Supporting Information

A Computational Study on the Reaction Mechanisms of Nickel-Catalyzed Diarylation of Alkenes

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Table S1. Cartesian Coordinates of the stationary points optimized at the B3LYP/6-31+G* level of theory in the gas phase.

Compound	Cartesian Coordinates		
CAT-1	28	1.148448000	0.127882000	0.206270000
	17	2.835652000	-0.791584000	-0.691086000
	17	1.389763000	2.204119000	-0.090447000
	6	-2.022087000	-0.821084000	-1.178520000
	6	-3.222097000	-0.147900000	-1.384927000
	6	-3.823542000	0.549059000	-0.330295000
	6	-3.221934000	0.562553000	0.932275000
	6	-2.022881000	-0.113946000	1.144191000
	6	-1.399628000	-0.814039000	0.088330000
	1	-1.548024000	-1.353451000	-1.999397000
	1	-3.687721000	-0.160431000	-2.366305000
	1	-4.758835000	1.078021000	-0.491693000
	1	-3.689598000	1.098779000	1.753153000
	1	-1.579401000	-0.107195000	2.135347000
	6	-0.118056000	-1.515983000	0.245493000
	6	0.690799000	-1.499595000	1.371498000
	1	0.180380000	-2.153158000	-0.584382000
	1	1.550811000	-2.157129000	1.429899000
	1	0.380348000	-1.033608000	2.305595000
CAT-2	28	1.021346000	-0.522804000	-0.037936000
	5	-2.578602000	0.006542000	-0.329718000
	8	-2.803366000	-1.323372000	-0.664114000
	8	-3.688376000	0.550880000	0.288574000
	6	-4.206741000	-1.640034000	-0.427943000
	6	-4.636050000	-0.511912000	0.586438000
	6	-4.299548000	-3.068813000	0.107273000
	1	-5.335644000	-3.325354000	0.360218000
	1	-3.955562000	-3.771794000	-0.659495000
	1	-3.678853000	-3.210019000	0.995486000
	6	-4.917317000	-1.547226000	-1.786888000
	1	-4.434020000	-2.235800000	-2.488418000
	1	-5.974809000	-1.824689000	-1.710142000
	1	-4.853583000	-0.537671000	-2.205523000
	6	-4.422829000	-0.898290000	2.057704000
	1	-4.564296000	-0.009134000	2.680934000
	1	-5.137331000	-1.663235000	2.382749000
	1	-3.408633000	-1.271864000	2.231776000

6	-6.051739000	0.031342000	0.393930000
1	-6.799168000	-0.755826000	0.552982000
1	-6.238850000	0.828345000	1.121494000
1	-6.192278000	0.451043000	-0.605084000
5	-1.089508000	0.870905000	-0.521862000
8	-1.221041000	2.272733000	-0.766968000
8	-0.199571000	0.773855000	0.724931000
6	-0.225308000	3.017301000	-0.053887000
6	0.036708000	2.134301000	1.227145000
6	-0.807769000	4.400055000	0.260655000
1	-0.131217000	4.982899000	0.898514000
1	-0.952139000	4.952748000	-0.674272000
1	-1.779203000	4.319390000	0.754019000
6	1.025700000	3.193854000	-0.936134000
1	0.717303000	3.642380000	-1.886865000
1	1.762826000	3.856604000	-0.467181000
1	1.506349000	2.238144000	-1.159093000
6	-1.013076000	2.350406000	2.326920000
1	-0.889624000	1.578132000	3.093801000
1	-0.890341000	3.328361000	2.805574000
1	-2.027747000	2.276759000	1.925863000
6	1.441167000	2.259324000	1.810804000
1	1.620129000	3.299546000	2.110206000
1	1.548202000	1.625475000	2.695187000
1	2.216089000	1.963874000	1.100441000
6	-0.844410000	0.627949000	-3.741767000
1	-1.677012000	1.245933000	-3.392781000
1	0.003929000	1.291027000	-3.945088000
1	-1.139415000	0.141302000	-4.680579000
6	-0.473236000	-0.434164000	-2.711364000
1	-1.315437000	-1.108540000	-2.520974000
1	0.362676000	-1.034406000	-3.090364000
8	-0.054247000	0.161571000	-1.476708000
6	4.631293000	-0.006521000	-1.541763000
6	5.944976000	0.305009000	-1.193149000
6	6.575249000	-0.398036000	-0.162834000
6	5.883591000	-1.410814000	0.512087000
6	4.570691000	-1.720608000	0.165361000
6	3.922367000	-1.020259000	-0.868934000
1	4.142402000	0.541279000	-2.344809000
1	6.474588000	1.091603000	-1.724177000
1	7.600002000	-0.161477000	0.112025000
1	6.370709000	-1.959062000	1.314249000
1	4.041035000	-2.496335000	0.705088000

	6	2.554732000	-1.318703000	-1.316822000
	6	1.683404000	-2.287312000	-0.848626000
	1	2.281497000	-0.808986000	-2.239664000
	1	0.831877000	-2.592571000	-1.451745000
	1	1.952239000	-2.944317000	-0.028823000
	8	1.942369000	-0.924153000	1.463083000
	6	1.182344000	-1.431585000	2.534872000
	1	0.337942000	-0.767642000	2.782110000
	1	0.746952000	-2.419956000	2.288480000
	6	2.087218000	-1.581853000	3.761113000
	1	2.514834000	-0.613309000	4.044303000
	1	1.516549000	-1.975107000	4.612717000
	1	2.915246000	-2.269060000	3.551445000
TS-cat-1	28	-0.658218000	-0.418567000	0.674570000
	5	1.886488000	-0.340656000	0.073242000
	8	2.381807000	-1.077553000	1.134201000
	8	2.428750000	-0.742100000	-1.125454000
	6	3.499470000	-1.886596000	0.651371000
	6	3.225231000	-1.945264000	-0.902228000
	6	3.465328000	-3.234652000	1.369455000
	1	4.256641000	-3.895960000	0.995541000
	1	3.630872000	-3.083779000	2.441932000
	1	2.503126000	-3.736530000	1.242443000
	6	4.778590000	-1.123940000	1.024094000
	1	4.800743000	-0.975612000	2.108907000
	1	5.677335000	-1.680629000	0.735477000
	1	4.809294000	-0.138180000	0.549381000
	6	2.355970000	-3.135689000	-1.327480000
	1	2.087091000	-3.015458000	-2.382318000
	1	2.893808000	-4.084432000	-1.217447000
	1	1.428280000	-3.179966000	-0.749375000
	6	4.472806000	-1.865513000	-1.781622000
	1	5.130473000	-2.725591000	-1.605230000
	1	4.176728000	-1.876875000	-2.836010000
	1	5.040181000	-0.949081000	-1.601872000
	5	0.946477000	1.182195000	0.220017000
	8	1.850262000	2.293548000	0.190391000
	8	-0.056344000	1.381503000	-0.812258000
	6	1.210840000	3.358695000	-0.550560000
	6	0.260585000	2.584355000	-1.550016000
	6	2.307232000	4.185715000	-1.226196000
	1	1.875641000	4.964656000	-1.867493000
	1	2.918492000	4.677636000	-0.461146000
	1	2.966615000	3.558143000	-1.830439000

6	0.440437000	4.249088000	0.441396000
1	1.139689000	4.615515000	1.201446000
1	-0.006569000	5.118103000	-0.056385000
1	-0.350507000	3.689684000	0.948751000
6	0.970563000	2.152887000	-2.844074000
1	0.310278000	1.477783000	-3.399377000
1	1.203297000	3.010281000	-3.487005000
1	1.894477000	1.610021000	-2.625696000
6	-1.039751000	3.313364000	-1.895335000
1	-0.834813000	4.262727000	-2.406338000
1	-1.640137000	2.691341000	-2.568724000
1	-1.636905000	3.519473000	-1.003271000
6	-0.058909000	1.770596000	3.882024000
1	-0.295209000	2.803397000	3.603770000
1	-1.002764000	1.241291000	4.059973000
1	0.499293000	1.787874000	4.826854000
6	0.775654000	1.099458000	2.798883000
1	1.713939000	1.644696000	2.649267000
1	1.036047000	0.069434000	3.069402000
8	0.069903000	1.115516000	1.543366000
6	-4.430717000	0.576457000	0.231151000
6	-5.559210000	0.409546000	-0.571753000
6	-5.995618000	-0.876306000	-0.900726000
6	-5.294963000	-1.990851000	-0.423532000
6	-4.166560000	-1.824606000	0.375723000
6	-3.715872000	-0.534918000	0.716834000
1	-4.091277000	1.577965000	0.485565000
1	-6.096102000	1.280474000	-0.938284000
1	-6.876376000	-1.011883000	-1.523085000
1	-5.631723000	-2.992976000	-0.676066000
1	-3.627302000	-2.696420000	0.730351000
6	-2.565048000	-0.290389000	1.599968000
6	-1.722736000	-1.231837000	2.185364000
1	-2.496309000	0.731971000	1.968242000
1	-1.145469000	-0.966764000	3.067014000
1	-1.824409000	-2.291893000	1.976816000
8	-0.980373000	-1.848681000	-0.343701000
6	-1.314609000	-1.600728000	-1.697202000
1	-2.223745000	-0.978203000	-1.759514000
1	-0.508392000	-1.056917000	-2.210762000
6	-1.576180000	-2.934708000	-2.399796000
1	-2.404955000	-3.469398000	-1.921944000
1	-1.834026000	-2.762554000	-3.453042000
1	-0.687282000	-3.574019000	-2.361368000

	28	-0.542072000	1.440483000	0.262773000
	5	-1.676351000	-0.077460000	0.035276000
	8	-2.888649000	-0.115212000	-0.621226000
	8	-1.340912000	-1.332960000	0.540028000
	6	-3.518400000	-1.403919000	-0.371926000
	6	-2.287481000	-2.310146000	0.009666000
	6	-4.271923000	-1.825006000	-1.633355000
	1	-4.716105000	-2.820822000	-1.511212000
	1	-5.081989000	-1.114187000	-1.827982000
	1	-3.619938000	-1.836739000	-2.510153000
	6	-4.510399000	-1.198361000	0.782730000
	1	-5.216919000	-0.409939000	0.503869000
	1	-5.079203000	-2.110738000	0.996486000
	1	-3.999967000	-0.881923000	1.698092000
	6	-1.613611000	-2.970253000	-1.202174000
	1	-0.667795000	-3.419901000	-0.880940000
	1	-2.239846000	-3.760911000	-1.631130000
	1	-1.392115000	-2.237766000	-1.984828000
	6	-2.559390000	-3.359205000	1.087249000
	1	-3.318334000	-4.076465000	0.751109000
	1	-1.639916000	-3.915852000	1.299661000
INT-cat-1	1	-2.901431000	-2.904376000	2.020319000
	5	2.054887000	0.153003000	0.491324000
	8	3.028893000	-0.679082000	0.978986000
	8	2.287411000	0.628220000	-0.767551000
	6	4.143080000	-0.616767000	0.028539000
	6	3.428184000	-0.119149000	-1.294827000
	6	4.775900000	-2.002926000	-0.058000000
	1	5.577534000	-2.015075000	-0.805751000
	1	5.212327000	-2.269195000	0.910497000
	1	4.042182000	-2.768699000	-0.320385000
	6	5.149030000	0.391736000	0.596816000
	1	5.453348000	0.066327000	1.597006000
	1	6.045079000	0.458316000	-0.029460000
	1	4.713633000	1.392787000	0.682953000
	6	2.854895000	-1.258972000	-2.145969000
	1	2.221193000	-0.830546000	-2.928736000
	1	3.651084000	-1.839711000	-2.624414000
	1	2.238403000	-1.938739000	-1.548847000
	6	4.257773000	0.823467000	-2.162683000
	1	5.159497000	0.319711000	-2.530487000
	1	3.666030000	1.137072000	-3.028649000
	1	4.555812000	1.721688000	-1.616858000
	6	0.469449000	1.254618000	3.490596000

	1	1.317489000	1.948387000	3.505453000
	1	-0.423500000	1.799105000	3.164718000
	1	0.300790000	0.895652000	4.513525000
	6	0.741496000	0.068553000	2.584169000
	1	1.645469000	-0.469005000	2.879057000
	1	-0.098085000	-0.627326000	2.548340000
	8	0.934957000	0.529036000	1.204557000
	8	-1.416796000	2.701294000	-0.553564000
	6	-2.758047000	3.121900000	-0.505769000
	1	-3.413153000	2.346625000	-0.929435000
	1	-3.089801000	3.297812000	0.533704000
	6	-2.905780000	4.416888000	-1.306536000
	1	-2.607544000	4.256888000	-2.349386000
	1	-3.947670000	4.765326000	-1.289733000
	1	-2.269107000	5.205854000	-0.888054000
	28	-0.253325000	0.938590000	0.475688000
	5	-1.818317000	-0.027479000	0.017381000
	8	-2.932426000	-0.206145000	0.822495000
	8	-1.943696000	-0.691647000	-1.190218000
	6	-3.822157000	-1.156515000	0.165839000
	6	-3.338917000	-1.091415000	-1.334749000
	6	-5.264269000	-0.710514000	0.403228000
	1	-5.968920000	-1.365279000	-0.124622000
	1	-5.492974000	-0.759208000	1.473658000
	1	-5.426809000	0.317330000	0.070992000
	6	-3.584034000	-2.522098000	0.826849000
	1	-3.756832000	-2.428648000	1.904392000
	1	-4.263746000	-3.287571000	0.434996000
	1	-2.554695000	-2.864069000	0.676052000
TS-cat-2	6	-4.034675000	0.003808000	-2.156001000
	1	-3.516609000	0.106155000	-3.115225000
	1	-5.084056000	-0.244336000	-2.354245000
	1	-3.987860000	0.972488000	-1.650031000
	6	-3.387050000	-2.418547000	-2.090931000
	1	-4.416843000	-2.790125000	-2.164097000
	1	-3.006967000	-2.273354000	-3.107983000
	1	-2.773236000	-3.184267000	-1.609505000
	5	2.363684000	-0.252074000	0.436393000
	8	3.317471000	-1.229804000	0.535015000
	8	2.710472000	0.811361000	-0.347011000
	6	4.522295000	-0.699792000	-0.114434000
	6	3.926603000	0.420113000	-1.062302000
	6	5.223242000	-1.850886000	-0.830425000
	1	6.100457000	-1.487531000	-1.378504000

1	5.564929000	-2.586784000	-0.094960000
1	4.557606000	-2.357669000	-1.533002000
6	5.414464000	-0.142745000	1.001322000
1	5.632375000	-0.941570000	1.717778000
1	6.364263000	0.229714000	0.602998000
1	4.923775000	0.673787000	1.541391000
6	3.481271000	-0.108750000	-2.431120000
1	2.901003000	0.667950000	-2.938475000
1	4.340994000	-0.365326000	-3.059591000
1	2.843590000	-0.993602000	-2.335759000
6	4.802140000	1.658597000	-1.231544000
1	5.756321000	1.396478000	-1.703835000
1	4.291309000	2.380815000	-1.876458000
1	5.006547000	2.146272000	-0.275437000
6	0.307063000	-0.815981000	3.313340000
1	1.070963000	-0.200313000	3.801192000
1	-0.588213000	-0.207793000	3.148401000
1	0.048249000	-1.642197000	3.987192000
6	0.816682000	-1.383025000	2.002440000
1	1.721539000	-1.980367000	2.136309000
1	0.056784000	-1.988544000	1.502424000
8	1.141310000	-0.293544000	1.077065000
8	-1.414001000	2.133483000	-0.157852000
6	-2.137908000	2.964173000	0.739468000
1	-2.874850000	2.375400000	1.307554000
1	-1.467076000	3.441125000	1.474938000
6	-2.852913000	4.052268000	-0.061668000
1	-3.548658000	3.604605000	-0.781347000
1	-3.420576000	4.715797000	0.605079000
1	-2.129584000	4.656103000	-0.622220000

	28	0.016235000	-0.052156000	-0.245949000
	5	-2.861453000	-0.485038000	0.083353000
	8	-3.992098000	-1.238098000	0.322635000
	8	-3.110904000	0.852350000	-0.077039000
	6	-5.138229000	-0.361190000	0.103503000
	6	-4.501531000	1.072458000	0.303611000
	6	-6.229087000	-0.734365000	1.104662000
	1	-7.084677000	-0.054109000	1.017394000
INT-cat-2	1	-6.582703000	-1.750859000	0.901128000
	1	-5.862578000	-0.704456000	2.133572000
	6	-5.625939000	-0.618054000	-1.328900000
	1	-5.864274000	-1.681320000	-1.437701000
	1	-6.528203000	-0.039587000	-1.556035000
	1	-4.857862000	-0.365284000	-2.067313000

	6	-4.495438000	1.536119000	1.766945000
	1	-3.872167000	2.431974000	1.850840000
	1	-5.504888000	1.782188000	2.115340000
	1	-4.075183000	0.772637000	2.429964000
	6	-5.077486000	2.167557000	-0.591306000
	1	-6.142088000	2.324676000	-0.379421000
	1	-4.551040000	3.108630000	-0.400693000
	1	-4.961761000	1.927636000	-1.650874000
	6	-1.404587000	-3.140330000	-1.245456000
	1	-2.346578000	-2.995113000	-1.785863000
	1	-0.587125000	-2.713088000	-1.835172000
	1	-1.236540000	-4.219783000	-1.134430000
	6	-1.451402000	-2.494593000	0.128077000
	1	-2.283008000	-2.875269000	0.727838000
	1	-0.514622000	-2.635068000	0.668696000
	8	-1.607223000	-1.040593000	0.018868000
	5	2.895599000	0.434826000	-0.209475000
	8	4.038497000	1.198318000	-0.325962000
	8	3.125465000	-0.841450000	0.231908000
	6	5.170384000	0.294811000	-0.143000000
	6	4.516207000	-0.895214000	0.667491000
	6	6.277012000	1.049559000	0.589689000
	1	7.122678000	0.385412000	0.804417000
	1	6.641637000	1.869108000	-0.038937000
	1	5.921993000	1.478208000	1.529935000
	6	5.645294000	-0.111331000	-1.544828000
	1	5.902061000	0.791646000	-2.108596000
	1	6.533291000	-0.751258000	-1.498428000
	1	4.862676000	-0.643903000	-2.095279000
	6	4.516238000	-0.671235000	2.186144000
	1	3.879883000	-1.428807000	2.654376000
	1	5.524468000	-0.757730000	2.606628000
	1	4.112701000	0.312338000	2.448339000
	6	5.068742000	-2.280856000	0.340725000
	1	6.135042000	-2.344505000	0.589653000
	1	4.536733000	-3.034192000	0.931100000
	1	4.939390000	-2.529420000	-0.715321000
	6	1.087730000	3.244577000	0.044975000
	1	0.151968000	2.911474000	0.505668000
	1	1.858496000	3.320711000	0.819978000
	1	0.937007000	4.242106000	-0.388905000
	6	1.501981000	2.277713000	-1.050313000
	1	0.735804000	2.196421000	-1.822896000
	1	2.455079000	2.563202000	-1.504320000

	8	1.648729000	0.919854000	-0.519114000
CAT-R	28	-0.312041000	-0.453499000	-0.706371000
	6	3.246453000	-1.731706000	0.290725000
	6	4.389493000	-1.258759000	0.937586000
	6	4.839211000	0.043968000	0.706003000
	6	4.129931000	0.864761000	-0.178807000
	6	2.986707000	0.392592000	-0.821101000
	6	2.520743000	-0.919631000	-0.602333000
	1	2.907386000	-2.749674000	0.473787000
	1	4.930897000	-1.910313000	1.619595000
	1	5.728718000	0.416399000	1.207567000
	1	4.466641000	1.881829000	-0.365396000
	1	2.444859000	1.052490000	-1.492520000
	6	1.318182000	-1.471215000	-1.264474000
	6	0.638856000	-0.912816000	-2.363655000
	1	1.135509000	-2.524897000	-1.041635000
	1	0.013561000	-1.553704000	-2.985196000
	1	1.004067000	-0.014271000	-2.860788000
	6	-1.316077000	0.782384000	0.340589000
	6	-1.142587000	-0.135867000	1.412415000
	6	-2.015708000	-1.226177000	1.553027000
	6	-3.051381000	-1.407719000	0.613283000
	6	-3.192334000	-0.565943000	-0.491325000
	6	-2.294436000	0.519145000	-0.653720000
	1	-0.388774000	0.061790000	2.167891000
	1	-3.740384000	-2.239866000	0.740725000
	1	-2.450854000	1.233129000	-1.456766000
	35	-0.501190000	2.537032000	0.455613000
	6	-4.287178000	-0.783543000	-1.508240000
	1	-4.983354000	0.064893000	-1.526285000
	1	-3.872415000	-0.882563000	-2.518842000
	1	-4.863469000	-1.687705000	-1.288224000
	6	-1.863412000	-2.180849000	2.713773000
	1	-0.948739000	-1.981807000	3.280617000
	1	-2.712566000	-2.093825000	3.404359000
	1	-1.831061000	-3.221812000	2.370571000
TS-OA	28	0.039028000	0.161003000	0.546588000
	6	-3.867941000	-0.768837000	0.911011000
	6	-5.056193000	-0.700547000	0.181110000
	6	-5.315271000	0.402214000	-0.636226000
	6	-4.371895000	1.433600000	-0.715733000
	6	-3.183129000	1.359024000	0.007556000
	6	-2.911174000	0.259563000	0.843852000
	1	-3.675737000	-1.631000000	1.546284000

	1	-5.778997000	-1.509755000	0.251761000
	1	-6.238901000	0.458762000	-1.206446000
	1	-4.559364000	2.294091000	-1.353546000
	1	-2.455438000	2.161260000	-0.082843000
	6	-1.681746000	0.151593000	1.661087000
	6	-0.814598000	1.199102000	1.998735000
	1	-1.624579000	-0.758498000	2.260392000
	1	-0.169639000	1.093370000	2.871155000
	1	-1.014024000	2.224848000	1.690011000
	6	1.606211000	-0.339846000	-0.298102000
	6	2.544688000	-1.138240000	0.384052000
	6	3.820658000	-0.626570000	0.606591000
	6	4.141302000	0.658738000	0.112642000
	6	3.227537000	1.437452000	-0.596587000
	6	1.938128000	0.912964000	-0.833841000
	1	2.264612000	-2.124526000	0.740352000
	1	5.145150000	1.045398000	0.280115000
	1	1.237697000	1.445143000	-1.470956000
	35	-0.053728000	-1.358105000	-1.284690000
	6	3.602336000	2.800161000	-1.132658000
	1	3.421049000	2.867508000	-2.212578000
	1	3.008946000	3.590409000	-0.654953000
	1	4.659593000	3.021212000	-0.954115000
	6	4.852503000	-1.420242000	1.376057000
	1	4.500323000	-2.434736000	1.588190000
	1	5.791515000	-1.498524000	0.814495000
	1	5.086991000	-0.940160000	2.335087000
INT-OA	28	0.257174000	-0.418032000	0.332267000
	6	2.970313000	1.731915000	-0.523772000
	6	4.259353000	1.548035000	-1.017334000
	6	5.136200000	0.668029000	-0.373883000
	6	4.715082000	-0.019311000	0.768544000
	6	3.426252000	0.166942000	1.266536000
	6	2.529711000	1.045883000	0.626233000
	1	2.286671000	2.407501000	-1.032872000
	1	4.579672000	2.085039000	-1.906054000
	1	6.141450000	0.520296000	-0.759196000
	1	5.393033000	-0.701190000	1.274794000
	1	3.122383000	-0.366330000	2.162585000
	6	1.144317000	1.254581000	1.090158000
	6	0.500573000	0.547158000	2.099587000
	1	0.637394000	2.121850000	0.671313000
	1	-0.446938000	0.903172000	2.490282000
	1	1.019441000	-0.183480000	2.719275000

	6	-1.510686000	0.124123000	0.089392000
	6	-1.816987000	1.305046000	-0.589019000
	6	-3.152351000	1.731257000	-0.683408000
	6	-4.149574000	0.964734000	-0.064775000
	6	-3.850402000	-0.216830000	0.624594000
	6	-2.511945000	-0.638686000	0.688759000
	1	-1.038698000	1.893949000	-1.069505000
	1	-5.185129000	1.296454000	-0.124016000
	1	-2.267420000	-1.564728000	1.203108000
	35	0.274102000	-2.162211000	-1.057971000
	6	-4.941373000	-1.047587000	1.263845000
	1	-5.069541000	-2.002606000	0.737848000
	1	-4.706549000	-1.283517000	2.309029000
	1	-5.903720000	-0.525000000	1.244433000
	6	-3.506913000	2.979144000	-1.461939000
	1	-2.669376000	3.684973000	-1.494580000
	1	-3.768731000	2.734260000	-2.500354000
	1	-4.367813000	3.495042000	-1.021695000
TS-MI	28	0.048116000	-0.603919000	0.083379000
	6	-3.715059000	0.125178000	1.226551000
	6	-4.904451000	0.678899000	0.753002000
	6	-4.872213000	1.736299000	-0.160010000
	6	-3.639191000	2.238663000	-0.591755000
	6	-2.451970000	1.681442000	-0.122480000
	6	-2.470235000	0.628965000	0.810451000
	1	-3.746397000	-0.703265000	1.930173000
	1	-5.856975000	0.277459000	1.089207000
	1	-5.798121000	2.165414000	-0.533706000
	1	-3.604778000	3.052096000	-1.311937000
	1	-1.502521000	2.060027000	-0.492687000
	6	-1.241671000	0.052119000	1.395326000
	6	-0.021629000	0.771600000	1.597206000
	1	-1.425319000	-0.788825000	2.065402000
	1	0.551597000	0.535149000	2.488890000
	1	0.012134000	1.822459000	1.322395000
	6	1.650904000	0.298838000	0.412000000
	6	2.654385000	-0.384913000	1.113504000
	6	4.003148000	-0.165531000	0.802756000
	6	4.319655000	0.785448000	-0.178475000
	6	3.331082000	1.506489000	-0.862627000
	6	1.986508000	1.271529000	-0.541248000
	1	2.391918000	-1.101847000	1.888619000
	1	5.366598000	0.977039000	-0.408996000
	1	1.207597000	1.836040000	-1.049785000

	35	-1.058523000	-2.133305000	-1.113050000
	6	3.704387000	2.499626000	-1.939954000
	1	3.833619000	1.997191000	-2.907892000
	1	2.929590000	3.263137000	-2.069295000
	1	4.646859000	3.007847000	-1.707241000
	6	5.092391000	-0.949058000	1.499878000
	1	4.758015000	-1.322492000	2.473727000
	1	5.393975000	-1.819001000	0.901261000
	1	5.987010000	-0.336588000	1.659249000
	28	-0.332025000	0.465324000	0.155286000
	6	3.378198000	0.005585000	1.178512000
	6	4.646658000	-0.187786000	0.633261000
	6	4.817111000	-1.036856000	-0.464536000
	6	3.708126000	-1.697812000	-1.003742000
	6	2.442105000	-1.505089000	-0.454604000
	6	2.253463000	-0.659577000	0.655279000
	1	3.250938000	0.676431000	2.025158000
	1	5.501577000	0.331569000	1.059019000
	1	5.804169000	-1.183358000	-0.895417000
	1	3.829305000	-2.352002000	-1.863541000
	1	1.587085000	-2.003886000	-0.904338000
	6	0.925422000	-0.464172000	1.283088000
	6	-0.000081000	-1.674702000	1.487627000
	1	0.990848000	0.173699000	2.171083000
	1	-0.131443000	-1.910313000	2.552470000
	1	0.386597000	-2.571825000	0.996232000
INT-MI	6	-1.315808000	-1.242641000	0.846732000
	6	-1.987832000	-0.115454000	1.385439000
	6	-3.205087000	0.344495000	0.806903000
	6	-3.698756000	-0.323384000	-0.304850000
	6	-3.049720000	-1.454159000	-0.864224000
	6	-1.868794000	-1.897639000	-0.285118000
	1	-1.670562000	0.304828000	2.338369000
	1	-4.623123000	0.025159000	-0.762375000
	1	-1.354270000	-2.764007000	-0.695407000
	35	0.646748000	2.139476000	-0.954910000
	6	-3.645290000	-2.142404000	-2.068947000
	1	-3.685327000	-1.464001000	-2.930777000
	1	-3.058908000	-3.019544000	-2.360449000
	1	-4.672471000	-2.472950000	-1.869580000
	6	-3.926249000	1.522303000	1.415131000
	1	-4.203680000	1.319243000	2.457679000
	1	-3.290115000	2.415948000	1.416884000
	1	-4.840911000	1.760043000	0.863129000

	28	-1.438159000	0.511073000	-0.164439000
	6	-2.694795000	-1.167201000	1.296849000
	6	-4.083558000	-1.042335000	1.375917000
	6	-4.863931000	-1.093696000	0.216397000
	6	-4.255808000	-1.243341000	-1.035452000
	6	-2.870247000	-1.370811000	-1.127519000
	6	-2.051350000	-1.377564000	0.041817000
	1	-2.102456000	-1.141872000	2.205752000
	1	-4.554203000	-0.892603000	2.343497000
	1	-5.943834000	-0.993840000	0.285675000
	1	-4.859187000	-1.251250000	-1.938748000
	1	-2.397469000	-1.500680000	-2.097542000
	6	-0.610483000	-1.207605000	-0.113767000
	6	0.393500000	-1.490904000	0.994318000
	1	-0.225844000	-1.445595000	-1.109119000
	1	0.383289000	-2.575576000	1.191024000
	1	0.089799000	-1.007101000	1.929827000
TS-con	6	1.804536000	-1.064632000	0.632929000
	6	2.644297000	-1.932287000	-0.081903000
	6	3.937740000	-1.550486000	-0.450786000
	6	4.380609000	-0.266902000	-0.094571000
	6	3.567047000	0.619594000	0.617528000
	6	2.279496000	0.199798000	0.985230000
	1	2.285646000	-2.926288000	-0.348054000
	1	5.384281000	0.046036000	-0.379953000
	1	1.636291000	0.879797000	1.539412000
	35	-0.458727000	2.471858000	-0.467126000
	6	4.055237000	1.996761000	1.005740000
	1	3.334700000	2.766854000	0.705457000
	1	4.185612000	2.081070000	2.092816000
	1	5.017305000	2.228707000	0.536537000
	6	4.841503000	-2.489630000	-1.218503000
	1	4.386990000	-3.480105000	-1.329492000
	1	5.053288000	-2.106267000	-2.225376000
	1	5.806925000	-2.618919000	-0.713341000
	28	-2.051786000	-0.158498000	-0.121592000
	6	-0.763894000	1.897230000	1.538379000
	6	-1.447695000	3.093503000	1.520238000
	6	-2.027363000	3.575383000	0.319227000
INT-con	6	-1.890537000	2.860966000	-0.855634000
	6	-1.177633000	1.633479000	-0.870492000
	6	-0.594367000	1.134119000	0.338569000
	1	-0.331958000	1.519737000	2.461545000
	1	-1.554368000	3.669496000	2.435630000

	1	-2.571567000	4.515931000	0.325670000
	1	-2.311511000	3.241173000	-1.782511000
	1	-0.920127000	1.197012000	-1.832918000
	6	-0.183305000	-0.256447000	0.328804000
	6	0.696234000	-0.878436000	-0.746528000
	1	-0.020121000	-0.692822000	1.316854000
	1	0.449769000	-0.479667000	-1.736717000
	1	0.495429000	-1.954431000	-0.782137000
	6	2.172284000	-0.638247000	-0.454095000
	6	2.972140000	-1.653486000	0.075549000
	6	4.331222000	-1.437645000	0.358415000
	6	4.872229000	-0.174426000	0.103095000
	6	4.093935000	0.868070000	-0.427138000
	6	2.744958000	0.621485000	-0.693674000
	1	2.536961000	-2.633788000	0.265488000
	1	5.924666000	0.005971000	0.318436000
	1	2.128920000	1.419578000	-1.104166000
	35	-3.410689000	-1.897745000	-0.053005000
	6	4.708167000	2.224239000	-0.694076000
	1	5.545204000	2.151926000	-1.400132000
	1	3.973844000	2.918499000	-1.116042000
	1	5.101322000	2.672658000	0.227361000
	6	5.185387000	-2.557231000	0.910217000
	1	4.694286000	-3.057778000	1.753491000
	1	5.377298000	-3.323486000	0.147352000
	1	6.155496000	-2.186345000	1.257426000
R2-KOEt	6	3.029838000	-1.249977000	-0.022147000
	6	2.407049000	-0.456681000	1.145797000
	1	2.658328000	-0.939251000	2.102836000
	1	2.848008000	0.557245000	1.154817000
	6	2.526089000	-0.590048000	-1.325556000
	1	2.982345000	0.413749000	-1.408400000
	1	2.861137000	-1.172768000	-2.195482000
	6	4.560673000	-1.145856000	0.050679000
	1	4.943938000	-1.586207000	0.981185000
	1	5.030545000	-1.681886000	-0.784366000
	1	4.897998000	-0.101731000	0.009065000
	6	2.600977000	-2.725548000	0.038206000
	1	1.513763000	-2.821128000	-0.018606000
	1	3.035708000	-3.290747000	-0.796766000
	1	2.938601000	-3.193087000	0.973346000
	8	0.992169000	-0.376352000	1.061906000
	8	1.117996000	-0.505644000	-1.387577000
	5	0.451373000	0.113000000	-0.259948000

	6	-1.151179000	-0.255733000	-0.279368000
	6	-2.177441000	0.702771000	-0.352509000
	6	-1.576718000	-1.597805000	-0.193560000
	6	-3.538328000	0.356373000	-0.341041000
	1	-1.915972000	1.756838000	-0.456187000
	6	-2.925067000	-1.954613000	-0.183027000
	1	-0.825207000	-2.381909000	-0.140021000
	6	-3.936817000	-0.981178000	-0.255320000
	1	-4.295102000	1.136880000	-0.417666000
	1	-3.202565000	-3.006807000	-0.121595000
	6	0.651990000	3.849394000	-1.112240000
	1	1.508918000	4.129818000	-0.486598000
	1	0.701411000	4.432142000	-2.040935000
	1	-0.267555000	4.137765000	-0.584065000
	6	0.670268000	2.353002000	-1.409496000
	1	1.571231000	2.103789000	-1.989317000
	1	-0.189486000	2.083560000	-2.042939000
	8	0.649532000	1.620923000	-0.197813000
	19	-0.433970000	1.464754000	2.181845000
	6	-5.397040000	-1.375916000	-0.252030000
	1	-6.048716000	-0.498390000	-0.329690000
	1	-5.633473000	-2.040765000	-1.093008000
	1	-5.668636000	-1.912967000	0.666615000
COM-1	28	0.157314000	-1.015041000	0.275211000
	6	1.837213000	-1.309733000	2.843693000
	6	1.233002000	-0.971613000	4.036591000
	6	0.351209000	0.134044000	4.110712000
	6	0.099214000	0.891775000	2.983013000
	6	0.736194000	0.585926000	1.756416000
	6	1.637663000	-0.514007000	1.671732000
	1	2.507290000	-2.163793000	2.783932000
	1	1.427495000	-1.563922000	4.927740000
	1	-0.126145000	0.381027000	5.055443000
	1	-0.582170000	1.736254000	3.026403000
	1	0.657480000	1.300355000	0.942304000
	6	2.089115000	-0.915842000	0.356855000
	6	2.679305000	0.057428000	-0.662852000
	1	2.585390000	-1.887681000	0.330047000
	1	2.164684000	1.023179000	-0.630825000
	1	2.509033000	-0.355092000	-1.663300000
	6	4.171017000	0.266406000	-0.450001000
	6	5.099284000	-0.601675000	-1.033005000
	6	6.479209000	-0.437763000	-0.834824000
	6	6.916033000	0.616432000	-0.026519000

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6	6.010677000	1.506158000	0.573979000
6	4.643227000	1.314910000	0.354827000
1	4.743107000	-1.417021000	-1.662046000
1	7.984395000	0.754277000	0.136727000
1	3.928173000	1.995541000	0.814131000
35	0.249716000	-2.547951000	-1.507313000
6	6.512354000	2.649186000	1.428821000
1	7.073698000	3.378980000	0.830301000
1	5.684285000	3.180876000	1.909540000
1	7.186078000	2.293329000	2.218487000
6	7.464699000	-1.381650000	-1.488476000
1	7.251272000	-2.426226000	-1.228503000
1	7.422736000	-1.307458000	-2.583087000
1	8.492738000	-1.163213000	-1.179886000
8	-1.879437000	-0.939131000	0.368710000
6	-2.493059000	-2.042280000	1.059172000
1	-2.114943000	-2.962755000	0.587557000
1	-3.576417000	-1.985757000	0.906166000
6	-2.176034000	-2.074429000	2.547359000
1	-2.649494000	-2.952594000	3.007536000
1	-1.096101000	-2.143444000	2.713897000
1	-2.551183000	-1.170771000	3.033704000
6	-5.586551000	1.020598000	0.216797000
6	-4.852842000	0.714287000	-1.105296000
1	-5.549314000	0.257997000	-1.825764000
1	-4.492853000	1.659126000	-1.547334000
6	-4.519046000	1.541025000	1.207836000
1	-4.218207000	2.553001000	0.885477000
1	-4.955298000	1.635232000	2.212474000
6	-6.636743000	2.116080000	-0.025881000
1	-7.406887000	1.775966000	-0.731022000
1	-7.144057000	2.387392000	0.909133000
1	-6.183772000	3.027296000	-0.436683000
6	-6.273408000	-0.241561000	0.764770000
1	-5.546006000	-1.028865000	0.980645000
1	-6.810798000	-0.018377000	1.695674000
1	-7.003716000	-0.636380000	0.044714000
8	-3.762158000	-0.174767000	-0.924425000
8	-3.388640000	0.698993000	1.313567000
5	-2.729602000	0.292236000	0.080606000
6	-1.755742000	1.425108000	-0.583516000
6	-1.517442000	2.663002000	0.040114000
6	-1.096219000	1.227463000	-1.811928000
6	-0.691027000	3.641266000	-0.522913000

	1	-1.979097000	2.861510000	1.004884000
	6	-0.259982000	2.192205000	-2.380659000
	1	-1.209229000	0.285840000	-2.345578000
	6	-0.048708000	3.426630000	-1.750639000
	1	-0.540850000	4.584903000	0.000794000
	1	0.238129000	1.980992000	-3.326186000
	19	-2.719026000	-2.142801000	-2.150513000
	6	0.811203000	4.494490000	-2.388397000
	1	1.623376000	4.056464000	-2.980123000
	1	0.221163000	5.128742000	-3.064771000
	1	1.259685000	5.152581000	-1.635352000
TS-pre-TM	28	-0.175143000	-0.604499000	0.119012000
	6	-1.863088000	-3.105457000	0.440636000
	6	-1.861835000	-3.961615000	-0.638889000
	6	-1.910165000	-3.454252000	-1.959425000
	6	-1.957165000	-2.089442000	-2.175593000
	6	-1.962384000	-1.187222000	-1.081982000
	6	-1.935040000	-1.688445000	0.255833000
	1	-1.803721000	-3.492992000	1.451274000
	1	-1.817469000	-5.035257000	-0.473748000
	1	-1.924250000	-4.141516000	-2.802260000
	1	-2.025931000	-1.698455000	-3.187130000
	1	-2.188913000	-0.141074000	-1.266750000
	6	-1.703742000	-0.739784000	1.327085000
	6	-2.562235000	0.500485000	1.614161000
	1	-1.365448000	-1.209381000	2.251693000
	1	-1.903946000	1.348281000	1.830125000
	1	-3.080613000	0.291156000	2.563142000
	6	-3.612223000	0.919692000	0.602618000
	6	-3.458990000	2.079171000	-0.163353000
	6	-4.439070000	2.484584000	-1.085317000
	6	-5.584329000	1.697302000	-1.230635000
	6	-5.773716000	0.529474000	-0.472366000
	6	-4.781426000	0.158272000	0.437851000
	1	-2.560563000	2.680798000	-0.040434000
	1	-6.352037000	1.999213000	-1.942411000
	1	-4.913813000	-0.744886000	1.031545000
	6	-7.023889000	-0.303406000	-0.649968000
	1	-7.068691000	-0.745142000	-1.654220000
	1	-7.063694000	-1.123352000	0.074767000
	1	-7.930404000	0.301808000	-0.523075000
	6	-4.263281000	3.761112000	-1.878062000
	1	-4.418914000	4.645432000	-1.245280000
	1	-3.252741000	3.839009000	-2.297073000

pre-TM	1	-4.977205000	3.819846000	-2.706782000
	8	1.305496000	-0.526284000	-1.219690000
	6	1.330111000	-0.849228000	-2.618321000
	1	0.925576000	-1.866096000	-2.706897000
	1	2.379100000	-0.859221000	-2.946900000
	6	0.535747000	0.105019000	-3.504919000
	1	0.543611000	-0.266346000	-4.538786000
	1	-0.505225000	0.171356000	-3.175535000
	1	0.975838000	1.102962000	-3.479144000
	6	4.753651000	1.875665000	-0.994225000
	6	4.440369000	0.894418000	0.155364000
	1	5.338512000	0.317300000	0.419808000
	1	4.141962000	1.464874000	1.050628000
	6	3.414237000	2.536345000	-1.393409000
	1	3.092811000	3.208285000	-0.578142000
	1	3.549452000	3.152824000	-2.292879000
	6	5.730175000	2.952751000	-0.498302000
	1	6.690185000	2.510236000	-0.201180000
	1	5.937303000	3.688478000	-1.286377000
	1	5.328014000	3.493738000	0.367624000
	6	5.362969000	1.127261000	-2.192331000
	1	4.673395000	0.369107000	-2.576225000
	1	5.588531000	1.821274000	-3.012452000
	1	6.300678000	0.629911000	-1.908399000
	8	3.415308000	-0.025975000	-0.189427000
	8	2.398480000	1.591799000	-1.673557000
	5	2.144214000	0.599986000	-0.644245000
	6	1.248196000	1.196941000	0.615331000
	6	0.523091000	2.406751000	0.440158000
	6	1.363800000	0.733937000	1.946432000
	6	0.006382000	3.122364000	1.513788000
	1	0.425728000	2.809518000	-0.565816000
	6	0.818277000	1.440846000	3.029115000
	1	1.922565000	-0.173956000	2.148468000
	6	0.152432000	2.652919000	2.835821000
	1	-0.508447000	4.066613000	1.339049000
	1	0.940274000	1.046441000	4.036199000
	19	3.082699000	-2.582300000	-0.334447000
	35	1.135166000	-2.828911000	1.908700000
	6	-0.403846000	3.443508000	3.996880000
	1	-1.501497000	3.473111000	3.969483000
	1	-0.106671000	3.007964000	4.956495000
	1	-0.054848000	4.483637000	3.974003000
pre-TM	28	0.364529000	0.290557000	-0.116604000

6	1.088119000	3.135170000	-0.383384000
6	0.970758000	3.655813000	-1.655771000
6	1.391284000	2.909129000	-2.782869000
6	1.907502000	1.636294000	-2.618047000
6	2.047551000	1.080391000	-1.322119000
6	1.679513000	1.846269000	-0.170046000
1	0.725350000	3.697147000	0.470568000
1	0.541240000	4.645374000	-1.787510000
1	1.308850000	3.340405000	-3.777976000
1	2.240716000	1.061800000	-3.478556000
1	2.611579000	0.160448000	-1.208059000
6	1.604433000	1.176203000	1.111336000
6	2.706658000	0.360927000	1.795764000
1	1.054013000	1.753958000	1.855185000
1	2.211660000	-0.338048000	2.480694000
1	3.254001000	1.066752000	2.440752000
6	3.718415000	-0.388806000	0.952630000
6	3.503513000	-1.721427000	0.583602000
6	4.434352000	-2.422426000	-0.199042000
6	5.595750000	-1.758487000	-0.609576000
6	5.849412000	-0.426860000	-0.245199000
6	4.901023000	0.241215000	0.536343000
1	2.591985000	-2.220729000	0.906775000
1	6.324811000	-2.290689000	-1.219497000
1	5.080327000	1.276207000	0.823769000
6	7.129573000	0.256029000	-0.672563000
1	7.338125000	0.088311000	-1.736157000
1	7.081381000	1.337170000	-0.505089000
1	7.991090000	-0.127910000	-0.109940000
6	4.194290000	-3.870840000	-0.563264000
1	4.354939000	-4.527925000	0.302053000
1	3.165674000	-4.034359000	-0.905826000
1	4.871819000	-4.201630000	-1.357707000
8	-0.919935000	-0.366968000	-1.450519000
6	-0.777396000	-0.714088000	-2.839415000
1	-0.522058000	0.212082000	-3.369533000
1	-1.753948000	-1.061808000	-3.195508000
6	0.283133000	-1.777642000	-3.096295000
1	0.352350000	-1.976398000	-4.174211000
1	1.267535000	-1.444905000	-2.749212000
1	0.020345000	-2.704498000	-2.581560000
6	-4.246062000	-2.774259000	-0.571554000
6	-4.193728000	-1.334446000	-0.018274000
1	-5.142123000	-0.814712000	-0.212888000

	1	-4.055647000	-1.367866000	1.075516000
	6	-2.835544000	-3.377412000	-0.385496000
	1	-2.657166000	-3.534792000	0.693036000
	1	-2.775290000	-4.358834000	-0.874761000
	6	-5.263195000	-3.595119000	0.236323000
	1	-6.275027000	-3.182339000	0.131725000
	1	-5.294632000	-4.635292000	-0.113006000
	1	-5.015756000	-3.608067000	1.305431000
	6	-4.639955000	-2.769992000	-2.058658000
	1	-3.922572000	-2.200728000	-2.657006000
	1	-4.673597000	-3.792996000	-2.455430000
	1	-5.633958000	-2.324523000	-2.199624000
	8	-3.149859000	-0.570106000	-0.608969000
	8	-1.809963000	-2.566899000	-0.933021000
	5	-1.804165000	-1.180043000	-0.520922000
	6	-1.097515000	-0.940727000	0.965571000
	6	-0.376386000	-1.995035000	1.597418000
	6	-1.371656000	0.190479000	1.774522000
	6	-0.023533000	-1.946171000	2.938908000
	1	-0.147456000	-2.884268000	1.013991000
	6	-0.996004000	0.247624000	3.126853000
	1	-1.936199000	1.034358000	1.384761000
	6	-0.343508000	-0.824015000	3.735749000
	1	0.495080000	-2.789805000	3.393014000
	1	-1.243294000	1.137214000	3.702254000
	19	-2.809497000	1.915483000	-1.381923000
	35	-2.173159000	3.761306000	0.908218000
	6	0.014498000	-0.801731000	5.203023000
	1	1.090916000	-0.953178000	5.355045000
	1	-0.262438000	0.149601000	5.668012000
	1	-0.501318000	-1.604358000	5.746160000
TS-TM	28	0.413095000	-0.100986000	-0.112666000
	6	0.046945000	-2.704975000	-1.589623000
	6	-0.519056000	-3.718198000	-0.840122000
	6	-0.134592000	-3.907313000	0.510983000
	6	0.818948000	-3.081813000	1.078805000
	6	1.407855000	-2.031330000	0.328486000
	6	1.043544000	-1.834431000	-1.039184000
	1	-0.251614000	-2.562869000	-2.626117000
	1	-1.278208000	-4.365587000	-1.269891000
	1	-0.592386000	-4.708342000	1.084796000
	1	1.143683000	-3.243208000	2.104235000
	1	2.261126000	-1.504408000	0.745327000
	6	1.430980000	-0.589796000	-1.689190000

6	2.867582000	-0.079045000	-1.888317000
1	0.863485000	-0.408826000	-2.606260000
1	2.805337000	1.001168000	-2.068070000
1	3.228345000	-0.518714000	-2.831577000
6	3.906192000	-0.353690000	-0.818684000
6	4.159173000	0.579117000	0.199713000
6	5.114266000	0.335188000	1.192849000
6	5.824185000	-0.875370000	1.155923000
6	5.608259000	-1.820421000	0.147206000
6	4.645045000	-1.541282000	-0.834805000
1	3.603719000	1.514513000	0.209240000
1	6.568940000	-1.078743000	1.924482000
1	4.463587000	-2.269402000	-1.624413000
6	6.404190000	-3.105594000	0.097038000
1	6.971649000	-3.261445000	1.020606000
1	5.752938000	-3.975571000	-0.050115000
1	7.121187000	-3.095002000	-0.734613000
6	5.402283000	1.359524000	2.268291000
1	6.389582000	1.818350000	2.124879000
1	4.660627000	2.165271000	2.262713000
1	5.400832000	0.905733000	3.267001000
8	-0.821198000	0.155344000	1.399886000
6	-0.508768000	0.015176000	2.809853000
1	-0.481167000	-1.064166000	2.988199000
1	-1.340352000	0.446657000	3.375289000
6	0.808959000	0.660149000	3.211953000
1	1.003399000	0.453206000	4.272106000
1	1.642822000	0.252504000	2.629343000
1	0.771869000	1.743545000	3.072947000
6	-3.518601000	3.277588000	0.938540000
6	-3.397588000	2.253105000	-0.205769000
1	-4.382983000	1.858437000	-0.479822000
1	-2.966283000	2.736469000	-1.093576000
6	-2.085247000	3.634429000	1.379595000
1	-1.570589000	4.187594000	0.579911000
1	-2.102162000	4.269065000	2.272917000
6	-4.217303000	4.540235000	0.408477000
1	-5.233739000	4.310640000	0.065013000
1	-4.300200000	5.300518000	1.195083000
1	-3.669947000	4.984403000	-0.432181000
6	-4.318767000	2.690546000	2.115755000
1	-3.841339000	1.794221000	2.524114000
1	-4.405457000	3.422227000	2.928680000
1	-5.334251000	2.419713000	1.800252000

	8	-2.584262000	1.128651000	0.150000000
	8	-1.316396000	2.478918000	1.710029000
	5	-1.371233000	1.385045000	0.845273000
	6	0.006814000	1.797069000	-0.651660000
	6	0.947169000	2.767323000	-0.226469000
	6	-0.540650000	2.010264000	-1.938409000
	6	1.316438000	3.853704000	-1.019535000
	1	1.386451000	2.683933000	0.765858000
	6	-0.176391000	3.092656000	-2.742354000
	1	-1.271856000	1.303491000	-2.327379000
	6	0.763501000	4.034967000	-2.298294000
	1	2.044405000	4.572622000	-0.645590000
	1	-0.622376000	3.205889000	-3.729519000
	19	-2.898335000	-1.564969000	0.163612000
	35	-4.160096000	-4.150019000	-0.641502000
	6	1.141735000	5.224336000	-3.148777000
	1	0.984339000	5.022243000	-4.213820000
	1	0.535757000	6.103754000	-2.889794000
	1	2.192125000	5.502036000	-3.005408000
INT-TM	28	0.610990000	-0.086933000	-0.332747000
	6	0.512217000	-3.057480000	-1.415529000
	6	0.064144000	-4.056869000	-0.566055000
	6	0.440190000	-4.052341000	0.794596000
	6	1.285169000	-3.059837000	1.269795000
	6	1.748154000	-2.034055000	0.415774000
	6	1.366324000	-2.010872000	-0.954077000
	1	0.218822000	-3.066909000	-2.463608000
	1	-0.594841000	-4.837089000	-0.935590000
	1	0.072169000	-4.832503000	1.454632000
	1	1.613584000	-3.075952000	2.306889000
	1	2.499233000	-1.338887000	0.780567000
	6	1.634875000	-0.814168000	-1.768642000
	6	3.044026000	-0.276300000	-2.077881000
	1	1.074238000	-0.842568000	-2.708225000
	1	2.901620000	0.664825000	-2.621648000
	1	3.508607000	-0.974912000	-2.791953000
	6	4.020083000	-0.041271000	-0.941752000
	6	4.063079000	1.197946000	-0.282649000
	6	4.972055000	1.442800000	0.752682000
	6	5.845013000	0.412507000	1.136327000
	6	5.837653000	-0.829998000	0.492794000
	6	4.919539000	-1.038031000	-0.548349000
	1	3.380117000	1.985431000	-0.595234000
	1	6.554317000	0.589437000	1.944162000

1	4.904438000	-1.999490000	-1.059878000
6	6.816403000	-1.915510000	0.882507000
1	7.252642000	-1.726861000	1.869440000
1	6.336222000	-2.900804000	0.906894000
1	7.644381000	-1.977842000	0.163392000
6	5.041405000	2.796448000	1.425026000
1	5.924086000	3.358567000	1.091515000
1	4.160173000	3.404499000	1.194345000
1	5.113625000	2.702538000	2.515462000
8	-0.531637000	0.284170000	1.451959000
6	0.193194000	0.218588000	2.723375000
1	0.516651000	-0.820691000	2.804436000
1	-0.520423000	0.427678000	3.525292000
6	1.371596000	1.174101000	2.777250000
1	1.905519000	1.030275000	3.725052000
1	2.076124000	0.984958000	1.960397000
1	1.037511000	2.213984000	2.725384000
6	-3.960083000	2.680170000	1.400472000
6	-3.585652000	1.854702000	0.158349000
1	-4.454226000	1.311165000	-0.225867000
1	-3.192218000	2.494842000	-0.639587000
6	-2.658392000	3.275804000	1.965143000
1	-2.262989000	4.045087000	1.291104000
1	-2.827076000	3.727252000	2.947804000
6	-4.889913000	3.829282000	0.974218000
1	-5.828941000	3.438899000	0.564206000
1	-5.144577000	4.462124000	1.833032000
1	-4.425850000	4.465428000	0.211046000
6	-4.662469000	1.799673000	2.452711000
1	-4.028625000	0.976216000	2.798337000
1	-4.938869000	2.395851000	3.330582000
1	-5.580163000	1.361859000	2.042338000
8	-2.578764000	0.860945000	0.455432000
8	-1.621614000	2.290401000	2.139112000
5	-1.581540000	1.198844000	1.331539000
6	0.107587000	1.484275000	-1.272790000
6	0.360161000	2.761002000	-0.729828000
6	-0.600032000	1.468100000	-2.493540000
6	-0.070640000	3.939443000	-1.357675000
1	0.906250000	2.857257000	0.207322000
6	-1.039691000	2.639465000	-3.118856000
1	-0.817662000	0.519734000	-2.983967000
6	-0.778419000	3.902862000	-2.565555000
1	0.158218000	4.902206000	-0.900359000

	1	-1.587238000	2.569901000	-4.058695000
	19	-2.306886000	-1.795120000	-0.228951000
	35	-3.664263000	-4.431801000	-0.420767000
	6	-1.208322000	5.170075000	-3.270952000
	1	-0.508837000	5.435817000	-4.075693000
	1	-2.198328000	5.061548000	-3.730170000
	1	-1.247107000	6.020172000	-2.580379000
	28	0.602520000	0.277324000	-0.559569000
	6	1.473200000	-0.388745000	-3.283722000
	6	1.244134000	-1.688922000	-3.703093000
	6	1.418430000	-2.777770000	-2.814189000
	6	1.822869000	-2.524816000	-1.510018000
	6	2.068663000	-1.205927000	-1.051586000
	6	1.927141000	-0.084305000	-1.954526000
	1	1.356355000	0.429194000	-3.992570000
	1	0.954880000	-1.874588000	-4.735751000
	1	1.265891000	-3.798112000	-3.157382000
	1	1.978911000	-3.352154000	-0.820939000
	1	2.592990000	-1.095796000	-0.108007000
	6	2.123293000	1.348169000	-1.554851000
	6	3.436091000	1.804482000	-0.863939000
	1	2.046780000	1.940434000	-2.467144000
	1	3.267060000	2.805997000	-0.451070000
	1	4.157424000	1.934580000	-1.682320000
	6	4.101911000	0.929230000	0.182392000
TS-RE	6	3.769251000	1.011713000	1.544188000
	6	4.395989000	0.207791000	2.502649000
	6	5.378723000	-0.699071000	2.076652000
	6	5.749962000	-0.795807000	0.731815000
	6	5.103387000	0.029905000	-0.200222000
	1	3.015659000	1.723654000	1.870785000
	1	5.870456000	-1.334578000	2.811935000
	1	5.378605000	-0.040352000	-1.251568000
	6	6.827800000	-1.758169000	0.285053000
	1	7.158542000	-2.398796000	1.109241000
	1	6.473428000	-2.407930000	-0.524695000
	1	7.707680000	-1.221610000	-0.093423000
	6	4.048195000	0.327803000	3.970018000
	1	4.848040000	0.834035000	4.526854000
	1	3.128728000	0.904011000	4.119292000
	1	3.908364000	-0.657206000	4.431282000
	8	-0.744422000	-0.201605000	0.921533000
	6	-0.129661000	-0.427999000	2.236093000
	1	-0.448717000	0.384870000	2.894080000

1	0.944844000	-0.337450000	2.060151000
6	-0.488212000	-1.789073000	2.802011000
1	0.033339000	-1.917817000	3.759819000
1	-1.563095000	-1.887466000	2.973340000
1	-0.190060000	-2.595763000	2.126889000
6	-4.823479000	0.706825000	0.647218000
6	-3.905721000	0.873830000	-0.576814000
1	-4.364529000	0.422702000	-1.462875000
1	-3.720211000	1.935105000	-0.787098000
6	-4.039537000	1.167703000	1.889316000
1	-3.927433000	2.259974000	1.891115000
1	-4.561714000	0.874872000	2.805395000
6	-6.043917000	1.629902000	0.474914000
1	-6.625909000	1.344192000	-0.409833000
1	-6.711958000	1.553325000	1.341517000
1	-5.752837000	2.682448000	0.364561000
6	-5.288569000	-0.754820000	0.788201000
1	-4.464871000	-1.475568000	0.828526000
1	-5.889397000	-0.877667000	1.697904000
1	-5.918828000	-1.034439000	-0.065770000
8	-2.621010000	0.237685000	-0.408630000
8	-2.717883000	0.607665000	1.972791000
5	-2.067186000	0.218552000	0.847448000
6	0.627094000	2.209894000	-0.828318000
6	0.744541000	3.043551000	0.305718000
6	-0.317579000	2.612807000	-1.804520000
6	-0.061505000	4.172441000	0.473178000
1	1.455656000	2.798982000	1.088389000
6	-1.123211000	3.736938000	-1.631284000
1	-0.419173000	2.032071000	-2.720415000
6	-1.010935000	4.546401000	-0.488557000
1	0.052010000	4.774218000	1.374039000
1	-1.842518000	4.001793000	-2.405661000
19	-1.458096000	-2.037130000	-1.633963000
35	-2.808640000	-3.674586000	0.474650000
6	-1.841703000	5.798653000	-0.327223000
1	-1.332407000	6.674909000	-0.752455000
1	-2.808314000	5.709203000	-0.836709000
1	-2.035409000	6.019211000	0.728943000
INT-RE	28	-0.316982000	1.545259000	-0.691892000
	6	0.963149000	-3.072742000	0.000863000
	6	-0.150716000	-3.807453000	0.426695000
	6	-0.998285000	-3.289081000	1.410279000
	6	-0.701107000	-2.045302000	1.980611000

6	0.409243000	-1.312643000	1.547163000
6	1.257577000	-1.812319000	0.545237000
1	1.615149000	-3.486618000	-0.766839000
1	-0.370152000	-4.772050000	-0.023158000
1	-1.885235000	-3.837839000	1.710143000
1	-1.348413000	-1.637675000	2.753525000
1	0.616637000	-0.338529000	1.983574000
6	2.508064000	-1.052622000	0.098538000
6	3.597580000	-1.183385000	1.201809000
1	2.883177000	-1.592345000	-0.783472000
1	3.537184000	-2.211108000	1.584420000
1	3.335492000	-0.537898000	2.049435000
6	5.037076000	-0.921009000	0.787090000
6	5.600120000	-1.554688000	-0.332612000
6	6.938426000	-1.362189000	-0.686197000
6	7.729256000	-0.519360000	0.111169000
6	7.206294000	0.118388000	1.238910000
6	5.856322000	-0.094063000	1.561161000
1	4.989107000	-2.217821000	-0.942156000
1	8.774102000	-0.362452000	-0.153678000
1	5.438891000	0.397361000	2.439771000
6	8.068272000	1.011499000	2.103567000
1	9.068896000	1.136027000	1.676402000
1	7.625501000	2.009262000	2.215970000
1	8.186622000	0.595538000	3.112680000
6	7.530807000	-2.041271000	-1.901001000
1	8.431673000	-2.611235000	-1.641319000
1	6.817561000	-2.733632000	-2.360695000
1	7.821683000	-1.307904000	-2.664505000
8	-1.772305000	2.144533000	0.503721000
6	-1.355281000	3.131119000	1.507331000
1	-0.357575000	2.814221000	1.817179000
1	-2.040385000	3.055129000	2.355028000
6	-1.338419000	4.534787000	0.929001000
1	-0.983213000	5.237885000	1.692644000
1	-0.662897000	4.591618000	0.069034000
1	-2.341492000	4.844976000	0.619346000
6	-5.684833000	0.769069000	0.613419000
6	-4.865419000	0.497278000	-0.656449000
1	-4.901284000	-0.564483000	-0.917064000
1	-5.233135000	1.098496000	-1.497658000
6	-5.437570000	2.227967000	1.024548000
1	-5.887010000	2.920149000	0.300971000
1	-5.859210000	2.440733000	2.012151000

6	-7.173431000	0.578366000	0.274095000
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6	-5.282422000	-0.200433000	1.743984000
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1	-5.935278000	-0.059911000	2.614620000
1	-5.358141000	-1.237979000	1.402555000
8	-3.454814000	0.824161000	-0.479370000
8	-4.030141000	2.545100000	1.107429000
5	-3.130637000	1.841173000	0.368503000
6	2.210235000	0.368582000	-0.383614000
6	2.913320000	1.484414000	0.025119000
6	1.208954000	0.535905000	-1.414355000
6	2.716635000	2.755719000	-0.588196000
1	3.677581000	1.402717000	0.789587000
6	1.033011000	1.811689000	-2.057585000
1	0.889099000	-0.367378000	-1.941504000
6	1.826722000	2.936125000	-1.629332000
1	3.322107000	3.594774000	-0.249939000
1	0.554151000	1.866742000	-3.037714000
19	-1.839840000	-1.376397000	-1.110813000
35	-4.258036000	-3.152243000	-0.694204000
6	1.712338000	4.250442000	-2.363744000
1	2.067020000	4.151485000	-3.399366000
1	0.672635000	4.597068000	-2.417136000
1	2.307441000	5.033403000	-1.881359000
6	3.188573000	-1.162000000	1.169593000
6	4.530169000	-1.536819000	1.088109000
6	5.088684000	-1.881086000	-0.147158000
6	4.289699000	-1.847085000	-1.291183000
6	2.944361000	-1.471925000	-1.202921000
6	2.371577000	-1.120649000	0.027750000
1	2.764528000	-0.892388000	2.135074000
1	5.138869000	-1.562868000	1.988828000
Product	1	6.132839000	-2.175827000	-0.214835000
1	4.709266000	-2.116129000	-2.257731000
1	2.343018000	-1.461959000	-2.107626000
6	0.913283000	-0.683757000	0.177416000
6	-0.021372000	-1.293071000	-0.911179000
1	0.566300000	-1.079362000	1.140918000
1	0.239641000	-2.353070000	-1.024734000
1	0.176514000	-0.810289000	-1.875436000
6	-1.496046000	-1.176399000	-0.584216000

	6	-2.093081000	-2.083402000	0.307794000
	6	-3.447113000	-1.996193000	0.641464000
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	6	-3.652167000	-0.053534000	-0.830223000
	6	-2.288532000	-0.171891000	-1.144971000
	1	-1.487941000	-2.878211000	0.742914000
	1	-5.270146000	-0.891198000	0.313692000
	1	-1.837937000	0.538198000	-1.836451000
	6	-4.486946000	1.043242000	-1.453284000
	1	-5.511525000	1.035091000	-1.066297000
	1	-4.058981000	2.033113000	-1.250770000
	1	-4.541398000	0.932512000	-2.544175000
	6	-4.085623000	-2.987076000	1.589681000
	1	-3.342635000	-3.672138000	2.011825000
	1	-4.584896000	-2.478440000	2.424122000
	1	-4.846162000	-3.593668000	1.080677000
	6	0.780857000	0.837588000	0.255689000
	6	0.062876000	1.439336000	1.295787000
	6	1.345481000	1.676357000	-0.717031000
	6	-0.087371000	2.827857000	1.363769000
	1	-0.396300000	0.815596000	2.059895000
	6	1.192703000	3.061270000	-0.650656000
	1	1.921638000	1.245351000	-1.532688000
	6	0.475930000	3.665763000	0.393995000
	1	-0.654788000	3.262316000	2.184821000
	1	1.643963000	3.684436000	-1.420973000
	6	0.345290000	5.169720000	0.480921000
	1	1.244124000	5.622667000	0.921443000
	1	0.208991000	5.619214000	-0.509753000
	1	-0.506971000	5.462282000	1.104064000
TS-con'	28	0.219469000	0.907614000	-0.284107000
	6	2.973095000	-1.617050000	0.985289000
	6	4.324850000	-1.916672000	0.819255000
	6	4.936956000	-1.729582000	-0.423756000
	6	4.185404000	-1.238307000	-1.496633000
	6	2.837301000	-0.928147000	-1.325636000
	6	2.200172000	-1.126684000	-0.084584000
	1	2.503494000	-1.761049000	1.955759000
	1	4.901661000	-2.292443000	1.660541000
	1	5.990450000	-1.962046000	-0.555594000
	1	4.656567000	-1.078804000	-2.463165000
	1	2.278751000	-0.519794000	-2.164294000
	6	0.768816000	-0.818872000	0.131521000
	6	-0.254309000	-1.189798000	-0.962378000

	1	0.430850000	-1.094538000	1.134300000
	1	-0.075568000	-2.227579000	-1.281619000
	1	-0.049294000	-0.607205000	-1.886672000
	6	-1.706060000	-0.975911000	-0.558592000
	6	-2.257443000	-1.662908000	0.535526000
	6	-3.586810000	-1.468264000	0.913918000
	6	-4.368788000	-0.558957000	0.179592000
	6	-3.852401000	0.140925000	-0.912213000
	6	-2.511572000	-0.080944000	-1.271581000
	1	-1.642468000	-2.366035000	1.093719000
	1	-5.405484000	-0.397420000	0.470988000
	1	-2.100482000	0.445937000	-2.132795000
	35	1.179808000	2.544545000	0.829612000
	6	-4.698440000	1.124537000	-1.687866000
	1	-5.739323000	1.109548000	-1.349130000
	1	-4.323715000	2.149308000	-1.569125000
	1	-4.690709000	0.899184000	-2.761498000
	6	-4.181722000	-2.212134000	2.087649000
	1	-5.036284000	-2.826931000	1.777917000
	1	-3.446267000	-2.873190000	2.557490000
	1	-4.544861000	-1.516619000	2.854677000
INT-con'	28	0.897072000	-1.065528000	0.605238000
	6	2.048596000	1.926442000	-1.572570000
	6	3.078738000	2.861139000	-1.660217000
	6	3.614836000	3.424566000	-0.498264000
	6	3.112406000	3.042972000	0.750928000
	6	2.086029000	2.104935000	0.838310000
	6	1.529585000	1.531656000	-0.323439000
	1	1.637368000	1.487482000	-2.478691000
	1	3.464135000	3.149339000	-2.634740000
	1	4.418861000	4.152759000	-0.564020000
	1	3.529539000	3.470380000	1.659046000
	1	1.723868000	1.807418000	1.819278000
	6	0.452955000	0.525772000	-0.283969000
	6	-0.559009000	0.467716000	0.828297000
	1	0.051750000	0.285068000	-1.270881000
	1	-0.442702000	1.292178000	1.537159000
	1	-0.323782000	-0.444399000	1.528829000
	6	-2.005851000	0.295441000	0.418908000
	6	-2.920987000	1.308445000	0.707862000
	6	-4.262278000	1.207034000	0.305930000
	6	-4.666299000	0.054554000	-0.374063000
	6	-3.768712000	-0.985656000	-0.666934000
	6	-2.437146000	-0.851183000	-0.262866000

	1	-2.589341000	2.198333000	1.240811000
	1	-5.705817000	-0.041048000	-0.684408000
	1	-1.726787000	-1.649223000	-0.474984000
	35	2.441969000	-2.518901000	0.044548000
	6	-4.243342000	-2.230611000	-1.381730000
	1	-4.794065000	-1.980374000	-2.296646000
	1	-3.404661000	-2.877009000	-1.659398000
	1	-4.920057000	-2.817708000	-0.747148000
	6	-5.233636000	2.329515000	0.593493000
	1	-5.154514000	2.672340000	1.632104000
	1	-5.037509000	3.197446000	-0.050016000
	1	-6.268539000	2.016907000	0.419801000
COM-2	28	-0.678833000	-1.045842000	0.213022000
	6	-3.873659000	-3.037482000	0.100849000
	6	-4.377526000	-4.240146000	-0.388384000
	6	-4.084725000	-4.648738000	-1.694783000
	6	-3.287385000	-3.835201000	-2.503899000
	6	-2.778726000	-2.631876000	-2.010898000
	6	-3.059586000	-2.206724000	-0.697207000
	1	-4.093254000	-2.730990000	1.120366000
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	1	-4.479015000	-5.586270000	-2.078399000
	1	-3.056997000	-4.137668000	-3.522706000
	1	-2.162226000	-2.018874000	-2.663290000
	6	-2.542198000	-0.945310000	-0.118934000
	6	-2.051616000	0.175283000	-0.989027000
	1	-3.102322000	-0.621886000	0.757653000
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	1	-0.884021000	0.175034000	-0.998498000
	6	-2.495182000	1.554612000	-0.550501000
	6	-3.225140000	2.357638000	-1.432381000
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	6	-3.445990000	4.046414000	0.266765000
	6	-2.703766000	3.267592000	1.166372000
	6	-2.231738000	2.020847000	0.741904000
	1	-3.428326000	1.998746000	-2.440544000
	1	-3.821121000	5.016691000	0.588903000
	1	-1.650600000	1.403215000	1.424178000
	35	-0.881604000	-2.089324000	2.281845000
	6	-2.419501000	3.755861000	2.568941000
	1	-2.846126000	3.078351000	3.319736000
	1	-1.339773000	3.811101000	2.756723000
	1	-2.842082000	4.751804000	2.740138000
	6	-4.529733000	4.454446000	-1.990302000

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1	-4.712583000	5.453961000	-1.581637000
8	1.339420000	-1.208383000	-0.047192000
6	1.671147000	-2.588729000	-0.352862000
1	1.237694000	-3.203495000	0.446129000
1	2.759110000	-2.689198000	-0.322590000
6	1.132337000	-3.037717000	-1.704299000
1	1.395007000	-4.090430000	-1.875359000
1	0.039214000	-2.960243000	-1.735963000
1	1.560869000	-2.428567000	-2.504294000
6	5.292695000	-0.179612000	-1.012626000
6	4.753849000	0.174834000	0.390903000
1	5.465806000	-0.158197000	1.161063000
1	4.666933000	1.271716000	0.471268000
6	4.169735000	0.144984000	-2.026130000
1	4.046858000	1.241073000	-2.082177000
1	4.456296000	-0.205068000	-3.027716000
6	6.522985000	0.691094000	-1.313002000
1	7.330300000	0.497128000	-0.594099000
1	6.917773000	0.478952000	-2.315087000
1	6.282416000	1.760861000	-1.268026000
6	5.680239000	-1.666114000	-1.088466000
1	4.820875000	-2.312567000	-0.891707000
1	6.067188000	-1.916628000	-2.084845000
1	6.463309000	-1.905158000	-0.355838000
8	3.496937000	-0.425927000	0.673332000
8	2.940537000	-0.467962000	-1.694171000
5	2.428352000	-0.180481000	-0.363834000
6	1.822868000	1.331150000	-0.228507000
6	1.250450000	1.976196000	-1.343137000
6	1.930538000	2.110991000	0.935277000
6	0.813884000	3.300768000	-1.296620000
1	1.178106000	1.427510000	-2.280971000
6	1.498054000	3.441558000	0.994940000
1	2.422729000	1.696037000	1.816785000
6	0.928032000	4.061456000	-0.122620000
1	0.385012000	3.758006000	-2.187495000
1	1.622972000	4.009656000	1.916433000
19	1.999302000	-1.042904000	2.676768000
6	0.458488000	5.497714000	-0.078172000
1	0.800308000	6.002724000	0.832362000
1	0.831964000	6.068088000	-0.937832000
1	-0.637474000	5.556580000	-0.101525000

	28	-0.813633000	-0.850842000	0.067009000
	6	-3.816511000	-3.150076000	0.101674000
	6	-4.193974000	-4.420556000	-0.330574000
	6	-3.906459000	-4.833942000	-1.635173000
	6	-3.241989000	-3.960890000	-2.502633000
	6	-2.862735000	-2.690561000	-2.069635000
	6	-3.147223000	-2.258958000	-0.759455000
	1	-4.026714000	-2.837705000	1.121165000
	1	-4.710310000	-5.090136000	0.352794000
	1	-4.199141000	-5.824424000	-1.974110000
	1	-3.013433000	-4.271873000	-3.519102000
	1	-2.339887000	-2.033915000	-2.759325000
	6	-2.798573000	-0.916325000	-0.250853000
	6	-2.310723000	0.144321000	-1.041517000
	1	-3.268505000	-0.657641000	0.693021000
	1	-2.298720000	0.009220000	-2.120602000
	1	-0.612685000	-0.350675000	-1.279160000
	6	-2.454994000	1.567044000	-0.636206000
	6	-2.745579000	2.512895000	-1.627587000
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TS-BHE	6	-2.637906000	3.311639000	1.054339000
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	1	-2.787375000	2.197344000	-2.669323000
	1	-3.157531000	5.267193000	0.307911000
	1	-2.146473000	1.262774000	1.481344000
	35	-1.198705000	-1.442714000	2.394634000
	6	-2.539372000	3.761840000	2.494630000
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	1	-3.437837000	5.863159000	-1.985316000
	8	1.143751000	-1.239885000	0.163084000
	6	1.361200000	-2.676568000	0.108278000
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	6	4.705818000	-0.259634000	0.435462000
	1	5.382247000	-0.629803000	1.220201000
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	1	7.278100000	-0.370579000	-0.606696000
	1	6.824749000	-0.457759000	-2.314918000
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	6	5.337476000	-2.317322000	-0.911042000
	1	4.400531000	-2.823887000	-0.665908000
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	6	1.908869000	1.211298000	-0.228057000
	6	1.330486000	1.826424000	-1.356343000
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	6	1.036516000	3.189227000	-1.395363000
	1	1.131708000	1.217569000	-2.235956000
	6	1.887608000	3.435349000	0.830030000
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	6	1.304048000	4.022405000	-0.297353000
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	1	2.133847000	4.056367000	1.690864000
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INT-BHE	28	0.520240000	0.992514000	0.039867000
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	6	2.235461000	5.579770000	-1.950175000
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	6	2.340304000	2.957801000	-0.914193000
	1	2.754227000	3.913976000	0.973734000
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1	4.581291000	-4.969231000	-1.750763000
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6	-1.990605000	2.264295000	0.503857000
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	1	0.342660000	-5.605586000	-2.383319000
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TS-PT	28	-1.403529000	1.126077000	-0.750406000
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6	4.146122000	-1.670647000	-1.295618000
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1	6.588198000	0.826853000	-1.139974000
1	6.125184000	-0.141357000	-2.552359000
8	2.937002000	-0.925077000	-1.381615000
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5	2.496982000	-0.248432000	-0.114508000
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INT-PT	28	-1.714772000	0.000036000	-1.235806000
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	1	3.567225000	-2.398977000	-0.578726000
	1	3.831063000	-1.460108000	0.907035000
	6	4.884251000	0.772374000	-0.335882000
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	1	5.679793000	1.344285000	-0.830375000
	6	6.176201000	-1.389242000	-0.318864000
	1	6.194730000	-2.445967000	-0.616570000
	1	7.068434000	-0.913536000	-0.744972000
	1	6.263819000	-1.345245000	0.774266000
	6	4.822234000	-0.767502000	-2.351203000
	1	3.908433000	-0.299207000	-2.726641000
	1	5.678621000	-0.254860000	-2.807302000
	1	4.837311000	-1.810965000	-2.693711000
	8	2.445411000	-0.690181000	-0.435821000
	8	3.657550000	1.412024000	-0.628151000
	5	2.469405000	0.758685000	-0.157290000
	6	2.025789000	1.151357000	1.346793000
	6	1.941321000	2.504833000	1.732809000
	6	1.777422000	0.205110000	2.351527000
	6	1.617359000	2.884736000	3.034298000
	1	2.140165000	3.277630000	0.992773000
	6	1.460711000	0.576342000	3.665144000
	1	1.836600000	-0.855396000	2.111445000
	6	1.370011000	1.923743000	4.029900000
	1	1.559201000	3.942661000	3.287725000
	1	1.283583000	-0.192476000	4.416402000
	19	0.371271000	-2.386218000	-0.681027000
	6	1.020012000	2.340471000	5.440396000
	1	1.792754000	2.991186000	5.869513000
	1	0.075745000	2.899805000	5.469030000
	1	0.911375000	1.471718000	6.098835000
Bypro	6	3.532179000	1.244367000	-0.000791000
	6	4.914698000	1.053841000	-0.000799000
	6	5.443705000	-0.238923000	-0.000014000
	6	4.572997000	-1.335751000	0.000785000

6	3.193418000	-1.143823000	0.000786000
6	2.640127000	0.153675000	-0.000024000
1	3.129972000	2.255482000	-0.001407000
1	5.577593000	1.915644000	-0.001414000
1	6.519610000	-0.392937000	-0.000004000
1	4.973273000	-2.346742000	0.001428000
1	2.540847000	-2.012222000	0.001460000
6	1.197447000	0.424006000	-0.000082000
6	0.197682000	-0.483813000	0.000097000
1	0.943548000	1.483281000	-0.000347000
1	0.452691000	-1.542977000	0.000229000
6	-1.245561000	-0.216389000	0.000070000
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6	-3.520937000	-1.132565000	-0.000280000
6	-4.026649000	0.169664000	-0.000052000
6	-3.174101000	1.289123000	0.000253000
6	-1.796043000	1.083198000	0.000305000
1	-1.721265000	-2.317012000	-0.000381000
1	-5.104920000	0.323043000	-0.000098000
1	-1.138596000	1.948553000	0.000577000
6	-3.754606000	2.685942000	0.000534000
1	-2.966801000	3.446517000	0.000732000
1	-4.384033000	2.856399000	-0.882283000
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6	-4.442744000	-2.332049000	-0.000575000
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1	-5.494622000	-2.027609000	-0.000587000
CAT-P	28	-1.092224000	-0.079529000	0.271489000
	6	-2.930800000	-0.495708000	0.161222000
	6	-3.439458000	0.126069000	-1.017288000
	6	-3.829516000	1.457257000	-0.987367000
	6	-3.726266000	2.184272000	0.229671000
	6	-3.225180000	1.614007000	1.390380000
	6	-2.804669000	0.248061000	1.371676000
	1	-3.544831000	-0.461740000	-1.924589000
	1	-4.056062000	3.221982000	0.247153000
	1	-2.645499000	-0.266322000	2.316950000
	35	-3.043816000	-2.465340000	0.265584000
	6	-3.160576000	2.389632000	2.685168000
	1	-3.797141000	1.930770000	3.453793000
	1	-2.139203000	2.411593000	3.085557000
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15	1.101731000	0.055637000	-0.002631000
6	2.092264000	-0.227363000	1.587533000
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6	3.539840000	-0.747488000	1.458946000
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6	3.411970000	-1.786975000	3.780618000
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1	4.328597000	0.110821000	3.287156000
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6	1.638605000	-1.274789000	-1.240709000
6	0.494327000	-1.515668000	-2.255041000
6	2.974107000	-1.077789000	-1.989429000
1	1.720570000	-2.182873000	-0.622426000
6	0.798890000	-2.686861000	-3.203644000
1	0.337392000	-0.602286000	-2.849424000
1	-0.444925000	-1.701680000	-1.720278000
6	3.276539000	-2.259250000	-2.931312000
1	2.920846000	-0.157126000	-2.587919000
1	3.803962000	-0.950621000	-1.287466000
6	2.136892000	-2.497618000	-3.931513000
1	-0.020232000	-2.796859000	-3.926506000
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1	2.063729000	-1.633130000	-4.609400000
6	1.662971000	1.721424000	-0.709058000
6	0.744855000	2.842933000	-0.167140000
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6	1.039742000	4.198995000	-0.829312000
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	1	-0.305509000	2.564200000	-0.312429000
	6	3.435771000	3.482662000	-1.216824000
	1	3.380484000	2.208470000	0.526653000
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	1	2.714580000	5.534845000	-1.219502000
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	6	-2.890495000	-0.606871000	-0.143970000
	6	-2.886067000	0.207005000	-1.304326000
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	1	-3.646183000	-0.908789000	1.870271000
	35	-2.359562000	-2.578168000	-0.361941000
	6	-5.153922000	1.363868000	2.219760000
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TS-OA-P	1	-4.323416000	3.151176000	-2.393161000
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	1	-4.085516000	1.711726000	-3.399726000
	15	1.087275000	0.127643000	0.026441000
	6	1.625245000	-0.144663000	1.825773000
	6	0.663242000	-1.148205000	2.505899000
	6	3.088248000	-0.550765000	2.101667000
	1	1.450369000	0.838642000	2.291759000
	6	0.943888000	-1.283093000	4.011899000
	1	0.764326000	-2.133804000	2.027509000
	1	-0.375663000	-0.833546000	2.342585000
	6	3.367684000	-0.682997000	3.611093000
	1	3.293475000	-1.518159000	1.621040000
	1	3.785713000	0.171978000	1.667783000
	6	2.404266000	-1.668706000	4.286306000
	1	0.263606000	-2.025500000	4.449891000
	1	0.722077000	-0.324716000	4.506353000

	1	4.408668000	-0.998002000	3.765361000
	1	3.267635000	0.305614000	4.085160000
	1	2.594194000	-1.707717000	5.367166000
	1	2.590428000	-2.681763000	3.897832000
	6	2.083838000	-1.070670000	-1.053703000
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	6	3.555290000	-0.731881000	-1.373928000
	1	2.065702000	-2.006226000	-0.471389000
	6	1.976688000	-2.430141000	-3.218359000
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	6	0.542789000	2.890149000	-0.110240000
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	6	0.889449000	4.304991000	-0.605250000
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INT-OA-P	28	0.608999000	-1.274222000	-0.511376000
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	6	4.603503000	0.865679000	0.559414000
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COM-3	28	0.523283000	-0.646493000	-0.413523000
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	6	4.389155000	0.940520000	2.991358000
	1	3.528259000	1.326414000	3.550230000
	1	4.780616000	0.078627000	3.549918000
	1	5.169528000	1.711062000	2.997957000
	6	2.602972000	4.144726000	-0.634678000
	1	3.506514000	3.747975000	-0.153007000
	1	2.854129000	4.364618000	-1.677764000
	1	2.351959000	5.089338000	-0.137196000
TS-TM-s	28	0.552609000	-0.751413000	-0.439096000
	35	1.440277000	-2.945761000	-0.512840000
	8	-1.327771000	-1.419463000	-0.824846000
	6	-1.651127000	-1.844849000	-2.173328000
	1	-0.774800000	-2.396937000	-2.521199000
	1	-1.796372000	-0.960292000	-2.799662000
	6	-2.891111000	-2.726408000	-2.186440000

1	-3.093840000	-3.061821000	-3.211439000
1	-2.742626000	-3.619222000	-1.566562000
1	-3.767802000	-2.180095000	-1.824864000
6	-4.164531000	0.971253000	1.015889000
6	-3.664897000	1.403507000	-0.378174000
1	-4.511433000	1.619627000	-1.040481000
1	-3.056335000	2.315973000	-0.293807000
6	-2.922506000	0.558835000	1.830839000
1	-2.325310000	1.451731000	2.058519000
1	-3.222711000	0.100682000	2.782338000
6	-4.844203000	2.162826000	1.709022000
1	-5.727432000	2.488868000	1.145684000
1	-5.179468000	1.893313000	2.718953000
1	-4.166201000	3.020725000	1.796639000
6	-5.153375000	-0.202324000	0.896123000
1	-4.691259000	-1.068265000	0.412150000
1	-5.511716000	-0.512834000	1.886554000
1	-6.028817000	0.085780000	0.300481000
8	-2.899424000	0.381576000	-1.003141000
8	-2.095716000	-0.392956000	1.152935000
5	-1.871850000	-0.206464000	-0.256109000
6	-0.285092000	1.073423000	-0.458508000
6	-0.130532000	1.961476000	0.628395000
6	-0.288990000	1.678520000	-1.740766000
6	0.000291000	3.341501000	0.460984000
1	-0.081004000	1.558073000	1.637275000
6	-0.160970000	3.053649000	-1.920552000
1	-0.422141000	1.058952000	-2.626404000
6	-0.007284000	3.913049000	-0.818793000
1	0.126039000	3.982602000	1.332489000
1	-0.170377000	3.470759000	-2.926861000
19	-0.804812000	-2.728832000	1.603296000
6	2.201853000	-0.032435000	0.106274000
6	3.118008000	0.461829000	-0.831070000
6	2.567820000	0.001459000	1.461376000
6	4.365204000	0.977075000	-0.443105000
1	2.867562000	0.454193000	-1.891414000
6	3.800451000	0.515751000	1.885736000
1	1.879344000	-0.366739000	2.224854000
6	4.689831000	1.005369000	0.919005000
1	5.650177000	1.414888000	1.232876000
6	5.348328000	1.470988000	-1.482918000
1	6.009707000	2.245874000	-1.077128000
1	5.987467000	0.653601000	-1.845513000

	1	4.831286000	1.888831000	-2.354829000
	6	4.176455000	0.522704000	3.352450000
	1	3.291952000	0.413675000	3.991790000
	1	4.860805000	-0.302307000	3.595615000
	1	4.681809000	1.454381000	3.635874000
	6	0.182294000	5.398635000	-1.015520000
	1	-0.038072000	5.957217000	-0.099188000
	1	1.219428000	5.626639000	-1.297729000
	1	-0.462129000	5.785182000	-1.814122000
INT-TM-s	28	-1.272415000	0.012208000	-0.892603000
	35	0.824174000	-0.144264000	-1.982648000
	8	3.969817000	0.289462000	-0.029564000
	6	4.959505000	0.256748000	-1.076561000
	1	4.468520000	-0.021570000	-2.015724000
	1	5.701850000	-0.514021000	-0.841099000
	6	5.614486000	1.623677000	-1.181084000
	1	6.384920000	1.610519000	-1.960895000
	1	4.881799000	2.394995000	-1.448449000
	1	6.088257000	1.905703000	-0.233845000
	6	2.109464000	-3.159533000	1.371268000
	6	2.718608000	-3.176205000	-0.042352000
	1	3.325725000	-4.074693000	-0.194571000
	1	1.928583000	-3.153975000	-0.802468000
	6	1.432387000	-1.791354000	1.565389000
	1	0.556387000	-1.697852000	0.911631000
	1	1.109402000	-1.661242000	2.603579000
	6	1.039084000	-4.260022000	1.467177000
	1	1.485267000	-5.250371000	1.313587000
	1	0.567023000	-4.261221000	2.457360000
	1	0.249352000	-4.124422000	0.718973000
	6	3.197830000	-3.389429000	2.437700000
	1	3.978427000	-2.622408000	2.402831000
	1	2.761043000	-3.377234000	3.443922000
	1	3.680523000	-4.363627000	2.292285000
	8	3.581996000	-2.052401000	-0.279580000
	8	2.316143000	-0.689302000	1.269609000
	5	3.276347000	-0.856221000	0.293392000
	6	-2.966973000	-0.570569000	-0.449250000
	6	-4.129059000	0.005567000	0.087100000
	6	-3.044546000	-1.912097000	-0.867533000
	6	-5.312706000	-0.729659000	0.198763000
	1	-4.116869000	1.038983000	0.424873000
	6	-4.235731000	-2.643245000	-0.772992000
	1	-2.168520000	-2.409119000	-1.294693000

	6	-5.390640000	-2.063876000	-0.233204000
	1	-6.199285000	-0.253556000	0.617872000
	1	-4.262335000	-3.677004000	-1.115932000
	19	1.647437000	1.849994000	0.381441000
	6	-1.350129000	1.585372000	0.070738000
	6	-1.195280000	2.800534000	-0.632318000
	6	-1.350007000	1.642518000	1.478996000
	6	-1.026535000	4.026244000	0.032882000
	1	-1.205335000	2.794058000	-1.720785000
	6	-1.160680000	2.850791000	2.174203000
	1	-1.504191000	0.729514000	2.050888000
	6	-0.977656000	4.031725000	1.437544000
	1	-0.835279000	4.974937000	1.964558000
	6	-0.920517000	5.321012000	-0.744610000
	1	-1.912956000	5.766711000	-0.896657000
	1	-0.310229000	6.063040000	-0.216074000
	1	-0.483894000	5.161305000	-1.737019000
	6	-1.203606000	2.884974000	3.687230000
	1	-2.231826000	3.035831000	4.043307000
	1	-0.846981000	1.945101000	4.123740000
	1	-0.596685000	3.702827000	4.093288000
	6	-6.683122000	-2.843193000	-0.126165000
	1	-7.066605000	-2.851583000	0.902582000
	1	-7.469159000	-2.408345000	-0.758289000
	1	-6.547156000	-3.884600000	-0.438789000
TS-RE-s	28	-1.184090000	-0.311151000	-0.891463000
	35	0.833351000	-0.426925000	-2.002591000
	8	3.752554000	1.144018000	-0.314228000
	6	4.646985000	1.380583000	-1.418528000
	1	4.265122000	0.858684000	-2.302773000
	1	5.629913000	0.960522000	-1.175875000
	6	4.745782000	2.877084000	-1.662664000
	1	5.444198000	3.077359000	-2.483695000
	1	3.771979000	3.297106000	-1.942937000
	1	5.107501000	3.397966000	-0.768650000
	6	3.161579000	-2.660971000	1.268050000
	6	3.659380000	-2.534358000	-0.182936000
	1	4.503137000	-3.208286000	-0.364920000
	1	2.855614000	-2.775575000	-0.888681000
	6	2.104939000	-1.563813000	1.489827000
	1	1.206141000	-1.770533000	0.896376000
	1	1.824925000	-1.504827000	2.547295000
	6	2.497143000	-4.035843000	1.451257000
	1	3.220264000	-4.843092000	1.281280000

1	2.109940000	-4.150117000	2.471492000
1	1.662372000	-4.177433000	0.754610000
6	4.329938000	-2.504504000	2.260521000
1	4.827882000	-1.534436000	2.161186000
1	3.973541000	-2.593669000	3.294361000
1	5.084216000	-3.284120000	2.096658000
8	4.120695000	-1.208019000	-0.486138000
8	2.578073000	-0.254137000	1.117870000
5	3.481002000	-0.147759000	0.080607000
6	-2.952006000	-0.513877000	-0.261784000
6	-4.026237000	-0.187133000	-1.120068000
6	-3.131723000	-1.632225000	0.586261000
6	-5.186083000	-0.959865000	-1.160598000
1	-3.954573000	0.680848000	-1.770242000
6	-4.292522000	-2.403727000	0.537683000
1	-2.348200000	-1.914066000	1.285390000
6	-5.345612000	-2.081779000	-0.332215000
1	-5.984292000	-0.687326000	-1.849785000
1	-4.382723000	-3.273931000	1.186785000
19	1.063736000	1.903203000	0.166932000
6	-1.910638000	0.883716000	0.331388000
6	-2.149415000	2.182503000	-0.211163000
6	-1.537857000	0.839258000	1.705212000
6	-1.959541000	3.352551000	0.530923000
1	-2.465674000	2.272378000	-1.247816000
6	-1.343819000	1.995433000	2.469505000
1	-1.390722000	-0.125750000	2.183868000
6	-1.533109000	3.254163000	1.869750000
1	-1.396801000	4.159015000	2.460800000
6	-2.234540000	4.709642000	-0.082607000
1	-3.209160000	5.095134000	0.245772000
1	-1.481427000	5.450995000	0.212760000
1	-2.254128000	4.660985000	-1.176779000
6	-0.975130000	1.896925000	3.935113000
1	-1.870403000	1.971627000	4.567146000
1	-0.491425000	0.941615000	4.166969000
1	-0.297837000	2.704268000	4.239261000
6	-6.620466000	-2.892544000	-0.350579000
1	-7.357269000	-2.498374000	0.363744000
1	-7.089949000	-2.878366000	-1.341074000
1	-6.433804000	-3.938256000	-0.079748000
INT-RE-s	28	-1.093062000	-0.973405000	-0.575886000
	35	0.712522000	-0.568535000	-1.935598000
	8	3.213602000	1.699988000	-0.381252000

6	3.989729000	2.060935000	-1.539964000
1	3.672986000	1.439654000	-2.385048000
1	5.046384000	1.848570000	-1.340985000
6	3.783012000	3.537472000	-1.833394000
1	4.385804000	3.835107000	-2.699506000
1	2.733020000	3.751433000	-2.067672000
1	4.082056000	4.153597000	-0.977595000
6	3.529729000	-2.050626000	1.400276000
6	3.944809000	-1.894877000	-0.073802000
1	4.911104000	-2.375980000	-0.258629000
1	3.195025000	-2.343739000	-0.736078000
6	2.264205000	-1.201454000	1.617965000
1	1.410276000	-1.634270000	1.082251000
1	2.017777000	-1.142868000	2.683966000
6	3.190110000	-3.526151000	1.670406000
1	4.069174000	-4.162750000	1.510480000
1	2.864706000	-3.669411000	2.708460000
1	2.389199000	-3.883443000	1.012379000
6	4.664194000	-1.591951000	2.336951000
1	4.928543000	-0.540953000	2.180478000
1	4.369595000	-1.710275000	3.387211000
1	5.568249000	-2.191144000	2.171931000
8	4.093298000	-0.517789000	-0.454166000
8	2.418135000	0.156494000	1.158489000
5	3.246669000	0.403372000	0.083217000
6	-2.844950000	-0.525737000	0.165657000
6	-3.854956000	-0.915089000	-0.785739000
6	-2.207912000	-1.594634000	0.911517000
6	-4.207337000	-2.232932000	-0.971976000
1	-4.384807000	-0.143063000	-1.338701000
6	-2.629709000	-2.948262000	0.700206000
1	-1.664325000	-1.383907000	1.833219000
6	-3.590279000	-3.286313000	-0.232790000
1	-4.982727000	-2.478587000	-1.695552000
1	-2.172741000	-3.729883000	1.305823000
19	0.424073000	1.830914000	0.141086000
6	-2.675838000	0.905126000	0.536539000
6	-2.792519000	1.923211000	-0.440189000
6	-2.378304000	1.305948000	1.856956000
6	-2.597691000	3.272222000	-0.130706000
1	-3.008512000	1.644108000	-1.468262000
6	-2.166917000	2.649948000	2.194324000
1	-2.325923000	0.553204000	2.639428000
6	-2.256084000	3.625873000	1.188460000

	1	-2.101346000	4.674090000	1.440961000
	6	-2.769982000	4.339574000	-1.190341000
	1	-3.777467000	4.774489000	-1.144313000
	1	-2.058581000	5.163332000	-1.056524000
	1	-2.636572000	3.932241000	-2.198318000
	6	-1.906173000	3.048226000	3.631382000
	1	-2.850082000	3.248574000	4.156021000
	1	-1.390260000	2.255745000	4.184947000
	1	-1.301044000	3.959858000	3.695454000
	6	-4.000685000	-4.718734000	-0.477631000
	1	-5.083386000	-4.855775000	-0.353243000
	1	-3.753364000	-5.035488000	-1.500525000
	1	-3.495004000	-5.402839000	0.212746000
	28	-0.867776000	-0.855544000	-0.338748000
	6	-2.366665000	1.713784000	1.594285000
	6	-3.596471000	2.368524000	1.595749000
	6	-4.106564000	2.901744000	0.408537000
	6	-3.376770000	2.775299000	-0.779609000
	6	-2.147596000	2.121820000	-0.783990000
	6	-1.618448000	1.577009000	0.405862000
	1	-1.975900000	1.291983000	2.517454000
	1	-4.158501000	2.459290000	2.521313000
	1	-5.066603000	3.410786000	0.406607000
	1	-3.770047000	3.185867000	-1.705717000
	1	-1.597722000	2.032622000	-1.716310000
	6	-0.338347000	0.855879000	0.468357000
	6	0.563203000	0.628852000	-0.594105000
	1	0.031261000	0.657569000	1.475881000
TS-BHE-noR2	1	0.370434000	1.124645000	-1.544504000
	1	0.253152000	-0.986515000	-1.219595000
	6	2.014165000	0.394202000	-0.306569000
	6	2.924652000	1.389990000	-0.682557000
	6	4.288649000	1.270776000	-0.387510000
	6	4.720678000	0.142321000	0.320496000
	6	3.830714000	-0.865841000	0.717300000
	6	2.475547000	-0.727284000	0.394296000
	1	2.569131000	2.268685000	-1.218129000
	1	5.778147000	0.040917000	0.561784000
	1	1.770251000	-1.507143000	0.673963000
	35	-2.203771000	-2.609084000	-0.320825000
	6	4.330423000	-2.082929000	1.463001000
	1	4.915296000	-1.797073000	2.345867000
	1	3.501950000	-2.715235000	1.797807000
	1	4.981913000	-2.697376000	0.828169000

	6	5.273273000	2.322027000	-0.848104000
	1	5.740137000	2.033755000	-1.799670000
	1	4.784141000	3.289780000	-1.003630000
	1	6.080044000	2.463589000	-0.120103000
INT-BHE-noR2	28	0.743958000	0.818249000	0.074865000
	6	2.720428000	-1.914228000	1.251000000
	6	4.033676000	-2.313564000	1.018886000
	6	4.526770000	-2.380105000	-0.288918000
	6	3.690628000	-2.050614000	-1.359018000
	6	2.372620000	-1.655340000	-1.129945000
	6	1.862135000	-1.577395000	0.183130000
	1	2.345622000	-1.851370000	2.270003000
	1	4.676102000	-2.567812000	1.857757000
	1	5.553042000	-2.686755000	-0.471627000
	1	4.064167000	-2.102359000	-2.378236000
	1	1.741076000	-1.419768000	-1.981733000
	6	0.492433000	-1.124553000	0.495560000
	6	-0.472474000	-0.751609000	-0.446456000
	1	0.188471000	-1.268410000	1.530238000
	1	-0.223595000	-0.844568000	-1.504967000
	1	-0.198233000	1.362881000	0.978751000
	6	-1.922526000	-0.605701000	-0.205002000
	6	-2.776783000	-0.556692000	-1.314744000
	6	-4.167652000	-0.449199000	-1.166502000
	6	-4.692564000	-0.385660000	0.126052000
	6	-3.864629000	-0.428961000	1.263082000
	6	-2.486894000	-0.533582000	1.083538000
	1	-2.351107000	-0.604919000	-2.315927000
	1	-5.769759000	-0.296711000	0.258861000
	1	-1.843787000	-0.549067000	1.959431000
	35	1.774450000	2.771357000	-0.053449000
	6	-4.468429000	-0.345710000	2.646901000
	1	-5.170682000	-1.169884000	2.825363000
	1	-3.697751000	-0.388000000	3.423418000
	1	-5.026473000	0.589586000	2.780443000
	6	-5.066698000	-0.410774000	-2.381741000
	1	-4.734268000	0.347801000	-3.100708000
	1	-5.068506000	-1.375620000	-2.905649000
	1	-6.101166000	-0.181365000	-2.105883000
COM-noR2	28	0.324701000	0.562389000	0.339474000
	6	1.872046000	-2.430967000	1.948078000
	6	3.027077000	-3.213255000	1.927420000
	6	3.453773000	-3.796563000	0.730503000
	6	2.705483000	-3.599265000	-0.435320000

6	1.555618000	-2.812320000	-0.414901000
6	1.120600000	-2.207204000	0.778569000
1	1.544464000	-1.975897000	2.880717000
1	3.589986000	-3.370794000	2.844476000
1	4.349875000	-4.412008000	0.708951000
1	3.021252000	-4.058854000	-1.368769000
1	0.993278000	-2.666943000	-1.329762000
6	-0.108650000	-1.391142000	0.878006000
6	-0.941231000	-1.014074000	-0.176703000
1	-0.505001000	-1.342614000	1.888648000
1	-0.636725000	-1.286963000	-1.181774000
1	-0.408602000	0.803392000	1.546371000
6	-2.364846000	-0.631520000	-0.076912000
6	-3.112204000	-0.565299000	-1.262185000
6	-4.477748000	-0.247065000	-1.255792000
6	-5.098395000	-0.005080000	-0.027845000
6	-4.382896000	-0.067829000	1.181713000
6	-3.024520000	-0.376431000	1.142199000
1	-2.613788000	-0.759829000	-2.210338000
1	-6.160047000	0.238036000	-0.005326000
1	-2.467540000	-0.412860000	2.074388000
35	1.442806000	0.315174000	-1.915619000
6	-5.083493000	0.204220000	2.494772000
1	-5.936955000	-0.470367000	2.640052000
1	-4.404741000	0.072913000	3.344085000
1	-5.472337000	1.230148000	2.534456000
6	-5.250679000	-0.168942000	-2.553801000
1	-4.880197000	0.646400000	-3.188711000
1	-5.155781000	-1.096440000	-3.132268000
1	-6.316728000	0.006912000	-2.374104000
8	1.181149000	2.180057000	0.680978000
6	0.761522000	3.057510000	1.700954000
1	0.784616000	2.563060000	2.686996000
1	-0.277473000	3.386362000	1.537143000
6	1.663824000	4.295248000	1.748456000
1	1.337342000	4.992890000	2.530800000
1	2.705014000	4.017771000	1.973251000
1	1.639170000	4.834917000	0.791109000
19	3.281063000	2.350641000	-0.687372000
TS-PT-noR2	28	-0.238676000	0.493016000	-0.124325000
	6	-2.167957000	-2.061207000	-1.882946000
	6	-3.466353000	-2.561094000	-1.767634000
	6	-3.969590000	-2.940068000	-0.516387000
	6	-3.144790000	-2.820294000	0.610835000

6	-1.851652000	-2.304853000	0.498964000
6	-1.331536000	-1.907089000	-0.754689000
1	-1.790627000	-1.766578000	-2.859838000
1	-4.082744000	-2.665885000	-2.657605000
1	-4.973492000	-3.346835000	-0.425157000
1	-3.508653000	-3.134398000	1.586770000
1	-1.245933000	-2.199142000	1.392623000
6	0.004887000	-1.292725000	-0.925828000
6	0.927634000	-1.085707000	0.132787000
1	0.367919000	-1.300464000	-1.951724000
1	0.697018000	-1.488092000	1.116929000
1	-0.345369000	0.978902000	-1.512130000
6	2.360249000	-0.777560000	-0.060299000
6	3.247338000	-0.978489000	1.008145000
6	4.617638000	-0.709013000	0.889817000
6	5.101235000	-0.230978000	-0.331570000
6	4.243807000	-0.014932000	-1.424277000
6	2.883811000	-0.284063000	-1.274067000
1	2.856095000	-1.349606000	1.954082000
1	6.164044000	-0.017314000	-0.438198000
1	2.215818000	-0.097833000	-2.111118000
35	-0.845179000	1.031885000	2.166614000
6	4.794509000	0.508055000	-2.732975000
1	5.550095000	-0.171226000	-3.148603000
1	4.003024000	0.624220000	-3.481130000
1	5.276808000	1.485451000	-2.602151000
6	5.543361000	-0.930276000	2.065679000
1	5.252779000	-0.309234000	2.922647000
1	5.520472000	-1.974880000	2.401851000
1	6.579701000	-0.684170000	1.810493000
8	-1.387941000	1.821582000	-1.103974000
6	-0.929587000	3.171936000	-0.988568000
1	0.020637000	3.291875000	-1.530305000
1	-0.736431000	3.410252000	0.067467000
6	-1.971840000	4.122567000	-1.568998000
1	-1.622707000	5.161320000	-1.503113000
1	-2.169395000	3.889431000	-2.621970000
1	-2.919903000	4.055200000	-1.018732000
19	-3.320441000	0.615297000	0.274862000
INT-PT-noR2	28	0.225590000	0.302960000	0.531339000
	6	-1.420158000	-2.276159000	-1.669185000
	6	-2.516937000	-3.138197000	-1.593182000
	6	-2.732264000	-3.916233000	-0.448238000
	6	-1.807228000	-3.832233000	0.604686000

6	-0.713789000	-2.968511000	0.530252000
6	-0.495750000	-2.145999000	-0.603827000
1	-1.269280000	-1.679253000	-2.566443000
1	-3.200698000	-3.210144000	-2.436499000
1	-3.577040000	-4.597530000	-0.390497000
1	-1.936529000	-4.452203000	1.489515000
1	-0.021034000	-2.919233000	1.364780000
6	0.583363000	-1.148809000	-0.702060000
6	1.643324000	-0.989606000	0.244528000
1	0.739309000	-0.781302000	-1.718682000
1	1.703362000	-1.692425000	1.079093000
1	-5.293659000	0.700105000	-1.473479000
6	2.948140000	-0.371868000	-0.080201000
6	4.082936000	-0.722328000	0.668698000
6	5.342889000	-0.164450000	0.410009000
6	5.462697000	0.766083000	-0.625905000
6	4.348853000	1.149351000	-1.393765000
6	3.107682000	0.580575000	-1.110260000
1	3.979390000	-1.452193000	1.471007000
1	6.435467000	1.208139000	-0.838184000
1	2.238269000	0.899597000	-1.680072000
35	-1.196581000	1.882009000	1.389382000
6	4.500687000	2.176490000	-2.494510000
1	5.249299000	1.863729000	-3.234022000
1	3.554938000	2.337697000	-3.022875000
1	4.827576000	3.145170000	-2.094142000
6	6.541942000	-0.567980000	1.240265000
1	6.404097000	-0.301561000	2.296391000
1	6.710261000	-1.651961000	1.200525000
1	7.455250000	-0.075425000	0.889246000
8	-4.546431000	0.893063000	-0.885923000
6	-4.082125000	2.242220000	-1.157177000
1	-3.674834000	2.281680000	-2.176218000
1	-3.258316000	2.396943000	-0.456400000
6	-5.179258000	3.277439000	-0.960997000
1	-4.778975000	4.283019000	-1.138057000
1	-6.011578000	3.123409000	-1.661249000
1	-5.573082000	3.240312000	0.060600000
19	-2.966678000	-0.626232000	0.691582000

Table S2. Imaginary frequencies (cm^{-1}) of the key saddle points calculated at the B3LYP/6-31+G* level of theory in the gas phase.

Species	Frequency	Species	Frequency
TS-cat-1	-75.2	TS-cat-2	-114.9
TS-OA	-78.6	TS-MI	-136.9
TS-con	-121.7	TS-pre-TM	-48.5
TS-TM	-233.2	TS-RE	-299.8
TS-con'	-129.5	TS-BHE	-361.7
TS-PT	-491.2	TS-OA-P	-78.8
TS-TM-s	-232.9	TS-RE-s	-278.7
TS-pre-TM-Na	-50.4	TS-TM-Na	-231.0
TS-RE-Na	-295.9	TS-BHE-noR2	-602.8
TS-PT-noR2	-1055.7		

Table S3. Electronic energies E (in a.u.), unscaled entropies S (cal·mol^{-1}·K^{-1}) and Gibbs free-energies G (in a.u.) calculated at the B3LYP/6-31+G* level of theory in the gas phase at 353 K, and electronic energies E' (in a.u.) obtained from the M06-SMD/6-311++G(3df,2p) single point calculations in toluene.

Species	E	S	G	E'
CAT-1	-2738.32454	121.125	-2738.23767	-2738.190349
K2OEt2	-1508.80487	130.417	-1508.72358	-1508.717618
K2Cl2	-2120.42324	90.525	-2120.46275	-2120.440292
B2pin2	-822.574	155.988	-822.26892	-822.2979516
CAT-2	-2949.36368	258.727	-2948.81346	-2948.859293
TS-cat-1	-2949.33893	255.588	-2948.7889	-2948.838867
INT-cat-1	-2639.72278	225.99	-2639.29927	-2639.367319
R1	-309.66127	87.217	-309.56644	-309.4980518
TS-cat-2	-2639.71856	219.742	-2639.29292	-2639.367589
INT-cat-2	-2639.73664	223.057	-2639.3095	-2639.400745
Bpin-OEt	-565.7916	124.584	-565.58834	-565.6082375
R3	-2882.025	106.491	-2881.92519	-2884.157693
CAT-R	-4699.90055	163.838	-4699.68511	-4701.902404
R2	-642.95891	133.867	-642.73907	-642.6991605
(R2-KOEt)2	-2794.76959	307.773	-2794.19345	-2794.188061
R2-KOEt	-1397.37071	168.059	-1397.09194	-1397.082006
Na2OEt2	-633.60094	121.544	-633.51345	-633.4702103
(R2-NaOEt)2	-1919.55163	299.497	-1918.96998	-1918.931823
R2-NaOEt	-959.75922	165.713	-959.47877	-959.4501858
CAT-R'	-5787.61371	234.403	-5787.20854	-5789.485584
TS-OA	-4699.89759	159.605	-4699.68077	-4701.892716
INT-OA	-4699.92621	167.706	-4699.71191	-4701.919544

TS-MI	-4699.90897	161.775	-4699.69235	-4701.907977
INT-MI	-4699.93993	157.549	-4699.71875	-4701.941898
TS-con	-4699.93567	158.455	-4699.71587	-4701.939588
INT-con	-4699.94181	164.566	-4699.72437	-4701.943099
COM-1	-6097.36008	284.697	-6096.83377	-6099.07475
TS-pre-TM	-6097.33015	277.815	-6096.80094	-6099.04635
pre-TM	-6097.33291	288.672	-6096.80819	-6099.054678
TS-TM	-6097.3183	286.851	-6096.79393	-6099.047839
INT-TM	-6097.33528	295.73	-6096.81341	-6099.060428
TS-RE	-6097.30155	295.478	-6096.78171	-6099.027881
INT-RE	-6097.35027	291.973	-6096.82536	-6099.074746
KBr-BpinOEt	-3698.20507	149.473	-3698.03754	-3700.347343
product	-890.95771	178.947	-890.62555	-890.5060375
COM-1-Na	-5659.75514	281.563	-5659.22679	-5661.447275
TS-pre-TM-Na	-5659.72626	276.711	-5659.19632	-5661.419088
pre-TM-Na	-5659.72898	284.035	-5659.20149	-5661.426613
TS-TM-Na	-5659.71867	284.446	-5659.19253	-5661.421298
INT-TM-Na	-5659.74617	290.427	-5659.22077	-5661.437234
TS-RE-Na	-5659.69756	287.389	-5659.17264	-5661.399516
INT-RE-Na	-5659.74762	292.402	-5659.22255	-5661.444707
NaBr-BpinOEt	-3260.60075	149.319	-3260.43283	-3262.719155
TS-con'	-4699.91623	162.195	-4699.69953	-4701.918106
INT-con'	-4699.92979	163.992	-4699.7129	-4701.931566
COM-2	-6097.34893	279.218	-6096.82061	-6099.063733
TS-BHE	-6097.33241	281.072	-6096.80853	-6099.0443
INT-BHE	-6097.33482	283.404	-6096.81035	-6099.04317
TS-PT	-6097.31382	287.765	-6096.79645	-6099.023798
INT-PT	-6097.33204	292.912	-6096.81055	-6099.046297
R2-KBr-EtOH	-3969.73834	185.582	-3969.45304	-3971.742159
Bypro	-619.36666	140.58	-619.15427	-619.046811
PCy3	-1047.18537	158.787	-1046.76253	-1046.838132
CAT-P	-5437.42774	236.195	-5436.88409	-5439.246529
TS-OA-P	-5437.4264	230.614	-5436.8806	-5439.242824
INT-OA-P	-5437.46515	236.918	-5436.92017	-5439.277576
COM-3	-5787.66183	237.595	-5787.25688	-5789.527193
TS-TM-s	-5787.64769	244.21	-5787.24777	-5789.515036
INT-TM-s	-5787.69069	257.527	-5787.29555	-5789.540126
TS-RE-s	-5787.67081	250.422	-5787.27339	-5789.532596
INT-RE-s	-5787.70542	250.057	-5787.30558	-5789.572
TS-BHE-noR2	-4699.91449	167.101	-4699.70355	-4701.9141
INT-BHE-noR2	-4699.925	167.59	-4699.71303	-4701.922691
COM-noR2	-5454.36869	202.8	-5454.09565	-5456.318252
TS-PT-noR2	-5454.34455	203.003	-5454.07467	-5456.299183

INT-PT-noR2	-5454.38258	213.119	-5454.11258	-5456.346019
K2Br2	-6343.47958	95.753	-6343.52211	-6348.088552
EtOH	-155.04563	67.214	-154.99674	-154.9990325

Table S4. Computed electronic energies (in a.u.) using the B3LYP/sdd+6-31+G* theoretical method, on the basis of the geometries B3LYP/6-31+G* optimized (E_1) and those itself optimized (E_2), respectively.

Species	E_1	E_2	ΔE
TS-OA	-3362.31300926	-3362.31341731	-0.00040805
INT-OA	-3362.34894796	-3362.34996082	-0.00101286
TS-MI	-3362.33135708	-3362.33354705	-0.00218997
INT-MI	-3362.36449969	-3362.36495978	-0.00046009
COM-1	-4759.76469726	-4759.76582577	-0.00112851
TS-TM	-4759.73367862	-4759.73384301	-0.00016439
INT-TM	-4759.75099123	-4759.75133348	-0.00034225
TS-RE	-4759.71152373	-4759.71298402	-0.00146029

Table S5. Activation barriers of some tested processes (in terms of electronic energies in kcal/mol), computed at the M06-SMD/6-311++G(3df,2p)//M06/6-31+G* and M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* levels of theory, respectively.

	$E_a^{M06//M06}$	$E_a^{M06//B3}$	ΔE_a
The barrier of oxidative addition (between **TS-OA** and **CAT-R**)	8.2	6.1	2.1
The barrier of migratory insertion (between **TS-MI** and **INT-OA**)	8.0	7.3	0.7
The barrier of transmetalation (between **TS-TM** and **pre-TM**)	4.6	4.3	0.3
The rate-determining barrier (between **TS-RE** and **COM-1**)	29.0	29.4	-0.4

Table S6. Relative free-energy data (in kcal/mol) calculated at the M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* level of theory (353 K), with and without entropy corrections (ΔG^{corr} and ΔG), for the main pathway. Released and added molecules are not shown for simplicity.

Species	ΔG^{corr}	ΔG
CAT-R	0 (ref.)	0 (ref.)
TS-OA	6.2	6.9
INT-OA	-10.8	-11.5
TS-MI	-3.1	-2.8
INT-MI	-22.3	-21.2

TS-con	-21.5	-20.6
INT-con	-24.2	-24.3
COM-1	-40.7	-34.8
TS-pre-TM	-22.2	-15.2
pre-TM	-28.4	-23.2
TS-TM	-24.6	-19.2
INT-TM	-32.5	-28.6
TS-RE	-13.4	-9.5
INT-RE	-40.3	-35.7
P + CAT-R	-57.7	-54.3

Table S7. Relative free-energy data (in kcal/mol) calculated at the M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* level of theory (353 K), with and without entropy corrections (ΔG^{corr} and ΔG), for the Heck coupling pathway. Released and added molecules are not shown for simplicity.

Species	ΔG^{corr}	ΔG
INT-MI	-22.3	-21.2
TS-con'	-9.4	-9.1
INT-con'	-17.4	-17.4
TS-BHE-noR2	-9.6	-10.2
INT-BHE-noR2	-14.3	-14.9
COM-noR2	-29.8	-25.2
TS-PT-noR2	-19.8	-15.2
INT-PT-noR2	-47.3	-44.5
Bypro + CAT-R	-45.1	-44.5
COM-2	-33.5	-26.8
TS-BHE	-23.6	-17.3
INT-BHE	-22.3	-16.2
TS-PT	-13.8	-8.5
INT-PT	-24.4	-20.0
Bypro + CAT-R	-19.0	-15.2

Table S8. Relative free-energy data (in kcal/mol) calculated at the M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* level of theory (353 K), with and without entropy corrections (ΔG^{corr} and ΔG), for the Suzuki coupling pathway. Released and added molecules are not shown for simplicity.

Species	ΔG^{corr}	ΔG
CAT-R	2.4	1.8
CAT-P	0 (new ref.)	0 (new ref)
TS-OA-P	2.7	3.1
INT-OA-P	-18.5	-19.3

COM-3	-17.0	-18.8
TS-TM-s	-11.2	-14.2
INT-TM-s	-27.6	-32.9
TS-RE-s	-22.7	-26.8
INT-RE-s	-46.0	-50.0
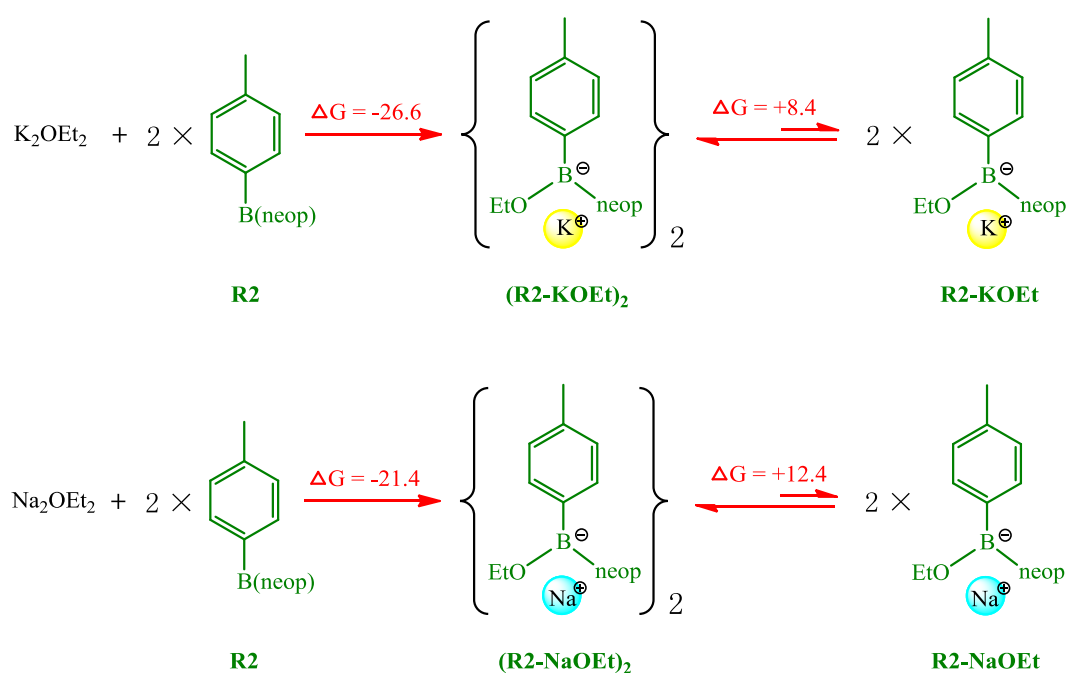
Figure S1. Generation of the active reagents of transmetalation from **R2** and KOEt or NaOEt, along with the relative free-energies (in kcal/mol) calculated by the M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* method at 353 K.
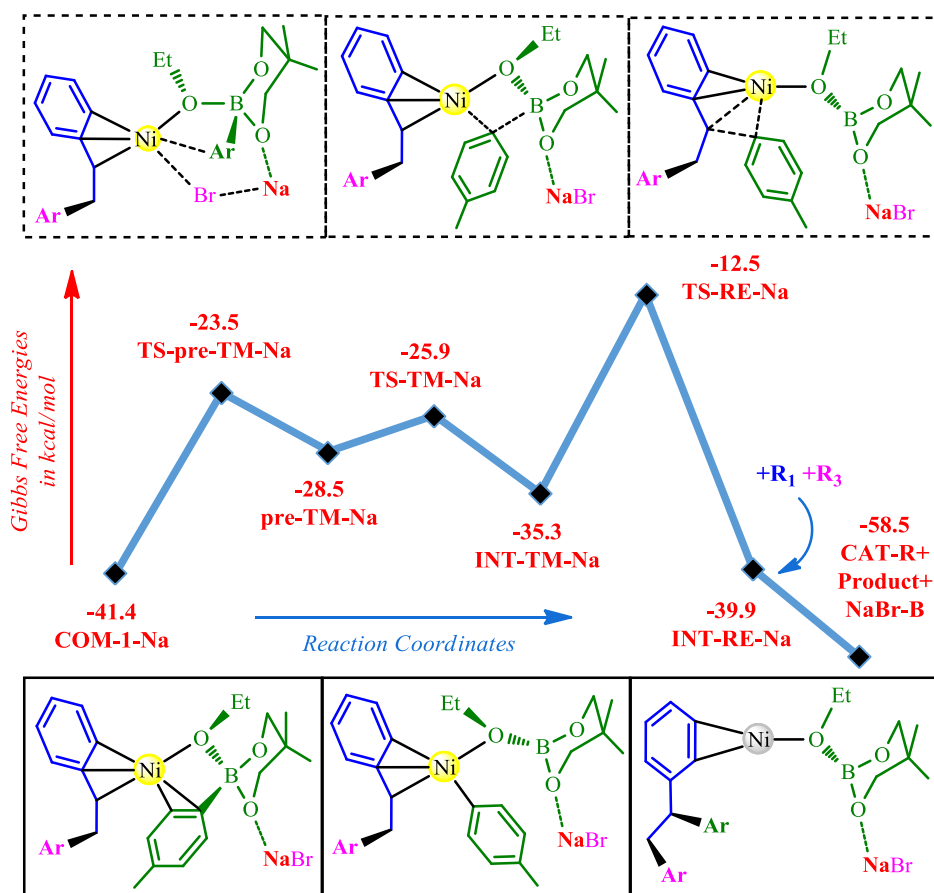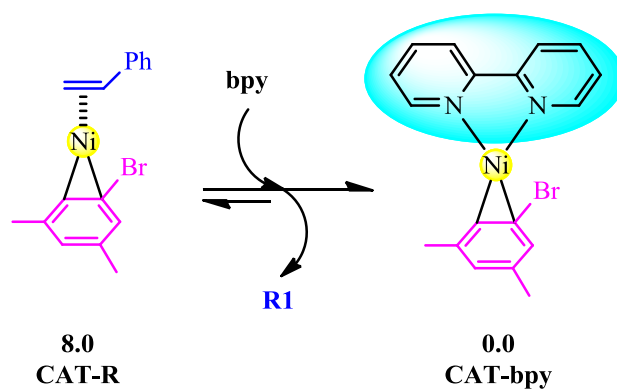
Figure S2. Mechanisms and free-energy variations of the transmetalation and reductive elimination processes involving the additive NaOEt instead of KOEt, calculated by the M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* method at 353 K.

Relative Free-Energies in kcal/mol

Figure S3. Ligand exchange of **R1** and **bpy** between **CAT-R** and **CAT-bpy**, along with the free-energy change (in kcal/mol) of this process calculated by the M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* method at 353 K.
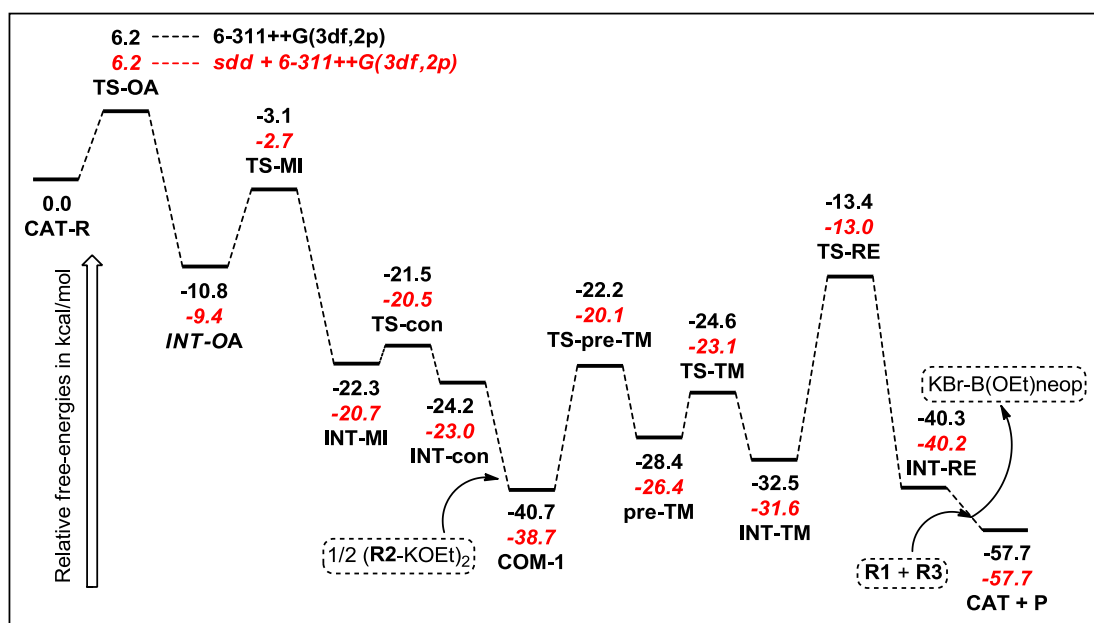
Figure S4. Relative free energies (in kcal/mol) of the main reaction obtained from the M06-SMD/6-311++G(3df,2p) and M06-SMD/sdd+6-311++G(3df,2p) single point calculations, respectively, on the basis of the geometries optimized at the B3LYP/6-31+G* level of theory at 353 K. The basis set of sdd+6-311++G(3df,2p) uses sdd for Ni and 6-311++G(3df,2p) for other atoms.
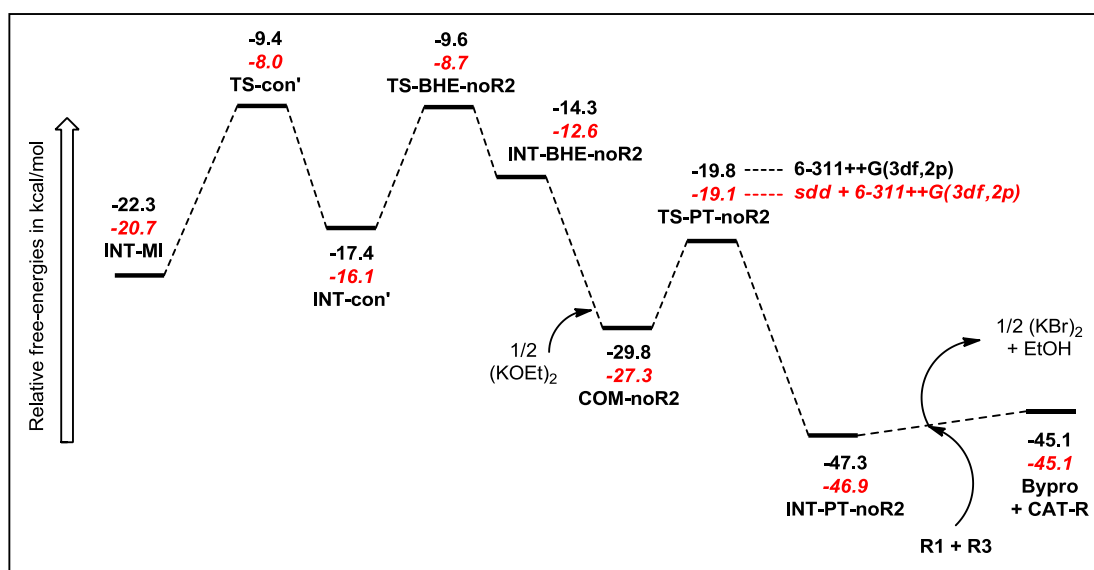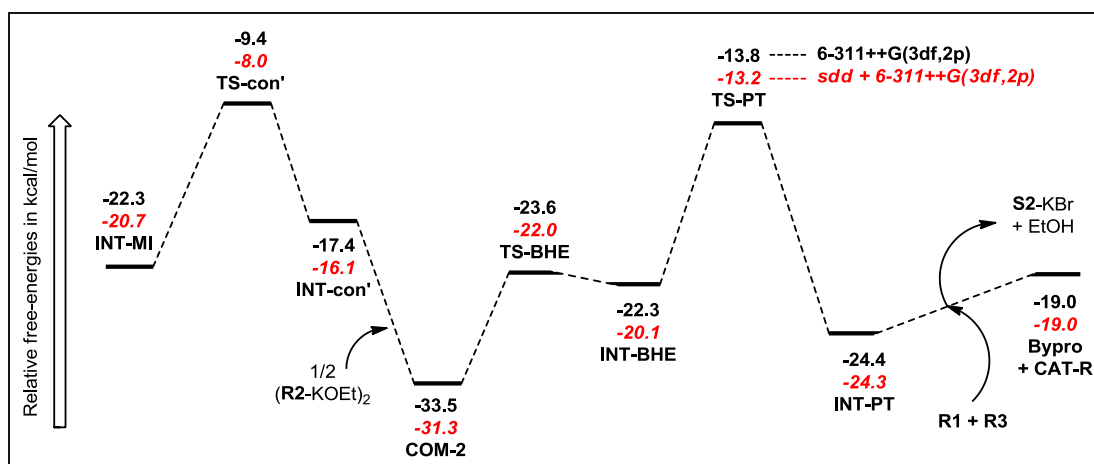
Figure S5. Relative free energies (in kcal/mol) of the Heck reaction in the absence of **R2**, obtained from the M06-SMD/6-311++G(3df,2p) and M06-SMD/sdd+ 6-311++G(3df,2p) single point calculations, respectively, on the basis of the geometries optimized at the B3LYP/6-31+G* level of theory at 353 K. The basis set of sdd+6-311++G(3df,2p) uses sdd for Ni and 6-311++G(3df,2p) for other atoms.
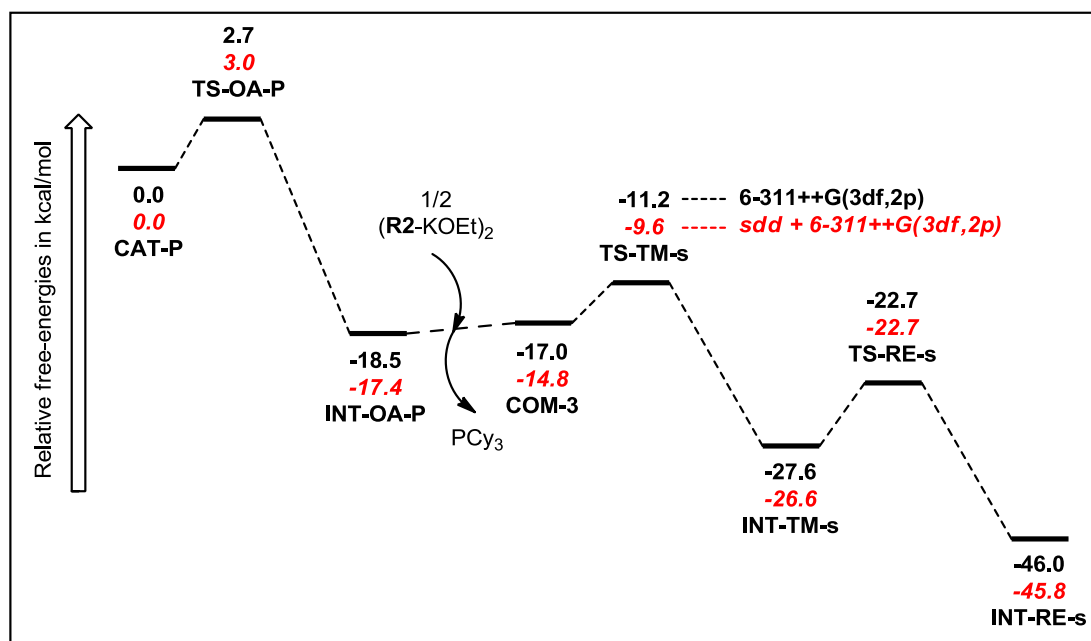
Figure S6. Relative free energies (in kcal/mol) of the Heck reaction in the presence of **R2**, obtained from the M06-SMD/6-311++G(3df,2p) and M06-SMD/sdd+ 6-311++G(3df,2p) single point calculations, respectively, on the basis of the geometries optimized at the B3LYP/6-31+G* level of theory at 353 K. The basis set of sdd+6-311++G(3df,2p) uses sdd for Ni and 6-311++G(3df,2p) for other atoms.

Figure S7. Relative free energies (in kcal/mol) of the Suzuki coupling reaction in the presence of PCy₃, obtained from the M06-SMD/6-311++G(3df,2p) and M06-SMD/ sdd+6-311++G(3df,2p) single point calculations, respectively, on the basis of the geometries optimized at the B3LYP/6-31+G* level of theory at 353 K. The basis set of sdd+6-311++G(3df,2p) uses sdd for Ni and 6-311++G(3df,2p) for other atoms.
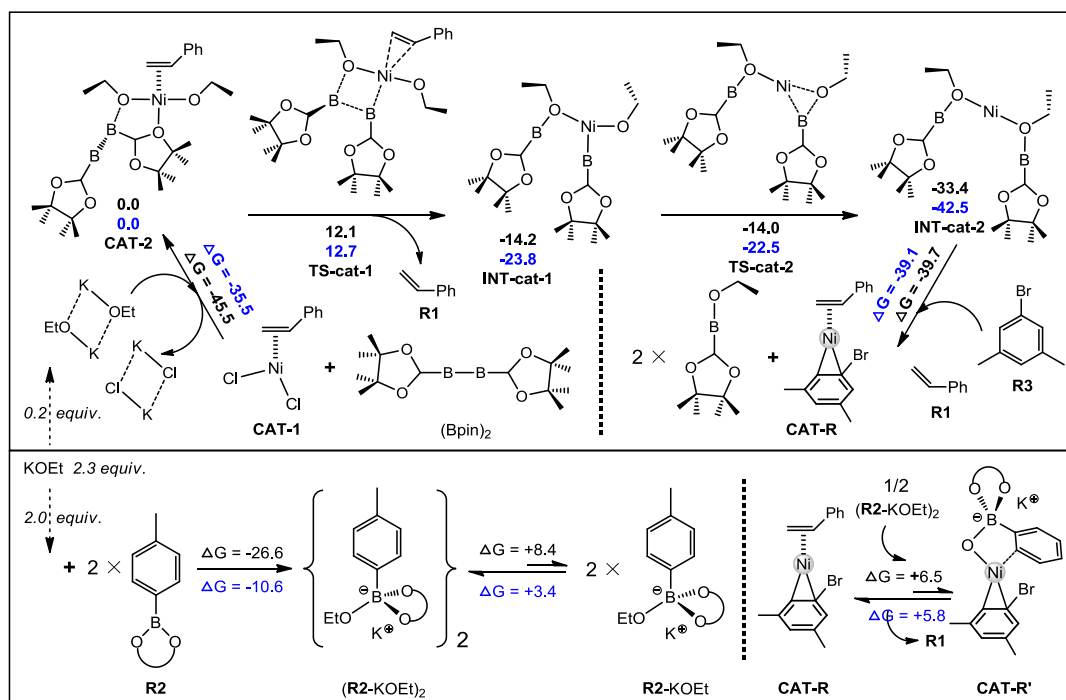
Figure S8. Relative free-energy data (in kcal/mol) calculated at the M06-SMD/6-311++G(3df,2p)//B3LYP/6-31+G* level of theory (353 K), with and without entropy corrections (in black and in blue), for the generation of the catalyst.