000307000	-1.719152000	-0.778954000
	H	3.291249000	-1.954860000	-0.112367000
	C	-5.268895000	-2.402061000	0.002525000
	C	-5.716671000	-1.166909000	-0.767877000
	H	-6.426065000	-1.523806000	-1.533741000
	H	-6.286504000	-0.544630000	-0.049750000
	O	-4.669842000	-0.501322000	-1.379431000
	H	-4.172489000	0.026894000	-0.704826000
	F	7.076131000	-1.877087000	1.054278000
	F	6.324971000	-0.181521000	-0.071544000
	F	5.222781000	-0.907488000	1.642406000
	F	-4.594969000	-3.269135000	-0.773032000
	F	-6.321433000	-3.051281000	0.525659000
	F	-4.444831000	-2.078947000	1.027228000
TS-2C	Ru	-1.870452000	-0.750403000	0.017208000
	C	-1.614228000	2.194858000	0.580369000
	O	-1.785483000	2.486142000	-0.616115000
	O	-1.494803000	0.988764000	1.013272000
	C	-1.599256000	3.255575000	1.657784000
	H	-2.600091000	3.281191000	2.119013000
	H	-0.871550000	3.001460000	2.438325000
	H	-1.373789000	4.237074000	1.227850000
	C	0.972881000	0.401530000	-0.127482000
	O	1.377111000	1.391051000	-0.733984000
	C	1.347926000	0.140264000	1.284053000
	C	2.324978000	0.953516000	1.878980000
	C	0.781215000	-0.915400000	2.013985000
	C	2.741734000	0.694885000	3.183334000

	H	2.750812000	1.769980000	1.296235000
	C	1.193907000	-1.169180000	3.320673000
	C	2.180724000	-0.366996000	3.903771000
	H	3.512903000	1.318532000	3.640769000
	H	0.750018000	-2.004538000	3.865815000
	H	2.516617000	-0.570665000	4.923615000
	C	0.114063000	-0.613095000	-0.805353000
	H	0.415919000	-1.675889000	-0.602506000
	C	-3.588156000	-0.354591000	-1.155263000
	C	-2.933366000	-1.483678000	-1.734350000
	C	-2.636723000	-2.639775000	-0.962380000
	C	-2.981762000	-2.583820000	0.415227000
	C	-3.750113000	-1.512039000	0.971721000
	C	-4.071297000	-0.380307000	0.199415000
	H	-3.717031000	0.555124000	-1.743775000
	H	-2.567243000	-1.427735000	-2.758458000
	H	-2.570063000	-3.351664000	1.073080000
	H	-3.958209000	-1.521123000	2.040903000
	C	-1.915843000	-3.817934000	-1.545222000
	H	-1.100381000	-3.489739000	-2.200766000
	H	-1.502542000	-4.442511000	-0.746338000
	H	-2.625295000	-4.416674000	-2.141229000
	C	-4.777362000	0.840167000	0.750174000
	C	-4.659310000	0.989533000	2.267715000
	C	-6.246610000	0.818561000	0.293533000
	H	-4.292467000	1.710708000	0.278894000
	H	-3.608927000	0.952221000	2.589326000
	H	-5.084035000	1.954476000	2.582930000
	H	-5.217974000	0.201705000	2.798306000
	H	-6.331306000	0.757387000	-0.802495000
	H	-6.776868000	-0.046625000	0.723054000
	H	-6.762872000	1.733097000	0.623339000
	H	0.032630000	-1.587733000	1.583568000
	C	0.585422000	-3.941649000	0.940721000
	O	-0.497495000	-3.761427000	1.526642000
	O	0.935453000	-3.339273000	-0.131196000
	C	1.611140000	-4.891497000	1.554530000
	H	2.182465000	-5.419607000	0.777160000
	H	2.324537000	-4.292630000	2.146159000
	H	1.123804000	-5.607236000	2.229947000
	S	0.285413000	-0.442357000	-2.557860000
	C	2.025099000	-0.487892000	-2.992172000
	H	2.044871000	-0.571982000	-4.086742000
	H	2.511924000	0.417649000	-2.617572000

	H	2.447009000	-1.377464000	-2.491231000
	C	-0.330419000	1.170423000	-3.070375000
	H	-0.805809000	0.985823000	-4.042789000
	H	-1.035722000	1.523173000	-2.300187000
	H	0.510778000	1.865976000	-3.146127000
	O	-0.414973000	-1.509493000	-3.312761000
	C	1.585893000	4.707529000	-0.032162000
	C	0.762013000	4.522374000	-1.298595000
	H	1.229849000	5.174619000	-2.057751000
	H	0.918592000	3.473890000	-1.595954000
	O	-0.577507000	4.863709000	-1.134473000
	H	-1.101014000	4.043121000	-0.993919000
	F	1.167364000	3.909885000	0.972295000
	F	1.542549000	5.968041000	0.424910000
	F	2.876963000	4.402925000	-0.269194000
	C	4.739721000	-1.064970000	-0.207088000
	C	3.884479000	-2.279755000	0.088816000
	H	4.574221000	-3.045702000	0.498529000
	H	3.194933000	-1.988219000	0.901137000
	O	3.217483000	-2.705120000	-1.054483000
	H	2.347041000	-3.106428000	-0.741762000
	F	4.003671000	-0.026099000	-0.662451000
	F	5.678210000	-1.312015000	-1.132681000
	F	5.363323000	-0.648545000	0.909218000
INT-2C	Ru	0.521454000	-0.778770000	0.702165000
	C	-0.894625000	-2.951027000	-0.686792000
	O	-1.826715000	-2.144159000	-0.764948000
	O	0.234702000	-2.682355000	-0.125096000
	C	-0.986233000	-4.332926000	-1.299453000
	H	-0.400799000	-4.333689000	-2.233266000
	H	-0.545537000	-5.088164000	-0.633331000
	H	-2.028711000	-4.586421000	-1.529946000
	C	1.858124000	-1.267867000	-1.882928000
	O	2.360007000	-2.163949000	-2.551689000
	C	0.612262000	-0.567982000	-2.321221000
	C	-0.156935000	-1.141105000	-3.344104000
	C	0.144900000	0.581845000	-1.649384000
	C	-1.395017000	-0.595469000	-3.671241000
	H	0.230609000	-2.026512000	-3.850648000
	C	-1.112432000	1.110136000	-1.974371000
	C	-1.881061000	0.519574000	-2.975191000
	H	-1.998470000	-1.050210000	-4.460523000
	H	-1.483642000	1.986085000	-1.444833000
	H	-2.862929000	0.933540000	-3.215318000

	C	2.310800000	-0.865971000	-0.520002000
	H	2.675985000	0.186701000	-0.487108000
	C	0.045726000	-1.505217000	2.667834000
	C	1.317884000	-0.861223000	2.687887000
	C	1.449574000	0.520577000	2.319058000
	C	0.302575000	1.156610000	1.803940000
	C	-0.960246000	0.484253000	1.756322000
	C	-1.142722000	-0.824644000	2.257584000
	H	-0.002468000	-2.564440000	2.919536000
	H	2.208317000	-1.421456000	2.971904000
	H	0.399118000	2.163404000	1.393231000
	H	-1.800342000	0.991038000	1.281434000
	C	2.766665000	1.229716000	2.422647000
	H	3.545444000	0.721156000	1.840827000
	H	2.679177000	2.267038000	2.083279000
	H	3.088092000	1.223923000	3.477074000
	C	-2.519114000	-1.458829000	2.240215000
	C	-3.450228000	-0.733556000	3.224333000
	C	-2.517985000	-2.966194000	2.490783000
	H	-2.916513000	-1.298748000	1.233076000
	H	-3.512045000	0.341966000	3.001605000
	H	-4.467768000	-1.145333000	3.146595000
	H	-3.105951000	-0.849769000	4.265470000
	H	-1.840720000	-3.496497000	1.805992000
	H	-2.223341000	-3.212953000	3.524700000
	H	-3.530589000	-3.361953000	2.325525000
	H	0.819683000	1.139278000	-0.993615000
	C	3.964969000	2.221002000	-0.638780000
	O	2.686153000	2.120979000	-0.622046000
	O	4.736187000	1.250086000	-0.604650000
	C	4.529474000	3.637548000	-0.705910000
	H	4.036410000	4.279519000	0.040269000
	H	5.615899000	3.634047000	-0.550733000
	H	4.306051000	4.067183000	-1.696323000
	S	3.639342000	-1.855493000	0.073481000
	O	4.029972000	-1.567119000	1.471629000
	C	3.154969000	-3.576425000	-0.059481000
	H	2.160752000	-3.649246000	0.399311000
	H	3.097321000	-3.839902000	-1.120809000
	H	3.923382000	-4.135600000	0.489711000
	C	5.047287000	-1.662489000	-1.011935000
	H	5.259628000	-0.579663000	-0.966444000
	H	5.854138000	-2.278972000	-0.593565000
	H	4.736411000	-1.981282000	-2.014722000

	C	-4.866595000	-1.144081000	-1.263845000
	C	-4.813980000	0.210923000	-0.569053000
	H	-5.920540000	-1.290024000	-1.558161000
	H	-4.268848000	-1.041914000	-2.187680000
	F	-5.227988000	1.180588000	-1.407589000
	F	-3.558997000	0.536557000	-0.180504000
	F	-5.582658000	0.255548000	0.527362000
	O	-4.448199000	-2.191463000	-0.456780000
	H	-3.475699000	-2.293269000	-0.588192000
	C	0.497939000	4.553538000	-0.446166000
	C	-0.935303000	4.650118000	0.045937000
	H	0.467013000	4.016139000	-1.412882000
	H	0.816490000	5.594180000	-0.660060000
	F	-1.720482000	5.222731000	-0.882459000
	F	-1.044981000	5.358646000	1.174156000
	F	-1.460891000	3.421775000	0.301785000
	O	1.296597000	3.925821000	0.495150000
	H	1.881848000	3.244245000	0.020263000
TS-3C	Ru	0.280335000	-0.266398000	-0.308922000
	C	2.185445000	0.018702000	2.115651000
	O	3.119376000	0.507374000	1.475179000
	O	1.088092000	-0.455958000	1.630638000
	C	2.253387000	-0.059196000	3.630741000
	H	1.427184000	0.533674000	4.053345000
	H	2.113924000	-1.100042000	3.961577000
	H	3.215629000	0.321045000	3.994604000
	C	-0.897804000	1.290203000	1.924049000
	O	-1.208023000	1.284950000	3.112341000
	C	0.123506000	2.201795000	1.357607000
	C	0.722986000	3.181621000	2.152628000
	C	0.586782000	1.916957000	0.048817000
	C	1.797965000	3.909475000	1.642789000
	H	0.352573000	3.339902000	3.167356000
	C	1.675760000	2.667922000	-0.435416000
	C	2.276234000	3.647545000	0.351493000
	H	2.277724000	4.676269000	2.256013000
	H	2.059143000	2.479607000	-1.438451000
	H	3.132086000	4.204746000	-0.036381000
	C	-1.417481000	0.329116000	0.896056000
	H	-2.086901000	0.850624000	0.176198000
	C	0.378419000	-2.437834000	-0.776911000
	C	-0.724275000	-1.869871000	-1.460871000
	C	-0.568548000	-0.768756000	-2.349666000
	C	0.735040000	-0.209789000	-2.457386000

	C	1.865743000	-0.791888000	-1.816497000
	C	1.693499000	-1.907412000	-0.958170000
	H	0.204898000	-3.259195000	-0.084375000
	H	-1.721572000	-2.264112000	-1.269584000
	H	0.861129000	0.706025000	-3.037716000
	H	2.846065000	-0.320599000	-1.898106000
	C	-1.739540000	-0.258072000	-3.138552000
	H	-1.498470000	0.688703000	-3.633336000
	H	-2.017144000	-0.998625000	-3.906623000
	H	-2.612278000	-0.098649000	-2.491441000
	C	2.900908000	-2.468310000	-0.232352000
	C	3.790964000	-3.223963000	-1.233721000
	C	2.558784000	-3.345781000	0.972517000
	H	3.468057000	-1.602257000	0.131555000
	H	4.116157000	-2.572528000	-2.057050000
	H	4.696192000	-3.590150000	-0.727124000
	H	3.258294000	-4.089235000	-1.661657000
	H	1.888316000	-2.822102000	1.667814000
	H	2.083920000	-4.293740000	0.669774000
	H	3.480635000	-3.602420000	1.515719000
	H	-0.281337000	1.844431000	-0.907109000
	C	-2.223639000	2.623011000	-1.825741000
	O	-0.972341000	2.458336000	-1.959002000
	O	-2.910492000	2.104172000	-0.915250000
	C	-2.920401000	3.461959000	-2.881903000
	H	-3.405913000	2.781773000	-3.601632000
	H	-3.709138000	4.073497000	-2.421516000
	H	-2.205366000	4.094329000	-3.423206000
	S	-2.390600000	-0.946275000	1.611171000
	O	-2.894434000	-1.933501000	0.627148000
	C	-1.390750000	-1.758469000	2.853923000
	H	-0.437885000	-1.994331000	2.365116000
	H	-1.223998000	-1.047598000	3.671125000
	H	-1.954046000	-2.649427000	3.159296000
	C	-3.773217000	-0.234020000	2.497923000
	H	-4.368829000	0.287308000	1.728519000
	H	-4.338281000	-1.071183000	2.927870000
	H	-3.360496000	0.451767000	3.247014000
	C	6.260773000	-0.245326000	-0.671721000
	C	5.524305000	1.076884000	-0.511001000
	H	5.679067000	1.405747000	0.531961000
	H	6.034166000	1.794952000	-1.176748000
	O	4.181967000	0.978804000	-0.850003000
	H	3.659095000	0.795564000	-0.024224000

	F	6.098008000	-0.762510000	-1.902202000
	F	7.579762000	-0.079526000	-0.468350000
	F	5.834648000	-1.176202000	0.206720000
	C	-6.323373000	-1.006766000	-0.470982000
	C	-5.224234000	-0.082412000	-0.952811000
	H	-4.304408000	-0.693472000	-0.999498000
	H	-5.493319000	0.215574000	-1.984558000
	O	-5.120100000	1.002032000	-0.082901000
	H	-4.396562000	1.584876000	-0.423875000
	F	-6.405008000	-2.080280000	-1.278378000
	F	-7.523312000	-0.411557000	-0.461331000
	F	-6.090679000	-1.457979000	0.777433000
INT-3C	C	-1.791630000	2.316227000	0.585904000
	C	-0.602178000	2.617211000	-0.135445000
	C	0.637102000	2.270909000	0.496641000
	C	0.674652000	1.626975000	1.743855000
	C	-0.539413000	1.358724000	2.469034000
	C	-1.762508000	1.762248000	1.908332000
	H	-2.764613000	2.513357000	0.134169000
	H	1.574887000	2.435724000	-0.034298000
	H	1.623816000	1.263956000	2.132177000
	H	-2.702543000	1.542190000	2.411796000
	C	-0.468946000	0.617661000	3.772804000
	H	-1.447447000	0.197467000	4.046238000
	H	0.268330000	-0.193544000	3.696878000
	H	-0.147528000	1.294849000	4.581970000
	C	-0.610112000	3.314465000	-1.482034000
	H	0.384564000	3.142699000	-1.926351000
	C	-0.787230000	4.827860000	-1.283017000
	H	-0.023740000	5.233802000	-0.601438000
	H	-0.708837000	5.363388000	-2.242407000
	H	-1.775787000	5.051104000	-0.848717000
	C	-1.642274000	2.744716000	-2.458561000
	H	-1.595067000	3.277853000	-3.420613000
	H	-1.444500000	1.679792000	-2.646248000
	H	-2.671185000	2.852543000	-2.077778000
	Ru	-0.673619000	0.475075000	0.345087000
	C	0.857870000	-1.913525000	1.362180000
	O	1.699309000	-1.205155000	1.930588000
	O	-0.309096000	-1.509683000	0.992577000
	C	1.159944000	-3.359795000	1.016435000
	H	2.143604000	-3.658671000	1.399497000
	H	0.373286000	-4.020296000	1.411650000
	H	1.140444000	-3.459466000	-0.080880000

	C	-1.683365000	-1.692637000	-1.452760000
	O	-2.238508000	-2.782586000	-1.565591000
	C	-0.369907000	-1.332031000	-1.994368000
	C	0.230022000	-2.058932000	-3.035751000
	C	0.257337000	-0.232092000	-1.358501000
	C	1.480218000	-1.667836000	-3.502479000
	H	-0.298871000	-2.916509000	-3.458988000
	C	1.522085000	0.134479000	-1.856677000
	C	2.117970000	-0.565939000	-2.909056000
	H	1.965611000	-2.211885000	-4.316115000
	H	2.082543000	0.950946000	-1.403357000
	H	3.110008000	-0.261967000	-3.253192000
	C	-2.264464000	-0.508275000	-0.707363000
	H	-2.667769000	0.245804000	-1.400990000
	S	-3.655775000	-0.946924000	0.287043000
	O	-4.256984000	0.184835000	1.026884000
	C	-4.934237000	-1.689546000	-0.742083000
	H	-4.464939000	-2.501500000	-1.312575000
	H	-5.740469000	-2.028283000	-0.077655000
	H	-5.289417000	-0.881883000	-1.395829000
	C	-3.149185000	-2.270258000	1.377093000
	H	-2.977357000	-3.160017000	0.759256000
	H	-2.201196000	-1.945035000	1.827199000
	H	-3.964896000	-2.391305000	2.101242000
	C	4.330527000	-1.325834000	0.175574000
	C	4.634959000	0.164287000	0.102285000
	H	5.163608000	-1.830938000	-0.342910000
	H	3.416223000	-1.485295000	-0.426001000
	F	5.780137000	0.487776000	0.714202000
	F	3.660829000	0.915650000	0.666165000
	F	4.738206000	0.566894000	-1.186440000
	O	4.236331000	-1.792813000	1.476864000
	H	3.326505000	-1.575421000	1.799594000
TS-10	C	-1.265514000	-2.017765000	1.172573000
	C	-0.497993000	-0.965367000	1.734129000
	C	0.923580000	-0.983685000	1.542146000
	C	1.549853000	-1.972661000	0.764124000
	C	0.760411000	-2.934101000	0.063241000
	C	-0.653551000	-2.955369000	0.306271000
	H	-2.349620000	-2.006209000	1.265617000
	H	1.519590000	-0.155432000	1.920315000
	H	2.618159000	-1.899945000	0.581667000
	H	-1.290717000	-3.631860000	-0.264007000
	C	1.396302000	-3.879892000	-0.911924000

	H	0.664623000	-4.233874000	-1.651659000
	H	2.234041000	-3.398985000	-1.432270000
	H	1.797486000	-4.754322000	-0.372862000
	C	-1.176779000	0.157464000	2.498723000
	H	-0.377788000	0.839821000	2.827949000
	C	-1.884879000	-0.407896000	3.739584000
	H	-1.197661000	-0.993216000	4.370702000
	H	-2.294868000	0.411281000	4.350645000
	H	-2.721882000	-1.061239000	3.446630000
	C	-2.141293000	0.957966000	1.613760000
	H	-2.611826000	1.763422000	2.198748000
	H	-1.606812000	1.409548000	0.768389000
	H	-2.941426000	0.310302000	1.227104000
	Ru	-0.086186000	-1.010906000	-0.405141000
	C	2.187910000	0.212285000	-1.944636000
	O	0.930495000	-0.076550000	-1.890092000
	O	3.074547000	-0.357295000	-1.302520000
	C	2.518889000	1.377638000	-2.854117000
	C	-2.831833000	-0.792825000	-1.548418000
	O	-3.211082000	-1.831700000	-1.001938000
	O	-1.594907000	-0.405239000	-1.606700000
	C	-3.807391000	0.156846000	-2.212527000
	H	3.553046000	1.302214000	-3.215521000
	H	1.811660000	1.443247000	-3.690754000
	H	2.420122000	2.304001000	-2.263369000
	H	-3.519205000	0.305961000	-3.264040000
	H	-3.744101000	1.140300000	-1.721558000
	H	-4.829317000	-0.235068000	-2.151273000
	C	0.895887000	3.109359000	0.154117000
	O	0.885514000	1.890312000	0.463687000
	C	-0.188826000	3.668316000	-0.718044000
	C	-0.605602000	5.005897000	-0.622025000
	C	-0.806104000	2.821039000	-1.651803000
	C	-1.624222000	5.490011000	-1.444318000
	H	-0.147612000	5.664892000	0.118312000
	C	-1.811699000	3.314361000	-2.485066000
	H	-0.485884000	1.783304000	-1.734790000
	C	-2.226327000	4.645795000	-2.382556000
	H	-1.951164000	6.528481000	-1.351203000
	H	-2.271964000	2.650466000	-3.219487000
	H	-3.019019000	5.026340000	-3.031525000
	C	1.911850000	3.993994000	0.583688000
	H	2.049790000	5.036536000	0.308311000
	S	3.164054000	3.406716000	1.560344000

	C	3.981952000	2.029397000	0.749742000
	H	4.631488000	1.506319000	1.462077000
	H	3.209237000	1.362899000	0.350216000
	H	4.566276000	2.487177000	-0.058479000
	C	2.449654000	2.635484000	3.024709000
	H	1.663573000	1.953659000	2.678821000
	H	3.251504000	2.120046000	3.569379000
	H	2.038726000	3.466189000	3.611881000
	O	4.142208000	4.439985000	1.950499000
	C	5.292717000	-3.180025000	-0.358544000
	C	5.804280000	-1.867364000	0.218574000
	H	6.512732000	-1.454646000	-0.526471000
	H	6.380580000	-2.122536000	1.122111000
	F	4.656795000	-2.995702000	-1.530914000
	F	4.422472000	-3.789916000	0.469136000
	F	6.311651000	-4.026520000	-0.576637000
	O	4.786772000	-0.988386000	0.568446000
	H	4.266022000	-0.727596000	-0.228690000
	C	-5.594866000	-0.843394000	1.243818000
	C	-6.874668000	-1.177043000	0.491236000
	H	-5.878044000	-0.657524000	2.292266000
	H	-5.222869000	0.113045000	0.826263000
	F	-7.486727000	-2.260527000	0.981752000
	F	-7.738796000	-0.146919000	0.560848000
	F	-6.627847000	-1.410511000	-0.814399000
	O	-4.663514000	-1.873253000	1.199504000
	H	-4.288166000	-1.927483000	0.287370000
INT-10	C	-2.541047000	-2.831511000	0.379704000
	C	-1.859203000	-2.377857000	1.521291000
	C	-0.470725000	-2.739560000	1.665379000
	C	0.174021000	-3.571471000	0.734139000
	C	-0.520676000	-4.030438000	-0.438121000
	C	-1.868130000	-3.628667000	-0.602686000
	H	-3.547412000	-2.480279000	0.170222000
	H	0.109092000	-2.338710000	2.497238000
	H	1.242607000	-3.757561000	0.837230000
	H	-2.382139000	-3.868568000	-1.534598000
	C	0.197851000	-4.821496000	-1.490433000
	H	-0.322414000	-4.756604000	-2.455771000
	H	1.218749000	-4.441389000	-1.630009000
	H	0.257156000	-5.882340000	-1.195356000
	C	-2.518131000	-1.547971000	2.603883000
	H	-1.805195000	-0.748222000	2.853432000
	C	-2.695310000	-2.410114000	3.866135000

	H	-1.740193000	-2.832999000	4.214232000
	H	-3.119939000	-1.809143000	4.685629000
	H	-3.382574000	-3.248617000	3.669972000
	C	-3.837552000	-0.900168000	2.183634000
	H	-4.178269000	-0.198392000	2.960612000
	H	-3.741107000	-0.368349000	1.228204000
	H	-4.629420000	-1.656702000	2.063278000
	Ru	-0.655623000	-1.859455000	-0.342490000
	C	2.211303000	-1.643419000	-0.986022000
	O	1.049541000	-1.793055000	-1.512562000
	O	2.416810000	-1.490987000	0.232061000
	C	3.355759000	-1.653443000	-1.975896000
	C	-2.644852000	-0.329245000	-1.976454000
	O	-3.437742000	-0.334512000	-1.017936000
	O	-1.520348000	-0.946501000	-2.002071000
	C	-2.949087000	0.465569000	-3.233940000
	H	4.279299000	-1.987300000	-1.486974000
	H	3.115972000	-2.277765000	-2.846526000
	H	3.511279000	-0.624095000	-2.329534000
	H	-2.801045000	-0.162552000	-4.124069000
	H	-2.236507000	1.302472000	-3.297257000
	H	-3.965562000	0.875819000	-3.207876000
	C	0.508134000	1.145541000	-0.027670000
	O	-0.254745000	0.153845000	0.259862000
	C	1.314330000	1.295832000	-1.277799000
	C	2.601605000	1.854709000	-1.179195000
	C	0.815999000	0.946323000	-2.540949000
	C	3.365853000	2.083864000	-2.323208000
	H	3.019197000	2.066028000	-0.196135000
	C	1.576809000	1.192937000	-3.684138000
	H	-0.150405000	0.455655000	-2.616227000
	C	2.848246000	1.766807000	-3.582230000
	H	4.372793000	2.493375000	-2.220854000
	H	1.174630000	0.923035000	-4.663463000
	H	3.441457000	1.950014000	-4.481700000
	C	0.629878000	2.211547000	0.865037000
	H	1.187115000	3.128491000	0.696481000
	S	0.017440000	2.116829000	2.442247000
	O	0.379236000	3.272488000	3.282378000
	C	0.604165000	0.588130000	3.178314000
	H	0.190573000	0.523685000	4.193105000
	H	0.289986000	-0.232512000	2.525816000
	H	1.700714000	0.671953000	3.157913000
	C	-1.768875000	1.944701000	2.368353000

	H	-2.001583000	1.182586000	1.615731000
	H	-2.141196000	1.689701000	3.368954000
	H	-2.120545000	2.933690000	2.050364000
	C	-3.439407000	3.251661000	-0.629913000
	C	-4.696167000	2.535971000	-0.146133000
	H	-4.440209000	2.105039000	0.843556000
	H	-5.443913000	3.328573000	0.027108000
	F	-3.614207000	3.863734000	-1.803850000
	F	-2.387610000	2.415305000	-0.767233000
	F	-3.068035000	4.191624000	0.274688000
	O	-5.199530000	1.614524000	-1.043151000
	H	-4.609047000	0.813695000	-1.041245000
	C	5.614323000	0.771939000	0.774845000
	C	4.779850000	0.202963000	1.915070000
	H	5.061094000	-0.863590000	2.006307000
	H	5.115267000	0.719620000	2.829549000
	F	5.355584000	0.160454000	-0.396101000
	F	5.393814000	2.085894000	0.591155000
	F	6.924893000	0.612158000	1.033523000
	O	3.416912000	0.400421000	1.744802000
	H	3.065248000	-0.292132000	1.123587000
TS-20	Ru	0.060498000	-0.941500000	-0.252926000
	C	-1.799236000	-1.943018000	1.912521000
	O	-2.827800000	-1.649509000	1.291669000
	O	-0.595824000	-1.815243000	1.465378000
	C	-1.873709000	-2.525467000	3.307722000
	H	-1.505965000	-3.563518000	3.286948000
	H	-1.218491000	-1.955284000	3.979863000
	H	-2.907167000	-2.507197000	3.674155000
	C	-1.437198000	1.380927000	1.062796000
	O	-1.205863000	0.661321000	0.016729000
	C	-0.934089000	1.026358000	2.418647000
	C	-1.804276000	1.060774000	3.519327000
	C	0.416950000	0.701745000	2.611588000
	C	-1.328298000	0.769976000	4.799150000
	H	-2.859886000	1.291495000	3.363215000
	C	0.888100000	0.417337000	3.893007000
	C	0.020065000	0.450418000	4.988884000
	H	-2.014015000	0.786362000	5.649501000
	H	1.945770000	0.180819000	4.027452000
	H	0.393172000	0.228185000	5.991670000
	C	-2.154091000	2.559666000	0.939453000
	H	-2.348719000	3.275544000	1.734413000
	C	0.489541000	-2.912464000	-1.071221000

	C	-0.476325000	-2.213386000	-1.856418000
	C	-0.163640000	-0.937779000	-2.442481000
	C	1.088737000	-0.354202000	-2.139170000
	C	1.977525000	-0.999671000	-1.240108000
	C	1.724976000	-2.315335000	-0.732698000
	H	0.201393000	-3.846965000	-0.586225000
	H	-1.482482000	-2.615554000	-1.977917000
	H	1.301997000	0.670938000	-2.434633000
	H	2.837045000	-0.442565000	-0.868679000
	C	-1.189214000	-0.221890000	-3.267506000
	H	-1.023703000	0.862917000	-3.243584000
	H	-1.110113000	-0.555381000	-4.316016000
	H	-2.199199000	-0.454666000	-2.904908000
	C	2.698110000	-2.978268000	0.223097000
	C	2.900418000	-2.155524000	1.504469000
	C	4.019447000	-3.267384000	-0.505917000
	H	2.249846000	-3.944743000	0.508204000
	H	1.958223000	-2.084618000	2.066930000
	H	3.652516000	-2.640669000	2.145991000
	H	3.231666000	-1.128655000	1.288910000
	H	3.859463000	-3.894121000	-1.397421000
	H	4.513843000	-2.341343000	-0.835215000
	H	4.715280000	-3.797685000	0.162268000
	H	1.116917000	0.707870000	1.773698000
	C	2.511886000	1.999034000	0.154397000
	O	3.140955000	1.149492000	0.852681000
	O	1.336658000	1.829108000	-0.254063000
	C	3.216946000	3.312415000	-0.175011000
	H	4.300948000	3.160810000	-0.266081000
	H	2.807645000	3.758190000	-1.092227000
	H	3.046784000	4.018070000	0.655402000
	S	-2.554097000	3.159515000	-0.614459000
	C	-3.549666000	1.947529000	-1.477160000
	H	-3.642797000	2.271712000	-2.521675000
	H	-3.103867000	0.951494000	-1.375825000
	H	-4.519966000	1.987266000	-0.969109000
	C	-1.028955000	3.339889000	-1.557614000
	H	-1.266004000	3.251592000	-2.625918000
	H	-0.717855000	4.365506000	-1.317008000
	H	-0.263072000	2.624735000	-1.204560000
	O	-3.270699000	4.447752000	-0.553023000
	C	6.046741000	0.371980000	-1.213412000
	C	6.131627000	0.271512000	0.304562000
	H	7.193401000	0.063892000	0.528381000

	H	5.555271000	-0.632777000	0.584256000
	F	6.798651000	1.360398000	-1.709304000
	F	4.780928000	0.585731000	-1.648106000
	F	6.458049000	-0.783244000	-1.784916000
	O	5.720053000	1.415566000	0.956073000
	H	4.719023000	1.380581000	1.015817000
	C	-5.772149000	-0.852094000	-1.199197000
	C	-4.713585000	-1.941025000	-1.146084000
	H	-4.907463000	-2.607094000	-2.004791000
	H	-4.881306000	-2.512885000	-0.217515000
	F	-7.004246000	-1.383663000	-1.183166000
	F	-5.676676000	-0.004507000	-0.157421000
	F	-5.663682000	-0.109406000	-2.320514000
	O	-3.425954000	-1.414397000	-1.213355000
	H	-3.073738000	-1.371313000	-0.277300000
INT-2O	Ru	-0.254815000	-0.937236000	-0.602691000
	C	-2.474131000	0.417423000	-1.967005000
	O	-3.217929000	-0.350709000	-1.342659000
	O	-1.187435000	0.387865000	-1.885636000
	C	-3.051675000	1.465442000	-2.893926000
	H	-3.869508000	1.984378000	-2.375927000
	H	-2.288119000	2.178255000	-3.227665000
	H	-3.488179000	0.960501000	-3.770630000
	C	0.867388000	1.751844000	-0.133243000
	O	1.175916000	0.549836000	-0.463932000
	C	-0.514318000	1.988896000	0.372481000
	C	-1.273492000	3.095051000	-0.029292000
	C	-1.084425000	1.016369000	1.216258000
	C	-2.595392000	3.223716000	0.396653000
	H	-0.839984000	3.827471000	-0.712664000
	C	-2.410020000	1.162528000	1.643803000
	C	-3.167286000	2.259807000	1.235856000
	H	-3.194249000	4.072962000	0.059936000
	H	-2.842765000	0.417695000	2.312914000
	H	-4.202432000	2.367506000	1.562172000
	C	1.742326000	2.823646000	-0.185207000
	H	1.470646000	3.817852000	0.167136000
	C	-1.432831000	-2.707032000	-1.141420000
	C	-0.260850000	-2.592976000	-1.941091000
	C	1.038814000	-2.492131000	-1.348297000
	C	1.129287000	-2.517981000	0.080080000
	C	-0.035748000	-2.561369000	0.864546000
	C	-1.343091000	-2.645491000	0.271712000
	H	-2.411014000	-2.661612000	-1.615610000

	H	-0.360978000	-2.489123000	-3.023519000
	H	2.093129000	-2.317253000	0.551039000
	H	0.085241000	-2.382363000	1.930319000
	C	2.267103000	-2.308094000	-2.189927000
	H	3.076802000	-1.865796000	-1.595898000
	H	2.608464000	-3.291241000	-2.556910000
	H	2.057027000	-1.677808000	-3.066487000
	C	-2.618380000	-2.577691000	1.095560000
	C	-2.370206000	-2.347755000	2.587932000
	C	-3.473477000	-3.834837000	0.869395000
	H	-3.184815000	-1.729972000	0.683145000
	H	-1.722896000	-1.482027000	2.786190000
	H	-3.328769000	-2.182453000	3.102723000
	H	-1.893851000	-3.225152000	3.054491000
	H	-3.745526000	-3.958095000	-0.188245000
	H	-2.945490000	-4.742558000	1.205176000
	H	-4.413218000	-3.753433000	1.435722000
	H	-0.443049000	0.232821000	1.646327000
	C	2.017021000	0.319108000	2.781174000
	O	1.219973000	-0.625247000	2.661646000
	O	3.171381000	0.388532000	2.230811000
	C	1.610619000	1.547619000	3.592851000
	H	2.458976000	1.922107000	4.184275000
	H	1.315752000	2.347792000	2.893616000
	H	0.757269000	1.322807000	4.246073000
	S	3.379241000	2.772164000	-0.692781000
	O	3.757336000	3.925348000	-1.534068000
	C	4.408010000	2.742948000	0.773414000
	H	4.258461000	3.728820000	1.234404000
	H	4.063064000	1.920519000	1.430887000
	H	5.446380000	2.621063000	0.440062000
	C	3.703159000	1.218585000	-1.513317000
	H	2.978325000	1.144524000	-2.331522000
	H	4.729235000	1.323980000	-1.887459000
	H	3.604012000	0.386419000	-0.803483000
	C	-6.448407000	0.874939000	0.149219000
	C	-5.825085000	-0.452554000	0.558731000
	H	-4.935888000	-0.202746000	1.168632000
	H	-6.554918000	-0.949316000	1.219300000
	F	-6.622685000	1.663795000	1.235167000
	F	-7.640599000	0.725868000	-0.437656000
	F	-5.661351000	1.555915000	-0.709128000
	O	-5.540524000	-1.273864000	-0.519921000
	H	-4.752684000	-0.894660000	-0.975858000

	C	6.228558000	-1.017908000	-0.051387000
	C	5.201529000	-1.631703000	0.885972000
	H	5.356491000	-2.726371000	0.832778000
	H	5.464535000	-1.304589000	1.908796000
	F	6.258202000	0.334057000	0.043835000
	F	5.965994000	-1.303548000	-1.341007000
	F	7.464417000	-1.461338000	0.221896000
	O	3.911697000	-1.274863000	0.530741000
	H	3.529415000	-0.627445000	1.255705000
TS-3O	Ru	0.492148000	1.604127000	-0.267358000
	C	2.460205000	0.132578000	-1.965192000
	O	3.353387000	0.408243000	-1.147502000
	O	1.262618000	0.594734000	-1.925134000
	C	2.720628000	-0.848870000	-3.090537000
	H	2.449629000	-1.851308000	-2.722630000
	H	2.098641000	-0.625119000	-3.967359000
	H	3.786074000	-0.861306000	-3.352603000
	C	-1.478169000	-0.398362000	-1.065091000
	O	-1.291357000	0.877245000	-1.053063000
	C	-0.429961000	-1.215615000	-0.429765000
	C	-0.213853000	-2.560552000	-0.736762000
	C	0.445896000	-0.510398000	0.439561000
	C	0.901952000	-3.217969000	-0.212218000
	H	-0.884965000	-3.083374000	-1.420801000
	C	1.558317000	-1.201770000	0.949685000
	C	1.797592000	-2.535575000	0.618242000
	H	1.086608000	-4.263647000	-0.469927000
	H	2.256090000	-0.698549000	1.615632000
	H	2.689652000	-3.033955000	0.998773000
	C	-2.594367000	-0.961045000	-1.670995000
	H	-2.906381000	-1.997784000	-1.590382000
	C	2.131040000	3.057580000	-0.263982000
	C	1.043950000	3.595280000	-1.024268000
	C	-0.256247000	3.672834000	-0.469014000
	C	-0.445687000	3.221613000	0.880536000
	C	0.641404000	2.716815000	1.624974000
	C	1.963762000	2.634416000	1.075936000
	H	3.088353000	2.883259000	-0.753553000
	H	1.195263000	3.842166000	-2.075965000
	H	-1.450654000	3.168949000	1.301004000
	H	0.434601000	2.286938000	2.601547000
	C	-1.431465000	4.122681000	-1.286044000
	H	-2.313723000	3.508291000	-1.059921000
	H	-1.680106000	5.171153000	-1.052064000

	H	-1.219868000	4.051100000	-2.362176000
	C	3.144792000	2.084487000	1.856114000
	C	2.759960000	1.466419000	3.202925000
	C	4.201767000	3.184092000	2.053484000
	H	3.595614000	1.301616000	1.230163000
	H	1.942958000	0.736598000	3.120130000
	H	3.631230000	0.949104000	3.630827000
	H	2.441514000	2.238834000	3.922861000
	H	4.547756000	3.596942000	1.093741000
	H	3.801486000	4.015951000	2.656753000
	H	5.078930000	2.775614000	2.578588000
	H	-0.129950000	0.177837000	1.367310000
	C	-1.943865000	0.227313000	2.670218000
	O	-0.672736000	0.290883000	2.644223000
	O	-2.682014000	0.459647000	1.688504000
	C	-2.563731000	-0.208697000	3.989574000
	H	-1.930370000	0.081414000	4.838307000
	H	-3.577374000	0.200414000	4.102512000
	H	-2.629617000	-1.309453000	3.981136000
	S	-3.814769000	0.041254000	-2.302940000
	O	-4.923260000	-0.703248000	-2.924190000
	C	-4.419111000	1.145455000	-1.026542000
	H	-4.971593000	0.505417000	-0.320909000
	H	-3.547133000	1.580624000	-0.520867000
	H	-5.067370000	1.891211000	-1.505873000
	C	-3.053282000	1.148053000	-3.503463000
	H	-2.767175000	0.499925000	-4.341390000
	H	-3.812553000	1.879529000	-3.810032000
	H	-2.176734000	1.609008000	-3.032344000
	C	-5.335359000	-1.589101000	2.008791000
	H	-6.404158000	-1.854278000	1.958430000
	H	-4.987905000	-1.810541000	3.037565000
	C	-4.608471000	-2.566653000	1.096274000
	O	-5.175770000	-0.262974000	1.640787000
	H	-4.213315000	0.014396000	1.728825000
	C	5.529895000	-2.778079000	-0.385195000
	C	5.789496000	-1.406685000	0.222169000
	H	6.544492000	-1.551551000	1.013108000
	H	6.247050000	-0.789742000	-0.574742000
	O	4.643224000	-0.846614000	0.763875000
	H	4.120920000	-0.446068000	0.024281000
	F	5.072758000	-3.657265000	0.525364000
	F	4.615536000	-2.723823000	-1.373147000
	F	6.660131000	-3.288325000	-0.907294000

	F	-4.902846000	-3.835025000	1.434322000
	F	-3.269546000	-2.433713000	1.169000000
	F	-4.953746000	-2.399191000	-0.194207000
INT-3O	Ru	-1.510910000	-0.589165000	0.039202000
	C	0.076507000	1.197372000	-1.881662000
	O	-0.200479000	2.232272000	-1.256610000
	O	-0.295694000	0.012569000	-1.558790000
	C	0.884240000	1.293161000	-3.167397000
	H	1.298860000	0.322805000	-3.468626000
	H	0.216426000	1.654022000	-3.966742000
	H	1.685121000	2.033196000	-3.039439000
	C	1.139803000	-1.102224000	1.103646000
	O	0.215969000	-1.702970000	0.429824000
	C	0.737009000	0.128828000	1.786023000
	C	1.515405000	0.798501000	2.746412000
	C	-0.509944000	0.635299000	1.340844000
	C	1.060552000	1.997056000	3.284433000
	H	2.470762000	0.379503000	3.068782000
	C	-0.919347000	1.870117000	1.871680000
	C	-0.154757000	2.534963000	2.830945000
	H	1.649692000	2.522423000	4.039188000
	H	-1.841271000	2.334950000	1.520323000
	H	-0.503499000	3.491890000	3.229480000
	C	2.448363000	-1.590102000	1.086683000
	H	3.315958000	-1.072997000	1.490549000
	C	-3.300333000	-0.461893000	-1.249534000
	C	-2.985166000	-1.851324000	-1.197796000
	C	-2.748781000	-2.461984000	0.054424000
	C	-2.956054000	-1.697778000	1.253448000
	C	-3.341003000	-0.337297000	1.170835000
	C	-3.545140000	0.317783000	-0.085577000
	H	-3.330692000	0.026814000	-2.224075000
	H	-2.785272000	-2.398171000	-2.119639000
	H	-2.751929000	-2.147746000	2.226043000
	H	-3.428637000	0.245491000	2.090022000
	C	-2.243621000	-3.872714000	0.153698000
	H	-1.487892000	-3.953349000	0.948262000
	H	-3.068442000	-4.562008000	0.399802000
	H	-1.792247000	-4.200700000	-0.793249000
	C	-4.057850000	1.742549000	-0.141477000
	C	-5.595574000	1.721370000	-0.185344000
	C	-3.467425000	2.573863000	-1.281566000
	H	-3.761606000	2.218919000	0.807943000
	H	-6.018556000	1.157211000	0.660917000

	H	-5.999630000	2.745415000	-0.151050000
	H	-5.951545000	1.247935000	-1.115259000
	H	-2.368387000	2.576670000	-1.244642000
	H	-3.786640000	2.193134000	-2.266117000
	H	-3.826012000	3.612695000	-1.211165000
	S	2.879883000	-2.683657000	-0.140395000
	O	4.312164000	-3.032525000	-0.135673000
	C	1.876763000	-4.171787000	-0.001230000
	H	2.164046000	-4.622334000	0.957338000
	H	0.823332000	-3.869060000	-0.008560000
	H	2.146965000	-4.825007000	-0.841703000
	C	2.404162000	-2.010080000	-1.744028000
	H	3.111566000	-1.187032000	-1.903307000
	H	2.531304000	-2.801238000	-2.494899000
	H	1.374975000	-1.623486000	-1.684107000
	C	2.519897000	3.139803000	0.056114000
	C	3.477305000	1.995565000	-0.240580000
	H	1.749318000	2.740714000	0.734914000
	H	3.112425000	3.883253000	0.619864000
	F	2.859115000	0.958249000	-0.863047000
	F	4.495295000	2.361708000	-1.028731000
	F	4.006221000	1.499382000	0.899844000
	O	1.995383000	3.705719000	-1.098423000
	H	1.098945000	3.308996000	-1.232619000

Table S2. Cartesian coordinates of the optimized stationary points involved in the annulation process

Names	Cartesian coordinates			
TS-4C	C	1.277093000	2.451701000	-1.255830000
	C	-0.054168000	2.605951000	-0.770426000
	C	-1.086442000	1.845388000	-1.429466000
	C	-0.763655000	0.866876000	-2.359665000
	C	0.608757000	0.607328000	-2.727004000
	C	1.603704000	1.485609000	-2.251905000
	H	2.076770000	3.057038000	-0.826708000
	H	-2.127135000	1.972035000	-1.127515000
	H	-1.545222000	0.215111000	-2.744371000
	H	2.642370000	1.332080000	-2.546878000
	C	0.947977000	-0.542076000	-3.633354000
	H	1.949369000	-0.927272000	-3.395813000
	H	0.214305000	-1.348372000	-3.500038000
	H	0.926714000	-0.225725000	-4.690133000

	C	-0.440659000	3.653668000	0.256224000
	H	-1.336673000	3.261454000	0.764954000
	C	-0.828619000	4.960294000	-0.454531000
	H	-1.625493000	4.795042000	-1.196158000
	H	-1.187033000	5.708168000	0.270087000
	H	0.038670000	5.388050000	-0.984073000
	C	0.624216000	3.888630000	1.328626000
	H	0.246787000	4.589113000	2.088849000
	H	0.888705000	2.946643000	1.829576000
	H	1.541170000	4.332482000	0.907790000
	Ru	0.626685000	0.541042000	-0.390204000
	C	-0.340446000	-2.264334000	-0.701453000
	O	-1.253333000	-1.830968000	-1.420914000
	O	0.633497000	-1.557379000	-0.253832000
	C	-0.314481000	-3.733870000	-0.314709000
	H	-1.339633000	-4.128449000	-0.312676000
	H	0.264226000	-4.293575000	-1.068132000
	H	0.156678000	-3.878513000	0.666729000
	C	2.022762000	-0.162616000	2.099354000
	O	2.942963000	-0.686782000	2.718745000
	C	0.618101000	-0.061009000	2.505536000
	C	0.150459000	-0.361708000	3.794671000
	C	-0.240524000	0.365845000	1.460896000
	C	-1.206571000	-0.226244000	4.069263000
	H	0.861958000	-0.692341000	4.555803000
	C	-1.603796000	0.503361000	1.770251000
	C	-2.076090000	0.207336000	3.053143000
	H	-1.597618000	-0.454439000	5.063501000
	H	-2.315843000	0.818982000	1.008510000
	H	-3.146089000	0.302675000	3.257439000
	C	2.179791000	0.471789000	0.731766000
	H	3.014167000	1.192392000	0.660617000
	S	3.658815000	-1.151001000	-0.171820000
	O	3.738398000	-1.078858000	-1.669411000
	C	5.310807000	-0.834476000	0.505704000
	H	5.223972000	-0.869190000	1.599615000
	H	6.016725000	-1.575168000	0.104410000
	H	5.587466000	0.173816000	0.169442000
	C	3.419679000	-2.870603000	0.340057000
	H	3.393853000	-2.892951000	1.436993000
	H	2.447012000	-3.153874000	-0.073113000
	H	4.238734000	-3.473182000	-0.076921000
	C	-3.923678000	-2.047662000	0.228546000
	C	-4.559857000	-0.716897000	-0.147299000

	H	-4.655420000	-2.563740000	0.873166000
	H	-3.041077000	-1.804296000	0.849463000
	F	-5.716381000	-0.862507000	-0.803174000
	F	-3.750951000	0.031418000	-0.934064000
	F	-4.812033000	0.017296000	0.961450000
	O	-3.633971000	-2.835664000	-0.875127000
	H	-2.779903000	-2.506169000	-1.250282000
INT-4C	C	0.049059000	1.094107000	-2.055923000
	C	1.229188000	1.795111000	-1.666060000
	C	1.108790000	2.666419000	-0.530244000
	C	-0.073438000	2.736693000	0.191796000
	C	-1.259302000	2.039225000	-0.223425000
	C	-1.194229000	1.267852000	-1.384523000
	H	0.079620000	0.468453000	-2.949465000
	H	1.986291000	3.226367000	-0.201988000
	H	-0.103124000	3.340673000	1.100398000
	H	-2.071700000	0.724135000	-1.731503000
	C	-2.551242000	2.184459000	0.557689000
	H	-3.329812000	1.665234000	-0.020199000
	Ru	0.839572000	0.209642000	-0.115484000
	C	-0.273386000	-1.144965000	2.232762000
	O	-1.060524000	-1.756850000	1.505511000
	O	0.619423000	-0.295735000	1.829374000
	C	-0.312741000	-1.320372000	3.736086000
	H	-0.761960000	-0.418221000	4.182332000
	H	0.704927000	-1.416853000	4.139188000
	H	-0.922513000	-2.192944000	4.000316000
	C	2.423071000	-2.055124000	-0.990460000
	O	2.631234000	-3.136027000	-1.516100000
	C	3.391746000	-1.209822000	-0.268311000
	C	4.743546000	-1.517849000	-0.078897000
	C	2.812316000	-0.034231000	0.249988000
	C	5.543256000	-0.637769000	0.648482000
	H	5.140065000	-2.444310000	-0.502344000
	C	3.620285000	0.828769000	1.001075000
	C	4.975605000	0.526627000	1.188413000
	H	6.602085000	-0.853909000	0.808588000
	H	3.202615000	1.729599000	1.457843000
	H	5.600213000	1.208609000	1.772695000
	C	1.083004000	-1.377879000	-1.004149000
	H	0.294349000	-1.844490000	-1.617355000
	C	2.483421000	1.769000000	-2.494542000
	H	2.545201000	0.841128000	-3.080010000
	H	2.504361000	2.621803000	-3.193371000

	H	3.375469000	1.822570000	-1.855093000
	C	-2.461032000	1.497195000	1.928248000
	H	-1.638101000	1.909741000	2.534133000
	H	-3.399743000	1.641156000	2.484875000
	H	-2.302488000	0.419219000	1.806630000
	C	-2.963666000	3.659210000	0.685698000
	H	-3.021621000	4.149886000	-0.298285000
	H	-3.952964000	3.732988000	1.162970000
	H	-2.255423000	4.229352000	1.308630000
	C	-3.246423000	-2.302063000	-0.878899000
	C	-4.346143000	-1.297734000	-0.567886000
	H	-3.301592000	-3.087283000	-0.102963000
	H	-3.510419000	-2.761558000	-1.846683000
	F	-4.355930000	-0.275919000	-1.453394000
	F	-4.204748000	-0.747847000	0.653138000
	F	-5.555280000	-1.879434000	-0.611945000
	O	-1.998816000	-1.701724000	-0.964517000
	H	-1.581922000	-1.685238000	-0.063875000
INT-4C'	Ru	-0.358426000	-1.307325000	0.169123000
	C	0.713543000	1.011727000	-0.465905000
	O	0.813717000	0.195129000	-1.423344000
	O	0.167289000	0.605373000	0.619810000
	C	1.178414000	2.431828000	-0.549474000
	H	0.293960000	3.080636000	-0.634378000
	H	1.721178000	2.707945000	0.364019000
	H	1.811548000	2.569044000	-1.434641000
	C	-2.788982000	-2.034811000	1.450691000
	C	-3.199242000	-1.645164000	0.081184000
	C	-4.494334000	-1.772288000	-0.435500000
	C	-2.148063000	-1.041610000	-0.662177000
	C	-4.763968000	-1.265251000	-1.704814000
	H	-5.267406000	-2.247669000	0.173575000
	C	-2.444586000	-0.526200000	-1.936776000
	C	-3.741555000	-0.641633000	-2.443608000
	H	-5.768206000	-1.342538000	-2.127773000
	H	-1.668611000	-0.030560000	-2.524356000
	H	-3.968964000	-0.235906000	-3.433276000
	C	2.764778000	-2.076697000	-0.270931000
	O	1.752252000	-2.098209000	0.421104000
	O	2.841440000	-1.405739000	-1.412924000
	H	2.035198000	-0.809272000	-1.529637000
	C	4.020179000	-2.806364000	0.092589000
	H	4.255674000	-3.541827000	-0.692779000
	H	4.855544000	-2.090390000	0.126099000

	H	3.896964000	-3.309152000	1.057717000
	C	-1.370124000	-1.559284000	1.663423000
	O	-3.450909000	-2.619606000	2.286524000
	H	-1.075720000	-1.271308000	2.688509000
	C	4.629113000	1.216037000	0.475051000
	C	5.122455000	1.163601000	-0.964005000
	H	4.385958000	1.718721000	-1.575424000
	H	6.069231000	1.725541000	-0.992371000
	F	5.485087000	0.647434000	1.327926000
	F	3.444238000	0.566292000	0.615074000
	F	4.427660000	2.486406000	0.859898000
	O	5.356647000	-0.134312000	-1.410185000
	H	4.504484000	-0.555998000	-1.618522000
	C	-2.976902000	2.819983000	0.116948000
	C	-3.237171000	1.742651000	1.153863000
	H	-4.064312000	2.098580000	1.787373000
	H	-3.592844000	0.856749000	0.598278000
	F	-2.588432000	3.982333000	0.656970000
	F	-1.988356000	2.442991000	-0.738672000
	F	-4.071914000	3.048492000	-0.622134000
	O	-2.135557000	1.495480000	1.969116000
	H	-1.367854000	1.230075000	1.430437000
TS-5C	Ru	-1.028325000	-0.095315000	0.956934000
	C	-0.671643000	1.605124000	-1.121727000
	O	0.405315000	1.070432000	-0.699009000
	O	-1.745478000	1.381864000	-0.486761000
	C	-0.668043000	2.489949000	-2.329646000
	H	-1.691476000	2.709217000	-2.656260000
	H	-0.129250000	3.415527000	-2.067290000
	H	-0.105097000	2.001310000	-3.138169000
	C	-3.201922000	-1.855855000	1.577513000
	O	-4.005264000	-2.423216000	2.293960000
	C	-2.964326000	-2.135606000	0.136937000
	C	-3.989883000	-2.625142000	-0.668364000
	C	-1.771260000	-1.607768000	-0.433981000
	C	-3.870858000	-2.563363000	-2.059581000
	H	-4.904604000	-2.979074000	-0.188239000
	C	-1.677627000	-1.538930000	-1.831886000
	C	-2.730728000	-1.993058000	-2.630883000
	H	-4.682020000	-2.922605000	-2.695968000
	H	-0.776290000	-1.155169000	-2.305773000
	H	-2.652897000	-1.901962000	-3.716418000
	C	-2.382316000	-0.681178000	2.012420000
	H	-2.668033000	-0.183428000	2.955437000

	C	1.033105000	-1.945995000	-0.585789000
	C	-0.157092000	-2.168645000	0.362892000
	H	-0.505731000	-3.204682000	0.358135000
	C	1.650851000	-1.046746000	1.469813000
	C	0.269303000	-1.574990000	1.640269000
	H	0.048621000	-2.043112000	2.599723000
	O	2.357861000	-0.481514000	2.277199000
	O	1.144053000	-2.299466000	-1.736261000
	N	2.003698000	-1.270280000	0.133104000
	C	3.249826000	-0.788616000	-0.452059000
	H	3.034922000	-0.534693000	-1.498134000
	H	3.516222000	0.122744000	0.095502000
	C	4.365021000	-1.804619000	-0.359800000
	C	4.515279000	-2.788260000	-1.347319000
	C	5.235420000	-1.794385000	0.738343000
	C	5.528853000	-3.743352000	-1.241272000
	H	3.824249000	-2.805805000	-2.193357000
	C	6.249483000	-2.749352000	0.843357000
	H	5.104492000	-1.037709000	1.515422000
	C	6.398884000	-3.724522000	-0.146917000
	H	5.641065000	-4.504970000	-2.016867000
	H	6.926005000	-2.731871000	1.701315000
	H	7.193525000	-4.470297000	-0.066143000
	C	0.443885000	2.148316000	2.417553000
	O	-0.534243000	1.394225000	2.402701000
	O	1.231282000	2.335033000	1.382682000
	H	0.949676000	1.772754000	0.590445000
	C	0.842974000	2.893083000	3.649821000
	H	1.698831000	2.355688000	4.091273000
	H	1.177226000	3.909642000	3.401026000
	H	0.016323000	2.911154000	4.368795000
	C	-5.021896000	1.729962000	-1.480062000
	C	-5.639136000	0.829211000	-0.420255000
	H	-5.808128000	1.929683000	-2.225676000
	H	-4.782968000	2.687122000	-0.976928000
	F	-6.685110000	1.435528000	0.165510000
	F	-6.070810000	-0.334689000	-0.926256000
	F	-4.745712000	0.536200000	0.551737000
	O	-3.932755000	1.143610000	-2.113527000
	H	-3.181857000	1.139043000	-1.485826000
	C	2.836504000	3.058176000	-1.599779000
	C	4.218993000	2.858409000	-1.003648000
	H	2.967909000	3.441095000	-2.622778000
	H	2.361841000	2.062826000	-1.656884000

	F	4.124926000	2.472683000	0.289849000
	F	4.879473000	1.893104000	-1.666387000
	F	4.965079000	3.967083000	-1.033679000
	O	2.071031000	3.983359000	-0.879710000
	H	1.952919000	3.648515000	0.023968000
INT-5C	Ru	-0.422275000	0.806035000	1.465892000
	C	0.409822000	0.620132000	-1.243415000
	O	-0.232114000	-0.423202000	-1.121416000
	O	0.565177000	1.432047000	-0.228332000
	C	1.075322000	1.059440000	-2.514556000
	H	2.167086000	1.081894000	-2.361354000
	H	0.823320000	0.369141000	-3.328329000
	H	0.748607000	2.080341000	-2.760144000
	C	-1.069554000	3.653921000	1.542355000
	O	-1.397033000	4.573149000	2.271577000
	C	-1.263561000	3.757825000	0.040194000
	C	-0.537321000	4.819518000	-0.525941000
	C	-2.063182000	2.944668000	-0.801451000
	C	-0.549374000	5.061568000	-1.898594000
	H	0.057824000	5.455364000	0.132775000
	C	-2.089501000	3.220683000	-2.174990000
	C	-1.328956000	4.254262000	-2.726091000
	H	0.040117000	5.881882000	-2.314020000
	H	-2.719070000	2.605376000	-2.817544000
	H	-1.360491000	4.432915000	-3.803498000
	C	-0.340517000	2.482471000	2.132274000
	H	0.168663000	2.704870000	3.091836000
	C	-3.200602000	0.609405000	-1.137468000
	C	-2.956765000	1.843791000	-0.238309000
	H	-3.962256000	2.280451000	-0.085528000
	C	-2.476257000	-0.209147000	0.866156000
	C	-2.455168000	1.224040000	1.042523000
	H	-2.878974000	1.588165000	1.986230000
	O	-1.892156000	-0.969940000	1.689117000
	O	-3.543489000	0.575526000	-2.293822000
	N	-2.959029000	-0.542362000	-0.369666000
	C	-2.971514000	-1.890038000	-0.934576000
	H	-2.857980000	-1.766540000	-2.019086000
	H	-2.091834000	-2.421599000	-0.553404000
	C	-4.248985000	-2.622378000	-0.598662000
	C	-5.404170000	-2.420913000	-1.367565000
	C	-4.304351000	-3.475317000	0.511115000
	C	-6.595614000	-3.068003000	-1.033616000
	H	-5.362100000	-1.748090000	-2.228022000

	C	-5.496123000	-4.123845000	0.845261000
	H	-3.407094000	-3.622919000	1.117262000
	C	-6.643337000	-3.921621000	0.073154000
	H	-7.490348000	-2.907970000	-1.640228000
	H	-5.529064000	-4.789629000	1.711101000
	H	-7.575181000	-4.429756000	0.332981000
	C	2.661803000	0.526565000	1.970804000
	O	1.532203000	0.161055000	2.300314000
	O	2.890544000	1.293261000	0.921764000
	H	2.031450000	1.484325000	0.429421000
	C	3.887344000	0.128435000	2.727898000
	H	4.492217000	-0.536258000	2.094651000
	H	4.492492000	1.019859000	2.949459000
	H	3.606728000	-0.393756000	3.648674000
	C	2.263716000	-2.639340000	0.383891000
	C	0.802298000	-3.045286000	0.478611000
	H	0.784543000	-4.059494000	0.908285000
	H	0.317925000	-2.362735000	1.201172000
	F	2.848967000	-2.634952000	1.593010000
	F	2.387381000	-1.374401000	-0.117708000
	F	2.978013000	-3.431598000	-0.419924000
	O	0.188062000	-3.070295000	-0.769087000
	H	0.046405000	-2.145944000	-1.057685000
	C	5.770142000	-1.237450000	-1.159329000
	C	4.692897000	-0.588000000	-2.011411000
	H	5.100486000	-0.485692000	-3.028296000
	H	3.846104000	-1.294450000	-2.047846000
	F	6.898652000	-0.521018000	-1.123289000
	F	5.349141000	-1.374763000	0.124507000
	F	6.064710000	-2.460269000	-1.617519000
	O	4.346429000	0.685859000	-1.552778000
	H	3.990017000	0.632272000	-0.650414000
TS-6C	Ru	-0.547245000	-0.238290000	1.169824000
	C	-1.213126000	0.625066000	-1.123252000
	O	-0.037642000	0.208220000	-0.889524000
	O	-2.030361000	0.544977000	-0.143015000
	C	-1.622430000	1.164767000	-2.451329000
	H	-2.676688000	1.463602000	-2.428363000
	H	-0.992942000	2.028080000	-2.707107000
	H	-1.474079000	0.387145000	-3.214781000
	C	-0.822370000	-2.386266000	2.831551000
	O	-0.926424000	-3.195235000	3.723911000
	C	-1.090715000	-2.691073000	1.365990000
	C	-2.401649000	-3.097816000	1.021398000

	C	-0.081992000	-2.595262000	0.361581000
	C	-2.738619000	-3.355205000	-0.295158000
	H	-3.141675000	-3.193856000	1.818865000
	C	-0.456581000	-2.891562000	-0.971161000
	C	-1.757164000	-3.243493000	-1.294086000
	H	-3.759577000	-3.631798000	-0.561391000
	H	0.298412000	-2.862032000	-1.754337000
	H	-2.020595000	-3.439947000	-2.334833000
	C	-0.490164000	-0.942911000	2.959601000
	H	0.005976000	-0.613605000	3.884561000
	C	2.309617000	-2.225078000	-0.488428000
	C	1.382296000	-2.269300000	0.732848000
	H	1.759183000	-3.047358000	1.415911000
	C	2.320096000	-0.058478000	0.362236000
	C	1.471914000	-0.851783000	1.313817000
	H	1.913543000	-0.777018000	2.311777000
	O	2.631515000	1.113166000	0.424081000
	O	2.599242000	-3.139176000	-1.224797000
	N	2.763633000	-0.923465000	-0.630684000
	C	3.649719000	-0.503324000	-1.712382000
	H	3.425447000	-1.149556000	-2.571023000
	H	3.380188000	0.532226000	-1.956588000
	C	5.108989000	-0.605280000	-1.328997000
	C	5.804483000	-1.808147000	-1.516577000
	C	5.766032000	0.485453000	-0.742943000
	C	7.142882000	-1.914883000	-1.131842000
	H	5.285542000	-2.662731000	-1.957291000
	C	7.104794000	0.377622000	-0.359157000
	H	5.217090000	1.415309000	-0.577768000
	C	7.795772000	-0.821762000	-0.554339000
	H	7.678978000	-2.854649000	-1.284839000
	H	7.610342000	1.233707000	0.094094000
	H	8.843715000	-0.904862000	-0.256191000
	C	-1.055086000	2.153077000	2.534517000
	O	-0.197730000	1.680278000	1.694635000
	O	-1.889560000	1.427201000	3.119529000
	H	-1.378324000	0.000872000	2.865085000
	C	-1.017311000	3.640156000	2.754823000
	H	-1.829510000	4.085868000	2.159157000
	H	-1.208042000	3.863832000	3.813020000
	H	-0.066881000	4.061065000	2.406083000
	C	-5.002593000	-0.965101000	-1.879063000
	C	-5.146379000	-0.237099000	-0.550388000
	H	-6.225532000	-0.221560000	-0.322722000

	H	-4.650719000	-0.867884000	0.210305000
	F	-3.708303000	-1.061595000	-2.265440000
	F	-5.475804000	-2.226680000	-1.777828000
	F	-5.663344000	-0.360576000	-2.869656000
	O	-4.657529000	1.062806000	-0.596390000
	H	-3.711649000	1.030921000	-0.353121000
	C	1.353317000	3.776684000	-0.631874000
	C	-0.055787000	4.287591000	-0.887529000
	H	1.430319000	2.788836000	-1.114806000
	H	2.022569000	4.472108000	-1.171826000
	F	-1.012592000	3.464455000	-0.404910000
	F	-0.269294000	5.492989000	-0.350356000
	F	-0.268485000	4.384696000	-2.220643000
	O	1.667302000	3.734692000	0.721840000
	H	1.760469000	2.797717000	0.968854000
INT-6C	Ru	-1.325719000	-1.107974000	-0.032172000
	C	-0.893737000	-0.465859000	2.364934000
	O	-0.035139000	-1.142755000	1.696979000
	O	-1.961126000	-0.163339000	1.750002000
	C	-0.628024000	-0.024762000	3.764327000
	H	-1.514396000	-0.208183000	4.387481000
	H	0.257287000	-0.531298000	4.165328000
	H	-0.446036000	1.061457000	3.747569000
	C	-4.428635000	-0.942814000	-0.990519000
	O	-5.128460000	-1.356144000	-1.895871000
	C	-4.749703000	0.360273000	-0.317499000
	C	-6.012133000	0.486692000	0.282341000
	C	-3.859343000	1.443325000	-0.306729000
	C	-6.373576000	1.663344000	0.933615000
	H	-6.703969000	-0.356822000	0.233949000
	C	-4.242991000	2.634137000	0.328224000
	C	-5.481259000	2.739519000	0.959018000
	H	-7.352317000	1.745993000	1.411566000
	H	-3.556332000	3.481550000	0.331878000
	H	-5.756095000	3.670544000	1.459890000
	C	-3.308986000	-1.777260000	-0.451217000
	H	-3.221873000	-2.665273000	-1.089842000
	C	-1.327450000	1.761686000	-0.161876000
	C	-2.536372000	1.412598000	-1.042068000
	H	-2.574774000	2.212533000	-1.809625000
	C	-0.601358000	0.293557000	-1.865784000
	C	-2.047162000	0.122939000	-1.711766000
	H	-2.597949000	-0.303031000	-2.550592000
	O	0.219014000	-0.021856000	-2.690699000

	O	-1.195089000	2.594981000	0.683583000
	N	-0.281959000	0.846449000	-0.550086000
	C	1.111849000	1.081497000	-0.124542000
	H	1.124365000	1.030229000	0.965593000
	H	1.688119000	0.235017000	-0.513505000
	C	1.667836000	2.405858000	-0.589897000
	C	1.996198000	3.383434000	0.357591000
	C	1.886495000	2.669127000	-1.950348000
	C	2.531847000	4.608158000	-0.044686000
	H	1.836956000	3.174960000	1.417131000
	C	2.413176000	3.898015000	-2.352757000
	H	1.649898000	1.904583000	-2.691609000
	C	2.736901000	4.870159000	-1.401759000
	H	2.787939000	5.360852000	0.704581000
	H	2.581307000	4.093613000	-3.414565000
	H	3.153689000	5.829361000	-1.718212000
	C	-0.658483000	-3.451946000	-0.558367000
	O	-1.357544000	-3.156875000	0.459173000
	O	-0.423781000	-2.482418000	-1.358195000
	H	-3.556307000	-2.062326000	0.583510000
	C	-0.087856000	-4.809397000	-0.783738000
	H	-0.306256000	-5.140184000	-1.809575000
	H	1.006913000	-4.734158000	-0.679992000
	H	-0.483184000	-5.525138000	-0.053288000
	C	3.447730000	0.047109000	2.616206000
	C	3.205660000	-1.347368000	2.057734000
	H	2.887621000	-1.245313000	1.008223000
	H	4.184774000	-1.853192000	2.051905000
	C	4.316606000	-0.902861000	-1.768305000
	C	3.074857000	-1.608056000	-2.279873000
	H	2.580836000	-0.929412000	-2.994864000
	H	3.423024000	-2.504117000	-2.828253000
	F	4.105166000	0.029907000	3.782107000
	F	2.277434000	0.706300000	2.846449000
	F	4.151851000	0.796174000	1.752928000
	F	4.986809000	-1.653264000	-0.878411000
	F	4.021727000	0.261663000	-1.164640000
	F	5.145403000	-0.635703000	-2.789865000
	O	2.300720000	-2.075611000	2.832513000
	H	1.412505000	-1.873559000	2.485437000
	O	2.251193000	-1.927982000	-1.194937000
	H	1.333282000	-2.039324000	-1.505037000
TS-7C	Ru	0.158049000	0.246083000	0.568990000
	C	-0.236715000	0.548661000	-1.886198000

	O	-0.023356000	1.541241000	-1.100826000
	O	-0.156064000	-0.600862000	-1.356073000
	C	-0.586871000	0.733176000	-3.323207000
	H	-0.446331000	1.776582000	-3.628264000
	H	0.004427000	0.042937000	-3.940881000
	H	-1.651775000	0.476041000	-3.433749000
	C	-0.798131000	-2.919041000	1.789407000
	O	-1.296308000	-3.568975000	2.685361000
	C	-0.422673000	-3.532551000	0.481435000
	C	-1.295895000	-4.487716000	-0.064240000
	C	0.762218000	-3.192143000	-0.194373000
	C	-1.019389000	-5.071120000	-1.296797000
	H	-2.201289000	-4.739775000	0.489286000
	C	1.048525000	-3.811237000	-1.418158000
	C	0.157039000	-4.729154000	-1.972706000
	H	-1.714277000	-5.794614000	-1.728667000
	H	1.969563000	-3.556509000	-1.942396000
	H	0.387558000	-5.187922000	-2.937110000
	C	-0.681413000	-1.423816000	1.916224000
	H	-0.674650000	-1.122643000	2.968532000
	C	2.331092000	-1.173764000	-0.521551000
	C	1.775137000	-2.249574000	0.426132000
	H	2.656361000	-2.856396000	0.717564000
	C	2.188665000	-0.213676000	1.635078000
	C	1.351206000	-1.431745000	1.643944000
	H	1.363996000	-1.936658000	2.610467000
	O	2.672966000	0.457235000	2.511421000
	O	2.741865000	-1.279717000	-1.640764000
	N	2.302554000	0.066174000	0.206228000
	C	3.066964000	1.238912000	-0.268556000
	H	2.688070000	1.476328000	-1.269373000
	H	2.795793000	2.057695000	0.409483000
	C	4.560555000	1.005365000	-0.286982000
	C	5.206331000	0.651338000	-1.480109000
	C	5.316942000	1.141143000	0.887580000
	C	6.585933000	0.436820000	-1.501360000
	H	4.619120000	0.532246000	-2.392432000
	C	6.696090000	0.922947000	0.865161000
	H	4.813815000	1.408239000	1.818148000
	C	7.333406000	0.570980000	-0.328163000
	H	7.078237000	0.163245000	-2.437550000
	H	7.276340000	1.032974000	1.784367000
	H	8.413067000	0.403368000	-0.344337000
	C	-1.331035000	1.637466000	2.022559000

	O	-1.781701000	0.944482000	1.034619000
	O	-0.087963000	1.548324000	2.222181000
	H	-1.610117000	-1.067189000	1.453757000
	C	-2.243213000	2.429040000	2.895698000
	H	-2.686688000	1.748386000	3.640853000
	H	-1.680042000	3.212259000	3.417665000
	H	-3.052170000	2.866042000	2.297819000
	C	-4.209823000	-1.791416000	-0.354425000
	C	-3.227235000	-1.148340000	-1.317280000
	H	-2.243848000	-1.621077000	-1.146006000
	H	-3.553785000	-1.413591000	-2.334466000
	F	-5.458542000	-1.343286000	-0.510403000
	F	-4.222040000	-3.126673000	-0.523343000
	F	-3.856361000	-1.553461000	0.931046000
	O	-3.196320000	0.244946000	-1.213037000
	H	-2.856652000	0.504858000	-0.335169000
	C	-2.346765000	4.442271000	-0.373656000
	C	-2.284632000	3.716192000	-1.708020000
	H	-2.615868000	2.676991000	-1.531915000
	H	-3.016834000	4.198943000	-2.373946000
	F	-2.213254000	5.766448000	-0.496098000
	F	-3.521919000	4.204746000	0.247364000
	F	-1.364868000	4.021130000	0.457268000
	O	-1.014309000	3.805532000	-2.277770000
	H	-0.449542000	3.176482000	-1.788837000
INT-7C	Ru	0.536848000	0.111634000	-0.982215000
	C	-1.423509000	1.010465000	-2.222256000
	O	-1.221858000	-0.251618000	-2.034754000
	O	-0.563262000	1.777773000	-1.710241000
	C	-2.619384000	1.506750000	-2.962229000
	H	-2.333700000	2.352940000	-3.601706000
	H	-3.077559000	0.699682000	-3.546757000
	H	-3.350321000	1.863068000	-2.220140000
	C	2.962544000	2.612284000	0.340271000
	O	4.130740000	2.823258000	0.099075000
	C	1.925677000	3.676046000	0.385998000
	C	2.230238000	4.925089000	-0.181459000
	C	0.649629000	3.444115000	0.936855000
	C	1.268191000	5.926938000	-0.233737000
	H	3.232046000	5.071294000	-0.589126000
	C	-0.311322000	4.460997000	0.882014000
	C	-0.007573000	5.687737000	0.292824000
	H	1.503878000	6.892381000	-0.686580000
	H	-1.304056000	4.278947000	1.295301000

	H	-0.771060000	6.468010000	0.249779000
	C	2.442799000	1.186065000	0.527489000
	H	3.281110000	0.491689000	0.640738000
	C	-0.891463000	1.394320000	1.087668000
	C	0.325873000	2.146567000	1.639695000
	H	0.027360000	2.389174000	2.676128000
	C	0.716418000	-0.234369000	1.653014000
	C	1.453738000	1.097213000	1.696899000
	H	2.024833000	1.158711000	2.634355000
	O	1.069497000	-1.303979000	2.073260000
	O	-1.983861000	1.823604000	0.839437000
	N	-0.534478000	0.009643000	0.987450000
	C	-1.590087000	-1.035237000	0.997973000
	H	-2.255171000	-0.799406000	0.164591000
	H	-1.068984000	-1.977040000	0.786139000
	C	-2.348015000	-1.091977000	2.302397000
	C	-3.587646000	-0.445981000	2.421597000
	C	-1.825114000	-1.783882000	3.406552000
	C	-4.289740000	-0.486154000	3.628293000
	H	-3.997513000	0.086769000	1.562978000
	C	-2.527565000	-1.819031000	4.612875000
	H	-0.863938000	-2.292806000	3.313821000
	C	-3.760242000	-1.169109000	4.726571000
	H	-5.256080000	0.017098000	3.709354000
	H	-2.113857000	-2.362518000	5.465730000
	H	-4.310855000	-1.200533000	5.669915000
	C	1.995241000	-1.535105000	-2.143549000
	O	1.503582000	-1.760590000	-0.980433000
	O	1.697444000	-0.414023000	-2.658572000
	H	2.052060000	1.021235000	-0.535398000
	C	2.864289000	-2.532785000	-2.836045000
	H	3.796354000	-2.042483000	-3.151986000
	H	3.087981000	-3.370926000	-2.165329000
	H	2.350263000	-2.893252000	-3.740533000
	C	4.749365000	-2.521516000	0.502088000
	C	3.628275000	-3.282744000	1.193882000
	H	4.112512000	-4.100954000	1.751424000
	H	3.175466000	-2.589865000	1.926148000
	C	-4.894903000	-1.247913000	-1.473316000
	C	-3.971370000	-2.329053000	-2.018467000
	H	-3.422256000	-2.740951000	-1.149583000
	H	-4.626530000	-3.128530000	-2.401771000
	F	4.286204000	-1.417795000	-0.146045000
	F	5.385370000	-3.260598000	-0.415541000

	F	5.655387000	-2.094924000	1.396472000
	F	-4.191397000	-0.215556000	-0.935279000
	F	-5.676166000	-1.737617000	-0.497660000
	F	-5.683050000	-0.723593000	-2.417339000
	O	-3.151090000	-1.880659000	-3.044213000
	H	-2.394567000	-1.384307000	-2.666844000
	O	2.707380000	-3.825155000	0.304937000
	H	2.140827000	-3.103373000	-0.038126000
3	C	3.263850000	1.566387000	-0.083695000
	O	4.216847000	2.316329000	-0.140218000
	C	3.403468000	0.084227000	-0.183779000
	C	4.687700000	-0.475385000	-0.077410000
	C	2.279801000	-0.751575000	-0.338881000
	C	4.858462000	-1.855102000	-0.091320000
	H	5.533085000	0.207003000	0.028307000
	C	2.463163000	-2.141381000	-0.351054000
	C	3.739348000	-2.688129000	-0.219886000
	H	5.857409000	-2.287191000	0.001066000
	H	1.594384000	-2.792608000	-0.456976000
	H	3.864042000	-3.773611000	-0.225657000
	C	1.861485000	2.077718000	0.194463000
	H	1.829285000	3.162281000	0.029408000
	C	-0.148623000	-0.579903000	0.494439000
	C	0.900520000	-0.177747000	-0.552279000
	H	0.502376000	-0.606246000	-1.490154000
	C	-0.584751000	1.650372000	-0.027861000
	C	0.784681000	1.354144000	-0.630183000
	H	0.811193000	1.721317000	-1.665809000
	O	-1.205351000	2.684638000	-0.073555000
	O	-0.285613000	-1.651644000	1.033302000
	N	-0.985257000	0.514466000	0.673878000
	C	-2.225241000	0.447327000	1.444875000
	H	-2.042655000	-0.239900000	2.281415000
	H	-2.411390000	1.456358000	1.835175000
	C	-3.386984000	-0.027961000	0.601168000
	C	-3.670246000	-1.397121000	0.495799000
	C	-4.159483000	0.891909000	-0.122091000
	C	-4.718435000	-1.839529000	-0.314730000
	H	-3.055482000	-2.113867000	1.045266000
	C	-5.207625000	0.448198000	-0.931697000
	H	-3.924998000	1.956838000	-0.054657000
	C	-5.489911000	-0.917688000	-1.028295000
	H	-4.934699000	-2.908112000	-0.388248000
	H	-5.807149000	1.171916000	-1.489171000

	H	-6.311731000	-1.263738000	-1.659887000
	H	1.678995000	1.901131000	1.271043000

Table S3. Cartesian coordinates of the optimized stationary points involved in the reaction pathway featuring Ru-carbene formation prior to C-H activation or subsequent to migratory insertion

Names	Cartesian coordinates			
TS-2CC	C	-0.137428000	0.919160000	-1.706704000
	C	1.267796000	1.061590000	-1.524560000
	C	1.674939000	2.004998000	-0.547369000
	C	0.759537000	2.896325000	0.088341000
	C	-0.622852000	2.776345000	-0.140931000
	C	-1.068635000	1.741845000	-1.023301000
	H	-0.521800000	0.131939000	-2.354813000
	H	2.731392000	2.048511000	-0.291271000
	H	1.136862000	3.612316000	0.816928000
	H	-2.131527000	1.555036000	-1.154444000
	C	-1.644494000	3.665238000	0.534885000
	H	-2.561799000	3.063745000	0.614484000
	Ru	0.179500000	0.654377000	0.488094000
	C	2.776981000	0.072275000	1.882536000
	O	1.524097000	0.305920000	2.040338000
	O	3.357710000	0.014772000	0.789760000
	C	3.558907000	-0.090772000	3.173661000
	C	-2.320834000	0.671641000	2.126131000
	O	-2.995784000	0.709669000	1.080134000
	O	-1.045324000	0.599871000	2.162948000
	C	-3.006549000	0.747228000	3.476931000
	H	4.363516000	-0.823580000	3.027638000
	H	4.019519000	0.878292000	3.427391000
	H	2.906700000	-0.392869000	4.002513000
	H	-3.303425000	1.794039000	3.653343000
	H	-2.338176000	0.429670000	4.286714000
	H	-3.926930000	0.145332000	3.469539000
	C	0.711757000	-2.108754000	-0.388844000
	O	0.618146000	-2.231639000	-1.605882000
	C	1.835589000	-2.730060000	0.373618000
	C	2.983883000	-3.099692000	-0.344501000
	C	1.799531000	-2.915666000	1.766542000
	C	4.085992000	-3.631811000	0.318442000
	H	3.005737000	-2.926939000	-1.420392000
	C	2.897629000	-3.468149000	2.424848000

	H	0.925766000	-2.617922000	2.345574000
	C	4.042388000	-3.821076000	1.703731000
	H	4.989847000	-3.872935000	-0.242751000
	H	2.865056000	-3.611726000	3.507121000
	H	4.907790000	-4.237244000	2.225281000
	C	-0.201936000	-1.253594000	0.406217000
	H	-0.634169000	-1.683881000	1.320185000
	S	-2.237956000	-1.780516000	-0.811074000
	O	-2.782823000	-0.772318000	-1.782818000
	C	-3.525878000	-2.269247000	0.368316000
	H	-4.328634000	-2.772954000	-0.183299000
	H	-3.066631000	-2.929905000	1.117261000
	H	-3.915588000	-1.352318000	0.821040000
	C	-2.083011000	-3.348896000	-1.711987000
	H	-1.768804000	-4.138151000	-1.014826000
	H	-3.067160000	-3.562798000	-2.151194000
	H	-1.314268000	-3.190963000	-2.474769000
	C	2.265491000	0.264594000	-2.307952000
	H	1.790357000	-0.607739000	-2.772170000
	H	2.702114000	0.893355000	-3.100668000
	H	3.087512000	-0.074252000	-1.667535000
	C	-1.238050000	4.103243000	1.944750000
	H	-0.391502000	4.808584000	1.926979000
	H	-2.077750000	4.621013000	2.433237000
	H	-0.953334000	3.238866000	2.562429000
	C	-1.939757000	4.869971000	-0.375480000
	H	-2.275188000	4.548800000	-1.373530000
	H	-2.730592000	5.496965000	0.064846000
	H	-1.040692000	5.494390000	-0.504271000
	C	5.929055000	1.247473000	-1.647633000
	C	6.290707000	0.082269000	-0.734723000
	H	7.226453000	-0.338506000	-1.140701000
	H	6.526191000	0.526831000	0.252072000
	F	4.867074000	1.947347000	-1.186704000
	F	5.623319000	0.847422000	-2.889960000
	F	6.959020000	2.109916000	-1.734124000
	O	5.322621000	-0.906882000	-0.683620000
	H	4.617237000	-0.629936000	-0.048061000
	C	-5.727270000	0.425813000	-0.661352000
	C	-6.773241000	-0.566619000	-1.124609000
	H	-4.799038000	0.184604000	-1.209984000
	H	-6.078906000	1.421373000	-1.001464000
	F	-6.402651000	-1.846710000	-0.890122000
	F	-7.956874000	-0.386265000	-0.524826000

	F	-6.965720000	-0.451043000	-2.452144000
	O	-5.582484000	0.343719000	0.723883000
	H	-4.655115000	0.601720000	0.941604000
INT-2CC	C	0.617564000	-0.166588000	-1.813288000
	C	-0.586739000	-0.897787000	-1.603826000
	C	-0.553482000	-1.847053000	-0.554609000
	C	0.660294000	-2.229228000	0.104108000
	C	1.844222000	-1.526752000	-0.125850000
	C	1.779894000	-0.423320000	-1.046848000
	H	0.616307000	0.659858000	-2.523423000
	H	-1.478456000	-2.354195000	-0.283336000
	H	0.620198000	-3.010341000	0.863097000
	H	2.661326000	0.197764000	-1.179216000
	C	3.141797000	-1.824842000	0.591506000
	H	3.743564000	-0.906584000	0.556956000
	Ru	0.130581000	0.158220000	0.386164000
	C	-2.346081000	-0.365772000	1.832738000
	O	-1.064170000	-0.294411000	1.978213000
	O	-2.940425000	-0.099138000	0.784218000
	C	-3.098469000	-0.827799000	3.064144000
	C	2.380764000	1.493131000	1.789953000
	O	2.970386000	1.655545000	0.710090000
	O	1.210802000	0.973697000	1.923898000
	C	3.048204000	1.902025000	3.089514000
	H	-3.416611000	-1.868893000	2.898192000
	H	-2.474621000	-0.779077000	3.964840000
	H	-4.004318000	-0.216959000	3.187353000
	H	4.035291000	1.417920000	3.145018000
	H	2.440736000	1.635273000	3.962478000
	H	3.222431000	2.989245000	3.073230000
	C	-1.234889000	2.428096000	-1.043266000
	O	-0.831741000	2.410230000	-2.199189000
	C	-2.569620000	2.987520000	-0.683883000
	C	-3.384476000	3.481476000	-1.715227000
	C	-3.033496000	3.014161000	0.641444000
	C	-4.646672000	3.993691000	-1.425611000
	H	-3.003909000	3.447304000	-2.737391000
	C	-4.295616000	3.531522000	0.929644000
	H	-2.414520000	2.618628000	1.447267000
	C	-5.103214000	4.018886000	-0.102486000
	H	-5.281026000	4.372301000	-2.230291000
	H	-4.654385000	3.548888000	1.961122000
	H	-6.094618000	4.418493000	0.124541000
	C	-0.412560000	1.895225000	0.077464000

	H	-0.122889000	2.651145000	0.829007000
	C	-1.817931000	-0.674452000	-2.427433000
	H	-1.818461000	0.332669000	-2.863684000
	H	-1.838014000	-1.403712000	-3.254755000
	H	-2.732371000	-0.814688000	-1.837488000
	C	2.941193000	-2.195187000	2.064208000
	H	2.449301000	-3.174575000	2.181824000
	H	3.918534000	-2.257814000	2.565778000
	H	2.331730000	-1.439248000	2.581967000
	C	3.913125000	-2.910192000	-0.178970000
	H	4.089705000	-2.609668000	-1.221715000
	H	4.894649000	-3.074995000	0.289251000
	H	3.359804000	-3.863766000	-0.178185000
	C	6.249178000	1.172016000	-0.224827000
	C	6.158007000	0.108060000	-1.309832000
	H	5.984720000	2.133200000	-0.704795000
	F	6.527788000	-1.102944000	-0.865854000
	F	6.947290000	0.422566000	-2.350421000
	O	5.474805000	0.874654000	0.886078000
	H	4.569778000	1.264978000	0.773648000
	H	7.314684000	1.224554000	0.059473000
	F	4.896736000	-0.019232000	-1.788254000
	C	-5.430585000	-2.082332000	-0.353436000
	C	-4.410108000	-3.212791000	-0.332531000
	H	-6.216943000	-2.398161000	-1.058875000
	H	-5.884965000	-2.061734000	0.658313000
	F	-5.008610000	-4.390602000	-0.094479000
	F	-3.734780000	-3.317995000	-1.487590000
	F	-3.477792000	-3.042712000	0.641543000
	O	-4.914476000	-0.868208000	-0.767719000
	H	-4.277794000	-0.524214000	-0.094559000
TS-3CC	C	2.643654000	2.869692000	-1.102645000
	C	3.021882000	1.953463000	-0.099796000
	C	2.140301000	1.790126000	0.998689000
	C	0.954119000	2.555771000	1.095691000
	C	0.599803000	3.469917000	0.103818000
	C	1.469099000	3.602839000	-0.999299000
	H	3.285778000	3.011719000	-1.972312000
	H	2.450122000	1.172999000	1.843172000
	H	0.303170000	2.418686000	1.959139000
	H	1.203305000	4.299207000	-1.798931000
	C	-0.657528000	4.288344000	0.201018000
	H	-1.211569000	4.270804000	-0.749866000
	Ru	0.910552000	-0.051669000	-0.359114000

	C	-0.903783000	-1.249812000	1.816730000
	O	-0.607403000	-0.068247000	1.442003000
	O	-0.274440000	-2.264546000	1.415009000
	C	-2.019179000	-1.426095000	2.819262000
	C	-1.159726000	0.057082000	-1.881829000
	O	-0.452864000	1.092166000	-1.755106000
	O	-0.758281000	-0.982936000	-1.231863000
	C	-2.403791000	-0.007515000	-2.706988000
	H	-2.599224000	-2.329547000	2.594767000
	H	-1.568825000	-1.555661000	3.816977000
	H	-2.672239000	-0.544510000	2.837882000
	H	-3.197042000	0.572244000	-2.210598000
	H	-2.732813000	-1.047612000	-2.822508000
	H	-2.216928000	0.456124000	-3.686111000
	C	3.016552000	-1.687065000	-1.494241000
	O	3.745704000	-2.091587000	-2.383222000
	C	3.216497000	-1.947513000	-0.043487000
	C	4.435844000	-2.442521000	0.427096000
	C	2.211610000	-1.482772000	0.840125000
	C	4.694214000	-2.453067000	1.798045000
	H	5.179753000	-2.771931000	-0.301862000
	C	2.507462000	-1.484988000	2.215942000
	C	3.734074000	-1.957048000	2.689508000
	H	5.647581000	-2.829977000	2.175512000
	H	1.751766000	-1.145566000	2.928082000
	H	3.939118000	-1.951423000	3.762837000
	C	1.875719000	-0.754537000	-1.749401000
	H	1.574093000	-0.683023000	-2.810646000
	C	4.390525000	1.297980000	-0.076252000
	H	4.268138000	0.312178000	0.394221000
	H	0.933752000	-1.782933000	0.820946000
	C	5.010425000	1.093705000	-1.460668000
	H	5.909348000	0.464076000	-1.382683000
	H	4.319400000	0.599761000	-2.157893000
	H	5.320145000	2.050724000	-1.910196000
	C	5.332199000	2.114055000	0.829274000
	H	4.925159000	2.214819000	1.846765000
	H	6.315889000	1.623771000	0.901370000
	H	5.484129000	3.127581000	0.424243000
	H	-0.420094000	5.344108000	0.416273000
	H	-1.320132000	3.913497000	0.991097000
	C	-4.222281000	2.555495000	0.342753000
	C	-3.008099000	1.670076000	0.503842000
	H	-3.354142000	0.633878000	0.341343000

	H	-2.316273000	1.931283000	-0.316142000
	O	-2.438287000	1.855596000	1.764676000
	H	-1.698120000	1.209146000	1.805333000
	F	-3.925271000	3.860838000	0.455039000
	F	-5.182696000	2.281034000	1.232372000
	F	-4.743493000	2.368014000	-0.892908000
	C	-2.474216000	-3.824308000	-0.602555000
	C	-3.683819000	-2.986629000	-0.220134000
	H	-1.787330000	-3.809594000	0.262406000
	H	-2.839928000	-4.854635000	-0.741023000
	F	-4.640791000	-2.999429000	-1.154154000
	F	-3.345887000	-1.684156000	-0.027428000
	F	-4.224354000	-3.424610000	0.933147000
	O	-1.881255000	-3.387040000	-1.784354000
	H	-1.372580000	-2.577277000	-1.579361000
INT-3C'	Ru	-0.145069000	1.049941000	1.235477000
	C	0.526620000	-1.463948000	1.018594000
	O	0.860471000	-0.978023000	2.136886000
	O	0.029927000	-0.670802000	0.148804000
	C	0.654562000	-2.917866000	0.684256000
	H	-0.332236000	-3.387768000	0.816517000
	H	0.940175000	-3.042703000	-0.369062000
	H	1.374427000	-3.404435000	1.354486000
	C	-2.432603000	1.652816000	-0.456894000
	C	-2.979501000	0.844006000	0.634308000
	C	-4.305968000	0.380937000	0.659545000
	C	-2.023663000	0.500282000	1.627354000
	C	-4.716773000	-0.427041000	1.713442000
	H	-4.990965000	0.658205000	-0.146146000
	C	-2.472323000	-0.330776000	2.676495000
	C	-3.795335000	-0.773875000	2.718811000
	H	-5.742400000	-0.800111000	1.758691000
	H	-1.772174000	-0.650076000	3.453764000
	H	-4.121723000	-1.417619000	3.541287000
	S	-0.156086000	2.983397000	-1.353467000
	O	0.920247000	3.886215000	-0.901039000
	C	0.469872000	1.552338000	-2.225489000
	H	1.177801000	1.069834000	-1.541332000
	H	-0.358093000	0.866957000	-2.462930000
	H	0.976411000	1.929349000	-3.123372000
	C	-1.139379000	3.857466000	-2.589173000
	H	-1.557073000	4.727155000	-2.064626000
	H	-0.442538000	4.181671000	-3.373805000
	H	-1.933744000	3.186087000	-2.934833000

	C	3.060708000	1.239993000	1.206724000
	O	1.983367000	1.646423000	0.795980000
	O	3.172153000	0.214798000	2.049212000
	H	2.272672000	-0.216727000	2.201477000
	C	4.369644000	1.847624000	0.805347000
	H	4.891872000	2.221969000	1.699829000
	H	5.008734000	1.072196000	0.356011000
	H	4.191785000	2.666900000	0.100107000
	C	-1.152848000	2.354173000	-0.001174000
	O	-2.878831000	1.708747000	-1.600738000
	H	-1.380501000	3.278073000	0.569922000
	C	3.847320000	-1.714514000	-1.102229000
	C	4.517049000	-2.331942000	0.117614000
	H	3.736339000	-2.900370000	0.656247000
	H	5.251801000	-3.058214000	-0.265060000
	F	4.713808000	-1.070592000	-1.890139000
	F	2.898446000	-0.811686000	-0.742048000
	F	3.234050000	-2.658889000	-1.833228000
	O	5.176018000	-1.396392000	0.909264000
	H	4.524122000	-0.935706000	1.468485000
	C	-2.867722000	-2.658126000	-1.192023000
	C	-2.556911000	-1.495607000	-2.117813000
	H	-2.910182000	-1.782654000	-3.120576000
	H	-3.158034000	-0.634233000	-1.780963000
	F	-2.258548000	-3.795431000	-1.571594000
	F	-2.460086000	-2.407852000	0.072539000
	F	-4.188477000	-2.892308000	-1.151258000
	O	-1.189127000	-1.220320000	-2.192114000
	H	-0.829107000	-1.049517000	-1.294297000
TS-4CC	Ru	0.738586000	-0.220685000	0.122932000
	C	0.149911000	1.698055000	1.857426000
	O	-0.772434000	1.037428000	1.242411000
	O	1.343644000	1.444752000	1.573562000
	C	-0.241766000	2.748110000	2.851034000
	H	0.642541000	3.187151000	3.328004000
	H	-0.822667000	3.523375000	2.324938000
	H	-0.902270000	2.303071000	3.610628000
	C	2.597449000	-2.391436000	-0.082129000
	O	2.781797000	-3.354248000	-0.815623000
	C	2.189042000	-2.464256000	1.358749000
	C	3.000814000	-3.013026000	2.345028000
	C	0.999152000	-1.755707000	1.685011000
	C	2.657501000	-2.839087000	3.692764000
	H	3.918532000	-3.536208000	2.065065000

	C	0.675072000	-1.588586000	3.044950000
	C	1.511567000	-2.110595000	4.032921000
	H	3.292079000	-3.259597000	4.475887000
	H	-0.255210000	-1.089991000	3.316991000
	H	1.257200000	-1.962783000	5.085357000
	C	2.624211000	-0.958211000	-0.486871000
	H	3.334403000	-0.358615000	0.108314000
	S	3.115605000	-0.650328000	-2.166195000
	O	3.381511000	0.774341000	-2.449460000
	C	4.578064000	-1.618926000	-2.574501000
	H	5.377145000	-1.213758000	-1.942687000
	H	4.362806000	-2.670197000	-2.345969000
	H	4.793545000	-1.438998000	-3.636183000
	C	1.863502000	-1.313718000	-3.259281000
	H	0.919749000	-0.816991000	-3.004958000
	H	2.190869000	-1.069607000	-4.278431000
	H	1.809165000	-2.395915000	-3.087825000
	C	-1.758185000	-1.636411000	1.064650000
	C	-0.380989000	-2.164170000	0.645860000
	H	-0.306489000	-3.232479000	0.888704000
	C	-1.536021000	-1.220813000	-1.218972000
	C	-0.256344000	-1.803037000	-0.784239000
	H	0.232434000	-2.491901000	-1.476001000
	O	-1.854424000	-0.801710000	-2.321108000
	O	-2.268627000	-1.659892000	2.162060000
	N	-2.358583000	-1.131327000	-0.080912000
	C	-3.656928000	-0.474670000	-0.077701000
	H	-3.804099000	-0.063869000	0.928806000
	H	-3.605068000	0.348255000	-0.800857000
	C	-4.784698000	-1.418773000	-0.426536000
	C	-5.440536000	-2.139974000	0.580309000
	C	-5.156237000	-1.614060000	-1.763623000
	C	-6.461689000	-3.036231000	0.255940000
	H	-5.135810000	-2.000451000	1.620442000
	C	-6.177454000	-2.510049000	-2.088007000
	H	-4.626075000	-1.067654000	-2.546927000
	C	-6.833635000	-3.221323000	-1.078895000
	H	-6.969914000	-3.591737000	1.048079000
	H	-6.463161000	-2.653781000	-3.133073000
	H	-7.634448000	-3.920309000	-1.332776000
	C	-0.342826000	1.857102000	-1.823204000
	O	0.609349000	1.137908000	-1.509622000
	O	-1.327393000	2.143594000	-0.995702000
	H	-1.184531000	1.675626000	-0.106465000

	C	-0.478552000	2.423300000	-3.198425000
	H	-1.187270000	1.776337000	-3.742091000
	H	-0.896350000	3.438929000	-3.170710000
	H	0.493633000	2.407576000	-3.704986000
	C	4.399372000	2.070749000	0.483060000
	C	5.779742000	1.678755000	0.000321000
	H	4.476711000	3.114613000	0.844438000
	H	3.736807000	2.055079000	-0.400965000
	F	6.169758000	2.469591000	-1.010038000
	F	6.703020000	1.758421000	0.964950000
	F	5.802873000	0.400620000	-0.456614000
	O	4.016955000	1.170860000	1.480813000
	H	3.081891000	1.343234000	1.706088000
	C	-3.507677000	3.118925000	1.301585000
	C	-4.755464000	3.000717000	0.441132000
	H	-3.821672000	3.491225000	2.288122000
	H	-3.093100000	2.104099000	1.436214000
	F	-4.433359000	2.672696000	-0.829072000
	F	-5.566145000	2.039822000	0.917138000
	F	-5.452082000	4.141741000	0.391257000
	O	-2.580482000	4.019430000	0.763562000
	H	-2.242896000	3.639301000	-0.064574000
INT-4CC	Ru	0.996687000	-0.694771000	0.262503000
	C	1.988240000	1.276864000	1.710991000
	O	0.752837000	1.194315000	1.400175000
	O	2.780972000	0.395667000	1.270110000
	C	2.461570000	2.376527000	2.614036000
	H	2.476450000	1.986717000	3.645038000
	H	3.480744000	2.685073000	2.347423000
	H	1.771883000	3.229196000	2.575320000
	C	1.872677000	-3.067973000	0.808738000
	O	2.887435000	-3.719960000	1.050945000
	C	1.119108000	-2.336242000	1.867326000
	C	1.846326000	-2.114721000	3.086291000
	C	-0.232089000	-1.845400000	1.755643000
	C	1.317106000	-1.372252000	4.107852000
	H	2.844874000	-2.547145000	3.150827000
	C	-0.739066000	-1.082942000	2.860810000
	C	0.009615000	-0.831339000	3.981638000
	H	1.895362000	-1.198970000	5.018311000
	H	-1.749828000	-0.681388000	2.801946000
	H	-0.413034000	-0.229631000	4.789108000
	C	1.512110000	-2.557467000	-0.557616000
	H	0.706223000	-3.062174000	-1.115213000

	S	2.872290000	-2.646799000	-1.693266000
	O	2.615114000	-1.962720000	-2.973875000
	C	4.357200000	-2.042757000	-0.901261000
	H	4.178116000	-1.022325000	-0.544572000
	H	4.597963000	-2.710949000	-0.067725000
	H	5.121015000	-2.041696000	-1.689791000
	C	3.241975000	-4.385316000	-1.989555000
	H	2.362912000	-4.795014000	-2.504522000
	H	4.126945000	-4.438225000	-2.637784000
	H	3.397838000	-4.855111000	-1.009268000
	C	-2.656649000	-1.993557000	0.993929000
	C	-1.204518000	-2.294515000	0.644012000
	H	-1.094914000	-3.367773000	0.434126000
	C	-1.996949000	-0.376789000	-0.538799000
	C	-0.858355000	-1.334803000	-0.487708000
	H	-0.745010000	-1.760839000	-1.496333000
	O	-2.109704000	0.605617000	-1.263469000
	O	-3.400421000	-2.610003000	1.720101000
	N	-2.990204000	-0.807177000	0.337640000
	C	-4.312885000	-0.194642000	0.464097000
	H	-4.705880000	-0.530654000	1.433436000
	H	-4.191302000	0.892452000	0.485522000
	C	-5.243678000	-0.598947000	-0.658960000
	C	-5.719884000	-1.916801000	-0.740764000
	C	-5.623678000	0.330037000	-1.636068000
	C	-6.556770000	-2.300262000	-1.790042000
	H	-5.431409000	-2.637698000	0.028262000
	C	-6.464862000	-0.055461000	-2.684327000
	H	-5.258404000	1.357110000	-1.570081000
	C	-6.930469000	-1.369895000	-2.765765000
	H	-6.924875000	-3.327982000	-1.843996000
	H	-6.756204000	0.676799000	-3.441473000
	H	-7.587432000	-1.669949000	-3.586024000
	C	0.609741000	1.575493000	-1.722546000
	O	1.159236000	0.489571000	-1.477061000
	O	0.139813000	2.380464000	-0.810673000
	H	0.267615000	1.991800000	0.107659000
	C	0.429496000	2.040308000	-3.129920000
	H	-0.607589000	1.792957000	-3.410341000
	H	0.563880000	3.127064000	-3.199816000
	H	1.119728000	1.510237000	-3.795605000
	C	3.891558000	2.923811000	-1.369928000
	C	4.363658000	1.481025000	-1.443871000
	H	3.503896000	0.880665000	-1.792069000

	H	5.139515000	1.445975000	-2.225495000
	C	-2.583059000	3.175023000	1.468828000
	C	-2.762606000	3.676291000	0.041734000
	H	-3.261201000	4.656176000	0.118576000
	H	-1.749476000	3.834930000	-0.366228000
	F	4.886143000	3.785324000	-1.140938000
	F	3.292247000	3.279301000	-2.524716000
	F	2.980708000	3.096473000	-0.383141000
	F	-2.037668000	1.937953000	1.500510000
	F	-1.765258000	3.990547000	2.158006000
	F	-3.745761000	3.099878000	2.134977000
	O	4.912055000	1.032881000	-0.243173000
	H	4.188483000	0.873910000	0.405571000
	O	-3.541832000	2.827854000	-0.737443000
	H	-3.010355000	2.039508000	-0.995572000
TS-5CC	Ru	0.827476000	-0.042965000	0.402259000
	C	1.668661000	-0.773692000	-2.048574000
	O	0.453403000	-0.420739000	-1.910779000
	O	2.380930000	-0.932636000	-1.013638000
	C	2.255428000	-0.942341000	-3.419816000
	H	3.088533000	-1.656119000	-3.410368000
	H	1.480671000	-1.247958000	-4.134672000
	H	2.652635000	0.035495000	-3.735603000
	C	2.268857000	1.438169000	2.081647000
	O	3.132833000	1.837737000	2.835489000
	C	2.112445000	1.909951000	0.652520000
	C	3.322259000	2.060357000	-0.088632000
	C	0.857023000	2.251432000	0.046063000
	C	3.303723000	2.443878000	-1.409235000
	H	4.263240000	1.831763000	0.411187000
	C	0.892160000	2.670516000	-1.318484000
	C	2.069865000	2.742249000	-2.030402000
	H	4.237075000	2.522903000	-1.967138000
	H	-0.034752000	2.970926000	-1.804816000
	H	2.048602000	3.063023000	-3.074496000
	C	1.395708000	0.227907000	2.219407000
	H	0.811051000	0.075338000	3.141318000
	S	2.793311000	-1.282741000	3.117525000
	O	2.322372000	-1.755885000	4.451276000
	C	2.850650000	-2.671874000	1.965637000
	H	1.807710000	-2.929102000	1.747354000
	H	3.379423000	-2.354980000	1.058683000
	H	3.370001000	-3.489187000	2.484835000
	C	4.537790000	-0.807579000	3.196636000

	H	4.574587000	0.099877000	3.810007000
	H	5.073818000	-1.643944000	3.667461000
	H	4.878711000	-0.614140000	2.169845000
	C	-1.583523000	2.966980000	0.028817000
	C	-0.448563000	2.377352000	0.867189000
	H	-0.284932000	3.007807000	1.754208000
	C	-2.084631000	0.709178000	0.302988000
	C	-0.875146000	0.937718000	1.144188000
	H	-1.112648000	0.687107000	2.187044000
	O	-2.726287000	-0.318113000	0.155410000
	O	-1.738803000	4.113338000	-0.324558000
	N	-2.415568000	1.911165000	-0.327588000
	C	-3.586022000	2.073955000	-1.183367000
	H	-3.360069000	2.901859000	-1.869168000
	H	-3.693881000	1.146187000	-1.760359000
	C	-4.845854000	2.360578000	-0.395840000
	C	-5.108631000	3.659388000	0.065354000
	C	-5.740719000	1.329029000	-0.085264000
	C	-6.252214000	3.918944000	0.823447000
	H	-4.403804000	4.461183000	-0.167323000
	C	-6.885234000	1.589419000	0.672277000
	H	-5.544722000	0.314496000	-0.431731000
	C	-7.143130000	2.884600000	1.128481000
	H	-6.450354000	4.933943000	1.176633000
	H	-7.573113000	0.773032000	0.904696000
	H	-8.038368000	3.089467000	1.720762000
	C	-0.913176000	-2.523619000	0.163746000
	O	-0.082472000	-1.895731000	0.833421000
	O	-1.094614000	-2.328685000	-1.122700000
	H	-0.541240000	-1.555077000	-1.469510000
	C	-1.799799000	-3.547184000	0.788106000
	H	-2.684390000	-3.003975000	1.157075000
	H	-2.150117000	-4.284821000	0.056863000
	H	-1.296155000	-4.018235000	1.641069000
	C	6.176483000	-0.032584000	-1.879265000
	C	5.897424000	-1.143202000	-0.877672000
	H	5.762778000	-2.073016000	-1.462922000
	H	6.806156000	-1.259498000	-0.266568000
	F	7.261909000	-0.321033000	-2.611501000
	F	6.381422000	1.150651000	-1.280951000
	F	5.140785000	0.128408000	-2.732921000
	O	4.824796000	-0.852923000	-0.041779000
	H	3.975262000	-0.852124000	-0.550134000
	C	-5.510767000	-2.928745000	-0.734755000

	C	-4.480427000	-2.370906000	-1.698236000
	H	-4.008653000	-1.511682000	-1.195216000
	H	-5.045867000	-2.000070000	-2.574286000
	F	-6.174734000	-3.974678000	-1.241847000
	F	-4.957936000	-3.331457000	0.425953000
	F	-6.421667000	-1.976434000	-0.434784000
	O	-3.557605000	-3.359937000	-2.060793000
	H	-2.668395000	-3.014108000	-1.889485000

Table S4. Electronic energies (E in au) and Gibbs free energies (G in au) calculated at the B3LYP+D3BJ/def2SVP level, single-point energies (E^{sp} in au) calculated at the B3LYP+D3BJ/def2TZVPP level, and imaginary frequencies (IF in cm^{-1}) of all the transition states, in the C-H activation process

Names	E	G	E^{sp}	IF
CAT(sol)	-1845.860884	-1845.494456	-1847.944811	--
1	-936.374969	-936.2199442	-937.1694523	--
TS-1C(sol)	-2782.255368	-2781.704591	-2785.117012	-37.0 i
INT-1C(sol)	-2782.276276	-2781.724545	-2785.135635	--
TS-2C(sol)	-2782.244165	-2781.690788	-2785.106745	-20.8 i
INT-2C(sol)	-2782.255156	-2781.704003	-2785.111057	--
TS-3C(sol)	-2782.246058	-2781.696989	-2785.096325	-931.9 i
HOAc(sol)	-681.38326	-681.3026773	-682.207193	--
INT-3C(sol)	-2100.859421	-2100.4150967	-2102.907671	--
CAT(nosol)	-940.931113	-940.6674368	-941.9338353	--
TS-1C(nosol)	-1877.323061	-1876.874529	-1879.106164	-15.0 i
INT-1C(nosol)	-1877.341508	-1876.891735	-1879.121968	--
TS-2C(nosol)	-1877.308146	-1876.859477	-1879.082901	-49.7 i
INT-2C(nosol)	-1877.311286	-1876.863648	-1879.086389	--
TS-3C(nosol)	-1877.303248	-1876.858895	-1879.075519	-730.6 i
HOAc(nosol)	-228.924281	-228.8920518	-229.205541	--
INT-3C(nosol)	-1648.388477	-1647.994882	-1649.894783	--
TS-1O(sol)	-2782.243337	-2781.694188	-2785.113814	-9.8 i
INT-1O(sol)	-2782.267004	-2781.713195	-2785.13132	--
TS-2O(sol)	-2782.232129	-2781.681995	-2785.102061	-54.2 i
INT-2O(sol)	-2782.246473	-2781.695642	-2785.11079	--
TS-3O(sol)	-2782.228537	-2781.681481	-2785.091935	-852.3 i
INT-3O(sol)	-2100.849087	-2100.40476	-2102.902823	--
TS-1O(nosol)	-1877.316548	-1876.869847	-1879.102777	-36.2 i
INT-1O(nosol)	-1877.329721	-1876.880931	-1879.112987	--
TS-2O(nosol)	-1877.284748	-1876.837226	-1879.080625	-62.5 i
INT-2O(nosol)	-1877.296168	-1876.848653	-1879.085244	--

TS-3O(nosol)	-1877.288613	-1876.844739	-1879.072497	-491.3 <i>i</i>
INT-3O(nosol)	-1648.376361	-1647.985206	-1649.888656	--

Table S5. Electronic energies (E in au) and Gibbs free energies (G in au) calculated at the B3LYP+D3BJ/def2SVP level, single-point energies (E^{sp} in au) calculated at the B3LYP+D3BJ/def2TZVPP level, and imaginary frequencies (IF in cm^{-1}) of all the transition states, in the annulation process

Names	E	G	E^{sp}	IF
<i>p</i> -cymene	-389.272904	-389.1121522	-389.7030918	--
2	-629.390372	-629.2535574	-630.098544	--
TS-4C(sol)	-2100.842588	-2100.402710	-2102.884143	-128.0 <i>i</i>
INT-4C(sol)	-1547.846643	-1547.481482	-1549.544781	--
INT-4C'(sol)	-1839.940384	-1839.670718	-1842.035218	--
TS-5C(sol)	-2469.369954	-2468.931323	-2472.145677	-321.0 <i>i</i>
INT-5C(sol)	-2469.387881	-2468.946167	-2472.163327	--
TS-6C(sol)	-2469.365826	-2468.929005	-2472.14297	-660.5 <i>i</i>
INT-6C(sol)	-2469.388277	-2468.944717	-2472.164798	--
TS-7C(sol)	-2469.375948	-2468.930319	-2472.14967	-301.0 <i>i</i>
INT-7C(sol)	-2469.430700	-2468.986145	-2472.203586	--
TS-4C(nosol)	-1648.374857	-1647.986912	-1649.875147	-145.5 <i>i</i>
INT-4C(nosol)	-1095.377349	-1095.064609	-1096.533546	--
INT-4C'(nosol)	-935.026202	-934.8582477	-936.0304002	--
TS-5C(nosol)	-1564.456446	-1564.119381	-1566.142684	-315.1 <i>i</i>
INT-5C(nosol)	-1564.46805	-1564.128155	-1566.158838	--
DMSO	-552.969052	-552.9217009	-553.3336217	--
TS-6C(nosol)	-1564.441662	-1564.107699	-1566.135927	-772.4 <i>i</i>
INT-6C(nosol)	-1564.466739	-1564.126604	-1566.157354	--
TS-7C(nosol)	-1564.452039	-1564.110700	-1566.142124	-321.5 <i>i</i>
INT-7C(nosol)	-1564.509353	-1564.167206	-1566.196857	--
3	-1012.889456	-1012.637732	-1014.016559	--

Table S6. Electronic energies (E in au) and Gibbs free energies (G in au) calculated at the B3LYP+D3BJ/def2SVP level, single-point energies (E^{sp} in au) calculated at the B3LYP+D3BJ/def2TZVPP level, and imaginary frequencies (IF in cm^{-1}) of all the transition states, in the reaction pathway featuring Ru-carbene formation prior to C-H activation or subsequent to migratory insertion

Names	E	G	E^{sp}	IF
TS-2CC	-2782.254932	-2781.706274	-2785.110744	-87.6 <i>i</i>

INT-2CC	-2229.258964	-2228.786233	-2231.766484	--
TS-3CC	-2229.229228	-2228.755091	-2231.731201	-901.7 <i>i</i>
INT-3C'	-2392.945678	-2392.597232	-2395.38359	--
TS-4CC	-3022.363604	-3021.846162	-3025.489221	-285.4 <i>i</i>
INT-4CC	-3022.40687	-3021.887744	-3025.529921	--
TS-5CC	-3022.387037	-3021.87021	-3025.508598	-131.5 <i>i</i>

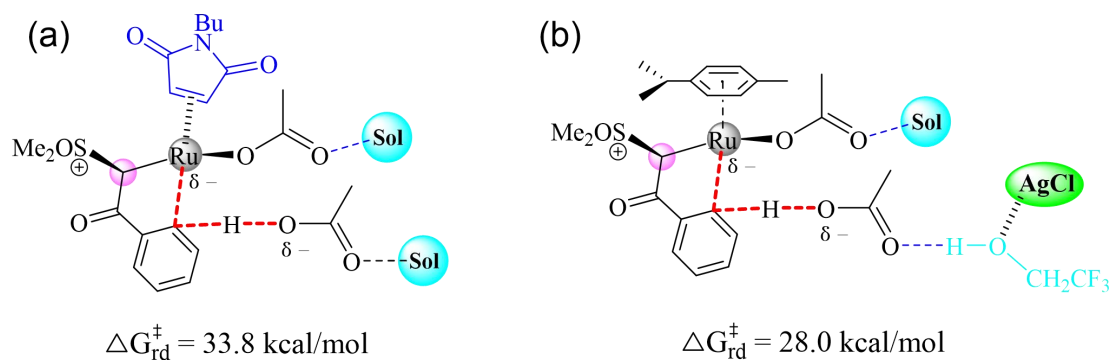


Figure S1. Two additional C-H activation transition states and their rate-determining free-energy barriers (a) for the case in which the *p*-cymene ligand is replaced by reactant **2**; (b) for the case in which AgCl mediates the reaction.