

Density Functional Theory Study on Mechanism and Selectivity of Nickel-Catalyzed Hydroboration of Vinylarenes

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Table S1. Cartesian coordinates of the optimized stationary points in the main reaction pathway, calculated at the B3LYP-D3(BJ)/def2SVP level.

Names	Cartesian Coordinates			
NiL(cod)	28	-0.096873000	-0.732739000	0.590338000
	6	-0.183517000	-1.093094000	2.606500000
	1	0.364209000	-0.273234000	3.087556000
	6	-1.479419000	-0.808299000	2.161751000
	1	-1.883932000	0.191125000	2.360012000
	6	0.319030000	-2.494281000	2.931732000
	1	0.982008000	-2.454754000	3.812284000
	1	-0.527809000	-3.130397000	3.231946000
	6	-2.514427000	-1.860531000	1.823037000
	1	-2.982531000	-2.273425000	2.740239000
	1	-3.326905000	-1.365805000	1.273153000
	6	1.075194000	-3.144188000	1.749659000
	1	2.142523000	-2.869735000	1.806213000
	1	1.055642000	-4.249008000	1.852370000
	6	-1.952336000	-3.014740000	0.959434000
	1	-2.766227000	-3.420779000	0.337419000
	1	-1.629256000	-3.849239000	1.601952000
	6	-0.798081000	-2.580614000	0.063634000
	1	-1.024087000	-2.575101000	-1.009384000
	6	0.557974000	-2.700816000	0.397630000
	1	1.272424000	-2.796914000	-0.424336000
	6	1.377660000	4.829271000	0.147984000
	6	0.748209000	3.829438000	-0.831381000
	6	0.378289000	2.473381000	-0.189119000
	6	-0.449866000	2.712268000	1.111787000
	6	0.260403000	3.651486000	2.082008000
	6	0.546169000	5.003064000	1.422368000
	6	1.590505000	1.630651000	0.158491000
	6	-0.473251000	1.625939000	-1.111356000
	8	-0.950373000	2.194170000	-2.245087000
	7	-0.835222000	0.416896000	-0.862340000

6	-1.711038000	1.178554000	-2.928047000
7	1.540434000	0.404331000	0.541023000
8	2.822376000	2.188179000	0.056933000
6	2.923910000	-0.073135000	0.697068000
6	-1.788380000	0.006468000	-1.909302000
6	-3.165508000	-0.222468000	-1.326914000
6	3.741409000	1.245146000	0.641675000
6	3.301880000	-1.047639000	-0.399714000
6	-3.869287000	-1.398912000	-1.600272000
6	-5.145838000	-1.604475000	-1.068599000
6	-5.730147000	-0.629864000	-0.257495000
6	4.204420000	-2.083016000	-0.136093000
6	4.590445000	-2.967179000	-1.148133000
6	4.075783000	-2.819433000	-2.437441000
6	-5.032397000	0.551298000	0.019272000
6	-3.758908000	0.751935000	-0.511995000
6	3.175737000	-1.782769000	-2.708644000
6	2.791304000	-0.903144000	-1.696569000
1	1.494636000	5.798179000	-0.364705000
1	2.388869000	4.490938000	0.416511000
1	-0.184123000	4.252682000	-1.233998000
1	1.412540000	3.665388000	-1.692887000
1	-1.415186000	3.153819000	0.810116000
1	-0.662554000	1.730285000	1.553749000
1	-0.356742000	3.779779000	2.985992000
1	1.206766000	3.190634000	2.417658000
1	-0.415954000	5.487789000	1.173760000
1	1.064184000	5.677150000	2.124128000
1	-1.173223000	0.904554000	-3.849010000
1	-2.693654000	1.594030000	-3.188496000
1	3.030958000	-0.567404000	1.672417000
1	-1.437516000	-0.929615000	-2.363683000
1	4.016555000	1.609916000	1.644712000
1	4.635939000	1.187088000	0.009047000
1	-3.405366000	-2.170899000	-2.219364000
1	-5.679700000	-2.533735000	-1.280894000
1	-6.724041000	-0.791774000	0.166097000
1	4.597676000	-2.210949000	0.876172000
1	5.286492000	-3.779096000	-0.924354000
1	4.368560000	-3.513664000	-3.228632000
1	-5.479890000	1.313260000	0.661769000
1	-3.208711000	1.664584000	-0.272958000
1	2.762685000	-1.667454000	-3.713751000
1	2.059163000	-0.120708000	-1.901577000

pre-com	28	-0.034232000	-0.303151000	-1.182689000
	6	1.686164000	-0.693261000	-2.034455000
	6	-4.579091000	2.535885000	0.857849000
	6	-3.223742000	2.170535000	1.475509000
	6	-2.238202000	1.546216000	0.464787000
	6	-2.134060000	2.441477000	-0.811217000
	6	-3.502691000	2.739611000	-1.416382000
	6	-4.428213000	3.404352000	-0.394058000
	6	-2.636846000	0.144846000	0.035597000
	6	-0.832921000	1.438141000	1.032047000
	8	-0.565086000	2.033092000	2.207963000
	7	0.142482000	0.861716000	0.431398000
	6	0.806976000	1.694124000	2.529967000
	7	-1.918901000	-0.597369000	-0.724886000
	8	-3.779619000	-0.392539000	0.510184000
	6	-2.542985000	-1.930164000	-0.799088000
	6	1.368871000	1.116759000	1.203198000
	6	2.316619000	2.056629000	0.480863000
	6	-3.912886000	-1.696387000	-0.103608000
	6	-1.660453000	-2.953665000	-0.115064000
	6	3.531926000	2.392701000	1.093567000
	6	4.440987000	3.236097000	0.455634000
	6	4.145996000	3.751536000	-0.811374000
	6	-1.303331000	-4.138281000	-0.765500000
	6	-0.503006000	-5.088619000	-0.124228000
	6	-0.055525000	-4.861471000	1.178569000
	6	2.938175000	3.417706000	-1.427243000
	6	2.026219000	2.575183000	-0.784320000
	6	-0.406020000	-3.677020000	1.835021000
	6	-1.201342000	-2.730212000	1.191290000
	1	-5.184504000	3.059280000	1.615555000
	1	-5.124648000	1.615097000	0.601231000
	1	-2.744647000	3.078807000	1.870472000
	1	-3.359026000	1.491610000	2.330251000
	1	-1.638038000	3.381559000	-0.517274000
	1	-1.470875000	1.927674000	-1.523335000
	1	-3.376074000	3.380398000	-2.303779000
	1	-3.957857000	1.799446000	-1.776857000
	1	-4.006096000	4.386841000	-0.114000000
	1	-5.416231000	3.603902000	-0.839884000
	1	0.786498000	0.950419000	3.341661000
	1	1.316507000	2.604027000	2.869956000
	1	-2.666364000	-2.210870000	-1.853671000
	1	1.891291000	0.162481000	1.369339000

	1	-4.750543000	-1.652725000	-0.816120000
	1	-4.135863000	-2.427256000	0.684242000
	1	3.781793000	1.966609000	2.069309000
	1	5.387990000	3.483126000	0.941636000
	1	4.859514000	4.406514000	-1.317103000
	1	-1.638708000	-4.310620000	-1.791159000
	1	-0.220120000	-6.003658000	-0.649399000
	1	0.577217000	-5.598738000	1.677758000
	1	2.704006000	3.807260000	-2.420981000
	1	1.104083000	2.272534000	-1.279101000
	1	-0.042658000	-3.484349000	2.846832000
	1	-1.450694000	-1.797379000	1.702177000
	6	0.586262000	-1.429157000	-2.611970000
	1	0.502414000	-2.508508000	-2.418232000
	6	2.587656000	-1.214011000	-0.995348000
	6	2.260671000	-2.336573000	-0.197844000
	6	3.788281000	-0.538524000	-0.686597000
	6	3.070992000	-2.733538000	0.863325000
	1	1.342700000	-2.887162000	-0.400512000
	6	4.598598000	-0.935338000	0.377953000
	1	4.071521000	0.331074000	-1.283906000
	6	4.245168000	-2.032333000	1.170227000
	1	2.777266000	-3.599873000	1.462552000
	1	5.513826000	-0.376376000	0.592221000
	1	4.877652000	-2.343734000	2.005308000
	1	0.293724000	-1.166699000	-3.638160000
	1	2.116550000	0.133204000	-2.615143000
TS1 ^{Ra}	28	0.233724000	0.196044000	0.706688000
	6	1.862856000	0.461949000	1.683618000
	6	0.766580000	1.136005000	2.417183000
	6	-3.998871000	-2.198878000	-2.343682000
	6	-2.530350000	-1.849982000	-2.617714000
	6	-1.752937000	-1.373366000	-1.367691000
	6	-1.978204000	-2.366309000	-0.170625000
	6	-3.457664000	-2.652666000	0.076092000
	6	-4.147082000	-3.183607000	-1.181406000
	6	-2.160486000	0.013722000	-0.910547000
	6	-0.256096000	-1.359817000	-1.617969000
	8	0.202457000	-2.060201000	-2.663311000
	7	0.634433000	-0.819423000	-0.859485000
	6	1.635149000	-1.861699000	-2.708694000
	7	-1.494083000	0.707115000	-0.069772000
	8	-3.287344000	0.556176000	-1.382204000
	6	-2.195237000	1.976528000	0.174347000

6	1.964078000	-1.242050000	-1.327436000
6	2.625561000	-2.217927000	-0.372564000
6	-3.490244000	1.803462000	-0.663756000
6	-1.315967000	3.148796000	-0.197849000
6	3.988362000	-2.501221000	-0.539130000
6	4.633079000	-3.412597000	0.298038000
6	3.920459000	-4.047765000	1.320535000
6	-1.029297000	4.146691000	0.739533000
6	-0.196230000	5.219174000	0.405809000
6	0.358039000	5.302054000	-0.873369000
6	2.563029000	-3.768081000	1.492619000
6	1.916970000	-2.859959000	0.648831000
6	0.077865000	4.307236000	-1.816435000
6	-0.751005000	3.237738000	-1.478317000
1	-4.432279000	-2.623052000	-3.264417000
1	-4.562069000	-1.282158000	-2.119617000
1	-2.014562000	-2.746792000	-2.989918000
1	-2.454270000	-1.091726000	-3.412578000
1	-1.444837000	-3.298985000	-0.422152000
1	-1.521868000	-1.923576000	0.727437000
1	-3.536328000	-3.380381000	0.900405000
1	-3.943424000	-1.730730000	0.435551000
1	-3.699879000	-4.155702000	-1.462130000
1	-5.214385000	-3.374959000	-0.983718000
1	1.852190000	-1.178710000	-3.544415000
1	2.112905000	-2.833070000	-2.884707000
1	-2.452931000	2.015744000	1.240239000
1	2.609471000	-0.358340000	-1.431424000
1	-4.362993000	1.665926000	-0.015710000
1	-3.653300000	2.597351000	-1.404601000
1	4.554849000	-1.986092000	-1.319834000
1	5.697052000	-3.619592000	0.160128000
1	4.424686000	-4.755013000	1.983242000
1	-1.454322000	4.074370000	1.743806000
1	0.026538000	5.987034000	1.150224000
1	1.014249000	6.135732000	-1.133799000
1	1.998758000	-4.252441000	2.292932000
1	0.864546000	-2.627293000	0.806882000
1	0.518616000	4.359750000	-2.814647000
1	-0.948072000	2.451296000	-2.211551000
8	-1.431010000	-0.497574000	2.516456000
6	-1.100979000	-1.446031000	3.464054000
1	-0.098051000	-1.263709000	3.918174000
1	-1.817899000	-1.489515000	4.314839000

	1	-1.053842000	-2.480450000	3.044997000
	1	-0.371972000	0.491541000	2.295152000
	1	0.683049000	2.225353000	2.306806000
	1	0.736786000	0.868981000	3.484916000
	1	2.297902000	-0.411404000	2.185449000
	6	2.829229000	1.190444000	0.846190000
	6	4.115065000	0.656218000	0.622869000
	6	2.499260000	2.390101000	0.176969000
	6	5.017481000	1.269431000	-0.248415000
	1	4.399819000	-0.261964000	1.140341000
	6	3.401487000	3.003830000	-0.689693000
	1	1.517779000	2.839524000	0.326073000
	6	4.665460000	2.445730000	-0.917218000
	1	6.005848000	0.826922000	-0.401274000
	1	3.108983000	3.927338000	-1.195332000
	1	5.369824000	2.928194000	-1.599211000
	6	-4.640224000	-0.006690000	3.004782000
	1	-5.628786000	0.447661000	2.814485000
	1	-4.817431000	-1.070505000	3.270977000
	1	-4.217476000	0.486764000	3.903902000
	8	-3.829727000	0.145382000	1.876291000
	1	-2.889425000	-0.149435000	2.129979000
INT1 ^{Ra}	28	0.001750000	0.267585000	0.898821000
	6	1.682910000	0.841611000	1.759282000
	6	1.310913000	2.029470000	2.661023000
	6	-3.817859000	-2.716596000	-2.156228000
	6	-2.404469000	-2.215713000	-2.479748000
	6	-1.695611000	-1.562366000	-1.272000000
	6	-1.767573000	-2.509913000	-0.024650000
	6	-3.192919000	-2.965479000	0.275400000
	6	-3.832051000	-3.642998000	-0.937871000
	6	-2.290108000	-0.227738000	-0.891491000
	6	-0.214198000	-1.328294000	-1.533760000
	8	0.307100000	-2.010463000	-2.562192000
	7	0.610766000	-0.639347000	-0.815123000
	6	1.687813000	-1.599741000	-2.668232000
	7	-1.735146000	0.532081000	-0.036154000
	8	-3.422199000	0.215678000	-1.453903000
	6	-2.506031000	1.777924000	0.084506000
	6	1.972400000	-0.978233000	-1.288799000
	6	2.686929000	-1.932732000	-0.345835000
	6	-3.766455000	1.446546000	-0.754363000
	6	-1.661725000	2.940383000	-0.390681000
	6	4.002437000	-2.311957000	-0.652408000

6	4.705784000	-3.182691000	0.178498000
6	4.102381000	-3.685549000	1.337005000
6	-1.270957000	3.940914000	0.505292000
6	-0.441746000	4.985771000	0.086532000
6	0.005230000	5.037349000	-1.235436000
6	2.794161000	-3.312508000	1.647915000
6	2.088719000	-2.443142000	0.809717000
6	-0.379325000	4.039251000	-2.137604000
6	-1.204658000	2.996788000	-1.715511000
1	-4.214409000	-3.240141000	-3.041487000
1	-4.481180000	-1.858867000	-1.972133000
1	-1.784426000	-3.065285000	-2.799069000
1	-2.427342000	-1.508043000	-3.322521000
1	-1.118946000	-3.376649000	-0.235570000
1	-1.344136000	-1.971585000	0.834632000
1	-3.166982000	-3.653609000	1.136118000
1	-3.780136000	-2.092388000	0.603513000
1	-3.276356000	-4.569535000	-1.174105000
1	-4.865648000	-3.947982000	-0.706948000
1	1.756897000	-0.862580000	-3.484045000
1	2.296738000	-2.480782000	-2.901708000
1	-2.772061000	1.908893000	1.139721000
1	2.566097000	-0.064528000	-1.394774000
1	-4.625369000	1.223926000	-0.108744000
1	-4.021382000	2.204185000	-1.506007000
1	4.490038000	-1.899574000	-1.540050000
1	5.731847000	-3.463155000	-0.071686000
1	4.653647000	-4.362456000	1.993956000
1	-1.603488000	3.886360000	1.544437000
1	-0.133856000	5.753659000	0.799696000
1	0.660722000	5.848011000	-1.561585000
1	2.314015000	-3.691879000	2.553022000
1	1.080852000	-2.129296000	1.076223000
1	-0.024970000	4.069322000	-3.170695000
1	-1.484394000	2.208858000	-2.420029000
8	-0.977051000	0.213229000	2.513004000
6	-0.527134000	-0.625085000	3.527545000
1	0.431060000	-0.290445000	3.973957000
1	-1.264817000	-0.655249000	4.355953000
1	-0.374895000	-1.680164000	3.201367000
1	0.880746000	2.857885000	2.076151000
1	2.207996000	2.433266000	3.168227000
1	0.569611000	1.753714000	3.419904000
1	2.120187000	0.031393000	2.364602000

	6	2.661876000	1.270987000	0.720385000
	6	3.964993000	0.745808000	0.657018000
	6	2.299400000	2.229146000	-0.251631000
	6	4.853367000	1.124278000	-0.353634000
	1	4.273377000	0.009085000	1.402191000
	6	3.180788000	2.608845000	-1.262071000
	1	1.298558000	2.661205000	-0.225569000
	6	4.464712000	2.050370000	-1.326345000
	1	5.855753000	0.688433000	-0.382961000
	1	2.861131000	3.342843000	-2.006716000
	1	5.157696000	2.344207000	-2.118760000
	6	-4.161073000	-0.219336000	3.327804000
	1	-5.254871000	-0.249833000	3.182004000
	1	-3.885125000	-1.120164000	3.914791000
	1	-3.936148000	0.663473000	3.960588000
	8	-3.531433000	-0.166358000	2.079391000
	1	-2.541248000	-0.044969000	2.227909000
INT1-1 ^{Ra}	28	-0.094690000	-0.082955000	0.971807000
	6	0.416694000	1.158018000	2.369967000
	6	-5.275358000	0.087537000	-0.988618000
	6	-4.058287000	-0.843807000	-1.050353000
	6	-2.902502000	-0.427324000	-0.100921000
	6	-3.455358000	-0.192749000	1.333289000
	6	-4.617626000	0.797433000	1.345305000
	6	-5.759182000	0.313685000	0.446538000
	6	-2.170965000	0.814969000	-0.569088000
	6	-1.870799000	-1.547536000	-0.076921000
	8	-2.233318000	-2.681982000	0.536318000
	7	-0.727713000	-1.527045000	-0.669400000
	6	-1.035567000	-3.518854000	0.558166000
	7	-1.013139000	1.145875000	-0.125956000
	8	-2.686894000	1.603173000	-1.522561000
	6	-0.480884000	2.242010000	-0.964698000
	6	-0.162547000	-2.882625000	-0.543463000
	6	1.334181000	-2.893629000	-0.331494000
	6	-1.768361000	2.720964000	-1.670620000
	6	0.594261000	1.693023000	-1.884868000
	6	2.117584000	-1.854773000	-0.847727000
	6	3.502511000	-1.865645000	-0.683425000
	6	4.124625000	-2.916851000	-0.004591000
	6	1.940702000	1.983882000	-1.646041000
	6	2.936559000	1.446913000	-2.466858000
	6	2.594309000	0.614023000	-3.532972000
	6	3.348011000	-3.961202000	0.503840000

6	1.961068000	-3.949702000	0.337871000
6	1.248729000	0.312944000	-3.772683000
6	0.256031000	0.845698000	-2.951373000
1	-6.082695000	-0.346182000	-1.600943000
1	-5.018205000	1.055033000	-1.444509000
1	-4.357735000	-1.859051000	-0.746053000
1	-3.674630000	-0.916309000	-2.079664000
1	-3.787587000	-1.169144000	1.716211000
1	-2.626082000	0.136824000	1.974780000
1	-4.969226000	0.931894000	2.380661000
1	-4.270217000	1.790138000	1.006250000
1	-6.158620000	-0.632177000	0.855587000
1	-6.591757000	1.035602000	0.455323000
1	-1.347180000	-4.551992000	0.364419000
1	-0.569360000	-3.400567000	1.544530000
1	-0.049638000	3.018173000	-0.319893000
1	-0.365673000	-3.384888000	-1.510566000
1	-2.222441000	3.591402000	-1.173298000
1	-1.644327000	2.922415000	-2.740874000
1	1.637155000	-1.025022000	-1.362080000
1	4.092845000	-1.037568000	-1.080982000
1	5.208980000	-2.921877000	0.130897000
1	2.218511000	2.617118000	-0.804233000
1	3.983019000	1.678221000	-2.256851000
1	3.372265000	0.186753000	-4.169835000
1	3.822405000	-4.786411000	1.040738000
1	1.367623000	-4.768553000	0.752620000
1	0.974265000	-0.351950000	-4.594796000
1	-0.787412000	0.577811000	-3.129339000
9	0.563466000	-1.461532000	1.934803000
6	1.739811000	1.682300000	1.927811000
6	2.789902000	0.772329000	1.659633000
6	2.005411000	3.054243000	1.751678000
6	4.036238000	1.219417000	1.233995000
1	2.585948000	-0.294921000	1.773555000
6	3.263340000	3.502369000	1.328484000
1	1.227404000	3.789727000	1.964912000
6	4.285082000	2.589467000	1.063276000
1	4.824710000	0.490454000	1.030244000
1	3.442212000	4.574436000	1.207688000
1	5.266578000	2.937916000	0.732369000
6	-0.633731000	2.184012000	2.751673000
1	-0.285105000	2.841290000	3.570993000
1	-0.919018000	2.842150000	1.914268000

	1	-1.553792000	1.693662000	3.105382000
	1	0.561282000	0.427550000	3.177196000
INT1-2 ^{Ra}	28	-0.694482000	0.194451000	-0.191212000
	6	-0.607601000	-0.222502000	-2.083201000
	6	-0.879579000	5.358991000	2.004181000
	6	-0.710264000	3.887784000	2.402888000
	6	-0.453136000	2.918503000	1.208191000
	6	0.667705000	3.484820000	0.297919000
	6	0.390929000	4.922646000	-0.136027000
	6	0.239592000	5.842434000	1.078328000
	6	-1.694490000	2.683222000	0.376188000
	6	-0.046989000	1.586525000	1.820136000
	8	1.178249000	1.512142000	2.349822000
	7	-0.846075000	0.594160000	2.024454000
	6	1.305096000	0.168348000	2.921114000
	7	-1.894310000	1.636453000	-0.343588000
	8	-2.654729000	3.611116000	0.347070000
	6	-3.240388000	1.710642000	-0.938677000
	6	-0.166324000	-0.298388000	2.982389000
	6	-0.449081000	-1.771382000	2.806993000
	6	-3.632283000	3.180150000	-0.634568000
	6	-4.185773000	0.685638000	-0.345654000
	6	-1.548545000	-2.211258000	2.060455000
	6	-1.844687000	-3.571556000	1.966961000
	6	-1.052123000	-4.511932000	2.630115000
	6	-5.247534000	0.206969000	-1.121151000
	6	-6.156725000	-0.708177000	-0.589059000
	6	-6.010436000	-1.156448000	0.725924000
	6	0.044578000	-4.078398000	3.379029000
	6	0.347516000	-2.717555000	3.460600000
	6	-4.955521000	-0.676855000	1.506719000
	6	-4.048747000	0.244333000	0.977130000
	1	-0.904987000	5.966981000	2.923303000
	1	-1.849980000	5.495993000	1.507180000
	1	0.164861000	3.792319000	3.064659000
	1	-1.583351000	3.532935000	2.972016000
	1	1.598152000	3.449773000	0.882884000
	1	0.819480000	2.809887000	-0.553694000
	1	1.214877000	5.266453000	-0.780094000
	1	-0.522399000	4.966053000	-0.755060000
	1	1.196423000	5.860278000	1.631474000
	1	0.043116000	6.878711000	0.759134000
	1	1.781290000	0.278370000	3.902303000
	1	1.928273000	-0.445779000	2.257791000

1	-3.167807000	1.536238000	-2.019529000
1	-0.581927000	-0.015265000	3.970168000
1	-3.535659000	3.839176000	-1.510294000
1	-4.630190000	3.284812000	-0.192300000
1	-2.169101000	-1.489399000	1.534108000
1	-2.699522000	-3.893154000	1.367106000
1	-1.281308000	-5.577522000	2.556522000
1	-5.347772000	0.529776000	-2.158845000
1	-6.969985000	-1.087753000	-1.211686000
1	-6.713355000	-1.883707000	1.139201000
1	0.678958000	-4.804188000	3.892506000
1	1.222788000	-2.398030000	4.031005000
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1	-3.210296000	0.590009000	1.583025000
9	0.616144000	-1.075352000	0.230697000
6	3.759822000	1.973207000	-1.632289000
6	4.807897000	1.562860000	-0.538825000
6	2.303202000	-3.492035000	-1.012379000
6	3.145285000	-3.372991000	0.310622000
5	2.171610000	-1.330810000	-0.193205000
5	2.983579000	0.161422000	-0.458065000
8	2.572668000	1.281472000	-1.174282000
8	4.321264000	0.269989000	-0.134746000
8	2.148694000	-2.118534000	-1.385868000
8	2.652524000	-2.157117000	0.875411000
6	0.914631000	-4.098184000	-0.767016000
1	0.295146000	-3.932441000	-1.660768000
1	0.966340000	-5.182053000	-0.579937000
1	0.420885000	-3.616876000	0.086431000
6	2.999046000	-4.230723000	-2.150793000
1	3.242017000	-5.266230000	-1.862936000
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6	2.936542000	-4.517789000	1.295268000
1	3.251689000	-5.477255000	0.854395000
1	3.540260000	-4.343606000	2.199827000
1	1.887078000	-4.593869000	1.599030000
6	4.645399000	-3.191741000	0.036467000
1	5.134031000	-2.882889000	0.972483000
1	5.119242000	-4.120227000	-0.318124000
1	4.815699000	-2.394990000	-0.700206000
6	3.490142000	3.467702000	-1.735113000
1	4.391760000	3.994802000	-2.084362000
1	2.685911000	3.652873000	-2.463197000

	1	3.190475000	3.900637000	-0.774623000
	6	4.085423000	1.404024000	-3.017152000
	1	3.217328000	1.553157000	-3.675905000
	1	4.956606000	1.898933000	-3.471344000
	1	4.278949000	0.323280000	-2.959304000
	6	4.769306000	2.462160000	0.700883000
	1	5.362067000	1.987023000	1.496070000
	1	5.189630000	3.459572000	0.502043000
	1	3.740332000	2.573065000	1.072689000
	6	6.238837000	1.419114000	-1.042512000
	1	6.613837000	2.374560000	-1.442649000
	1	6.893109000	1.114554000	-0.212108000
	1	6.313072000	0.654041000	-1.825783000
	6	-0.266947000	0.975796000	-2.947516000
	1	-0.145496000	0.681920000	-4.007487000
	1	-1.035654000	1.766686000	-2.919871000
	1	0.685913000	1.408970000	-2.615638000
	6	-1.850941000	-0.976738000	-2.406290000
	6	-2.183812000	-2.123502000	-1.650215000
	6	-2.719119000	-0.618793000	-3.454720000
	6	-3.331889000	-2.861824000	-1.920105000
	1	-1.517753000	-2.432429000	-0.843612000
	6	-3.865695000	-1.369567000	-3.736077000
	1	-2.482814000	0.243145000	-4.081934000
	6	-4.183682000	-2.489671000	-2.967707000
	1	-3.563643000	-3.739967000	-1.311931000
	1	-4.514162000	-1.074076000	-4.565756000
	1	-5.083724000	-3.070800000	-3.181682000
	1	0.242931000	-0.918123000	-2.051340000
TS2 ^{Ra}	6	-0.128973000	4.455164000	-1.624203000
	6	-0.956716000	3.181695000	-1.491453000
	6	-1.712776000	3.097470000	-0.134535000
	6	-2.561250000	4.390153000	0.044018000
	6	-1.803874000	5.702181000	-0.203156000
	6	-1.021427000	5.693640000	-1.519422000
	6	-0.757264000	2.878998000	1.036645000
	6	-2.614973000	1.879237000	-0.155541000
	8	-3.901255000	2.072537000	0.164226000
	7	-2.260929000	0.667298000	-0.400736000
	6	-4.574574000	0.806692000	-0.015696000
	7	-0.410781000	1.756742000	1.535237000
	8	-0.287981000	4.000826000	1.633297000
	6	0.330369000	2.056483000	2.784652000
	6	-3.416183000	-0.212173000	-0.102355000

6	-3.253120000	-1.018081000	1.169348000
6	0.662131000	3.555869000	2.622556000
6	1.541837000	1.228301000	3.140296000
6	-3.788241000	-2.311892000	1.220191000
6	-3.803014000	-3.026392000	2.420585000
6	-3.276510000	-2.455036000	3.581816000
6	2.617223000	1.079556000	2.256099000
6	3.774477000	0.414588000	2.659254000
6	3.881706000	-0.098260000	3.955411000
6	-2.713367000	-1.176389000	3.528739000
6	-2.697274000	-0.462008000	2.329233000
6	2.809954000	0.035985000	4.841221000
6	1.646167000	0.691609000	4.430576000
1	0.399895000	4.433077000	-2.590269000
1	0.648450000	4.471979000	-0.843637000
1	-1.720808000	3.156904000	-2.285813000
1	-0.327282000	2.297916000	-1.615958000
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1	-3.027864000	4.395651000	1.039993000
1	-2.537182000	6.525653000	-0.203144000
1	-1.113811000	5.891838000	0.629081000
1	-1.727260000	5.695407000	-2.370607000
1	-0.423324000	6.615236000	-1.607745000
1	-5.157770000	0.864877000	-0.948407000
1	-5.244312000	0.645297000	0.837266000
1	-0.402461000	1.925689000	3.601823000
1	-3.571391000	-0.899508000	-0.936699000
1	0.529973000	4.151083000	3.534754000
1	1.676893000	3.706034000	2.221884000
1	-4.190045000	-2.762409000	0.309609000
1	-4.221810000	-4.035228000	2.446046000
1	-3.285468000	-3.012838000	4.521253000
1	2.543848000	1.458733000	1.240308000
1	4.589128000	0.288015000	1.943158000
1	4.792187000	-0.614095000	4.270792000
1	-2.270349000	-0.735927000	4.425331000
1	-2.221182000	0.516793000	2.281392000
1	2.877001000	-0.372639000	5.852521000
1	0.808038000	0.795547000	5.126075000
28	-0.411714000	0.022162000	-0.712650000
6	-0.760058000	-0.821959000	-2.459531000
9	1.434585000	1.680433000	-0.535713000
6	1.826446000	-3.348173000	0.276855000
6	1.107837000	-2.744446000	1.535035000

	6	4.031781000	0.188714000	-1.723022000
	6	3.150483000	0.079166000	-3.020862000
	5	1.816127000	0.456532000	-1.155772000
	5	0.980082000	-1.273610000	-0.217007000
	8	1.351248000	-2.478617000	-0.784449000
	8	0.973153000	-1.349899000	1.159382000
	8	3.068188000	-0.048431000	-0.679722000
	8	1.887012000	0.570009000	-2.563804000
	6	4.596290000	1.600525000	-1.508599000
	1	5.012686000	1.661220000	-0.491775000
	1	5.397499000	1.837157000	-2.224907000
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	6	3.620926000	0.956383000	-4.177805000
	1	4.641975000	0.685146000	-4.489958000
	1	2.953222000	0.816924000	-5.041528000
	1	3.603622000	2.019798000	-3.906704000
	6	2.970309000	-1.364759000	-3.502075000
	1	2.187033000	-1.378681000	-4.274882000
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	1	2.646141000	-2.015817000	-2.680398000
	6	5.158157000	-0.831291000	-1.630715000
	1	5.884140000	-0.676584000	-2.444355000
	1	5.690397000	-0.714982000	-0.674125000
	1	4.783711000	-1.858307000	-1.688431000
	6	3.346370000	-3.212773000	0.345102000
	1	3.770282000	-3.870863000	1.117535000
	1	3.775255000	-3.503884000	-0.624450000
	1	3.633243000	-2.173691000	0.549004000
	6	1.440405000	-4.784040000	-0.054707000
	1	1.953266000	-5.101524000	-0.974771000
	1	1.744545000	-5.461426000	0.758355000
	1	0.360534000	-4.896727000	-0.211001000
	6	1.899150000	-2.829159000	2.830499000
	1	1.331286000	-2.344851000	3.637330000
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	1	2.860772000	-2.312439000	2.751627000
	6	-0.302226000	-3.291486000	1.745209000
	1	-0.286142000	-4.334150000	2.095757000
	1	-0.805427000	-2.680246000	2.502447000
	1	-0.899802000	-3.235284000	0.826568000
	6	-1.831591000	-1.861663000	-2.424649000
	6	-3.101246000	-1.664789000	-3.006977000
	6	-1.587807000	-3.118507000	-1.833653000
	6	-4.086398000	-2.656802000	-2.966090000

	1	-3.328185000	-0.719809000	-3.501779000
	6	-2.567167000	-4.107480000	-1.787394000
	1	-0.598193000	-3.298754000	-1.420249000
	6	-3.831437000	-3.882060000	-2.345993000
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	1	-2.341843000	-5.066989000	-1.313864000
	1	-4.600248000	-4.657839000	-2.313288000
	1	0.195526000	-1.300940000	-2.690945000
	6	-1.011786000	0.316607000	-3.436185000
	1	-1.180258000	-0.084412000	-4.453907000
	1	-1.898646000	0.913917000	-3.175729000
	1	-0.139555000	0.977081000	-3.485314000
INT2 ^{Ra}	6	4.150363000	-0.181129000	1.624773000
	6	3.249077000	0.049069000	0.412098000
	6	2.918722000	1.533101000	0.118095000
	6	4.239998000	2.353474000	0.086999000
	6	5.086757000	2.145876000	1.344871000
	6	5.422335000	0.666044000	1.553126000
	6	1.962827000	2.187472000	1.101462000
	6	2.217394000	1.614632000	-1.225139000
	8	2.599244000	2.606534000	-2.039829000
	7	1.292744000	0.835008000	-1.655128000
	6	1.800286000	2.526686000	-3.235628000
	7	1.133847000	3.102722000	0.791064000
	8	2.038487000	1.817084000	2.404309000
	6	0.483336000	3.545242000	2.036113000
	6	0.841250000	1.337327000	-2.970883000
	6	-0.625343000	1.703697000	-2.952275000
	6	0.938866000	2.476461000	3.066492000
	6	-1.015905000	3.705244000	1.924436000
	6	-1.517658000	1.098379000	-3.844058000
	6	-2.864312000	1.468626000	-3.858475000
	6	-3.325952000	2.450326000	-2.978467000
	6	-1.805034000	2.713272000	1.325447000
	6	-3.187712000	2.876467000	1.233719000
	6	-3.804671000	4.019733000	1.749943000
	6	-2.441838000	3.045719000	-2.074538000
	6	-1.098166000	2.671235000	-2.054520000
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	6	-1.639377000	4.851698000	2.435332000
	1	4.402049000	-1.253160000	1.660230000
	1	3.599317000	0.048851000	2.547624000
	1	3.760664000	-0.330634000	-0.483428000
	1	2.330762000	-0.533476000	0.508408000

	1	4.811830000	2.023298000	-0.795466000
	1	4.002351000	3.415229000	-0.067594000
	1	6.009278000	2.743177000	1.257378000
	1	4.545996000	2.528163000	2.226832000
	1	6.045450000	0.317938000	0.708658000
	1	6.026897000	0.534346000	2.465699000
	1	2.474636000	2.358145000	-4.087488000
	1	1.274786000	3.482429000	-3.364073000
	1	0.908173000	4.530519000	2.299037000
	1	0.991553000	0.545985000	-3.716719000
	1	1.298702000	2.892028000	4.016639000
	1	0.154055000	1.728411000	3.257922000
	1	-1.154692000	0.328756000	-4.530334000
	1	-3.552869000	0.989332000	-4.558848000
	1	-4.378472000	2.743510000	-2.988152000
	1	-1.348311000	1.817664000	0.908410000
	1	-3.772889000	2.105427000	0.733266000
	1	-4.888089000	4.142317000	1.675192000
	1	-2.800726000	3.797319000	-1.369966000
	1	-0.417175000	3.116408000	-1.323370000
	1	-3.495452000	5.910215000	2.757755000
	1	-1.029680000	5.635105000	2.894706000
	28	0.118064000	-0.678639000	-0.905279000
	6	0.503287000	-1.951895000	-2.316371000
	9	0.139371000	0.164233000	1.081014000
	6	-3.700885000	-2.406720000	-0.775007000
	6	-3.922900000	-0.938515000	-0.254220000
	6	-0.839618000	-2.435792000	3.204972000
	6	0.374211000	-3.121418000	2.460473000
	5	-0.117270000	-1.127705000	1.497399000
	5	-1.665859000	-1.362676000	-0.556267000
	8	-2.285997000	-2.598758000	-0.559952000
	8	-2.613498000	-0.352038000	-0.451841000
	8	-1.209202000	-1.374284000	2.288831000
	8	0.910724000	-2.017414000	1.686750000
	6	-0.430847000	-1.754286000	4.512389000
	1	-1.265158000	-1.128298000	4.860802000
	1	-0.193166000	-2.487651000	5.296906000
	1	0.444586000	-1.105453000	4.362094000
	6	1.479753000	-3.633151000	3.373735000
	1	1.099026000	-4.416047000	4.047676000
	1	2.283067000	-4.069555000	2.762064000
	1	1.915895000	-2.826457000	3.976469000
	6	-0.071736000	-4.219903000	1.493897000

	1	0.792055000	-4.553109000	0.901894000
	1	-0.454446000	-5.092885000	2.042346000
	1	-0.847236000	-3.862923000	0.802811000
	6	-2.042468000	-3.341064000	3.426285000
	1	-1.768837000	-4.203797000	4.052888000
	1	-2.838402000	-2.783620000	3.941835000
	1	-2.441180000	-3.708672000	2.473707000
	6	-4.465808000	-3.483123000	-0.016652000
	1	-5.552403000	-3.328506000	-0.106099000
	1	-4.224802000	-4.471790000	-0.435328000
	1	-4.202285000	-3.490214000	1.048104000
	6	-3.952004000	-2.545507000	-2.280015000
	1	-3.598207000	-3.531677000	-2.613802000
	1	-5.021250000	-2.462116000	-2.524338000
	1	-3.401919000	-1.776557000	-2.841428000
	6	-4.247382000	-0.876873000	1.239037000
	1	-4.195233000	0.166719000	1.577602000
	1	-5.259338000	-1.257061000	1.444937000
	1	-3.514081000	-1.443327000	1.821836000
	6	-4.948956000	-0.136242000	-1.045930000
	1	-5.936710000	-0.622195000	-1.006375000
	1	-5.050293000	0.870217000	-0.614283000
	1	-4.649066000	-0.016214000	-2.092870000
	6	-0.192712000	-3.300991000	-2.471749000
	1	0.310093000	-3.898830000	-3.254816000
	1	-0.179985000	-3.889125000	-1.544596000
	1	-1.244053000	-3.182360000	-2.755384000
	6	1.986625000	-2.114202000	-2.143324000
	6	2.909030000	-1.510858000	-3.019901000
	6	2.515173000	-2.909585000	-1.107971000
	6	4.287004000	-1.672049000	-2.861071000
	1	2.536156000	-0.913774000	-3.855902000
	6	3.889441000	-3.082058000	-0.947801000
	1	1.830310000	-3.370047000	-0.399493000
	6	4.788465000	-2.459999000	-1.820460000
	1	4.973693000	-1.188488000	-3.561212000
	1	4.263453000	-3.699925000	-0.127040000
	1	5.865843000	-2.589949000	-1.693427000
	1	0.313568000	-1.363924000	-3.230425000
TS3 ^{Ra}	6	4.152478000	-0.194378000	1.599313000
	6	3.254262000	0.036609000	0.384612000
	6	2.922514000	1.520606000	0.092206000
	6	4.243397000	2.341450000	0.062372000
	6	5.087631000	2.134106000	1.322038000

6	5.423714000	0.654413000	1.531211000
6	1.967373000	2.176132000	1.076120000
6	2.221649000	1.600167000	-1.251405000
8	2.603944000	2.591611000	-2.067573000
7	1.298685000	0.818409000	-1.680135000
6	1.809319000	2.505375000	-3.265814000
7	1.148956000	3.101670000	0.769204000
8	2.031856000	1.793810000	2.377140000
6	0.494776000	3.540850000	2.012804000
6	0.848917000	1.317925000	-2.998068000
6	-0.617937000	1.684530000	-2.980239000
6	0.943639000	2.467935000	3.042943000
6	-1.004200000	3.703208000	1.897820000
6	-1.516189000	1.056284000	-3.850038000
6	-2.864255000	1.420868000	-3.860417000
6	-3.321865000	2.421478000	-2.999828000
6	-1.790990000	2.726637000	1.271407000
6	-3.173709000	2.890602000	1.180324000
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6	-1.086395000	2.672198000	-2.102403000
6	-3.016415000	4.993343000	2.358059000
6	-1.630168000	4.835216000	2.437293000
1	4.405479000	-1.266127000	1.633986000
1	3.599416000	0.033786000	2.521436000
1	3.769287000	-0.340579000	-0.510216000
1	2.336620000	-0.547778000	0.473858000
1	4.816788000	2.011135000	-0.818997000
1	4.005652000	3.403054000	-0.092912000
1	6.010089000	2.731838000	1.236871000
1	4.544943000	2.516236000	2.203010000
1	6.049317000	0.307032000	0.688314000
1	6.026219000	0.523218000	2.445238000
1	2.486702000	2.331227000	-4.114224000
1	1.285369000	3.460829000	-3.402374000
1	0.919860000	4.524478000	2.281009000
1	0.998917000	0.523929000	-3.740994000
1	1.313480000	2.881669000	3.990174000
1	0.150568000	1.730716000	3.242669000
1	-1.156984000	0.271349000	-4.520484000
1	-3.557341000	0.922320000	-4.542653000
1	-4.375622000	2.710349000	-3.006592000
1	-1.332779000	1.842718000	0.832208000
1	-3.756334000	2.132010000	0.658079000

	1	-4.876372000	4.142713000	1.651090000
	1	-2.786317000	3.810492000	-1.431103000
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	28	0.104758000	-0.689342000	-0.942249000
	6	0.472928000	-1.962728000	-2.354378000
	9	0.139871000	0.181122000	1.022856000
	6	-3.707698000	-2.432578000	-0.722184000
	6	-3.927872000	-0.950648000	-0.240509000
	6	-0.805169000	-2.335118000	3.281173000
	6	0.393284000	-3.044076000	2.531869000
	5	-0.085414000	-1.061862000	1.557135000
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	8	-2.286939000	-2.609195000	-0.534269000
	8	-2.627252000	-0.363084000	-0.480850000
	8	-1.169532000	-1.275552000	2.357452000
	8	0.931148000	-1.956642000	1.732554000
	6	-0.377249000	-1.645394000	4.577609000
	1	-1.201814000	-1.007924000	4.928361000
	1	-0.139613000	-2.374177000	5.366177000
	1	0.503448000	-1.007028000	4.413491000
	6	1.505221000	-3.551370000	3.439263000
	1	1.126056000	-4.322188000	4.127729000
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	6	-0.072322000	-4.149971000	1.584033000
	1	0.784535000	-4.501799000	0.993056000
	1	-0.462529000	-5.010052000	2.147178000
	1	-0.846067000	-3.793177000	0.890568000
	6	-2.017762000	-3.222125000	3.519802000
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	6	-4.448143000	-3.490754000	0.084970000
	1	-5.537532000	-3.345984000	0.015095000
	1	-4.209287000	-4.490040000	-0.309094000
	1	-4.162139000	-3.464345000	1.143672000
	6	-3.992857000	-2.619470000	-2.215844000
	1	-3.635334000	-3.611410000	-2.527651000
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	1	-3.464814000	-1.862516000	-2.813461000
	6	-4.224572000	-0.847356000	1.256236000
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	1	-5.229483000	-1.228450000	1.492823000
	1	-3.477075000	-1.392264000	1.841669000
	6	-4.972681000	-0.175506000	-1.035083000
	1	-5.958508000	-0.661475000	-0.961798000
	1	-5.067296000	0.843419000	-0.631934000
	1	-4.693512000	-0.086613000	-2.090961000
	6	-0.243190000	-3.300848000	-2.517914000
	1	0.251758000	-3.904828000	-3.301538000
	1	-0.246274000	-3.892846000	-1.592737000
	1	-1.291447000	-3.163275000	-2.806374000
	6	1.950515000	-2.146539000	-2.161224000
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	6	4.268534000	-1.735730000	-2.840137000
	1	2.544405000	-0.956876000	-3.866294000
	6	3.820375000	-3.133878000	-0.929181000
	1	1.746631000	-3.396848000	-0.419995000
	6	4.742179000	-2.526320000	-1.788545000
	1	4.973410000	-1.262982000	-3.529563000
	1	4.172547000	-3.753690000	-0.100175000
	1	5.815506000	-2.669364000	-1.642603000
	1	0.305209000	-1.375728000	-3.273269000
INT3 ^{Ra}	6	0.637486000	2.168833000	-4.542085000
	6	1.523205000	2.167222000	-3.290425000
	6	0.911899000	1.328474000	-2.153028000
	6	0.577425000	-0.099165000	-2.655501000
	6	-0.321756000	-0.073775000	-3.885320000
	6	0.298763000	0.751658000	-5.015309000
	6	-0.316579000	1.983790000	-1.539205000
	6	1.816861000	1.236589000	-0.933189000
	8	2.814397000	2.135680000	-0.840061000
	7	1.596803000	0.476993000	0.074887000
	6	3.281230000	2.086261000	0.526797000
	7	-0.939717000	1.456728000	-0.550594000
	8	-0.659402000	3.249068000	-1.861887000
	6	-1.750836000	2.515887000	0.090499000
	6	2.609556000	0.809495000	1.105416000
	6	3.606532000	-0.303543000	1.346664000
	6	-1.790657000	3.583148000	-1.016749000
	6	-1.001880000	2.863380000	1.365812000
	6	3.845049000	-0.779684000	2.639568000
	6	4.787609000	-1.787504000	2.864183000
	6	5.510049000	-2.319237000	1.793980000
	6	-1.196850000	2.049162000	2.493334000

	6	-0.393563000	2.215410000	3.623694000
	6	0.608618000	3.191177000	3.642653000
	6	5.287147000	-1.837176000	0.499669000
	6	4.339463000	-0.838788000	0.278632000
	6	0.801555000	4.007040000	2.524300000
	6	0.004463000	3.836742000	1.387355000
	1	1.145721000	2.731346000	-5.342195000
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	1	1.528069000	-0.607834000	-2.881685000
	1	0.111343000	-0.672275000	-1.842045000
	1	-0.510232000	-1.109144000	-4.209070000
	1	-1.305578000	0.346440000	-3.607249000
	1	1.222173000	0.251178000	-5.359506000
	1	-0.377821000	0.793212000	-5.884746000
	1	2.943722000	3.002717000	1.031706000
	1	4.377160000	2.039346000	0.520735000
	1	-2.747173000	2.126545000	0.334922000
	1	2.081609000	1.039030000	2.041674000
	1	-2.703973000	3.503457000	-1.626223000
	1	-1.670055000	4.615819000	-0.668453000
	1	3.276542000	-0.368304000	3.477273000
	1	4.953702000	-2.160329000	3.877573000
	1	6.243778000	-3.110149000	1.965966000
	1	-1.967172000	1.275083000	2.471230000
	1	-0.548310000	1.572416000	4.493269000
	1	1.234337000	3.319767000	4.529282000
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	1	4.147901000	-0.490362000	-0.738782000
	1	1.575479000	4.778703000	2.534186000
	1	0.194377000	4.455018000	0.507236000
	28	-0.472384000	-0.207190000	0.283752000
	6	-0.333735000	-2.029160000	1.038440000
	6	-4.316761000	-1.127190000	1.427884000
	6	-4.372788000	-1.436644000	-0.112775000
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	8	-2.979702000	-1.507042000	-0.461992000
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	1	-6.418949000	-0.691986000	1.784279000
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	1	-4.789590000	-0.480648000	-1.995767000
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	6	-5.043505000	-2.755340000	-0.477882000
	1	-6.093404000	-2.771227000	-0.144850000
	1	-5.028938000	-2.887379000	-1.570229000
	1	-4.517435000	-3.608034000	-0.030336000
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	1	0.625379000	-2.910312000	2.814580000
	1	1.275702000	-1.332287000	2.353080000
	6	0.411835000	-2.729209000	-0.052030000
	6	1.800105000	-2.952364000	-0.011117000
	6	-0.275788000	-3.159390000	-1.211981000
	6	2.477747000	-3.528961000	-1.089309000
	1	2.364496000	-2.666361000	0.874636000
	6	0.398816000	-3.736609000	-2.284894000
	1	-1.353890000	-2.996675000	-1.267272000
	6	1.788058000	-3.917904000	-2.239504000
	1	3.558694000	-3.677626000	-1.021099000
	1	-0.163960000	-4.049688000	-3.169420000
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	1	-1.269368000	-2.593902000	1.192142000
TS4 ^{Ra}	6	-5.541571000	-1.116813000	-1.079639000
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	6	-3.353821000	0.105117000	-0.590000000
	6	-2.845238000	-0.326806000	-1.998641000
	6	-3.487823000	-1.631366000	-2.459211000
	6	-5.015845000	-1.533014000	-2.456745000
	6	-2.804431000	-0.849273000	0.456489000
	6	-2.697025000	1.438887000	-0.259429000
	8	-3.468587000	2.530129000	-0.092598000
	7	-1.435137000	1.583067000	-0.113377000
	6	-2.562091000	3.643415000	0.118043000
	7	-1.548422000	-1.052588000	0.619011000
	8	-3.630003000	-1.406008000	1.371131000
	6	-1.359112000	-1.736346000	1.918221000
	6	-1.171535000	2.976515000	0.290573000
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	6	-2.789780000	-2.226055000	2.222702000

	6	-0.785087000	-0.712316000	2.879740000
	6	1.188910000	3.842511000	0.124443000
	6	2.298370000	4.246177000	-0.622032000
	6	2.191595000	4.389484000	-2.005615000
	6	0.592273000	-0.684969000	3.126806000
	6	1.143306000	0.321130000	3.925464000
	6	0.327871000	1.315278000	4.471064000
	6	0.972364000	4.128652000	-2.641396000
	6	-0.130258000	3.715548000	-1.894795000
	6	-1.048545000	1.298564000	4.218679000
	6	-1.601188000	0.289058000	3.428421000
	1	-6.634912000	-0.982063000	-1.110809000
	1	-5.346532000	-1.921554000	-0.352933000
	1	-5.183956000	1.017658000	-1.231215000
	1	-5.248678000	0.426269000	0.430635000
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	1	-1.745755000	-0.412474000	-1.956546000
	1	-3.112038000	-1.886582000	-3.462694000
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	1	-5.329470000	-0.787148000	-3.210035000
	1	-5.465443000	-2.492314000	-2.760901000
	1	-2.898718000	4.197914000	1.003385000
	1	-2.613903000	4.299238000	-0.763961000
	1	-0.648447000	-2.562640000	1.794371000
	1	-0.879801000	2.952703000	1.353571000
	1	-2.937991000	-3.277424000	1.931383000
	1	-3.105919000	-2.081096000	3.262861000
	1	1.285026000	3.691673000	1.201819000
	1	3.254853000	4.412947000	-0.122982000
	1	3.062775000	4.686482000	-2.593702000
	1	1.237521000	-1.417928000	2.639067000
	1	2.220908000	0.335638000	4.102495000
	1	0.761838000	2.104280000	5.090155000
	1	0.889549000	4.224182000	-3.726492000
	1	-1.064237000	3.464363000	-2.404329000
	1	-1.693241000	2.073576000	4.641000000
	1	-2.674902000	0.296201000	3.222946000
	28	-0.167500000	-0.105733000	-0.272034000
	6	1.604426000	0.331555000	-2.783671000
	1	0.588370000	0.255827000	-3.199898000
	6	1.542104000	0.476029000	-1.266154000
	1	2.093505000	1.202489000	-3.256930000
	1	2.136895000	-0.578337000	-3.096803000
	6	2.537456000	-3.155100000	0.018299000

	6	1.658681000	-3.584173000	-1.213633000
	5	1.087827000	-1.442891000	-0.575213000
	8	1.832118000	-1.993116000	0.486892000
	8	1.131351000	-2.329871000	-1.663293000
	6	2.603015000	-4.176569000	1.148174000
	1	3.039608000	-5.125938000	0.799526000
	1	3.237589000	-3.789417000	1.959960000
	1	1.608453000	-4.382665000	1.566405000
	6	3.950405000	-2.719331000	-0.377112000
	1	4.401867000	-2.177503000	0.466474000
	1	4.588817000	-3.579124000	-0.632453000
	1	3.928121000	-2.026523000	-1.227535000
	6	0.463331000	-4.460350000	-0.816287000
	1	-0.219070000	-4.530129000	-1.676238000
	1	0.765543000	-5.477646000	-0.525022000
	1	-0.092242000	-4.003744000	0.015824000
	6	2.430220000	-4.241484000	-2.351869000
	1	2.915771000	-5.171245000	-2.014979000
	1	1.740043000	-4.492347000	-3.171686000
	1	3.198667000	-3.568671000	-2.752763000
	6	2.840707000	0.713946000	-0.572783000
	6	2.838944000	0.985058000	0.810894000
	6	4.083648000	0.717697000	-1.228435000
	6	4.012323000	1.263990000	1.502543000
	1	1.883003000	0.957707000	1.336735000
	6	5.268242000	0.990480000	-0.534634000
	1	4.131233000	0.507786000	-2.298165000
	6	5.244658000	1.268621000	0.833210000
	1	3.971756000	1.474820000	2.575406000
	1	6.220152000	0.984457000	-1.073385000
	1	6.170567000	1.480442000	1.373707000
	1	0.964429000	1.391715000	-1.063602000
INT4 ^{Ra}	6	-5.631733000	-0.700366000	-0.359886000
	6	-4.849773000	0.549761000	0.059099000
	6	-3.331392000	0.409247000	-0.176167000
	6	-3.049893000	-0.031057000	-1.647989000
	6	-3.827719000	-1.288855000	-2.023363000
	6	-5.331592000	-1.106905000	-1.805235000
	6	-2.685859000	-0.589996000	0.764039000
	6	-2.595873000	1.726387000	0.041906000
	8	-3.309213000	2.869832000	0.021542000
	7	-1.329096000	1.831504000	0.187405000
	6	-2.359329000	3.959706000	0.125304000
	7	-1.435456000	-0.884960000	0.726434000

	8	-3.405549000	-1.128046000	1.774079000
	6	-1.110057000	-1.683525000	1.927689000
	6	-0.988128000	3.258421000	0.326252000
	6	0.119887000	3.619960000	-0.636965000
	6	-2.516465000	-2.037192000	2.468140000
	6	-0.245368000	-0.853440000	2.853454000
	6	1.431769000	3.737534000	-0.165242000
	6	2.493753000	3.928145000	-1.052018000
	6	2.247442000	4.018081000	-2.422979000
	6	1.071300000	-1.237175000	3.124088000
	6	1.872151000	-0.462572000	3.967418000
	6	1.369520000	0.711108000	4.531643000
	6	0.939105000	3.902504000	-2.904393000
	6	-0.116789000	3.694576000	-2.016770000
	6	0.056786000	1.109596000	4.251672000
	6	-0.746015000	0.328817000	3.420629000
	1	-6.709278000	-0.508067000	-0.230886000
	1	-5.379479000	-1.532184000	0.316853000
	1	-5.192603000	1.413824000	-0.529312000
	1	-5.041272000	0.788678000	1.115584000
	1	-3.332963000	0.806277000	-2.307862000
	1	-1.963577000	-0.190975000	-1.752180000
	1	-3.610038000	-1.549008000	-3.071536000
	1	-3.459063000	-2.133980000	-1.415766000
	1	-5.704153000	-0.324700000	-2.491941000
	1	-5.873576000	-2.032053000	-2.060933000
	1	-2.654316000	4.591370000	0.973907000
	1	-2.413487000	4.551692000	-0.799467000
	1	-0.545759000	-2.573149000	1.625523000
	1	-0.616151000	3.411049000	1.351946000
	1	-2.816662000	-3.064787000	2.210920000
	1	-2.631403000	-1.875798000	3.547302000
	1	1.631213000	3.638068000	0.903933000
	1	3.515012000	3.979231000	-0.669891000
	1	3.076413000	4.159209000	-3.120084000
	1	1.483886000	-2.113294000	2.623067000
	1	2.902824000	-0.766753000	4.160044000
	1	1.999604000	1.321046000	5.183670000
	1	0.744941000	3.951818000	-3.978240000
	1	-1.129373000	3.562580000	-2.407112000
	1	-0.340784000	2.030478000	4.685825000
	1	-1.767574000	0.648359000	3.199217000
	28	-0.136798000	0.126619000	-0.205375000
	6	1.952468000	0.315057000	-2.808355000

	1	0.971868000	0.292694000	-3.302282000
	6	1.781052000	0.213227000	-1.289951000
	1	2.467744000	1.244821000	-3.098886000
	1	2.518201000	-0.539649000	-3.208138000
	6	1.810156000	-3.420454000	-0.562959000
	6	0.729209000	-3.405893000	-1.709668000
	5	1.068678000	-1.255183000	-0.917079000
	8	1.617687000	-2.147649000	0.055281000
	8	0.669694000	-2.026252000	-2.048867000
	6	1.622774000	-4.521253000	0.476292000
	1	1.681700000	-5.518872000	0.012972000
	1	2.414893000	-4.453376000	1.237926000
	1	0.654055000	-4.435531000	0.987145000
	6	3.245008000	-3.458499000	-1.105456000
	1	3.933011000	-3.210288000	-0.284245000
	1	3.515338000	-4.445725000	-1.510983000
	1	3.385137000	-2.703951000	-1.892284000
	6	-0.662672000	-3.840973000	-1.228877000
	1	-1.391181000	-3.601906000	-2.017919000
	1	-0.716766000	-4.919965000	-1.018808000
	1	-0.956168000	-3.283894000	-0.330481000
	6	1.113124000	-4.208427000	-2.949986000
	1	1.269668000	-5.270837000	-2.703531000
	1	0.306741000	-4.144999000	-3.696619000
	1	2.027708000	-3.813755000	-3.410502000
	6	3.022720000	0.428378000	-0.477693000
	6	2.903253000	0.785107000	0.877784000
	6	4.315381000	0.297012000	-1.008476000
	6	4.025884000	1.014841000	1.669266000
	1	1.898753000	0.880681000	1.299460000
	6	5.445362000	0.518650000	-0.214386000
	1	4.446175000	0.020285000	-2.055894000
	6	5.310186000	0.884238000	1.127117000
	1	3.897416000	1.298292000	2.716693000
	1	6.441174000	0.408492000	-0.652798000
	1	6.193899000	1.063717000	1.744558000
	1	1.148322000	1.123946000	-1.025106000
(R)-3	6	-1.034000000	2.899475000	-0.578915000
	1	-0.307673000	3.517403000	-1.129695000
	6	-0.927708000	1.434367000	-1.012695000
	1	-2.040037000	3.307668000	-0.768101000
	1	-0.810149000	3.025074000	0.491015000
	6	1.945309000	-0.921602000	-0.365887000
	6	2.261164000	0.230408000	0.666307000

	5	0.421371000	0.748128000	-0.572333000
	8	1.012223000	-0.272736000	-1.266632000
	8	1.054499000	1.030260000	0.606135000
	6	3.142859000	-1.415412000	-1.164789000
	1	3.906979000	-1.843209000	-0.497402000
	1	2.821038000	-2.201400000	-1.863941000
	1	3.599266000	-0.607878000	-1.751086000
	6	1.197072000	-2.099282000	0.262772000
	1	0.828405000	-2.753106000	-0.540798000
	1	1.848605000	-2.690561000	0.922601000
	1	0.326501000	-1.754745000	0.839391000
	6	3.416864000	1.130888000	0.226648000
	1	3.435895000	2.023166000	0.869263000
	1	4.386129000	0.618472000	0.313704000
	1	3.289312000	1.463400000	-0.813776000
	6	2.467795000	-0.233962000	2.101854000
	1	3.327079000	-0.918888000	2.171407000
	1	2.669656000	0.635093000	2.745442000
	1	1.577422000	-0.742916000	2.491858000
	6	-1.989549000	0.509529000	-0.431439000
	6	-2.310871000	-0.687168000	-1.096631000
	6	-2.610980000	0.766646000	0.800246000
	6	-3.228186000	-1.589060000	-0.556855000
	1	-1.824199000	-0.911445000	-2.049241000
	6	-3.530388000	-0.135870000	1.343648000
	1	-2.374315000	1.680512000	1.347197000
	6	-3.844388000	-1.317420000	0.668961000
	1	-3.464901000	-2.509583000	-1.096738000
	1	-4.004192000	0.089022000	2.302739000
	1	-4.564141000	-2.021494000	1.093407000
	1	-0.997274000	1.365368000	-2.110944000
pre-com ⁿ BuOH	28	-0.320559000	0.379761000	-0.397397000
	6	-1.470083000	0.301647000	-1.980812000
	6	-0.167855000	0.864978000	-2.265584000
	6	2.537857000	-1.191938000	4.400309000
	6	1.089337000	-0.769502000	4.121393000
	6	0.753239000	-0.653365000	2.616338000
	6	1.201342000	-1.953321000	1.870560000
	6	2.664720000	-2.295420000	2.135475000
	6	2.930603000	-2.457703000	3.633532000
	6	1.421433000	0.539672000	1.954829000
	6	-0.742391000	-0.532150000	2.379949000
	8	-1.566637000	-0.853987000	3.391187000
	7	-1.290679000	-0.239647000	1.257063000

6	-2.913579000	-0.612682000	2.917261000
7	1.189972000	0.932552000	0.756366000
8	2.300077000	1.259504000	2.668495000
6	1.958872000	2.168436000	0.512243000
6	-2.740374000	-0.447231000	1.383917000
6	-3.219221000	-1.647150000	0.587688000
6	2.851802000	2.259685000	1.773964000
6	1.012722000	3.327989000	0.293222000
6	-4.598090000	-1.876935000	0.481339000
6	-5.085260000	-2.968875000	-0.236769000
6	-4.194627000	-3.844887000	-0.866866000
6	1.094929000	4.101986000	-0.868641000
6	0.210357000	5.163851000	-1.080079000
6	-0.766074000	5.461695000	-0.126977000
6	-2.820018000	-3.622095000	-0.764704000
6	-2.333930000	-2.530352000	-0.038505000
6	-0.856447000	4.691014000	1.036986000
6	0.026429000	3.631332000	1.242951000
1	2.653249000	-1.350770000	5.485057000
1	3.219314000	-0.373689000	4.126278000
1	0.406230000	-1.522527000	4.540703000
1	0.860181000	0.179817000	4.628465000
1	0.549317000	-2.771612000	2.220343000
1	1.021036000	-1.807655000	0.798870000
1	2.916874000	-3.219609000	1.590418000
1	3.312514000	-1.507533000	1.714899000
1	2.347815000	-3.316933000	4.014335000
1	3.991897000	-2.694157000	3.813644000
1	-3.281678000	0.303458000	3.404525000
1	-3.539513000	-1.466368000	3.204855000
1	2.577803000	2.017942000	-0.376823000
1	-3.266136000	0.445677000	1.014747000
1	3.887123000	1.969749000	1.555600000
1	2.810230000	3.231247000	2.282934000
1	-5.298359000	-1.176717000	0.944870000
1	-6.162941000	-3.130252000	-0.317004000
1	-4.572818000	-4.696041000	-1.438027000
1	1.847226000	3.857305000	-1.622185000
1	0.278019000	5.752918000	-1.997570000
1	-1.463600000	6.285441000	-0.295092000
1	-2.116492000	-4.296954000	-1.256615000
1	-1.262550000	-2.341842000	0.016894000
1	-1.627958000	4.909045000	1.778986000
1	-0.064581000	3.018723000	2.143424000

	8	2.040404000	-1.375654000	-1.276760000
	1	1.377826000	-0.644481000	-1.240311000
	1	-0.077025000	1.946744000	-2.438070000
	1	0.476381000	0.297453000	-2.951607000
	1	-1.686600000	-0.704907000	-2.362144000
	6	-2.678226000	1.094339000	-1.701701000
	6	-3.955159000	0.499310000	-1.774279000
	6	-2.616478000	2.437841000	-1.262794000
	6	-5.106832000	1.194990000	-1.402356000
	1	-4.035143000	-0.535068000	-2.115474000
	6	-3.766418000	3.132216000	-0.894224000
	1	-1.649563000	2.935026000	-1.190565000
	6	-5.023746000	2.516445000	-0.951943000
	1	-6.079150000	0.698144000	-1.465700000
	1	-3.677379000	4.167150000	-0.552604000
	1	-5.924220000	3.062261000	-0.659633000
	8	4.099249000	0.035873000	-0.163897000
	1	3.451408000	-0.608525000	-0.517275000
	6	1.562675000	-2.391036000	-2.139411000
	1	0.465255000	-2.467917000	-2.044234000
	1	1.776335000	-2.136875000	-3.197179000
	6	5.140226000	0.183045000	-1.106617000
	1	5.656793000	1.129998000	-0.865891000
	1	5.894478000	-0.623269000	-0.996337000
	6	2.229160000	-3.710823000	-1.782448000
	1	1.974004000	-3.961914000	-0.737438000
	1	3.322035000	-3.558927000	-1.805197000
	6	1.848213000	-4.870514000	-2.707669000
	1	2.460615000	-5.748314000	-2.440888000
	1	2.125850000	-4.615065000	-3.746323000
	6	0.368113000	-5.256410000	-2.655548000
	1	-0.283566000	-4.443807000	-3.013291000
	1	0.162746000	-6.139305000	-3.280987000
	1	0.059964000	-5.499308000	-1.624388000
	6	4.656313000	0.215560000	-2.556874000
	1	5.534381000	0.373694000	-3.209291000
	1	4.250356000	-0.776782000	-2.822465000
	6	3.591625000	1.274968000	-2.844786000
	1	2.719361000	1.085947000	-2.202922000
	1	3.980561000	2.270261000	-2.559657000
	6	3.133061000	1.291477000	-4.300791000
	1	2.345910000	2.043355000	-4.466553000
	1	3.966692000	1.513144000	-4.988277000
	1	2.716036000	0.312590000	-4.590390000

TS1 ⁿ BuOH	28	-0.448318000	0.276617000	-0.295378000
	6	-1.663316000	0.290352000	-1.780981000
	6	-0.356884000	0.813842000	-2.239687000
	6	2.426158000	-1.236706000	4.470644000
	6	0.967245000	-0.902575000	4.133026000
	6	0.684945000	-0.757787000	2.617743000
	6	1.282931000	-1.978804000	1.830028000
	6	2.747021000	-2.236029000	2.177176000
	6	2.939050000	-2.443135000	3.680103000
	6	1.272311000	0.506256000	2.023875000
	6	-0.803676000	-0.779169000	2.325678000
	8	-1.602778000	-1.319623000	3.254912000
	7	-1.369140000	-0.436132000	1.219883000
	6	-2.958874000	-1.210811000	2.761775000
	7	0.955494000	0.974928000	0.878024000
	8	2.208829000	1.170167000	2.709127000
	6	1.769897000	2.170004000	0.603469000
	6	-2.776045000	-0.864959000	1.263836000
	6	-3.045739000	-2.033661000	0.333802000
	6	2.691057000	2.236385000	1.849388000
	6	0.895279000	3.377029000	0.358843000
	6	-4.376233000	-2.388521000	0.071016000
	6	-4.673853000	-3.463565000	-0.767896000
	6	-3.639167000	-4.192649000	-1.362867000
	6	0.995256000	4.087402000	-0.842523000
	6	0.174110000	5.192761000	-1.085510000
	6	-0.754824000	5.598435000	-0.124562000
	6	-2.311524000	-3.842598000	-1.106949000
	6	-2.015175000	-2.770974000	-0.260009000
	6	-0.862321000	4.892068000	1.078424000
	6	-0.044556000	3.787051000	1.314994000
	1	2.494331000	-1.431205000	5.553737000
	1	3.064395000	-0.366657000	4.263194000
	1	0.323131000	-1.715113000	4.498008000
	1	0.648328000	0.011397000	4.658142000
	1	0.670380000	-2.860099000	2.086879000
	1	1.175104000	-1.774287000	0.754616000
	1	3.083001000	-3.122027000	1.614216000
	1	3.357858000	-1.395582000	1.808721000
	1	2.391712000	-3.350938000	3.996392000
	1	4.001667000	-2.620888000	3.912494000
	1	-3.456972000	-0.407672000	3.326434000
	1	-3.469015000	-2.165453000	2.938392000
	1	2.375753000	1.956409000	-0.283094000

1	-3.419775000	-0.025296000	0.966249000
1	3.730160000	2.002842000	1.590854000
1	2.619753000	3.179412000	2.407711000
1	-5.187849000	-1.803305000	0.512582000
1	-5.715687000	-3.725505000	-0.967630000
1	-3.868450000	-5.027887000	-2.028714000
1	1.716283000	3.762148000	-1.596378000
1	0.256302000	5.733764000	-2.030979000
1	-1.400631000	6.458745000	-0.314854000
1	-1.496100000	-4.395504000	-1.576371000
1	-0.977672000	-2.484444000	-0.092380000
1	-1.595855000	5.196958000	1.828368000
1	-0.148494000	3.223914000	2.246198000
8	1.644796000	-0.824211000	-1.316480000
1	0.641057000	0.208024000	-1.621686000
1	-0.253881000	1.902773000	-2.333614000
1	0.003879000	0.329248000	-3.159571000
1	-1.955133000	-0.679535000	-2.201952000
6	-2.809575000	1.158009000	-1.467235000
6	-4.123015000	0.649659000	-1.545410000
6	-2.653068000	2.485264000	-1.009653000
6	-5.224626000	1.416209000	-1.160147000
1	-4.271785000	-0.368072000	-1.911965000
6	-3.753343000	3.251184000	-0.629907000
1	-1.656030000	2.918993000	-0.937127000
6	-5.048229000	2.722563000	-0.693944000
1	-6.229755000	0.991238000	-1.231841000
1	-3.593594000	4.272984000	-0.277145000
1	-5.908734000	3.325363000	-0.393738000
8	3.745533000	0.041596000	-0.096863000
1	2.964922000	-0.378143000	-0.591988000
6	1.600061000	-1.854942000	-2.239805000
1	0.551510000	-2.061253000	-2.557100000
1	2.143009000	-1.602047000	-3.184495000
6	4.892407000	0.043112000	-0.905516000
1	5.549588000	0.863289000	-0.554976000
1	5.477315000	-0.893577000	-0.779447000
6	2.215675000	-3.149203000	-1.690369000
1	1.621700000	-3.485805000	-0.820953000
1	3.214669000	-2.895583000	-1.295432000
6	2.337159000	-4.287606000	-2.707782000
1	2.966182000	-5.088529000	-2.281688000
1	2.882155000	-3.919293000	-3.596215000
6	0.999568000	-4.888341000	-3.145188000

	1	0.343316000	-4.136140000	-3.610181000
	1	1.140257000	-5.702131000	-3.874639000
	1	0.459604000	-5.310674000	-2.280479000
	6	4.608986000	0.235339000	-2.398189000
	1	5.578491000	0.317091000	-2.923687000
	1	4.120120000	-0.669754000	-2.797514000
	6	3.734303000	1.446720000	-2.724230000
	1	2.756946000	1.298103000	-2.242267000
	1	4.179839000	2.354734000	-2.276462000
	6	3.523907000	1.653371000	-4.222865000
	1	2.870906000	2.517579000	-4.426778000
	1	4.478654000	1.824167000	-4.748335000
	1	3.050834000	0.767065000	-4.677419000
pre-com ^{iPrOH}	28	-0.495891000	0.279083000	-0.633496000
	6	-1.858289000	0.304375000	-2.043223000
	6	-0.650699000	1.011196000	-2.411810000
	6	3.183001000	-1.581589000	3.376929000
	6	1.682445000	-1.262506000	3.413870000
	6	1.083373000	-0.967003000	2.021057000
	6	1.468303000	-2.107053000	1.023242000
	6	2.973458000	-2.347136000	0.983878000
	6	3.516521000	-2.688554000	2.372599000
	6	1.556393000	0.357668000	1.445887000
	6	-0.434472000	-0.927031000	2.048605000
	8	-1.062999000	-1.382420000	3.144779000
	7	-1.172461000	-0.567974000	1.062015000
	6	-2.479853000	-1.182150000	2.918203000
	7	1.119275000	0.861882000	0.350697000
	8	2.461905000	1.073406000	2.125609000
	6	1.742358000	2.186877000	0.162531000
	6	-2.571582000	-0.868325000	1.400719000
	6	-3.124978000	-2.016347000	0.576860000
	6	2.776797000	2.237771000	1.316919000
	6	0.684736000	3.268031000	0.206420000
	6	-4.490770000	-2.318948000	0.668600000
	6	-5.038366000	-3.366741000	-0.071279000
	6	-4.224805000	-4.122693000	-0.922742000
	6	0.549782000	4.182180000	-0.842615000
	6	-0.429030000	5.179544000	-0.796256000
	6	-1.281759000	5.272641000	0.305699000
	6	-2.863597000	-3.826867000	-1.017232000
	6	-2.315442000	-2.781667000	-0.267610000
	6	-1.154567000	4.360940000	1.359071000
	6	-0.179531000	3.365530000	1.306781000

	1	3.505796000	-1.872850000	4.389878000
	1	3.743295000	-0.672375000	3.114809000
	1	1.135663000	-2.126751000	3.819321000
	1	1.484082000	-0.418809000	4.091490000
	1	0.940278000	-3.020029000	1.346789000
	1	1.088533000	-1.828434000	0.032824000
	1	3.188842000	-3.156731000	0.267622000
	1	3.472513000	-1.447601000	0.590290000
	1	3.074755000	-3.643498000	2.713108000
	1	4.607058000	-2.844260000	2.331428000
	1	-2.804141000	-0.338577000	3.546981000
	1	-3.009819000	-2.095354000	3.215720000
	1	2.255314000	2.195331000	-0.807273000
	1	-3.187673000	0.023244000	1.211469000
	1	3.799829000	2.112652000	0.945600000
	1	2.685815000	3.126585000	1.954544000
	1	-5.136955000	-1.709398000	1.306109000
	1	-6.106110000	-3.586274000	0.004496000
	1	-4.653797000	-4.936879000	-1.511693000
	1	1.207543000	4.100858000	-1.711354000
	1	-0.530866000	5.879859000	-1.628424000
	1	-2.052228000	6.046287000	0.339478000
	1	-2.219679000	-4.406798000	-1.682921000
	1	-1.259557000	-2.535034000	-0.361100000
	1	-1.828499000	4.418369000	2.216893000
	1	-0.100024000	2.642538000	2.122479000
	8	2.075550000	-0.866032000	-2.056188000
	6	1.789106000	-1.709491000	-3.167197000
	1	1.461783000	-1.082820000	-4.020381000
	1	1.268999000	-0.351058000	-1.814267000
	1	-0.659143000	2.109855000	-2.431558000
	1	-0.074178000	0.601933000	-3.253471000
	1	-2.063901000	-0.654202000	-2.536955000
	6	-3.060235000	0.942045000	-1.483724000
	6	-4.286809000	0.245860000	-1.451371000
	6	-3.028247000	2.220292000	-0.878339000
	6	-5.413667000	0.780710000	-0.825090000
	1	-4.342920000	-0.742875000	-1.912448000
	6	-4.153270000	2.753596000	-0.253543000
	1	-2.100824000	2.791472000	-0.881231000
	6	-5.356957000	2.037129000	-0.213183000
	1	-6.345107000	0.207543000	-0.814122000
	1	-4.086492000	3.741406000	0.210644000
	1	-6.238016000	2.456834000	0.278614000

	6	5.370367000	0.277563000	-1.425366000
	1	5.273309000	0.383455000	-2.526214000
	8	4.102061000	0.458071000	-0.821904000
	1	3.433669000	-0.073515000	-1.308356000
	6	0.664352000	-2.684235000	-2.825741000
	1	-0.227440000	-2.134591000	-2.491119000
	1	0.389200000	-3.292988000	-3.701651000
	1	0.975513000	-3.360537000	-2.013015000
	6	3.081603000	-2.413527000	-3.549417000
	1	2.931733000	-3.056400000	-4.430095000
	1	3.869350000	-1.681550000	-3.784445000
	1	3.432528000	-3.043393000	-2.715992000
	6	5.937327000	-1.111097000	-1.127022000
	1	5.251255000	-1.896347000	-1.477598000
	1	6.910421000	-1.260539000	-1.622589000
	1	6.075803000	-1.240312000	-0.041196000
	6	6.282767000	1.387141000	-0.919511000
	1	7.283249000	1.321250000	-1.374160000
	1	5.855812000	2.374103000	-1.154839000
	1	6.395954000	1.312544000	0.174811000
TS1 ^{iPrOH}	28	-0.509155000	0.198003000	-0.479607000
	6	-1.973170000	0.230981000	-1.722245000
	6	-0.812169000	0.902556000	-2.348135000
	6	3.234821000	-1.346598000	3.635884000
	6	1.721071000	-1.108102000	3.561488000
	6	1.180288000	-0.909892000	2.123898000
	6	1.719449000	-2.038862000	1.173754000
	6	3.233502000	-2.204632000	1.267462000
	6	3.684528000	-2.473712000	2.703257000
	6	1.570586000	0.427088000	1.526571000
	6	-0.331987000	-1.032984000	2.081062000
	8	-0.919887000	-1.689205000	3.090358000
	7	-1.102331000	-0.672615000	1.113024000
	6	-2.344857000	-1.661256000	2.841074000
	7	1.027432000	0.933078000	0.486734000
	8	2.561148000	1.126270000	2.090301000
	6	1.685406000	2.210591000	0.170719000
	6	-2.448976000	-1.211499000	1.363453000
	6	-2.799626000	-2.337612000	0.408530000
	6	2.802484000	2.282200000	1.245040000
	6	0.689628000	3.347956000	0.189982000
	6	-4.126322000	-2.786445000	0.351743000
	6	-4.487848000	-3.829783000	-0.502251000
	6	-3.524206000	-4.432490000	-1.317614000

6	0.517165000	4.160514000	-0.935457000
6	-0.414252000	5.203537000	-0.925260000
6	-1.181569000	5.444501000	0.216560000
6	-2.201205000	-3.987596000	-1.267428000
6	-1.840352000	-2.947905000	-0.406586000
6	-1.016200000	4.635965000	1.346363000
6	-0.089430000	3.593839000	1.329874000
1	3.496885000	-1.583681000	4.680210000
1	3.769654000	-0.422975000	3.374538000
1	1.203462000	-1.984312000	3.976719000
1	1.433612000	-0.247816000	4.186131000
1	1.212917000	-2.975237000	1.464110000
1	1.426341000	-1.785440000	0.144931000
1	3.533205000	-3.029814000	0.601010000
1	3.713200000	-1.299270000	0.863037000
1	3.256953000	-3.433298000	3.049767000
1	4.780233000	-2.584738000	2.748250000
1	-2.792564000	-0.936763000	3.538657000
1	-2.748932000	-2.663033000	3.030997000
1	2.136196000	2.109100000	-0.824152000
1	-3.188631000	-0.407398000	1.243847000
1	3.797609000	2.163826000	0.802650000
1	2.752429000	3.178501000	1.877695000
1	-4.888056000	-2.300479000	0.967945000
1	-5.526799000	-4.165942000	-0.540580000
1	-3.806925000	-5.242727000	-1.993793000
1	1.111384000	3.965186000	-1.831640000
1	-0.545043000	5.824523000	-1.814415000
1	-1.913816000	6.255111000	0.224427000
1	-1.440647000	-4.442077000	-1.906548000
1	-0.814843000	-2.582652000	-0.398762000
1	-1.622415000	4.810914000	2.238139000
1	0.018393000	2.950455000	2.206978000
8	1.414528000	-0.651690000	-1.955880000
6	1.219682000	-1.606611000	-2.947936000
1	0.138531000	-1.638399000	-3.229316000
1	0.323342000	0.335187000	-1.981216000
1	-0.804605000	2.000276000	-2.347922000
1	-0.597063000	0.532900000	-3.361912000
1	-2.262826000	-0.724199000	-2.177432000
6	-3.108257000	0.966137000	-1.142768000
6	-4.373364000	0.350262000	-1.044062000
6	-2.974552000	2.264577000	-0.603425000
6	-5.445213000	0.985577000	-0.413731000

	1	-4.507066000	-0.646946000	-1.468478000
	6	-4.045411000	2.899753000	0.022099000
	1	-2.015152000	2.777388000	-0.662582000
	6	-5.288400000	2.264150000	0.130019000
	1	-6.413043000	0.479823000	-0.354031000
	1	-3.903243000	3.902746000	0.432102000
	1	-6.126096000	2.764246000	0.622083000
	6	4.680514000	0.233388000	-1.859165000
	1	4.299938000	0.462978000	-2.876434000
	8	3.611890000	0.244649000	-0.942938000
	1	2.792606000	-0.174881000	-1.370993000
	6	1.575005000	-3.014128000	-2.449078000
	1	0.955573000	-3.285819000	-1.581090000
	1	1.424428000	-3.777591000	-3.230933000
	1	2.629447000	-3.050755000	-2.129751000
	6	1.997994000	-1.262533000	-4.225666000
	1	1.776706000	-1.963077000	-5.048861000
	1	1.743154000	-0.243909000	-4.558822000
	1	3.083526000	-1.290215000	-4.035117000
	6	5.355972000	-1.139641000	-1.907620000
	1	4.624842000	-1.919065000	-2.169844000
	1	6.168923000	-1.167078000	-2.652108000
	1	5.778512000	-1.391211000	-0.920825000
	6	5.664731000	1.330278000	-1.464179000
	1	6.524727000	1.371241000	-2.151311000
	1	5.170312000	2.314719000	-1.470448000
	1	6.047196000	1.144722000	-0.446317000

Table S2. Cartesian coordinates of the optimized stationary points involved in the discussion of selectivity, calculated at the B3LYP-D3(BJ)/def2SVP level

Names	Cartesian Coordinates			
TS1 ^{Ra}	28	0.233724000	0.196044000	0.706688000
	6	1.862856000	0.461949000	1.683618000
	6	0.766580000	1.136005000	2.417183000
	6	-3.998871000	-2.198878000	-2.343682000
	6	-2.530350000	-1.849982000	-2.617714000
	6	-1.752937000	-1.373366000	-1.367691000
	6	-1.978204000	-2.366309000	-0.170625000
	6	-3.457664000	-2.652666000	0.076092000
	6	-4.147082000	-3.183607000	-1.181406000
	6	-2.160486000	0.013722000	-0.910547000
	6	-0.256096000	-1.359817000	-1.617969000

	8	0.202457000	-2.060201000	-2.663311000
	7	0.634433000	-0.819423000	-0.859485000
	6	1.635149000	-1.861699000	-2.708694000
	7	-1.494083000	0.707115000	-0.069772000
	8	-3.287344000	0.556176000	-1.382204000
	6	-2.195237000	1.976528000	0.174347000
	6	1.964078000	-1.242050000	-1.327436000
	6	2.625561000	-2.217927000	-0.372564000
	6	-3.490244000	1.803462000	-0.663756000
	6	-1.315967000	3.148796000	-0.197849000
	6	3.988362000	-2.501221000	-0.539130000
	6	4.633079000	-3.412597000	0.298038000
	6	3.920459000	-4.047765000	1.320535000
	6	-1.029297000	4.146691000	0.739533000
	6	-0.196230000	5.219174000	0.405809000
	6	0.358039000	5.302054000	-0.873369000
	6	2.563029000	-3.768081000	1.492619000
	6	1.916970000	-2.859959000	0.648831000
	6	0.077865000	4.307236000	-1.816435000
	6	-0.751005000	3.237738000	-1.478317000
	1	-4.432279000	-2.623052000	-3.264417000
	1	-4.562069000	-1.282158000	-2.119617000
	1	-2.014562000	-2.746792000	-2.989918000
	1	-2.454270000	-1.091726000	-3.412578000
	1	-1.444837000	-3.298985000	-0.422152000
	1	-1.521868000	-1.923576000	0.727437000
	1	-3.536328000	-3.380381000	0.900405000
	1	-3.943424000	-1.730730000	0.435551000
	1	-3.699879000	-4.155702000	-1.462130000
	1	-5.214385000	-3.374959000	-0.983718000
	1	1.852190000	-1.178710000	-3.544415000
	1	2.112905000	-2.833070000	-2.884707000
	1	-2.452931000	2.015744000	1.240239000
	1	2.609471000	-0.358340000	-1.431424000
	1	-4.362993000	1.665926000	-0.015710000
	1	-3.653300000	2.597351000	-1.404601000
	1	4.554849000	-1.986092000	-1.319834000
	1	5.697052000	-3.619592000	0.160128000
	1	4.424686000	-4.755013000	1.983242000
	1	-1.454322000	4.074370000	1.743806000
	1	0.026538000	5.987034000	1.150224000
	1	1.014249000	6.135732000	-1.133799000
	1	1.998758000	-4.252441000	2.292932000
	1	0.864546000	-2.627293000	0.806882000

	1	0.518616000	4.359750000	-2.814647000
	1	-0.948072000	2.451296000	-2.211551000
	8	-1.431010000	-0.497574000	2.516456000
	6	-1.100979000	-1.446031000	3.464054000
	1	-0.098051000	-1.263709000	3.918174000
	1	-1.817899000	-1.489515000	4.314839000
	1	-1.053842000	-2.480450000	3.044997000
	1	-0.371972000	0.491541000	2.295152000
	1	0.683049000	2.225353000	2.306806000
	1	0.736786000	0.868981000	3.484916000
	1	2.297902000	-0.411404000	2.185449000
	6	2.829229000	1.190444000	0.846190000
	6	4.115065000	0.656218000	0.622869000
	6	2.499260000	2.390101000	0.176969000
	6	5.017481000	1.269431000	-0.248415000
	1	4.399819000	-0.261964000	1.140341000
	6	3.401487000	3.003830000	-0.689693000
	1	1.517779000	2.839524000	0.326073000
	6	4.665460000	2.445730000	-0.917218000
	1	6.005848000	0.826922000	-0.401274000
	1	3.108983000	3.927338000	-1.195332000
	1	5.369824000	2.928194000	-1.599211000
	6	-4.640224000	-0.006690000	3.004782000
	1	-5.628786000	0.447661000	2.814485000
	1	-4.817431000	-1.070505000	3.270977000
	1	-4.217476000	0.486764000	3.903902000
	8	-3.829727000	0.145382000	1.876291000
	1	-2.889425000	-0.149435000	2.129979000
TS1 ^{Rb}	28	0.122411000	-0.664623000	0.181467000
	6	-0.205938000	-1.966571000	1.697074000
	1	-0.458324000	-2.951720000	1.284663000
	6	1.191192000	-1.522645000	1.498495000
	6	0.058976000	4.639427000	-1.841981000
	6	-0.625596000	3.333506000	-2.270410000
	6	-0.443001000	2.164797000	-1.272113000
	6	-0.803296000	2.649841000	0.172230000
	6	-0.017778000	3.893695000	0.571068000
	6	-0.288108000	5.041071000	-0.405540000
	6	0.973704000	1.615448000	-1.258823000
	6	-1.370770000	1.007957000	-1.603357000
	8	-2.390060000	1.216189000	-2.439811000
	7	-1.244756000	-0.178788000	-1.134876000
	6	-3.227055000	0.024368000	-2.351899000
	7	1.332119000	0.517985000	-0.694178000

	8	1.956111000	2.330426000	-1.827678000
	6	2.793598000	0.389970000	-0.769969000
	6	-2.255675000	-1.035016000	-1.804890000
	6	-2.798237000	-2.130236000	-0.920410000
	6	3.169627000	1.543854000	-1.733085000
	6	3.240170000	-0.979244000	-1.220101000
	6	-2.302109000	-3.430680000	-1.085511000
	6	-2.714043000	-4.467229000	-0.245199000
	6	-3.636437000	-4.208813000	0.771732000
	6	4.487918000	-1.469981000	-0.817855000
	6	4.922410000	-2.730727000	-1.235148000
	6	4.106533000	-3.515551000	-2.054216000
	6	-4.140492000	-2.915600000	0.937213000
	6	-3.722881000	-1.877627000	0.101804000
	6	2.858424000	-3.031246000	-2.457456000
	6	2.428449000	-1.768433000	-2.045535000
	1	-0.242754000	5.435240000	-2.542576000
	1	1.149339000	4.535098000	-1.936816000
	1	-1.709151000	3.501164000	-2.350147000
	1	-0.281617000	3.029278000	-3.271038000
	1	-1.881114000	2.862395000	0.162563000
	1	-0.672315000	1.819603000	0.879225000
	1	-0.303040000	4.179351000	1.596254000
	1	1.063584000	3.669283000	0.606405000
	1	-1.358435000	5.309538000	-0.345153000
	1	0.279200000	5.941620000	-0.118786000
	1	-3.614261000	-0.194604000	-3.353678000
	1	-4.030718000	0.261470000	-1.643581000
	1	3.192484000	0.572181000	0.240751000
	1	-1.730209000	-1.524378000	-2.645484000
	1	3.972744000	2.193013000	-1.362450000
	1	3.419064000	1.182315000	-2.742271000
	1	-1.572288000	-3.629951000	-1.875475000
	1	-2.314219000	-5.474564000	-0.384134000
	1	-3.962171000	-5.014244000	1.434604000
	1	5.116688000	-0.866766000	-0.157773000
	1	5.895706000	-3.105667000	-0.909931000
	1	4.439861000	-4.506062000	-2.372500000
	1	-4.858077000	-2.707114000	1.733994000
	1	-4.089700000	-0.864075000	0.264368000
	1	2.212596000	-3.644003000	-3.090995000
	1	1.443732000	-1.400329000	-2.338378000
	1	-0.561307000	-1.903350000	2.737177000
	8	-2.031851000	0.044103000	1.834886000

	6	-2.635396000	-0.216268000	3.050809000
	1	-2.008346000	-0.861617000	3.709764000
	1	-2.830269000	0.708412000	3.638963000
	1	-3.614029000	-0.743289000	2.957718000
	1	-1.095192000	-1.032520000	1.432565000
	6	1.838080000	-0.559880000	2.409875000
	6	1.107086000	0.479056000	3.029712000
	6	3.230959000	-0.595964000	2.619027000
	6	1.750337000	1.436085000	3.812566000
	1	0.029425000	0.544756000	2.860352000
	6	3.873802000	0.367806000	3.401192000
	1	3.812044000	-1.399979000	2.159017000
	6	3.137759000	1.392653000	4.001432000
	1	1.161810000	2.232363000	4.276473000
	1	4.956072000	0.312585000	3.548599000
	1	3.637164000	2.147123000	4.614115000
	1	1.885581000	-2.249191000	1.058171000
	6	-4.386701000	2.200615000	1.189266000
	1	-5.174591000	2.700970000	0.598995000
	1	-4.879999000	1.715502000	2.055620000
	1	-3.729948000	2.999055000	1.597724000
	8	-3.698017000	1.297066000	0.376328000
	1	-2.996612000	0.803296000	0.945643000
TS1 ^{Sa}	28	0.069880000	0.364757000	-0.729440000
	6	0.350180000	2.107677000	-1.718111000
	1	0.761626000	2.870291000	-1.046102000
	6	1.233182000	0.987429000	-2.111346000
	1	1.042254000	0.571580000	-3.110781000
	6	-2.774187000	-4.398655000	0.584362000
	6	-2.434284000	-3.108014000	1.341146000
	6	-1.807269000	-1.996616000	0.461197000
	6	-2.671779000	-1.793678000	-0.826618000
	6	-2.901361000	-3.101877000	-1.575469000
	6	-3.593548000	-4.132786000	-0.680902000
	6	-0.375696000	-2.312210000	0.059911000
	6	-1.782093000	-0.672768000	1.207920000
	8	-2.590614000	-0.516975000	2.259519000
	7	-1.029313000	0.321871000	0.910593000
	6	-2.538599000	0.901997000	2.594344000
	7	0.467733000	-1.476417000	-0.439779000
	8	0.081316000	-3.559457000	0.250383000
	6	1.782445000	-2.130720000	-0.517261000
	6	-1.204551000	1.345367000	1.972788000
	6	-1.075288000	2.761765000	1.472702000

6	1.397196000	-3.619228000	-0.347612000
6	2.726538000	-1.631168000	0.562358000
6	0.102460000	3.468864000	1.753121000
6	0.304994000	4.752593000	1.242024000
6	-0.676809000	5.342216000	0.441458000
6	4.091073000	-1.924431000	0.455125000
6	4.981946000	-1.537317000	1.456215000
6	4.518393000	-0.844596000	2.577525000
6	-1.854911000	4.643715000	0.162286000
6	-2.057736000	3.360115000	0.672578000
6	3.158899000	-0.543844000	2.688258000
6	2.267029000	-0.935462000	1.687518000
1	-3.329521000	-5.064371000	1.265264000
1	-1.848270000	-4.927049000	0.315000000
1	-3.357388000	-2.681256000	1.758156000
1	-1.774338000	-3.324766000	2.195120000
1	-3.627870000	-1.362433000	-0.494179000
1	-2.203013000	-1.016231000	-1.443889000
1	-3.506729000	-2.895481000	-2.472682000
1	-1.939294000	-3.507345000	-1.939417000
1	-4.590368000	-3.746023000	-0.401938000
1	-3.762380000	-5.074996000	-1.227576000
1	-2.582191000	0.997261000	3.685360000
1	-3.404126000	1.367307000	2.104609000
1	2.234208000	-1.938950000	-1.499899000
1	-0.384946000	1.176677000	2.695490000
1	1.304532000	-4.145306000	-1.310817000
1	2.058622000	-4.177757000	0.325121000
1	0.876969000	2.999738000	2.366655000
1	1.230878000	5.288688000	1.463519000
1	-0.521889000	6.343835000	0.032870000
1	4.464966000	-2.441638000	-0.431841000
1	6.045781000	-1.761972000	1.351330000
1	5.216379000	-0.534163000	3.358603000
1	-2.621002000	5.095469000	-0.472212000
1	-2.960221000	2.805174000	0.417072000
1	2.788216000	0.004202000	3.558075000
1	1.211846000	-0.677481000	1.766765000
6	2.655166000	0.934895000	-1.732386000
6	3.156003000	1.569189000	-0.574643000
6	3.574549000	0.217432000	-2.524338000
6	4.506413000	1.502674000	-0.241639000
1	2.470734000	2.119128000	0.073145000
6	4.928213000	0.147209000	-2.189303000

	1	3.214743000	-0.273745000	-3.433366000
	6	5.404799000	0.793983000	-1.046871000
	1	4.862202000	1.999105000	0.664367000
	1	5.616842000	-0.409128000	-2.831241000
	1	6.462746000	0.740935000	-0.780102000
	1	-0.132014000	2.603805000	-2.574147000
	8	-2.228678000	1.267053000	-1.659984000
	6	-2.534384000	1.234190000	-3.006037000
	1	-2.766716000	0.207191000	-3.378251000
	1	-3.409796000	1.867917000	-3.274324000
	1	-1.692808000	1.595753000	-3.642560000
	1	-0.853705000	1.683841000	-1.407785000
	6	-5.354258000	1.181511000	-0.698989000
	1	-6.196721000	1.110792000	0.011229000
	1	-5.535596000	0.431013000	-1.497256000
	1	-5.409006000	2.181762000	-1.176350000
	8	-4.151365000	0.968840000	-0.019129000
	1	-3.380842000	1.074868000	-0.686603000
TS1 ^{Sb}	28	0.057807000	-0.859355000	-0.352354000
	6	-1.307550000	-2.160920000	-0.641640000
	6	-0.111420000	-2.861538000	-0.114685000
	6	2.474439000	4.466721000	0.277918000
	6	1.730981000	3.644205000	-0.781601000
	6	1.030029000	2.363210000	-0.249015000
	6	0.210012000	2.692955000	1.051641000
	6	1.023922000	3.474102000	2.079975000
	6	1.589894000	4.765666000	1.489954000
	6	2.012440000	1.256510000	0.070153000
	6	0.016645000	1.858178000	-1.255140000
	8	-0.449894000	2.750375000	-2.139778000
	7	-0.528854000	0.690364000	-1.290235000
	6	-1.331260000	2.036270000	-3.033591000
	7	1.764702000	0.001469000	0.042068000
	8	3.242938000	1.616708000	0.450071000
	6	2.988393000	-0.732366000	0.442308000
	6	-1.643079000	0.736100000	-2.256708000
	6	-3.002333000	0.781094000	-1.583789000
	6	3.913158000	0.411514000	0.908555000
	6	3.484512000	-1.582233000	-0.704213000
	6	-4.143923000	0.581923000	-2.371593000
	6	-5.419057000	0.701855000	-1.817547000
	6	-5.563916000	1.014829000	-0.463498000
	6	3.503072000	-2.976006000	-0.577907000
	6	3.929389000	-3.780229000	-1.639007000

6	4.339135000	-3.195439000	-2.839610000
6	-4.429734000	1.197254000	0.329314000
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6	4.321859000	-1.802779000	-2.975086000
6	3.895837000	-1.003393000	-1.913530000
1	2.810482000	5.405799000	-0.192039000
1	3.375860000	3.932356000	0.605905000
1	0.942812000	4.272776000	-1.217588000
1	2.406893000	3.372909000	-1.608128000
1	-0.668159000	3.282499000	0.737771000
1	-0.137649000	1.745643000	1.485814000
1	0.374434000	3.689704000	2.943924000
1	1.831602000	2.827070000	2.452272000
1	0.757165000	5.427922000	1.187505000
1	2.166406000	5.315649000	2.251373000
1	-0.782429000	1.853597000	-3.971139000
1	-2.212022000	2.659756000	-3.225781000
1	2.695094000	-1.378690000	1.281137000
1	-1.588921000	-0.141727000	-2.914380000
1	3.956092000	0.468210000	2.003630000
1	4.918464000	0.393177000	0.468554000
1	-4.034725000	0.327437000	-3.430335000
1	-6.301093000	0.540403000	-2.441899000
1	-6.559906000	1.095860000	-0.022455000
1	3.164868000	-3.427213000	0.357908000
1	3.937212000	-4.867294000	-1.528339000
1	4.671041000	-3.822542000	-3.670606000
1	-4.534027000	1.407085000	1.395286000
1	-2.274863000	1.193342000	0.404807000
1	4.640503000	-1.340421000	-3.912682000
1	3.876749000	0.084306000	-2.027752000
8	1.008425000	-1.950145000	2.190249000
6	0.888617000	-3.011342000	3.066104000
1	0.710572000	-2.683677000	4.114603000
1	0.031459000	-3.681510000	2.814908000
1	1.791506000	-3.666708000	3.094926000
1	0.512644000	-2.200328000	0.805451000
1	0.557010000	-3.302303000	-0.866132000
1	-0.334072000	-3.608248000	0.663914000
6	-2.496597000	-2.066402000	0.234198000
6	-2.358979000	-1.806303000	1.615214000
6	-3.795055000	-2.230867000	-0.278353000
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	6	-4.915542000	-2.141303000	0.547714000
	1	-3.924123000	-2.426877000	-1.345735000
	6	-4.765789000	-1.885445000	1.913357000
	1	-3.347811000	-1.515705000	3.505870000
	1	-5.913451000	-2.266981000	0.120208000
	1	-5.642836000	-1.814094000	2.561451000
	1	-1.553895000	-2.328328000	-1.699657000
	6	1.210123000	0.542092000	4.350791000
	1	1.393087000	1.578634000	4.686514000
	1	0.156140000	0.300093000	4.602253000
	1	1.850882000	-0.119739000	4.971044000
	8	1.480021000	0.444132000	2.984110000
	1	1.259863000	-0.502302000	2.686724000
TSI'	28	-0.087755000	0.127006000	0.687247000
	6	1.594098000	-0.241126000	1.849216000
	6	0.628478000	0.788129000	2.283722000
	6	-5.536823000	0.061996000	-1.351379000
	6	-4.116003000	-0.391650000	-1.711510000
	6	-3.116733000	-0.437410000	-0.509249000
	6	-3.776201000	-1.192685000	0.686295000
	6	-5.150182000	-0.632199000	1.045891000
	6	-6.103911000	-0.698066000	-0.149436000
	6	-2.696820000	0.952089000	-0.086340000
	6	-1.888444000	-1.202654000	-0.977302000
	8	-2.142547000	-2.403339000	-1.515567000
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	6	-1.514431000	2.709331000	0.681006000
	6	0.034609000	-1.774708000	-1.915546000
	6	1.526851000	-1.896267000	-1.789957000
	6	-2.897415000	3.185836000	0.157467000
	6	-0.317024000	3.298622000	-0.034609000
	6	2.306809000	-0.734618000	-1.863667000
	6	3.697747000	-0.814233000	-1.887298000
	6	4.330330000	-2.058533000	-1.844352000
	6	0.423703000	4.328634000	0.553779000
	6	1.535029000	4.868929000	-0.100485000
	6	1.917049000	4.377689000	-1.350691000
	6	3.560368000	-3.221293000	-1.775678000
	6	2.166161000	-3.139554000	-1.748669000
	6	1.182688000	3.345469000	-1.943492000
	6	0.071846000	2.809540000	-1.290726000

1	-6.178644000	-0.089667000	-2.235044000
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1	-4.160265000	-1.415011000	-2.109138000
1	-3.698648000	0.243127000	-2.509858000
1	-3.882342000	-2.241308000	0.365531000
1	-3.073900000	-1.207939000	1.531047000
1	-5.555406000	-1.206076000	1.894792000
1	-5.059442000	0.411982000	1.394109000
1	-6.258605000	-1.758127000	-0.421354000
1	-7.094436000	-0.294335000	0.116888000
1	-0.917076000	-3.646465000	-2.644244000
1	-0.550780000	-3.568580000	-0.850228000
1	-1.410151000	2.897205000	1.759439000
1	-0.148435000	-1.362814000	-2.929174000
1	-3.525870000	3.637957000	0.936830000
1	-2.819886000	3.870715000	-0.698240000
1	1.819286000	0.242022000	-1.892423000
1	4.290226000	0.100191000	-1.917508000
1	5.421015000	-2.118341000	-1.852007000
1	0.142523000	4.698462000	1.543404000
1	2.112104000	5.664432000	0.376191000
1	2.792723000	4.788826000	-1.857960000
1	4.044635000	-4.199970000	-1.732843000
1	1.578707000	-4.056327000	-1.679083000
1	1.487195000	2.943712000	-2.912619000
1	-0.472093000	1.977458000	-1.740611000
1	1.734232000	-1.032914000	2.600586000
8	0.638629000	-2.641964000	0.907795000
6	1.525768000	-3.511154000	1.510506000
1	1.976212000	-3.107664000	2.451905000
1	1.047816000	-4.473645000	1.803797000
1	2.385366000	-3.772215000	0.854044000
1	1.053583000	-1.185189000	1.101481000
1	0.970537000	1.830800000	2.285277000
1	0.016783000	0.544847000	3.161900000
6	2.926804000	0.209409000	1.326645000
6	3.085431000	1.441480000	0.668999000
6	4.064824000	-0.588783000	1.512181000
6	4.341642000	1.874569000	0.246281000
1	2.215824000	2.071679000	0.486986000
6	5.324133000	-0.161456000	1.084293000
1	3.957928000	-1.560676000	1.999811000
6	5.472086000	1.077470000	0.456163000
1	4.434107000	2.841894000	-0.254282000

	1	6.195272000	-0.801923000	1.244473000
	1	6.457428000	1.416218000	0.126462000
	6	-0.988135000	-2.179913000	3.704888000
	1	-1.814351000	-1.830380000	4.349801000
	1	-0.802268000	-3.244039000	3.960834000
	1	-0.082808000	-1.613099000	4.010760000
	8	-1.332540000	-1.992788000	2.366799000
	1	-0.572793000	-2.339878000	1.774995000
INT1 ^s	28	0.099888000	-0.890542000	0.119732000
	6	-1.539651000	-1.894235000	-0.148621000
	6	-1.276845000	-3.404875000	-0.187098000
	6	2.566052000	4.399328000	-0.090964000
	6	1.922439000	3.451170000	-1.111743000
	6	1.222838000	2.219360000	-0.483511000
	6	0.272113000	2.680333000	0.674181000
	6	0.980912000	3.569398000	1.691264000
	6	1.592002000	4.800809000	1.020088000
	6	2.199278000	1.205628000	0.065878000
	6	0.346829000	1.504300000	-1.497210000
	8	0.059636000	2.186783000	-2.614034000
	7	-0.227654000	0.354345000	-1.361508000
	6	-0.699016000	1.298881000	-3.460943000
	7	1.907701000	-0.019122000	0.259687000
	8	3.434920000	1.596115000	0.412088000
	6	3.097065000	-0.709714000	0.800899000
	6	-1.190979000	0.214570000	-2.480222000
	6	-2.628757000	0.440220000	-2.045507000
	6	4.030271000	0.472214000	1.119894000
	6	3.560926000	-1.735637000	-0.212989000
	6	-3.664813000	-0.092305000	-2.824185000
	6	-4.998748000	0.151492000	-2.493976000
	6	-5.311158000	0.928490000	-1.374681000
	6	2.961459000	-3.003838000	-0.190285000
	6	3.288819000	-3.957360000	-1.155321000
	6	4.217592000	-3.654396000	-2.156324000
	6	-4.284109000	1.452681000	-0.589734000
	6	-2.950051000	1.209517000	-0.922528000
	6	4.811289000	-2.390057000	-2.190213000
	6	4.479766000	-1.434019000	-1.225393000
	1	2.921091000	5.294258000	-0.627951000
	1	3.450481000	3.923392000	0.353650000
	1	1.152997000	4.001664000	-1.671128000
	1	2.665783000	3.116917000	-1.852127000
	1	-0.558191000	3.235129000	0.205191000

1	-0.138765000	1.786831000	1.161367000
1	0.252897000	3.866710000	2.463409000
1	1.749598000	2.974882000	2.208803000
1	0.780800000	5.419967000	0.593752000
1	2.107424000	5.430113000	1.763718000
1	-0.016934000	0.901710000	-4.229737000
1	-1.507833000	1.869976000	-3.931296000
1	2.774332000	-1.224502000	1.711880000
1	-1.094810000	-0.785217000	-2.923148000
1	4.008174000	0.717673000	2.190202000
1	5.063876000	0.356694000	0.773150000
1	-3.425019000	-0.714275000	-3.691732000
1	-5.796662000	-0.277269000	-3.104996000
1	-6.354111000	1.105624000	-1.103072000
1	2.218515000	-3.217988000	0.580196000
1	2.814791000	-4.941516000	-1.127228000
1	4.476275000	-4.401768000	-2.910397000
1	-4.518079000	2.028313000	0.307509000
1	-2.158295000	1.586798000	-0.278332000
1	5.533566000	-2.144267000	-2.972684000
1	4.936973000	-0.442517000	-1.275977000
8	0.573774000	-1.649072000	1.778601000
6	0.093932000	-2.650236000	2.609206000
1	0.472984000	-2.493324000	3.640981000
1	-1.010033000	-2.689227000	2.681039000
1	0.437019000	-3.662529000	2.304445000
1	-0.964280000	-3.814031000	0.779907000
1	-0.488031000	-3.644090000	-0.920495000
1	-2.182178000	-3.964973000	-0.491653000
6	-2.678396000	-1.485288000	0.761157000
6	-2.494322000	-0.653715000	1.880274000
6	-3.994206000	-1.882315000	0.462176000
6	-3.574914000	-0.229156000	2.657486000
1	-1.481666000	-0.338215000	2.133920000
6	-5.078699000	-1.460321000	1.232104000
1	-4.171387000	-2.512861000	-0.413398000
6	-4.875142000	-0.626794000	2.336042000
1	-3.397556000	0.420138000	3.519569000
1	-6.091106000	-1.772940000	0.962023000
1	-5.722644000	-0.290574000	2.939000000
1	-1.878171000	-1.645188000	-1.164902000
6	0.622106000	0.623725000	4.286192000
1	0.770091000	1.630507000	4.713829000
1	-0.469977000	0.429993000	4.272110000

	1	1.073341000	-0.103751000	4.992672000
	8	1.195515000	0.579912000	3.010569000
	1	0.941471000	-0.284697000	2.568042000
INT1-1 ^s	28	-0.109091000	0.103562000	-0.910953000
	6	0.418143000	-1.081314000	-2.341624000
	6	-5.346134000	-0.270427000	0.853482000
	6	-4.141419000	0.663259000	1.023390000
	6	-2.950074000	0.326747000	0.086698000
	6	-3.447669000	0.183257000	-1.380442000
	6	-4.603751000	-0.807402000	-1.500516000
	6	-5.778557000	-0.393189000	-0.610105000
	6	-2.217574000	-0.937218000	0.487770000
	6	-1.933397000	1.457389000	0.179867000
	8	-2.288059000	2.626510000	-0.370233000
	7	-0.819615000	1.412284000	0.824761000
	6	-1.111184000	3.485780000	-0.269368000
	7	-1.044533000	-1.218040000	0.052238000
	8	-2.749420000	-1.804469000	1.359986000
	6	-0.524500000	-2.384411000	0.797184000
	6	-0.270993000	2.780473000	0.817059000
	6	1.232526000	2.824925000	0.661283000
	6	-1.821179000	-2.920948000	1.445886000
	6	0.546022000	-1.921912000	1.768911000
	6	2.012317000	1.756485000	1.119177000
	6	3.401387000	1.793335000	1.000136000
	6	4.031539000	2.901853000	0.428319000
	6	1.895866000	-2.172073000	1.502136000
	6	2.886954000	-1.705706000	2.370329000
	6	2.536752000	-0.984573000	3.512747000
	6	3.258433000	3.976275000	-0.019380000
	6	1.867153000	3.937619000	0.099544000
	6	1.188416000	-0.723317000	3.780930000
	6	0.200293000	-1.185218000	2.912235000
	1	-6.177679000	0.110833000	1.468287000
	1	-5.094362000	-1.267033000	1.245640000
	1	-4.441859000	1.695461000	0.784129000
	1	-3.791720000	0.663843000	2.067281000
	1	-3.771291000	1.181061000	-1.712294000
	1	-2.592940000	-0.102624000	-2.011082000
	1	-4.919227000	-0.869793000	-2.554204000
	1	-4.263314000	-1.820754000	-1.220284000
	1	-6.169149000	0.578408000	-0.963605000
	1	-6.606046000	-1.115380000	-0.700840000
	1	-1.455763000	4.492945000	-0.006303000

	1	-0.600831000	3.461119000	-1.240447000
	1	-0.091022000	-3.102884000	0.089259000
	1	-0.516811000	3.209356000	1.809085000
	1	-2.258078000	-3.759644000	0.883245000
	1	-1.712942000	-3.195217000	2.501674000
	1	1.526479000	0.883989000	1.551035000
	1	3.988724000	0.941097000	1.347878000
	1	5.119478000	2.928270000	0.328586000
	1	2.180872000	-2.715843000	0.601978000
	1	3.935653000	-1.902622000	2.137824000
	1	3.310701000	-0.612281000	4.187859000
	1	3.739295000	4.846892000	-0.472244000
	1	1.276714000	4.780685000	-0.268395000
	1	0.907850000	-0.144006000	4.663510000
	1	-0.845510000	-0.945298000	3.115404000
	9	0.571753000	1.563122000	-1.725429000
	6	1.806929000	-1.512622000	-1.986191000
	6	2.806325000	-0.565724000	-1.676150000
	6	2.157019000	-2.875070000	-1.946715000
	6	4.090253000	-0.975198000	-1.320627000
	1	2.536793000	0.492543000	-1.682271000
	6	3.447512000	-3.286132000	-1.595610000
	1	1.400945000	-3.624247000	-2.201475000
	6	4.420505000	-2.336059000	-1.274509000
	1	4.840057000	-0.221327000	-1.067148000
	1	3.692245000	-4.351631000	-1.572512000
	1	5.428798000	-2.651667000	-0.994648000
	6	0.299434000	-0.402507000	-3.702550000
	1	0.635388000	-1.082468000	-4.508764000
	1	-0.744779000	-0.121137000	-3.917413000
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	1	-0.251564000	-1.958425000	-2.310546000
INT1-2 ^S	28	0.870808000	0.484433000	0.586088000
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	6	-0.393683000	5.557351000	-1.182835000
	6	-0.300508000	4.185648000	-1.861000000
	6	-0.045369000	3.025113000	-0.865429000
	6	-1.074865000	3.087158000	0.294484000
	6	-1.098686000	4.453216000	0.972474000
	6	-1.405382000	5.564364000	-0.033893000
	6	1.356951000	3.045775000	-0.288060000
	6	-0.164084000	1.694785000	-1.604227000
	8	-1.224296000	1.502425000	-2.394412000
	7	0.713339000	0.755238000	-1.568293000

6	-1.133230000	0.097899000	-2.842918000
7	1.822693000	2.106517000	0.452962000
8	2.218111000	4.013198000	-0.625189000
6	3.291238000	2.276017000	0.564641000
6	0.368153000	-0.175252000	-2.657388000
6	0.871922000	-1.588028000	-2.505404000
6	3.452637000	3.737138000	0.091943000
6	3.971882000	1.230117000	-0.300957000
6	1.820552000	-1.919480000	-1.533565000
6	2.367771000	-3.202181000	-1.486329000
6	1.986297000	-4.165948000	-2.422107000
6	4.623059000	0.141089000	0.287034000
6	5.185269000	-0.861434000	-0.508589000
6	5.097992000	-0.786052000	-1.898644000
6	1.045900000	-3.837437000	-3.403288000
6	0.490519000	-2.558647000	-3.440423000
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6	3.890784000	1.301546000	-1.700552000
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1	-2.058805000	2.860860000	-0.131425000
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1	3.515494000	4.447190000	0.930209000
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1	0.731439000	-4.586536000	-4.133654000
1	-0.250647000	-2.316488000	-4.206626000
1	4.367890000	0.360755000	-3.581580000
1	3.363980000	2.130331000	-2.177988000

9	-0.206987000	-1.067744000	0.461275000
6	-4.387191000	1.228900000	1.255335000
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6	-1.862166000	-3.769671000	0.995681000
6	-2.269910000	-3.645363000	-0.516490000
5	-1.742326000	-1.547045000	0.337302000
5	-2.863003000	-0.234538000	0.357023000
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8	-3.974609000	-0.308574000	-0.463888000
8	-1.988542000	-2.420463000	1.446898000
8	-1.762709000	-2.354908000	-0.855446000
6	-0.402707000	-4.217689000	1.162825000
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1	-0.274097000	-5.289937000	0.948151000
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	6	2.182373000	-0.398282000	2.804812000
	6	2.271312000	-1.725333000	2.333114000
	6	3.265098000	0.103524000	3.551441000
	6	3.403579000	-2.500093000	2.577789000
	1	1.441903000	-2.134480000	1.757272000
	6	4.397829000	-0.676236000	3.807195000
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	6	4.476887000	-1.981297000	3.313800000
	1	3.447847000	-3.522402000	2.192677000
	1	5.221238000	-0.262455000	4.395573000
	1	5.361623000	-2.592399000	3.508046000
	1	1.170367000	1.474940000	2.843961000
TS2 ^S	6	3.341992000	-3.026615000	-1.891143000
	6	2.874703000	-1.581528000	-2.030436000
	6	3.581355000	-0.635908000	-1.017236000
	6	5.119348000	-0.782304000	-1.194754000
	6	5.631493000	-2.229485000	-1.190072000
	6	4.847075000	-3.137290000	-2.141267000
	6	3.150735000	-0.893912000	0.427376000
	6	3.149739000	0.789227000	-1.305875000
	8	4.120562000	1.680166000	-1.545660000
	7	1.945655000	1.240773000	-1.295373000
	6	3.477723000	2.928886000	-1.879031000
	7	2.132325000	-0.394396000	1.013354000
	8	4.003321000	-1.628781000	1.180995000
	6	2.317459000	-0.642466000	2.463357000
	6	2.011813000	2.711924000	-1.430868000
	6	1.675217000	3.445197000	-0.146533000
	6	3.366894000	-1.771334000	2.468327000
	6	1.104483000	-0.955317000	3.296784000
	6	1.287477000	4.790707000	-0.218879000
	6	1.092307000	5.536712000	0.945285000
	6	1.278949000	4.941092000	2.196534000
	6	0.146950000	-1.873407000	2.859013000
	6	-0.918794000	-2.222960000	3.688463000
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	1	1.792327000	-1.510109000	-1.909361000
	1	5.361181000	-0.322585000	-2.164907000
	1	5.643533000	-0.186910000	-0.433424000
	1	6.698051000	-2.216768000	-1.469207000
	1	5.576291000	-2.636015000	-0.171561000
	1	5.054558000	-2.847658000	-3.187912000
	1	5.186597000	-4.180193000	-2.032433000
	1	3.574498000	3.078757000	-2.965626000
	1	3.987959000	3.737245000	-1.341636000
	1	2.771238000	0.280776000	2.869690000
	1	1.321941000	3.043087000	-2.217866000
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	1	2.891201000	-2.764101000	2.515747000
	1	1.139033000	5.260803000	-1.195545000
	1	0.787757000	6.583575000	0.875579000
	1	1.122218000	5.521499000	3.108638000
	1	0.206725000	-2.288628000	1.855727000
	1	-1.671652000	-2.919569000	3.317799000
	1	-1.865345000	-1.949800000	5.615711000
	1	1.748945000	3.109163000	3.245582000
	1	2.059701000	1.783472000	1.165265000
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	6	-3.334198000	0.952425000	1.216135000
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	6	-2.352977000	-3.422326000	0.071297000
	6	-2.676643000	-3.029411000	-1.421151000
	5	-0.971346000	-1.694786000	-0.550593000
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	8	-0.995161000	0.805415000	1.310850000
	8	-1.688863000	-2.248441000	0.559348000
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	6	-1.368862000	-4.598217000	0.178022000
	1	-1.038435000	-4.686043000	1.224120000
	1	-1.833968000	-5.550943000	-0.117022000
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INT2 ^s	6	4.107136000	-0.146422000	1.684808000
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6	5.387280000	0.688375000	1.617462000
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TS3 ^S	6	4.123594000	-0.332609000	1.621667000
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INT3 ^s	6	-0.615975000	-4.891633000	1.493829000
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	6	1.458216000	-1.414028000	3.459678000
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6	2.976771000	-3.701952000	1.054142000
6	2.199511000	-2.748856000	0.387839000
6	-0.039683000	3.957372000	-2.095223000
6	-0.899038000	2.937764000	-1.687386000
1	-4.300277000	-3.129871000	-3.011399000
1	-4.499983000	-1.732755000	-1.947169000
1	-1.854660000	-3.019444000	-2.823399000
1	-2.469510000	-1.449388000	-3.341316000
1	-1.167718000	-3.348660000	-0.283799000
1	-1.288406000	-1.927205000	0.775328000
1	-3.188902000	-3.530253000	1.151850000
1	-3.774507000	-1.961447000	0.586256000
1	-3.361784000	-4.472914000	-1.148924000
1	-4.923723000	-3.799359000	-0.659263000
1	1.718388000	-0.547678000	-3.536586000
1	2.275658000	-2.214035000	-3.142515000
1	-2.813589000	2.064915000	1.020116000
1	2.476729000	0.065097000	-1.348839000
1	-4.576132000	1.438961000	-0.388888000
1	-3.772853000	2.346501000	-1.741869000
1	4.612881000	-1.351004000	-1.562918000
1	5.991611000	-3.052279000	-0.394181000
1	4.946346000	-4.563697000	1.294737000
1	-1.772526000	4.137301000	1.374494000
1	-0.237893000	5.959594000	0.656763000
1	0.881895000	5.843454000	-1.567357000
1	2.513648000	-4.347313000	1.804498000
1	1.143428000	-2.635885000	0.629480000
1	0.457325000	3.894729000	-3.066056000
1	-1.065254000	2.077159000	-2.340462000
8	-2.220725000	-0.263734000	2.901133000
6	-1.747055000	-1.368074000	3.637065000
1	-0.921746000	-1.084433000	4.314573000
1	-2.576336000	-1.755793000	4.248168000
1	-1.388208000	-2.186837000	2.985161000
1	-1.469001000	0.134411000	2.397120000
1	0.312487000	2.515359000	2.133808000
1	-0.008684000	1.198374000	3.339698000
1	1.939007000	-0.069658000	2.602223000
6	2.654205000	1.322132000	1.093356000
6	3.980821000	0.811632000	1.100887000
6	2.348424000	2.348601000	0.170184000
6	4.908992000	1.296437000	0.168507000
6	3.285838000	2.821748000	-0.743913000

	1	1.340908000	2.762574000	0.154650000
	6	4.577656000	2.284486000	-0.761816000
	1	5.923362000	0.886282000	0.179854000
	1	3.001196000	3.609487000	-1.446142000
	1	5.322435000	2.640998000	-1.477762000
	6	-5.550457000	-0.067994000	2.479555000
	1	-6.500989000	0.213616000	1.997866000
	1	-5.670787000	-1.098751000	2.870559000
	1	-5.401407000	0.603971000	3.347211000
	8	-4.517724000	0.036677000	1.533990000
	1	-3.664515000	-0.121223000	2.002043000
	6	4.405263000	-0.229597000	2.104244000
	1	5.467471000	-0.484913000	1.980988000
	1	4.257656000	0.129070000	3.136726000
	1	3.826669000	-1.159836000	2.004049000
TS1 ^R -1a	28	0.042550000	0.242386000	0.743222000
	6	1.635052000	0.627593000	1.747240000
	6	0.497081000	1.326600000	2.391749000
	6	-3.935567000	-2.624645000	-2.152352000
	6	-2.518086000	-2.147632000	-2.493196000
	6	-1.767982000	-1.526843000	-1.293021000
	6	-1.848059000	-2.476589000	-0.047593000
	6	-3.281543000	-2.896815000	0.266450000
	6	-3.951374000	-3.557778000	-0.939173000
	6	-2.309762000	-0.167510000	-0.890918000
	6	-0.293512000	-1.329204000	-1.594703000
	8	0.200409000	-1.870771000	-2.714757000
	7	0.550848000	-0.728975000	-0.827904000
	6	1.579602000	-1.439487000	-2.808878000
	7	-1.712286000	0.603697000	-0.066973000
	8	-3.455989000	0.275870000	-1.414537000
	6	-2.494161000	1.839175000	0.091403000
	6	1.900308000	-0.929584000	-1.383111000
	6	2.717523000	-1.917638000	-0.572122000
	6	-3.761077000	1.534612000	-0.751995000
	6	-1.668327000	3.028151000	-0.346640000
	6	4.074467000	-2.081133000	-0.885019000
	6	4.852999000	-3.015778000	-0.202759000
	6	4.284277000	-3.795183000	0.810414000
	6	-1.401593000	4.076579000	0.539744000
	6	-0.595406000	5.150806000	0.150440000
	6	-0.049341000	5.185876000	-1.134317000
	6	2.936451000	-3.628451000	1.134418000
	6	2.155226000	-2.694473000	0.445994000

6	-0.313202000	4.142544000	-2.028571000
6	-1.113876000	3.070679000	-1.634318000
1	-4.353943000	-3.134148000	-3.035958000
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1	-1.920669000	-3.006581000	-2.833134000
1	-2.540218000	-1.431346000	-3.328555000
1	-1.228143000	-3.360919000	-0.274711000
1	-1.412881000	-1.949351000	0.814004000
1	-3.261508000	-3.584959000	1.127324000
1	-3.848101000	-2.010083000	0.595941000
1	-3.418570000	-4.494774000	-1.187808000
1	-4.988234000	-3.841625000	-0.695955000
1	1.627933000	-0.639696000	-3.564266000
1	2.189256000	-2.293918000	-3.125602000
1	-2.769977000	1.931389000	1.149412000
1	2.427506000	0.033440000	-1.414425000
1	-4.627943000	1.357704000	-0.105877000
1	-3.973947000	2.281618000	-1.527944000
1	4.528934000	-1.455483000	-1.657968000
1	5.910510000	-3.128811000	-0.453050000
1	4.894019000	-4.523136000	1.350536000
1	-1.818463000	4.041786000	1.549370000
1	-0.386236000	5.957608000	0.856602000
1	0.587343000	6.020229000	-1.437257000
1	2.485585000	-4.223534000	1.931987000
1	1.109532000	-2.551877000	0.716490000
1	0.117908000	4.159875000	-3.032328000
1	-1.296058000	2.245520000	-2.327832000
8	-1.616890000	-0.410031000	2.574084000
6	-1.260408000	-1.273571000	3.590506000
1	-0.290764000	-0.993448000	4.067609000
1	-2.005027000	-1.314289000	4.417617000
1	-1.126297000	-2.326139000	3.241815000
1	-0.601724000	0.624414000	2.299155000
1	0.382568000	2.397765000	2.178847000
1	0.447233000	1.157802000	3.478942000
1	2.048810000	-0.194301000	2.339049000
6	2.621271000	1.315893000	0.893912000
6	3.983386000	0.914321000	0.870874000
6	2.212230000	2.337643000	0.009147000
6	4.848653000	1.491570000	-0.070034000
6	3.089357000	2.908274000	-0.909614000
1	1.174376000	2.670793000	0.025316000
6	4.416850000	2.471703000	-0.966666000

	1	5.893002000	1.166575000	-0.089379000
	1	2.729272000	3.689469000	-1.583344000
	1	5.114673000	2.902187000	-1.689164000
	6	-4.855399000	-0.172777000	2.966068000
	1	-5.876211000	0.175768000	2.728026000
	1	-4.944335000	-1.223568000	3.315255000
	1	-4.494729000	0.425624000	3.827852000
	8	-4.039132000	-0.039562000	1.839632000
	1	-3.079443000	-0.226350000	2.129925000
	6	4.517746000	-0.091160000	1.859152000
	1	5.589116000	-0.273119000	1.693411000
	1	4.390284000	0.268389000	2.893983000
	1	4.002848000	-1.059547000	1.792042000
TS1 ^S -1a	28	-0.115728000	0.751435000	-0.327459000
	6	1.228395000	1.944655000	-0.960208000
	6	0.337354000	2.714804000	-0.061584000
	6	-3.813179000	-3.870610000	-0.913471000
	6	-2.650720000	-3.103485000	-1.554494000
	6	-1.771124000	-2.271855000	-0.569065000
	6	-1.426484000	-3.114449000	0.717694000
	6	-2.642369000	-3.816619000	1.321042000
	6	-3.357475000	-4.694849000	0.292859000
	6	-2.466903000	-1.006790000	-0.130372000
	6	-0.437003000	-1.974191000	-1.217708000
	8	0.106971000	-3.015053000	-1.871867000
	7	0.294233000	-0.915944000	-1.146144000
	6	1.323055000	-2.537079000	-2.484883000
	7	-1.948124000	0.144882000	0.071006000
	8	-3.781462000	-1.125048000	0.135307000
	6	-2.993066000	1.049211000	0.602380000
	6	1.628018000	-1.254923000	-1.686372000
	6	2.646778000	-1.490334000	-0.584966000
	6	-4.269609000	0.183148000	0.514474000
	6	-3.044660000	2.347998000	-0.163836000
	6	3.991411000	-1.642136000	-0.950753000
	6	4.959470000	-1.925267000	0.010331000
	6	4.592978000	-2.058578000	1.353269000
	6	-3.045090000	3.565016000	0.525478000
	6	-3.061511000	4.774525000	-0.173781000
	6	-3.065090000	4.776574000	-1.571059000
	6	3.256133000	-1.902000000	1.721236000
	6	2.281611000	-1.617982000	0.759054000
	6	-3.060721000	3.562993000	-2.266810000
	6	-3.055707000	2.356486000	-1.565000000

1	-4.251582000	-4.529800000	-1.680992000
1	-4.602711000	-3.173056000	-0.603524000
1	-1.978442000	-3.829258000	-2.030776000
1	-3.017842000	-2.440184000	-2.354897000
1	-0.683998000	-3.869242000	0.413690000
1	-0.956464000	-2.435959000	1.445821000
1	-2.300704000	-4.421917000	2.176519000
1	-3.343434000	-3.069637000	1.726502000
1	-2.668603000	-5.491741000	-0.043534000
1	-4.222145000	-5.201094000	0.752047000
1	1.109817000	-2.338421000	-3.547881000
1	2.090141000	-3.314118000	-2.390876000
1	-2.689723000	1.276359000	1.634073000
1	1.981075000	-0.445683000	-2.337847000
1	-4.801188000	0.086257000	1.470191000
1	-4.969514000	0.523226000	-0.263627000
1	4.288145000	-1.511616000	-1.994572000
1	6.006168000	-2.022844000	-0.286539000
1	5.351351000	-2.273683000	2.109998000
1	-2.996049000	3.558456000	1.615829000
1	-3.054007000	5.719322000	0.374931000
1	-3.064165000	5.722054000	-2.118700000
1	2.959721000	-1.986920000	2.768779000
1	1.252577000	-1.453308000	1.081979000
1	-3.055047000	3.558257000	-3.359493000
1	-3.031607000	1.410235000	-2.111941000
8	-0.792816000	1.793238000	2.240862000
6	-0.421791000	2.725036000	3.188881000
1	0.172521000	3.564883000	2.756993000
1	-1.294056000	3.205989000	3.690990000
1	0.208271000	2.298907000	4.002129000
1	-0.302434000	2.068955000	0.884588000
1	-0.382694000	3.366882000	-0.570326000
1	0.857223000	3.285662000	0.719693000
6	2.688098000	1.784463000	-0.767006000
6	3.332476000	1.600491000	0.487017000
6	3.493133000	1.785209000	-1.925547000
6	4.724923000	1.448693000	0.515192000
6	4.877188000	1.626536000	-1.877942000
1	3.004778000	1.934034000	-2.893384000
6	5.503553000	1.463084000	-0.642587000
1	5.208727000	1.294282000	1.483230000
1	5.461932000	1.639457000	-2.801527000
1	6.586753000	1.334878000	-0.578132000

	6	0.301977000	-0.885734000	3.833453000
	1	0.503579000	-1.960699000	3.989276000
	1	1.269527000	-0.351188000	3.927568000
	1	-0.341359000	-0.548258000	4.672020000
	8	-0.297301000	-0.705268000	2.583446000
	1	-0.508281000	0.284544000	2.468906000
	6	2.580051000	1.554524000	1.790447000
	1	3.174000000	1.038391000	2.557728000
	1	2.363298000	2.566274000	2.169920000
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	1	1.000861000	2.086092000	-2.027618000
pre-com-1b	28	0.330402000	-0.199198000	0.966535000
	6	-1.089404000	-0.311922000	2.340192000
	6	0.079051000	-1.098979000	2.665046000
	6	4.371889000	1.817775000	-2.474866000
	6	2.856533000	1.698372000	-2.675280000
	6	2.127785000	1.226917000	-1.400592000
	6	2.525903000	2.126377000	-0.189389000
	6	4.038471000	2.218764000	-0.009464000
	6	4.722514000	2.715686000	-1.285336000
	6	2.418747000	-0.225819000	-1.066491000
	6	0.616197000	1.316771000	-1.530037000
	8	0.101226000	1.932392000	-2.603801000
	7	-0.211236000	0.879260000	-0.651046000
	6	-1.338449000	1.790854000	-2.507693000
	7	1.918666000	-0.825103000	-0.049933000
	8	3.139048000	-0.963429000	-1.918615000
	6	2.252634000	-2.259536000	-0.144216000
	6	-1.567274000	1.277348000	-1.059903000
	6	-2.175346000	2.313744000	-0.136150000
	6	3.231574000	-2.296213000	-1.347629000
	6	0.972686000	-3.050904000	-0.315265000
	6	-3.511976000	2.687477000	-0.334123000
	6	-4.114257000	3.633258000	0.494993000
	6	-3.385883000	4.215348000	1.538178000
	6	0.661818000	-4.109345000	0.542738000
	6	-0.543852000	-4.805076000	0.407785000
	6	-1.449270000	-4.448106000	-0.593313000
	6	-2.053489000	3.848058000	1.737727000
	6	-1.448825000	2.904027000	0.902320000
	6	-1.142315000	-3.394682000	-1.462129000
	6	0.058572000	-2.700711000	-1.320874000
	1	4.824071000	2.209986000	-3.400226000
	1	4.798418000	0.815834000	-2.313104000

	1	2.440152000	2.680733000	-2.944960000
	1	2.626679000	1.017748000	-3.507578000
	1	2.095637000	3.126320000	-0.367205000
	1	2.037726000	1.712159000	0.704914000
	1	4.259167000	2.888425000	0.837881000
	1	4.430044000	1.224546000	0.258431000
	1	4.400386000	3.752119000	-1.497071000
	1	5.815102000	2.748480000	-1.144815000
	1	-1.655169000	1.066230000	-3.273421000
	1	-1.796072000	2.767405000	-2.708448000
	1	2.764975000	-2.571003000	0.775472000
	1	-2.218512000	0.391075000	-1.049935000
	1	4.266543000	-2.439651000	-1.018037000
	1	2.950276000	-3.017294000	-2.126028000
	1	-4.098360000	2.208586000	-1.122440000
	1	-5.160247000	3.906140000	0.335974000
	1	-3.858114000	4.950576000	2.194086000
	1	1.360709000	-4.377096000	1.339210000
	1	-0.779831000	-5.621641000	1.093991000
	1	-2.396575000	-4.982798000	-0.693222000
	1	-1.478771000	4.293769000	2.553290000
	1	-0.418997000	2.593200000	1.075514000
	1	-1.850220000	-3.104884000	-2.241899000
	1	0.278615000	-1.862988000	-1.986327000
	8	3.090422000	-0.175508000	2.648800000
	6	3.067030000	0.989405000	3.440512000
	1	2.393445000	0.882153000	4.310105000
	1	4.085632000	1.169945000	3.816255000
	1	2.749182000	1.881919000	2.869339000
	1	2.181086000	-0.357865000	2.312675000
	1	0.017997000	-2.190779000	2.548704000
	1	0.634177000	-0.820073000	3.571152000
	1	-1.283822000	0.612981000	2.898647000
	6	6.169121000	-1.008107000	1.476438000
	1	6.903218000	-1.478377000	0.802244000
	1	6.543519000	0.008276000	1.715001000
	1	6.156645000	-1.590976000	2.418088000
	8	4.919051000	-0.987578000	0.837325000
	1	4.251991000	-0.657087000	1.483062000
	6	-2.213535000	-0.848699000	1.603450000
	1	-2.046426000	-1.824750000	1.130782000
	6	-3.401577000	-0.217551000	1.400789000
	1	-3.570059000	0.734982000	1.912294000
	6	-4.467468000	-0.646255000	0.505261000

	6	-4.359029000	-1.772793000	-0.344256000
	6	-5.662700000	0.103989000	0.428402000
	6	-5.388398000	-2.125250000	-1.213931000
	1	-3.450437000	-2.374903000	-0.319441000
	6	-6.691371000	-0.248807000	-0.444920000
	1	-5.771302000	0.981413000	1.070629000
	6	-6.564209000	-1.366593000	-1.275723000
	1	-5.273144000	-3.003864000	-1.855355000
	1	-7.603199000	0.353992000	-0.476961000
	1	-7.368774000	-1.644476000	-1.960559000
TS1 ^R -1b	28	-0.246149000	-0.007795000	-0.886283000
	6	1.260513000	0.225263000	-2.068223000
	6	0.232921000	-0.567523000	-2.781602000
	6	-4.408810000	0.568515000	3.052399000
	6	-2.881478000	0.712770000	3.059236000
	6	-2.240913000	0.642610000	1.652635000
	6	-2.978816000	1.616174000	0.665208000
	6	-4.491231000	1.406545000	0.675337000
	6	-5.072875000	1.549221000	2.082634000
	6	-2.273145000	-0.750846000	1.057590000
	6	-0.794256000	1.103948000	1.678692000
	8	-0.414302000	1.865933000	2.711421000
	7	0.081996000	0.926039000	0.750079000
	6	0.987144000	2.176846000	2.522331000
	7	-1.610583000	-1.088470000	0.020620000
	8	-3.024604000	-1.700036000	1.627776000
	6	-1.856768000	-2.505022000	-0.275752000
	6	1.273619000	1.727872000	1.067380000
	6	1.461925000	2.877499000	0.097903000
	6	-2.940341000	-2.872963000	0.772883000
	6	-0.554960000	-3.273378000	-0.203624000
	6	2.720495000	3.487657000	0.009460000
	6	2.929641000	4.562781000	-0.856502000
	6	1.880159000	5.034802000	-1.651027000
	6	-0.143945000	-4.081087000	-1.268962000
	6	1.079295000	-4.757529000	-1.220163000
	6	1.903383000	-4.632723000	-0.099638000
	6	0.623281000	4.430615000	-1.566710000
	6	0.413324000	3.359451000	-0.694309000
	6	1.498831000	-3.828705000	0.972177000
	6	0.280613000	-3.151948000	0.916647000
	1	-4.778009000	0.732464000	4.078151000
	1	-4.682507000	-0.459785000	2.776401000
	1	-2.616953000	1.692808000	3.480975000

1	-2.423855000	-0.045791000	3.713207000
1	-2.732380000	2.643999000	0.982060000
1	-2.579227000	1.443380000	-0.345864000
1	-4.947739000	2.138394000	-0.011062000
1	-4.712220000	0.412588000	0.252850000
1	-4.916739000	2.584271000	2.440083000
1	-6.162551000	1.384108000	2.067665000
1	1.560787000	1.605764000	3.267815000
1	1.126807000	3.252266000	2.687390000
1	-2.286877000	-2.569561000	-1.283120000
1	2.161119000	1.081551000	1.015424000
1	-3.920667000	-3.002262000	0.299680000
1	-2.681119000	-3.733363000	1.403914000
1	3.548716000	3.105130000	0.612489000
1	3.917299000	5.025747000	-0.920214000
1	2.044134000	5.869035000	-2.337174000
1	-0.782882000	-4.169112000	-2.151384000
1	1.391647000	-5.377921000	-2.063438000
1	2.862974000	-5.153518000	-0.062957000
1	-0.201297000	4.786062000	-2.188935000
1	-0.563681000	2.878237000	-0.656058000
1	2.142755000	-3.718268000	1.847589000
1	-0.015990000	-2.502514000	1.743870000
8	-2.289254000	0.420591000	-2.299521000
6	-2.404702000	1.513394000	-3.134707000
1	-1.467972000	1.713982000	-3.707609000
1	-3.211790000	1.408057000	-3.894748000
1	-2.621386000	2.459510000	-2.581459000
1	-0.978707000	-0.275530000	-2.408926000
1	0.407044000	-1.650402000	-2.844228000
1	-0.011011000	-0.166229000	-3.776978000
1	1.467928000	1.235023000	-2.443500000
6	-5.206935000	-1.122151000	-2.456681000
1	-5.949876000	-1.900605000	-2.208349000
1	-5.753216000	-0.156488000	-2.509843000
1	-4.830367000	-1.338797000	-3.477512000
8	-4.191840000	-1.122311000	-1.495674000
1	-3.469752000	-0.481553000	-1.809524000
6	2.354586000	-0.425781000	-1.378086000
1	2.203797000	-1.482441000	-1.126035000
6	3.496118000	0.192153000	-0.976838000
1	3.641325000	1.233260000	-1.282043000
6	4.547837000	-0.366713000	-0.133563000
6	4.494022000	-1.671169000	0.407452000

	6	5.668301000	0.426899000	0.193870000
	6	5.510771000	-2.151207000	1.228642000
	1	3.640685000	-2.311423000	0.182690000
	6	6.685419000	-0.054501000	1.018946000
	1	5.734044000	1.438950000	-0.215651000
	6	6.614644000	-1.348051000	1.543323000
	1	5.443463000	-3.165788000	1.631253000
	1	7.541018000	0.584539000	1.252799000
	1	7.409515000	-1.728227000	2.189183000
TS1 ^S -1b	28	-0.329369000	0.913171000	-0.365120000
	6	1.001383000	2.148235000	-1.026896000
	6	0.036279000	2.886262000	-0.178716000
	6	-4.308426000	-3.179121000	-1.415736000
	6	-3.008785000	-2.489201000	-1.838373000
	6	-2.086016000	-2.059499000	-0.651093000
	6	-1.940512000	-3.227704000	0.393830000
	6	-3.254066000	-3.920958000	0.760265000
	6	-4.036326000	-4.360125000	-0.479981000
	6	-2.645083000	-0.841196000	0.041868000
	6	-0.695353000	-1.817406000	-1.191926000
	8	-0.148722000	-2.887520000	-1.797437000
	7	0.064541000	-0.781500000	-1.105308000
	6	1.129429000	-2.468254000	-2.322078000
	7	-2.123538000	0.321402000	0.148684000
	8	-3.846044000	-1.008836000	0.620298000
	6	-3.032344000	1.181360000	0.941070000
	6	1.421568000	-1.183537000	-1.525135000
	6	2.331631000	-1.414680000	-0.328870000
	6	-4.125591000	0.185254000	1.387493000
	6	-3.515070000	2.355505000	0.121076000
	6	3.682122000	-1.703968000	-0.573148000
	6	4.561921000	-1.944735000	0.479874000
	6	4.099678000	-1.894545000	1.798584000
	6	-3.284345000	3.660879000	0.568187000
	6	-3.716467000	4.756572000	-0.184734000
	6	-4.381055000	4.554066000	-1.396598000
	6	2.757772000	-1.604723000	2.048095000
	6	1.870681000	-1.366245000	0.991645000
	6	-4.613669000	3.251502000	-1.851874000
	6	-4.183276000	2.160307000	-1.095950000
	1	-4.828680000	-3.523356000	-2.324800000
	1	-4.975261000	-2.459177000	-0.919049000
	1	-2.422053000	-3.187564000	-2.453327000
	1	-3.213210000	-1.604937000	-2.464271000

1	-1.264667000	-3.968420000	-0.056465000
1	-1.447458000	-2.809212000	1.283081000
1	-3.012998000	-4.795582000	1.386794000
1	-3.875115000	-3.253483000	1.373764000
1	-3.457484000	-5.128772000	-1.025195000
1	-4.985871000	-4.835052000	-0.184285000
1	1.008253000	-2.282180000	-3.401623000
1	1.854860000	-3.272647000	-2.154725000
1	-2.451626000	1.549939000	1.796327000
1	1.859305000	-0.402092000	-2.159760000
1	-4.036577000	-0.077774000	2.450088000
1	-5.148331000	0.510163000	1.156245000
1	4.059851000	-1.713428000	-1.598915000
1	5.615910000	-2.137276000	0.270819000
1	4.789467000	-2.069029000	2.627671000
1	-2.740475000	3.811856000	1.503838000
1	-3.525814000	5.771339000	0.172760000
1	-4.715593000	5.409113000	-1.988910000
1	2.384448000	-1.559397000	3.073712000
1	0.829519000	-1.139334000	1.222017000
1	-5.130045000	3.087727000	-2.800921000
1	-4.360130000	1.144465000	-1.460407000
8	-0.421753000	1.573781000	2.191693000
6	0.711544000	1.898934000	2.917289000
1	1.212983000	2.818698000	2.534901000
1	0.490779000	2.102585000	3.988551000
1	1.489959000	1.102146000	2.901090000
1	-0.370842000	2.150377000	0.836288000
1	-0.752711000	3.437747000	-0.703391000
1	0.502649000	3.540445000	0.575586000
6	-0.955740000	-1.132395000	3.938663000
1	-1.339156000	-2.140597000	4.174396000
1	0.109142000	-1.105536000	4.250032000
1	-1.498902000	-0.412260000	4.584512000
8	-1.134459000	-0.876376000	2.575355000
1	-0.844158000	0.082935000	2.395207000
6	2.353818000	1.928212000	-0.551496000
1	2.476249000	1.927647000	0.536922000
6	3.434602000	1.668782000	-1.325928000
1	3.301637000	1.670650000	-2.414989000
6	4.778247000	1.335902000	-0.858397000
6	5.151773000	1.374297000	0.501607000
6	5.752709000	0.920672000	-1.788735000
6	6.429186000	1.000672000	0.907262000

	1	4.424335000	1.684550000	1.253211000
	6	7.032349000	0.540097000	-1.382523000
	1	5.489027000	0.887896000	-2.849817000
	6	7.379659000	0.575214000	-0.029338000
	1	6.686960000	1.033653000	1.968958000
	1	7.763885000	0.216375000	-2.127656000
	1	8.380811000	0.279798000	0.293351000
	1	0.904891000	2.253926000	-2.116864000

Table S3. Imaginary frequency of all the transition states in this work, calculated at the B3LYP-D3(BJ)/def2SVP level.

Names	I. F. ($i\text{ cm}^{-1}$)	Names	I. F. ($i\text{ cm}^{-1}$)
TS1^{Ra}	-698.89	TS2^{Ra}	-49.57
TS3^{Ra}	-39.47	TS4^{Ra}	-131.64
TS1^{Rb}	-720.43	TS1^{Sa}	-739.48
TS1^{Sb}	-514.31	TS1'	-622.78
TS1^{nBuOH}	-752.75	TS1^{iPrOH}	-747.99
TS2^S	-45.58	TS3^S	-36.23
TS4^S	-146.28	TS1^R-1a	-666.15
TS1^S-1a	-604.25	TS1^R-1b	-586.33
TS1^S-1b	-730.22		

Table S4. Electronic energies (E in au), Gibbs free energies (G in au) and entropies (S in $\text{cal}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) calculated at the B3LYP-D3(BJ)/def2SVP level and single-point energies (E' in au) calculated at the B3LYP-D3(BJ)/def2TZVPP level

Names	E	G	S	E'
NiL(cod)	-3009.510229	-3008.927662	190.988	-3011.381469
cod	-311.843142	-311.693778	81.955	-312.1957986
1	-309.456371	-309.3536755	80.814	-309.8045595
(MeOH)₂	-231.2859203	-231.2118567	82.884	-231.5767947
pre-com	-3238.46183	-3237.826408	227.35	-3240.611211
TS1^{Ra}	-3238.431132	-3237.800903	224.243	-3240.573807
INT1^{Ra}	-3238.461873	-3237.824678	222.905	-3240.603586
[Me₄N]F	-313.972209	-313.83788	79.652	-314.3708889
[Me₄N]OMe·MeOH	-444.8976534	-444.6816907	115.24	-445.4349617
INT1-1^{Ra}	-3107.53426	-3106.982274	193.765	-3109.531068
B₂pin₂	-822.017072	-821.696901	128.313	-822.9579185
FBpin	-510.773021	-510.628689	98.367	-511.4257187
INT1-2^{Ra}	-3929.589946	-3928.692352	276.305	-3932.502704

TS2^{Ra}	-3929.580223	-3928.681699	273.232	-3932.48665
INT2^{Ra}	-3929.591155	-3928.693996	278.284	-3932.501769
TS3^{Ra}	-3929.591091	-3928.694095	276.371	-3932.502386
INT3^{Ra}	-3418.753374	-3418.032738	233.835	-3421.088957
TS4^{Ra}	-3418.746716	-3418.026315	233.835	-3421.082263
INT4^{Ra}	-3418.753959	-3418.030331	233.969	-3421.088452
(R)-3	-721.115723	-720.8296977	126.658	-721.9291277
TS1[']	-3238.405607	-3237.774017	220.369	-3240.548974
TS1^{Rb}	-3238.425657	-3237.794446	221.813	-3240.569319
TS1^{Sa}	-3238.42488	-3237.794149	222.346	-3240.567539
TS1^{Sb}	-3238.426341	-3237.795523	223.805	-3240.569764
pre-com^{nBuOH}	-3474.220046	-3473.420628	257.571	-3476.631286
TS1^{nBuOH}	-3474.190423	-3473.395131	253.591	-3476.593457
pre-com^{iPrOH}	-3395.649841	-3394.905854	245.454	-3397.973974
TS1^{iPrOH}	-3395.618473	-3394.87782	240.177	-3397.934878
pre-com-1a	-3277.75645	-3277.093883	232.079	-3279.948408
TS1^{R-1a}	-3277.725294	-3277.067361	227.953	-3279.910526
TS1^{S-1a}	-3277.724793	-3277.065509	224.91	-3279.90857
pre-com-1b	-3315.820385	-3315.154597	238.533	-3318.055924
TS1^{R-1b}	-3315.788391	-3315.127256	235.084	-3318.0177
TS1^{S-1b}	-3395.618473	-3394.87782	240.177	-3397.934878
INT1^S	-3238.4621	-3237.823952	222.04	-3240.604194
INT1-1^S	-3107.532718	-3106.981401	194.993	-3109.528491
INT1-2^S	-3929.586494	-3928.687722	273.849	-3932.497501
TS2^S	-3929.566939	-3928.668869	273.186	-3932.474475
INT2^S	-3929.597331	-3928.698809	276.775	-3932.506243
TS3^S	-3929.595875	-3928.698368	276.622	-3932.50922
INT3^S	-3418.753273	-3418.03193	233.053	-3421.092501
TS4^S	-3418.742484	-3418.020863	229.261	-3421.075324
INT4^S	-3418.75425	-3418.029982	232.67	-3421.086167
(S)-3	-721.115723	-720.8296977	126.658	-721.9291277