

Supporting Information

A Computational Study on Ligand Assisted vs. Ligand Participated Mechanism for CO₂ Hydrogenation: Importance of Bifunctional Ligand Based Catalysts

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1. Gaussian full references

Gaussian 09 Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

2. Intermediates of the reactions catalyzed by Mn-AMP

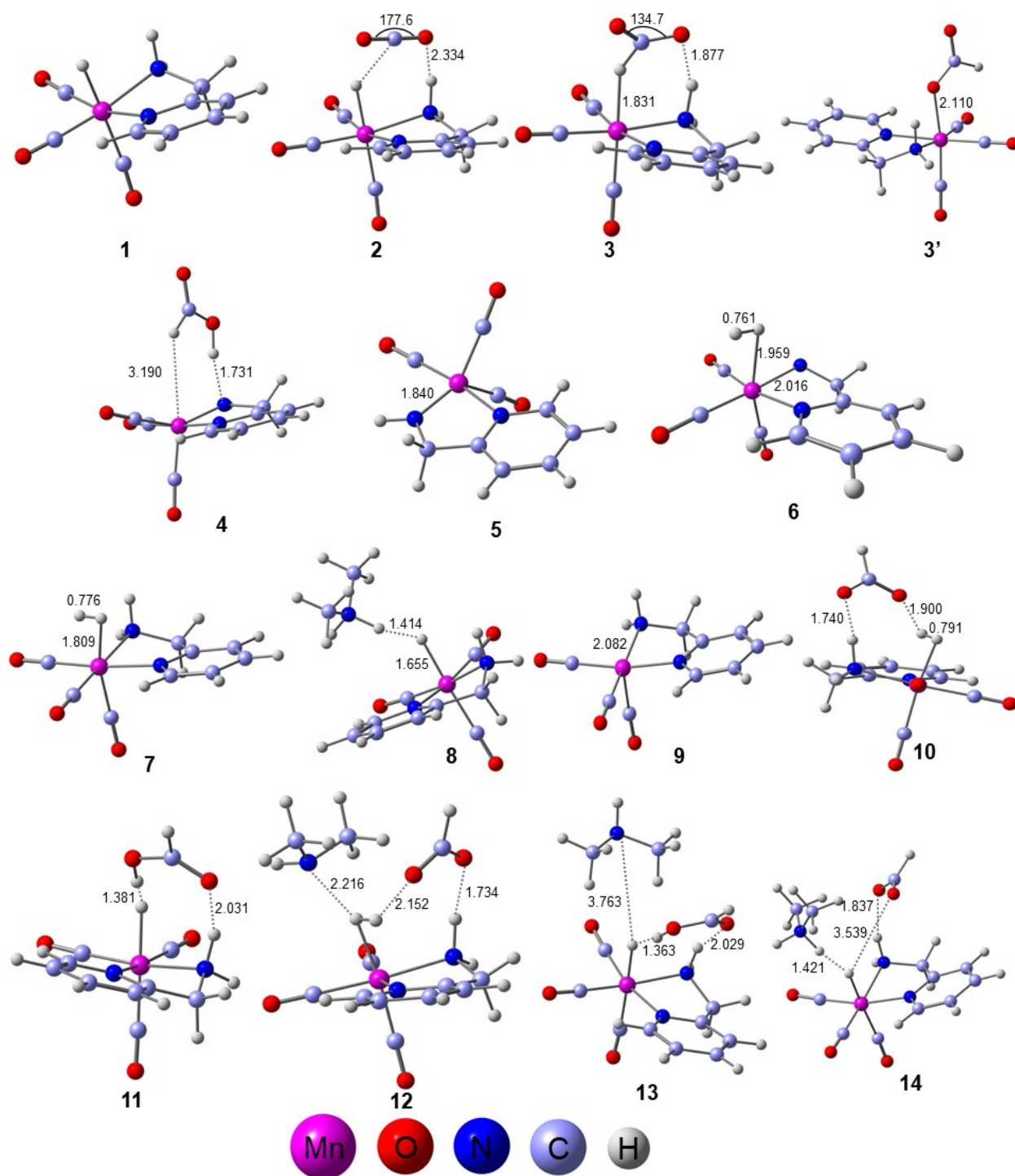


Figure S1: Optimized geometries of intermediates for CO₂ hydrogenation catalyzed by **Mn-AMP** complex. Bond lengths and bond angles are in Å and °, respectively.

3. Transition states of the reaction catalyzed by Mn-AMP

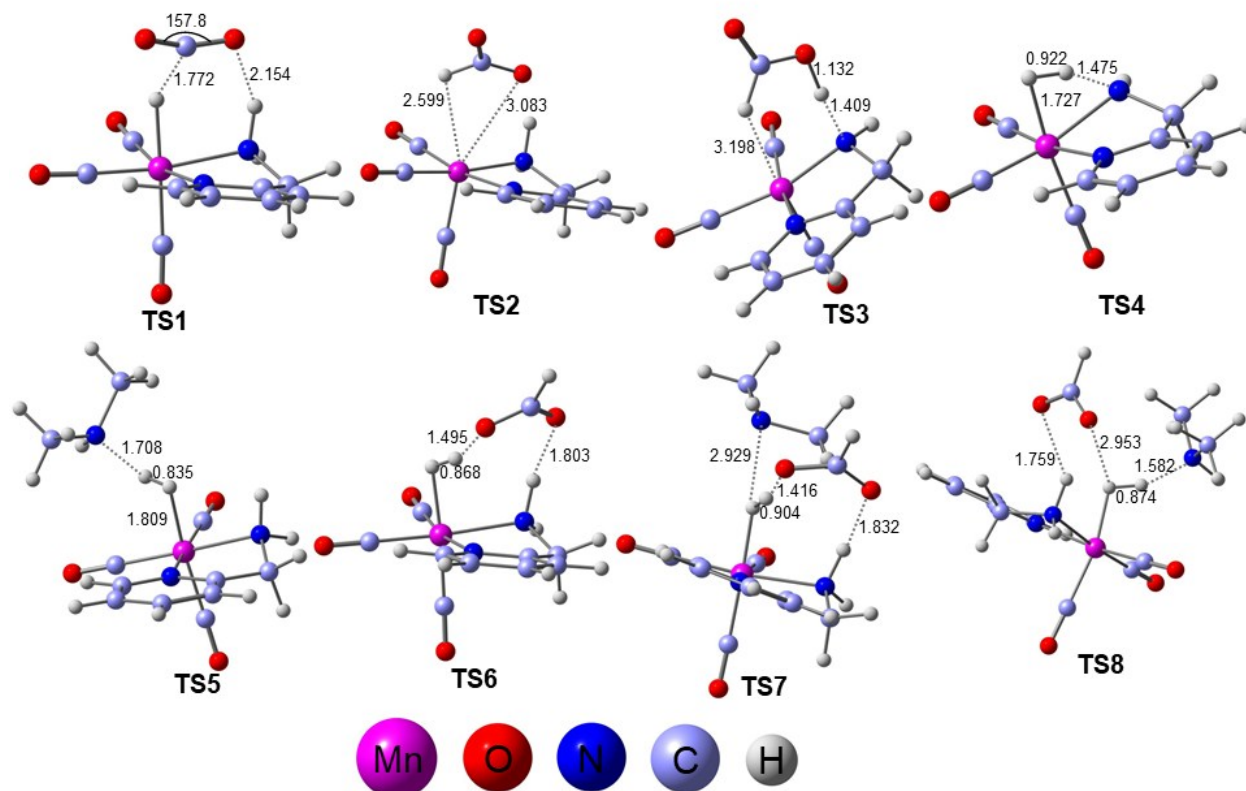


Figure S2: Optimized geometries of transition states for CO₂ hydrogenation catalyzed by **Mn-AMP** complex. Bond lengths and bond angles are in Å and °, respectively.

4. Total reaction free energy barrier for all the modelled complexes

Table S1: The calculated total reaction free energy barriers (in kcal/mol) for CO₂ hydrogenation via Ligand assisted (presence of external base) and ligand participated mechanisms.

Complexes	Ligand Participated Mechanism	Ligand Assisted Mechanism (Presence of external base)
Mn-AMP	38.9	38.4
Mn-MAMP	38.4	32.3
Mn-AMI	38.4	36.4
Mn-MAMI	37.8	-
Mn-AMIM	37.0	37.7
Mn-MAMIM	37.8	-
Mn-AMNHC	35.8	35.8
Mn-MAMNHC	35.3	36.0

5. Comparison between catalytic activity of Mn-MAMP and Mn-MAMP'

To understand the role of N-H functionality, we have substituted the N-H group by N-Me group to model **Mn-MAMP** and **Mn-MAMP'** complexes. The substituted methyl group can be directed towards the formate anion (**Mn-MAMP'**) or far from the formate anion (**Mn-MAMP**) as shown in Figure S3.

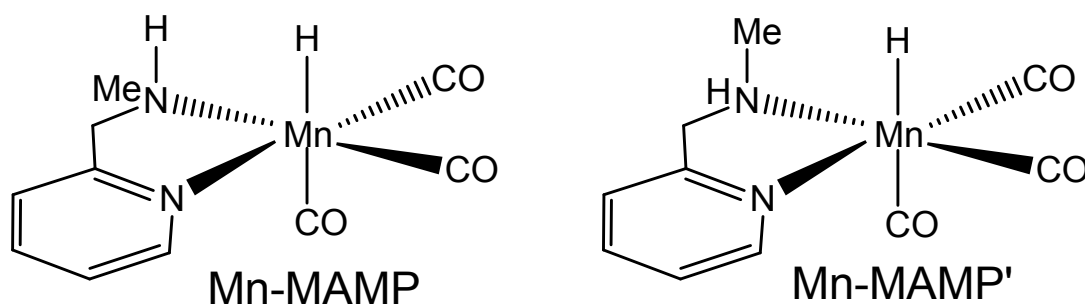


Figure S3: Structure of **Mn-MAMP** and **Mn-MAMP'** (Isomer of each other)

Our reaction free energy profile for CO₂ hydrogenation catalyzed by **Mn-MAMP** complex shows that hydride transfer is the rate determining steps (RDS), whereas hydrogenation by **Mn-MAMP'** shows that heterolytic H₂ cleavage is the RDS. Our calculated total reaction free energy barriers are same for **Mn-AMP** (21.3 kcal/mol) and **Mn-MAMP** (21.3 kcal/mol). This suggests that the presence of methyl group away from the formate anion does not affect the N-H $\cdots$ O hydrogen-bonding interactions between N-H and formate anion. On the other hand, **Mn-MAMP'** requires a total reaction free energy barrier of 25.4 kcal/mol, where Me-group is directed towards the formate anion. Therefore, the total reaction free energy barrier is 4.1 kcal/mol lower when catalyzed by **Mn-MAMP** complex over **Mn-MAMP'** complex. This shows the importance of

N-H functionality which forms N-H $\cdots$ O hydrogen-bonding interactions between N-H and formate anion when catalyzed via ligand assisted mechanism.

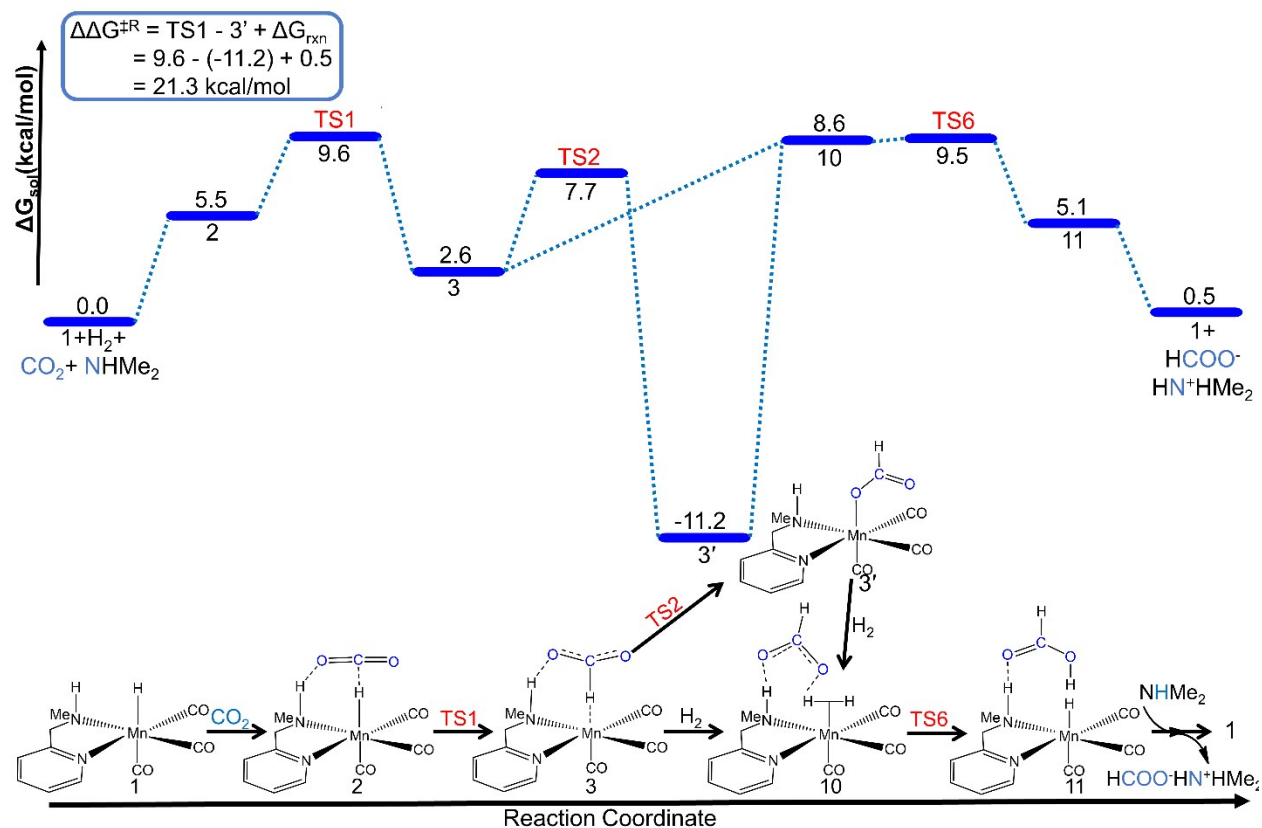


Figure S4: Reaction free energy profile diagram of CO₂ hydrogenation via ligand assisted mechanism catalyzed by **Mn-MAMP** complex. $\Delta\Delta G^{\ddagger R}$ and ΔG_{rxn} denote the total free energy barrier and total reaction free energy, respectively.

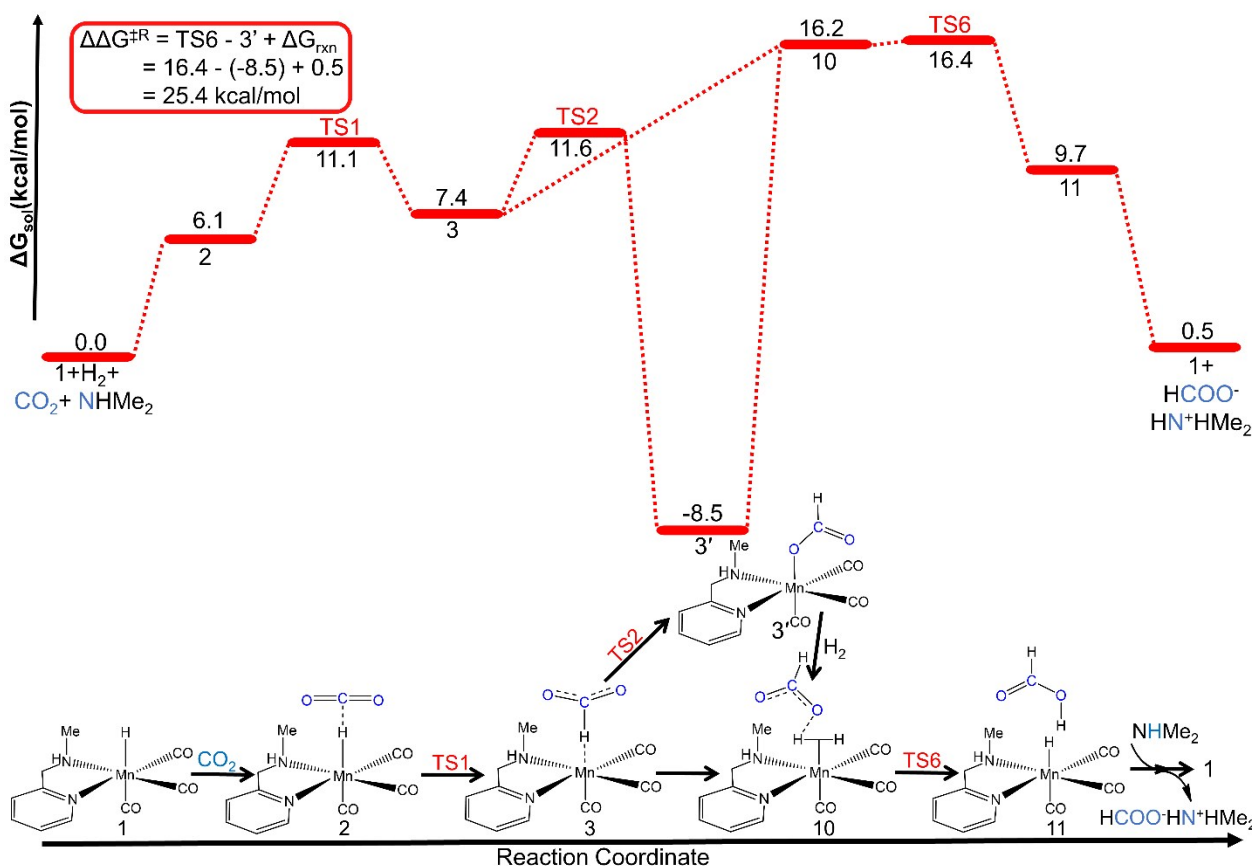


Figure S5: Reaction free energy profile diagram of CO₂ hydrogenation via ligand assisted mechanism catalyzed by **Mn-MAMP'** complex. $\Delta\Delta G^{\ddagger R}$ and ΔG_{rxn} denote the total free energy barrier and total reaction free energy, respectively.

6. Effect of temperature on rate of the reaction

Table S2: Stepwise reaction kinetic model for all barriers at different temperatures. All the temperatures are in Kelvin (K) and all the rate constant are in $\text{M}^{-1}\text{S}^{-1}$.

Temp (K)	TS1 (Hydride transfer step)	TS2 (Isomerisation step)	TS3 (N–H bond breaking)	TS4 (Heterolytic H_2 cleavage)	TS5 (Base assisted H_2 cleavage)	TS6 (Formate assisted H_2 cleavage)	TS7 (Formate assisted H_2 cleavage presence of external base)	TS8 (Base assisted H_2 cleavage presence of formate)
298.15	4.52×10^5	1.20×10^9	4.95×10^7	2.53×10^7	1.60×10^8	barrierless	1.28×10^3	5.52×10^2
323.15	1.75×10^6	2.52×10^9	1.33×10^8	7.17×10^7	3.93×10^8	barrierless	7.78×10^3	3.59×10^3
398.15	5.60×10^6	4.78×10^9	3.12×10^8	1.76×10^8	8.53×10^8	barrierless	3.67×10^4	1.79×10^4
423.15	1.53×10^7	8.35×10^9	6.54×10^8	3.82×10^8	1.67×10^9	barrierless	1.41×10^5	7.19×10^4

Table S3: Overall reaction kinetic model for all possible pathways at different temperatures. All the temperatures are in Kelvin (K) and all the rate constant are in $\text{M}^{-1}\text{S}^{-1}$.

Temp(K)	Ligand Participated	Ligand assisted (H_2 cleavage by base)	Ligand assisted (Formate anion assisted H_2 cleavage)	Formate vs base (formate assisted H_2 cleavage)	Formate vs base (base assisted H_2 cleavage)
298.15	1.25×10^{-16}	2.89×10^{-16}	1.91×10^{-3}	6.87×10^{-8}	2.97×10^{-8}
323.15	2.25×10^{-14}	4.88×10^{-14}	3.27×10^{-2}	2.61×10^{-6}	1.20×10^{-6}
398.15	1.93×10^{-12}	3.96×10^{-12}	3.76×10^{-1}	5.90×10^{-5}	2.88×10^{-5}
423.15	8.98×10^{-11}	1.76×10^{-10}	3.09	8.69×10^{-4}	4.45×10^{-4}

7. Cartesian coordinates and energies (in Hartree) in solvent phase for all the species.

H₂

1	0.000000000	0.000000000	0.371975000
1	0.000000000	0.000000000	-0.371975000

-1.180462

CO₂

6	0.000000000	0.000000000	0.000000000
8	0.000000000	0.000000000	1.169170000
8	0.000000000	0.000000000	-1.169170000

-188.602354

HCOOH

1	-0.697225000	-1.344426000	0.000000000
8	-1.035930000	-0.429889000	0.000000000
8	1.168302000	0.098528000	0.000000000
6	0.000000000	0.422739000	0.000000000
1	-0.361756000	1.458882000	0.000000000

-189.773891

[HCOO]⁻

8	-1.135907000	-0.216634000	0.000000000
8	1.136006000	-0.215165000	0.000000000
6	0.000000000	0.333019000	0.000000000
1	-0.000788000	1.456276000	0.000000000

-189.316431

NHMe₂

6	-1.217219000	-0.224597000	0.020228000
1	-2.096131000	0.422525000	-0.057703000
1	-1.277962000	-0.974169000	-0.777226000
1	-1.262213000	-0.759186000	0.986407000
7	-0.000003000	0.569559000	-0.152629000
6	1.217226000	-0.224573000	0.020211000
1	1.277892000	-0.974186000	-0.777200000
1	2.096138000	0.422515000	-0.057707000
1	1.262301000	-0.759235000	0.986390000
1	-0.000044000	1.329841000	0.522812000

-135.121262

[HNHMe₂]⁺

6	1.260183000	-0.276550000	0.000000000
1	2.114339000	0.399392000	0.000033000
1	1.264393000	-0.898214000	0.894376000

1	1.264385000	-0.898151000	-0.894423000
7	0.000000000	0.541528000	0.000004000
6	-1.260183000	-0.276550000	0.000000000
1	-1.264390000	-0.898218000	0.894373000
1	-2.114339000	0.399392000	0.000038000
1	-1.264388000	-0.898147000	-0.894425000
1	0.000000000	1.160932000	-0.815794000
1	0.000000000	1.160923000	0.815791000

-135.554309

[HCOO-HNMe₂⁺]

7	-0.977068000	-0.006849000	0.157652000
1	-0.497614000	-0.056233000	1.064546000
8	1.309513000	0.110596000	-1.117992000
8	1.760865000	-0.096787000	1.088714000
6	2.096277000	0.016491000	-0.114649000
1	3.180915000	0.039608000	-0.353897000
6	-1.786496000	1.236387000	0.072229000
1	-2.211872000	1.309557000	-0.929639000
1	-2.586309000	1.210356000	0.814505000
1	-1.133999000	2.090488000	0.257518000
6	-1.741866000	-1.257964000	-0.085688000
1	-2.162545000	-1.221179000	-1.091627000
1	-1.059035000	-2.104211000	-0.002125000
1	-2.543752000	-1.350878000	0.648668000
1	-0.116832000	0.050477000	-0.508642000

-324.903231

1-Mn-AMP

25	-0.975293000	0.028255000	-0.216439000
6	-1.158363000	-0.298633000	1.563307000
8	-1.347769000	-0.446204000	2.702817000
6	-2.661672000	-0.368411000	-0.648799000
8	-3.741890000	-0.637343000	-0.989669000
6	-1.359045000	1.763736000	-0.098327000
8	-1.600155000	2.903535000	-0.076257000
7	1.105681000	0.263914000	-0.126423000
6	1.773576000	1.433365000	-0.154892000
1	1.167315000	2.329826000	-0.200036000
6	3.163363000	1.509957000	-0.134007000
1	3.647108000	2.480121000	-0.158641000
6	3.902095000	0.325973000	-0.089288000
1	4.987154000	0.347001000	-0.079334000
6	3.215850000	-0.887869000	-0.065577000
1	3.748187000	-1.832935000	-0.038107000
6	1.820407000	-0.882066000	-0.078476000
6	1.004954000	-2.145995000	-0.002981000
1	1.560538000	-2.995662000	-0.413880000
1	0.787995000	-2.363570000	1.049216000

7	-0.286990000	-1.925405000	-0.685995000
1	-0.941392000	-2.660788000	-0.430293000
1	-0.166527000	-1.979914000	-1.694712000
1	-0.827365000	0.339732000	-1.777198000

-787.464881

2-Mn-AMP

25	-1.224461000	0.024114000	0.027369000
6	-1.818567000	-1.690792000	0.148722000
8	-2.259843000	-2.760364000	0.273745000
6	-2.766597000	0.713995000	-0.550677000
8	-3.738993000	1.209541000	-0.955214000
6	-1.588064000	0.449291000	1.719767000
8	-1.793191000	0.775485000	2.818951000
7	0.839455000	-0.521374000	0.365607000
6	1.514221000	-0.367779000	1.521156000
1	0.955946000	0.057177000	2.346535000
6	2.853193000	-0.719296000	1.664158000
1	3.348515000	-0.572367000	2.617436000
6	3.529513000	-1.246494000	0.561956000
1	4.576120000	-1.524789000	0.633658000
6	2.836397000	-1.401482000	-0.638147000
1	3.326315000	-1.797109000	-1.521676000
6	1.491177000	-1.033918000	-0.701121000
6	0.665406000	-1.220721000	-1.949671000
1	1.301624000	-1.183656000	-2.840493000
1	0.198076000	-2.211448000	-1.912675000
7	-0.419439000	-0.218229000	-1.986760000
1	-1.119474000	-0.490984000	-2.671797000
1	-0.051839000	0.685435000	-2.275403000
1	-0.703953000	1.563646000	-0.064620000
6	1.705703000	2.510098000	-0.514065000
8	1.782254000	2.923717000	0.575723000
8	1.672997000	2.113005000	-1.615654000

-976.056939

TS1-Mn-AMP

25	-1.093536000	-0.118998000	0.040933000
6	-1.485417000	-1.856823000	0.356160000
8	-1.778203000	-2.956036000	0.588480000
6	-2.747639000	0.293188000	-0.534759000
8	-3.794875000	0.589333000	-0.935232000
6	-1.472436000	0.413267000	1.715542000
8	-1.704713000	0.795881000	2.786062000
7	0.997943000	-0.392032000	0.358703000
6	1.675340000	-0.062323000	1.476235000
1	1.087529000	0.348101000	2.287663000
6	3.052248000	-0.219182000	1.595810000
1	3.547057000	0.066638000	2.517188000

6	3.765752000	-0.733804000	0.511499000
1	4.842096000	-0.861828000	0.565744000
6	3.070323000	-1.073098000	-0.648308000
1	3.586968000	-1.467208000	-1.517029000
6	1.686995000	-0.895766000	-0.690784000
6	0.861961000	-1.276886000	-1.894006000
1	1.456974000	-1.200433000	-2.810097000
1	0.543379000	-2.320158000	-1.787936000
7	-0.354733000	-0.435926000	-1.943189000
1	-1.024673000	-0.833394000	-2.596949000
1	-0.112893000	0.499737000	-2.274423000
1	-0.755431000	1.555390000	-0.270923000
6	0.663839000	2.537212000	-0.638706000
8	0.810180000	3.098450000	0.397375000
8	0.872499000	2.251012000	-1.778842000

-976.051691

3-Mn-AMP

25	-0.981071000	-0.197452000	0.037378000
6	-1.250904000	-1.971267000	0.154099000
8	-1.414835000	-3.112390000	0.230433000
6	-2.700079000	0.117207000	-0.460679000
8	-3.783385000	0.323967000	-0.799699000
6	-1.389252000	0.059223000	1.789149000
8	-1.657701000	0.236677000	2.897782000
7	1.069841000	-0.348173000	0.311983000
6	1.734665000	-0.103999000	1.460056000
1	1.131308000	0.149701000	2.322138000
6	3.120501000	-0.159551000	1.548250000
1	3.606107000	0.049904000	2.494427000
6	3.854205000	-0.476757000	0.403054000
1	4.937992000	-0.521569000	0.434323000
6	3.171216000	-0.726045000	-0.786217000
1	3.703899000	-0.965045000	-1.700297000
6	1.778542000	-0.657935000	-0.798243000
6	0.962197000	-0.946087000	-2.029065000
1	1.517852000	-0.682583000	-2.934410000
1	0.743671000	-2.018866000	-2.070365000
7	-0.320787000	-0.214513000	-1.933048000
1	-0.976726000	-0.574354000	-2.622642000
1	-0.154967000	0.786004000	-2.140414000
1	-0.763019000	1.617570000	-0.078679000
6	0.001674000	2.494162000	-0.354523000
8	0.242966000	3.212091000	0.617892000
8	0.343042000	2.497234000	-1.552204000

-976.063178

TS2-Mn-AMP

25	-0.983976000	-0.188215000	0.038854000
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6	-1.479207000	-1.867153000	0.381315000
8	-1.781116000	-2.964511000	0.577069000
6	-2.664313000	0.290969000	-0.498559000
8	-3.714895000	0.596093000	-0.857297000
6	-1.362797000	0.300082000	1.757372000
8	-1.643528000	0.566709000	2.843493000
7	1.035386000	-0.456074000	0.317852000
6	1.717911000	-0.150299000	1.442969000
1	1.129443000	0.165098000	2.294492000
6	3.102429000	-0.223750000	1.521655000
1	3.601449000	0.042774000	2.446117000
6	3.818008000	-0.631274000	0.393424000
1	4.901188000	-0.691659000	0.416709000
6	3.117984000	-0.958226000	-0.766238000
1	3.636598000	-1.280141000	-1.662752000
6	1.726482000	-0.866805000	-0.771105000
6	0.900706000	-1.264305000	-1.963957000
1	1.435070000	-1.049413000	-2.894510000
1	0.721636000	-2.344310000	-1.924551000
7	-0.405666000	-0.575906000	-1.909915000
1	-1.076556000	-1.048194000	-2.510318000
1	-0.307336000	0.394471000	-2.223359000
1	-0.448007000	2.332542000	0.486577000
6	0.243176000	2.690888000	-0.326361000
8	1.067382000	3.565179000	-0.001158000
8	0.056607000	2.172443000	-1.471905000

-976.055021

3'-Mn-AMP

25	-0.776206000	-0.413996000	0.058851000
6	-0.556073000	-2.133185000	0.550376000
8	-0.406227000	-3.236911000	0.866176000
6	-2.502859000	-0.688975000	-0.414734000
8	-3.597382000	-0.858438000	-0.743546000
6	-1.249561000	0.072331000	1.737079000
8	-1.548343000	0.387922000	2.808628000
7	1.307320000	-0.002837000	0.275922000
6	1.869365000	0.654479000	1.307397000
1	1.209966000	0.923447000	2.123459000
6	3.220654000	0.984414000	1.339756000
1	3.624310000	1.515576000	2.194305000
6	4.023631000	0.626064000	0.255084000
1	5.080351000	0.873073000	0.242155000
6	3.442565000	-0.047362000	-0.818573000
1	4.029602000	-0.333330000	-1.684862000
6	2.081143000	-0.351427000	-0.774919000
6	1.391580000	-1.113565000	-1.878457000
1	1.889922000	-0.942057000	-2.837828000
1	1.450556000	-2.185640000	-1.660046000
7	-0.039294000	-0.739059000	-1.916571000

1	-0.557174000	-1.401043000	-2.489753000
1	-0.156213000	0.186341000	-2.333821000
1	-2.444521000	2.195384000	0.310328000
6	-1.652942000	2.480459000	-0.415124000
8	-1.656331000	3.623511000	-0.893843000
8	-0.792073000	1.560420000	-0.684664000

-976.084805

TS3-Mn-AMP

25	-1.064903000	-0.188604000	0.013918000
6	-1.657875000	-1.661177000	-0.774505000
8	-1.997862000	-2.616184000	-1.334524000
6	-2.665320000	0.643855000	-0.216600000
8	-3.675257000	1.174119000	-0.391993000
6	-1.556936000	-0.780856000	1.668923000
8	-1.883075000	-1.138332000	2.719361000
7	0.887405000	-0.850761000	0.135880000
6	1.438436000	-1.558137000	1.148123000
1	0.778888000	-1.823127000	1.964756000
6	2.774653000	-1.932840000	1.156252000
1	3.169402000	-2.496758000	1.993652000
6	3.583304000	-1.563136000	0.076051000
1	4.633827000	-1.834791000	0.053872000
6	3.019715000	-0.837367000	-0.969368000
1	3.612665000	-0.528058000	-1.823358000
6	1.665153000	-0.499991000	-0.915391000
6	0.956280000	0.245949000	-2.006509000
1	1.629453000	0.992125000	-2.450463000
1	0.702904000	-0.469186000	-2.802595000
7	-0.256667000	0.857190000	-1.445120000
1	-0.860448000	1.151538000	-2.211133000
1	0.142857000	2.072420000	-0.874575000
1	0.993190000	1.976032000	1.152326000
6	1.029369000	2.988300000	0.702265000
8	1.519712000	3.924802000	1.329210000
8	0.521980000	3.075882000	-0.497203000

-976.051910

4-Mn-AMP

25	-0.810346000	-0.655958000	-0.111914000
6	-0.679133000	-2.414528000	-0.342792000
8	-0.553714000	-3.547385000	-0.556772000
6	-2.578308000	-0.668862000	-0.500303000
8	-3.701847000	-0.674252000	-0.770782000
6	-1.135559000	-0.847166000	1.664559000
8	-1.350258000	-0.923413000	2.800695000
7	1.230051000	-0.421163000	0.119363000
6	1.975595000	-0.853284000	1.161847000
1	1.441588000	-1.370931000	1.949240000

6	3.346919000	-0.655107000	1.230900000
1	3.900463000	-1.019736000	2.088754000
6	3.982913000	0.020550000	0.182464000
1	5.053562000	0.196620000	0.207484000
6	3.219703000	0.463440000	-0.892840000
1	3.672801000	0.990736000	-1.725701000
6	1.842507000	0.222107000	-0.899521000
6	0.939562000	0.627473000	-2.024820000
1	1.162745000	1.662901000	-2.324136000
1	1.165616000	-0.002760000	-2.898674000
7	-0.447704000	0.459277000	-1.598231000
1	-1.070322000	0.568572000	-2.396235000
1	-0.803807000	2.001954000	-0.892390000
1	-0.620897000	2.230267000	1.245641000
6	-0.818232000	3.152487000	0.672386000
8	-0.921804000	4.240146000	1.211186000
8	-0.934292000	2.978889000	-0.636245000

-976.050080

5-Mn-AMP

25	0.968371000	0.154877000	-0.000057000
6	1.237001000	-1.049596000	1.304415000
8	1.382804000	-1.774467000	2.200793000
6	2.699368000	0.656352000	-0.000149000
8	3.807654000	0.993509000	-0.000203000
6	1.237005000	-1.050011000	-1.304159000
8	1.382827000	-1.775175000	-2.200297000
7	-1.079558000	-0.135520000	0.000005000
6	-1.719536000	-1.326303000	0.000078000
1	-1.085152000	-2.205065000	0.000128000
6	-3.103325000	-1.428451000	0.000091000
1	-3.571283000	-2.406487000	0.000148000
6	-3.864586000	-0.252846000	0.000026000
1	-4.949104000	-0.296987000	0.000029000
6	-3.207975000	0.973651000	-0.000043000
1	-3.760028000	1.907819000	-0.000092000
6	-1.809677000	0.999915000	-0.000049000
6	-0.999005000	2.259622000	-0.000103000
1	-1.271611000	2.863806000	-0.880619000
1	-1.271481000	2.863773000	0.880478000
7	0.409880000	1.908406000	-0.000201000
1	0.985228000	2.746091000	-0.000248000

-786.282661

6-Mn-AMP

25	-0.950897000	0.042301000	-0.276583000
6	-1.125914000	-0.288893000	1.463509000
8	-1.213113000	-0.553158000	2.587672000
6	-2.681292000	-0.396879000	-0.575835000

8	-3.776083000	-0.720796000	-0.763235000
6	-1.333325000	1.809131000	-0.082362000
8	-1.600121000	2.924904000	0.094439000
7	1.107032000	0.251834000	-0.137152000
6	1.799187000	1.410694000	-0.125898000
1	1.211913000	2.320274000	-0.157870000
6	3.186810000	1.454037000	-0.082710000
1	3.695807000	2.411361000	-0.079381000
6	3.893484000	0.247023000	-0.047990000
1	4.978646000	0.242383000	-0.018559000
6	3.181575000	-0.949145000	-0.057366000
1	3.692270000	-1.906187000	-0.035512000
6	1.783706000	-0.919169000	-0.097936000
6	0.920852000	-2.147763000	-0.068060000
1	1.448159000	-2.970761000	-0.576923000
1	0.847533000	-2.449543000	0.996062000
7	-0.366824000	-1.844859000	-0.681367000
1	-1.027279000	-2.570054000	-0.409157000
1	-0.729531000	0.618358000	-2.188301000
1	-0.562496000	-0.124012000	-2.189266000

-787.433144

TS4-Mn-AMP

25	-0.977168000	0.023453000	-0.262450000
6	-1.074137000	-0.188650000	1.534734000
8	-1.133693000	-0.341211000	2.680560000
6	-2.706509000	-0.442665000	-0.465818000
8	-3.809377000	-0.770035000	-0.599560000
6	-1.373771000	1.785045000	-0.217991000
8	-1.627446000	2.916644000	-0.213460000
7	1.105159000	0.252816000	-0.148812000
6	1.785133000	1.416396000	-0.141202000
1	1.191878000	2.321454000	-0.187487000
6	3.173177000	1.472810000	-0.077242000
1	3.672698000	2.435094000	-0.074272000
6	3.890305000	0.274548000	-0.023176000
1	4.974802000	0.280164000	0.023277000
6	3.189276000	-0.929575000	-0.037397000
1	3.708804000	-1.881399000	-0.003996000
6	1.793520000	-0.910123000	-0.097088000
6	0.943285000	-2.154263000	-0.079568000
1	1.507669000	-2.988520000	-0.522066000
1	0.774826000	-2.415580000	0.983011000
7	-0.293224000	-1.878472000	-0.790170000
1	-0.969175000	-2.628642000	-0.694854000
1	-0.768277000	0.076112000	-1.979057000
1	-0.505109000	-0.789736000	-1.722256000

-787.421289

7-Mn-AMP

25	-0.958199000	0.024275000	-0.308149000
6	-1.079646000	-0.198852000	1.497437000
8	-1.145064000	-0.321724000	2.637912000
6	-2.722204000	-0.422415000	-0.517779000
8	-3.824912000	-0.728547000	-0.632719000
6	-1.370029000	1.797475000	-0.126586000
8	-1.636247000	2.909815000	-0.001504000
7	1.107231000	0.255506000	-0.163106000
6	1.775424000	1.427480000	-0.204805000
1	1.175662000	2.324112000	-0.297015000
6	3.162106000	1.498781000	-0.142523000
1	3.650422000	2.465650000	-0.181059000
6	3.892350000	0.313334000	-0.036443000
1	4.976258000	0.332490000	0.008155000
6	3.205453000	-0.899025000	0.005304000
1	3.735450000	-1.842046000	0.083158000
6	1.812368000	-0.894273000	-0.053526000
6	0.996684000	-2.154599000	0.051724000
1	1.539729000	-3.010990000	-0.357285000
1	0.798418000	-2.362554000	1.108543000
7	-0.311074000	-1.953830000	-0.623630000
1	-0.971642000	-2.654760000	-0.292813000
1	-0.207554000	-2.128936000	-1.623078000
1	-0.379569000	0.337797000	-1.993810000
1	-1.120554000	0.136856000	-2.110257000

-787.897586

TS5-Mn-AMP

25	-0.299104000	-0.808248000	0.068189000
6	0.513291000	-2.158199000	0.970370000
8	1.030450000	-3.009526000	1.551330000
6	-1.761738000	-1.822928000	-0.314407000
8	-2.687591000	-2.456495000	-0.581500000
6	-1.046177000	-0.197535000	1.603098000
8	-1.536912000	0.194810000	2.572128000
7	1.398568000	0.415850000	0.141715000
6	1.563790000	1.474806000	0.959162000
1	0.771391000	1.660550000	1.672797000
6	2.683183000	2.297731000	0.903057000
1	2.766382000	3.136817000	1.584207000
6	3.673140000	2.020885000	-0.041772000
1	4.556893000	2.645771000	-0.118145000
6	3.504379000	0.928473000	-0.891633000
1	4.246607000	0.682170000	-1.643089000
6	2.359060000	0.141872000	-0.770171000
6	2.131931000	-1.086562000	-1.611416000
1	2.626834000	-0.995008000	-2.582493000
1	2.565243000	-1.951809000	-1.098284000
7	0.674379000	-1.330124000	-1.751637000

1	0.518563000	-2.297224000	-2.029902000
1	0.300417000	-0.760088000	-2.509400000
1	-0.854583000	0.527138000	-0.969763000
1	-1.590863000	0.817352000	-0.600149000
7	-2.882821000	1.676544000	-0.286429000
1	-3.377859000	1.287240000	0.513630000
6	-2.416319000	3.034380000	0.027630000
1	-1.778786000	3.388186000	-0.788882000
1	-3.245316000	3.742591000	0.155996000
1	-1.822445000	3.011621000	0.944955000
6	-3.732199000	1.602426000	-1.483665000
1	-3.144005000	1.909270000	-2.354606000
1	-4.059752000	0.570290000	-1.632570000
1	-4.613616000	2.253016000	-1.411760000

-923.008909

8-Mn-AMP

25	0.623023000	0.920787000	0.014717000
6	0.055493000	2.459846000	0.814139000
8	-0.265737000	3.437034000	1.347225000
6	2.193181000	1.591488000	-0.542143000
8	3.207633000	1.986070000	-0.942828000
6	1.359463000	0.267757000	1.505102000
8	1.844392000	-0.216941000	2.445512000
7	-1.281970000	-0.045971000	0.247513000
6	-1.582534000	-0.966751000	1.183657000
1	-0.811601000	-1.173809000	1.916638000
6	-2.806739000	-1.626890000	1.226870000
1	-2.994749000	-2.360880000	2.002459000
6	-3.764912000	-1.324726000	0.256948000
1	-4.727775000	-1.825279000	0.252564000
6	-3.461492000	-0.365568000	-0.708630000
1	-4.178220000	-0.099898000	-1.478396000
6	-2.214694000	0.262271000	-0.680041000
6	-1.847663000	1.363261000	-1.643178000
1	-2.406976000	1.264846000	-2.579060000
1	-2.122634000	2.322795000	-1.190743000
7	-0.384304000	1.376645000	-1.860605000
1	-0.104606000	2.267587000	-2.264483000
1	-0.120223000	0.657895000	-2.530641000
1	1.090138000	-0.448813000	-0.788326000
1	1.407025000	-1.740332000	-0.309738000
7	1.680054000	-2.755734000	-0.129413000
1	1.837261000	-2.838545000	0.877885000
6	0.542885000	-3.634141000	-0.535429000
1	0.353120000	-3.480121000	-1.597989000
1	0.805088000	-4.675325000	-0.346273000
1	-0.338070000	-3.353456000	0.042182000
6	2.957311000	-3.021823000	-0.857696000
1	2.784557000	-2.861945000	-1.922360000

1	3.714344000	-2.326125000	-0.494881000
1	3.269173000	-4.050513000	-0.676072000

-923.019320

9-Mn-AMP

25	-0.939180000	0.003928000	-0.283317000
6	-1.216911000	-0.167907000	1.476680000
8	-1.355138000	-0.288582000	2.614721000
6	-2.691390000	-0.415712000	-0.650914000
8	-3.785266000	-0.695353000	-0.869435000
6	-1.354142000	1.786789000	-0.194573000
8	-1.630802000	2.901890000	-0.126820000
7	1.096061000	0.250665000	-0.138399000
6	1.754833000	1.429894000	-0.188682000
1	1.145794000	2.322095000	-0.255321000
6	3.141266000	1.513111000	-0.160267000
1	3.620466000	2.484190000	-0.205628000
6	3.884436000	0.333541000	-0.077444000
1	4.968893000	0.362978000	-0.058115000
6	3.210838000	-0.886070000	-0.025540000
1	3.751915000	-1.824067000	0.033535000
6	1.817600000	-0.893775000	-0.052683000
6	1.013260000	-2.160026000	0.051410000
1	1.554935000	-3.010367000	-0.371496000
1	0.820994000	-2.376705000	1.107237000
7	-0.299339000	-1.950169000	-0.611031000
1	-0.954180000	-2.672278000	-0.315052000
1	-0.195470000	-2.070215000	-1.621861000

-786.726108

10-Mn-AMP

25	1.125021000	-0.052315000	-0.110372000
6	1.700685000	-1.106690000	1.244401000
8	2.060694000	-1.788063000	2.102081000
6	2.663683000	0.921870000	-0.093625000
8	3.627944000	1.553342000	-0.062570000
6	1.788314000	-1.214124000	-1.342923000
8	2.221381000	-1.954351000	-2.115669000
7	-0.776768000	-0.880057000	-0.035809000
6	-1.280790000	-1.776771000	-0.906414000
1	-0.602784000	-2.152015000	-1.662606000
6	-2.602205000	-2.205033000	-0.859052000
1	-2.958895000	-2.925568000	-1.586163000
6	-3.440933000	-1.684568000	0.129116000
1	-4.479817000	-1.991920000	0.192459000
6	-2.922937000	-0.754953000	1.027924000
1	-3.542856000	-0.316837000	1.802628000
6	-1.586114000	-0.371432000	0.918212000
6	-0.943928000	0.597590000	1.872605000

1	-1.679637000	1.320388000	2.239824000
1	-0.565961000	0.039775000	2.737220000
7	0.190633000	1.272030000	1.204585000
1	0.817392000	1.646889000	1.913521000
1	-0.184957000	2.093880000	0.675002000
1	-2.544600000	3.574370000	-1.452077000
6	-1.770609000	2.901186000	-1.018869000
8	-1.699674000	1.734521000	-1.490978000
8	-1.052617000	3.390408000	-0.096714000
1	0.786357000	0.944050000	-1.528652000
1	0.040365000	1.001754000	-1.270747000

-977.234395

TS6-Mn-AMP

25	1.120139000	-0.063475000	-0.099975000
6	1.714461000	-1.092268000	1.264415000
8	2.092635000	-1.763745000	2.123816000
6	2.638723000	0.934932000	-0.110457000
8	3.589630000	1.588380000	-0.108486000
6	1.793055000	-1.228853000	-1.317227000
8	2.235326000	-1.965294000	-2.089820000
7	-0.783759000	-0.890687000	-0.027101000
6	-1.289572000	-1.781573000	-0.902114000
1	-0.607170000	-2.168049000	-1.648769000
6	-2.618420000	-2.189278000	-0.871911000
1	-2.977005000	-2.903907000	-1.603933000
6	-3.462371000	-1.653960000	0.103558000
1	-4.507280000	-1.943122000	0.151684000
6	-2.941119000	-0.733525000	1.010705000
1	-3.563945000	-0.286977000	1.778174000
6	-1.596314000	-0.373667000	0.920171000
6	-0.946881000	0.582188000	1.883064000
1	-1.679217000	1.299541000	2.266629000
1	-0.561313000	0.011964000	2.736125000
7	0.183312000	1.264467000	1.213057000
1	0.814110000	1.632551000	1.922205000
1	-0.194750000	2.090841000	0.696616000
1	-2.643218000	3.406825000	-1.409675000
6	-1.763155000	2.857185000	-1.014870000
8	-1.119697000	3.406111000	-0.075882000
8	-1.517262000	1.736690000	-1.554115000
1	0.722120000	0.818945000	-1.540384000
1	-0.018183000	1.067593000	-1.307087000

-977.234683

11-Mn-AMP

25	-1.208848000	-0.027733000	-0.052149000
6	-1.870358000	1.292041000	1.006833000
8	-2.347812000	2.142285000	1.638239000

6	-2.681036000	-1.045249000	0.034020000
8	-3.604215000	-1.748429000	0.080810000
6	-1.758723000	0.738904000	-1.571386000
8	-2.099216000	1.201565000	-2.582238000
7	0.722215000	0.783433000	-0.083883000
6	1.278660000	1.465912000	-1.103728000
1	0.649257000	1.632646000	-1.969238000
6	2.589850000	1.929410000	-1.073174000
1	2.987329000	2.471143000	-1.924123000
6	3.367084000	1.671350000	0.058000000
1	4.397129000	2.008785000	0.113145000
6	2.796462000	0.963097000	1.114654000
1	3.366718000	0.732303000	2.008205000
6	1.470895000	0.538795000	1.014529000
6	0.765667000	-0.191555000	2.126372000
1	1.480847000	-0.755509000	2.734260000
1	0.275893000	0.543105000	2.776058000
7	-0.279064000	-1.058088000	1.542146000
1	-0.923680000	-1.357007000	2.269572000
1	0.172369000	-1.894287000	1.165095000
1	3.171221000	-2.891330000	-1.164103000
6	2.206418000	-2.534047000	-0.777096000
8	1.828790000	-2.757344000	0.365153000
8	1.544129000	-1.851030000	-1.693297000
1	-0.661045000	-1.207560000	-1.013346000
1	0.640168000	-1.534717000	-1.343117000

-977.239509

12-Mn-AMP

25	0.164212000	1.056344000	-0.150639000
6	-0.711223000	2.534852000	-0.723747000
8	-1.280121000	3.472356000	-1.081551000
6	1.744287000	1.629808000	-0.846480000
8	2.740629000	1.984035000	-1.306223000
6	0.537462000	1.823119000	1.453802000
8	0.794064000	2.312569000	2.467701000
7	-1.610597000	0.149554000	0.436046000
6	-2.061149000	0.047492000	1.702296000
1	-1.478705000	0.549666000	2.464450000
6	-3.207141000	-0.665216000	2.033680000
1	-3.524814000	-0.719487000	3.068728000
6	-3.918839000	-1.302276000	1.013967000
1	-4.815237000	-1.872207000	1.236483000
6	-3.451920000	-1.201887000	-0.294040000
1	-3.967352000	-1.691481000	-1.113346000
6	-2.291481000	-0.470303000	-0.550969000
6	-1.749185000	-0.285322000	-1.941751000
1	-1.965911000	-1.165702000	-2.555701000
1	-2.253537000	0.572336000	-2.402344000
7	-0.296658000	-0.013193000	-1.882774000

1	-0.013335000	0.461297000	-2.737197000
1	0.211208000	-0.930467000	-1.869103000
1	0.716312000	-4.250503000	-0.840028000
6	0.494526000	-3.157879000	-0.859909000
8	-0.085952000	-2.669510000	0.141856000
8	0.866726000	-2.536062000	-1.902831000
1	1.249873000	-0.220009000	0.467480000
1	0.599389000	-0.635824000	0.307795000
7	3.332790000	-0.646430000	1.095521000
1	4.059230000	-0.084214000	1.530463000
6	2.911027000	-1.702484000	2.018348000
1	2.040888000	-2.220826000	1.599789000
1	3.696336000	-2.454627000	2.211363000
1	2.614627000	-1.258053000	2.973936000
6	3.815394000	-1.169752000	-0.184327000
1	4.622074000	-1.916232000	-0.075748000
1	2.985078000	-1.644506000	-0.719117000
1	4.186518000	-0.345290000	-0.800333000

-1112.344991

TS7-Mn-AMP

25	0.079266000	1.099556000	-0.053113000
6	-0.832626000	2.596946000	-0.493618000
8	-1.403966000	3.568560000	-0.755148000
6	1.645506000	1.775780000	-0.658484000
8	2.638525000	2.196488000	-1.072578000
6	0.405265000	1.689944000	1.622095000
8	0.635377000	2.053861000	2.696295000
7	-1.662763000	0.053793000	0.406830000
6	-2.111627000	-0.221952000	1.646133000
1	-1.553298000	0.208153000	2.468219000
6	-3.223174000	-1.024236000	1.879803000
1	-3.541184000	-1.217061000	2.898147000
6	-3.895758000	-1.573661000	0.786465000
1	-4.760614000	-2.213091000	0.931399000
6	-3.430779000	-1.293540000	-0.497449000
1	-3.916868000	-1.708678000	-1.373808000
6	-2.314534000	-0.471765000	-0.653527000
6	-1.768185000	-0.090465000	-2.003251000
1	-1.990595000	-0.865910000	-2.743381000
1	-2.251695000	0.836043000	-2.333397000
7	-0.314303000	0.153216000	-1.880888000
1	0.012012000	0.670591000	-2.693687000
1	0.164274000	-0.764715000	-1.887850000
1	0.190586000	-4.108249000	-0.459051000
6	0.309243000	-3.013070000	-0.576540000
8	0.209976000	-2.344293000	0.509721000
8	0.520592000	-2.554827000	-1.720645000
1	1.052963000	-0.212521000	0.386839000
1	0.584945000	-0.985936000	0.375044000

7	3.921520000	-0.694155000	0.662226000
1	4.875519000	-0.385919000	0.831869000
6	3.603137000	-1.796319000	1.571256000
1	2.545797000	-2.059456000	1.465189000
1	4.198051000	-2.709200000	1.381497000
1	3.775433000	-1.482970000	2.606055000
6	3.782934000	-1.069595000	-0.745377000
1	4.387823000	-1.951493000	-1.026199000
1	2.736074000	-1.305797000	-0.961165000
1	4.077501000	-0.229406000	-1.381247000

-1112.342875

13-Mn-AMP

25	0.020253000	1.178448000	-0.062380000
6	-0.939089000	2.616935000	-0.622546000
8	-1.510136000	3.578821000	-0.936422000
6	1.601870000	1.851557000	-0.566318000
8	2.645015000	2.239576000	-0.896963000
6	0.232481000	1.790028000	1.603334000
8	0.403290000	2.144126000	2.697663000
7	-1.680256000	0.021119000	0.340933000
6	-2.192587000	-0.238484000	1.559773000
1	-1.693383000	0.229234000	2.399535000
6	-3.293384000	-1.066782000	1.752705000
1	-3.663105000	-1.242550000	2.756711000
6	-3.888941000	-1.662948000	0.639014000
1	-4.743198000	-2.322725000	0.752355000
6	-3.359561000	-1.400561000	-0.623731000
1	-3.783743000	-1.850466000	-1.515104000
6	-2.259615000	-0.549707000	-0.738592000
6	-1.653463000	-0.178902000	-2.066073000
1	-1.822502000	-0.970287000	-2.803724000
1	-2.136643000	0.734277000	-2.432617000
7	-0.217325000	0.107880000	-1.869793000
1	0.152297000	0.588731000	-2.685971000
1	0.276056000	-0.783659000	-1.784765000
1	0.131137000	-4.157809000	0.227992000
6	0.254142000	-3.104931000	-0.062670000
8	0.423221000	-2.331142000	0.993688000
8	0.230778000	-2.734741000	-1.228586000
1	0.901033000	-0.064787000	0.451850000
1	0.555929000	-1.355157000	0.724554000
7	4.528458000	-0.980275000	0.046958000
1	5.379710000	-1.535577000	0.078287000
6	4.013982000	-0.810420000	1.407715000
1	3.155794000	-0.130892000	1.387417000
1	3.678651000	-1.755897000	1.872014000
1	4.787650000	-0.368271000	2.043195000
6	3.561925000	-1.631231000	-0.838223000
1	3.210690000	-2.609932000	-0.464713000

1	2.682848000	-0.988459000	-0.947176000
1	4.004410000	-1.778496000	-1.828367000

-1112.348842

TS8-Mn-AMP

25	-0.170635000	-1.103876000	-0.170853000
6	0.761080000	-2.505090000	-0.840497000
8	1.371455000	-3.392026000	-1.259769000
6	-1.729334000	-1.701833000	-0.869319000
8	-2.722553000	-2.070130000	-1.333003000
6	-0.480461000	-1.951547000	1.397117000
8	-0.700301000	-2.487559000	2.399190000
7	1.580083000	-0.150431000	0.427832000
6	2.076968000	-0.132244000	1.682514000
1	1.536311000	-0.707594000	2.423484000
6	3.218850000	0.579382000	2.025784000
1	3.575090000	0.562452000	3.049601000
6	3.879090000	1.307864000	1.031072000
1	4.772319000	1.879027000	1.263311000
6	3.364942000	1.294775000	-0.261193000
1	3.836156000	1.858439000	-1.059145000
6	2.208818000	0.558573000	-0.532003000
6	1.629905000	0.461884000	-1.915488000
1	1.765466000	1.410160000	-2.444295000
1	2.175935000	-0.313174000	-2.466820000
7	0.202797000	0.083743000	-1.848094000
1	-0.060618000	-0.365724000	-2.722014000
1	-0.379724000	0.949495000	-1.777394000
1	-1.289603000	4.149606000	-0.701724000
6	-0.752656000	3.199344000	-0.940346000
8	0.367459000	3.019842000	-0.404241000
8	-1.359954000	2.409625000	-1.729095000
1	-1.547896000	0.273506000	0.678378000
1	-0.731196000	0.396843000	0.392395000
7	-2.944670000	0.686142000	1.295442000
1	-3.328680000	-0.060863000	1.870626000
6	-2.617713000	1.848877000	2.132210000
1	-2.084646000	2.583361000	1.521393000
1	-3.512101000	2.325420000	2.555919000
1	-1.958864000	1.535411000	2.946603000
6	-3.856921000	0.996172000	0.183064000
1	-4.779894000	1.482996000	0.528101000
1	-3.337322000	1.655424000	-0.518684000
1	-4.116570000	0.070994000	-0.336822000

-1112.343688

14-Mn-AMP

25	-0.330077000	1.272631000	-0.099449000
6	-1.641883000	2.202674000	-0.952283000

8	-2.466538000	2.847814000	-1.455069000
6	0.987129000	2.363097000	-0.608801000
8	1.891527000	3.020691000	-0.934542000
6	-0.524042000	2.133413000	1.454083000
8	-0.604565000	2.666167000	2.485540000
7	-1.589779000	-0.332847000	0.377137000
6	-2.122487000	-0.590408000	1.586996000
1	-1.920242000	0.135719000	2.364834000
6	-2.887160000	-1.723088000	1.847363000
1	-3.290003000	-1.881851000	2.841483000
6	-3.107466000	-2.637108000	0.814340000
1	-3.691149000	-3.536409000	0.983279000
6	-2.554627000	-2.375910000	-0.437927000
1	-2.689500000	-3.063312000	-1.266305000
6	-1.805252000	-1.213009000	-0.624389000
6	-1.210619000	-0.834945000	-1.953886000
1	-1.002327000	-1.729082000	-2.551396000
1	-1.937849000	-0.224262000	-2.502371000
7	0.006010000	-0.029132000	-1.725980000
1	0.240529000	0.464046000	-2.584372000
1	0.786767000	-0.682497000	-1.543219000
1	1.815163000	-4.146678000	-1.307043000
6	1.680404000	-3.129727000	-0.864814000
8	1.359485000	-3.074724000	0.348327000
8	1.878307000	-2.156820000	-1.656107000
1	2.153185000	0.380221000	0.912012000
1	0.748928000	0.394692000	0.691476000
7	3.186710000	0.201006000	1.075057000
1	3.553249000	1.024822000	1.556419000
6	3.310333000	-1.002481000	1.954130000
1	2.792563000	-1.829110000	1.461856000
1	4.367368000	-1.226757000	2.103274000
1	2.835276000	-0.779971000	2.910678000
6	3.846473000	0.058002000	-0.259329000
1	4.906489000	-0.152019000	-0.110272000
1	3.352247000	-0.758394000	-0.790640000
1	3.720120000	0.993791000	-0.805060000

-1112.350914

1-Mn-MAMP

25	-0.867188000	0.298922000	-0.194377000
6	-1.085995000	0.067650000	1.595209000
8	-1.296519000	-0.014582000	2.737446000
6	-2.591369000	0.112530000	-0.615266000
8	-3.700549000	-0.005135000	-0.949051000
6	-1.048300000	2.071065000	-0.139977000
8	-1.157716000	3.230791000	-0.155498000
7	1.225496000	0.320489000	-0.125413000
6	2.016070000	1.406332000	-0.227882000
1	1.511812000	2.360245000	-0.321106000

6	3.406001000	1.331030000	-0.221576000
1	3.992058000	2.239499000	-0.305732000
6	4.012336000	0.077781000	-0.114899000
1	5.093277000	-0.019224000	-0.114715000
6	3.198566000	-1.050503000	-0.016268000
1	3.624441000	-2.045341000	0.060507000
6	1.812162000	-0.891945000	-0.017214000
6	0.862955000	-2.047862000	0.135662000
1	1.320071000	-2.984733000	-0.206916000
1	0.614781000	-2.167679000	1.197759000
7	-0.396226000	-1.752755000	-0.579264000
1	-0.201768000	-1.761817000	-1.578979000
1	-0.695604000	0.514086000	-1.769479000
6	-1.426843000	-2.775501000	-0.302267000
1	-2.297610000	-2.586142000	-0.930911000
1	-1.053839000	-3.788449000	-0.499583000
1	-1.728025000	-2.699715000	0.745002000

-826.749661

2-Mn-MAMP

25	-1.081726000	0.287198000	0.118906000
6	-1.753686000	-0.559669000	1.580361000
8	-2.249674000	-1.032506000	2.521318000
6	-2.648966000	0.478435000	-0.713465000
8	-3.640594000	0.627065000	-1.304599000
6	-1.218621000	1.924301000	0.811044000
8	-1.283708000	3.013833000	1.217447000
7	0.922437000	0.020987000	0.668344000
6	1.741794000	0.959949000	1.181617000
1	1.309184000	1.940637000	1.335746000
6	3.074182000	0.708047000	1.494400000
1	3.687647000	1.502660000	1.904215000
6	3.591410000	-0.567710000	1.259569000
1	4.627994000	-0.797528000	1.484374000
6	2.750031000	-1.540728000	0.721279000
1	3.111068000	-2.542135000	0.512094000
6	1.422389000	-1.214107000	0.443034000
6	0.437451000	-2.213570000	-0.095714000
1	0.946729000	-3.002126000	-0.663963000
1	-0.079655000	-2.692064000	0.745488000
7	-0.584528000	-1.521124000	-0.907621000
1	-0.135458000	-1.194650000	-1.761487000
1	-0.522530000	1.051753000	-1.167251000
6	1.837136000	1.044390000	-2.329564000
8	2.028568000	2.159214000	-2.038321000
8	1.685115000	-0.074595000	-2.641412000
6	-1.681428000	-2.437119000	-1.284991000
1	-1.299013000	-3.352904000	-1.753186000
1	-2.249605000	-2.699779000	-0.389655000
1	-2.346390000	-1.930240000	-1.984964000

-1015.343258

TS1-Mn-MAMP

25	0.953459000	0.141149000	-0.271054000
6	1.384099000	-0.993125000	-1.619314000
8	1.705458000	-1.677110000	-2.501046000
6	2.640118000	0.345451000	0.299377000
8	3.715009000	0.506783000	0.707492000
6	1.090596000	1.613649000	-1.281930000
8	1.166348000	2.596292000	-1.896337000
7	-1.110966000	-0.068766000	-0.529156000
6	-1.937107000	0.823024000	-1.110697000
1	-1.474509000	1.714611000	-1.514929000
6	-3.313324000	0.633789000	-1.187699000
1	-3.931506000	1.385558000	-1.665426000
6	-3.865639000	-0.523051000	-0.634130000
1	-4.935918000	-0.699217000	-0.668774000
6	-3.015219000	-1.446334000	-0.026879000
1	-3.401651000	-2.354347000	0.423713000
6	-1.644169000	-1.190831000	0.002705000
6	-0.651100000	-2.150223000	0.596369000
1	-1.117482000	-2.772551000	1.369910000
1	-0.285902000	-2.819946000	-0.192134000
7	0.510879000	-1.401540000	1.121351000
1	0.196460000	-0.880381000	1.941283000
1	0.599355000	1.175967000	0.940825000
6	-0.669242000	1.738786000	2.034604000
8	-0.859353000	2.828536000	1.609590000
8	-0.800679000	0.799454000	2.754905000
6	1.594490000	-2.316610000	1.540557000
1	1.224513000	-3.087373000	2.227756000
1	2.019556000	-2.796263000	0.656083000
1	2.375933000	-1.741426000	2.038070000

-1015.336718

3-Mn-MAMP

25	0.890011000	0.166358000	-0.272746000
6	1.236165000	-0.720406000	-1.796905000
8	1.453775000	-1.292577000	-2.776884000
6	2.642675000	0.192036000	0.204832000
8	3.753936000	0.213597000	0.515100000
6	1.068799000	1.783500000	-1.084950000
8	1.190496000	2.814032000	-1.590217000
7	-1.170147000	0.072162000	-0.495209000
6	-1.972114000	1.076894000	-0.903606000
1	-1.482493000	1.996869000	-1.196120000
6	-3.356530000	0.959686000	-0.941124000
1	-3.956508000	1.799292000	-1.272825000
6	-3.940223000	-0.242857000	-0.536680000

1	-5.018366000	-0.365574000	-0.545496000
6	-3.114648000	-1.282379000	-0.110872000
1	-3.528018000	-2.228184000	0.221902000
6	-1.733324000	-1.094364000	-0.106015000
6	-0.764476000	-2.165636000	0.306363000
1	-1.221684000	-2.854601000	1.025958000
1	-0.476002000	-2.750720000	-0.575285000
7	0.457554000	-1.539345000	0.860165000
1	0.194159000	-1.107288000	1.765188000
1	0.602623000	1.081278000	1.295031000
6	-0.166375000	1.273118000	2.189134000
8	-0.503091000	2.456697000	2.255372000
8	-0.418665000	0.252028000	2.856825000
6	1.511619000	-2.548767000	1.106861000
1	1.124325000	-3.384752000	1.700596000
1	1.884191000	-2.928202000	0.152675000
1	2.334637000	-2.081952000	1.648547000

-1015.347842

TS2-Mn-MAMP

25	-0.866256000	0.018853000	0.303078000
6	-1.256436000	-1.237301000	1.507656000
8	-1.479171000	-2.072829000	2.272742000
6	-2.625520000	0.217839000	-0.149880000
8	-3.736684000	0.341325000	-0.427095000
6	-1.031431000	1.346547000	1.551146000
8	-1.154999000	2.175654000	2.341329000
7	1.176566000	-0.145723000	0.482827000
6	1.983369000	0.682577000	1.178834000
1	1.498962000	1.458125000	1.757720000
6	3.367830000	0.567061000	1.159619000
1	3.971226000	1.262203000	1.731834000
6	3.946839000	-0.444134000	0.390142000
1	5.025037000	-0.558976000	0.347784000
6	3.117000000	-1.300658000	-0.331715000
1	3.527612000	-2.091859000	-0.949371000
6	1.736133000	-1.126449000	-0.262667000
6	0.767968000	-2.017813000	-0.985012000
1	1.212089000	-2.416339000	-1.904434000
1	0.514979000	-2.871001000	-0.343682000
7	-0.477038000	-1.272535000	-1.269145000
1	-0.252552000	-0.523206000	-1.949630000
1	-0.985845000	2.171766000	-1.120750000
6	0.005602000	2.234210000	-1.661948000
8	0.594243000	3.330634000	-1.590054000
8	0.367082000	1.173852000	-2.256707000
6	-1.526559000	-2.159227000	-1.815095000
1	-1.143668000	-2.748819000	-2.655708000
1	-1.876404000	-2.836244000	-1.032291000
1	-2.364271000	-1.554174000	-2.162402000

-1015.339740

3'-Mn-MAMP

25	-0.735858000	-0.152213000	0.352751000
6	-0.602084000	-1.541297000	1.490677000
8	-0.510732000	-2.438368000	2.216813000
6	-2.509770000	-0.424083000	0.111364000
8	-3.639700000	-0.594888000	-0.059564000
6	-1.057937000	1.010764000	1.702176000
8	-1.259503000	1.756419000	2.562533000
7	1.376729000	0.142414000	0.317527000
6	2.038551000	1.122308000	0.960691000
1	1.449039000	1.753636000	1.614083000
6	3.404969000	1.332502000	0.803495000
1	3.891266000	2.135643000	1.345559000
6	4.115157000	0.501030000	-0.064709000
1	5.180352000	0.640671000	-0.218507000
6	3.430390000	-0.508759000	-0.739681000
1	3.943232000	-1.169113000	-1.430750000
6	2.060963000	-0.665164000	-0.520956000
6	1.260298000	-1.760500000	-1.174189000
1	1.716666000	-2.066389000	-2.123077000
1	1.252254000	-2.637345000	-0.515422000
7	-0.142362000	-1.329073000	-1.359382000
1	-0.164033000	-0.582655000	-2.058521000
1	-2.201968000	2.471004000	-0.458380000
6	-1.444458000	2.351629000	-1.261922000
8	-1.404757000	3.179595000	-2.182666000
8	-0.664632000	1.332350000	-1.140198000
6	-0.998749000	-2.443264000	-1.819180000
1	-0.577602000	-2.933166000	-2.705123000
1	-1.094243000	-3.176506000	-1.014998000
1	-1.988490000	-2.055714000	-2.062582000

-1015.369860

10-Mn-MAMP

25	1.058218000	-0.256463000	-0.237208000
6	1.649687000	-1.075006000	1.265056000
8	2.026267000	-1.605283000	2.217209000
6	2.684213000	0.510779000	-0.521187000
8	3.716546000	0.994961000	-0.694484000
6	1.516854000	-1.698857000	-1.249365000
8	1.817472000	-2.615054000	-1.883411000
7	-0.890496000	-0.882912000	0.106867000
6	-1.538396000	-1.859653000	-0.556655000
1	-0.962513000	-2.415184000	-1.285998000
6	-2.880254000	-2.149009000	-0.337856000
1	-3.355961000	-2.943858000	-0.900892000
6	-3.584984000	-1.395166000	0.602854000

1	-4.635481000	-1.589281000	0.793997000
6	-2.918264000	-0.379816000	1.285724000
1	-3.430731000	0.237802000	2.015300000
6	-1.569743000	-0.149580000	1.014873000
6	-0.766125000	0.902932000	1.723122000
1	-1.408375000	1.728619000	2.051628000
1	-0.309696000	0.464852000	2.619963000
7	0.310215000	1.390848000	0.833152000
1	-0.161821000	2.005456000	0.128922000
1	-2.666031000	3.064300000	-2.115645000
6	-1.855066000	2.475974000	-1.629601000
8	-1.765402000	1.259297000	-1.944747000
8	-1.118849000	3.105364000	-0.812374000
1	0.729823000	0.531279000	-1.778959000
1	-0.028153000	0.593217000	-1.557116000
6	1.252786000	2.256301000	1.576483000
1	0.715639000	3.046474000	2.114638000
1	1.824584000	1.662141000	2.293964000
1	1.942714000	2.722531000	0.872028000

-1016.518760

TS6-Mn-MAMP

25	0.404020000	-0.790619000	-0.032208000
6	0.002729000	-1.847478000	1.384135000
8	-0.239955000	-2.576186000	2.252174000
6	2.174837000	-1.109676000	0.096574000
8	3.319354000	-1.277094000	0.153841000
6	0.206755000	-2.144975000	-1.200591000
8	0.078321000	-2.945365000	-2.029182000
7	-1.536893000	-0.060387000	-0.255291000
6	-2.404749000	-0.387842000	-1.233638000
1	-2.074398000	-1.140278000	-1.938492000
6	-3.659293000	0.200863000	-1.352143000
1	-4.319306000	-0.101599000	-2.157395000
6	-4.034497000	1.178124000	-0.427584000
1	-5.003234000	1.662845000	-0.494105000
6	-3.134756000	1.529559000	0.576643000
1	-3.377223000	2.294029000	1.306962000
6	-1.897191000	0.886714000	0.636862000
6	-0.878151000	1.178664000	1.697492000
1	-1.001635000	2.195508000	2.089824000
1	-1.019631000	0.483501000	2.534497000
7	0.478505000	0.964939000	1.150770000
1	0.696193000	1.742770000	0.500093000
1	3.508996000	3.013803000	-1.760528000
6	2.606543000	2.512713000	-1.364529000
8	1.941862000	3.039213000	-0.466425000
8	2.362213000	1.376033000	-1.944738000
1	0.666092000	0.094659000	-1.394768000
1	1.420558000	0.764471000	-1.550785000

6	1.493717000	1.050849000	2.222239000
1	2.486026000	1.039304000	1.771363000
1	1.380894000	1.974998000	2.802130000
1	1.394866000	0.191703000	2.889931000

-1016.517380

11-Mn-MAMP

25	1.119864000	-0.227351000	-0.191734000
6	1.793051000	-1.021925000	1.295690000
8	2.280894000	-1.556579000	2.204433000
6	2.662898000	0.557442000	-0.650049000
8	3.639210000	1.089699000	-0.985532000
6	1.479238000	-1.623384000	-1.252135000
8	1.695301000	-2.508638000	-1.973818000
7	-0.854273000	-0.797998000	0.212380000
6	-1.545021000	-1.776213000	-0.405391000
1	-1.010116000	-2.338650000	-1.160700000
6	-2.875423000	-2.057645000	-0.112977000
1	-3.383681000	-2.855620000	-0.642631000
6	-3.528161000	-1.290470000	0.854345000
1	-4.568746000	-1.475547000	1.100926000
6	-2.818871000	-0.274222000	1.493056000
1	-3.288459000	0.353303000	2.243050000
6	-1.482881000	-0.058860000	1.152929000
6	-0.630800000	0.986299000	1.816792000
1	-1.247228000	1.806839000	2.204311000
1	-0.105067000	0.533821000	2.667179000
7	0.384555000	1.471642000	0.859407000
1	-0.123348000	2.009720000	0.151835000
1	-3.148484000	2.236954000	-2.272605000
6	-2.185055000	1.993592000	-1.803021000
8	-1.726931000	2.632324000	-0.864936000
8	-1.619191000	0.947823000	-2.377531000
1	0.575430000	0.488437000	-1.535830000
1	-0.716934000	0.735647000	-1.952952000
6	1.353790000	2.372955000	1.516193000
1	2.009586000	2.805848000	0.759799000
1	0.846123000	3.184075000	2.053372000
1	1.961495000	1.801003000	2.221589000

-1016.524463

1-Mn-AMI

25	-0.823308000	0.023700000	-0.215317000
6	-0.955309000	-0.260421000	1.576249000
8	-1.107581000	-0.404581000	2.721786000
6	-2.472003000	-0.533323000	-0.610816000
8	-3.531114000	-0.903257000	-0.925837000
6	-1.312062000	1.734998000	-0.165177000
8	-1.597994000	2.864330000	-0.182962000

7	1.243952000	0.428979000	-0.142269000
6	2.066846000	1.536021000	-0.163945000
1	1.668150000	2.537936000	-0.203956000
6	3.375721000	1.123900000	-0.134733000
1	4.306559000	1.668193000	-0.143323000
7	3.331932000	-0.258341000	-0.098908000
1	4.130100000	-0.877870000	-0.075329000
6	2.030377000	-0.637128000	-0.102128000
6	1.461813000	-2.017930000	-0.033729000
1	2.108391000	-2.746155000	-0.535486000
1	1.361929000	-2.322493000	1.014109000
7	0.101870000	-1.953902000	-0.620702000
1	0.150801000	-2.030553000	-1.633610000
1	-0.709577000	0.268694000	-1.814858000
1	-0.456722000	-2.736039000	-0.289684000

-765.413160

2-Mn-AMI

25	1.080971000	-0.090716000	-0.010031000
6	1.855885000	1.517558000	0.337169000
8	2.413672000	2.508381000	0.587890000
6	2.503485000	-0.806469000	-0.814860000
8	3.395041000	-1.314765000	-1.366248000
6	1.476892000	-0.830487000	1.560688000
8	1.683694000	-1.353418000	2.580757000
7	-0.843742000	0.559669000	0.576538000
6	-1.680802000	0.425412000	1.665955000
1	-1.382990000	-0.125587000	2.544462000
6	-2.862740000	1.072337000	1.406030000
1	-3.762703000	1.196807000	1.986834000
7	-2.728143000	1.601145000	0.134145000
1	-3.429128000	2.130226000	-0.366091000
6	-1.498672000	1.272018000	-0.329805000
6	-0.875912000	1.613711000	-1.644510000
1	-1.627788000	1.681054000	-2.438417000
1	-0.371083000	2.583539000	-1.573551000
7	0.152966000	0.581177000	-1.912214000
1	-0.284010000	-0.249432000	-2.304180000
1	0.404814000	-1.530708000	-0.325828000
6	-2.114358000	-2.168588000	-0.621173000
8	-2.092945000	-2.821864000	0.346980000
8	-2.184944000	-1.531960000	-1.602226000
1	0.822200000	0.924105000	-2.595930000

-954.007116

TS1-Mn-AMI

25	-0.977460000	-0.065858000	0.020679000
6	-1.588913000	-1.749496000	0.325144000
8	-2.028487000	-2.803289000	0.545003000

6	-2.491880000	0.533858000	-0.718595000
8	-3.449276000	0.962330000	-1.222291000
6	-1.399957000	0.577037000	1.632588000
8	-1.630898000	1.047585000	2.670976000
7	1.008308000	-0.544167000	0.543120000
6	1.866804000	-0.309740000	1.598620000
1	1.531715000	0.167914000	2.506052000
6	3.118480000	-0.762890000	1.267431000
1	4.051548000	-0.770499000	1.807845000
7	3.009820000	-1.258123000	-0.020127000
1	3.761530000	-1.649217000	-0.571203000
6	1.723580000	-1.112991000	-0.419320000
6	1.104115000	-1.475640000	-1.730791000
1	1.831795000	-1.396057000	-2.545837000
1	0.737145000	-2.507439000	-1.706254000
7	-0.055997000	-0.567746000	-1.916258000
1	0.278008000	0.324650000	-2.275603000
1	-0.444587000	1.470067000	-0.279484000
6	1.200661000	2.468121000	-0.559594000
8	1.260744000	2.988945000	0.493694000
8	1.405351000	2.122630000	-1.671857000
1	-0.702375000	-0.957866000	-2.596727000

-953.999432

3-Mn-AMI

25	-0.829060000	-0.203055000	0.006209000
6	-1.179541000	-1.959088000	-0.108878000
8	-1.388127000	-3.093274000	-0.187031000
6	-2.485556000	0.248450000	-0.587833000
8	-3.531707000	0.543139000	-0.977491000
6	-1.334343000	-0.123177000	1.748223000
8	-1.636778000	-0.063040000	2.860327000
7	1.146241000	-0.471179000	0.435250000
6	1.959738000	-0.485049000	1.552992000
1	1.561793000	-0.366947000	2.548392000
6	3.258446000	-0.648253000	1.149931000
1	4.183725000	-0.701371000	1.700721000
7	3.218855000	-0.733745000	-0.232006000
1	4.016539000	-0.850248000	-0.842260000
6	1.932366000	-0.626040000	-0.625429000
6	1.351076000	-0.681743000	-1.997971000
1	2.003913000	-0.201504000	-2.733833000
1	1.206508000	-1.723943000	-2.300805000
7	0.023992000	-0.019448000	-1.911189000
1	0.167718000	1.004436000	-1.983749000
1	-0.523145000	1.616659000	0.117630000
6	0.216243000	2.529777000	-0.055066000
8	0.371127000	3.197747000	0.970366000
8	0.639911000	2.622331000	-1.225130000
1	-0.560142000	-0.314569000	-2.689868000

-954.015348

TS2-Mn-AMI

25	-0.929608000	0.021231000	0.040431000
6	-1.994859000	-1.261765000	-0.579597000
8	-2.644553000	-2.116260000	-1.007761000
6	-2.172689000	1.318002000	-0.307075000
8	-2.946865000	2.138687000	-0.539549000
6	-1.533836000	-0.219321000	1.746860000
8	-1.912851000	-0.389511000	2.822068000
7	0.718982000	-1.110983000	0.304419000
6	1.339023000	-1.791596000	1.338851000
1	0.894158000	-1.866934000	2.318350000
6	2.531960000	-2.284994000	0.886043000
1	3.308443000	-2.853782000	1.371740000
7	2.626809000	-1.894273000	-0.440398000
1	3.399584000	-2.092592000	-1.062183000
6	1.520408000	-1.194057000	-0.757687000
6	1.123653000	-0.579348000	-2.056874000
1	1.981723000	-0.129527000	-2.567697000
1	0.700501000	-1.344355000	-2.716280000
7	0.080579000	0.423129000	-1.734653000
1	0.533840000	1.324706000	-1.430015000
1	2.333557000	1.346297000	0.449393000
6	2.021256000	2.415102000	0.341247000
8	2.610451000	3.253041000	1.056207000
8	1.091708000	2.631114000	-0.505239000
1	-0.488821000	0.611607000	-2.556074000

-954.010553

3'-Mn-AMI

25	-0.813091000	-0.212548000	0.008748000
6	-1.048022000	-1.923901000	0.514015000
8	-1.175580000	-3.028870000	0.836632000
6	-2.504240000	-0.072791000	-0.638477000
8	-3.572215000	0.026913000	-1.067606000
6	-1.302004000	0.408579000	1.633624000
8	-1.601976000	0.803679000	2.678497000
7	1.219911000	-0.294339000	0.441377000
6	2.057639000	0.089858000	1.470311000
1	1.675942000	0.502311000	2.391093000
6	3.356161000	-0.134990000	1.093164000
1	4.294505000	0.034337000	1.596534000
7	3.291239000	-0.662700000	-0.184449000
1	4.081042000	-0.935611000	-0.753504000
6	1.989236000	-0.746789000	-0.541629000
6	1.402633000	-1.292369000	-1.803783000
1	2.024186000	-1.052805000	-2.672789000
1	1.329290000	-2.382923000	-1.735164000

7	0.030872000	-0.738739000	-1.920646000
1	0.059764000	0.191187000	-2.342846000
1	0.282358000	2.533073000	0.903303000
6	0.165256000	2.667323000	-0.192081000
8	0.569750000	3.717263000	-0.715181000
8	-0.392292000	1.688439000	-0.813704000
1	-0.535430000	-1.334331000	-2.519259000

-954.034983

10-Mn-AMI

25	0.982777000	0.113340000	-0.112004000
6	1.824677000	-0.757064000	1.229941000
8	2.342215000	-1.325864000	2.089130000
6	2.144990000	1.513437000	-0.032102000
8	2.873601000	2.405525000	0.033794000
6	1.959921000	-0.769647000	-1.364363000
8	2.573948000	-1.350546000	-2.150223000
7	-0.539041000	-1.245307000	-0.121692000
6	-0.911764000	-2.349366000	-0.866041000
1	-0.271716000	-2.768260000	-1.626583000
6	-2.159608000	-2.747511000	-0.466514000
1	-2.799560000	-3.551648000	-0.792275000
7	-2.535023000	-1.865148000	0.532981000
1	-3.414545000	-1.872969000	1.030965000
6	-1.536550000	-0.974212000	0.710041000
6	-1.453591000	0.153513000	1.681041000
1	-2.403105000	0.695560000	1.732437000
1	-1.230223000	-0.233827000	2.680934000
7	-0.355907000	1.051977000	1.233700000
1	-0.793985000	1.863747000	0.739478000
1	-3.340038000	2.985926000	-1.343802000
6	-2.494599000	2.426872000	-0.881829000
8	-2.325627000	1.232822000	-1.247281000
8	-1.797935000	3.062529000	-0.034351000
1	-0.349943000	0.866658000	-1.230795000
1	0.357043000	0.987373000	-1.545802000
1	0.115965000	1.431437000	2.051015000

-955.186209

TS6-Mn-AMI

25	-1.006414000	0.087555000	0.079614000
6	-1.838153000	-0.957693000	-1.135735000
8	-2.376941000	-1.633066000	-1.904983000
6	-2.262148000	1.385442000	-0.033479000
8	-3.048185000	2.230962000	-0.104721000
6	-1.826202000	-0.725468000	1.468545000
8	-2.329145000	-1.251173000	2.367823000
7	0.641296000	-1.133282000	0.138647000
6	1.162460000	-2.103932000	0.970923000

1	0.619504000	-2.472283000	1.827217000
6	2.409709000	-2.450038000	0.520103000
1	3.140526000	-3.153809000	0.884857000
7	2.634857000	-1.669140000	-0.600666000
1	3.469650000	-1.674925000	-1.170550000
6	1.547705000	-0.890899000	-0.798637000
6	1.286710000	0.100834000	-1.882377000
1	2.195781000	0.649348000	-2.150490000
1	0.927696000	-0.415922000	-2.778873000
7	0.225239000	1.014166000	-1.385194000
1	0.692405000	1.821948000	-0.935259000
1	3.405441000	2.715862000	1.230928000
6	2.428011000	2.349368000	0.858887000
8	1.929162000	1.377062000	1.523366000
8	1.929231000	2.901426000	-0.147433000
1	0.555247000	1.124615000	1.245957000
1	-0.337369000	1.108437000	1.281010000
1	-0.299788000	1.378278000	-2.176439000

-955.185074

11-Mn-AMI

25	1.079676000	0.121596000	-0.050900000
6	1.922784000	-1.185944000	0.885011000
8	2.512705000	-2.013005000	1.449588000
6	2.365050000	1.341224000	0.201898000
8	3.166318000	2.169739000	0.353828000
6	1.738025000	-0.382106000	-1.634102000
8	2.123700000	-0.688800000	-2.687010000
7	-0.667573000	-0.977536000	-0.248205000
6	-1.300285000	-1.734965000	-1.212914000
1	-0.857965000	-1.905091000	-2.182164000
6	-2.505539000	-2.167387000	-0.721069000
1	-3.290257000	-2.766975000	-1.153914000
7	-2.593477000	-1.654768000	0.561679000
1	-3.364984000	-1.784760000	1.201587000
6	-1.465700000	-0.947693000	0.809926000
6	-1.057236000	-0.229533000	2.053126000
1	-1.919631000	0.208939000	2.565702000
1	-0.568516000	-0.928089000	2.741575000
7	-0.068473000	0.795791000	1.636746000
1	-0.585976000	1.621882000	1.330144000
1	-3.659520000	2.447251000	-0.981302000
6	-2.663927000	2.178806000	-0.599800000
8	-1.902032000	1.678684000	-1.553674000
8	-2.342172000	2.336376000	0.570932000
1	-0.967329000	1.449980000	-1.209585000
1	0.360497000	1.308733000	-0.887163000
1	0.501258000	1.065464000	2.434319000

-955.189506

1-Mn-MAMI

25	-0.745894000	0.298563000	-0.203728000
6	-0.909749000	0.069131000	1.592552000
8	-1.084564000	-0.037680000	2.738896000
6	-2.445734000	-0.078644000	-0.588623000
8	-3.541671000	-0.326773000	-0.897161000
6	-1.054972000	2.052449000	-0.188418000
8	-1.221253000	3.204743000	-0.227153000
7	1.348727000	0.503505000	-0.148536000
6	2.279256000	1.518353000	-0.233949000
1	1.984441000	2.552285000	-0.325434000
6	3.539623000	0.976628000	-0.189163000
1	4.520510000	1.422581000	-0.230529000
7	3.356620000	-0.389989000	-0.079957000
1	4.088016000	-1.085574000	-0.028413000
6	2.023268000	-0.633426000	-0.055581000
6	1.312109000	-1.938104000	0.083477000
1	1.890584000	-2.769373000	-0.339132000
1	1.141951000	-2.154594000	1.145260000
7	-0.013805000	-1.788842000	-0.559747000
1	0.121582000	-1.779785000	-1.569015000
1	-0.614262000	0.482736000	-1.808381000
6	-0.921452000	-2.901302000	-0.216104000
1	-0.467704000	-3.879284000	-0.421798000
1	-1.174452000	-2.836621000	0.844828000
1	-1.838309000	-2.802001000	-0.798309000

-804.697889

2-Mn-MAMI

25	-0.984215000	0.324515000	0.073873000
6	-1.818470000	-0.589380000	1.405571000
8	-2.412964000	-1.123675000	2.252117000
6	-2.441897000	0.554369000	-0.926926000
8	-3.358339000	0.723846000	-1.626000000
6	-1.147362000	1.931663000	0.824975000
8	-1.201008000	2.999741000	1.286002000
7	0.950700000	-0.018431000	0.840749000
6	1.929951000	0.690795000	1.506741000
1	1.779180000	1.713847000	1.814443000
6	3.033864000	-0.109411000	1.664230000
1	3.994778000	0.065587000	2.121088000
7	2.706866000	-1.319019000	1.077447000
1	3.308486000	-2.128230000	1.009525000
6	1.444525000	-1.223980000	0.595325000
6	0.637696000	-2.253971000	-0.121684000
1	1.272068000	-2.947359000	-0.688466000
1	0.059248000	-2.842569000	0.600763000
7	-0.324401000	-1.534990000	-0.988950000
1	0.194975000	-1.142922000	-1.772200000
1	-0.263813000	1.129165000	-1.135408000

6	2.257544000	1.177746000	-1.868586000
8	2.349017000	2.307466000	-1.586070000
8	2.212670000	0.047360000	-2.173475000
6	-1.371088000	-2.433768000	-1.512941000
1	-0.944222000	-3.317977000	-2.003627000
1	-2.010570000	-2.752703000	-0.686527000
1	-1.980518000	-1.884934000	-2.231959000

-993.291839

TS1-Mn-MAMI

25	0.815146000	0.131868000	-0.252327000
6	1.336621000	-1.057458000	-1.498226000
8	1.681359000	-1.818445000	-2.300054000
6	2.466862000	0.265726000	0.467675000
8	3.517230000	0.369159000	0.942981000
6	1.095191000	1.557513000	-1.326679000
8	1.245855000	2.481805000	-2.004211000
7	-1.181606000	-0.000430000	-0.724610000
6	-2.122682000	0.737145000	-1.414950000
1	-1.861221000	1.638803000	-1.944862000
6	-3.345555000	0.135141000	-1.274218000
1	-4.323781000	0.393019000	-1.645310000
7	-3.129936000	-0.980493000	-0.484960000
1	-3.835014000	-1.639027000	-0.183579000
6	-1.816036000	-1.029526000	-0.176778000
6	-1.068646000	-2.033902000	0.629259000
1	-1.682310000	-2.452628000	1.434047000
1	-0.745489000	-2.861169000	-0.011542000
7	0.141551000	-1.353206000	1.155474000
1	-0.174994000	-0.738417000	1.921788000
1	0.353772000	1.308877000	1.007779000
6	-0.755047000	1.688143000	1.881624000
8	-0.844401000	2.856098000	1.618482000
8	-1.159594000	0.793356000	2.585687000
6	1.117090000	-2.324649000	1.693731000
1	0.645518000	-3.013880000	2.403761000
1	1.550405000	-2.896238000	0.870510000
1	1.914023000	-1.781727000	2.202555000

-993.284065

3-Mn-MAMI

25	0.761398000	0.079361000	-0.295147000
6	1.199274000	-1.200873000	-1.473216000
8	1.469040000	-2.034794000	-2.226795000
6	2.465304000	0.210243000	0.318439000
8	3.547603000	0.306313000	0.709788000
6	1.028684000	1.410508000	-1.502738000
8	1.175947000	2.261400000	-2.267975000
7	-1.238644000	-0.023853000	-0.671732000

6	-2.187351000	0.684541000	-1.385460000
1	-1.922781000	1.525502000	-2.006639000
6	-3.420057000	0.142834000	-1.134807000
1	-4.406602000	0.403256000	-1.483012000
7	-3.202935000	-0.905786000	-0.256414000
1	-3.914382000	-1.508418000	0.134710000
6	-1.879042000	-0.976940000	-0.003655000
6	-1.121161000	-1.933133000	0.849909000
1	-1.695511000	-2.244943000	1.729777000
1	-0.872399000	-2.832650000	0.274806000
7	0.144137000	-1.254680000	1.235005000
1	-0.108690000	-0.564195000	1.967313000
1	0.383912000	1.398602000	0.940893000
6	-0.384857000	1.842192000	1.730534000
8	-0.648734000	3.025122000	1.503003000
8	-0.722894000	1.030285000	2.615934000
6	1.117535000	-2.215787000	1.798927000
1	0.662700000	-2.823700000	2.589561000
1	1.484106000	-2.871573000	1.006113000
1	1.959121000	-1.663806000	2.217906000

-993.300274

TS2-Mn-MAMI

25	-0.624499000	-0.234078000	0.335691000
6	-0.522298000	-1.842786000	1.128401000
8	-0.444815000	-2.882861000	1.629779000
6	-2.378389000	-0.459567000	-0.061473000
8	-3.498081000	-0.593316000	-0.314266000
6	-1.018058000	0.600675000	1.894649000
8	-1.245114000	1.140629000	2.890050000
7	1.390065000	0.108488000	0.513183000
6	2.237309000	0.843921000	1.318326000
1	1.877109000	1.392565000	2.174318000
6	3.511780000	0.743221000	0.825303000
1	4.447715000	1.165752000	1.152932000
7	3.421713000	-0.064362000	-0.295526000
1	4.188673000	-0.331488000	-0.897470000
6	2.129587000	-0.428491000	-0.448652000
6	1.509643000	-1.308882000	-1.478533000
1	2.006596000	-1.218407000	-2.451058000
1	1.577697000	-2.357119000	-1.165100000
7	0.073712000	-0.938960000	-1.558117000
1	0.017160000	-0.042853000	-2.061602000
1	-1.646822000	2.148871000	-0.161885000
6	-0.954409000	2.566920000	-0.950998000
8	-0.929035000	3.819654000	-1.109616000
8	-0.282081000	1.694206000	-1.562507000
6	-0.704809000	-1.954846000	-2.298539000
1	-0.241898000	-2.187340000	-3.264621000
1	-0.769634000	-2.867679000	-1.702354000

1 -1.711698000 -1.574011000 -2.470629000

-993.294109

3'-Mn-MAMI

25	-0.545282000	-0.220766000	0.342265000
6	-0.195766000	-1.664614000	1.355720000
8	0.039889000	-2.598600000	1.999133000
6	-2.255830000	-0.744525000	0.067553000
8	-3.350783000	-1.071683000	-0.110308000
6	-1.008368000	0.769420000	1.781892000
8	-1.277913000	1.411347000	2.705047000
7	1.428110000	0.381579000	0.396125000
6	2.191149000	1.328374000	1.048680000
1	1.782584000	1.950996000	1.829299000
6	3.458920000	1.312353000	0.526387000
1	4.340486000	1.890841000	0.751644000
7	3.448887000	0.340786000	-0.459272000
1	4.231537000	0.080309000	-1.043879000
6	2.208705000	-0.198177000	-0.504735000
6	1.690141000	-1.295527000	-1.371171000
1	2.156964000	-1.292408000	-2.363211000
1	1.898730000	-2.267473000	-0.908600000
7	0.217194000	-1.131076000	-1.452926000
1	0.020914000	-0.334464000	-2.063762000
1	-2.383876000	2.202396000	-0.225415000
6	-1.637175000	2.240807000	-1.046547000
8	-1.734276000	3.124084000	-1.910135000
8	-0.722853000	1.334078000	-1.005927000
6	-0.433868000	-2.335897000	-2.009902000
1	0.035594000	-2.648114000	-2.950405000
1	-0.363860000	-3.151124000	-1.286010000
1	-1.486337000	-2.117908000	-2.193531000

-993.319934

10-Mn-MAMI

25	0.968046000	-0.080275000	-0.261160000
6	1.798324000	-0.759592000	1.192828000
8	2.311271000	-1.202209000	2.126051000
6	2.274967000	1.161409000	-0.511975000
8	3.108804000	1.943730000	-0.668812000
6	1.785137000	-1.283035000	-1.353912000
8	2.293219000	-2.065165000	-2.033131000
7	-0.660861000	-1.274484000	0.036971000
6	-1.198375000	-2.424385000	-0.508330000
1	-0.671361000	-3.008339000	-1.246498000
6	-2.437961000	-2.630340000	0.037240000
1	-3.176446000	-3.399856000	-0.120125000
7	-2.641242000	-1.583654000	0.920540000
1	-3.469913000	-1.431688000	1.479300000

6	-1.551684000	-0.787371000	0.890226000
6	-1.259322000	0.444101000	1.674043000
1	-2.161362000	1.044509000	1.840626000
1	-0.854662000	0.167273000	2.655119000
7	-0.233364000	1.220274000	0.930336000
1	-0.763655000	1.800924000	0.239024000
1	-3.340442000	2.591313000	-1.963591000
6	-2.486396000	2.104283000	-1.439969000
8	-2.303234000	0.877139000	-1.656036000
8	-1.795232000	2.849287000	-0.681389000
6	0.442854000	2.183515000	1.829231000
1	-0.289739000	2.787762000	2.377591000
1	1.075582000	1.653235000	2.545228000
1	1.066133000	2.850227000	1.232170000
1	-0.354432000	0.512842000	-1.490020000
1	0.363541000	0.629957000	-1.784501000

-994.470021

TS6-Mn-MAMI

25	0.986935000	-0.120008000	-0.237282000
6	1.814218000	-0.831626000	1.198676000
8	2.355584000	-1.289660000	2.113308000
6	2.350384000	1.019443000	-0.578239000
8	3.213776000	1.752384000	-0.814483000
6	1.648006000	-1.374738000	-1.358361000
8	2.041860000	-2.185908000	-2.082577000
7	-0.757621000	-1.160322000	0.115525000
6	-1.405418000	-2.269744000	-0.389896000
1	-0.959859000	-2.892570000	-1.149590000
6	-2.631580000	-2.378213000	0.212916000
1	-3.434167000	-3.088483000	0.095572000
7	-2.714802000	-1.312849000	1.093085000
1	-3.499386000	-1.097601000	1.692936000
6	-1.567353000	-0.603783000	1.006933000
6	-1.142791000	0.600823000	1.774839000
1	-1.990637000	1.255978000	2.007757000
1	-0.685170000	0.292284000	2.722392000
7	-0.121088000	1.308629000	0.960788000
1	-0.656435000	1.856653000	0.263266000
1	-3.460188000	2.148149000	-1.977074000
6	-2.466803000	1.890939000	-1.560185000
8	-1.962923000	0.802930000	-2.008987000
8	-1.954987000	2.660021000	-0.717126000
6	0.638957000	2.272191000	1.786697000
1	-0.032762000	2.944351000	2.334581000
1	1.266842000	1.732250000	2.499505000
1	1.279875000	2.868766000	1.136455000
1	-0.615179000	0.640072000	-1.676485000
1	0.296077000	0.622251000	-1.684426000

-994.466818

11-Mn-MAMI

25	-1.048073000	0.160999000	-0.230914000
6	-1.875093000	0.715882000	1.286956000
8	-2.450770000	1.077706000	2.229069000
6	-2.426946000	-0.828161000	-0.801487000
8	-3.292000000	-1.490317000	-1.206891000
6	-1.549554000	1.575398000	-1.203678000
8	-1.830189000	2.491599000	-1.861307000
7	0.802705000	0.995232000	0.321589000
6	1.567577000	2.098391000	-0.000146000
1	1.227480000	2.837662000	-0.708555000
6	2.746714000	2.042765000	0.698226000
1	3.603351000	2.697100000	0.724141000
7	2.684135000	0.881704000	1.449437000
1	3.401283000	0.538931000	2.073815000
6	1.497086000	0.281113000	1.197758000
6	0.936555000	-0.971749000	1.782397000
1	1.725815000	-1.689051000	2.038999000
1	0.381922000	-0.735863000	2.698844000
7	-0.017620000	-1.527751000	0.795221000
1	0.551591000	-1.926745000	0.044976000
1	3.679207000	-1.384040000	-2.267163000
6	2.677609000	-1.344061000	-1.815608000
8	1.941537000	-0.394408000	-2.360651000
8	2.327668000	-2.101482000	-0.919799000
6	-0.853006000	-2.593520000	1.381403000
1	-0.243426000	-3.371585000	1.858649000
1	-1.525672000	-2.158120000	2.124332000
1	-1.453597000	-3.046544000	0.591448000
1	1.005268000	-0.365419000	-1.954401000
1	-0.331561000	-0.386723000	-1.614271000

-994.473282

1-Mn-AMIM

25	-0.876793000	0.015697000	-0.202811000
6	-1.019333000	-0.224377000	1.593345000
8	-1.165384000	-0.339673000	2.743192000
6	-2.544513000	-0.487290000	-0.598573000
8	-3.613841000	-0.825888000	-0.915557000
6	-1.304482000	1.743396000	-0.191214000
8	-1.553752000	2.881151000	-0.234475000
7	1.185238000	0.330096000	-0.131331000
6	2.031120000	1.530747000	-0.253941000
1	1.705575000	2.305969000	0.442533000
6	3.463099000	1.013597000	0.034808000
1	3.748487000	1.178207000	1.081355000
7	3.301466000	-0.431975000	-0.236444000
1	3.969853000	-1.088417000	0.146785000

6	1.960935000	-0.702121000	-0.134778000
6	1.374531000	-2.081623000	-0.074014000
1	1.984559000	-2.792578000	-0.641503000
1	1.365813000	-2.409565000	0.971183000
7	-0.022602000	-2.009072000	-0.560903000
1	-0.049204000	-2.130151000	-1.569597000
1	-0.736674000	0.222836000	-1.812612000
1	1.933081000	1.924353000	-1.273402000
1	4.219613000	1.455973000	-0.615579000
1	-0.574332000	-2.761108000	-0.157219000

-766.593059

2-Mn-AMIM

25	-1.132631000	0.070752000	0.031846000
6	-1.848992000	-1.529456000	-0.447491000
8	-2.358235000	-2.541973000	-0.715323000
6	-2.576836000	1.049501000	-0.350730000
8	-3.482307000	1.738259000	-0.603361000
6	-1.552873000	-0.044605000	1.757639000
8	-1.778555000	-0.081583000	2.900255000
7	0.790336000	-0.720959000	0.255648000
6	1.583228000	-1.143948000	1.425085000
1	1.007438000	-1.834097000	2.045293000
6	2.852368000	-1.792061000	0.811141000
1	2.779527000	-2.886056000	0.788362000
7	2.821040000	-1.242336000	-0.562484000
1	3.330875000	-1.711043000	-1.300549000
6	1.539037000	-0.817041000	-0.792662000
6	0.999882000	-0.445286000	-2.142273000
1	1.774700000	0.030751000	-2.752392000
1	0.690472000	-1.364207000	-2.652123000
7	-0.186039000	0.421529000	-1.952458000
1	0.100147000	1.396703000	-1.935332000
1	-0.486425000	1.505003000	0.456079000
6	2.044439000	2.301762000	0.254167000
8	2.208880000	2.212720000	1.407208000
8	1.927269000	2.406407000	-0.906655000
1	1.821536000	-0.260382000	2.027340000
1	3.770491000	-1.506864000	1.327822000
1	-0.828271000	0.309914000	-2.731826000

-955.185887

TS1-Mn-AMIM

25	-0.972704000	-0.174666000	-0.007335000
6	-1.230253000	-1.954507000	0.217083000
8	-1.417315000	-3.085638000	0.392904000
6	-2.635633000	0.153365000	-0.604523000
8	-3.693379000	0.407473000	-1.009084000
6	-1.383759000	0.249366000	1.687396000

8	-1.609774000	0.562279000	2.780852000
7	1.094943000	-0.324884000	0.351684000
6	1.926330000	-0.199717000	1.562820000
1	1.476693000	-0.755010000	2.388598000
6	3.311046000	-0.754324000	1.136080000
1	3.466921000	-1.779693000	1.491587000
7	3.197694000	-0.728044000	-0.340023000
1	3.779415000	-1.345628000	-0.892033000
6	1.869399000	-0.626145000	-0.641164000
6	1.295688000	-0.879895000	-2.004154000
1	1.930195000	-0.435457000	-2.778351000
1	1.267554000	-1.961273000	-2.174849000
7	-0.083263000	-0.339750000	-2.036585000
1	-0.038837000	0.637439000	-2.321480000
1	-0.788778000	1.533466000	-0.226506000
6	0.408867000	2.546080000	-0.311188000
8	0.529195000	3.007588000	0.788398000
8	0.806569000	2.498756000	-1.450903000
1	1.971119000	0.859528000	1.847792000
1	4.140456000	-0.131160000	1.474666000
1	-0.645234000	-0.835812000	-2.723002000

-955.179756

3-Mn-AMIM

25	-0.909224000	-0.148141000	0.005745000
6	-1.348062000	-1.881461000	-0.094893000
8	-1.605444000	-3.006749000	-0.163065000
6	-2.569451000	0.389877000	-0.500509000
8	-3.618345000	0.739396000	-0.835702000
6	-1.318575000	-0.057953000	1.771373000
8	-1.559585000	0.005463000	2.898419000
7	1.054791000	-0.498169000	0.328301000
6	1.929710000	-0.430441000	1.517271000
1	1.549443000	-1.073906000	2.312785000
6	3.317362000	-0.879990000	0.987982000
1	3.526182000	-1.930833000	1.219752000
7	3.136021000	-0.703921000	-0.467923000
1	3.790008000	-1.081623000	-1.139432000
6	1.810140000	-0.634607000	-0.721385000
6	1.175550000	-0.664411000	-2.076174000
1	1.813632000	-0.181987000	-2.822915000
1	1.027898000	-1.706637000	-2.375437000
7	-0.143970000	0.003470000	-1.950986000
1	0.008606000	1.021755000	-2.045924000
1	-0.534281000	1.683883000	0.112310000
6	0.378249000	2.422247000	-0.035434000
8	0.783409000	2.897490000	1.031402000
8	0.707063000	2.581663000	-1.230249000
1	1.939793000	0.604703000	1.876218000
1	4.135683000	-0.261043000	1.359015000

1	-0.760577000	-0.298128000	-2.701577000
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-955.197968

TS2-Mn-AMIM

25	-1.021876000	-0.025824000	0.028032000
6	-1.880696000	-1.143223000	-1.048795000
8	-2.386085000	-1.885812000	-1.778596000
6	-2.401469000	1.171526000	0.000613000
8	-3.260603000	1.941226000	-0.028668000
6	-1.661360000	-0.852839000	1.518187000
8	-2.058726000	-1.383416000	2.462893000
7	0.741571000	-0.917808000	0.113968000
6	1.350774000	-1.951703000	0.977691000
1	0.902608000	-2.922834000	0.738112000
6	2.853959000	-1.902457000	0.607709000
1	3.310062000	-2.890646000	0.532277000
7	2.800634000	-1.234586000	-0.709560000
1	3.631106000	-0.813192000	-1.104508000
6	1.619059000	-0.593809000	-0.801185000
6	1.225019000	0.350879000	-1.885776000
1	2.043221000	1.039775000	-2.110749000
1	0.985941000	-0.226990000	-2.784348000
7	0.017053000	1.058571000	-1.410116000
1	0.314040000	1.864392000	-0.804929000
1	2.142204000	2.816562000	2.034149000
6	1.855151000	2.455798000	1.018692000
8	2.696842000	1.767937000	0.391030000
8	0.691491000	2.788945000	0.624640000
1	1.166016000	-1.734287000	2.030629000
1	3.425569000	-1.288467000	1.312313000
1	-0.514655000	1.421979000	-2.196998000

-955.198150

3'-Mn-AMIM

25	-0.636223000	-0.459222000	0.017290000
6	-0.328097000	-2.211105000	0.274640000
8	-0.103979000	-3.336432000	0.434919000
6	-2.341631000	-0.747351000	-0.526692000
8	-3.424989000	-0.921592000	-0.892700000
6	-1.128026000	-0.211588000	1.737138000
8	-1.419554000	-0.041450000	2.843618000
7	1.349503000	-0.001718000	0.337493000
6	2.067566000	0.622752000	1.463889000
1	1.930081000	0.044887000	2.379943000
6	3.542741000	0.667300000	0.989037000
1	4.123491000	-0.174688000	1.384669000
7	3.372239000	0.533191000	-0.473763000
1	4.153062000	0.274296000	-1.062421000
6	2.135937000	0.005022000	-0.691421000

6	1.647460000	-0.511540000	-2.011540000
1	2.080957000	0.058185000	-2.839505000
1	1.965180000	-1.553367000	-2.119896000
7	0.165773000	-0.456998000	-2.002676000
1	-0.149423000	0.467013000	-2.301138000
1	-2.419513000	2.036107000	0.575586000
6	-1.644874000	2.438288000	-0.111946000
8	-1.703015000	3.629430000	-0.453568000
8	-0.746502000	1.596039000	-0.486017000
1	1.656849000	1.626786000	1.622902000
1	4.046734000	1.601079000	1.243300000
1	-0.216594000	-1.139686000	-2.651722000

-955.216311

10-AMIM

25	-1.035335000	0.082232000	0.116564000
6	-1.835695000	-0.805134000	-1.234699000
8	-2.319818000	-1.387705000	-2.104741000
6	-2.303060000	1.390316000	0.112763000
8	-3.099663000	2.225420000	0.088980000
6	-1.908428000	-0.917765000	1.356905000
8	-2.455983000	-1.572761000	2.134070000
7	0.582122000	-1.135893000	0.043755000
6	1.014025000	-2.328420000	0.795914000
1	0.446178000	-3.199463000	0.448311000
6	2.525235000	-2.449443000	0.464957000
1	2.834655000	-3.474823000	0.255966000
7	2.628619000	-1.602368000	-0.743931000
1	3.526084000	-1.220570000	-1.013001000
6	1.531927000	-0.799898000	-0.771239000
6	1.337892000	0.348522000	-1.707036000
1	2.250994000	0.947641000	-1.776761000
1	1.115449000	-0.048418000	-2.703032000
7	0.200847000	1.163350000	-1.212716000
1	0.603597000	1.975476000	-0.690712000
1	3.178569000	3.120340000	1.372925000
6	2.365656000	2.530023000	0.891004000
8	2.316875000	1.297823000	1.148863000
8	1.580227000	3.174570000	0.132239000
1	0.823517000	-2.198824000	1.863550000
1	3.149494000	-2.040375000	1.266986000
1	-0.428162000	0.990282000	1.564657000
1	0.271132000	0.861604000	1.245922000
1	-0.307663000	1.547711000	-2.005365000

-956.369305

TS6-Mn-AMIM

25	-1.074511000	0.123183000	0.119811000
6	-1.904615000	-0.772659000	-1.198479000

8	-2.412999000	-1.358739000	-2.054489000
6	-2.354978000	1.419421000	0.140830000
8	-3.157615000	2.249547000	0.134352000
6	-1.904392000	-0.876424000	1.390775000
8	-2.427101000	-1.528496000	2.187448000
7	0.577905000	-1.050360000	0.037311000
6	1.092401000	-2.160426000	0.859284000
1	0.490932000	-3.057211000	0.673177000
6	2.561421000	-2.333995000	0.384682000
1	2.831043000	-3.377225000	0.210652000
7	2.555135000	-1.568722000	-0.882350000
1	3.422139000	-1.221458000	-1.270470000
6	1.452637000	-0.777505000	-0.879183000
6	1.162917000	0.307797000	-1.868301000
1	2.072874000	0.863056000	-2.114953000
1	0.770411000	-0.140697000	-2.786671000
7	0.145039000	1.196043000	-1.254013000
1	0.685176000	1.923619000	-0.738933000
1	3.637676000	2.555386000	1.202702000
6	2.623062000	2.203378000	0.904966000
8	2.120841000	1.271201000	1.589122000
8	2.100544000	2.781738000	-0.092659000
1	1.017991000	-1.908078000	1.919388000
1	3.272419000	-1.891790000	1.090411000
1	-0.421994000	1.068381000	1.586240000
1	0.356777000	1.021182000	1.396849000
1	-0.379281000	1.666987000	-1.987939000

-956.364376

11-Mn-AMIM

25	-1.153784000	0.118807000	0.053939000
6	-1.911020000	-1.250135000	-0.864656000
8	-2.437008000	-2.123925000	-1.421987000
6	-2.532806000	1.241243000	-0.172798000
8	-3.394651000	2.008496000	-0.315174000
6	-1.732833000	-0.432720000	1.652413000
8	-2.066728000	-0.769544000	2.713943000
7	0.699339000	-0.836297000	0.177765000
6	1.358996000	-1.658816000	1.206868000
1	0.817088000	-2.606931000	1.304463000
6	2.797721000	-1.865360000	0.663418000
1	3.157154000	-2.888756000	0.783855000
7	2.622227000	-1.524074000	-0.767159000
1	3.425482000	-1.230647000	-1.308465000
6	1.458786000	-0.812868000	-0.868097000
6	0.997468000	-0.105388000	-2.106385000
1	1.836454000	0.369962000	-2.625100000
1	0.554008000	-0.845629000	-2.781145000
7	-0.041242000	0.867912000	-1.702476000
1	0.427973000	1.718068000	-1.389112000

1	3.575612000	2.426221000	1.018390000
6	2.580844000	2.173122000	0.623689000
8	2.289951000	2.294436000	-0.558783000
8	1.783562000	1.730344000	1.577798000
1	1.335317000	-1.149805000	2.172931000
1	3.510729000	-1.178538000	1.134048000
1	-0.485007000	1.392257000	0.891362000
1	0.851193000	1.512116000	1.217919000
1	-0.627631000	1.105792000	-2.497624000

-956.370878

1-Mn-MAMIM

25	-0.788627000	0.307200000	-0.196430000
6	-0.974852000	0.072929000	1.595893000
8	-1.152235000	-0.035987000	2.741919000
6	-2.500998000	0.011590000	-0.604428000
8	-3.602690000	-0.186766000	-0.929327000
6	-1.016403000	2.072914000	-0.172467000
8	-1.131919000	3.232012000	-0.204779000
7	1.294807000	0.400871000	-0.126217000
6	2.269272000	1.491784000	-0.306140000
1	2.042619000	2.326750000	0.359851000
6	3.636843000	0.826694000	-0.007150000
1	3.953129000	1.001420000	1.028714000
7	3.309301000	-0.601475000	-0.214427000
1	3.904310000	-1.313915000	0.189344000
6	1.948446000	-0.712281000	-0.092273000
6	1.199687000	-2.004816000	0.024759000
1	1.743746000	-2.831556000	-0.448353000
1	1.083953000	-2.244734000	1.088495000
7	-0.149383000	-1.814005000	-0.553417000
1	-0.062018000	-1.813720000	-1.567631000
1	-0.621662000	0.496503000	-1.805075000
6	-1.076880000	-2.893533000	-0.161797000
1	-0.667081000	-3.887541000	-0.382719000
1	-1.277350000	-2.816078000	0.909524000
1	-2.016275000	-2.764920000	-0.700847000
1	2.203534000	1.852019000	-1.340417000
1	4.429778000	1.152270000	-0.682588000

-805.877816

2-Mn-MAMIM

25	-1.038421000	-0.295847000	0.140263000
6	-1.814678000	-0.439686000	-1.495459000
8	-2.360292000	-0.560801000	-2.517307000
6	-2.511842000	0.214039000	1.009660000
8	-3.439092000	0.564753000	1.622340000
6	-1.261457000	-2.001405000	0.599134000
8	-1.356980000	-3.113478000	0.933719000

7	0.891349000	-0.563826000	-0.602516000
6	1.829574000	-1.702402000	-0.606388000
1	1.347108000	-2.592360000	-1.015718000
6	3.021511000	-1.206773000	-1.466238000
1	2.956788000	-1.573236000	-2.497880000
7	2.818649000	0.259347000	-1.424611000
1	3.241196000	0.841178000	-2.137096000
6	1.509423000	0.466826000	-1.075797000
6	0.796115000	1.779096000	-1.188074000
1	1.483640000	2.622300000	-1.049067000
1	0.377715000	1.853312000	-2.198953000
7	-0.321790000	1.803001000	-0.218463000
1	0.066556000	2.025692000	0.695103000
1	-0.343971000	-0.148111000	1.606409000
6	2.147075000	0.598380000	2.258386000
8	2.431161000	-0.493647000	2.560309000
8	1.906706000	1.708407000	1.968529000
6	-1.328563000	2.826653000	-0.562361000
1	-0.875549000	3.816527000	-0.702735000
1	-1.838779000	2.529915000	-1.481815000
1	-2.064676000	2.880611000	0.240780000
1	2.125576000	-1.918342000	0.426004000
1	3.992503000	-1.481204000	-1.050384000

-994.471356

TS1-Mn-MAMIM

25	-0.863511000	-0.256956000	-0.149534000
6	-1.378387000	0.237364000	-1.797668000
8	-1.708180000	0.553445000	-2.862422000
6	-2.534998000	-0.152952000	0.530561000
8	-3.597530000	-0.093086000	0.987040000
6	-1.041798000	-2.020694000	-0.497550000
8	-1.130078000	-3.154938000	-0.706719000
7	1.126168000	-0.232886000	-0.589838000
6	2.140103000	-1.279192000	-0.832163000
1	1.825256000	-1.938220000	-1.643273000
6	3.429753000	-0.483124000	-1.165457000
1	3.610920000	-0.427548000	-2.245061000
7	3.086510000	0.852649000	-0.633754000
1	3.620792000	1.673039000	-0.882938000
6	1.739275000	0.906188000	-0.486927000
6	0.943626000	2.137662000	-0.196108000
1	1.514759000	2.855007000	0.404133000
1	0.688986000	2.620773000	-1.146015000
7	-0.309365000	1.725033000	0.481395000
1	-0.057225000	1.531983000	1.461408000
1	-0.413981000	-0.751593000	1.528125000
6	0.782682000	-0.586954000	2.370974000
8	1.070482000	-1.756948000	2.378029000
8	1.002686000	0.531138000	2.760861000

6	-1.320510000	2.802873000	0.452264000
1	-0.907686000	3.749977000	0.819575000
1	-1.675872000	2.938428000	-0.571041000
1	-2.162899000	2.515219000	1.080833000
1	2.247027000	-1.876020000	0.079951000
1	4.316983000	-0.884645000	-0.673846000

-994.464819

3-Mn-MAMIM

25	-0.819303000	-0.204476000	-0.220770000
6	-1.303855000	0.582660000	-1.753626000
8	-1.595399000	1.104226000	-2.743722000
6	-2.525895000	-0.245708000	0.398752000
8	-3.609374000	-0.283735000	0.798821000
6	-0.970235000	-1.871879000	-0.925187000
8	-1.045573000	-2.934151000	-1.369721000
7	1.162972000	-0.096756000	-0.594230000
6	2.198163000	-1.076948000	-0.983960000
1	1.922564000	-1.581090000	-1.911992000
6	3.488183000	-0.225051000	-1.118443000
1	3.707487000	0.029557000	-2.161835000
7	3.106843000	0.987839000	-0.365869000
1	3.653851000	1.836819000	-0.399189000
6	1.760655000	1.006531000	-0.253606000
6	0.936903000	2.149804000	0.241738000
1	1.474603000	2.742152000	0.990332000
1	0.701898000	2.806076000	-0.603658000
7	-0.327322000	1.592683000	0.785732000
1	-0.087714000	1.205513000	1.716267000
1	-0.409300000	-1.037563000	1.405867000
6	0.496145000	-1.124186000	2.161592000
8	1.002748000	-2.251473000	2.169731000
8	0.717534000	-0.075096000	2.803524000
6	-1.352086000	2.647197000	0.952691000
1	-0.954982000	3.501832000	1.512562000
1	-1.689844000	2.985953000	-0.029317000
1	-2.202698000	2.233347000	1.494742000
1	2.279722000	-1.825716000	-0.188265000
1	4.362168000	-0.704023000	-0.674482000

-994.482582

TS2-Mn-MAMIM

25	-0.942433000	-0.246812000	0.141747000
6	-1.804757000	-1.052599000	-1.181871000
8	-2.313146000	-1.575078000	-2.080913000
6	-2.398052000	0.751544000	0.606012000
8	-3.308937000	1.388169000	0.917259000
6	-1.397923000	-1.551470000	1.326962000
8	-1.680334000	-2.388968000	2.068927000

7	0.887467000	-0.953784000	-0.114668000
6	1.650394000	-2.108058000	0.407490000
1	1.306577000	-3.018117000	-0.097449000
6	3.118814000	-1.769115000	0.050554000
1	3.683991000	-2.630962000	-0.306950000
7	2.927902000	-0.770395000	-1.022185000
1	3.685525000	-0.153447000	-1.284537000
6	1.678532000	-0.278318000	-0.907055000
6	1.126387000	0.877952000	-1.665690000
1	1.856492000	1.690238000	-1.735411000
1	0.878001000	0.540894000	-2.678534000
7	-0.108297000	1.313092000	-0.978037000
1	0.183587000	1.870852000	-0.140301000
1	2.003990000	2.007236000	2.853080000
6	1.700760000	1.989476000	1.780269000
8	2.580087000	1.696870000	0.934618000
8	0.479738000	2.267157000	1.547623000
6	-0.952180000	2.153379000	-1.852337000
1	-0.368117000	2.963645000	-2.304377000
1	-1.388370000	1.540348000	-2.644935000
1	-1.757836000	2.588960000	-1.260530000
1	1.490915000	-2.224388000	1.480287000
1	3.645449000	-1.309297000	0.894120000

-994.482498

3'-Mn-MAMIM

25	-0.768264000	-0.015534000	0.275454000
6	-0.979778000	-1.409640000	1.388177000
8	-1.090821000	-2.320647000	2.095319000
6	-2.532407000	0.044199000	-0.148085000
8	-3.651743000	0.094781000	-0.432709000
6	-0.987290000	1.172454000	1.618195000
8	-1.112440000	1.921072000	2.491691000
7	1.286800000	-0.093533000	0.453428000
6	2.285374000	0.735426000	1.156002000
1	2.056136000	0.796921000	2.221614000
6	3.633783000	0.027835000	0.863402000
1	3.941351000	-0.621546000	1.691741000
7	3.277310000	-0.782539000	-0.320946000
1	3.862795000	-1.552422000	-0.616680000
6	1.921141000	-0.892124000	-0.345789000
6	1.153454000	-1.830266000	-1.224924000
1	1.667757000	-1.997877000	-2.178357000
1	1.075497000	-2.797506000	-0.715580000
7	-0.210951000	-1.285455000	-1.418245000
1	-0.153370000	-0.522803000	-2.097481000
1	0.092007000	2.975384000	-0.066794000
6	0.047421000	2.603861000	-1.112367000
8	0.414619000	3.352658000	-2.030875000
8	-0.393143000	1.404150000	-1.254557000

6	-1.150599000	-2.310817000	-1.918093000
1	-0.756583000	-2.823384000	-2.803808000
1	-1.334665000	-3.044524000	-1.129778000
1	-2.094413000	-1.828732000	-2.175370000
1	2.257902000	1.749079000	0.739141000
1	4.441717000	0.724745000	0.635283000

-994.501100

10-Mn-MAMIM

25	1.005857000	-0.130401000	-0.258401000
6	1.812629000	-0.803778000	1.207396000
8	2.301677000	-1.246102000	2.153803000
6	2.386296000	1.009361000	-0.587963000
8	3.267192000	1.728497000	-0.788236000
6	1.717110000	-1.433636000	-1.308953000
8	2.159603000	-2.278130000	-1.959225000
7	-0.689934000	-1.175077000	0.113862000
6	-1.282806000	-2.413488000	-0.423346000
1	-0.786036000	-3.278787000	0.030879000
6	-2.776530000	-2.317308000	-0.013630000
1	-3.174622000	-3.258728000	0.368474000
7	-2.725154000	-1.287561000	1.048429000
1	-3.562651000	-0.768892000	1.279524000
6	-1.555288000	-0.613583000	0.897065000
6	-1.186779000	0.640513000	1.616834000
1	-2.047814000	1.310562000	1.720033000
1	-0.847389000	0.371593000	2.623992000
7	-0.082861000	1.302266000	0.880317000
1	-0.547425000	1.902699000	0.160009000
1	-3.147468000	2.763246000	-1.988633000
6	-2.350216000	2.232826000	-1.418700000
8	-2.387960000	0.974489000	-1.406030000
8	-1.490456000	2.967974000	-0.844357000
6	0.659945000	2.227142000	1.766361000
1	-0.025368000	2.908638000	2.284558000
1	1.230670000	1.662998000	2.508089000
1	1.350221000	2.819926000	1.164952000
1	-1.144305000	-2.466535000	-1.505449000
1	-3.399849000	-1.967833000	-0.843356000
1	0.394430000	0.583094000	-1.813997000
1	-0.299803000	0.458523000	-1.485322000

-995.654134

TS6-Mn-MAMIM

25	1.023001000	-0.177867000	-0.226639000
6	1.803882000	-0.721974000	1.305254000
8	2.313021000	-1.079954000	2.280829000
6	2.508255000	0.697939000	-0.772887000
8	3.451574000	1.262835000	-1.134296000

6	1.491732000	-1.690300000	-1.098855000
8	1.764736000	-2.664369000	-1.659415000
7	-0.802798000	-0.895348000	0.323146000
6	-1.610469000	-2.067073000	-0.056216000
1	-1.167111000	-2.968222000	0.382394000
6	-3.016247000	-1.762518000	0.530929000
1	-3.455677000	-2.616589000	1.049166000
7	-2.713866000	-0.663462000	1.477820000
1	-3.446587000	-0.025435000	1.759480000
6	-1.486538000	-0.174273000	1.150976000
6	-0.869074000	1.074724000	1.692700000
1	-1.621057000	1.846562000	1.893447000
1	-0.358983000	0.842892000	2.634808000
7	0.126722000	1.532202000	0.693309000
1	-0.444646000	1.937486000	-0.067121000
1	-3.463328000	1.589523000	-2.197546000
6	-2.439122000	1.452399000	-1.794892000
8	-1.842217000	0.395158000	-2.191047000
8	-1.990976000	2.320946000	-1.011860000
6	0.993064000	2.594453000	1.245569000
1	0.399162000	3.405379000	1.684812000
1	1.647315000	2.173647000	2.013004000
1	1.609212000	3.003642000	0.443927000
1	-1.622664000	-2.174775000	-1.142602000
1	-3.709224000	-1.414063000	-0.242057000
1	0.425979000	0.393722000	-1.734265000
1	-0.459843000	0.341974000	-1.760555000

-995.651289

11-Mn-MAMIM

25	1.085993000	-0.198309000	-0.213760000
6	1.855511000	-0.634113000	1.369806000
8	2.390513000	-0.929511000	2.358275000
6	2.536975000	0.623209000	-0.868785000
8	3.450086000	1.177475000	-1.327970000
6	1.495083000	-1.745148000	-1.011088000
8	1.718168000	-2.747013000	-1.556895000
7	-0.812308000	-0.808936000	0.394976000
6	-1.605829000	-2.035698000	0.201628000
1	-1.125133000	-2.858695000	0.743458000
6	-2.996494000	-1.684775000	0.794013000
1	-3.416731000	-2.488091000	1.401578000
7	-2.672666000	-0.500458000	1.622247000
1	-3.405735000	0.155362000	1.860270000
6	-1.469762000	-0.022739000	1.182775000
6	-0.855299000	1.273270000	1.611139000
1	-1.613810000	2.053360000	1.750880000
1	-0.350859000	1.116186000	2.572112000
7	0.153626000	1.656704000	0.599717000
1	-0.372772000	1.995616000	-0.207889000

1	-3.603075000	1.166638000	-2.374622000
6	-2.593504000	1.176820000	-1.938950000
8	-1.874158000	0.156880000	-2.367467000
8	-2.222865000	2.039582000	-1.153796000
6	1.037477000	2.734039000	1.084389000
1	0.465311000	3.595666000	1.451894000
1	1.665926000	2.349997000	1.891722000
1	1.681735000	3.057096000	0.265545000
1	-1.645938000	-2.299306000	-0.857425000
1	-3.714781000	-1.416913000	0.010491000
1	0.415125000	0.235894000	-1.671958000
1	-0.928556000	0.175267000	-1.977372000

-995.653507

1-Mn-AMNHC

25	-0.796032000	0.017014000	-0.188910000
6	-0.958286000	-0.229082000	1.594516000
8	-1.095820000	-0.340742000	2.747786000
6	-2.444186000	-0.534894000	-0.670065000
8	-3.493428000	-0.881793000	-1.037382000
6	-1.245097000	1.730543000	-0.156384000
8	-1.484714000	2.873032000	-0.179237000
6	1.154470000	0.397657000	-0.134924000
7	1.995491000	1.459656000	-0.177725000
1	1.672250000	2.415376000	-0.217546000
6	3.332871000	1.070566000	-0.189779000
1	4.145007000	1.778431000	-0.231231000
6	3.333292000	-0.288663000	-0.149695000
1	4.145813000	-0.997713000	-0.145062000
7	1.996244000	-0.672501000	-0.119987000
6	1.436071000	-2.009284000	0.007285000
1	2.078127000	-2.723608000	-0.515789000
1	1.374079000	-2.284915000	1.064270000
7	0.070224000	-1.945025000	-0.537179000
1	0.081391000	-2.082166000	-1.544647000
1	-0.600005000	0.240818000	-1.760373000
1	-0.492696000	-2.691523000	-0.137691000

-765.390693

2-Mn-AMNHC

25	1.090617000	-0.103240000	0.049740000
6	1.964456000	1.333642000	-0.613480000
8	2.557051000	2.262723000	-0.995549000
6	2.379153000	-1.334886000	-0.228220000
8	3.172375000	-2.172519000	-0.384598000
6	1.561115000	0.185096000	1.733755000
8	1.803608000	0.361456000	2.861797000
6	-0.653234000	0.829284000	0.245310000
7	-1.400972000	1.412698000	1.213695000

1	-1.088165000	1.503514000	2.169341000
6	-2.649504000	1.811554000	0.745459000
1	-3.384915000	2.283034000	1.377233000
6	-2.687876000	1.472672000	-0.571126000
1	-3.460311000	1.597340000	-1.313159000
7	-1.461919000	0.875131000	-0.849656000
6	-0.956900000	0.397300000	-2.129449000
1	-1.780435000	-0.040943000	-2.699699000
1	-0.531477000	1.233545000	-2.691575000
7	0.114905000	-0.567250000	-1.832986000
1	-0.273142000	-1.501678000	-1.734352000
1	0.275694000	-1.348216000	0.638274000
6	-2.376555000	-2.013085000	0.409508000
8	-2.572884000	-1.755270000	1.531301000
8	-2.215717000	-2.282329000	-0.719330000
1	0.773842000	-0.591591000	-2.606419000

-953.984337

TS1-Mn-AMNHC

25	-0.939915000	-0.117285000	0.022186000
6	-1.498618000	-1.831815000	0.032652000
8	-1.872749000	-2.933083000	0.066866000
6	-2.464348000	0.591396000	-0.657901000
8	-3.418468000	1.084255000	-1.098883000
6	-1.394118000	0.197135000	1.714648000
8	-1.633219000	0.432340000	2.829295000
6	0.965043000	-0.591538000	0.460361000
7	1.792441000	-0.587069000	1.532532000
1	1.487158000	-0.334303000	2.461327000
6	3.097804000	-0.921738000	1.188662000
1	3.898459000	-0.960419000	1.909573000
6	3.089422000	-1.151488000	-0.152249000
1	3.881479000	-1.432980000	-0.827773000
7	1.780002000	-0.944681000	-0.570929000
6	1.224527000	-1.107211000	-1.909760000
1	1.985877000	-0.836183000	-2.646350000
1	0.928506000	-2.148951000	-2.060784000
7	0.024559000	-0.260887000	-1.980596000
1	0.283143000	0.698521000	-2.208749000
1	-0.387157000	1.479145000	0.007315000
6	0.973524000	2.612449000	-0.239301000
8	1.047810000	3.092636000	0.841202000
8	1.237050000	2.428196000	-1.385238000
1	-0.601406000	-0.602135000	-2.704879000

-953.975489

3-Mn-AMNHC

25	-0.819044000	-0.231206000	0.003734000
6	-1.049132000	-1.997969000	-0.153437000

8	-1.173200000	-3.144727000	-0.253658000
6	-2.505599000	0.151469000	-0.605692000
8	-3.567871000	0.389351000	-0.989588000
6	-1.314081000	-0.229134000	1.738491000
8	-1.594265000	-0.218041000	2.860676000
6	1.131772000	-0.450506000	0.411856000
7	1.965726000	-0.497610000	1.474919000
1	1.649081000	-0.442779000	2.432785000
6	3.294542000	-0.588344000	1.084585000
1	4.107039000	-0.624692000	1.792170000
6	3.292332000	-0.604290000	-0.277432000
1	4.102351000	-0.661706000	-0.986733000
7	1.961519000	-0.519727000	-0.659703000
6	1.396990000	-0.536242000	-2.003730000
1	2.054766000	0.020296000	-2.676290000
1	1.306995000	-1.567850000	-2.352335000
7	0.055227000	0.063663000	-1.899720000
1	0.144837000	1.096502000	-1.937729000
1	-0.613507000	1.584681000	0.169966000
6	0.063947000	2.555223000	0.026619000
8	0.184080000	3.188525000	1.077350000
8	0.463434000	2.721106000	-1.142940000
1	-0.514803000	-0.239516000	-2.685932000

-953.990302

TS2-Mn-AMNHC

25	-0.765064000	-0.338128000	0.003708000
6	-0.912730000	-2.096254000	0.213577000
8	-0.962089000	-3.245372000	0.338657000
6	-2.481328000	-0.184259000	-0.654559000
8	-3.555570000	-0.107520000	-1.064113000
6	-1.265881000	-0.020318000	1.715808000
8	-1.550263000	0.181410000	2.816582000
6	1.187669000	-0.346098000	0.431321000
7	2.013265000	-0.164818000	1.486777000
1	1.686275000	0.016757000	2.425641000
6	3.345391000	-0.216094000	1.109174000
1	4.153413000	-0.079960000	1.809573000
6	3.354954000	-0.447610000	-0.234928000
1	4.172986000	-0.555806000	-0.928932000
7	2.027131000	-0.526432000	-0.619406000
6	1.479804000	-0.766153000	-1.949225000
1	2.077967000	-0.222374000	-2.685128000
1	1.508886000	-1.835018000	-2.173747000
7	0.081253000	-0.307565000	-1.911221000
1	0.054356000	0.725760000	-2.015457000
1	-1.348184000	2.245515000	0.013870000
6	-0.394570000	2.798499000	-0.229113000
8	-0.126700000	3.772159000	0.502971000
8	0.261819000	2.344540000	-1.216691000

1	-0.448049000	-0.741975000	-2.663119000
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-953.981018

3'-Mn-AMNHC

25	0.544587000	0.473442000	0.022624000
6	0.084085000	2.190484000	0.244538000
8	-0.237729000	3.295866000	0.389078000
6	2.217617000	0.900797000	-0.594651000
8	3.269288000	1.175059000	-0.987029000
6	1.073583000	0.315167000	1.731648000
8	1.373384000	0.192217000	2.844507000
6	-1.348521000	-0.126615000	0.398434000
7	-2.076161000	-0.625334000	1.422409000
1	-1.708290000	-0.745411000	2.355439000
6	-3.359994000	-0.977998000	1.024479000
1	-4.083280000	-1.402821000	1.701680000
6	-3.440388000	-0.684378000	-0.301977000
1	-4.249574000	-0.799256000	-1.005357000
7	-2.200718000	-0.166984000	-0.657348000
6	-1.782715000	0.349999000	-1.956572000
1	-2.229535000	-0.261283000	-2.744950000
1	-2.120165000	1.383492000	-2.066258000
7	-0.311738000	0.324038000	-1.975623000
1	0.028927000	-0.603886000	-2.233824000
1	2.595500000	-1.802384000	0.576959000
6	1.855785000	-2.306915000	-0.080960000
8	2.045590000	-3.489132000	-0.405036000
8	0.854102000	-1.584304000	-0.442497000
1	0.038274000	0.992554000	-2.657154000

-954.007587

10-Mn-AMNHC

25	0.999776000	0.144354000	-0.120704000
6	1.789681000	-0.908898000	1.114327000
8	2.273828000	-1.601149000	1.901395000
6	2.254798000	1.468039000	0.080714000
8	3.048142000	2.293553000	0.221363000
6	1.880146000	-0.683102000	-1.464486000
8	2.418877000	-1.241778000	-2.321565000
6	-0.560498000	-1.119369000	-0.159326000
7	-1.040941000	-2.132569000	-0.912883000
1	-0.573911000	-2.488532000	-1.734669000
6	-2.266322000	-2.585430000	-0.440225000
1	-2.814181000	-3.382379000	-0.916326000
6	-2.553749000	-1.829675000	0.655076000
1	-3.402392000	-1.838932000	1.320026000
7	-1.493296000	-0.948651000	0.804314000
6	-1.305422000	0.075856000	1.824740000
1	-2.265128000	0.563303000	2.017025000

1	-0.942650000	-0.389358000	2.744954000
7	-0.306470000	1.026196000	1.306734000
1	-0.824327000	1.801562000	0.822187000
1	-3.359131000	2.987236000	-1.311298000
6	-2.521244000	2.386558000	-0.887515000
8	-2.283265000	1.273591000	-1.421899000
8	-1.906438000	2.910558000	0.093019000
1	-0.258380000	0.900116000	-1.198649000
1	0.424119000	1.284111000	-1.323036000
1	0.193038000	1.437109000	2.091901000

-955.162741

TS6-Mn-AMNHC

25	-1.036393000	0.118942000	0.082147000
6	-1.837186000	-1.026406000	-1.047669000
8	-2.349131000	-1.779593000	-1.765545000
6	-2.323538000	1.401329000	-0.108531000
8	-3.132676000	2.219163000	-0.226772000
6	-1.794173000	-0.626175000	1.528735000
8	-2.236352000	-1.120479000	2.479913000
6	0.609109000	-1.041207000	0.162777000
7	1.186809000	-1.953317000	0.975865000
1	0.769185000	-2.269204000	1.839540000
6	2.436711000	-2.343891000	0.510163000
1	3.057154000	-3.052943000	1.033996000
6	2.642348000	-1.658576000	-0.648079000
1	3.476001000	-1.655398000	-1.331932000
7	1.510807000	-0.877755000	-0.838356000
6	1.179224000	-0.012658000	-1.964669000
1	2.095514000	0.445500000	-2.346134000
1	0.707411000	-0.604946000	-2.753257000
7	0.218491000	0.979209000	-1.456356000
1	0.755314000	1.748542000	-1.019320000
1	3.534383000	2.518623000	1.203517000
6	2.531906000	2.226973000	0.834387000
8	1.888965000	1.434297000	1.613015000
8	2.142007000	2.678051000	-0.262079000
1	0.585219000	1.244661000	1.263330000
1	-0.344090000	1.277693000	1.212117000
1	-0.307941000	1.369121000	-2.234544000

-955.156867

11-Mn-AMNHC

25	1.108212000	0.130755000	-0.065708000
6	1.958028000	-1.067322000	0.984431000
8	2.526370000	-1.847128000	1.635082000
6	2.339735000	1.450549000	0.095514000
8	3.100957000	2.323545000	0.179152000
6	1.784235000	-0.499873000	-1.584877000

8	2.167892000	-0.913234000	-2.604161000
6	-0.566816000	-0.982220000	-0.165241000
7	-1.183466000	-1.813863000	-1.038910000
1	-0.782955000	-2.070042000	-1.929800000
6	-2.433725000	-2.218424000	-0.583712000
1	-3.076568000	-2.872802000	-1.150081000
6	-2.606014000	-1.624038000	0.627880000
1	-3.427002000	-1.662232000	1.325955000
7	-1.455927000	-0.879224000	0.859619000
6	-1.113134000	-0.097601000	2.043691000
1	-2.028751000	0.333266000	2.457334000
1	-0.643947000	-0.747887000	2.787225000
7	-0.144635000	0.921026000	1.618249000
1	-0.654387000	1.724134000	1.246339000
1	-3.791703000	2.160985000	-1.101668000
6	-2.769738000	2.005763000	-0.727713000
8	-1.998559000	1.461924000	-1.652322000
8	-2.428605000	2.308632000	0.407478000
1	-1.046163000	1.325979000	-1.318321000
1	0.321487000	1.246829000	-1.019464000
1	0.413018000	1.226396000	2.410796000

-955.163405

1-Mn-MAMNHC

25	-0.714614000	0.296590000	-0.182322000
6	-0.919785000	0.064942000	1.598173000
8	-1.086004000	-0.037309000	2.748481000
6	-2.413806000	-0.042008000	-0.676844000
8	-3.497202000	-0.240295000	-1.055434000
6	-0.967095000	2.050857000	-0.142035000
8	-1.077175000	3.212860000	-0.156761000
6	1.266572000	0.469118000	-0.130232000
7	2.219149000	1.429644000	-0.211068000
1	2.003954000	2.413705000	-0.278251000
6	3.505060000	0.894311000	-0.222335000
1	4.389702000	1.506748000	-0.290153000
6	3.356213000	-0.455023000	-0.142696000
1	4.085036000	-1.249622000	-0.122605000
7	1.984943000	-0.686299000	-0.088875000
6	1.273469000	-1.940383000	0.076175000
1	1.844458000	-2.753712000	-0.384459000
1	1.136737000	-2.155713000	1.141261000
7	-0.058517000	-1.762421000	-0.527279000
1	0.047585000	-1.781062000	-1.540067000
1	-0.491947000	0.488987000	-1.754634000
6	-0.974454000	-2.854250000	-0.131239000
1	-0.540310000	-3.843124000	-0.325364000
1	-1.200387000	-2.759446000	0.933033000
1	-1.902497000	-2.755408000	-0.694256000

-804.675128

2-Mn-MAMNHC

25	-0.990282000	-0.320139000	0.083467000
6	-1.913463000	-0.029905000	-1.442687000
8	-2.537773000	0.112281000	-2.417596000
6	-2.345606000	-0.062509000	1.242935000
8	-3.184130000	0.081715000	2.037636000
6	-1.204932000	-2.080466000	0.067604000
8	-1.278051000	-3.245001000	0.072939000
6	0.793601000	-0.418603000	-0.793740000
7	1.721119000	-1.342673000	-1.143795000
1	1.578964000	-2.335664000	-1.029139000
6	2.892434000	-0.758115000	-1.617623000
1	3.744799000	-1.337101000	-1.934545000
6	2.693008000	0.586694000	-1.570330000
1	3.334596000	1.409529000	-1.842583000
7	1.408287000	0.765361000	-1.066768000
6	0.669929000	1.997543000	-0.857332000
1	1.367757000	2.809675000	-0.627294000
1	0.105356000	2.251508000	-1.760596000
7	-0.292786000	1.746100000	0.229554000
1	0.225144000	1.734923000	1.106273000
1	-0.147105000	-0.564487000	1.420856000
6	2.430092000	-0.063534000	2.086075000
8	2.703187000	-1.199021000	2.089456000
8	2.192919000	1.083682000	2.092478000
6	-1.308272000	2.819370000	0.300057000
1	-0.847387000	3.813853000	0.350831000
1	-1.950874000	2.762649000	-0.581108000
1	-1.920498000	2.664972000	1.188619000

-993.269228

TS1-Mn-MAMNHC

25	0.856710000	0.165231000	-0.264229000
6	1.511154000	-1.094851000	-1.374969000
8	1.947092000	-1.889319000	-2.104596000
6	2.417868000	0.518901000	0.585086000
8	3.395918000	0.778424000	1.154240000
6	1.055551000	1.503235000	-1.423394000
8	1.127769000	2.396404000	-2.165818000
6	-1.063776000	-0.168981000	-0.761853000
7	-2.047276000	0.418885000	-1.483728000
1	-1.900962000	1.247196000	-2.042563000
6	-3.270983000	-0.222263000	-1.321103000
1	-4.171738000	0.109939000	-1.811464000
6	-3.046944000	-1.257693000	-0.467610000
1	-3.713077000	-2.006987000	-0.070704000
7	-1.695927000	-1.203938000	-0.144757000
6	-0.929505000	-2.102992000	0.703315000

1	-1.586562000	-2.529372000	1.468846000
1	-0.507101000	-2.912690000	0.099788000
7	0.182110000	-1.325558000	1.274481000
1	-0.201059000	-0.705774000	1.989836000
1	0.224531000	1.317012000	0.791470000
6	-1.148200000	1.908082000	1.748374000
8	-1.337470000	2.957921000	1.232205000
8	-1.309070000	1.016246000	2.521187000
6	1.202194000	-2.201587000	1.887482000
1	0.763551000	-2.888996000	2.621445000
1	1.698793000	-2.778415000	1.103929000
1	1.945473000	-1.576930000	2.383451000

-993.259643

3-Mn-MAMNHC

25	-0.756242000	0.027730000	0.319511000
6	-1.069009000	-1.379076000	1.378051000
8	-1.251207000	-2.297037000	2.059805000
6	-2.497872000	0.121076000	-0.243354000
8	-3.600027000	0.191401000	-0.580064000
6	-1.026017000	1.210872000	1.655966000
8	-1.156673000	1.976070000	2.513196000
6	1.221526000	-0.056003000	0.641797000
7	2.176932000	0.551448000	1.380463000
1	1.980351000	1.273758000	2.058996000
6	3.446824000	0.092603000	1.058189000
1	4.338401000	0.468488000	1.533488000
6	3.279353000	-0.843697000	0.082917000
1	3.995602000	-1.445208000	-0.453451000
7	1.913409000	-0.912965000	-0.149200000
6	1.180922000	-1.777855000	-1.059858000
1	1.776426000	-1.950190000	-1.961717000
1	0.973887000	-2.736052000	-0.574409000
7	-0.098945000	-1.106359000	-1.358020000
1	0.113213000	-0.331886000	-2.017069000
1	-0.479881000	1.470201000	-0.782073000
6	0.222598000	2.043513000	-1.556705000
8	0.423774000	3.210318000	-1.215271000
8	0.562630000	1.350067000	-2.535831000
6	-1.042011000	-2.043724000	-2.010929000
1	-0.574957000	-2.550704000	-2.863329000
1	-1.377659000	-2.788706000	-1.286299000
1	-1.904955000	-1.480628000	-2.365740000

-993.274500

TS2-Mn-MAMNHC

25	-0.888811000	-0.068012000	0.270831000
6	-1.831217000	-1.423868000	-0.381760000
8	-2.404560000	-2.316864000	-0.843472000

6	-2.336453000	1.075919000	0.207846000
8	-3.257222000	1.768320000	0.188376000
6	-1.239121000	-0.550765000	1.984242000
8	-1.431883000	-0.888541000	3.071928000
6	0.838405000	-1.076415000	0.230707000
7	1.632238000	-1.805046000	1.048887000
1	1.392961000	-2.026561000	2.005408000
6	2.814289000	-2.170070000	0.426282000
1	3.580539000	-2.743270000	0.922792000
6	2.758135000	-1.654870000	-0.835545000
1	3.463789000	-1.697491000	-1.649789000
7	1.543685000	-0.995698000	-0.925150000
6	0.960555000	-0.301275000	-2.063709000
1	1.746695000	0.234549000	-2.605472000
1	0.490257000	-1.026399000	-2.734402000
7	-0.064889000	0.612245000	-1.533646000
1	0.427026000	1.438490000	-1.094748000
1	2.430490000	1.296660000	0.510327000
6	2.023648000	2.327499000	0.657454000
8	2.607595000	3.058029000	1.484843000
8	1.001712000	2.617480000	-0.051320000
6	-0.940762000	1.099918000	-2.622712000
1	-0.350918000	1.477357000	-3.466259000
1	-1.588718000	0.290975000	-2.968454000
1	-1.559095000	1.911642000	-2.240498000

-993.266649

3'-Mn-MAMNHC

25	-0.735580000	0.007454000	0.272871000
6	-0.998591000	-1.382764000	1.370360000
8	-1.141564000	-2.293416000	2.075183000
6	-2.498721000	0.080311000	-0.237810000
8	-3.609084000	0.136630000	-0.550132000
6	-0.978165000	1.197306000	1.596473000
8	-1.098983000	1.963157000	2.458315000
6	1.263932000	-0.100709000	0.533849000
7	2.238956000	0.510929000	1.243590000
1	2.056571000	1.221741000	1.937652000
6	3.503828000	0.060777000	0.885041000
1	4.406099000	0.441380000	1.335827000
6	3.313568000	-0.873357000	-0.086091000
1	4.017609000	-1.470720000	-0.643042000
7	1.939756000	-0.950650000	-0.280860000
6	1.205111000	-1.854805000	-1.154526000
1	1.779413000	-2.023528000	-2.071013000
1	1.051931000	-2.811793000	-0.647174000
7	-0.111462000	-1.250197000	-1.417599000
1	0.007814000	-0.481570000	-2.082750000
1	0.515089000	2.847111000	-0.041779000
6	0.291258000	2.566399000	-1.092378000

8	0.639811000	3.330097000	-2.005742000
8	-0.322680000	1.446312000	-1.246225000
6	-1.058722000	-2.241103000	-1.974205000
1	-0.633580000	-2.771383000	-2.834594000
1	-1.320318000	-2.962465000	-1.196962000
1	-1.962880000	-1.720278000	-2.289339000

-993.292300

10-Mn-MAMNHC

25	0.983062000	-0.071811000	-0.283273000
6	1.762901000	-0.829891000	1.156921000
8	2.246538000	-1.324946000	2.081274000
6	2.379256000	1.093133000	-0.516178000
8	3.273037000	1.808675000	-0.659874000
6	1.687260000	-1.316298000	-1.390089000
8	2.108507000	-2.138112000	-2.085437000
6	-0.679571000	-1.144327000	0.071142000
7	-1.322291000	-2.233673000	-0.400103000
1	-0.972026000	-2.806454000	-1.154562000
6	-2.540780000	-2.425327000	0.239158000
1	-3.205683000	-3.236267000	-0.010225000
6	-2.654577000	-1.422130000	1.152474000
1	-3.436429000	-1.188863000	1.857217000
7	-1.501575000	-0.660057000	1.029902000
6	-1.098732000	0.520160000	1.777525000
1	-1.985382000	1.111188000	2.028788000
1	-0.590143000	0.220640000	2.699512000
7	-0.167238000	1.275832000	0.920362000
1	-0.777655000	1.787142000	0.235844000
1	-3.459153000	2.370748000	-2.008932000
6	-2.560441000	1.911306000	-1.535976000
8	-2.235401000	0.759835000	-1.922206000
8	-1.975334000	2.619881000	-0.659236000
6	0.549706000	2.298353000	1.715159000
1	-0.148759000	2.907323000	2.301882000
1	1.261768000	1.817137000	2.389936000
1	1.094068000	2.953471000	1.034444000
1	-0.264766000	0.475835000	-1.502301000
1	0.436443000	0.796125000	-1.697872000

-994.445987

TS6-Mn-MAMNHC

25	0.982167000	-0.120582000	-0.246435000
6	1.765935000	-0.830397000	1.209766000
8	2.272110000	-1.299933000	2.140025000
6	2.396967000	0.976771000	-0.603483000
8	3.296683000	1.661927000	-0.844140000
6	1.586291000	-1.435002000	-1.313180000
8	1.933989000	-2.299810000	-2.001551000

6	-0.735235000	-1.079516000	0.155205000
7	-1.446662000	-2.145859000	-0.270926000
1	-1.125500000	-2.777360000	-0.990618000
6	-2.686716000	-2.221193000	0.352030000
1	-3.402159000	-2.996584000	0.130710000
6	-2.746276000	-1.167053000	1.211244000
1	-3.521412000	-0.846317000	1.888558000
7	-1.540975000	-0.491871000	1.072339000
6	-1.061734000	0.682981000	1.781862000
1	-1.909690000	1.330818000	2.026389000
1	-0.558450000	0.379552000	2.705311000
7	-0.091364000	1.354060000	0.897298000
1	-0.664570000	1.856000000	0.193199000
1	-3.470217000	1.926630000	-2.076590000
6	-2.470421000	1.723148000	-1.642859000
8	-1.891562000	0.674172000	-2.084406000
8	-2.026323000	2.520262000	-0.783889000
6	0.687722000	2.362014000	1.651001000
1	0.030796000	3.038738000	2.210942000
1	1.365492000	1.860672000	2.345840000
1	1.276482000	2.949728000	0.946501000
1	-0.504628000	0.548927000	-1.662387000
1	0.384298000	0.605972000	-1.665795000

-994.444197

11-Mn-MAMNHC

25	1.058184000	0.152037000	0.237381000
6	1.922837000	0.635442000	-1.272105000
8	2.500920000	0.964945000	-2.226911000
6	2.363786000	-0.924737000	0.881579000
8	3.174703000	-1.624901000	1.329983000
6	1.593272000	1.567769000	1.172057000
8	1.882185000	2.505016000	1.800372000
6	-0.669735000	1.007291000	-0.338610000
7	-1.396487000	2.117751000	-0.068042000
1	-1.081886000	2.840553000	0.562914000
6	-2.627838000	2.108080000	-0.714527000
1	-3.347035000	2.904319000	-0.609815000
6	-2.673448000	0.949461000	-1.426189000
1	-3.438448000	0.539994000	-2.066384000
7	-1.469386000	0.299449000	-1.181694000
6	-0.985393000	-0.951071000	-1.748722000
1	-1.838692000	-1.606175000	-1.954298000
1	-0.449099000	-0.749711000	-2.681643000
7	-0.045501000	-1.536625000	-0.782174000
1	-0.612228000	-1.925299000	-0.024121000
1	-3.805880000	-1.271450000	2.111587000
6	-2.774240000	-1.277901000	1.732474000
8	-2.071237000	-0.278874000	2.235136000
8	-2.365214000	-2.119271000	0.943880000

6	0.759437000	-2.615387000	-1.388961000
1	0.129368000	-3.377617000	-1.865006000
1	1.434496000	-2.188188000	-2.134117000
1	1.357088000	-3.086125000	-0.607754000
1	-1.110985000	-0.289589000	1.897670000
1	0.265407000	-0.324671000	1.618168000

-994.448233

1-Mn-MAMP'

25	-0.959254000	0.148475000	-0.113266000
6	-1.170461000	0.290557000	1.686973000
8	-1.385606000	0.449812000	2.820671000
6	-2.637630000	-0.342475000	-0.468076000
8	-3.709374000	-0.689509000	-0.762796000
6	-1.334497000	1.859017000	-0.436257000
8	-1.569078000	2.968401000	-0.704802000
7	1.115367000	0.387028000	-0.094094000
6	1.797205000	1.487352000	-0.466884000
1	1.201929000	2.341679000	-0.765083000
6	3.187906000	1.544346000	-0.480761000
1	3.683577000	2.458122000	-0.789312000
6	3.912673000	0.412240000	-0.102190000
1	4.997938000	0.418454000	-0.108896000
6	3.211631000	-0.732007000	0.277567000
1	3.731319000	-1.638050000	0.571098000
6	1.816558000	-0.707378000	0.276294000
6	0.978559000	-1.875003000	0.722848000
1	1.529068000	-2.817889000	0.617489000
1	0.731821000	-1.745916000	1.782543000
7	-0.291117000	-1.885775000	-0.039690000
1	-0.806039000	0.077427000	-1.696614000
6	-0.139026000	-2.543833000	-1.358193000
1	0.576282000	-1.974988000	-1.954108000
1	0.211318000	-3.578696000	-1.250223000
1	-1.100454000	-2.529549000	-1.871308000
1	-0.970192000	-2.417774000	0.500032000

-826.748844

2-Mn-MAMP'

25	1.175858000	-0.054988000	0.127385000
6	1.907306000	1.167719000	1.256721000
8	2.436891000	1.876403000	2.014034000
6	2.703548000	-0.522305000	-0.667893000
8	3.661850000	-0.852079000	-1.240885000
6	1.298778000	-1.411481000	1.275285000
8	1.352274000	-2.334746000	1.983556000
7	-0.805008000	0.421322000	0.583576000
6	-1.638530000	-0.290167000	1.367684000
1	-1.214073000	-1.159932000	1.853754000

6	-2.976876000	0.046694000	1.547010000
1	-3.601802000	-0.566359000	2.186905000
6	-3.484475000	1.166710000	0.884910000
1	-4.525953000	1.452116000	0.992634000
6	-2.624270000	1.910015000	0.077613000
1	-2.973752000	2.786418000	-0.457925000
6	-1.291330000	1.515164000	-0.043035000
6	-0.276178000	2.299222000	-0.829724000
1	-0.760789000	2.909544000	-1.601429000
1	0.244494000	2.976477000	-0.143261000
7	0.729611000	1.376858000	-1.402893000
1	0.556763000	-1.166809000	-0.828619000
6	-1.884399000	-2.354078000	-1.087795000
8	-1.552119000	-3.201228000	-0.353719000
8	-2.248206000	-1.521479000	-1.825148000
6	0.283551000	0.800672000	-2.693319000
1	-0.617284000	0.211523000	-2.522298000
1	0.077971000	1.587901000	-3.430605000
1	1.062428000	0.136891000	-3.069155000
1	1.575044000	1.915712000	-1.576860000

-1015.341559

TS1-Mn-MAMP'

25	0.774430000	-0.535469000	-0.226539000
6	0.620855000	-2.249222000	-0.810903000
8	0.591686000	-3.328159000	-1.243341000
6	2.489976000	-0.672781000	0.264721000
8	3.594097000	-0.701995000	0.625300000
6	1.222193000	0.099029000	-1.835327000
8	1.532217000	0.548566000	-2.861674000
7	-1.250933000	-0.076567000	-0.371443000
6	-1.821613000	0.726998000	-1.288957000
1	-1.164376000	1.131541000	-2.048210000
6	-3.177831000	1.039985000	-1.273425000
1	-3.585342000	1.693256000	-2.036867000
6	-3.980920000	0.507913000	-0.262929000
1	-5.040813000	0.736721000	-0.217244000
6	-3.391527000	-0.316198000	0.696169000
1	-3.973866000	-0.740151000	1.507368000
6	-2.027050000	-0.590279000	0.609601000
6	-1.301525000	-1.486140000	1.578520000
1	-1.836871000	-1.552283000	2.533333000
1	-1.236871000	-2.494176000	1.154949000
7	0.079164000	-0.974605000	1.748108000
1	0.936399000	0.992648000	0.235217000
6	1.137705000	2.855950000	0.423098000
8	0.460656000	3.220126000	-0.479610000
8	1.857956000	2.866946000	1.364406000
6	0.127575000	0.166215000	2.694449000
1	-0.489020000	0.974459000	2.298487000

1	-0.251945000	-0.124885000	3.682152000
1	1.154554000	0.520201000	2.775646000
1	0.649849000	-1.725068000	2.131235000

-1015.333522

3-Mn-MAMP'

25	0.833202000	-0.384588000	-0.221375000
6	0.870317000	-2.051919000	-0.901569000
8	0.897586000	-3.111791000	-1.362974000
6	2.586121000	-0.431970000	0.256689000
8	3.691055000	-0.444381000	0.589351000
6	1.238923000	0.322094000	-1.845790000
8	1.502367000	0.772154000	-2.875111000
7	-1.214282000	-0.136686000	-0.378793000
6	-1.845605000	0.657550000	-1.265070000
1	-1.221275000	1.166133000	-1.986647000
6	-3.225002000	0.840940000	-1.250474000
1	-3.685645000	1.491584000	-1.984969000
6	-3.981104000	0.187646000	-0.276955000
1	-5.057988000	0.314737000	-0.233885000
6	-3.327855000	-0.623197000	0.652822000
1	-3.875906000	-1.134796000	1.436522000
6	-1.945177000	-0.766076000	0.571598000
6	-1.149793000	-1.634174000	1.509057000
1	-1.670319000	-1.766361000	2.463916000
1	-1.016305000	-2.623683000	1.059517000
7	0.194090000	-1.030394000	1.695790000
1	0.774460000	1.323394000	0.389103000
6	0.722749000	2.523744000	0.523362000
8	-0.045734000	3.055194000	-0.282552000
8	1.452964000	2.897454000	1.445901000
6	0.179480000	0.049846000	2.717289000
1	-0.555540000	0.801036000	2.425939000
1	-0.082709000	-0.349810000	3.702829000
1	1.158325000	0.527547000	2.751853000
1	0.819990000	-1.761473000	2.028566000

-1015.339398

TS2-Mn-MAMP'

25	0.796858000	-0.364017000	-0.245253000
6	0.794870000	-1.849844000	-1.248649000
8	0.775010000	-2.810161000	-1.890512000
6	2.524129000	-0.603176000	0.279446000
8	3.608727000	-0.761046000	0.636822000
6	1.298614000	0.598564000	-1.702458000
8	1.619867000	1.159001000	-2.658656000
7	-1.226771000	0.005347000	-0.422889000
6	-1.784501000	0.993691000	-1.147780000
1	-1.111167000	1.589872000	-1.750214000

6	-3.150441000	1.255929000	-1.126977000
1	-3.549928000	2.064598000	-1.727917000
6	-3.973101000	0.470416000	-0.318733000
1	-5.041818000	0.652918000	-0.273136000
6	-3.397802000	-0.549952000	0.438644000
1	-4.000067000	-1.176008000	1.087755000
6	-2.022639000	-0.759113000	0.359847000
6	-1.314576000	-1.862302000	1.097774000
1	-1.883575000	-2.175779000	1.979521000
1	-1.223252000	-2.729917000	0.435940000
7	0.052314000	-1.404808000	1.459998000
1	1.958970000	2.128557000	0.102695000
6	1.192701000	2.566217000	0.779270000
8	0.807928000	3.745566000	0.679897000
8	0.809527000	1.724201000	1.654235000
6	0.059830000	-0.648202000	2.740455000
1	-0.598230000	0.214353000	2.647994000
1	-0.273565000	-1.291024000	3.563058000
1	1.066601000	-0.278920000	2.928476000
1	0.624801000	-2.235850000	1.598052000

-1015.331076

3'-Mn-MAMP'

25	0.738936000	-0.399128000	-0.210840000
6	0.563207000	-2.102517000	-0.771862000
8	0.458233000	-3.188195000	-1.162581000
6	2.460269000	-0.677084000	0.279850000
8	3.547634000	-0.865042000	0.623832000
6	1.230762000	0.119048000	-1.872370000
8	1.549407000	0.458356000	-2.930418000
7	-1.297353000	-0.002056000	-0.424603000
6	-1.841118000	0.789516000	-1.366351000
1	-1.171136000	1.155997000	-2.134184000
6	-3.188499000	1.138494000	-1.364037000
1	-3.578964000	1.778353000	-2.147295000
6	-4.003828000	0.659614000	-0.337012000
1	-5.056813000	0.919498000	-0.298190000
6	-3.438526000	-0.149902000	0.648350000
1	-4.033008000	-0.529811000	1.472277000
6	-2.082002000	-0.465289000	0.571558000
6	-1.392234000	-1.360963000	1.566492000
1	-1.934131000	-1.380487000	2.518737000
1	-1.378090000	-2.382970000	1.172463000
7	0.013644000	-0.917988000	1.746184000
1	2.618840000	2.042120000	-0.126202000
6	1.680321000	2.408426000	0.342774000
8	1.630272000	3.579314000	0.748925000
8	0.720190000	1.555736000	0.414571000
6	0.134879000	0.139782000	2.779647000
1	-0.438896000	1.010526000	2.466531000

1	-0.226713000	-0.225293000	3.747964000
1	1.180398000	0.437235000	2.860595000
1	0.545797000	-1.722749000	2.070379000

-1015.364727

10-Mn-MAMP'

25	-0.316156000	0.568613000	0.202640000
6	0.306193000	1.652489000	1.516677000
8	0.707411000	2.364868000	2.330807000
6	-2.029715000	0.761651000	0.811238000
8	-3.087613000	0.899670000	1.241998000
6	-0.497228000	1.993550000	-0.913812000
8	-0.619342000	2.896929000	-1.620698000
7	1.618693000	0.053532000	-0.378973000
6	2.264833000	0.499623000	-1.474012000
1	1.739620000	1.226112000	-2.081698000
6	3.536766000	0.057443000	-1.822391000
1	4.013829000	0.447375000	-2.714282000
6	4.164759000	-0.889663000	-1.010966000
1	5.153821000	-1.261751000	-1.257629000
6	3.495461000	-1.357179000	0.119725000
1	3.943482000	-2.099263000	0.771629000
6	2.225396000	-0.861255000	0.411040000
6	1.447278000	-1.265477000	1.634553000
1	1.742997000	-2.263215000	1.977064000
1	1.663672000	-0.559687000	2.443929000
7	-0.005114000	-1.199514000	1.335334000
1	-4.801537000	-1.292498000	-1.813960000
6	-3.787918000	-1.292583000	-1.344452000
8	-3.601499000	-2.086538000	-0.389788000
8	-2.954975000	-0.475623000	-1.846982000
6	-0.492983000	-2.447556000	0.684605000
1	0.074894000	-2.608477000	-0.234649000
1	-0.346007000	-3.307628000	1.347961000
1	-1.549759000	-2.334906000	0.431266000
1	-0.497942000	-1.107681000	2.221369000
1	-0.540754000	-0.528338000	-1.126141000
1	-1.336389000	-0.404194000	-1.121335000

-1016.505900

TS6-Mn-MAMP'

25	0.277046000	0.734167000	-0.146505000
6	-0.421273000	2.028946000	-1.197781000
8	-0.845847000	2.889266000	-1.848417000
6	1.967933000	1.078171000	-0.664014000
8	3.061348000	1.277888000	-0.987238000
6	0.408889000	1.830172000	1.267879000
8	0.529329000	2.477775000	2.221465000
7	-1.626834000	-0.041812000	0.378644000

6	-2.248621000	0.145199000	1.557682000
1	-1.763177000	0.813258000	2.258677000
6	-3.445205000	-0.487754000	1.882687000
1	-3.903598000	-0.306576000	2.848346000
6	-4.021341000	-1.353530000	0.950389000
1	-4.949654000	-1.870105000	1.172276000
6	-3.385070000	-1.537187000	-0.277146000
1	-3.801432000	-2.193790000	-1.033588000
6	-2.194357000	-0.856138000	-0.533920000
6	-1.493212000	-0.902522000	-1.863921000
1	-1.769077000	-1.812829000	-2.409775000
1	-1.811295000	-0.042207000	-2.462776000
7	-0.031672000	-0.811712000	-1.653579000
1	4.791489000	-1.601703000	1.678838000
6	3.837005000	-1.676831000	1.129421000
8	3.764653000	-2.293298000	0.069765000
8	2.897787000	-0.982518000	1.719218000
6	0.564204000	-2.135747000	-1.362083000
1	0.133960000	-2.508561000	-0.429940000
1	0.344315000	-2.846092000	-2.169890000
1	1.639628000	-2.029654000	-1.228960000
1	0.369512000	-0.458045000	-2.519750000
1	0.855829000	-0.470171000	0.970917000
1	1.875020000	-0.802619000	1.179290000

-1016.505516

11-Mn-MAMP'

25	-0.294584000	0.747454000	0.114797000
6	0.432347000	2.171984000	0.982109000
8	0.858935000	3.122584000	1.495292000
6	-1.960309000	1.079462000	0.688848000
8	-3.044521000	1.253840000	1.066537000
6	-0.562183000	1.644844000	-1.407811000
8	-0.749876000	2.183749000	-2.420582000
7	1.612558000	-0.077832000	-0.413216000
6	2.166941000	-0.049154000	-1.639445000
1	1.612362000	0.484196000	-2.402123000
6	3.379282000	-0.667751000	-1.931302000
1	3.781893000	-0.613557000	-2.936601000
6	4.043781000	-1.355091000	-0.913657000
1	4.986521000	-1.857033000	-1.106600000
6	3.468606000	-1.392663000	0.356383000
1	3.946657000	-1.922732000	1.173375000
6	2.255683000	-0.738005000	0.574997000
6	1.594482000	-0.681591000	1.929136000
1	1.925487000	-1.517346000	2.557711000
1	1.891305000	0.249225000	2.425099000
7	0.122718000	-0.662052000	1.770157000
1	-4.741181000	-2.115628000	-1.518075000
6	-3.824195000	-1.859139000	-0.966341000

8	-3.613853000	-2.209824000	0.181829000
8	-3.009263000	-1.132000000	-1.722214000
6	-0.438458000	-2.018735000	1.566745000
1	-0.006025000	-2.441445000	0.657939000
1	-0.211250000	-2.672902000	2.418567000
1	-1.515726000	-1.942246000	1.421821000
1	-0.278586000	-0.276234000	2.622061000
1	-0.873506000	-0.551849000	-0.703606000
1	-2.167524000	-0.881380000	-1.222931000

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