

Activation of a (cyclooctadiene)rhodium(I) complex supported by a chiral ferrocenyl phosphine thioether ligand for hydrogenation catalysis: a combined *parahydrogen* NMR and DFT study.

Ekaterina M. Kozinets,^{a,b,c} Marianna Fekete,^d Oleg A. Filippov,^c Natalia V. Belkova*,^c Elena S. Shubina,^c Rinaldo Poli*,^{a,b,e} Simon Duckett*,^d and Eric Manoury*,^{a,b}

SUPPORTING INFORMATION

Sample preparation for experiments with *parahydrogen*.

2.5 mg of either $[\text{RhCl}(\text{P},\text{StBu})(\text{COD})]$ (**1**) or $[\text{Rh}(\text{P},\text{StBu})(\text{COD})]\text{BF}_4$ (**2**) were dissolved in 0.5 mL of d_4 -methanol and 20 μL pyridine (75 fold) was added into the solution. The combine solution was taken up by syringe and transferred to a Young's tap NMR tube. The sample in NMR tube was degassed on a high-vacuum line via three 'cool'-pump-thaw cycles (the sample was cooled to -78°C rather than frozen in liquid N_2 to avoid cracking of the NMR tube upon thawing). *Parahydrogen*, at pressure of 3 atmospheres was then admitted to the NMR tube.

Polarization step

The sample was shaken (to replenish $p\text{-H}_2$ in solution) for approximately 10 seconds in the magnetic field about 65 G, and rapidly (within 5 seconds) inserted into the NMR spectrometer, after which spectra were immediately acquired.

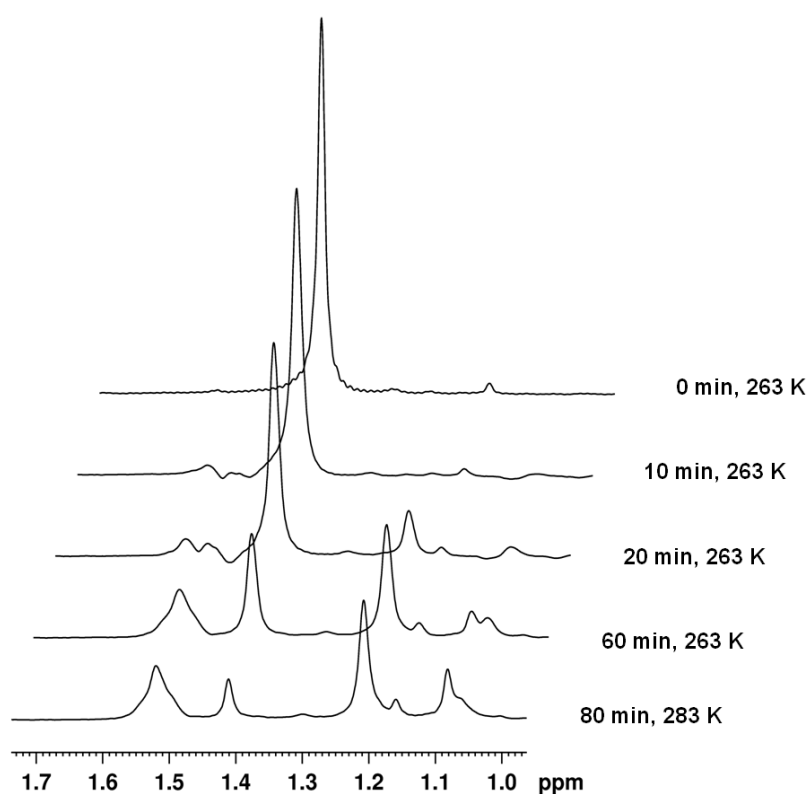


Figure S1. Spectrum showing the resonance at δ 1.54 assigned to complex **3**, $[\text{Rh}(\eta^5\text{-C}_8\text{H}_{13})(\text{P},\text{StBu})]$ and also those of the products of hydrogenation of COD.

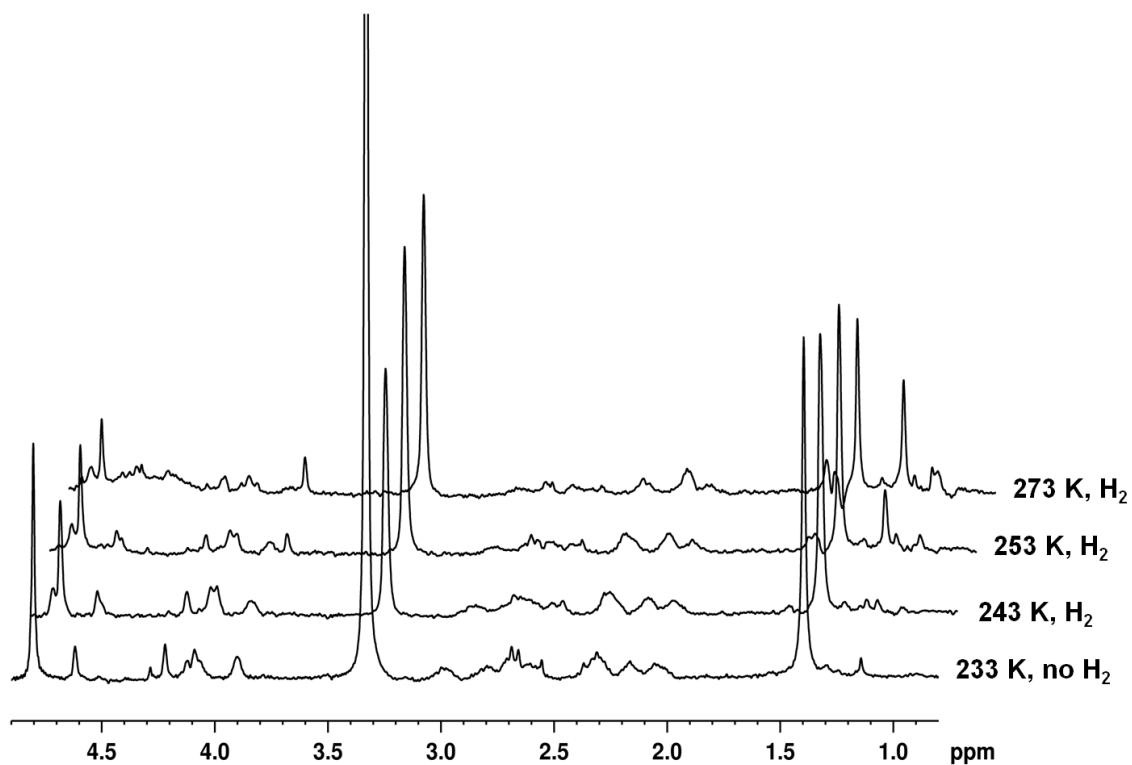


Figure S2. ^1H NMR spectra of **2** before and after reaction with H_2 , recorded at different temperature. We can see a decrease in the intensity of the proton signal of $-\text{CH}=$ in COD at 4.8 ppm, and formation of new products which ^1H signals appear around 4.8, 4.2, 3.8, 1.6 and 1.2 ppm.

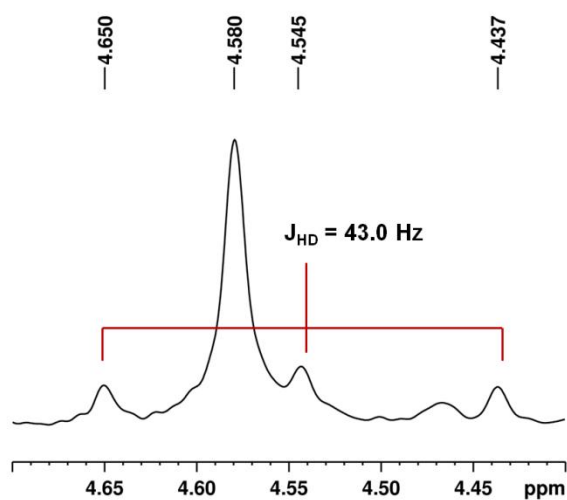
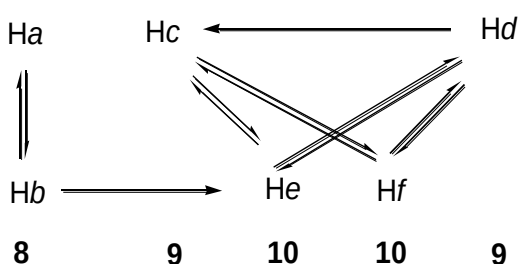


Figure S3. ^1H NMR spectrum of H_2 (at δ 4.580) and HD (δ 4.650, 4.545 and 4.437).

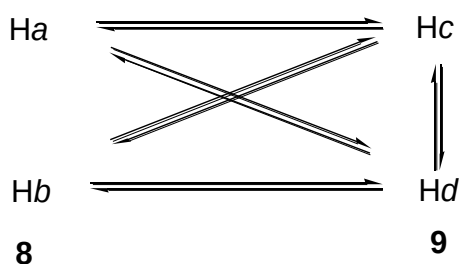
Kinetics of hydride exchange

The ligand exchange studies were completed using the EXSY protocol¹. A selected resonance was probed and the magnetization flow was followed as a function of the reaction time between zero and 1 second, in steps typically of 0.1 seconds. The intensity data was then simulated using a differential model, based on a least-mean squares fit to experiment, in order to extract the associated experimental site-exchange rate constants. Table S1 lists the constraints that were used (eg $k_{Ha \rightarrow Hb} = k_{Hb \rightarrow Ha}$ for the mutual site exchange). In order to improve the data specificity and accuracy, the exchange process was followed in separate experiments from each site (where possible). Under these conditions the total error was minimized in the rate constant fitting process using the solver routine in excel. The jack-knife method² was then used to estimate the individual rate constant errors which are included as (1) where this signals +/- for the 95 % confidence limit. These data are listed in Table S2 and Table S3 Exchange rates as a function of pyridine excess and solvent.

Complex 1



Complex 2



Scheme S1 : Hydride exchange pathways for products found in the chemistry of compounds **1** and **2**.

Table S1: List of constraints that were used for the calculation of the exchange rate constants.

$H_a \rightarrow H_b = 0$	$H_b \rightarrow H_e = H_a \rightarrow H_f$
$H_a \rightarrow H_c = 0$	$H_d \rightarrow H_a = H_c \rightarrow H_b$
$H_a \rightarrow H_e = 0$	$H_d \rightarrow H_b = H_c \rightarrow H_a$
$H_b \rightarrow H_c = 0$	$H_d \rightarrow H_e = H_c \rightarrow H_f$
$H_b \rightarrow H_d = 0$	$H_d \rightarrow H_f = H_c \rightarrow H_e$
$H_b \rightarrow H_f = 0$	$H_f \rightarrow H_a = H_e \rightarrow H_b$
$H_e \rightarrow H_a = 0$	$H_f \rightarrow H_b = H_e \rightarrow H_a$
$H_e \rightarrow H_b = 0$	$H_f \rightarrow H_c = H_e \rightarrow H_d$
$H_e \rightarrow H_f = 0$	$H_f \rightarrow H_d = H_e \rightarrow H_c$
	$H_f \rightarrow H_e = H_e \rightarrow H_f$

Table S2: Observed hydride site exchange rate constants at 273 K based on **1** as a function of pyridine excess:

$K_{X \rightarrow Y} / s^{-1}$	15 fold pyridine	45 fold pyridine	75 fold pyridine
$k_{Ha \rightarrow Hf}$	$0.34 s^{-1}$	$1.17 s^{-1}$	$1.29 s^{-1}$
$k_{Hc \rightarrow Ha}$	$0.05 s^{-1}$	$0.11 s^{-1}$	$0.11 s^{-1}$
$k_{Hc \rightarrow Hb}$	$0.05 s^{-1}$	$0.11 s^{-1}$	$0.11 s^{-1}$
$k_{Hc \rightarrow He}$	$0.42 s^{-1}$	$0.35 s^{-1}$	$0.41 s^{-1}$
$k_{Hc \rightarrow Hf}$	$0.42 s^{-1}$	$0.53 s^{-1}$	$0.42 s^{-1}$
$k_{He \rightarrow Hc}$	$2.89 s^{-1}$	$19.67 s^{-1}$	$31.33 s^{-1}$
$k_{He \rightarrow Hd}$	$2.89 s^{-1}$	$21.77 s^{-1}$	$31.65 s^{-1}$

¹ K.D. Atkinson, M.J. Cowley, P.I.P. Elliott, S.B. Duckett, G.G.R. Green, J. Lopez-Serrano, A.C.J. Whitwood, *JACS*, **2009**, *131*, 13362-13368 ;

² D. C. Harris, *J. Chem. Educ.*, **1998**, *75*, 119

Table S3: Observed hydride site exchange rate constants at 273 K based on a sample of **2** for the indicated pyridine excess:

$K_{X \rightarrow Y}$	8 fold pyridine	75 fold pyridine	173 fold pyridine
$k_{Ha \rightarrow Hc}$	0.00 s^{-1}	$1.19(1) \text{ s}^{-1}$	1.23 s^{-1}
$k_{Ha \rightarrow Hd}$	1.47 s^{-1}	$1.10(1) \text{ s}^{-1}$	0.02 s^{-1}
$k_{Hc \rightarrow Ha}$	0.14 s^{-1}	$0.167(2) \text{ s}^{-1}$	0.12 s^{-1}
$k_{Hd \rightarrow Ha}$	0.06 s^{-1}	$0.160(3) \text{ s}^{-1}$	0.02 s^{-1}
$k_{Hc \rightarrow Hd}$	0.29 s^{-1}	$0.785(6) \text{ s}^{-1}$	0.39 s^{-1}

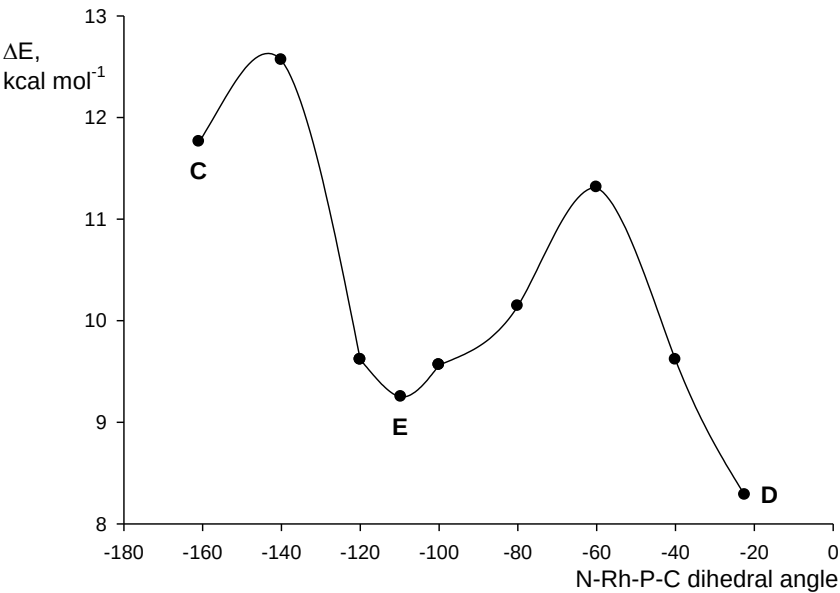
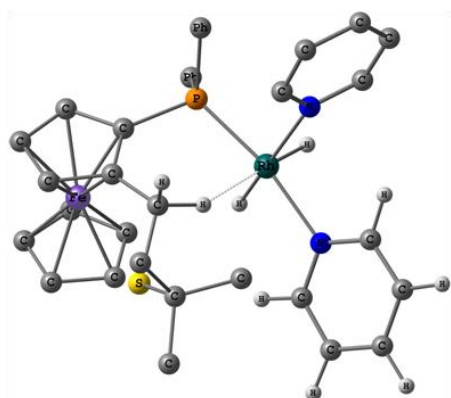
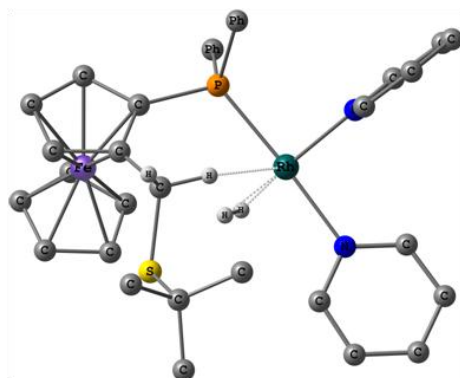


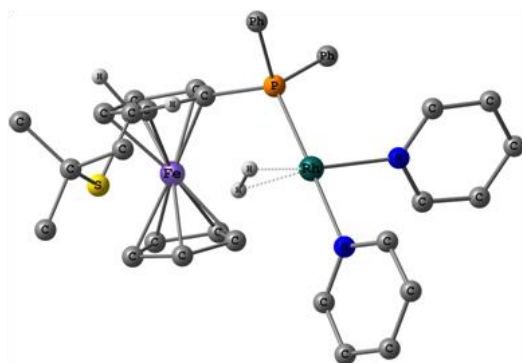
Figure S4. Relaxed potential energy surface scan results (dihedral N-Rh-P-C taken as reaction coordinate). Energies are relative to **V^{Pv}** adduct.



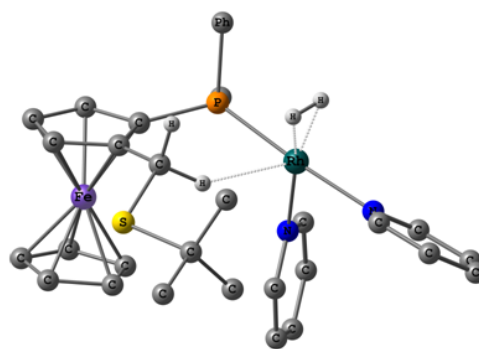
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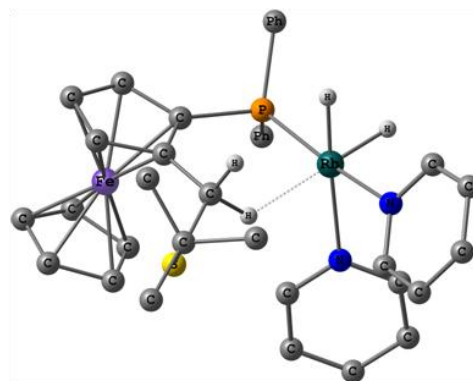
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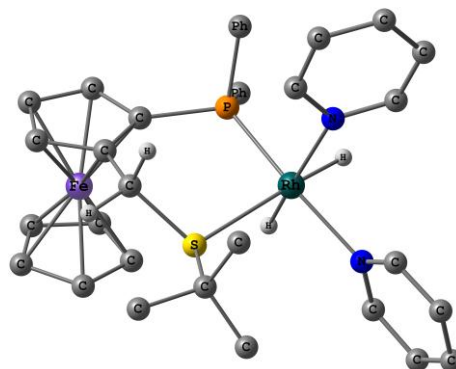
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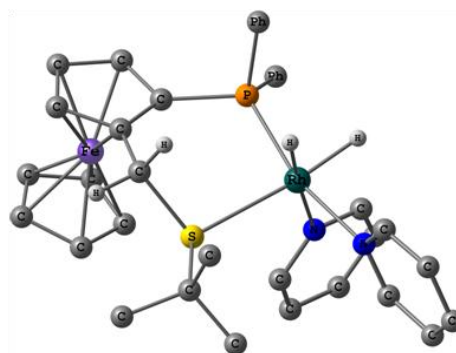
C



A



V



IV

Figure S5. M06 optimized geometries of selected complexes. Ph ligands, hydrogen atoms of aromatics and ^tBu group are omitted for clarity.

Table S5. Cartesian coordinates of all optimized structures.

a) B3LYP computed complexes				1	2.583062000	-14.888416000	16.764943000	6	2.970428000	-12.121230000	17.005805000
				1	0.216813000	-15.843455000	17.635929000	1	3.570714000	-12.584334000	16.220762000
I-MeCN				1	-1.309451000	-13.759380000	18.367644000	1	3.576467000	-12.056944000	17.914160000
E= -2285.86078243 Ha				6	0.520969000	-14.288221000	14.075920000	6	0.250879000	-12.252688000	20.910867000
45	1.828209000	-9.342315000	18.388692000	6	-0.753771000	-14.696745000	14.569760000	6	-0.089147000	-12.533803000	22.234760000
26	0.189314000	-13.501536000	15.998087000	6	-1.516930000	-13.523059000	14.845904000	6	-1.154879000	-11.866354000	22.843500000
15	0.082012000	-10.868011000	18.439454000	6	-0.714617000	-12.389243000	14.521670000	6	-1.875282000	-10.914009000	22.121052000
16	2.538432000	-10.404709000	16.398050000	6	0.545437000	-12.861302000	14.046810000	6	-1.536259000	-10.630317000	20.795408000
6	0.492772000	-12.540391000	17.828475000	1	1.333842000	-14.946258000	13.799466000	6	-0.473097000	-11.301542000	20.171767000
6	1.752994000	-12.946577000	17.249282000	1	-1.072725000	-15.716737000	14.736057000	1	1.074880000	-12.787347000	20.447899000
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6	-0.135436000	-6.437557000	20.878342000
1	0.270613000	-5.446733000	20.655448000
1	-1.227502000	-6.380535000	20.887690000
1	0.214329000	-6.748508000	21.866919000
6	0.338598000	-7.602643000	15.144919000
6	0.311395000	-7.394750000	19.874173000
1	2.296295000	-10.048238000	18.876796000
1	2.682228000	-8.415268000	17.687020000

II-MeOH

E=	-2252.96735932	Ha	
45	1.238861000	-9.137990000	17.801972000
26	0.017034000	-12.934408000	15.339476000
15	-0.275836000	-10.999228000	18.348510000
16	2.747630000	-10.414765000	16.638059000
6	0.039183000	-12.508854000	17.393290000
6	1.361420000	-12.882459000	16.947638000
6	1.272814000	-14.202101000	16.401290000
6	-0.077800000	-14.645395000	16.502250000
6	-0.841713000	-13.604776000	17.102700000
1	2.094996000	-14.757385000	15.968911000
1	-0.463067000	-15.589351000	16.141526000
1	-1.906427000	-13.620073000	17.290532000
6	0.676733000	-12.933314000	13.365736000
6	-0.575610000	-13.607552000	13.465289000
6	-1.536456000	-12.686473000	13.976682000
6	-0.880207000	-11.438670000	14.188518000
6	0.491063000	-11.590277000	13.810593000
1	1.608249000	-13.368124000	13.030134000
1	-0.756819000	-14.646827000	13.227472000
1	-2.574555000	-12.900488000	14.190107000
1	-1.359539000	-10.500072000	14.576578000
1	1.269284000	-10.839710000	13.851870000
6	2.663665000	-12.179169000	17.206551000
1	3.457344000	-12.701656000	16.671566000
1	2.898034000	-12.189159000	18.275242000
6	0.066341000	-12.892584000	20.463877000
6	0.235783000	-13.245712000	21.806148000
6	0.277965000	-12.259973000	22.792254000
6	0.155955000	-10.914121000	22.434907000
6	-0.003559000	-10.556162000	21.096855000
6	-0.057203000	-11.544300000	20.097372000
1	0.030582000	-13.670341000	19.708451000
1	0.331512000	-14.292895000	22.077188000
1	0.407811000	-12.536860000	23.833997000
1	0.192255000	-10.142589000	23.198276000
1	-0.083109000	-9.507675000	20.825717000
6	-3.023297000	-11.313129000	19.041151000
6	-4.384525000	-11.025842000	18.921699000
6	-4.828392000	-10.088227000	17.986389000

6	-3.905448000	-9.435082000	17.167228000
6	-2.541885000	-9.721303000	17.281682000
6	-2.086803000	-10.670029000	18.215727000
1	-2.690215000	-12.027446000	19.787457000
1	-5.097905000	-11.531436000	19.565544000
1	-5.887132000	-9.863837000	17.900906000
1	-4.244296000	-8.702712000	16.440104000
1	-1.831471000	-9.2122863000	16.634913000
6	4.580602000	-9.968813000	16.965215000
6	4.783904000	-8.598231000	16.305260000
6	5.448640000	-11.017334000	16.249437000
1	5.445339000	-11.985822000	16.755543000
1	5.147676000	-11.158185000	15.206463000
1	6.484339000	-10.662407000	16.249571000
1	4.593685000	-8.637324000	15.227855000
1	5.825748000	-8.294249000	16.450511000
1	4.143882000	-7.834515000	16.752393000
6	4.892973000	-9.914237000	18.462611000
1	4.722592000	-10.874596000	18.958116000
1	5.952508000	-9.664510000	18.590446000
1	4.296710000	-9.150825000	18.965580000
1	0.308786000	-9.262668000	15.157153000
1	-1.051078000	-7.880271000	18.431581000
6	0.733710000	-7.334134000	15.046925000
1	0.622591000	-6.491104000	15.728011000
1	1.790470000	-7.450125000	14.790137000
1	0.140829000	-7.155776000	14.144830000
6	0.147580000	-6.431757000	19.126336000
1	-0.650002000	-6.018398000	19.749313000
1	1.084366000	-6.447632000	19.680191000
1	0.268042000	-5.839151000	18.215589000
8	0.239043000	-8.497912000	15.744921000
8	-0.160747000	-7.809474000	18.808523000
1	2.266393000	-7.949474000	17.683797000
1	1.953574000	-9.421235000	19.108381000

II-Py

E=	-2518.11503414	Ha	
45	1.662191000	-9.579656000	18.982662000
26	0.008489000	-12.743363000	15.410215000
15	-0.031251000	-11.442126000	18.909906000
16	2.526940000	-10.217890000	16.893687000
6	0.214590000	-12.610475000	17.517637000
6	1.489543000	-12.832651000	16.873218000
6	1.406003000	-14.067019000	16.154477000
6	0.096802000	-14.602285000	16.323796000
6	-0.640601000	-13.704629000	17.141729000
1	2.198483000	-14.496422000	15.555592000
1	-0.283473000	-15.06591000	15.868604000
1	-1.674513000	-13.821728000	17.434381000
6	0.462872000	-12.643537000	13.385372000
6	-0.848677000	-13.174328000	13.568799000
6	-1.633623000	-12.191846000	14.241404000
6	-0.804018000	-11.053614000	14.471113000
6	0.492439000	-11.332706000	13.946170000
1	1.296595000	-13.159272000	12.928511000
1	-1.181292000	-14.160437000	13.274722000
1	-2.669544000	-12.301002000	14.532452000
1	-1.104200000	-10.133820000	14.951540000
1	1.345814000	-10.671211000	13.985782000
6	2.765189000	-12.050211000	16.996485000
1	3.428232000	-12.332593000	16.177092000
1	3.267820000	-12.262803000	17.943408000
6	-0.913005000	-13.570254000	20.584450000
6	-0.794995000	-14.478458000	21.635017000
6	0.323805000	-14.443705000	22.472253000
6	1.320767000	-13.494745000	22.252246000
6	1.202415000	-12.582345000	21.199711000
6	0.085786000	-12.607630000	20.352322000
1	-1.791921000	-13.608580000	19.949615000
1	-1.576294000	-15.214649000	21.799211000
1	0.414764000	-15.153104000	23.289257000
1	2.194172000	-13.461257000	22.897017000
1	1.983780000	-11.850689000	21.030622000
6	-2.464259000	-10.703170000	20.125194000
6	-3.797505000	-10.292420000	20.149253000
6	-4.526244000	-10.193707000	18.961346000
6	-3.912057000	-10.514240000	17.750413000
6	-2.576589000	-10.924459000	17.723233000
6	-1.833022000	-11.024881000	18.909069000
1	-1.922225000	-10.798452000	21.060745000
1	-4.271475000	-10.062609000	21.099162000
1	-5.565732000	-9.881149000	18.982243000
1	-4.474626000	-10.455292000	16.822919000
1	-2.116258000	-11.191065000	16.779973000
6	4.304347000	-9.596098000	16.599012000
6	4.195955000	-8.065419000	16.553348000
6	4.750148000	-10.117554000	15.222512000
1	4.879623000	-11.202879000	15.200626000
1	4.048493000	-9.830716000	14.433714000
1	5.723072000	-9.676295000	14.981568000

	3.496929000	-7.732421000	15.779174000
1	5.181669000	-7.651290000	16.315759000
1	3.877378000	-7.657072000	17.514733000
6	5.262770000	-10.049716000	17.702848000
1	5.370988000	-11.137912000	17.734439000
1	6.255300000	-9.629212000	17.504697000
1	4.930111000	-9.701788000	18.682772000
6	0.407171000	-7.943534000	23.448526000
6	1.675546000	-8.469205000	23.202781000
6	1.980739000	-8.938683000	21.930170000
7	1.093169000	-8.911746000	20.910874000
6	-0.131981000	-8.401323000	21.153094000
6	-0.510094000	-7.910808000	22.399917000
1	0.141986000	-7.568241000	24.431783000
1	2.428871000	-8.515647000	23.981644000
1	2.956624000	-9.342791000	21.695545000
1	-0.820796000	-8.395747000	20.318037000
1	-1.510267000	-7.513378000	22.534445000
6	-0.744568000	-5.653216000	16.835311000
6	0.231190000	-5.479655000	17.816691000
6	0.822913000	-6.598747000	18.388348000
7	0.492624000	-7.859842000	18.041880000
6	-0.450205000	-8.020707000	17.095518000
6	-1.090146000	-9.053068000	16.469312000
1	-1.223020000	-4.798549000	16.367590000
1	0.537837000	-4.485509000	18.135622000
1	1.592266000	-6.502763000	19.146542000
1	-0.696431000	-9.044422000	16.843916000
1	1.844639000	-7.145139000	19.173959000
1	2.638225000	-10.581404000	19.627580000
1	2.868137000	-8.598274000	19.141718000

1	5.311251000	-11.353251000	18.005266000	8	-0.155814000	-7.884105000	19.052056000	IV-MeCN
1	6.417253000	-10.125988000	17.380214000	1	2.178700000	-7.952652000	17.734110000	E= -2287.05337098 Ha
1	4.932275000	-9.629124000	18.214212000	1	0.623234000	-8.850972000	16.712774000	45 1.462467000 -9.468242000 17.598648000
7	2.788807000	-10.175678000	19.746427000					26 -0.137727000 -13.167418000 15.183656000
7	0.707767000	-8.097756000	19.075553000	III-Py				15 -0.031923000 -11.124810000 18.154682000
6	3.801161000	-10.911348000	22.042649000	E= -2518.11557409 Ha				16 2.852227000 -10.979571000 16.031509000
1	3.065834000	-11.522551000	22.573847000	45 1.836851000 -9.841001000 18.887420000				6 0.092836000 -12.665153000 17.198506000
1	4.711281000	-11.497299000	21.887259000	26 -0.310592000 -12.463093000 15.569351000				6 1.311360000 -13.241318000 16.681738000
1	4.045268000	-10.033885000	22.647773000	15 0.207587000 -11.760072000 19.019102000				6 0.999831000 -14.559410000 16.220148000
1	-0.476752000	-6.108113000	20.287681000	16 2.704366000 -10.561401000 16.805494000				6 -0.388384000 -14.802815000 16.437390000
1	-0.375233000	-5.207430000	19.682903000	6 0.234638000 -12.831734000 17.544030000				6 -0.952601000 -13.639030000 17.028621000
1	-1.539694000	-6.326435000	20.424079000	6 1.370419000 -13.020961000 16.668376000				1 1.701074000 -15.240838000 15.756684000
1	-0.019785000	-5.933087000	21.265675000	6 1.027465000 -14.046636000 15.731529000				1 -0.927574000 -15.697632000 16.157703000
6	3.246420000	-10.495416000	20.760124000	6 -0.295579000 -14.949247000 16.012381000				1 -1.989754000 -13.494110000 17.296852000
6	0.182770000	-7.222597000	19.618422000	6 -0.789008000 -13.747959000 17.117201000				6 0.018352000 -13.648110000 13.164438000
1	0.948041000	-8.906946000	16.756634000	1 1.663630000 -14.399206000 14.929959000				6 -1.354361000 -13.528000000 13.535035000
1	2.707405000	-8.347112000	17.665124000	1 -0.846743000 -15.236308000 15.450903000				6 -1.567929000 -12.204946000 14.022315000
				1 -1.776656000 -13.831349000 17.547420000				6 -0.323278000 -11.506354000 13.948815000
				6 -0.605614000 -12.061479000 13.548348000				6 0.655510000 -12.397581000 13.417745000
III-MeOH				6 -1.860781000 -12.174625000 14.217996000				1 0.496894000 -14.541309000 12.786218000
E= -2252.97045076 Ha				6 -1.910589000 -11.177682000 15.236700000				1 -2.095088000 -14.314810000 13.488128000
45 1.274964000 -9.199817000 18.044620000				6 -0.684535000 -10.446015000 15.194654000				1 -2.497847000 -11.815058000 14.412471000
15 -0.253605000 -11.088690000 18.467141000				6 0.120194000 -10.991728000 14.151140000				1 -0.133747000 -10.495715000 14.278006000
16 2.695668000 -10.426469000 16.682124000				1 -0.255339000 -12.695526000 12.745062000				1 1.701823000 -12.171272000 13.269917000
6 0.109371000 -12.574192000 17.506471000				1 -2.623838000 -12.913593000 14.014147000				6 2.703413000 -12.681184000 16.742120000
6 1.442741000 -12.923222000 17.067919000				1 -2.716681000 -11.026005000 15.940892000				1 3.364513000 -13.329789000 16.165736000
6 1.369840000 -14.227017000 16.483231000				1 -0.399134000 -9.639492000 15.855012000				1 3.060475000 -12.652153000 17.776592000
6 0.020090000 -14.681943000 16.550316000				1 1.115228000 -10.665607000 13.883038000				6 0.224826000 -13.050143000 20.237693000
6 -0.760428000 -13.668474000 17.172654000				6 2.737266000 -12.407698000 16.769908000				6 0.387409000 -13.445103000 21.569123000
1 2.199956000 -14.761654000 16.040224000				1 3.321603000 -12.697607000 15.895003000				6 0.515908000 -12.488671000 22.575527000
1 -0.353207000 -15.616117000 16.153412000				1 3.263632000 -12.761068000 17.661611000				6 0.487681000 -11.130169000 22.247901000
1 -1.827743000 -13.697227000 17.342798000				6 1.031186000 -14.245531000 20.144487000				6 0.340579000 -10.731852000 20.920166000
6 0.437645000 -13.220732000 13.421016000				6 1.269439000 -15.135581000 21.195746000				6 0.202376000 -11.688812000 19.899904000
6 -0.958521000 -13.254932000 13.712244000				6 0.895721000 -14.802681000 22.498268000				1 0.114890000 -13.807271000 19.469772000
6 -1.323824000 -11.996894000 14.275818000				6 0.273451000 -13.576114000 22.744157000				1 0.409966000 -14.502663000 21.814431000
6 -0.151296000 -11.183001000 14.329804000				6 0.039563000 -12.684011000 21.696867000				1 0.639594000 -12.797544000 23.609065000
6 0.935858000 -11.939449000 13.801019000				6 0.418593000 -13.003716000 20.380657000				1 0.588321000 -10.379233000 23.025837000
1 1.020269000 -14.034088000 13.010146000				1 1.306347000 -14.531261000 19.134253000				1 0.340296000 -9.675013000 20.674366000
1 -1.617100000 -14.100025000 13.563548000				1 1.733890000 -16.095711000 20.990356000				6 -2.707003000 -12.105072000 19.106727000
1 -2.309389000 -11.719494000 14.623427000				1 1.072529000 -15.498201000 23.312937000				6 -4.065626000 -10.704468000 19.002785000
1 -0.085971000 -10.177906000 13.721633000				1 -0.042196000 -13.318530000 23.751083000				6 -4.557446000 -10.071890000 17.861347000
1 1.960886000 -11.605595000 13.724976000				1 -0.473384000 -11.749479000 21.902054000				6 -3.684387000 -9.746897000 16.819984000
6 2.720064000 -12.170975000 17.317211000				6 -2.537341000 -12.170473000 19.671752000				6 -2.327081000 -10.050669000 16.922587000
1 3.534690000 -12.674436000 16.794757000				6 -3.879940000 -11.795382000 19.737623000				6 -1.823549000 -10.691752000 18.065613000
1 2.960812000 -12.140286000 18.384306000				6 -4.295016000 -10.519671000 19.328007000				1 -2.341478000 -11.506425000 20.001223000
6 0.179968000 -12.988047000 20.563668000				6 -3.319740000 -9.618577000 18.855421000				1 -4.736212000 -10.959066000 19.817897000
6 0.286381000 -13.367504000 21.905290000				6 -1.975248000 -9.991778000 18.790484000				1 -5.613248000 -9.831096000 17.783033000
6 0.036632000 -12.445290000 22.922043000				1 -1.567308000 -11.273090000 19.191847000				1 -4.061914000 -9.252968000 15.929109000
6 -0.322094000 -11.133978000 22.594963000				1 -2.247192000 -13.162358000 20.002636000				1 -1.656090000 -9.789017000 16.113960000
6 -0.422841000 -10.748465000 21.255909000				1 -4.616939000 -12.501045000 20.109484000				6 4.717800000 -10.662706000 16.121471000
6 -0.178152000 -11.674873000 20.221172000				1 -5.320141000 -10.229921000 19.380670000				6 4.917162000 -9.346920000 15.351685000
1 0.365220000 -13.720199000 19.785184000				1 -3.618363000 -8.623927000 18.537371000				6 5.461977000 -11.793352000 15.394043000
1 0.559855000 -14.388864000 22.152332000				1 -1.236924000 -9.288775000 18.420997000				1 5.423186000 -12.739704000 15.939623000
1 0.115747000 -12.744420000 23.962489000				6 4.521957000 -10.119237000 16.422564000				1 5.071703000 -11.951718000 14.384203000
1 -0.528116000 -10.412681000 23.380292000				6 4.635581000 -8.596809000 16.571832000				1 6.519318000 -11.519739000 15.305968000
1 -0.710248000 -9.727569000 21.016340000				6 4.756734000 -10.505357000 14.951869000				1 4.622507000 -9.451290000 14.302969000
6 -3.052117000 -11.323741000 18.966404000				1 4.685395000 -11.582726000 14.778950000				1 5.978161000 -9.074814000 15.377710000
6 -4.392403000 -11.001025000 18.745913000				1 4.053293000 -9.997929000 14.286188000				1 4.345334000 -8.527949000 15.792694000
6 -4.740267000 -10.053640000 17.780064000				1 5.770003000 -10.202626000 14.666170000				6 5.199419000 -10.540297000 17.571579000
6 -3.742653000 -9.429785000 17.028175000				1 3.897186000 -8.073036000 15.956853000				1 5.055636000 -11.471125000 18.127917000
6 -2.399465000 -9.751428000 17.243932000				1 5.631939000 -8.287270000 16.238081000				1 6.273639000 -10.320511000 17.578215000
6 -2.039100000 -10.704167000 18.215188000				1 4.504902000 -8.278980000 17.607791000				1 4.677988000 -9.742815000 18.104127000
1 -2.797462000 -12.053636000 19.728220000				6 5.513002000 -10.837445000 17.342640000				7 0.516230000 -8.461373000 15.866263000
1 -5.165127000 -11.489196000 19.332040000				1 5.466663000 -11.924967000 17.234588000				7 2.746864000 -7.824105000 17.692696000
1 -5.783457000 -9.802327000 17.615384000				1 6.530239000 -10.529246000 17.074608000				6 -0.371407000 -6.881332000 13.978641000
1 -4.006461000 -8.695447000 16.272849000				1 5.038603000 -10.58805000 18.390830000				1 -1.120214000 -6.197609000 14.388356000
1 -1.629104000 -9.279003000 16.640540000				6 -0.072700000 -7.274574000 22.623469000				1 0.449947000 -6.297165000 13.554552000
6 4.538321000 -9.927875000 16.771235000				6 0.466472000 -8.540696000 22.843918000				1 -0.828906000 -7.475445000 13.182366000
6 4.604984000 -8.498717000 16.215209000				6 0.986734000 -9.252517000 21.766758000				6 4.111985000 -5.667764000 18.263156000
6 5.302184000 -10.874934000 15.829906000				7 0.990970000 -8.772002000 20.506460000				1 4.684883000 -5.334316000 17.393610000
1 5.359590000 -11.898130000 16.209895000				6 0.471673000 -7.541039000 20.298174000				1 3.432290000 -4.867648000 18.570022000
1 4.865323000 -10.893212000 14.827172000				6 -0.065441000 -6.770193000 21.323391000				1 4.803116000 -5.878536000 19.084273000
1 6.331522000 -10.512677000 15.738240000				1 -0.484973000 -6.694677000 23.442994000				6 0.130071000 -7.758607000 15.030676000
1 4.197590000 -8.439301000 15.201174000				1 0.490267000 -8.980942000 23.834938000				6 3.350699000 -6.867973000 17.938106000
1 5.655659000 -8.192254000 16.174268000				1 1.415070000 -10.237144000 21.902764000				1 2.172911000 -10.002068000 18.841764000
1 4.066021000 -7.789813000 16.846477000				1 0.506017000 -7.180527000 19.278675000				1 0.594704000 -8.666932000 18.597880000
6 5.087438000 -9.997951000 18.196623000				1 -0.466207000 -5.788485000 21.095486000				
1 5.061583000 -11.013855000 18.600788000				6 5.618305000 -11.252409000 22.014091000				IV-MeOH
1 6.134870000 -9.675312000 18.188915000				6 5.339409000 -9.918012000 2				

6	0.509002000	-13.477486000	13.438651000	6	0.473816000	-14.675592000	21.332513000
6	-0.857907000	-13.792090000	13.698403000	6	0.947323000	-14.170766000	22.543694000
6	-1.510281000	-12.602975000	14.140248000	6	1.213349000	-12.805608000	22.664104000
6	-0.546318000	-11.551257000	14.150375000	6	1.015100000	-11.952333000	21.577673000
6	0.702788000	-12.091293000	13.716048000	6	0.530295000	-12.448354000	20.355268000
1	1.270024000	-14.173432000	13.112516000	1	-0.110455000	-14.237544000	19.318058000
1	-1.311237000	-14.769910000	13.609072000	1	0.268097000	-15.736519000	21.226379000
1	-2.544824000	-12.518368000	14.443032000	1	1.111137000	-14.835905000	23.386125000
1	-0.729718000	-10.534597000	14.465757000	1	1.583764000	-12.402270000	23.602016000
1	1.639003000	-11.557194000	13.631804000	1	1.244567000	-10.897654000	21.676414000
6	2.801430000	-12.339299000	17.089099000	6	-2.171145000	-10.889796000	20.430719000
1	3.516645000	-12.955103000	16.542392000	6	-3.496177000	-10.480657000	20.600667000
1	3.114426000	-12.289136000	18.137144000	6	-4.225963000	-9.987944000	19.518071000
6	0.267797000	-12.601230000	20.482175000	6	-3.622884000	-9.901584000	18.261206000
6	0.346818000	-12.884864000	21.849626000	6	-2.297426000	-10.303121000	18.089137000
6	0.112886000	-11.882305000	22.789447000	6	-1.557506000	-10.807610000	19.170925000
6	-0.198253000	-10.587733000	22.361289000	1	-1.623891000	-11.282224000	21.280599000
6	-0.266990000	-10.297579000	21.000350000	1	-3.958201000	-10.558066000	21.580306000
6	-0.037864000	-11.304462000	20.046389000	1	-5.258178000	-9.678376000	19.651048000
1	0.438587000	-13.395233000	19.763756000	1	-4.184560000	-9.522718000	17.412129000
1	0.586352000	-13.892950000	22.174380000	1	-1.842047000	-10.237897000	17.108762000
1	0.171156000	-12.105234000	23.850409000	6	4.724830000	-10.049798000	16.589374000
1	-0.383488000	-9.802995000	23.088577000	6	4.863381000	-8.531787000	16.403430000
1	-0.495564000	-9.286154000	20.678395000	6	5.247048000	-10.764679000	15.332855000
6	-2.908895000	-11.146707000	18.790383000	1	5.227168000	-11.853531000	15.427013000
6	-4.264816000	-10.921888000	18.544057000	1	4.681316000	-10.479407000	14.441169000
6	-4.659419000	-10.948411000	17.490868000	1	6.292957000	-10.479075000	15.174086000
6	-3.694222000	-9.094811000	16.683760000	1	4.363297000	-8.187774000	15.507534000
6	-2.337586000	-9.709016000	16.926054000	1	5.922886000	-8.281463000	16.282703000
6	-1.934118000	-10.545339000	17.977821000	1	4.485402000	-7.983942000	17.267761000
1	-2.614269000	-11.779337000	19.621455000	6	5.478657000	-10.521979000	17.838172000
1	-5.010481000	-11.388667000	19.180456000	1	5.387114000	-11.601392000	17.989563000
1	-5.714257000	-9.917639000	17.304413000	1	6.545535000	-10.299186000	17.719188000
1	-3.998113000	-8.838659000	15.868177000	1	5.122114000	-10.168800000	18.737936000
1	-1.588732000	-9.231488000	16.304672000	6	4.675075000	-5.883921000	20.577092000
6	4.746969000	-10.204074000	16.591327000	6	4.722301000	-7.173451000	21.105533000
6	4.937042000	-8.918028000	15.769419000	6	3.912489000	-8.162103000	20.554913000
6	5.606061000	-11.323760000	15.984023000	7	3.075880000	-7.934112000	19.518518000
1	5.580656000	-12.239639000	16.579581000	6	3.035795000	-6.683542000	19.015454000
1	5.300044000	-11.558067000	14.960230000	6	3.812431000	-5.639269000	19.510117000
1	6.649044000	-10.989996000	15.953757000	1	5.292702000	-5.091103000	20.987011000
1	4.760968000	-9.100034000	14.704999000	1	5.372765000	-7.419714000	21.937882000
1	5.969310000	-8.569525000	15.882223000	1	3.914677000	-9.171267000	20.946557000
1	4.272348000	-8.109758000	16.086526000	1	2.357948000	-6.520820000	18.187255000
6	5.106751000	-9.993406000	18.067150000	1	3.734463000	-4.655596000	19.059673000
1	4.969400000	-10.905250000	18.651151000	6	-1.216587000	-5.955643000	16.817633000
1	6.160599000	-9.704719000	18.149595000	6	-1.367244000	-6.338229000	18.149710000
1	4.500096000	-9.213050000	18.536149000	6	-0.572191000	-7.366929000	18.651400000
1	1.142411000	-9.025164000	14.912704000	7	0.348465000	-8.011343000	17.907215000
1	3.375673000	-7.510696000	17.981145000	6	0.483342000	-7.639364000	16.618271000
6	0.342496000	-7.219081000	15.129258000	6	-0.273086000	-6.624489000	16.036612000
1	-0.409576000	-6.806182000	15.802310000	1	-1.819956000	-5.157486000	16.396526000
1	1.270103000	-6.646361000	15.217035000	1	-2.089219000	-5.854318000	18.798619000
1	-0.030221000	-7.177171000	14.101627000	1	-0.663126000	-7.694864000	19.680321000
6	2.007592000	-6.127265000	18.323744000	1	1.226481000	-8.181199000	16.042244000
1	2.703301000	-5.296367000	18.177978000	1	-0.117937000	-6.368955000	14.993455000
1	1.044204000	-5.884548000	17.879501000	1	2.604274000	-10.515383000	19.696455000
1	1.874632000	-6.341270000	19.386771000	1	1.022614000	-9.222344000	20.271971000
8	0.539748000	-8.589956000	15.532208000				
8	2.502799000	-7.298827000	17.624376000				
1	0.198911000	-8.361193000	18.478635000				
1	1.815257000	-9.468280000	19.094830000				

IV-Py

E= -2518.12394505	Ha	
45	1.702213000	-9.540445000
26	-0.157804000	-12.353132000
15	0.213674000	-11.283565000
16	2.859610000	-10.349849000
6	0.211794000	-12.394564000
6	1.395561000	-12.760985000
6	1.078058000	-13.915432000
6	-0.285934000	-14.259844000
6	-0.827935000	-13.318175000
1	1.756719000	-14.417114000
1	-0.827073000	-15.064809000
1	-1.845525000	-13.293711000
6	0.080696000	-12.225047000
6	-1.280867000	-12.505078000
6	-1.776184000	-11.434616000
6	-0.719060000	-10.490768000
6	0.429509000	-10.979230000
1	0.740983000	-12.863110000
1	-1.830564000	-13.392153000
1	-2.770845000	-11.365830000
1	-0.773934000	-9.568611000
1	1.398470000	-10.502524000
6	2.779761000	-12.193128000
1	3.398034000	-12.607426000
1	3.219979000	-12.469147000
6	0.260179000	-13.822297000

V-MeCN

E= -2287.05708788	Ha	
45	1.673704000	-9.596244000
26	-0.096356000	-12.976640000
15	0.064942000	-11.179538000
16	3.015810000	-11.042324000
6	0.158182000	-12.681014000
6	1.355072000	-13.257763000
6	0.988763000	-14.512448000
6	-0.405815000	-14.721384000
6	-0.923519000	-13.597675000
1	1.662854000	-15.172814000
1	-0.980667000	-15.563985000
1	-1.956192000	-13.439154000
6	0.008676000	-13.246270000
6	-1.351273000	-13.110594000
6	-1.500291000	-11.836159000
6	-0.230457000	-11.183270000
6	0.700803000	-12.054132000
1	0.444068000	-14.113553000
1	-2.124643000	-13.858932000
1	-2.405960000	-11.444892000
1	-0.003725000	-10.210709000
1	1.752150000	-11.854765000
6	2.715107000	-12.778727000
1	3.403316000	-13.420892000
1	3.127638000	-12.845970000
6	0.460093000	-13.149738000
6	0.540443000	-13.588014000
6	0.298777000	-12.700303000
6	-0.020434000	-11.366503000
6	-0.092105000	-10.924649000

V-MeOH

E= -2252.98173546	Ha	
45	1.367640000	-9.351306000
26	3.942736000	-8.189203000
15	3.227903000	-10.317614000
16	2.171347000	-6.922872000
6	4.307835000	-9.240441000
6	4.528875000	-7.824703000
6	5.557353000	-7.421369000
6	5.969089000	-8.553368000
6	5.199894000	-9.671316000
1	5.934768000	-6.412337000
1	6.702058000	-8.552028000
1	5.252860000	-10.670045000
6	3.405285000	-6.733830000
6	3.753055000	-7.944504000
6	2.868422000	-8.969826000
6	1.971468000	-8.388856000
6	2.303043000	-7.008256000
1	3.908084000	-5.782331000
1	4.567665000	-8.069737000
1	2.889636000	-10.007676000
1	1.188894000	-8.907349000
1	1.821854000	-6.303715000
6	4.006414000	-6.927469000
1	4.298511000	-5.900662000
1	4.454877000	-7.203579000
6	5.530112000	-10.326382000
6	6.271098000	-10.755793000
6	5.778454000	-11.763020000
6	4.540428000	-12.351432000
6	3.795329000	-11.925018000
6	4.284894000	-10.904546000
1	5.931697000	-9.553789000
1	7.237523000	-10.305586000
1	6.357936000	-12.097368000
1	4.161129000	-13.150355000
1	2.846400000	-12.404920000
6	4.024386000	-12.768671000
6	3.876948000	-13.885934000
6	2.700813000	-14.068292000
6	1.669345000	-13.132807000
6	1.810878000	-12.016047000
6	2.992526000	-11.819232000
1	4.940636000	-12.645198000
1	4.679447000	-14.614312000

1	2.585923000	-14.939730000	13.653184000
1	0.748487000	-13.275295000	13.832940000
1	0.997529000	-11.305355000	15.305692000
6	1.982920000	-5.742418000	18.987778000
6	0.474792000	-5.698776000	19.273236000
6	2.467423000	-4.349294000	18.558098000
1	3.545099000	-4.318188000	18.376410000
1	1.950649000	-4.002215000	17.658835000
1	2.258528000	-3.637647000	19.364793000
1	-0.086111000	-5.332376000	18.407326000
1	0.291534000	-5.005078000	20.100791000
1	0.084166000	-6.678407000	19.557349000
6	2.750707000	-6.240460000	20.218106000
1	3.834005000	-6.206814000	20.069741000
1	2.526029000	-5.582506000	21.065700000
1	2.466731000	-7.261129000	20.480844000
1	2.592968000	-10.168201000	20.139218000
1	-1.129960000	-9.547218000	18.694290000
6	0.854220000	-9.877065000	21.041444000
1	0.092174000	-9.098321000	20.995911000
1	0.404971000	-10.849551000	20.810324000
1	1.282279000	-9.897735000	22.048024000
6	-1.582191000	-8.111360000	17.415938000
1	-2.530373000	-7.836373000	17.885814000
1	-1.071301000	-7.217052000	17.064630000
1	-1.750289000	-8.790331000	16.576296000
8	1.864776000	-9.528800000	20.077242000
8	-0.714477000	-8.224346000	18.403466000
1	0.811106000	-10.799886000	17.765545000
1	0.953254000	-9.317667000	16.321610000

V-Py

E=	-2518.12369046	Ha
45	0.657329000	0.998410000
26	-1.313061000	-1.057012000
15	-1.009247000	-0.564805000
16	1.954144000	0.138183000
6	-1.019406000	-1.562387000
6	0.123491000	-1.961472000
6	-0.343668000	-2.881076000
1	-1.747476000	-3.056254000
6	-2.169508000	-2.243573000
1	0.272556000	-3.339783000
1	-2.389107000	-3.660954000
1	-3.184699000	-2.130667000
6	-1.259033000	-0.548319000
6	-2.596458000	-0.470607000
6	-2.624451000	0.487391000
6	-1.302366000	1.004012000
6	-0.459760000	0.364712000
1	-0.908544000	-1.206227000
1	-3.433758000	-1.063439000
1	-3.486139000	0.752683000
1	-0.982804000	1.726323000
1	0.602955000	0.525513000
6	1.581218000	-1.660015000
1	2.125554000	-2.010226000
1	1.967563000	-2.202968000
6	-0.728625000	-3.194761000
6	-0.702043000	-4.129452000
6	-0.941420000	-3.725422000
6	-1.206446000	-2.379833000
6	-1.225650000	-1.444691000
6	-0.990773000	-1.843546000
1	-0.562710000	-3.526640000
1	-0.506691000	-5.174326000
1	-0.931192000	-4.453713000
1	-1.403768000	-2.060457000
1	-1.434950000	-0.402486000
6	-3.785450000	-0.716425000
6	-5.094527000	-0.232281000
6	-5.366234000	1.078253000
6	-4.321542000	1.905228000
6	-3.010926000	1.424536000
6	-2.727852000	0.106036000
1	-3.590283000	-1.733896000
1	-5.899404000	-0.879625000
1	-6.384262000	1.455089000
1	-4.523389000	2.929514000
1	-2.202763000	2.077217000
6	3.839411000	0.198458000
6	4.166281000	1.697188000
6	4.226537000	-0.486275000
1	4.112879000	-1.572986000
1	3.644146000	-0.099737000
1	5.284253000	-0.284696000
1	3.665302000	2.157625000
1	5.246734000	1.818818000
1	3.877150000	2.240785000
6	4.575412000	-0.450403000
1	4.344298000	-1.516801000

1	5.657628000	-0.365202000	-0.431813000
1	4.329965000	0.034791000	0.669315000
6	3.256870000	5.180610000	1.651944000
6	2.007687000	5.195088000	1.032564000
6	1.346150000	3.990661000	0.811531000
7	1.863248000	2.794902000	1.168567000
6	3.073533000	2.790029000	1.763981000
6	3.797467000	3.950250000	2.022910000
1	3.795181000	6.104057000	1.840445000
1	1.541080000	6.124035000	0.723255000
1	0.371963000	3.962524000	0.341134000
1	3.465808000	1.818022000	2.035647000
1	4.766654000	3.880281000	2.505037000
6	2.876356000	-1.183048000	4.895268000
6	2.206541000	0.036645000	4.992141000
6	1.648825000	0.591258000	3.843697000
7	1.732674000	0.008991000	2.630049000
6	2.375861000	-1.170313000	2.549203000
6	2.958924000	-1.798287000	3.647131000
1	3.319215000	-1.644845000	5.772172000
1	2.108332000	0.553414000	5.940903000
1	1.112494000	1.533169000	3.881082000
1	2.419377000	-1.620750000	1.564994000
1	3.462016000	-2.750587000	3.518666000
1	-0.148302000	1.758384000	-0.191548000
1	-0.325511000	1.626102000	1.886088000

b) M06 computed complexes and transition states

I-Py

E=	-2515.65847247	Ha
45	1.790483000	-9.364456000
26	0.206536000	-13.425921000
15	0.083265000	-10.882627000
16	2.508019000	-10.423690000
6	0.469435000	-12.549240000
6	1.731690000	-12.954033000
6	1.637719000	-14.364582000
6	0.403099000	-14.837269000
6	-0.345551000	-13.725944000
1	2.464623000	-14.958440000
1	0.044590000	-15.856862000
1	-1.361595000	-13.760370000
6	0.435393000	-14.078252000
6	-0.881031000	-11.022807000
6	-1.492485000	-13.119223000
6	-0.553956000	-12.077898000
6	0.637135000	-12.669898000
1	1.167548000	-14.814390000
1	-1.320678000	-15.340479000
1	-2.482322000	-12.992246000
1	-0.705348000	-11.608731000
1	1.548745000	-12.140266000
6	2.937708000	-12.122341000
1	3.527409000	-12.59854000
1	3.564899000	-12.028450000
6	0.245002000	-12.124591000
6	-0.075020000	-12.315819000
6	-1.130196000	-11.608731000
6	-1.863830000	-10.713279000
6	-1.548320000	-10.529376000
6	-0.491530000	-11.223431000
1	1.073262000	-12.677828000
1	0.494560000	-13.024003000
1	-1.384416000	-11.762647000
1	-2.692243000	-10.163574000
1	-2.131097000	-9.820932000
6	-2.625337000	-11.011727000
6	-3.711728000	-10.580534000
6	-3.595915000	-9.455965000
6	-2.395222000	-8.756155000
6	-1.307012000	-9.186448000
6	-1.409454000	-10.321644000
1	-2.729186000	-11.889092000
1	-4.653166000	-11.122669000
1	-4.446404000	-9.124611000
1	-2.303840000	-7.877389000
1	-0.352512000	-8.657210000
6	4.129521000	-9.888380000
6	3.940993000	-8.419721000
6	4.291282000	-10.694003000
1	4.388569000	-11.770930000
1	3.451280000	-10.527530000
1	5.208710000	-10.370832000
1	3.022348000	-8.258237000
1	4.786793000	-8.090029000
1	3.911452000	-7.789714000
6	5.318376000	-10.082924000
1	5.505037000	-11.139311000
1	6.22088000	-9.691815000

1	5.186494000	-9.542337000	17.495005000
6	4.930422000	-5.701216000	19.329743000
6	5.196033000	-6.988576000	19.782913000
6	4.339095000	-8.017042000	19.416855000
7	3.265854000	-7.823306000	18.633147000
6	3.011731000	-6.575925000	18.203581000
6	3.814793000	-5.491816000	18.526369000
1	5.581656000	-4.874062000	19.599072000
1	6.053665000	-7.200388000	20.414205000
1	4.501754000	-9.039953000	19.754792000
1	2.133994000	-6.463465000	17.568250000
1	3.566208000	-4.504369000	18.149603000
6	-0.006733000	-7.280788000	22.429398000
6	0.919049000	-8.313757000	22.515107000
6	1.394302000	-8.887233000	21.345183000
7	0.987639000	-8.488920000	20.128120000
6	0.088905000	-7.492238000	20.049306000
6	-0.427735000	-6.862711000	21.172062000
1	-0.398239000	-6.812097000	23.328314000
1	1.271441000	-8.681775000	23.478882000
1	2.109537000	-9.707123000	21.365671000
1	-0.224531000	-7.210664000	19.045395000
1	-1.152644000	-6.063113000	21.053786000

II-Py

E=	-2516.82106107	Ha	
45	1.699339000	-9.593173000	19.009991000
26	0.081598000	-12.749521000	15.511049000
15	0.001616000	-11.410444000	18.930842000
16	2.460540000	-10.230479000	16.895586000
6	0.247066000	-12.597723000	17.566941000
6	1.521937000	-12.843541000	16.941402000
6	1.427637000	-14.079008000	16.231008000
6	0.108401000	-14.588123000	16.385157000
6	-0.621460000	-13.675655000	17.190816000
1	2.217910000	-14.515821000	15.628969000
1	-0.286820000	-15.482203000	15.917142000
1	-1.668048000	-13.761991000	17.463155000
6	0.509675000	-12.796948000	13.520908000
6	-0.851742000	-13.150608000	13.745750000
6	-1.491204000	-12.055068000	14.390928000
6	-0.521639000	-11.024935000	14.563788000
6	0.715148000	-11.484361000	13.030759000
1	1.266849000	-13.437672000	14.083867000
1	-1.309013000	-14.103737000	13.507379000
1	-2.528063000	-12.025592000	14.708097000
1	-0.687189000	-10.053838000	15.108069000
1	1.651767000	-10.937957000	14.042893000
6	2.776260000	-12.038913000	17.018436000
1	3.419322000	-12.312528000	16.171382000
1	3.323233000	-12.220030000	17.952073000
6	-0.937588000	-13.491788000	20.600574000
6	-0.843428000	-14.389936000	21.655411000
6	0.266729000	-14.365761000	22.497432000
6	1.280349000	-13.441213000	22.279526000
6	1.185671000	-12.538224000	21.222710000
6	0.076165000	-12.551530000	20.734343000
1	-1.811281000	-13.519557000	19.951571000
1	-1.637098000	-15.114699000	21.819513000
1	0.339542000	-15.071695000	23.321000000
1	2.151589000	-13.421981000	22.929846000
1	1.983785000	-11.820341000	21.043994000
6	-2.448544000	-10.631640000	20.055437000
6	-3.749622000	-10.141874000	20.013992000
6	-4.399659000	-9.977153000	18.792950000
6	-3.744979000	-10.316716000	17.613470000
6	-2.443062000	-10.806562000	17.653620000
6	-1.775806000	-10.963806000	18.872064000
1	-1.959596000	-10.777699000	21.018290000
1	-4.263983000	-9.899575000	20.941273000
1	-5.418231000	-9.598710000	18.764131000
1	-4.251485000	-10.210503000	16.656063000
1	-1.935491000	-11.090358000	16.734421000
6	4.175670000	-9.556486000	16.945970000
6	4.020432000	-8.042131000	16.505782000
6	4.521404000	-10.018499000	15.084621000
1	4.615250000	-11.107120000	14.998311000
1	3.782701000	-9.667764000	14.353827000
1	5.493459000	-9.592854000	14.804878000
1	3.229035000	-7.712029000	15.819378000
1	4.963247000	-7.590584000	16.172046000
1	3.796956000	-7.664188000	17.509276000
6	5.216491000	-10.013236000	17.501268000
1	3.579414000	-11.096784000	17.466413000
1	6.174327000	-9.533074000	17.260955000
1	4.938559000	-9.730258000	18.522487000
1	0.335890000	-8.217049000	23.505061000
6	1.637319000	-8.638284000	23.528845000
6	1.996167000	-9.001407000	21.970515000
7	1.130313000	-8.965072000	20.940601000
6	-0.121727000	-8.539921000	21.180204000

1	-0.557469000	-8.166464000	22.442023000	1	0.526158000	-7.139251000	19.198969000	6	-0.662764000	-7.532968000	18.752811000
1	0.025098000	-7.931814000	24.506513000	1	-0.637040000	-5.843230000	20.972884000	7	0.310676000	-8.086760000	18.012134000
1	2.375751000	-8.689228000	24.052972000	6	5.544613000	-11.304521000	21.945283000	6	0.403756000	-7.721135000	16.723900000
1	3.002126000	-9.334614000	21.733228000	6	5.277595000	-9.964475000	21.686015000	6	-0.464730000	-6.815458000	16.130084000
1	-0.793649000	-8.514535000	20.324863000	6	4.231474000	-9.643404000	20.832486000	1	-2.168921000	-5.536339000	16.471478000
1	-1.585672000	-7.840808000	22.575982000	7	3.460354000	-10.569906000	20.327961000	1	-2.337902000	-6.201559000	18.888178000
6	-0.797288000	-5.785407000	16.836828000	6	3.725277000	-11.859263000	20.497811000	1	-0.7175237000	-7.855694000	19.790950000
6	0.155247000	-5.547575000	17.822285000	6	4.749375000	-12.270039000	21.340183000	1	1.205316000	-8.186721000	16.147937000
6	0.783375000	-6.629435000	18.422904000	1	6.357788000	-11.589689000	22.607462000	1	-0.347336000	-6.563613000	15.079933000
7	0.509845000	-7.902102000	18.094173000	1	5.869846000	-9.172701000	22.134878000	1	2.618738000	-10.583068000	19.756095000
6	-0.407108000	-8.120466000	17.143215000	1	3.992884000	-8.606532000	20.60651000	1	1.065171000	-9.296388000	20.381204000
6	-1.085466000	-7.100277000	16.491353000	1	3.083622000	-12.593324000	20.014140000				
1	-1.305379000	-4.958735000	16.347390000	1	4.910164000	-13.330186000	21.513435000	V-Py			
1	0.414962000	-4.537129000	18.123457000	1	0.821712000	-9.134347000	17.870478000	E=	-2516.83380293	Ha	
1	1.539694000	-6.489786000	19.193918000	1	2.665592000	-8.511764000	18.566350000	45	0.655176000	1.011813000	0.861044000
1	-0.601774000	-9.164376000	16.911100000					26	-1.319816000	-1.044784000	-2.766500000
1	-1.825352000	-7.343044000	15.733254000	IV-Py				15	-0.991788000	-0.538314000	0.673070000
1	2.705515000	-10.598327000	19.630591000	E=	-2516.83220866	Ha		16	1.879060000	0.224844000	-1.265518000
1	2.937482000	-8.625922000	19.173707000	45	1.715999000	-9.580135000	18.989384000	6	-1.002252000	-1.541669000	-0.831283000
				26	-0.052156000	-12.366930000	15.492128000	6	0.127265000	-1.917953000	-1.645188000
III-Py				15	0.227938000	-11.294046000	18.971537000	6	-0.347933000	-2.829170000	-2.639205000
E = -2516.82484859	Ha			16	2.791661000	-10.335366000	16.799619000	6	-1.744269000	-3.019538000	-2.454811000
45	1.829059000	-9.825042000	18.821775000	6	0.237351000	-12.388971000	17.529701000	6	-2.153449000	-2.228396000	-1.350247000
26	-0.311034000	-12.431113000	15.646871000	6	1.435275000	-12.770476000	16.831092000	1	0.260254000	-3.260666000	-3.427804000
15	0.231851000	-11.729765000	19.006837000	6	1.131636000	-13.922565000	16.045644000	1	-2.394679000	-3.612839000	-3.086806000
16	2.701649000	-10.576992000	16.774420000	6	-0.240717000	-14.250129000	16.235806000	1	-3.167964000	-2.116863000	-0.983593000
6	0.229191000	-12.815766000	17.557819000	6	-0.799215000	-13.300983000	17.134322000	6	-1.241758000	-0.503706000	-4.732015000
6	3.149048000	-13.010570000	16.670768000	1	1.824171000	-14.423183000	15.376784000	6	-2.585817000	-0.481807000	-4.259679000
6	0.977224000	-14.011966000	15.722325000	1	-0.780061000	-15.043601000	15.731610000	6	-2.658068000	0.438358000	-3.174857000
6	-0.347499000	-14.440203000	16.012282000	1	-1.830384000	-13.261695000	17.407499000	6	-1.356847000	0.987635000	-2.981495000
6	-0.812114000	-13.708433000	17.137322000	6	0.264567000	-12.266675000	13.481497000	6	-0.482008000	0.046769000	-3.941942000
1	1.596413000	-14.352772000	14.898831000	6	-1.110419000	-12.514283000	13.758994000	1	-0.856885000	-1.135462000	-5.523948000
1	-0.925180000	-15.153534000	15.436177000	6	-1.604046000	-11.434915000	14.544279000	1	-3.397902000	-1.098267000	-4.626969000
1	-1.804247000	-13.769644000	17.571089000	6	-0.531526000	-10.518797000	14.747677000	1	-3.535154000	0.651946000	-2.573034000
6	-0.626208000	-11.995963000	13.676171000	6	0.623664000	-11.032141000	14.092151000	1	-1.069426000	1.694026000	-2.209490000
6	-1.864467000	-12.103338000	14.371930000	1	0.930499000	-12.927082000	12.938527000	1	0.584081000	0.588052000	-4.020121000
6	-1.868558000	-11.138776000	15.420045000	1	-1.669393000	-13.395738000	13.467178000	6	1.571307000	-1.567413000	-1.506002000
6	-0.631051000	-10.430272000	15.367124000	1	-2.608832000	-11.346984000	14.943327000	1	2.075089000	-1.855796000	-2.435307000
6	0.135494000	-10.962310000	14.290177000	1	-0.580807000	-9.598167000	15.318326000	1	2.039445000	-2.128589000	-0.682876000
1	-0.304083000	-12.622767000	12.852956000	1	1.610233000	-10.581534000	14.098009000	6	-0.642704000	-3.149140000	1.719051000
1	-2.642313000	-12.831803000	14.174983000	6	2.794985000	-12.169054000	16.953767000	6	-0.534774000	-4.068345000	2.761675000
1	-2.649742000	-11.002825000	16.161375000	1	3.341042000	-12.565620000	16.153648000	6	-0.706542000	-3.654799000	4.077780000
1	-0.303209000	-9.656168000	16.051239000	1	3.247046000	-12.424319000	17.921872000	6	-0.995872000	-2.319046000	4.355021000
1	1.139716000	-10.657735000	14.016023000	6	0.248241000	-13.846752000	20.200486000	6	-1.103598000	-1.400963000	3.318969000
6	2.712773000	-12.413119000	16.761788000	6	0.412035000	-14.716547000	21.275046000	6	-0.922790000	-1.807814000	1.991794000
1	3.296053000	-12.718535000	15.884937000	6	0.782536000	-14.228778000	22.522644000	1	-0.518945000	-3.483543000	0.689539000
1	3.241216000	-12.762438000	17.659977000	6	1.000006000	-12.864600000	22.693404000	1	-0.324990000	-5.111982000	2.539704000
6	1.126347000	-14.174588000	20.04831000	6	0.854875000	-11.994994000	21.618771000	1	-0.626711000	-4.374319000	4.888978000
6	1.462557000	-15.028068000	21.152886000	6	0.466796000	-12.474214000	20.361119000	1	-1.141614000	-1.994148000	5.382775000
6	1.148582000	-14.684441000	22.463790000	1	-0.400763000	-14.249833000	19.233271000	1	-1.330315000	-0.356799000	3.537913000
6	0.475955000	-13.492643000	22.722354000	1	0.249009000	-15.781752000	21.131246000	6	-3.743968000	-0.755250000	1.191193000
6	0.143525000	-12.437333000	21.677465000	1	0.908525000	-14.910847000	23.359632000	6	-5.060982000	-0.308439000	1.189735000
6	0.478850000	-12.959142000	20.355839000	1	1.297537000	-12.475429000	23.664086000	6	-5.358318000	0.988166000	0.780338000
1	1.365416000	-14.461948000	19.080942000	1	1.057539000	-10.933620000	21.751102000	6	-4.333863000	1.840994000	0.382155000
1	1.959334000	-15.971904000	20.940403000	6	-2.126822000	-10.641536000	20.374920000	6	-3.015382000	1.096040000	0.385171000
1	1.407420000	-15.352703000	23.281100000	6	-3.402048000	-10.092903000	20.483535000	6	-2.708091000	0.392032000	0.777881000
1	0.198024000	-13.234804000	23.741669000	6	-4.071427000	-9.641162000	19.349703000	1	-3.522313000	-1.769695000	1.520530000
1	-0.102900000	-11.723199000	21.890518000	6	-3.462092000	-9.739469000	18.101394000	1	-5.856070000	-0.974917000	1.514573000
6	-2.495308000	-12.154167000	19.641529000	6	-2.184408000	-10.726321000	17.991738000	1	-6.388069000	1.336500000	0.782309000
6	-3.832851000	-11.779125000	19.704854000	6	-1.507965000	-10.736739000	19.125785000	1	-4.559279000	2.859604000	0.075917000
6	-4.216539000	-10.490265000	19.342133000	1	-1.616022000	-11.000464000	21.267084000	1	-2.214223000	2.069752000	0.085902000
6	-3.158071000	-9.573406000	18.922645000	1	-3.877581000	-10.028333000	21.459150000	6	3.753783000	0.304508000	-1.372742000
6	-1.291280000	-9.948991000	18.855968000	1	-5.069837000	-9.220116000	19.439101000	6	0.062968000	1.791593000	-1.505947000
6	-1.525075000	-11.244201000	19.203796000	1	-3.978735000	-9.391398000	17.209103000	6	4.223263000	-0.416129000	-2.630439000
1	-2.204727000	-13.160427000	19.941084000	1	-1.702644000	-10.345144000	17.019284000	1	1.455279000	-1.505847000	-2.548801000
1	-4.578218000	-12.495220000	20.042183000	6	4.623034000	-9.981440000	16.570809000	1	6.682144000	-0.086108000	-3.517676000
1	-5.263108000	-10.200477000	19.392546000	6	4.727143000	-8.463364000	16.518377000	1	5.283759000	-0.184004000	-2.793874000
1	-3.551437000	-8.564196000	18.643600000	6	5.061798000	-10.563574000	15.232437000	1	3.607532000	2.212118000	-2.410290000
1	-1.166250000	-9.237721000	18.520195000	1	5.001848000	-11.657040000	15.201771000	1	5.149828000	1.925501000	-1.580415000
6	4.531186000	-10.198114000	16.468507000	1	4.467393000	-10.157953000	14.405105000	1	3.713400000	2.366517000	-0.642303000
6	4.701406000	-8.699995000	16.667245000	1	6.112527000	-10.298613000	15.055156000	6	4.411690000	-0.285072000	-0.136967000
6	4.786334000	-10.547229000	15.005593000	1	4.065411000	-8.038062000	15.751935000	1	4.205554000	-1.358074000	-0.037071000
1	4.644076000	-11.612068000	14.788542000	1	5.756286000	-8.83983000	16.259423000	1	5.051708000	-0.170471000	-0.210924000
1	4.139252000	-9.966382000	14.338132000	1	4.488057000	-8.008901000	17.484314000	1	4.075839000	0.217895000	0.777333000
1	5.828681000	-10.307314000	14.759308000	6	5.452523000	-10.543583000	17.713268000				

1	2.905889000	-1.945606000	5.745875000	1	-1.647684000	5.756679000	1.383358000	C			
1	2.023282000	0.399529000	5.918711000	1	0.162901000	1.071835000	2.452735000	E= -2516.81506285 Ha			
1	1.250832000	1.541469000	3.848424000	1	1.312854000	-0.261771000	1.521617000	45	1.649884000	-9.699086000	19.169522000
1	2.218595000	-1.717424000	1.509800000					26	-0.113983000	-12.202621000	15.544885000
1	2.988497000	-3.020579000	3.478285000	B				15	0.124866000	-11.424820000	19.029349000
1	-0.208298000	1.774296000	-0.178934000	E= -2516.81409565 Ha				16	3.715218000	-12.445975000	15.547585000
1	-0.315405000	1.644577000	1.900513000	45	0.310410000	1.035959000	0.841930000	6	0.122246000	-12.462374000	17.545317000
				26	-1.687631000	-0.741146000	-2.605732000	6	1.307904000	-12.877734000	16.829968000
A				15	-1.278621000	-0.567750000	0.820647000	6	0.924126000	-13.917130000	15.935287000
E= -2516.81041082 Ha				16	2.028092000	-0.109374000	-2.954945000	6	-0.474450000	-14.143412000	16.069547000
45	0.489421000	0.936310000	0.964531000	6	-1.181497000	-1.415080000	-0.775783000	6	-0.974647000	-13.256073000	17.058594000
26	-1.669908000	-1.331485000	-2.580911000	6	-0.034342000	-1.424746000	-1.655921000	1	1.584519000	-14.400696000	15.222764000
15	-1.127948000	-0.654155000	0.851619000	6	-0.348985000	-2.276905000	-2.756926000	1	-1.065832000	-14.833306000	15.478857000
16	1.655830000	0.610954000	-3.216250000	6	-1.664642000	-2.785585000	-2.575646000	1	-2.005365000	-13.178417000	17.387288000
6	-0.872872000	-1.536621000	-0.720552000	6	-2.183657000	-2.260627000	-1.362535000	6	0.477970000	-11.742677000	13.654579000
6	0.155441000	-1.218392000	-1.687024000	1	0.296205000	-2.447614000	-3.611894000	6	-0.909080000	-12.065809000	13.673608000
6	0.149586000	-2.242399000	-2.675979000	1	-2.203618000	-3.413436000	-3.275462000	6	-1.563506000	-11.154630000	14.550403000
6	-0.856971000	-3.190097000	-2.340561000	1	-3.181237000	-2.425931000	-0.970662000	6	-0.578457000	-10.266828000	15.071537000
6	-1.487672000	-2.763770000	-1.142515000	6	-1.600456000	0.229926000	-4.392453000	6	0.685047000	-10.632069000	14.521940000
1	0.769928000	-2.248988000	-3.565480000	2	-9.065610000	-0.297132000	-4.171278000	1	1.254304000	-12.282518000	13.124744000
1	-1.133451000	-4.057634000	-2.928373000	6	-3.417117000	0.276277000	-2.970185000	1	-1.377679000	-12.890581000	13.149839000
1	-2.288271000	-3.285308000	-0.628652000	6	-2.427536000	1.160442000	-2.455027000	1	-2.618955000	-11.159712000	14.800374000
6	-1.960703000	-0.653358000	-4.479025000	6	-1.304784000	1.131825000	-3.329687000	1	-0.754221000	-9.475968000	15.792828000
2	-9.54338000	-1.613106000	-4.134765000	1	-0.929435000	-0.043151000	-5.198954000	1	1.649139000	-10.187631000	14.749390000
6	-3.660665000	-1.128350000	-2.996792000	1	-3.402915000	-1.041389000	-4.782955000	6	2.686813000	-12.355326000	17.056508000
6	-3.106121000	0.132912000	-2.638098000	1	-4.367596000	0.046771000	-2.499823000	1	3.169207000	-12.932281000	17.861509000
6	-2.054489000	0.427451000	-3.556457000	1	-2.503093000	1.724396000	-1.532839000	1	2.622746000	-11.306818000	17.390444000
1	-1.224537000	-0.748484000	-5.268975000	1	-0.367841000	1.661194000	-3.191377000	6	0.274507000	-14.029844000	20.139805000
1	-3.111488000	-2.568061000	-4.622277000	6	1.286073000	-0.764143000	-1.426167000	6	0.466279000	-14.933743000	21.182074000
1	-4.458950000	-1.642835000	-2.474140000	1	1.993039000	-1.473188000	-0.970083000	6	0.749627000	-14.478445000	22.464639000
1	-3.417069000	0.734244000	-1.787845000	1	1.193403000	0.099114000	-0.728676000	6	0.851174000	-13.111359000	22.707600000
1	-1.416817000	1.306213000	-3.562444000	6	-0.562842000	-3.156838000	-1.658510000	6	0.673316000	-12.207153000	21.667443000
6	1.111704000	-0.070642000	-1.609399000	6	-0.261807000	-4.125263000	2.624317000	6	0.373922000	-12.654945000	20.373398000
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6	-0.026182000	-2.956203000	1.990226000	6	-1.195857000	-1.618830000	3.398848000	1	0.897469000	-15.188597000	23.274138000
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6	-1.867872000	-1.981167000	3.213877000	1	-0.260975000	-4.602548000	4.722099000	6	-3.361960000	-10.049437000	20.704937000
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6	-5.504392000	0.810005000	1.127987000	1	-3.673763000	-2.148125000	1.363851000	1	-2.011366000	-10.689032000	17.138035000
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1	-6.530199000	1.164860000	1.186456000	6	4.512767000	0.506814000	-3.731575000	1	6.630589000	-11.106032000	17.530052000
1	-4.675272000	2.554040000	2.084485000	6	4.259359000	-1.676389000	-2.538318000	1	6.505278000	-12.539108000	14.837130000
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1	5.281361000	0.740750000	-2.164269000	6	1.736530000	3.236600000	-0.715319000	1	5.574368000	-5.213721000	20.049312000
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6	4.609970000	3.645423000	1.140669000	6	2.783916000	2.878865000	1.306433000	1	4.691569000	-9.280166000	18.964522000
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7	2.243302000	2.178890000	1.089863000	1	2.606531000	4.660892000	-2.057421000	6	-0.709901000	-6.366220000	16.529160000

15	-1.073300000	-0.671985000	0.727831000	6	0.534063000	-13.366333000	15.569536000	1	-1.127347000	-4.061833000	-2.932996000
16	1.913879000	-0.194901000	-2.977272000	6	-0.875341000	-13.177787000	15.593838000	1	-2.280130000	-3.293925000	-0.631004000
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6	-2.391649000	1.235885000	-2.382414000	1	-2.025210000	-9.592914000	15.072216000	1	2.011356000	-0.350505000	-1.024049000
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1	-6.457693000	0.821463000	1.877361000	6	6.343357000	-12.112718000	15.628360000	1	4.793932000	-1.479347000	-3.206535000
1	-4.743946000	2.557713000	1.423339000	6	5.423087000	-14.260114000	16.502519000	1	3.432825000	0.229050000	-5.420635000
1	-2.389333000	1.889778000	0.982948000	1	4.710644000	-14.754313000	17.173672000	1	5.019472000	0.574671000	-4.708149000
6	3.750114000	-0.520164000	0.916487000	1	5.245742000	-14.619596000	15.482886000	1	3.759187000	1.823067000	-4.701363000
6	4.356358000	0.578104000	-3.781881000	1	6.428214000	-14.580977000	16.808511000	6	4.207142000	0.971458000	-2.128787000
6	4.055349000	-1.883921000	-3.521413000	1	6.178454000	-12.435058000	14.593161000	1	3.856719000	0.684135000	-1.127076000
1	3.593291000	-2.702580000	-2.956086000	1	7.356493000	-12.419101000	15.918872000	1	5.281307000	0.745245000	-2.175021000
1	3.702080000	-1.942902000	-4.556625000	1	6.297610000	-11.017475000	15.661917000	1	4.081360000	2.054946000	-2.239462000
1	5.140030000	-2.059044000	-3.518169000	6	5.561778000	-12.249131000	17.996971000	6	4.613123000	3.641640000	1.137402000
1	3.944026000	0.562343000	-4.798071000	1	4.847989000	-12.679198000	18.711969000	6	4.360301000	2.671739000	2.101221000
1	5.441239000	0.430016000	-3.858712000	1	6.566580000	-12.545485000	18.823623000	6	3.170377000	1.962458000	2.044358000
1	4.179491000	1.573187000	-3.354095000	1	5.496031000	-11.155445000	18.051985000	7	2.247349000	2.173585000	1.088371000
6	4.286543000	-0.426087000	-1.494455000	6	4.021086000	-5.079662000	18.698972000	6	2.498939000	3.110033000	0.157388000
1	3.881095000	-1.213622000	-0.847238000	6	3.548633000	-5.683515000	17.539068000	6	3.662740000	3.864578000	0.148640000
1	5.378316000	-0.548145000	-1.509058000	6	2.835510000	-6.868288000	17.644762000	1	5.536038000	4.214949000	1.157391000
1	4.061842000	0.547112000	-1.038777000	7	2.577314000	-7.452878000	18.827165000	1	5.072973000	2.462124000	2.892843000
6	3.884342000	4.576351000	0.430763000	6	3.032379000	-6.864237000	19.945412000	1	2.930934000	1.195965000	2.776054000
6	3.526755000	3.809960000	-0.672427000	6	3.758648000	-5.682627000	19.923825000	1	1.735167000	3.249272000	-0.6707034000
6	2.551090000	2.835315000	-0.526323000	1	4.586818000	-4.153227000	18.649269000	1	3.814778000	4.608652000	-0.627617000
7	1.940314000	2.591164000	0.648468000	1	3.729242000	-5.249529000	16.560422000	6	-2.352240000	4.843610000	-0.447246000
6	2.292259000	3.333995000	1.710652000	1	2.452210000	-7.378328000	16.763172000	6	-2.252663000	3.720511000	-1.259615000
6	3.252497000	4.332818000	1.644308000	1	2.799052000	-7.370878000	20.880260000	6	-1.416221000	2.687398000	-0.862758000
1	4.641095000	5.351485000	0.345336000	1	4.109510000	-5.248594000	20.855073000	7	-0.693519000	2.720518000	0.269552000
1	3.989212000	3.962910000	-1.643355000	6	-2.007691000	-6.673981000	21.219292000	6	-0.786329000	3.813432000	1.040854000
1	2.245695000	2.210991000	-1.368586000	6	-1.382018000	-7.728829000	21.872839000	6	-1.603243000	4.889800000	0.724390000
1	1.780760000	3.112903000	2.645414000	6	-0.406343000	-8.449900000	21.200955000	1	-3.001411000	5.670926000	-0.721119000
1	3.495181000	4.906487000	2.533526000	7	-0.034052000	-8.161789000	19.941691000	1	-2.815125000	3.630472000	-2.185155000
6	2.049275000	-0.022327000	5.207724000	6	-0.626580000	-7.125926000	19.321559000	1	-1.337110000	1.778517000	-1.457685000
6	0.912697000	0.761783000	5.039545000	6	-1.618720000	-6.366042000	19.920690000	1	-0.188562000	3.807091000	1.951431000
6	0.459028000	1.014378000	3.754289000	1	-2.784232000	-6.098620000	21.715910000	1	-1.647576000	5.747226000	1.389167000
7	1.088858000	0.542049000	2.663320000	1	-1.647099000	-8.003856000	22.889076000	1	0.169743000	1.062871000	2.452555000
6	2.186250000	-0.214919000	2.827276000	1							

6	-3.354718000	0.468775000	-3.090062000	1	-3.561104000	-0.879020000	-4.726547000	6	1.103477000	-0.836058000	-2.157819000
6	-2.350473000	1.291090000	-2.506376000	1	-4.408187000	0.176390000	-2.382144000	1	0.775783000	0.183780000	-2.388884000
6	-1.186974000	1.223489000	-3.324172000	1	-2.495155000	1.814719000	-1.469202000	1	1.768832000	-1.183071000	-2.956501000
1	-0.775064000	0.064979000	-5.195995000	1	-0.415049000	1.741788000	-3.220987000	6	-0.328556000	-2.905978000	1.707343000
1	-3.312462000	-0.812986000	-4.927077000	6	1.330576000	-1.097693000	-1.629967000	6	-0.008237000	-3.613484000	2.861608000
1	-4.339383000	0.279628000	-2.677133000	1	1.976934000	-1.985372000	-1.585625000	6	-0.269015000	-3.064878000	4.114598000
1	-2.449518000	1.847689000	-1.582203000	1	1.438243000	-0.552621000	-0.677351000	6	-0.853273000	-1.804660000	4.219021000
1	-0.240820000	1.719137000	-3.133876000	6	0.513299000	-3.037856000	1.483910000	6	-1.175772000	-1.090254000	3.705250000
6	1.277953000	-1.056377000	-1.462443000	6	0.604575000	-3.993178000	2.391744000	6	-0.924238000	-1.642729000	1.804429000
1	1.908286000	-1.922635000	-1.209336000	6	0.274687000	-3.886232000	3.738917000	1	-0.125046000	-3.339061000	0.728845000
1	1.298483000	-0.364743000	-0.598255000	6	-0.517153000	-2.826688000	4.177139000	1	0.442487000	-4.599369000	2.780734000
6	-0.392065000	-3.109499000	1.540542000	6	-0.970807000	-1.873586000	3.272523000	1	-0.020538000	-3.624167000	5.013063000
6	-0.025998000	-4.072069000	2.480660000	6	-0.634557000	-1.968384000	1.917209000	1	-1.064059000	-1.379193000	5.196976000
6	-0.156196000	-3.806480000	3.838774000	1	0.402500000	-3.136258000	0.427607000	1	-1.641457000	-0.108169000	3.153307000
6	-0.660372000	-2.577306000	4.263441000	1	1.205907000	-4.828739000	2.041980000	6	-3.956123000	-0.899044000	5.151420000
6	-1.020813000	-1.614461000	3.329664000	1	0.623810000	-4.634018000	4.446531000	6	-5.277261000	-0.465588000	0.816002000
6	-0.889123000	-1.873539000	1.959766000	1	-0.790979000	-2.747596000	5.226830000	6	-5.583178000	0.840760000	0.440625000
1	-0.300979000	-3.327950000	0.476873000	1	-1.600130000	-1.054664000	3.621772000	6	-4.567181000	1.720404000	0.078843000
1	0.351378000	-5.035324000	2.145941000	6	-3.752556000	-1.263271000	1.430163000	6	-3.243670000	1.291303000	0.080405000
1	0.123060000	-4.560854000	4.570160000	6	-5.086005000	-0.950339000	1.665990000	6	-2.933434000	-0.024076000	0.431675000
1	-0.773234000	-2.370874000	5.325334000	6	-5.505061000	0.378531000	1.649377000	1	-3.718508000	-1.914947000	1.129972000
1	-1.412707000	-0.652203000	3.663176000	6	-4.587344000	1.396764000	1.412606000	1	-6.069247000	-1.145846000	1.118790000
6	-3.911781000	-1.218150000	1.412945000	6	-3.250813000	1.085933000	1.177449000	1	-6.616875000	1.176900000	0.444372000
6	-5.272888000	-0.974742000	1.556614000	6	-2.827004000	-0.246227000	1.167050000	1	-4.804319000	2.744990000	-0.195805000
6	-5.777290000	0.308567000	1.363787000	1	-3.426374000	-2.302572000	1.459941000	1	-2.442676000	1.981951000	-0.180292000
6	-4.916561000	1.351584000	1.038334000	1	-5.800738000	-1.744438000	1.867126000	6	3.685826000	0.014657000	-1.179666000
6	-3.553621000	1.110549000	0.896918000	1	-6.548778000	0.619948000	1.834542000	6	4.511456000	0.234840000	0.080855000
6	-3.039767000	-0.176865000	1.069941000	1	-4.910062000	2.434919000	1.415744000	6	3.432955000	1.325186000	-1.905985000
1	-3.524433000	-2.224463000	1.568976000	1	-2.519978000	1.787341000	1.007248000	1	2.865783000	1.183529000	-2.833400000
1	-5.940735000	-1.790132000	1.822797000	6	3.718759000	-0.577852000	-3.142437000	1	2.892980000	2.039938000	-1.273806000
1	-6.841894000	0.496725000	1.477512000	6	4.323849000	0.410294000	-4.131982000	1	4.396783000	1.774535000	-2.180531000
1	-5.304604000	2.357627000	0.900577000	6	3.788544000	-1.991539000	-3.703261000	1	4.079387000	1.008278000	0.723923000
1	-2.885306000	1.935303000	0.654853000	1	3.319721000	-2.727353000	-3.037523000	1	5.517952000	0.563574000	-0.207369000
6	3.831575000	-0.586629000	-2.678458000	1	3.294475000	-2.051859000	-4.679350000	1	4.618049000	-0.690333000	0.660821000
6	4.513274000	0.316627000	-3.714987000	1	4.837913000	-2.291415000	-3.829547000	6	4.393684000	-0.988946000	-2.080665000
6	4.121219000	-2.033746000	-2.972490000	1	3.799211000	0.388292000	-5.094620000	1	3.844967000	-1.190743000	-3.007163000
1	3.597878000	-2.708879000	-2.283760000	1	5.374593000	0.152077000	-4.316543000	1	5.369480000	-0.578624000	-2.371958000
1	3.826155000	-2.295554000	-3.994434000	1	4.288059000	1.436402000	-3.743640000	1	4.565281000	-1.939704000	-1.564150000
1	5.196929000	-2.229699000	-2.864766000	6	4.445388000	-0.485755000	-1.807085000	6	3.743130000	3.698556000	3.001510000
1	4.157928000	0.095083000	-4.728541000	1	4.017804000	-1.155261000	-1.050493000	6	3.157425000	4.145927000	1.822948000
1	5.596550000	0.141690000	-3.693527000	1	5.496102000	-0.777452000	-1.941484000	6	2.265830000	3.315048000	1.160027000
1	4.336370000	1.380590000	-3.513159000	1	4.431942000	0.537132000	-1.410505000	7	1.960879000	2.087341000	1.606807000
6	4.300073000	-0.190746000	-1.279894000	6	4.023937000	4.460538000	0.786290000	6	2.519079000	1.663136000	2.753237000
1	3.840307000	-0.818775000	-0.506178000	6	3.879184000	3.537847000	-0.243822000	6	3.411953000	2.434661000	3.479308000
1	5.386978000	-0.332656000	-1.206232000	6	2.815257000	2.649419000	-0.205062000	1	4.442747000	4.327940000	3.544564000
1	4.081126000	0.859553000	-1.047981000	7	1.922201000	2.638754000	0.801397000	1	3.377649000	5.129665000	1.420040000
6	3.554631000	4.762834000	0.171412000	6	2.064818000	3.531074000	1.793290000	1	1.770478000	3.628672000	0.244071000
6	3.204626000	3.897127000	-0.858222000	6	3.096691000	4.458203000	1.821983000	1	2.236957000	0.662234000	3.084741000
6	2.274502000	2.898064000	-0.610582000	1	4.844223000	5.173203000	0.780337000	1	3.837263000	2.046887000	4.399717000
7	1.704086000	2.729841000	0.595877000	1	4.573153000	3.504479000	-1.079264000	1	-0.551523000	1.681216000	1.427955000
6	2.043632000	3.568985000	1.586177000	1	2.650938000	1.923095000	-1.005047000	1	0.100543000	1.756579000	-0.386555000
6	2.961369000	4.594874000	1.417044000	1	1.319349000	3.490461000	2.584980000	[[P,(StBu)Rh(η ² -H ₂)(py)] ⁺ E= -2268.70780656 Ha			
1	4.276375000	5.558098000	0.005598000	1	3.165524000	5.163712000	2.644191000				
1	3.636835000	3.992178000	-1.850039000	6	2.012269000	0.060124000	5.242331000	45	1.450877000	-9.614120000	18.579765000
1	1.978399000	2.195246000	-1.393074000	6	0.858753000	0.820503000	5.082003000	26	-0.385917000	-11.495768000	15.391746000
1	1.553225000	3.408872000	2.543959000	6	0.396918000	1.070921000	3.799131000	15	0.127639000	-11.440653000	18.797846000
1	3.199509000	5.248219000	2.250673000	7	1.030157000	0.614013000	2.704019000	16	2.941588000	-10.730995000	17.070073000
6	2.879347000	-0.820570000	4.617831000	6	2.143530000	-0.120405000	2.861134000	6	-0.093243000	-12.306893000	17.233595000
6	2.042949000	0.274994000	4.800473000	6	2.662597000	-0.420947000	4.111714000	6	0.988139000	-12.637286000	16.346944000
6	1.360749000	0.782154000	3.704872000	1	2.398371000	-0.155230000	6.235022000	6	0.432571000	-13.351375000	15.240551000
7	1.476176000	0.263738000	2.471497000	1	0.316188000	1.214255000	5.936003000	6	-0.974365000	-13.450454000	15.431718000
6	2.281421000	-0.795482000	2.305025000	1	-0.508863000	1.648303000	3.161778000	6	-1.304302000	-12.806525000	16.655844000
6	2.99035000	-1.369564000	3.345788000	1	2.618819000	-0.469233000	1.945495000	1	0.991965000	-13.715940000	14.385295000
1	3.426060000	-1.245059000	5.455549000	1	3.564408000	-1.020129000	4.188913000	1	-1.679964000	-13.892090000	14.737891000
1	1.911682000	0.730721000	5.777276000	1	-0.507523000	1.356162000	-0.654921000	1	-2.298631000	-12.675686000	17.069959000
1	0.675424000	1.622535000	3.809129000	1	0.157275000	1.864865000	-0.738618000	6	-0.181875000	-10.665299000	13.541260000
1	2.339794000	-1.205593000	1.296894000	[[P,(StBu)Rh(H)(H ₂ (py))] ⁺ E= -2268.68974963 Ha			6	-1.546507000	-10.646545000	13.947303000	
1	3.633164000	-2.227296000	3.155623000				6	-1.637818000	-9.902152000	15.157977000	
1	-0.444025000	1.676880000	-0.444782000	45	0.509458000	0.791486000	0.714918000	6	-0.327593000	-9.454317000	15.496577000
1	-0.857559000	2.180381000	0.872432000	26	-1.832891000	-1.506546000	-2.937733000	6	0.573165000	-9.929403000	14.499350000
TS _{D-D'} E= -2516.81663833 Ha			15	-1.215106000	-0.605722000	0.329386000	1	0.217605000	-11.184246000	12.677930000	
			16	2.075684000	-0.758616000	-0.591777000	1	-2.364592000	-11.152181000	13.447833000	
45	0.376284000	1.141713000	0.804044000	6	-1.120641000	-1.730838000	-1.069576000	1	-2.540391000	-9.736713000	15.735893000
26	-1.756220000	-0.671607000	-2.619871000	6	-0.046345000	-1.779702000	-2.032652000	1	-0.048376000	-8.902879000	16.3934

6	-3.564122000	-11.820872000	20.566085000	6	5.417294000	-11.992368000	17.024697000	6	3.523375000	-6.128740000	16.878034000
6	-4.243671000	-10.709221000	20.079941000	1	5.005886000	-13.002862000	16.940082000	6	2.797210000	-7.291660000	17.090127000
6	-3.597270000	-9.810603000	19.234018000	1	5.530351000	-11.569078000	16.019249000	7	2.594470000	-7.804884000	18.314585000
6	-2.270068000	-10.023914000	18.880765000	1	6.420241000	-12.090853000	17.458891000	6	3.104837000	-7.150911000	19.372859000
6	-1.581935000	-11.142969000	19.362096000	1	5.427315000	-9.251105000	17.092954000	6	3.845455000	-5.986381000	19.245529000
1	-1.712222000	-12.917207000	20.587437000	1	6.288996000	-9.910242000	18.495757000	1	4.639017000	-4.554268000	17.840603000
1	-4.066332000	-12.520560000	21.229197000	1	4.754833000	-9.063735000	18.733965000	1	3.658983000	-5.755357000	15.867652000
1	-5.279242000	-10.538636000	20.362908000	6	4.360220000	-11.710367000	19.295123000	1	2.365096000	-7.846178000	16.259122000
1	-4.126287000	-8.939179000	18.855959000	1	3.812473000	-12.660542000	19.246053000	1	2.918004000	-7.598103000	20.347721000
1	-1.761812000	-9.319422000	18.221402000	1	5.333093000	-11.916196000	19.762150000	1	4.241959000	-5.500254000	20.131558000
6	4.592937000	-11.085925000	17.929784000	1	3.797420000	-11.030903000	19.947270000	1	0.258547000	-8.589507000	19.246966000
6	5.293879000	-9.741366000	18.065210000	6	4.062368000	-5.465471000	17.974036000	1	0.647766000	-8.943379000	19.927594000