Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

A Computational Study of the Enantioselective Addition of *n*-BuLi to Benzaldehyde in the Presence of a Chiral Lithium N,P-Amide.

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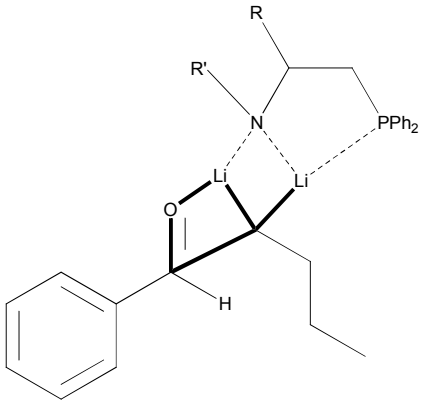

Fig S1. Schematic picture of the TS in the ligand-mediated addition of *n*-BuLi to benzaldehyde. Lines in bold were held fixed in the initial DFT optimizations.

Cartesian coordinates:
***(S)*-TS 1A**
File: FFMin_ValiPr_mixed_A2B2C2D1_1Solv_31_ext_TS1_NC.out
Energy(B3LYP/6-31g**): -1848.143410 au
Nuc.Rep. Energy: 4605.470256 au
G= -1847.486 au, ZPE= 1943.46 kJ/mol
Energy in solvent (SM8): -1848.22017 au
Dispersion energy: -68.8556 kcal/mol

N	1.670564	2.378451	0.196736
Li	0.283561	1.360518	1.188850
O	-0.579720	3.556776	-2.432912
C	-1.715375	3.085083	-2.165997
Li	0.068140	3.113887	-0.728486
C	-1.779137	2.938349	0.476066
C	-2.983024	2.069515	0.830545
H	-2.659432	1.032215	1.009665
O	-0.504298	-0.433518	1.518438
C	-0.991656	-1.318774	0.510210
H	-0.577730	-0.990039	-0.443258
H	-0.664549	-2.346393	0.712107
H	-2.087332	-1.287003	0.463618
C	-0.968936	-0.793174	2.820950
H	-0.620241	-1.799332	3.087280
H	-0.560329	-0.062751	3.519708
H	-2.065088	-0.766207	2.861520
H	-3.674235	2.016857	-0.022706
C	-5.293997	5.423127	-2.294029

C	-5.368402	4.030446	-2.322332
C	-4.200236	3.271758	-2.272712
C	-2.948982	3.898022	-2.192592
C	-2.882199	5.299524	-2.182393
C	-4.048038	6.055254	-2.227388
H	-6.203451	6.016573	-2.327914
H	-6.334229	3.537186	-2.384816
H	-4.253231	2.186624	-2.307769
H	-1.906978	5.773835	-2.142121
H	-3.991682	7.140012	-2.212238
H	-1.068950	2.921386	1.331165
H	-1.882152	1.995261	-2.182617
H	-2.083260	3.993769	0.409449
C	-3.800294	2.530138	2.056700
C	-5.005804	1.636648	2.370063
H	-4.142224	3.559332	1.882822
H	-3.141845	2.575005	2.935649
H	-5.560886	1.995013	3.243995
H	-5.704319	1.601689	1.525606
H	-4.694793	0.605114	2.579249
C	2.498309	3.343726	0.932853
C	1.761209	3.862307	2.187297
H	2.346770	4.614989	2.725127
P	1.255870	2.478284	3.335150
H	3.418881	2.854010	1.303152
H	0.819803	4.349187	1.905665
C	-0.764331	4.794114	6.844656
C	0.450236	4.148161	7.069146
C	1.087937	3.463288	6.033561
C	0.516574	3.410908	4.754628
C	-0.714771	4.055121	4.542890
C	-1.344448	4.746520	5.575913
H	-1.257963	5.327209	7.652339
H	0.908571	4.177739	8.054118
H	2.034902	2.970216	6.226253
H	-1.188561	4.014204	3.565144
H	-2.293171	5.242402	5.390080
C	5.206401	0.759312	5.102187
C	5.158719	2.104353	4.732537
C	3.988839	2.644326	4.199740
C	2.847880	1.846458	4.022074
C	2.912983	0.495373	4.393144
C	4.080115	-0.045120	4.933172
H	6.118945	0.340103	5.516428
H	6.033870	2.735278	4.860465
H	3.968184	3.693421	3.923025
H	2.042170	-0.139867	4.254709
H	4.110766	-1.093678	5.215644
C	3.025794	4.544828	0.065978
C	2.498972	1.499012	-0.648524
H	3.326500	2.065164	-1.113799
C	3.153109	0.340915	0.138722
H	2.383251	-0.343090	0.522096
H	3.839203	-0.244519	-0.487296
H	3.720916	0.712283	0.997381
C	1.671630	0.930291	-1.810487

H	2.259224	0.235019	-2.420789
H	0.804242	0.369360	-1.431455
H	1.292109	1.723274	-2.462613
H	3.426413	4.086464	-0.847732
C	1.946701	5.546648	-0.370293
H	2.380829	6.315763	-1.019058
H	1.145585	5.077990	-0.951769
H	1.496089	6.064691	0.484424
C	4.195270	5.281870	0.740679
H	4.658797	5.996070	0.050785
H	3.869588	5.852454	1.619175
H	4.974028	4.582491	1.066598

***(R)*-TS 1A**
File: FFMin_ValiPr_mixed_A2B2C2D1_1Solv_27_TS2_NC.out
Energy(B3LYP/6-31g**): -1848.144217 au
Nuc.Rep. Energy: 4620.928340 au
G= -1847.487 au, ZPE= 1943.06 kJ/mol
Energy in solvent (SM8): -1848.221906 au
Dispersion energy: -68.9454 kcal/mol

N	1.985407	2.101167	0.279861
Li	0.627239	1.097838	1.343807
O	-0.583530	3.028763	-2.223522
C	-1.711012	2.639879	-1.859042
Li	0.269020	2.725471	-0.528768
C	-1.324088	2.558582	0.997228
C	-2.782896	2.206357	1.309514
H	-2.952961	1.121831	1.204311
O	-0.007289	-0.727228	1.604218
C	-1.015271	-1.271680	0.752217
H	-1.359330	-0.462832	0.106309
H	-0.608674	-2.090833	0.143878
H	-1.858257	-1.645730	1.346680
C	0.490390	-1.661060	2.556390
H	0.984992	-2.505764	2.057351
H	1.210050	-1.129789	3.181676
H	-0.324426	-2.041496	3.185907
H	-3.452226	2.670787	0.569190
H	-2.392056	3.320613	-1.327142
H	-0.763445	2.328652	1.927785
H	-1.242384	3.663135	0.935790
C	-3.274834	2.627590	2.709748
C	-4.734990	2.260745	2.997015
H	-3.137947	3.711561	2.824081
H	-2.627079	2.165332	3.467338
H	-5.038626	2.567898	4.004177
H	-5.415975	2.743901	2.285869
H	-4.895115	1.178338	2.919563
C	2.788141	3.086582	1.016737
C	2.012710	3.606391	2.249778
H	2.541691	4.435740	2.731404
P	1.682438	2.252333	3.493010
H	3.712849	2.621476	1.409052
H	1.030010	3.978571	1.937763
C	-0.742857	4.232802	6.948215
C	-0.336045	2.898641	7.011969

C	0.392924	2.340786	5.965544
C	0.743330	3.104530	4.838788
C	0.326888	4.442281	4.787134
C	-0.412467	4.999305	5.833035
H	-1.316993	4.668599	7.760875
H	-0.590381	2.291838	7.876521
H	0.700280	1.299358	6.024661
H	0.575903	5.060686	3.931673
H	-0.727239	6.037512	5.773356
C	5.853956	1.641377	5.486394
C	5.292203	0.644524	4.691686
C	4.040385	0.841249	4.105489
C	3.337882	2.037765	4.298834
C	3.914530	3.033271	5.103036
C	5.162053	2.837233	5.690825
H	6.825647	1.488809	5.947622
H	5.824546	-0.288460	4.529223
H	3.608117	0.059997	3.487108
H	3.378542	3.961570	5.279647
H	5.594344	3.616467	6.312378
C	3.303393	4.286453	0.142352
C	2.831466	1.241651	-0.562182
H	3.617754	1.831606	-1.069682
C	3.570561	0.133212	0.223633
H	4.259026	-0.430907	-0.418948
H	4.157553	0.550174	1.047813
H	2.848683	-0.577824	0.648459
C	1.999103	0.599472	-1.680013
H	2.605915	-0.071674	-2.299174
H	1.179275	0.000032	-1.258618
H	1.561781	1.362330	-2.333014
H	3.715368	3.826121	-0.765216
C	2.205723	5.260182	-0.307991
H	2.616320	6.017803	-0.985115
H	1.404736	4.754599	-0.858152
H	1.756726	5.793141	0.538535
C	4.457874	5.048435	0.813873
H	4.907066	5.770230	0.122031
H	4.123223	5.612561	1.692867
H	5.249366	4.365184	1.142171
C	-3.442317	-1.058539	-3.123183
C	-4.195233	-0.158087	-2.368048
C	-3.627189	1.043125	-1.950897
C	-2.298023	1.351344	-2.279427
C	-1.551856	0.445998	-3.052956
C	-2.121559	-0.752344	-3.467389
H	-3.884905	-1.995386	-3.449658
H	-5.223307	-0.391101	-2.107013
H	-4.210526	1.746910	-1.366414
H	-0.532286	0.702417	-3.318582
H	-1.540997	-1.450117	-4.063751

***(S)*-TS 2A**
File: FFMin_PGiPr_mixed_A2B2C2D2_1Solv_70_TS1_NC.out
Energy(B3LYP/6-31g**): -1961.248649 au
Nuc.Rep. Energy: 5080.985682 au

G= -1960.596 au, ZPE= 1933.93 kJ/mol
Energy in solvent (SM8): -1961.336675 au
Dispersion energy: -70.8451 kcal/mol

7	-1.619113000	-2.190748000	0.034742000
3	-0.330346000	-1.256390000	-1.110137000
8	0.711505000	-3.698909000	2.388001000
6	1.878616000	-3.326060000	2.136256000
3	0.057576000	-3.135125000	0.684372000
6	1.850284000	-2.633238000	-0.561986000
6	2.980217000	-1.605609000	-0.644866000
1	2.574940000	-0.582464000	-0.577230000
8	0.303747000	0.544183000	-1.659568000
6	0.422064000	1.694540000	-0.824601000
1	-0.200769000	1.526569000	0.054264000
1	0.071823000	2.590143000	-1.353496000
1	1.463533000	1.843067000	-0.512705000
6	1.035548000	0.680020000	-2.879540000
1	0.670347000	1.543668000	-3.449142000
1	0.868773000	-0.230431000	-3.455332000
1	2.106389000	0.798909000	-2.678587000
1	3.645590000	-1.702811000	0.225716000
6	5.131003000	-6.035783000	1.561099000
6	5.381769000	-4.676598000	1.750143000
6	4.319578000	-3.794351000	1.934996000
6	2.998889000	-4.263764000	1.927465000
6	2.754945000	-5.635227000	1.752371000
6	3.816173000	-6.513083000	1.566223000
1	5.957935000	-6.724552000	1.412450000
1	6.402799000	-4.306209000	1.754595000
1	4.510060000	-2.736279000	2.092127000
1	1.728639000	-5.987835000	1.761103000
1	3.624326000	-7.572793000	1.424150000
1	1.234623000	-2.513941000	-1.484360000
1	2.164801000	-2.268316000	2.257471000
1	2.267655000	-3.644154000	-0.681565000
6	3.859815000	-1.698953000	-1.910481000
6	4.986319000	-0.661072000	-1.976776000
1	4.288677000	-2.708665000	-1.961200000
1	3.220786000	-1.605227000	-2.800427000
1	5.583832000	-0.766473000	-2.889359000
1	5.667416000	-0.759491000	-1.123197000
1	4.591591000	0.363081000	-1.958205000
6	-2.553031000	-3.124784000	-0.609143000
6	-3.045511000	-2.671228000	-2.025184000
1	-3.600604000	-1.737643000	-1.890476000
15	-1.699562000	-2.192450000	-3.233569000
1	-3.485542000	-3.178345000	-0.022961000
1	-3.745867000	-3.391211000	-2.468370000
6	-0.843318000	-5.724227000	-6.149524000
6	-0.125974000	-4.528667000	-6.212518000
6	-0.405658000	-3.500851000	-5.315321000
6	-1.413702000	-3.639903000	-4.346178000
6	-2.121369000	-4.847995000	-4.289614000
6	-1.836197000	-5.881385000	-5.184084000
1	-0.623859000	-6.530039000	-6.844185000
1	0.654683000	-4.398410000	-6.956701000

1	0.162442000	-2.575297000	-5.371068000
1	-2.887272000	-5.000985000	-3.537560000
1	-2.392695000	-6.812319000	-5.121730000
6	-4.050075000	0.786752000	-5.945700000
6	-4.061401000	-0.571800000	-6.262938000
6	-3.359519000	-1.484069000	-5.475797000
6	-2.631944000	-1.050004000	-4.358038000
6	-2.619551000	0.320126000	-4.054601000
6	-3.328644000	1.230797000	-4.837615000
1	-4.597914000	1.495184000	-6.560549000
1	-4.620381000	-0.924313000	-7.125611000
1	-3.375690000	-2.538104000	-5.734561000
1	-2.049866000	0.672871000	-3.198324000
1	-3.311557000	2.287891000	-4.586703000
6	-1.087474000	-7.229924000	-0.662443000
6	-2.353314000	-6.931201000	-0.158640000
6	-2.813088000	-5.613770000	-0.149196000
6	-2.024526000	-4.562267000	-0.637424000
6	-0.754566000	-4.882128000	-1.142681000
6	-0.289383000	-6.198120000	-1.155929000
1	-0.727984000	-8.255035000	-0.672392000
1	-2.984961000	-7.724925000	0.231361000
1	-3.801937000	-5.395192000	0.247368000
1	-0.117691000	-4.103747000	-1.548436000
1	0.695252000	-6.412438000	-1.561892000
6	-2.264398000	-1.467826000	1.143409000
1	-2.815575000	-2.179818000	1.790143000
6	-3.296763000	-0.409734000	0.693683000
1	-3.770598000	0.084929000	1.551461000
1	-4.097098000	-0.856796000	0.094885000
1	-2.813622000	0.361402000	0.078235000
6	-1.207899000	-0.806681000	2.040442000
1	-1.677760000	-0.216789000	2.835391000
1	-0.571873000	-0.123973000	1.460487000
1	-0.562520000	-1.553884000	2.513160000

***(R)*-TS 2A**

File: FFMin_PGiPr_mixed_A2B2C2D2_1Solv_49_TS2_ext_NC.out
Energy(B3LYP/6-31g**): -1961.252428 au
Nuc.Rep. Energy: 5135.280619 au
G= -1960.600 au, ZPE= 1936.49 kJ/mol
Energy in solvent (SM8): -1961.335642 au
Dispersion energy: -73.4250 kcal/mol

7	-2.039120000	-2.351474000	-0.731264000
3	-0.603928000	-1.496749000	-1.775271000
8	0.247927000	-3.371233000	1.937285000
6	1.399652000	-3.043577000	1.517123000
3	-0.472765000	-3.213499000	0.244736000
6	1.386540000	-3.211848000	-0.934924000
6	2.824042000	-2.893655000	-1.321223000
1	3.021845000	-1.813735000	-1.237569000
8	0.421270000	0.125258000	-2.171449000
6	1.311059000	0.698577000	-1.209415000
1	1.358172000	0.021194000	-0.357158000
1	0.942037000	1.679747000	-0.883305000
1	2.314317000	0.811926000	-1.638233000

6	0.310031000	0.915865000	-3.353246000
1	-0.063358000	1.919735000	-3.113379000
1	-0.396129000	0.416220000	-4.016463000
1	1.284904000	1.004164000	-3.850088000
1	3.513771000	-3.373015000	-0.611127000
1	2.157864000	-3.817057000	1.326164000
1	0.735546000	-2.890997000	-1.772228000
1	1.243728000	-4.302797000	-0.896073000
6	3.228172000	-3.344258000	-2.741406000
6	4.676355000	-3.002266000	-3.110820000
1	3.069210000	-4.427054000	-2.831483000
1	2.547400000	-2.878929000	-3.469298000
1	4.923774000	-3.329437000	-4.126958000
1	5.385487000	-3.483878000	-2.427274000
1	4.854868000	-1.921363000	-3.058911000
6	-2.764980000	-3.454510000	-1.380621000
6	-3.338074000	-3.080567000	-2.784138000
1	-4.182100000	-2.404437000	-2.621497000
15	-2.125460000	-2.136803000	-3.868862000
1	-3.665091000	-3.708131000	-0.793034000
1	-3.736156000	-3.953273000	-3.313429000
6	-1.469372000	-4.771260000	-7.661309000
6	-0.395178000	-4.175402000	-7.002536000
6	-0.617965000	-3.390398000	-5.869090000
6	-1.916380000	-3.185829000	-5.379910000
6	-2.990501000	-3.789259000	-6.056229000
6	-2.768221000	-4.576347000	-7.184776000
1	-1.298133000	-5.385673000	-8.540481000
1	0.618080000	-4.323981000	-7.365006000
1	0.225107000	-2.940100000	-5.351646000
1	-4.006646000	-3.635850000	-5.704036000
1	-3.609680000	-5.037016000	-7.695024000
6	-4.619154000	1.518957000	-5.377198000
6	-3.922301000	0.732510000	-6.293733000
6	-3.199753000	-0.382278000	-5.865632000
6	-3.164043000	-0.737224000	-4.507986000
6	-3.857071000	0.073724000	-3.591547000
6	-4.580594000	1.184698000	-4.022944000
1	-5.185336000	2.382422000	-5.713554000
1	-3.943040000	0.981338000	-7.351398000
1	-2.671215000	-0.984212000	-6.597692000
1	-3.834904000	-0.161207000	-2.531106000
1	-5.116869000	1.788929000	-3.296330000
6	-0.382493000	-7.102326000	-1.157020000
6	-0.953655000	-6.529714000	-0.018160000
6	-1.722469000	-5.372172000	-0.128590000
6	-1.937124000	-4.746165000	-1.369820000
6	-1.369959000	-5.343286000	-2.501716000
6	-0.600586000	-6.505836000	-2.396990000
1	0.218816000	-8.003197000	-1.077227000
1	-0.803777000	-6.982417000	0.957749000
1	-2.168558000	-4.942549000	0.765749000
1	-1.523909000	-4.915104000	-3.485183000
1	-0.169542000	-6.941633000	-3.294396000
6	-2.944142000	-1.475435000	0.029551000
1	-3.881452000	-1.293641000	-0.536212000

6	-2.290446000	-0.103099000	0.243201000
1	-2.929232000	0.558182000	0.839287000
1	-2.089301000	0.398718000	-0.711183000
1	-1.338182000	-0.209185000	0.777428000
6	-3.369310000	-2.059552000	1.394525000
1	-4.085351000	-1.406337000	1.909927000
1	-2.494001000	-2.191165000	2.041836000
1	-3.848292000	-3.037806000	1.277152000
6	2.980874000	0.830034000	2.515085000
6	3.819579000	-0.141253000	1.965435000
6	3.312587000	-1.395030000	1.627306000
6	1.954862000	-1.691387000	1.815885000
6	1.124854000	-0.715966000	2.391604000
6	1.632269000	0.534668000	2.733952000
1	3.378306000	1.804216000	2.786421000
1	4.873443000	0.074426000	1.811274000
1	3.974961000	-2.153118000	1.222983000
1	0.087843000	-0.971842000	2.582539000
1	0.979634000	1.278418000	3.183612000

***(S)*-TS 3A**
File: FFMin_PAiPr_mixed_A2B2C2D1_1Solv_R_24_TS1_NC.out
Energy(B3LYP/6-31g**): -2000.571952 au
Nuc.Rep. Energy: 5338.068472 au
G= -1999.890 au, ZPE= 2010.87 kJ/mol
Energy in solvent (SM8): -2000.655402 au
Dispersion energy: -75.8964 kcal/mol

N	1.412195	2.914563	-0.205200
Li	-0.019113	1.934233	0.836358
O	-1.281228	3.266836	-2.563748
C	-2.012648	2.404922	-2.013867
Li	-0.295056	3.635287	-1.004951
C	-1.996639	3.197938	0.452809
C	-3.014438	2.433688	1.299877
H	-2.502660	1.669582	1.907211
O	-0.445119	0.021488	1.341980
C	-1.175464	-0.853414	0.486707
H	-1.082967	-0.472098	-0.530590
H	-0.761878	-1.869168	0.529242
H	-2.234988	-0.879653	0.771824
C	-0.475734	-0.415606	2.700411
H	0.010714	-1.394834	2.800476
H	0.060537	0.328141	3.289138
H	-1.509653	-0.486420	3.061889
H	-3.703204	1.877707	0.647672
C	-6.275956	2.463390	-2.321114
C	-5.618589	1.291551	-1.943788
C	-4.230340	1.283702	-1.825526
C	-3.486827	2.442115	-2.088780
C	-4.153813	3.612564	-2.477572
C	-5.540461	3.622558	-2.587059
H	-7.358836	2.473804	-2.410299
H	-6.187209	0.387915	-1.743001
H	-3.712961	0.371450	-1.537835
H	-3.565854	4.498353	-2.693882
H	-6.054654	4.532482	-2.883564

H	-1.251697	3.659360	1.135279
H	-1.593825	1.424164	-1.737904
H	-2.488674	4.051081	-0.037613
C	-3.871556	3.292961	2.253177
C	-4.875878	2.475044	3.073218
H	-4.407124	4.046886	1.660297
H	-3.211977	3.848844	2.932602
H	-5.472518	3.111227	3.736371
H	-5.570845	1.931102	2.422067
H	-4.365092	1.734367	3.701419
C	2.234748	3.912437	0.475526
C	1.499347	4.520099	1.686616
H	2.104213	5.299745	2.163477
P	1.050807	3.201137	2.932742
H	3.162586	3.465939	0.876735
H	0.568233	4.997109	1.361239
C	-1.045719	5.486100	6.418069
C	-1.316766	5.821470	5.091966
C	-0.659479	5.166654	4.050821
C	0.291209	4.167181	4.315999
C	0.546955	3.832616	5.655341
C	-0.112750	4.487352	6.694417
H	-1.558216	5.996704	7.228313
H	-2.043952	6.595422	4.862667
H	-0.896972	5.439525	3.027399
H	1.275162	3.062569	5.891001
H	0.106513	4.216181	7.723606
C	5.261531	2.060211	4.569217
C	4.835640	3.388799	4.634634
C	3.574572	3.742206	4.162224
C	2.716807	2.774099	3.614676
C	3.156242	1.445380	3.556806
C	4.420661	1.089132	4.030681
H	6.246257	1.785917	4.936589
H	5.488017	4.149591	5.053989
H	3.249665	4.776540	4.228343
H	2.511555	0.685645	3.124751
H	4.747185	0.054559	3.974232
C	2.770000	5.084217	-0.440135
C	2.235039	2.048839	-1.069867
H	2.930500	2.654866	-1.683103
C	3.112352	1.038582	-0.295453
H	2.475927	0.321041	0.239054
H	3.763456	0.472839	-0.974380
H	3.754658	1.528149	0.442355
C	1.361538	1.277486	-2.067783
H	1.974872	0.654943	-2.728971
H	0.678161	0.599469	-1.537571
H	0.758736	1.947951	-2.686528
H	3.481159	5.678841	0.147341
H	3.345143	4.629724	-1.254008
C	-0.367366	7.607531	-2.032764
C	0.355175	8.008906	-0.907369
C	1.376989	7.204291	-0.404646
C	1.707532	5.983692	-1.013129
C	0.982706	5.602985	-2.154682

C	-0.050089	6.401022	-2.655469
H	-1.164881	8.233073	-2.423606
H	0.122870	8.952391	-0.420433
H	1.933781	7.528695	0.471310
H	1.240649	4.679823	-2.666039
H	-0.601319	6.071541	-3.530653

***(R)*-TS 3A**

File: FFMin_PAiPr_mixed_A2B2C2D1_1Solv_R_24_TS2_NC.out
Energy(B3LYP/6-31g**): -2000.572111 au
Nuc.Rep. Energy: 5318.952464 au
G= -1999.895 au, ZPE= 2010.07 kJ/mol
Energy in solvent (SM8): -2000.657773 au
Dispersion energy: -74.9842 kcal/mol

N	1.783740	2.725633	0.073361
Li	0.563147	1.678641	1.263473
O	-1.103250	2.668373	-2.266799
C	-2.081550	2.170206	-1.669141
Li	-0.043046	3.079231	-0.746237
C	-1.550161	2.745003	0.941984
C	-2.892791	2.232424	1.475270
H	-2.877230	1.133485	1.565413
O	0.322265	-0.155574	1.900933
C	-0.573318	-1.065572	1.262914
H	-1.136637	-0.497642	0.522774
H	-0.018637	-1.873232	0.768231
H	-1.265568	-1.499082	1.995918
C	1.096857	-0.762144	2.929566
H	1.756311	-1.538140	2.519072
H	1.695054	0.026568	3.387345
H	0.444375	-1.209556	3.690617
H	-3.695224	2.448524	0.754119
H	-2.857624	2.815459	-1.236058
H	-0.877191	2.760960	1.823601
H	-1.660563	3.820065	0.696956
C	-3.330827	2.810713	2.836548
C	-4.672891	2.262376	3.335678
H	-3.384941	3.904951	2.759318
H	-2.551829	2.603341	3.582604
H	-4.947546	2.687074	4.307652
H	-5.484132	2.492071	2.634008
H	-4.638825	1.171813	3.449982
C	2.475410	3.869663	0.663421
C	1.628211	4.511701	1.781913
H	2.072229	5.457100	2.114815
P	1.432104	3.357432	3.240040
H	3.429862	3.566741	1.133217
H	0.624007	4.734591	1.403492
C	-1.430702	5.515123	6.218447
C	-1.153644	6.120242	4.994653
C	-0.281784	5.512919	4.087962
C	0.320649	4.283234	4.389844
C	0.025382	3.681284	5.625128
C	-0.834784	4.292338	6.533250
H	-2.109855	5.988907	6.921369
H	-1.615402	7.070197	4.739822

H	-0.080260	6.004854	3.142446
H	0.476359	2.724335	5.876969
H	-1.046276	3.811502	7.484267
C	5.609467	3.797671	5.264913
C	4.679792	4.833481	5.378057
C	3.422300	4.713081	4.790783
C	3.072602	3.554482	4.079995
C	4.012012	2.519712	3.978915
C	5.274186	2.641050	4.563291
H	6.589511	3.893248	5.723800
H	4.935281	5.736617	5.925785
H	2.703575	5.521262	4.891165
H	3.757739	1.615628	3.432456
H	5.992284	1.830969	4.471678
C	2.927842	4.987417	-0.354363
C	2.701868	1.879872	-0.704711
H	3.335696	2.491556	-1.376134
C	3.677750	1.045035	0.157609
H	3.120975	0.317624	0.763425
H	4.390286	0.489006	-0.465272
H	4.260521	1.673283	0.838313
C	1.907439	0.936815	-1.616637
H	2.570293	0.271263	-2.181677
H	1.233032	0.302296	-1.025212
H	1.296011	1.495474	-2.332182
H	3.551307	5.707547	0.190666
H	3.582213	4.513923	-1.094623
C	-0.326492	7.029063	-2.350554
C	0.307157	7.619507	-1.255436
C	1.362812	6.966949	-0.619375
C	1.814076	5.713687	-1.060919
C	1.173870	5.140236	-2.171414
C	0.111511	5.787139	-2.807639
H	-1.148943	7.536388	-2.846828
H	-0.019189	8.592819	-0.898318
H	1.854378	7.439797	0.227970
H	1.526595	4.185764	-2.551875
H	-0.371718	5.313377	-3.656429
C	-3.148632	-1.955375	-2.096286
C	-4.001750	-1.082076	-1.419312
C	-3.649980	0.257696	-1.267027
C	-2.434523	0.735707	-1.779977
C	-1.591314	-0.145988	-2.476464
C	-1.944883	-1.482291	-2.628891
H	-3.424233	-2.999463	-2.217866
H	-4.942876	-1.444498	-1.015543
H	-4.318024	0.938268	-0.749397
H	-0.669023	0.239339	-2.895898
H	-1.288406	-2.158382	-3.169565

***(S)*-TS 4A**
File: FFMin_PGM_mixed_A2B2C2D1_1Solv_12_TS1_ext_NC.out
Energy(B3LYP/6-31g**): -1882.617472 au
Nuc.Rep. Energy: 4575.033574 au
G= -1882.019 au, ZPE= 1783.9 kJ/mol
Energy in solvent (SM8): -1882.706283 au

Dispersion energy: -61.9097 kcal/mol

7	-1.535311000	-2.238144000	-0.107123000
3	-0.195871000	-1.235826000	-1.156662000
8	0.730498000	-3.928495000	2.155020000
6	1.903943000	-3.533661000	2.041254000
3	0.102162000	-3.130099000	0.528744000
6	1.881447000	-2.382715000	-0.659239000
6	2.978973000	-1.328848000	-0.457782000
1	2.530189000	-0.331583000	-0.322071000
8	0.193886000	0.698955000	-1.237693000
6	0.134445000	1.587690000	-0.126845000
1	-0.322953000	1.043905000	0.700447000
1	-0.477338000	2.466420000	-0.367732000
1	1.140772000	1.916776000	0.162749000
6	0.749581000	1.306704000	-2.401768000
1	0.153063000	2.175831000	-2.703710000
1	0.724067000	0.563138000	-3.198620000
1	1.786291000	1.616676000	-2.220441000
1	3.520546000	-1.523527000	0.480606000
6	5.214770000	-6.103264000	1.261483000
6	5.434923000	-4.767684000	1.599162000
6	4.351355000	-3.930134000	1.850943000
6	3.042722000	-4.424858000	1.766207000
6	2.828577000	-5.773039000	1.438156000
6	3.911382000	-6.605143000	1.183672000
1	6.058929000	-6.756334000	1.059495000
1	6.447541000	-4.381639000	1.663689000
1	4.513952000	-2.889450000	2.116763000
1	1.809720000	-6.142528000	1.387263000
1	3.746464000	-7.646398000	0.923751000
1	1.448078000	-2.195406000	-1.674486000
1	2.165684000	-2.485625000	2.264484000
1	2.366848000	-3.359977000	-0.819622000
6	4.024505000	-1.230211000	-1.587203000
6	5.102061000	-0.164803000	-1.356790000
1	4.499225000	-2.212497000	-1.713422000
1	3.505519000	-1.026581000	-2.535490000
1	5.818438000	-0.122507000	-2.184686000
1	5.669184000	-0.364614000	-0.439549000
1	4.659539000	0.833590000	-1.253191000
6	-2.551994000	-3.009316000	-0.801517000
6	-3.223574000	-2.215373000	-1.976498000
1	-3.721635000	-1.338830000	-1.549143000
15	-1.957848000	-1.551702000	-3.189705000
1	-3.392732000	-3.236674000	-0.117068000
1	-3.996743000	-2.802687000	-2.484664000
6	-3.975179000	2.353822000	-4.768410000
6	-3.783422000	2.141217000	-3.402299000
6	-3.204982000	0.956843000	-2.951036000
6	-2.818195000	-0.049744000	-3.854008000
6	-3.006958000	0.181923000	-5.224404000
6	-3.580241000	1.372062000	-5.675093000
1	-4.425598000	3.277022000	-5.121353000
1	-4.086213000	2.899199000	-2.684834000
1	-3.055511000	0.814545000	-1.883651000
1	-2.712674000	-0.572331000	-5.946544000

1	-3.722451000	1.527003000	-6.741352000
6	-1.920220000	-4.414064000	-6.861433000
6	-3.141617000	-4.096962000	-6.263810000
6	-3.180918000	-3.249846000	-5.158298000
6	-1.998791000	-2.709136000	-4.628406000
6	-0.779627000	-3.038834000	-5.236482000
6	-0.738889000	-3.883440000	-6.346518000
1	-1.891448000	-5.074128000	-7.723798000
1	-4.065086000	-4.508615000	-6.661785000
1	-4.139679000	-2.999665000	-4.713840000
1	0.144934000	-2.635615000	-4.831791000
1	0.215111000	-4.128567000	-6.804638000
6	-1.225953000	-6.914210000	-2.197362000
6	-0.316692000	-5.862226000	-2.119857000
6	-0.729456000	-4.603987000	-1.672638000
6	-2.056791000	-4.369192000	-1.291003000
6	-2.958426000	-5.439965000	-1.377973000
6	-2.553428000	-6.696043000	-1.825060000
1	-0.906263000	-7.893038000	-2.543827000
1	0.719506000	-6.012267000	-2.410784000
1	-0.001319000	-3.801034000	-1.636299000
1	-3.993538000	-5.285335000	-1.081576000
1	-3.273204000	-7.508651000	-1.875884000
6	-2.145221000	-1.375345000	0.892493000
1	-1.365493000	-0.898530000	1.506076000
1	-2.801364000	-1.918761000	1.601155000
1	-2.769932000	-0.546478000	0.489916000

***(R)*-TS 4A**
File: FFMin_PGM_mixed_A2B2C2D1_1Solv_27_TS2_NC.out
Energy(B3LYP/6-31g**): -1882.615767 au
Nuc.Rep. Energy: 4559.405136 au
G= -1882.018 au, ZPE= 1782.5 kJ/mol
Energy in solvent (SM8): -1882.708628 au
Dispersion energy: -61.7562 kcal/mol

7	-1.711178000	-1.547803000	-0.359311000
3	-0.356791000	-0.656107000	-1.484145000
8	0.365723000	-3.661752000	1.760525000
6	1.588829000	-3.661138000	1.560298000
3	-0.082063000	-2.423026000	0.359837000
6	1.748736000	-1.588769000	-0.554817000
6	2.364498000	-0.336204000	0.088396000
1	1.609356000	0.460221000	0.195678000
8	-0.045103000	1.244674000	-1.904621000
6	-0.315267000	2.342013000	-1.037587000
1	-0.773968000	1.938339000	-0.135014000
1	-1.007215000	3.049844000	-1.513213000
1	0.612313000	2.865182000	-0.772601000
6	0.543272000	1.646580000	-3.138278000
1	-0.122230000	2.332563000	-3.677221000
1	0.687197000	0.745511000	-3.736088000
1	1.512623000	2.131134000	-2.965437000
1	2.665535000	-0.573983000	1.119809000
1	2.010220000	-4.191897000	0.690712000
1	1.531665000	-1.363512000	-1.631267000
1	2.553934000	-2.332947000	-0.670732000

6	3.586756000	0.266487000	-0.632704000
6	4.185637000	1.492541000	0.066361000
1	4.355930000	-0.512714000	-0.728052000
1	3.301500000	0.530155000	-1.662090000
1	5.051643000	1.891587000	-0.473884000
1	4.515050000	1.244624000	1.082658000
1	3.449239000	2.301920000	0.152849000
6	-2.665146000	-2.470274000	-0.959507000
6	-3.312403000	-1.919044000	-2.277553000
1	-3.874397000	-1.015271000	-2.018766000
15	-2.037669000	-1.381803000	-3.543279000
1	-3.528864000	-2.618169000	-0.282709000
1	-4.032322000	-2.624946000	-2.708226000
6	-4.259394000	1.962422000	-5.939747000
6	-3.713002000	0.874118000	-6.618002000
6	-3.077371000	-0.151528000	-5.916258000
6	-2.975179000	-0.111178000	-4.517423000
6	-3.514613000	1.000844000	-3.846666000
6	-4.155485000	2.021000000	-4.548499000
1	-4.758626000	2.756571000	-6.487319000
1	-3.785090000	0.815701000	-7.700961000
1	-2.666702000	-0.993152000	-6.463824000
1	-3.438185000	1.072230000	-2.764229000
1	-4.575630000	2.863355000	-4.005583000
6	-1.588385000	-4.927587000	-6.527941000
6	-2.860689000	-4.599009000	-6.054531000
6	-3.024819000	-3.537844000	-5.166845000
6	-1.918826000	-2.791729000	-4.729796000
6	-0.648000000	-3.131545000	-5.215260000
6	-0.481757000	-4.189632000	-6.109416000
1	-1.461472000	-5.757771000	-7.216944000
1	-3.726224000	-5.171573000	-6.377855000
1	-4.022390000	-3.289166000	-4.816309000
1	0.220085000	-2.568934000	-4.880146000
1	0.511548000	-4.440658000	-6.471720000
6	-1.038278000	-6.470711000	-1.533248000
6	-2.329641000	-6.286684000	-1.037668000
6	-2.838200000	-5.000053000	-0.862556000
6	-2.076828000	-3.864797000	-1.172982000
6	-0.781958000	-4.067073000	-1.671543000
6	-0.267592000	-5.353304000	-1.850083000
1	-0.638376000	-7.471538000	-1.668152000
1	-2.941389000	-7.146951000	-0.778932000
1	-3.843107000	-4.871099000	-0.466697000
1	-0.155504000	-3.215645000	-1.920021000
1	0.738775000	-5.477704000	-2.241148000
6	-2.402376000	-0.563867000	0.458472000
1	-1.672833000	0.059024000	0.997841000
1	-3.053693000	-1.014879000	1.234111000
1	-3.058398000	0.142250000	-0.099028000
6	4.451868000	-2.118697000	4.319879000
6	4.879314000	-2.729787000	3.139738000
6	3.942300000	-3.224094000	2.235384000
6	2.572513000	-3.106698000	2.505904000
6	2.148667000	-2.493295000	3.695439000
6	3.085628000	-2.001765000	4.596333000

1	5.181841000	-1.733909000	5.026282000
1	5.940061000	-2.820256000	2.927433000
1	4.265797000	-3.700982000	1.313792000
1	1.084165000	-2.419646000	3.892172000
1	2.757192000	-1.528316000	5.516795000

***(S)*-TS 5A**

File: FFMin_PAM_mixed_A2B1C1D4_1Solv_R_56_TS1_NC.out
Energy(B3LYP/6-31g**): -1921.943614 au
Nuc.Rep. Energy: 4855.912688 au
G= -1921.315 au, ZPE= 1861.97 kJ/mol
Energy in solvent (SM8): -1922.027796 au
Dispersion energy: -68.3219 kcal/mol

N	1.250840	3.106729	-0.384654
Li	-0.275920	2.384092	0.700508
O	-1.306840	3.284158	-2.607986
C	-1.901623	2.425560	-1.920404
Li	-0.348548	4.048142	-1.133922
C	-2.008821	3.844880	0.379731
C	-3.025476	3.398359	1.431565
H	-2.509710	2.905871	2.273879
O	-0.580056	0.406330	0.900031
C	0.542253	-0.472908	0.810953
H	1.287480	0.018747	0.186600
H	0.968129	-0.664137	1.803694
H	0.245740	-1.425871	0.352784
C	-1.629751	-0.130849	1.699846
H	-1.287258	-0.309042	2.728193
H	-2.440241	0.598025	1.707477
H	-1.991285	-1.078523	1.278034
H	-3.694419	2.634464	1.003575
C	-6.130523	1.825251	-1.983621
C	-5.296332	0.874046	-1.393238
C	-3.920005	1.082858	-1.365612
C	-3.364590	2.239687	-1.930929
C	-4.207675	3.186021	-2.531186
C	-5.583465	2.979543	-2.551610
H	-7.205288	1.667347	-2.002025
H	-5.720146	-0.025783	-0.956321
H	-3.262819	0.346338	-0.909955
H	-3.764028	4.070542	-2.976473
H	-6.235673	3.716446	-3.011668
H	-1.286903	4.533383	0.872095
H	-1.339701	1.601574	-1.449700
H	-2.524209	4.450430	-0.381982
C	-3.918691	4.513162	2.019044
C	-4.913416	4.015556	3.074109
H	-4.462805	4.994070	1.195210
H	-3.280642	5.296047	2.452809
H	-5.535414	4.829849	3.462639
H	-5.586132	3.256216	2.657484
H	-4.394672	3.561109	3.927326
C	2.333656	3.872998	0.198541
C	1.911547	4.522281	1.531360
H	2.747743	5.054872	2.000715
P	1.144805	3.298899	2.714294

H	3.195378	3.210844	0.420455
H	1.128270	5.271215	1.359627
C	0.213824	6.053293	6.358399
C	-0.767103	5.735675	5.419386
C	-0.462539	4.896562	4.347500
C	0.830518	4.375927	4.189351
C	1.808256	4.701702	5.140635
C	1.500933	5.532403	6.217247
H	-0.023788	6.699201	7.199059
H	-1.773194	6.132074	5.524884
H	-1.236261	4.641218	3.628552
H	2.812367	4.299369	5.045194
H	2.268189	5.773081	6.948327
C	4.587672	0.526324	4.200093
C	4.915337	1.686770	3.500733
C	3.910431	2.544792	3.049978
C	2.558698	2.251642	3.281515
C	2.245154	1.076638	3.984680
C	3.247062	0.224796	4.445915
H	5.370872	-0.140255	4.549629
H	5.956280	1.929412	3.305307
H	4.189228	3.445114	2.513494
H	1.202789	0.832237	4.176146
H	2.982502	-0.675367	4.993938
C	2.961214	4.974664	-0.750158
C	1.767336	2.204295	-1.403660
H	2.593373	1.559054	-1.036537
H	0.974199	1.536367	-1.765423
H	2.170012	2.698508	-2.311608
C	0.004030	7.813131	-2.144235
C	0.833506	8.136383	-1.069532
C	1.803938	7.234169	-0.631530
C	1.974210	5.991399	-1.257064
C	1.142548	5.687023	-2.350830
C	0.163345	6.584659	-2.787347
H	-0.754183	8.513909	-2.481702
H	0.723822	9.094262	-0.568367
H	2.442094	7.498405	0.208180
H	1.278650	4.747124	-2.879572
H	-0.468240	6.319600	-3.630581
H	3.779645	5.474150	-0.216840
H	3.414722	4.452478	-1.599800

***(R)*-TS 5A**
File: FFMin_PAM_mixed_A2B1C1D4_1Solv_R_58_TS2_NC.out
Energy(B3LYP/6-31g**): -1921.945087 au
Nuc.Rep. Energy: 4891.537114 au
G= -1921.316 au, ZPE= 1863.74 kJ/mol
Energy in solvent (SM8): -1922.030954 au
Dispersion energy: -68.6687 kcal/mol

N	1.785988	1.612891	0.124057
Li	0.257180	1.335929	1.341012
O	-0.718283	3.791229	-0.883601
C	-1.604479	3.361084	-0.096231
Li	0.219536	2.159535	-0.982525
C	-1.422061	0.810335	-0.176161

C	-1.585579	0.482344	-1.661449
H	-0.598388	0.344054	-2.142403
O	-0.082871	0.010025	2.826349
C	0.416227	-1.322386	2.713314
H	1.399410	-1.258594	2.245378
H	0.509579	-1.782670	3.705378
H	-0.246375	-1.938049	2.091082
C	-1.377526	0.063460	3.423748
H	-1.354639	-0.369800	4.431725
H	-1.656718	1.116500	3.490929
H	-2.113777	-0.473092	2.811986
H	-2.057915	1.327403	-2.186629
H	-1.408548	3.324030	0.986685
H	-0.831411	-0.004239	0.285584
H	-2.398867	0.801686	0.318273
C	-2.419243	-0.780084	-1.969499
C	-2.595699	-1.057833	-3.465903
H	-3.403737	-0.663289	-1.497473
H	-1.949284	-1.646439	-1.483803
H	-3.200782	-1.954237	-3.640665
H	-3.093853	-0.219622	-3.966871
H	-1.628976	-1.210119	-3.960370
C	2.810549	2.613193	0.364196
C	2.172435	3.906963	0.908297
H	2.932621	4.663092	1.134638
P	1.135521	3.545096	2.419064
H	3.538045	2.256618	1.123952
H	1.493437	4.321572	0.157066
C	-0.847868	7.601862	3.574705
C	-0.766741	7.208909	2.238793
C	-0.132121	6.017008	1.889696
C	0.443331	5.196917	2.875779
C	0.346502	5.598809	4.217824
C	-0.290715	6.790278	4.562625
H	-1.344113	8.529968	3.844056
H	-1.200915	7.830403	1.460638
H	-0.098012	5.722830	0.845135
H	0.778439	4.981619	4.999741
H	-0.349687	7.084564	5.607199
C	4.372766	2.686828	5.653116
C	4.401727	3.900867	4.962706
C	3.433166	4.181481	4.001910
C	2.419706	3.252868	3.715465
C	2.398722	2.040237	4.417456
C	3.370577	1.758182	5.379994
H	5.129910	2.468385	6.401048
H	5.180174	4.628741	5.174529
H	3.458951	5.132465	3.477327
H	1.619233	1.314903	4.200863
H	3.343306	0.813193	5.915903
C	3.717051	2.952859	-0.880976
C	2.370814	0.310874	-0.148678
H	3.075311	-0.031547	0.639828
H	1.579798	-0.449880	-0.228246
H	2.946058	0.236277	-1.094278
C	1.513973	4.383797	-4.324693

C	2.180030	5.283770	-3.493214
C	2.900863	4.821555	-2.391771
C	2.974287	3.454889	-2.092236
C	2.302679	2.559661	-2.943453
C	1.582188	3.017861	-4.048716
H	0.954306	4.742134	-5.183903
H	2.141005	6.349289	-3.703307
H	3.420130	5.532891	-1.753759
H	2.378478	1.492249	-2.755435
H	1.082411	2.305165	-4.699979
H	4.467861	3.689990	-0.570578
H	4.269013	2.042996	-1.142985
C	-5.762043	3.346723	-1.099178
C	-5.356102	3.047947	0.204136
C	-4.001831	3.036493	0.522196
C	-3.038866	3.322935	-0.455641
C	-3.453039	3.628248	-1.759188
C	-4.808852	3.637420	-2.077713
H	-6.819427	3.358048	-1.349065
H	-6.096858	2.828758	0.968135
H	-3.680188	2.810899	1.536350
H	-2.698444	3.874082	-2.499309
H	-5.126394	3.877836	-3.088525