

Supporting Information

Flexible Proton Responsive Ligand-based Mn(I)-Complexes for CO₂ Hydrogenation: A DFT Study

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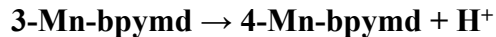
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S1. Deprotonation free energy of 3:

Example-



$$\Delta G^* = 20.39 \text{ kcal/mol}$$

where solvation free energy of H^+ is taken 265.9 kcal/mol.^[1-3]

At pH 8.3 deprotonation free energy of 3 calculated as:^[4-5]

$$\Delta G = RT \ln \left(\frac{Q}{K_{eq}} \right)$$

where, R ($0.00198588 \times 10^{-3} \text{ kcal K}^{-1} \text{ mol}^{-1}$) is the universal gas constant, T is the temperature (298.15 K), Q is the reaction quotient and K_{eq} is the equilibrium constant.

at equilibrium

$$\Delta G^* = RT \ln K_{eq}$$

$$K_{eq} = e^{\left(-\frac{\Delta G^*}{RT} \right)} = e^{\left(-\frac{20.39 \text{ kcal mol}^{-1}}{0.00198588 \times 10^{-3} \text{ kcal K}^{-1} \text{ mol}^{-1} \times 298.15 \text{ K}} \right)}$$
$$= 1.10678 \times 10^{-15}$$

$$\Delta G = RT \ln \left(\frac{Q}{K_{eq}} \right) = (298.15 \text{ K} \times 1.9 \text{ kcal K}^{-1} \text{ mol}^{-1}) \times \ln \frac{10^{-8.3}}{1.10678 \times 10^{-15}}$$

$$\Delta G = 9.1 \text{ kcal mol}^{-1}$$

S2. (a) Optimized geometries of 2

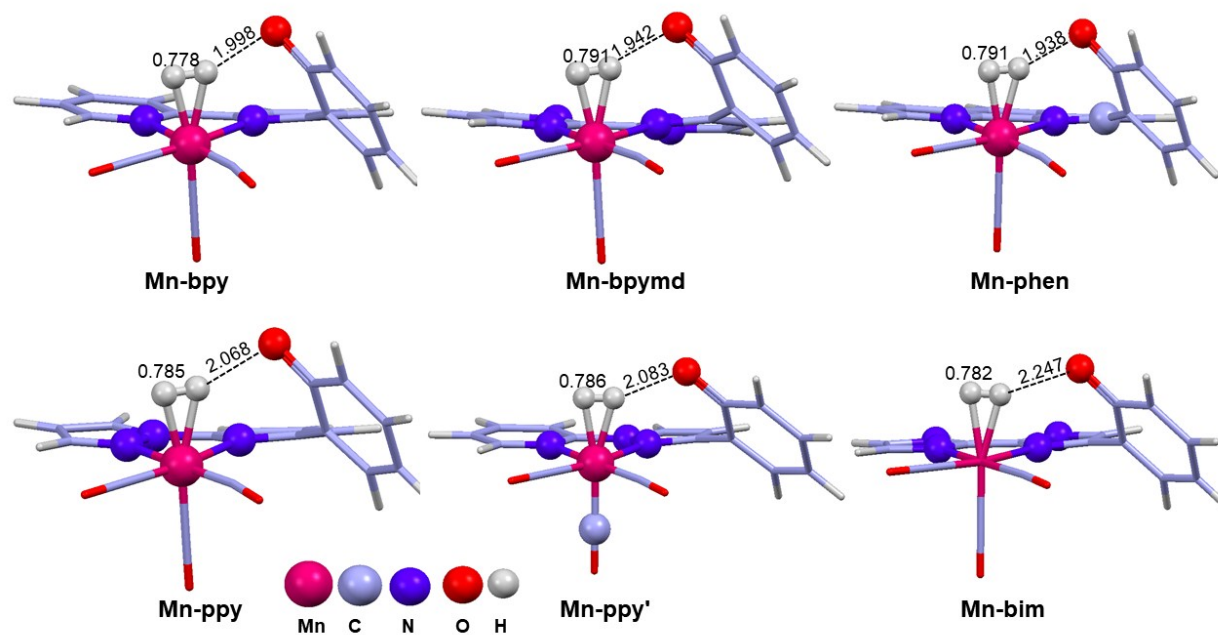


Figure S1. Optimized geometries of intermediate **2** of all the Mn-complexes. Bond lengths are in Å.

(b) Optimized geometries of TS1

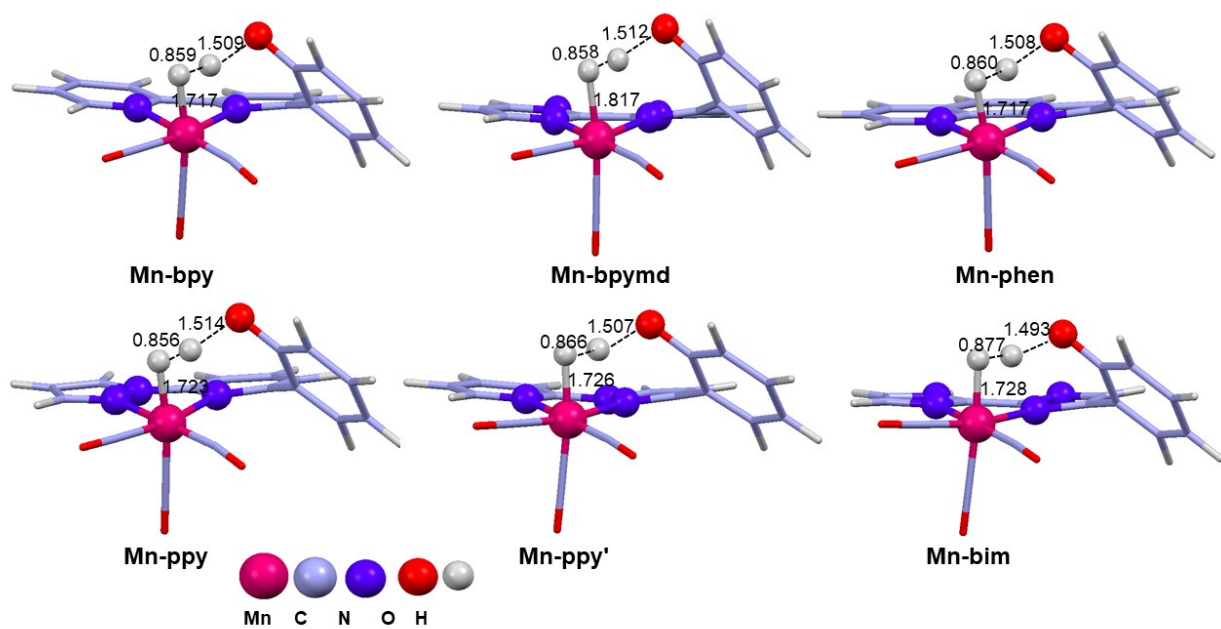


Figure S2. Optimized geometries of TS1 for all the Mn-complexes. Bond lengths are in Å.

(c) Optimized geometries of TS1-H₂O

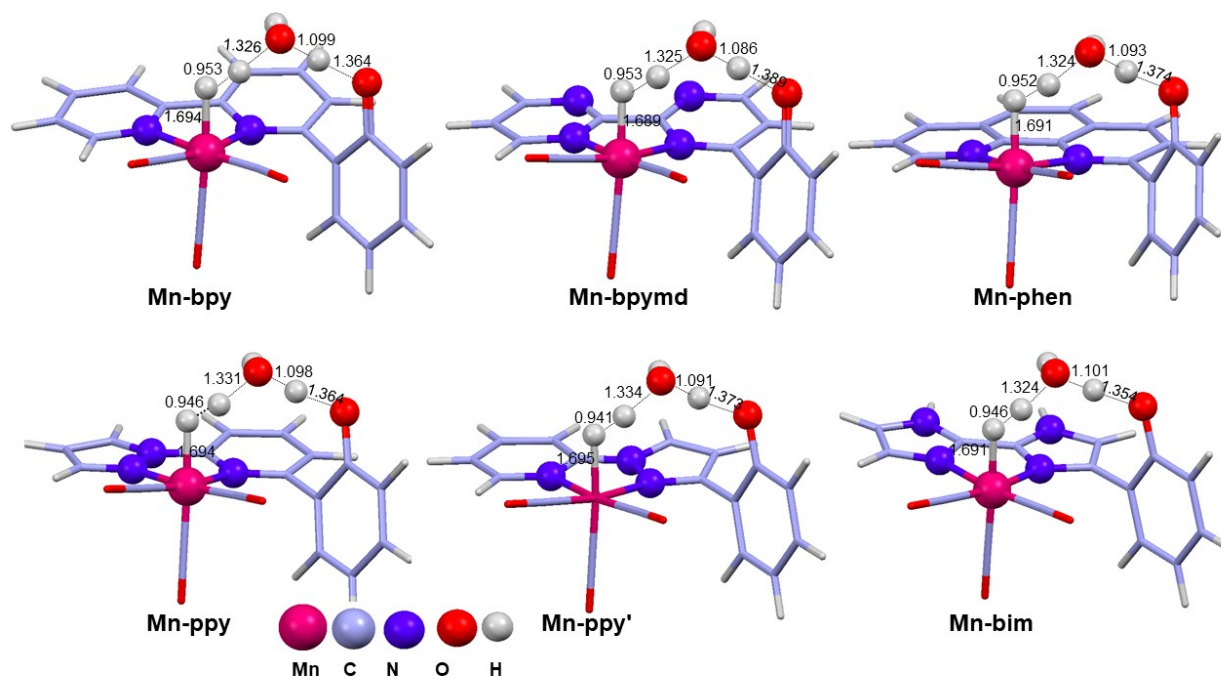


Figure S3. Optimized geometries of TS1-H₂O for all the Mn-complexes. Bond lengths are in Å.

(d) Optimized geometries of 3

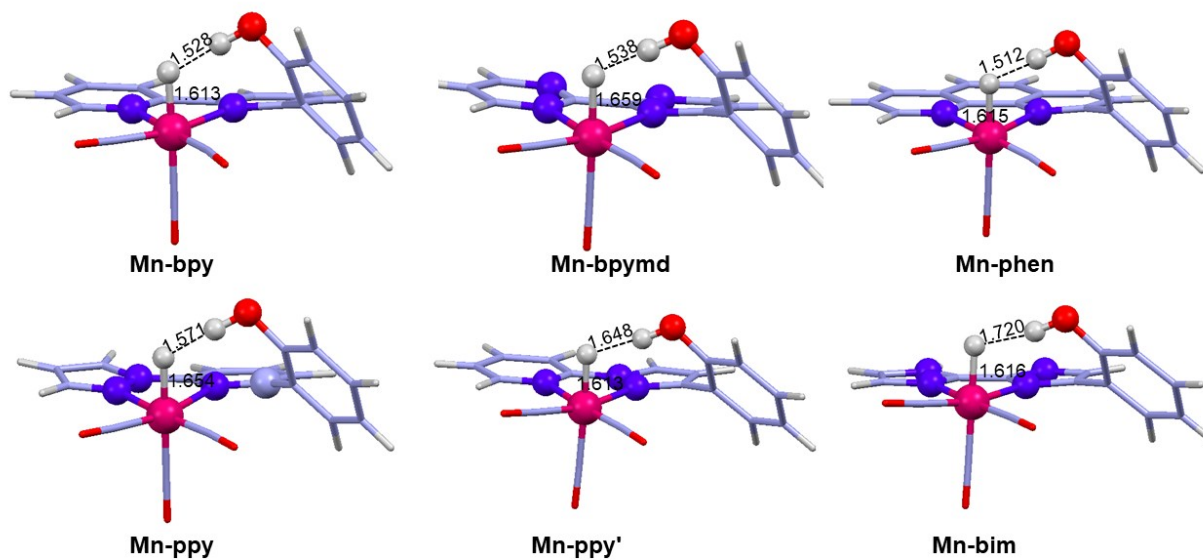


Figure S4. Optimized geometries of intermediate **3** for all the Mn-complexes. Bond lengths are in Å.

(e) Optimized geometries of 4

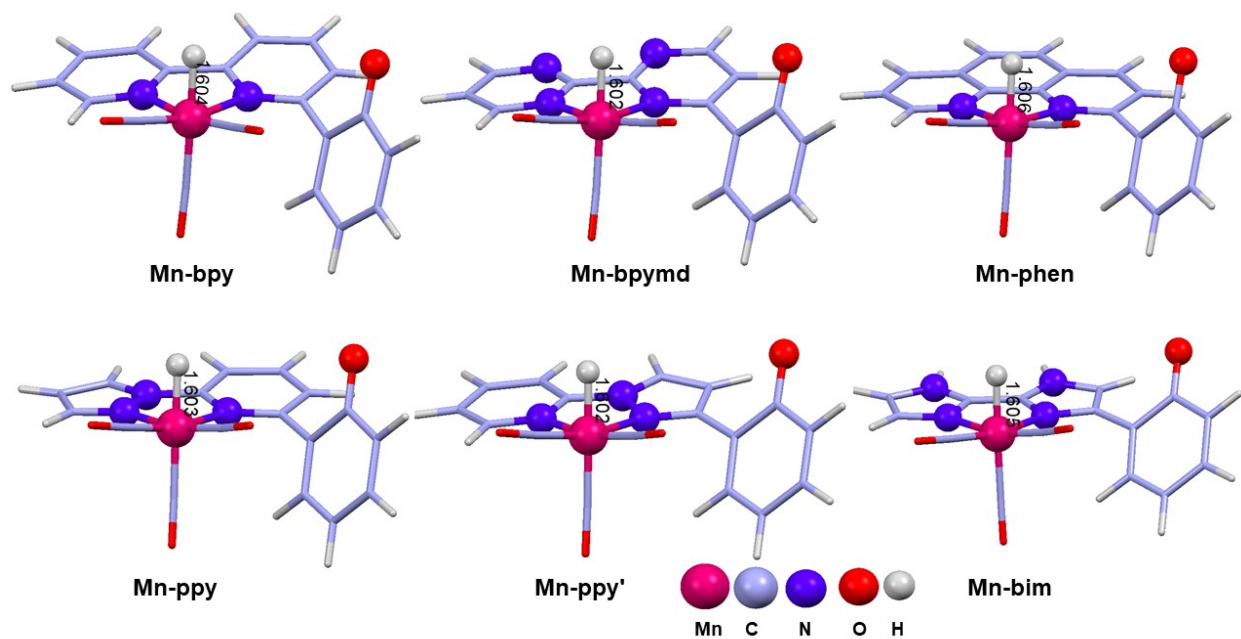


Figure S5. Optimized geometries of intermediate 4 for all the Mn-complexes. Bond lengths are in Å.

(f) Optimized geometries of 5

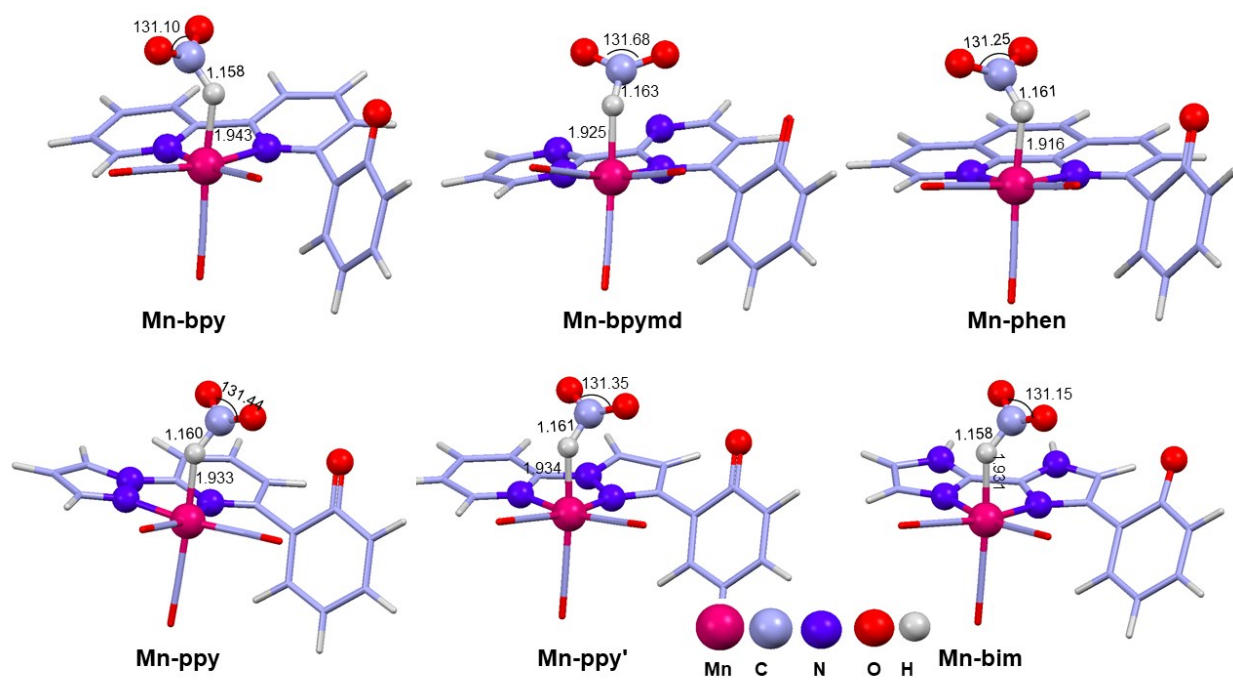


Figure S6. Optimized geometries of intermediate **5** for all the Mn-complexes. Bond lengths are in Å.

(g) Optimized geometries of **6**

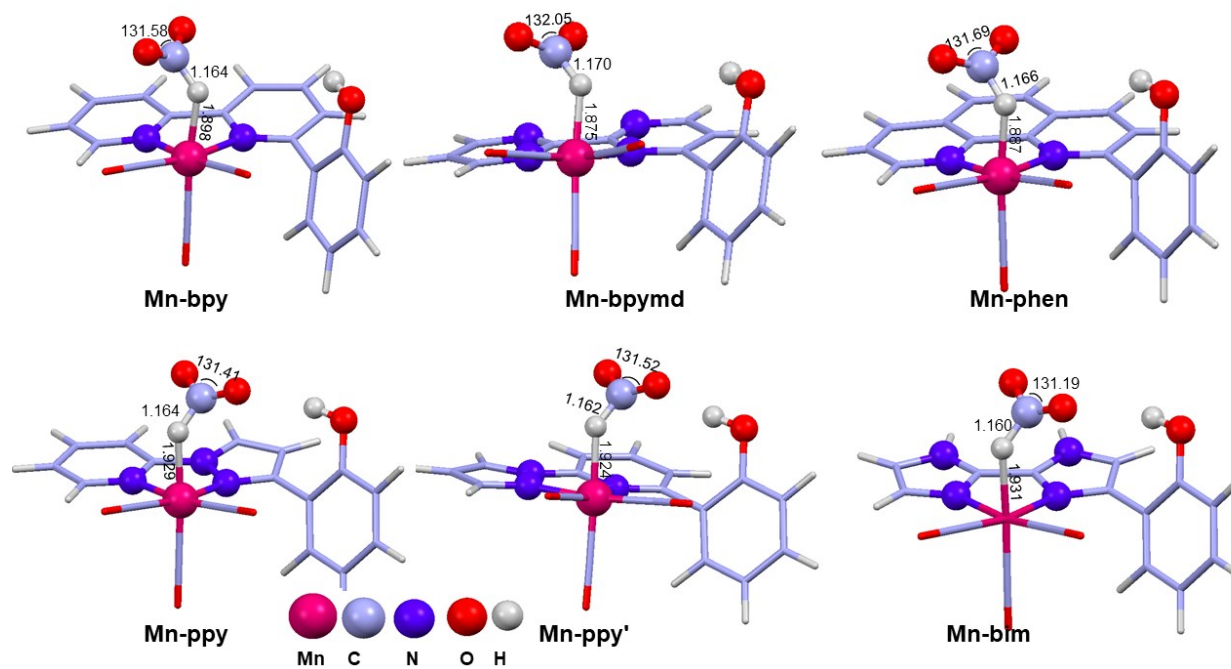


Figure S7. Optimized geometries of intermediate **6** for all the Mn-complexes. Bond lengths are in Å.

(h) Optimized geometries of 3-CO₂

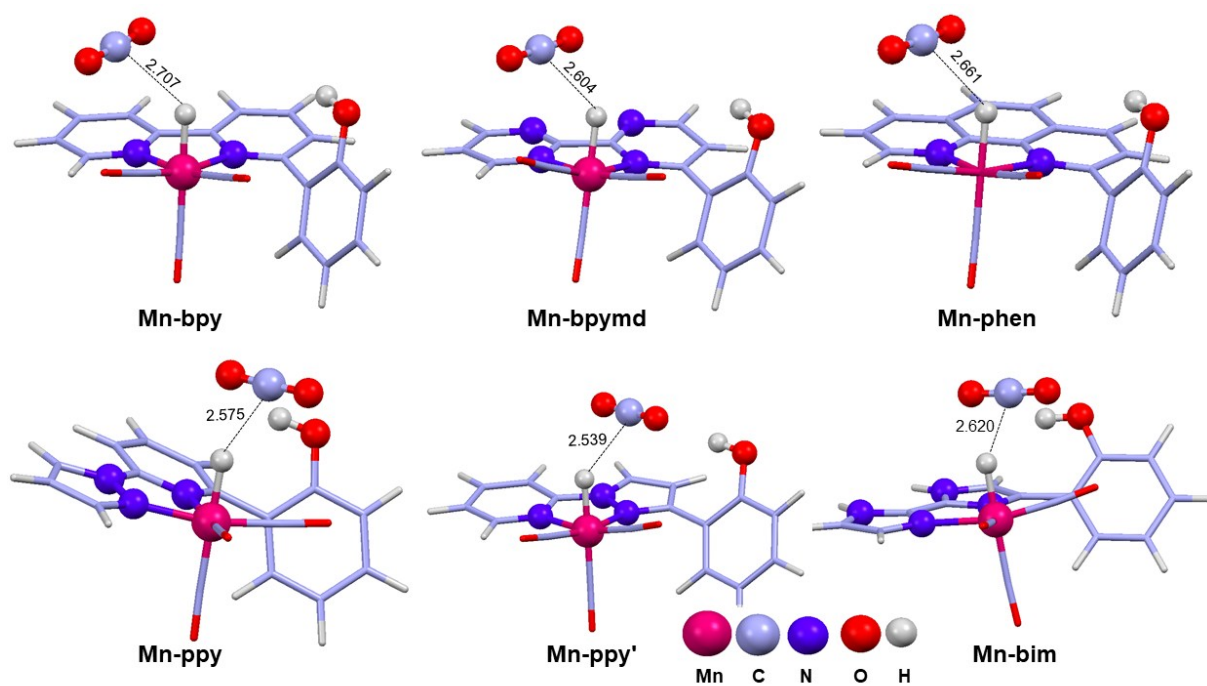


Figure S8. Optimized geometries of intermediate 3-CO₂ for all the Mn-complexes. Bond lengths are in Å.

(i) Optimized geometries of 4-CO₂

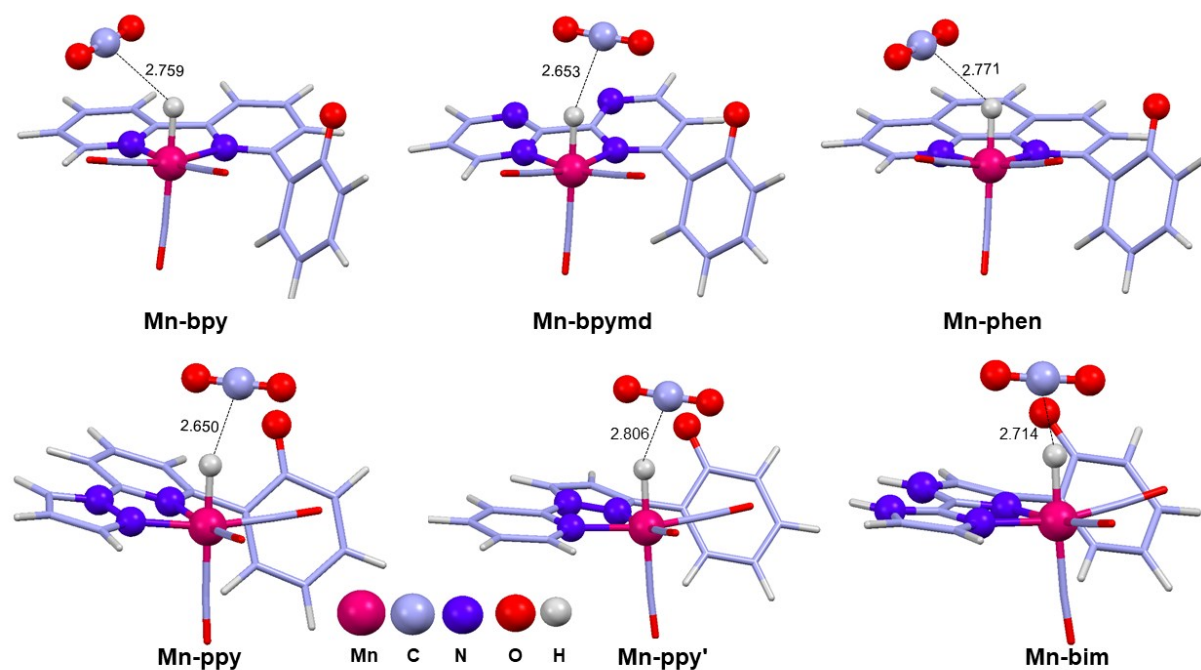


Figure S9. Optimized geometries of intermediate 4-CO₂ for all the Mn-complexes. Bond lengths are in Å.

(j) Optimized geometries of TS2

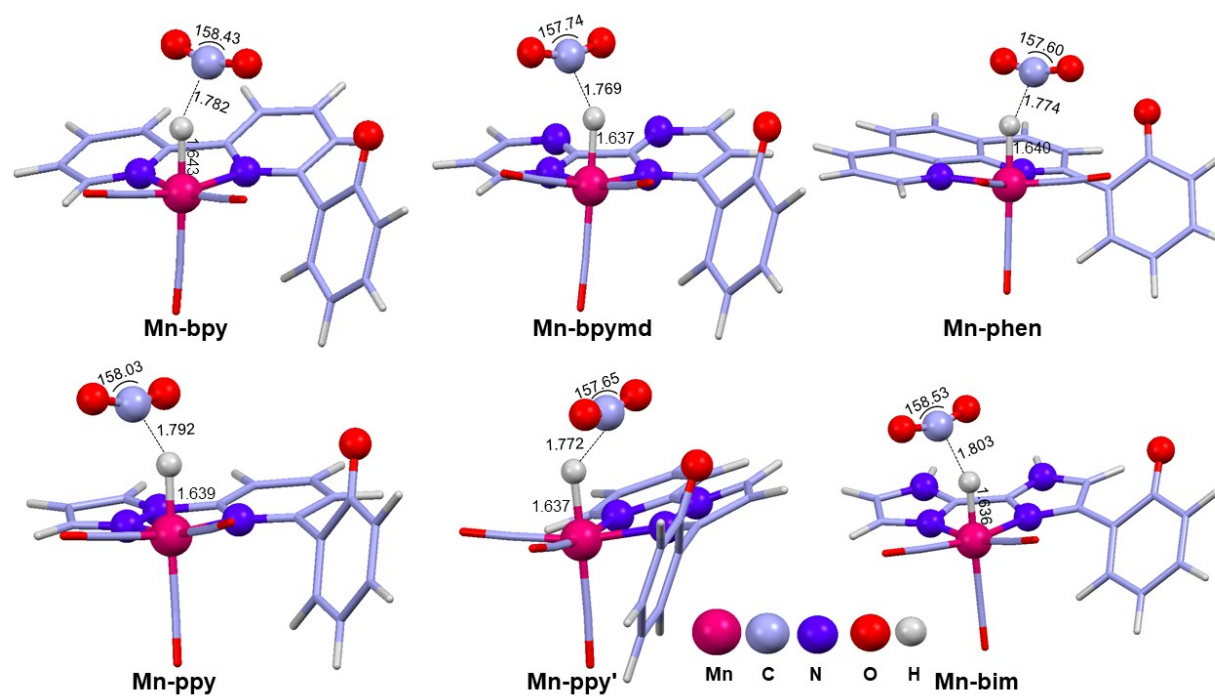


Figure S10. Optimized geometries of TS2 for all the Mn-complexes. Bond lengths are in Å.

(k) Optimized geometries of TS3

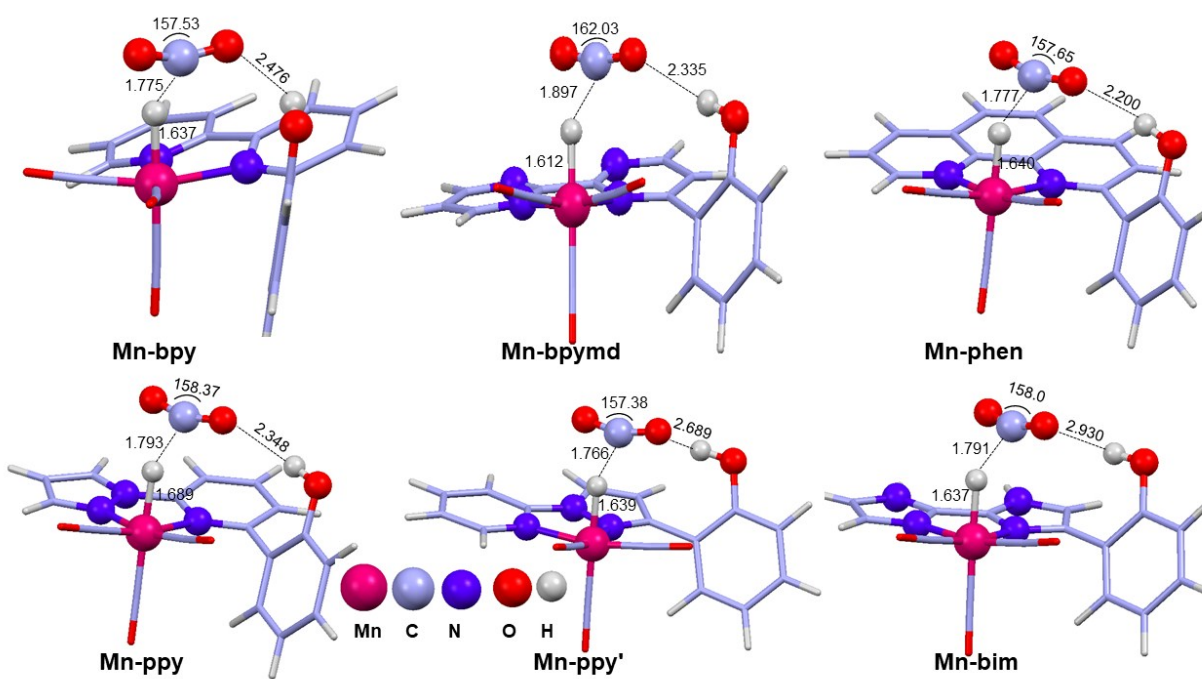


Figure S11. Optimized geometries of TS3 for all the Mn-complexes. Bond lengths are in Å.

S3. Relative reaction free energies for heterolytic H₂ cleavage and water splitting

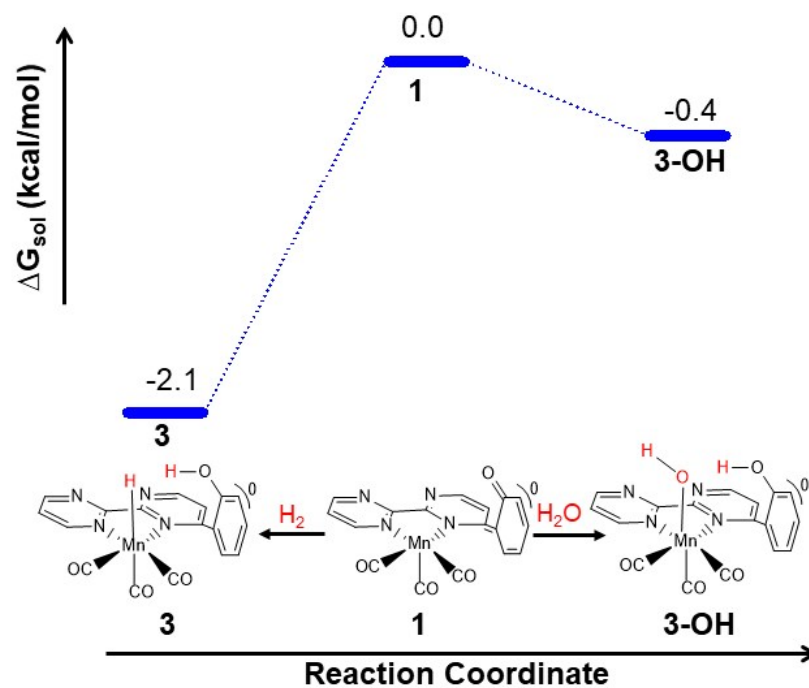


Figure S12. Relative reaction free energies for heterolytic H₂ cleavage and water splitting.

S4. Relaxed energy scan on the Mn-H and Mn-O bonds

We have investigated the relaxed energy scan for the desorption of formate from intermediate **5** (Figure S13). The relaxed energy scan suggests that the direct desorption of formate is favorable. Further, we find the reabsorbed of formate to more stable conformation **5'** (Figure S14) is a favourable process. Further, we have reabsorbed formate to a more stable conformation **5'** and it is also a favourable process (Figure S14). This agrees well with our calculated reaction free energy. In this process, we also find a new conformer **5''** (Figure S15), which is 0.79 kcal/mol less stable compared to **5'**.

Similarly, we have studied for **6** and **6'**. However, we are not able to optimize the intermediates related to formate desorption from **6**. However, the formate reabsorption is (**6**→**6'**) found to be a favourable process. In this process, we find another conformer **6''**, which is 0.71 kcal/mol less stable compared to **6'**. These results suggest the formation of **5'** and **6'** are favourable and the total free energy barrier of the reaction depends upon the stability of **5'/6'**.

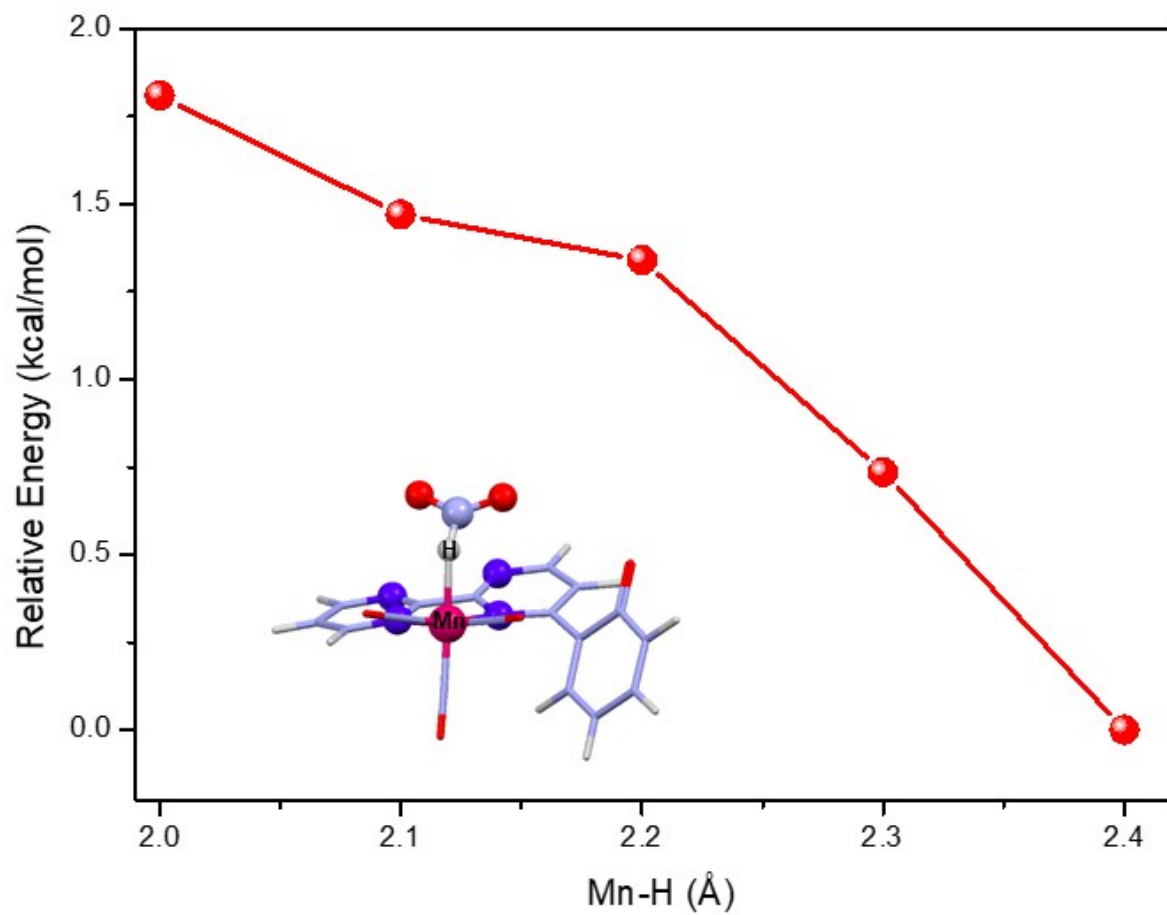


Figure S13. Relaxed scan energy profile for Mn-H bond of intermediate 5.

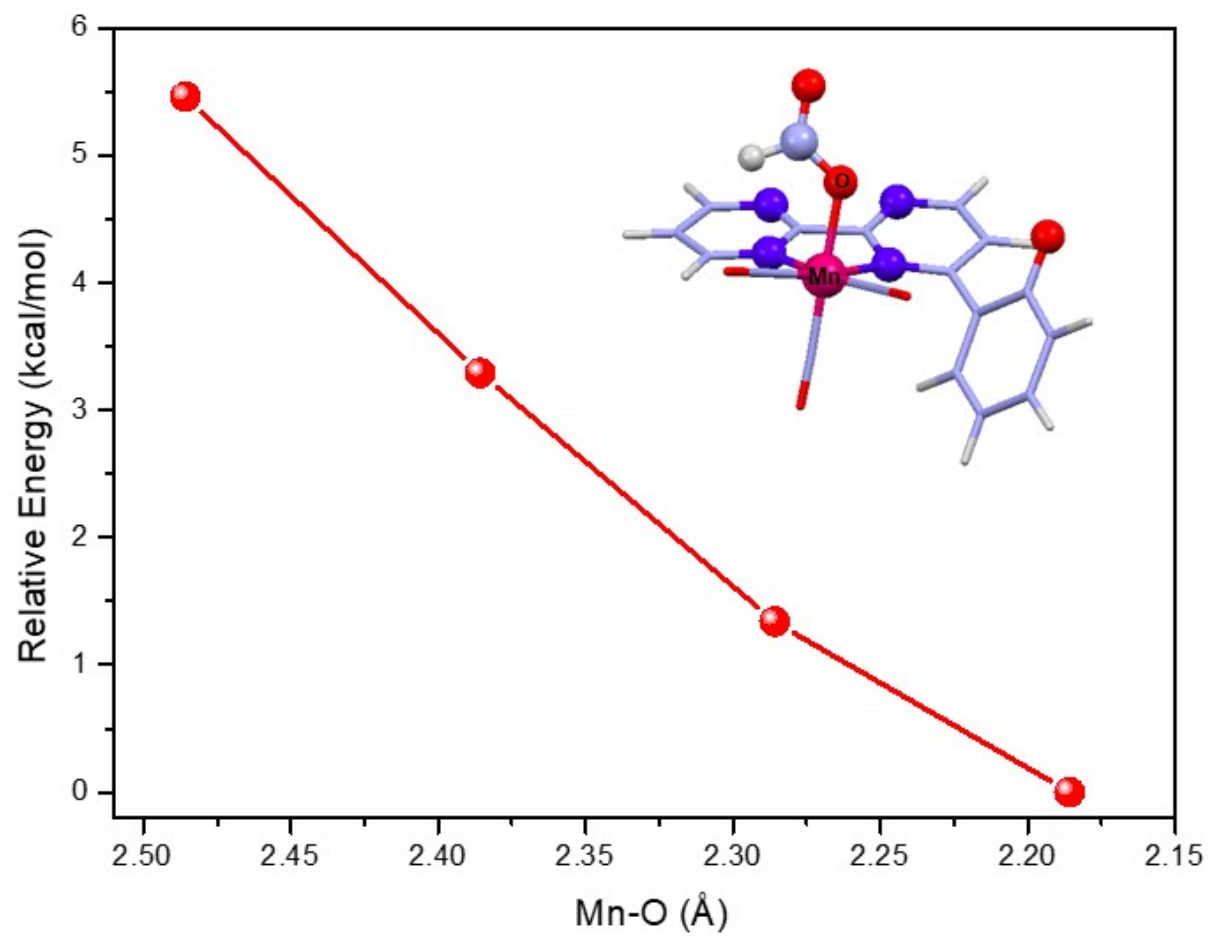


Figure S14. Relaxed scan energy profile for Mn-O bond of intermediate 5'.

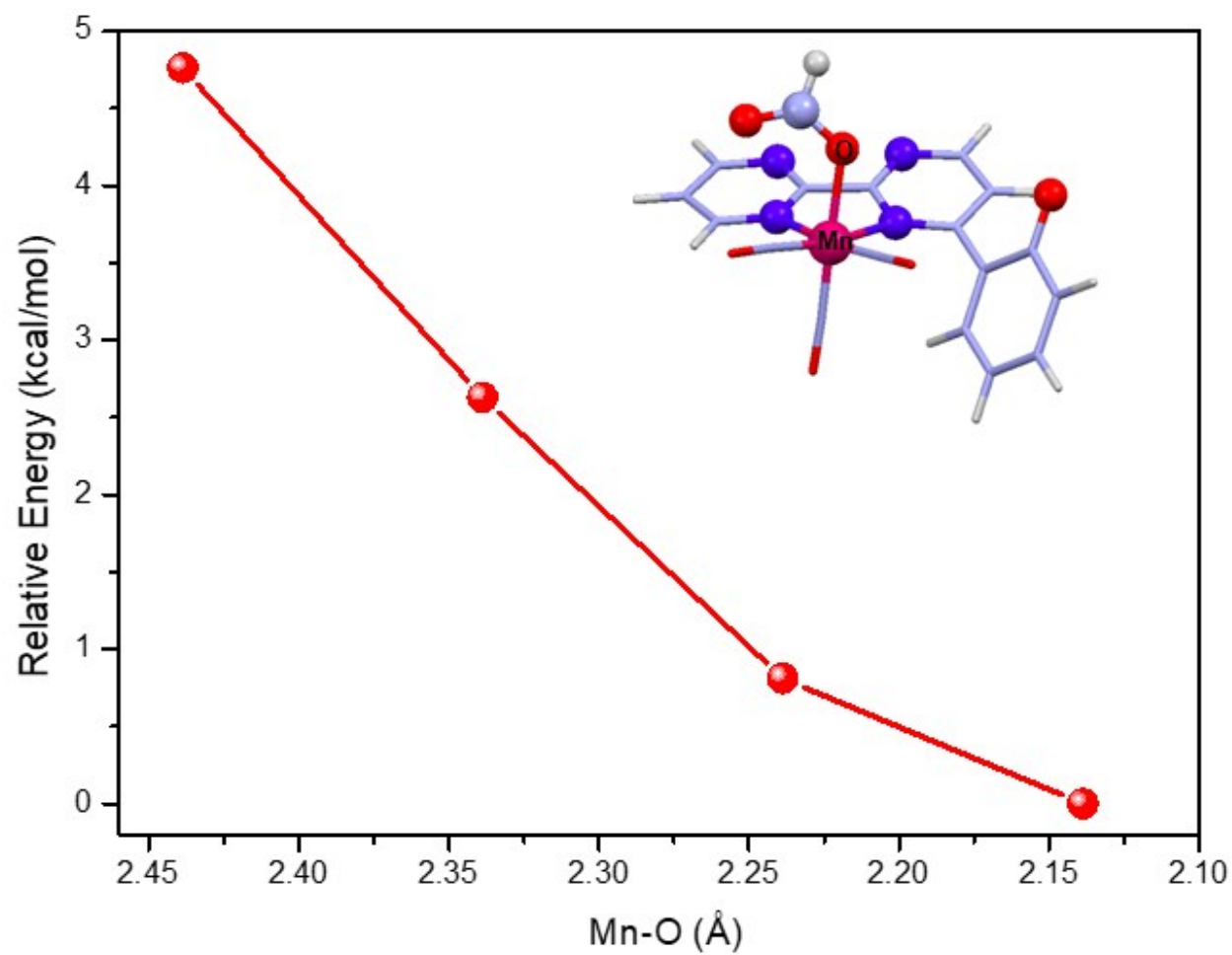


Figure S15. Relaxed scan energy profile for Mn-O bond of intermediate 5''.

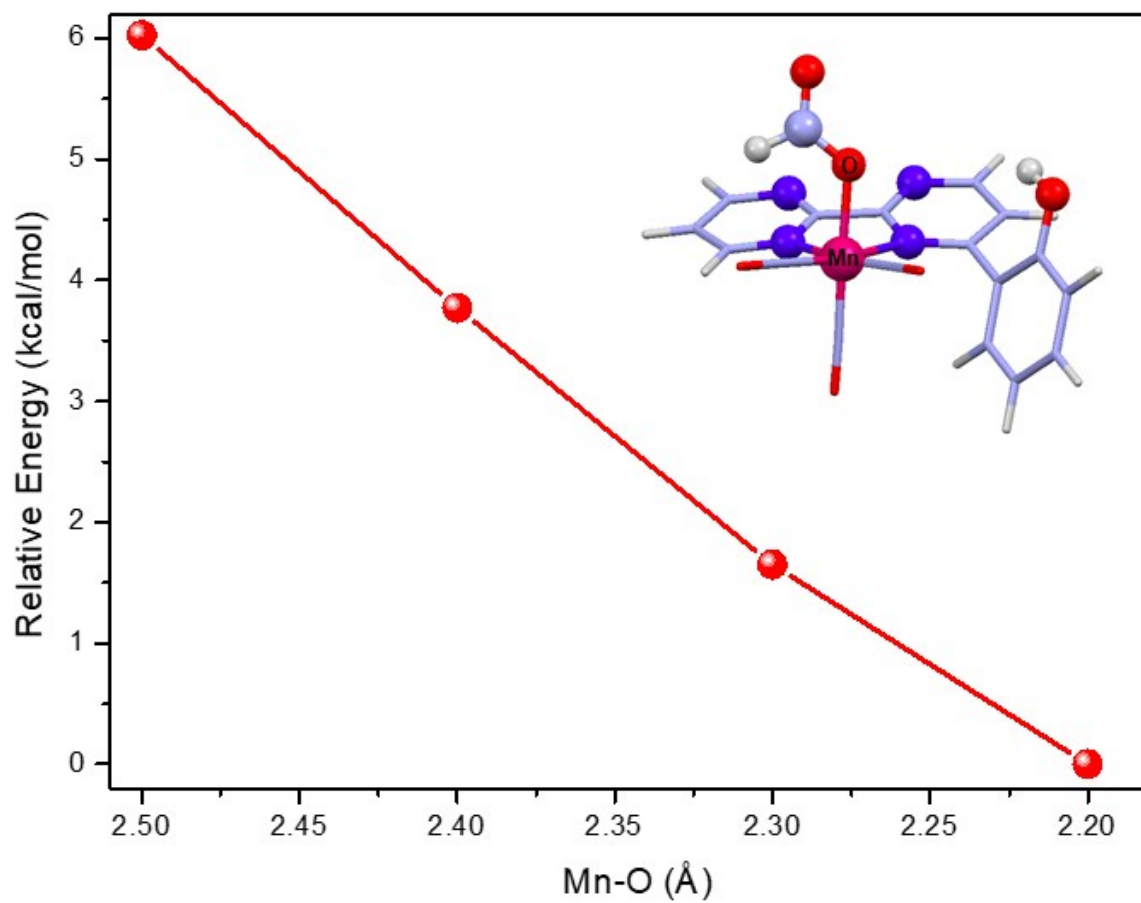


Figure S16. Relaxed scan energy profile for Mn-O bond of intermediate 6'.

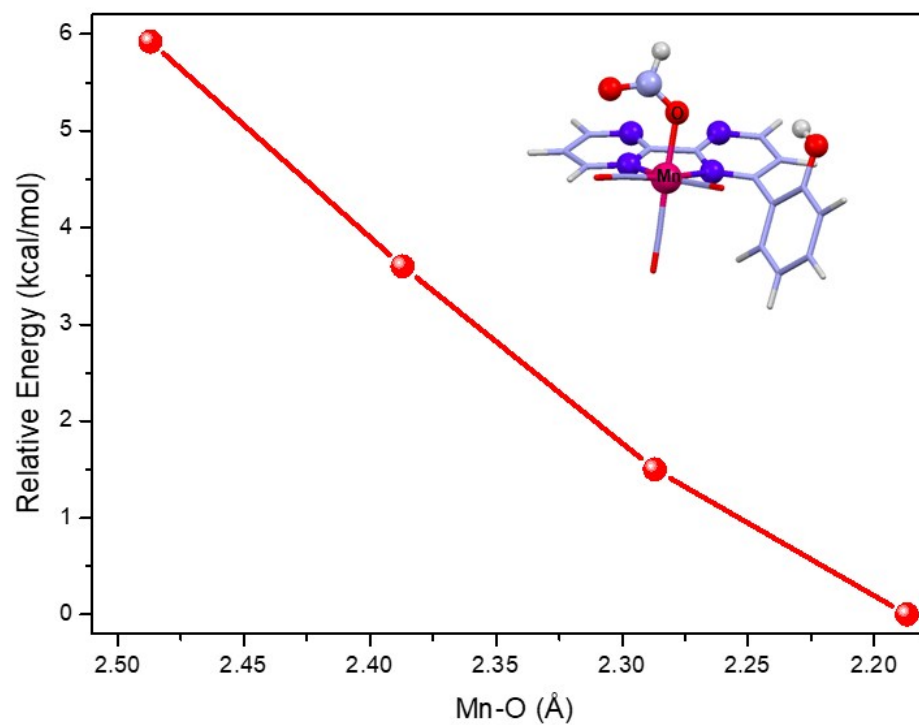


Figure S15. Relaxed scan energy profile for Mn-O bond of intermediate 6''.

S5. Gaussian full reference (reference number 14 in the manuscript)

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.

S6. Reference

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3. C. P. Kelly, C. J. Cramer, D G. Truhlar, *J. Phys. Chem. B* 2006, **110**, 16066–16081.
4. C. Hou, J. Jiang, S. Zhang, G. Wang, Z. Zhang, Z. Ke, C. Zhao, *ACS Catal.* 2014, **4**, 2990–2997
5. W. -H. Wang, J. F. Hull, J. T. Muckerman, E. Fujita, Y. Himeda, *Energy Environ. Sci.* 2012, **5**, 7923–7926.

S7. Cartesian coordinates and absolute free energies (in Hartree) in solvent phase for all the species.

H₂

1	0.000000000	0.000000000	0.372025000
1	0.000000000	0.000000000	-0.372025000

-1.177691

CO₂

6	0.000000000	0.000000000	0.000000000
8	0.000000000	0.000000000	1.169387000
8	0.000000000	0.000000000	-1.169387000

-188.596126

H₂O

8	0.000000000	0.000000000	0.118456000
1	0.000000000	0.766366000	-0.473823000
1	0.000000000	-0.766366000	-0.473823000

-76.444798

HCOO⁻

8	-1.132798000	-0.220762000	0.000000000
8	1.132857000	-0.220181000	0.000000000
6	0.000000000	0.345085000	0.000000000
1	-0.000473000	1.457030000	0.000000000

-189.336109

HCOOH

8	1.117216000	-0.091331000	0.000123000
8	-1.143880000	-0.267056000	0.000088000
6	-0.126866000	0.405520000	-0.000260000
1	-0.108196000	1.502015000	0.000301000
1	1.082701000	-1.068033000	-0.000429000

-189.777421

Mn-bpy

1

25	0.586814000	-0.981313000	-0.396601000
8	1.613950000	-3.563544000	-1.450191000

8	0.346372000	-2.162224000	2.275773000
7	2.434229000	-0.225503000	-0.013033000
7	0.095027000	1.005578000	0.024373000
6	1.223908000	-2.556169000	-1.042593000
6	-1.083012000	-1.557358000	-0.925998000
8	-2.052915000	-2.044742000	-1.313648000
6	0.410536000	-1.702991000	1.216092000
6	2.496112000	1.128573000	0.037540000
6	3.719681000	1.788007000	0.195776000
1	3.761821000	2.868977000	0.235560000
6	4.886879000	1.039402000	0.326054000
1	5.841076000	1.539493000	0.456309000
6	4.809176000	-0.354140000	0.301605000
1	5.689249000	-0.976952000	0.413820000
6	3.564365000	-0.946176000	0.128091000
1	3.456965000	-2.023616000	0.104365000
6	1.193416000	1.818705000	-0.034403000
6	-1.141284000	1.567543000	0.081922000
6	-1.298214000	2.960451000	-0.031088000
1	-2.298908000	3.373265000	0.003836000
6	-0.186729000	3.779554000	-0.150527000
1	-0.297873000	4.856234000	-0.229665000
6	1.084397000	3.202253000	-0.131860000
1	1.967626000	3.824707000	-0.196843000
6	-3.439132000	0.775993000	-0.589717000
6	-2.328734000	0.727124000	0.326583000
6	-4.560987000	-0.043652000	-0.252553000
6	-2.376443000	-0.081303000	1.475925000
1	-5.408380000	-0.036454000	-0.934413000
6	-4.578526000	-0.846535000	0.882176000
6	-3.484877000	-0.874045000	1.766597000
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1	-5.453763000	-1.459458000	1.087335000
1	-3.504109000	-1.490489000	2.659999000
8	-3.415527000	1.485111000	-1.686370000

-1244.927338

2

25	0.433637000	-1.066151000	0.058508000
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8	1.270896000	-3.910601000	-0.026280000
8	1.020737000	-0.906339000	2.955925000
7	2.306305000	-0.316087000	-0.368869000
7	0.055498000	0.997019000	0.033560000
6	0.953125000	-2.800091000	-0.000304000
6	-1.242913000	-1.686843000	0.466880000
8	-2.201273000	-2.234832000	0.806336000
6	0.790284000	-0.976166000	1.828575000
6	2.442844000	1.021173000	-0.184577000
6	3.685970000	1.647956000	-0.324543000
6	4.799074000	0.889028000	-0.675680000
1	5.767874000	1.363709000	-0.792227000
6	4.645112000	-0.481908000	-0.883427000
1	5.478983000	-1.113376000	-1.168483000
6	3.384495000	-1.044015000	-0.712697000
1	3.231813000	-2.106135000	-0.856565000
6	1.191468000	1.745868000	0.108204000
6	-1.151484000	1.606994000	0.139112000
6	-1.231763000	2.975000000	0.451664000
1	-2.210022000	3.432818000	0.542709000
6	-0.073293000	3.724730000	0.606700000
1	-0.124743000	4.780957000	0.850728000
6	1.160159000	3.108454000	0.402465000
6	-2.613984000	0.247734000	-1.407243000
6	-2.394151000	0.851101000	-0.116211000
6	-3.866745000	-0.417214000	-1.581288000
6	-3.395743000	0.825416000	0.869155000
1	-4.051053000	-0.891711000	-2.542356000
6	-4.824939000	-0.465237000	-0.576265000
6	-4.602475000	0.159911000	0.664955000
1	-3.198983000	1.312130000	1.821893000
1	-5.761303000	-0.989148000	-0.755697000
1	-5.353153000	0.124395000	1.448498000
8	-1.731351000	0.305344000	-2.368703000
1	0.378808000	-1.291290000	-1.700729000
1	-0.193434000	-0.751278000	-1.654296000
1	2.076185000	3.680649000	0.473913000
1	3.783153000	2.715611000	-0.173999000

-1246.095932

TS1

25	0.424307000	-1.055418000	0.102444000
8	1.199030000	-3.902870000	-0.126980000
8	1.201009000	-0.950482000	2.958322000
7	2.283149000	-0.304170000	-0.394353000
7	0.042424000	1.002788000	0.041151000
6	0.907575000	-2.787034000	-0.030024000
6	-1.223329000	-1.642849000	0.615542000
8	-2.175096000	-2.144972000	1.041609000
6	0.892346000	-0.986899000	1.845681000
6	2.424679000	1.032003000	-0.202856000
6	3.669551000	1.656273000	-0.340893000
6	4.780105000	0.895560000	-0.696022000
1	5.750725000	1.367388000	-0.809281000
6	4.621498000	-0.474010000	-0.910598000
1	5.453837000	-1.106510000	-1.198014000
6	3.359187000	-1.033232000	-0.741681000
1	3.202151000	-2.094442000	-0.888466000
6	1.175227000	1.757506000	0.095461000
6	-1.166170000	1.612218000	0.126059000
6	-1.253142000	2.985661000	0.412881000
1	-2.232077000	3.444925000	0.487714000
6	-0.096892000	3.740208000	0.559791000
1	-0.152414000	4.800680000	0.783511000
6	1.139075000	3.124792000	0.366366000
6	-2.563681000	0.137376000	-1.371927000
6	-2.403594000	0.850126000	-0.137955000
6	-3.806159000	-0.517709000	-1.584647000
6	-3.463172000	0.910448000	0.785013000
1	-3.932563000	-1.068099000	-2.513339000
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6	-4.665153000	0.246102000	0.555316000
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1	-5.461770000	0.280998000	1.292110000
8	-1.604561000	0.081221000	-2.282037000
1	0.221220000	-1.219551000	-1.594805000
1	-0.441728000	-0.684461000	-1.700574000
1	2.052587000	3.702522000	0.423498000

1	3.770653000	2.722580000	-0.182672000
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-1246.096518

TS1-H₂O

25	-0.562898000	-1.052170000	0.261469000
8	-1.544976000	-3.596488000	1.392432000
8	-0.465776000	-2.102857000	-2.506608000
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6	-1.165004000	-2.600425000	0.937677000
6	1.094507000	-1.692687000	0.616717000
8	2.068352000	-2.255468000	0.891341000
6	-0.502446000	-1.685550000	-1.428186000
6	-2.541724000	1.045926000	-0.192193000
6	-3.775392000	1.688988000	-0.351347000
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6	1.074364000	1.511464000	-0.403043000
6	1.228958000	2.905907000	-0.403642000
1	2.227914000	3.319481000	-0.480257000
6	0.114554000	3.726187000	-0.296772000
1	0.218513000	4.806213000	-0.277550000
6	-1.145745000	3.136574000	-0.226255000
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6	2.289229000	0.668604000	-0.517523000
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1	5.152808000	-0.079693000	1.169223000
6	4.670823000	-0.759829000	-0.823564000
6	3.722925000	-0.770872000	-1.858682000
1	1.797663000	-0.025838000	-2.489673000
1	5.601744000	-1.310056000	-0.937165000

1	3.908238000	-1.322342000	-2.775345000
8	2.965932000	1.247808000	1.722545000
1	-0.731386000	-0.471949000	1.844311000
1	-0.069641000	0.175501000	2.066752000
8	0.684013000	1.110100000	2.631921000
1	1.685044000	1.172110000	2.177706000
1	0.236273000	1.942738000	2.409300000

-1322.526919

3

25	0.482975000	-1.087613000	0.095321000
8	1.332144000	-3.868073000	-0.352635000
8	1.086865000	-1.073165000	3.008163000
7	2.341099000	-0.274614000	-0.327200000
7	0.045763000	0.988093000	0.035604000
6	1.013798000	-2.766920000	-0.148748000
6	-1.142929000	-1.772484000	0.423744000
8	-2.123395000	-2.348601000	0.671871000
6	0.854338000	-1.050319000	1.870696000
6	2.433735000	1.071862000	-0.203148000
6	3.658580000	1.734699000	-0.356919000
6	4.804855000	0.998937000	-0.641062000
1	5.759277000	1.500316000	-0.764360000
6	4.701077000	-0.386770000	-0.768571000
1	5.562682000	-1.005432000	-0.993649000
6	3.454711000	-0.979681000	-0.601121000
1	3.340497000	-2.052586000	-0.690516000
6	1.161833000	1.769027000	0.062652000
6	-1.164930000	1.586222000	0.144650000
6	-1.281518000	2.960491000	0.398362000
1	-2.269544000	3.396923000	0.488916000
6	-0.138133000	3.743457000	0.503896000
1	-0.210021000	4.806976000	0.706930000
6	1.101015000	3.143706000	0.306212000
6	-2.700635000	0.180219000	-1.285246000
6	-2.416975000	0.814175000	-0.056772000
6	-3.950232000	-0.407581000	-1.501405000
6	-3.405466000	0.820074000	0.941425000
1	-4.141640000	-0.882003000	-2.458949000

6	-4.918081000	-0.394823000	-0.495945000
6	-4.642697000	0.210360000	0.736355000
1	-3.187463000	1.307367000	1.887425000
1	-5.881917000	-0.863507000	-0.672209000
1	-5.387388000	0.213927000	1.526295000
8	-1.784546000	0.153464000	-2.320718000
1	0.215780000	-1.109889000	-1.495654000
1	-0.927871000	-0.222495000	-1.985658000
1	2.004646000	3.738032000	0.344981000
1	3.717928000	2.811435000	-0.263178000

-1246.107898

4

25	0.577130000	-1.042250000	-0.351536000
8	1.654994000	-3.566667000	-1.397002000
8	0.323255000	-2.103121000	2.412182000
7	2.434618000	-0.214414000	-0.020666000
7	0.086423000	1.003731000	0.013095000
6	1.230641000	-2.572921000	-0.955105000
6	-1.028062000	-1.609151000	-0.905003000
8	-2.000700000	-2.068344000	-1.352586000
6	0.414631000	-1.634739000	1.349386000
6	2.484975000	1.138262000	0.035877000
6	3.704966000	1.812162000	0.190834000
1	3.734606000	2.893281000	0.238922000
6	4.883622000	1.081478000	0.302628000
1	5.833237000	1.592331000	0.425142000
6	4.818713000	-0.313056000	0.268161000
1	5.706226000	-0.928401000	0.365495000
6	3.577017000	-0.916373000	0.107183000
1	3.485467000	-1.995287000	0.079407000
6	1.179465000	1.819733000	-0.031736000
6	-1.145284000	1.568867000	0.075671000
6	-1.307419000	2.961691000	-0.016486000
1	-2.310169000	3.370947000	0.021553000
6	-0.198436000	3.787397000	-0.133133000
1	-0.311409000	4.864312000	-0.208230000
6	1.068887000	3.208475000	-0.118349000
1	1.951758000	3.831893000	-0.180438000

6	-3.425050000	0.745763000	-0.644758000
6	-2.345251000	0.730409000	0.304794000
6	-4.566297000	-0.045218000	-0.306055000
6	-2.436107000	-0.024422000	1.484019000
1	-5.393958000	-0.058092000	-1.012056000
6	-4.629494000	-0.795615000	0.863935000
6	-3.561884000	-0.794992000	1.778414000
1	-1.603573000	0.000970000	2.181606000
1	-5.518463000	-1.388258000	1.070400000
1	-3.611445000	-1.372747000	2.696482000
8	-3.365706000	1.411139000	-1.771312000
1	0.749651000	-0.550463000	-1.868810000

-1245.646007

TS2

25	-0.496360000	-1.107675000	0.262558000
8	-1.567616000	-3.331403000	1.861266000
8	-0.085400000	-2.811847000	-2.130383000
7	-2.341334000	-0.441133000	-0.350318000
7	-0.016092000	0.809198000	-0.542563000
6	-1.149917000	-2.468182000	1.200475000
6	1.101824000	-1.469882000	1.000815000
8	2.063736000	-1.759619000	1.584584000
6	-0.233490000	-2.104366000	-1.219596000
6	-2.411577000	0.867666000	-0.692177000
6	-3.628397000	1.458108000	-1.059634000
1	-3.670017000	2.504056000	-1.336286000
6	-4.784652000	0.685178000	-1.084296000
1	-5.732757000	1.129562000	-1.369539000
6	-4.699482000	-0.668228000	-0.750453000
1	-5.569249000	-1.315554000	-0.767679000
6	-3.461709000	-1.188165000	-0.390773000
1	-3.353926000	-2.233978000	-0.130240000
6	-1.126040000	1.588424000	-0.691337000
6	1.207934000	1.390329000	-0.633332000
6	1.333420000	2.785061000	-0.758808000
1	2.326471000	3.214134000	-0.812393000
6	0.202530000	3.584293000	-0.836394000
1	0.289031000	4.662359000	-0.928118000

6	-1.050962000	2.974389000	-0.825786000
1	-1.950358000	3.571536000	-0.904852000
6	3.515079000	0.815008000	0.238347000
6	2.427954000	0.555167000	-0.670473000
6	4.667036000	-0.019686000	0.088546000
6	2.529376000	-0.458786000	-1.636703000
1	5.498091000	0.148120000	0.770192000
6	4.737652000	-1.025377000	-0.869463000
6	3.666697000	-1.257520000	-1.750530000
1	1.697285000	-0.609798000	-2.317796000
1	5.635565000	-1.636307000	-0.937451000
1	3.723646000	-2.032035000	-2.509370000
8	3.455508000	1.731188000	1.167703000
1	-0.766898000	-0.269217000	1.639246000
6	-0.777828000	1.276277000	2.527293000
8	-1.936591000	1.533463000	2.484118000
8	0.369289000	1.396252000	2.804734000

-1434.228935

5

25	-0.420172000	-0.981677000	-0.033635000
8	-1.521411000	-3.630888000	0.716387000
8	0.119170000	-1.978267000	-2.745468000
7	-2.221187000	-0.195022000	-0.581407000
7	0.106475000	1.027306000	-0.322079000
6	-1.109343000	-2.590714000	0.430201000
6	1.171073000	-1.589516000	0.638471000
8	2.093866000	-2.097375000	1.109371000
6	-0.067033000	-1.583322000	-1.675127000
6	-2.277133000	1.159408000	-0.590285000
6	-3.482512000	1.829833000	-0.824533000
1	-3.519136000	2.911674000	-0.826138000
6	-4.638386000	1.092709000	-1.066277000
1	-5.579238000	1.601222000	-1.250247000
6	-4.565989000	-0.301499000	-1.078487000
1	-5.436910000	-0.916641000	-1.273945000
6	-3.339539000	-0.904295000	-0.829644000
1	-3.238538000	-1.982437000	-0.829114000
6	-0.989241000	1.842168000	-0.367043000

6	1.340552000	1.586272000	-0.212061000
6	1.482761000	2.972351000	-0.029108000
1	2.480255000	3.381470000	0.076192000
6	0.365420000	3.793556000	-0.022708000
1	0.466480000	4.866173000	0.108429000
6	-0.891971000	3.222967000	-0.218287000
1	-1.776865000	3.845776000	-0.239869000
6	3.547869000	0.747551000	0.682284000
6	2.550521000	0.752054000	-0.356171000
6	4.705914000	-0.052146000	0.429606000
6	2.734415000	0.012342000	-1.536817000
1	5.470900000	-0.083743000	1.202136000
6	4.858519000	-0.788301000	-0.740319000
6	3.873073000	-0.764551000	-1.743760000
1	1.969349000	0.064285000	-2.306262000
1	5.755359000	-1.388480000	-0.879095000
1	3.997966000	-1.327530000	-2.663563000
8	3.395873000	1.396336000	1.805535000
1	-0.644144000	-0.317810000	1.778135000
6	-1.504495000	-0.223255000	2.547683000
8	-1.737148000	-1.262007000	3.204360000
8	-2.003480000	0.919740000	2.615178000

-1434.250559

5'

25	-0.512837000	-0.967972000	-0.091803000
8	-1.573149000	-3.685391000	0.392970000
8	-0.180414000	-1.560368000	-2.962351000
7	-2.354554000	-0.119634000	-0.457983000
7	0.008503000	1.083725000	-0.261239000
6	-1.169222000	-2.617108000	0.199626000
6	1.117864000	-1.652216000	0.339417000
8	2.078284000	-2.225271000	0.633981000
6	-0.288192000	-1.321935000	-1.833358000
6	-2.391818000	1.230660000	-0.363424000
6	-3.600237000	1.928551000	-0.486122000
1	-3.623202000	3.008254000	-0.413443000
6	-4.777918000	1.223725000	-0.718205000
1	-5.719337000	1.754287000	-0.817556000

6	-4.725037000	-0.166196000	-0.831532000
1	-5.613172000	-0.757960000	-1.022531000
6	-3.493156000	-0.796025000	-0.693634000
1	-3.410832000	-1.872761000	-0.774902000
6	-1.085965000	1.892287000	-0.168535000
6	1.243450000	1.635328000	-0.178349000
6	1.401953000	3.005408000	0.094177000
1	2.405274000	3.407318000	0.170149000
6	0.289087000	3.820406000	0.235620000
1	0.399284000	4.880362000	0.441779000
6	-0.978118000	3.259517000	0.081998000
1	-1.860777000	3.880194000	0.166604000
6	3.463882000	0.717332000	0.589195000
6	2.450379000	0.816471000	-0.427910000
6	4.621903000	-0.045143000	0.242631000
6	2.618510000	0.198217000	-1.677009000
1	5.400448000	-0.145421000	0.995764000
6	4.760925000	-0.660551000	-0.997362000
6	3.759859000	-0.545472000	-1.977665000
1	1.840023000	0.316406000	-2.425423000
1	5.660193000	-1.235517000	-1.208914000
1	3.873879000	-1.013888000	-2.950518000
8	3.329564000	1.262709000	1.770142000
1	-0.124047000	-2.009023000	2.778246000
6	-0.641283000	-1.041587000	2.920548000
8	-0.924307000	-0.680340000	4.085991000
8	-0.910685000	-0.367788000	1.865483000

-1434.270550

TS3

25	-0.583916000	-1.059047000	0.051573000
8	-1.597921000	-3.485213000	1.369992000
8	-0.460228000	-2.235472000	-2.669979000
7	-2.469899000	-0.284936000	-0.250726000
7	-0.149076000	0.952136000	-0.442532000
6	-1.203587000	-2.542797000	0.813761000
6	1.052742000	-1.654525000	0.494618000
8	2.039440000	-2.151956000	0.853688000
6	-0.504772000	-1.745648000	-1.617883000

6	-2.543684000	1.061661000	-0.369917000
6	-3.775007000	1.711534000	-0.521850000
1	-3.821678000	2.788308000	-0.624072000
6	-4.944547000	0.957808000	-0.563780000
1	-5.905185000	1.447881000	-0.684549000
6	-4.856976000	-0.431628000	-0.464200000
1	-5.737449000	-1.062974000	-0.507417000
6	-3.601941000	-1.010501000	-0.310631000
1	-3.490859000	-2.085450000	-0.236805000
6	-1.244526000	1.757651000	-0.380662000
6	1.068880000	1.532657000	-0.552587000
6	1.227041000	2.924484000	-0.530741000
1	2.224075000	3.341306000	-0.620463000
6	0.111167000	3.744041000	-0.402121000
1	0.215653000	4.823467000	-0.367882000
6	-1.144717000	3.151306000	-0.342209000
1	-2.032412000	3.764927000	-0.256631000
6	3.320756000	0.675465000	0.195458000
6	2.274276000	0.684703000	-0.744536000
6	4.473589000	-0.081874000	-0.037181000
6	2.408140000	-0.084437000	-1.912468000
1	5.259629000	-0.082290000	0.711599000
6	4.585976000	-0.839604000	-1.202131000
6	3.550664000	-0.846986000	-2.146420000
1	1.597973000	-0.073411000	-2.634954000
1	5.482001000	-1.430127000	-1.369512000
1	3.635485000	-1.437341000	-3.053262000
8	3.266529000	1.364058000	1.389075000
1	-0.706296000	-0.441176000	1.563009000
6	0.207441000	0.326812000	2.877358000
8	0.479322000	-0.617983000	3.544781000
8	0.154909000	1.471626000	2.565109000
1	2.387885000	1.751418000	1.531832000

-1434.689485

6			
25	-0.431370000	-0.996587000	-0.075043000
8	-1.508102000	-3.677829000	0.593286000
8	0.031419000	-1.848136000	-2.855988000

7	-2.258140000	-0.193118000	-0.514756000
7	0.080002000	1.026922000	-0.332022000
6	-1.105713000	-2.626698000	0.338220000
6	1.171770000	-1.645833000	0.517864000
8	2.101926000	-2.179002000	0.943837000
6	-0.131397000	-1.515866000	-1.761986000
6	-2.310288000	1.161000000	-0.531352000
6	-3.521154000	1.835666000	-0.716380000
1	-3.555086000	2.917313000	-0.729209000
6	-4.692051000	1.102317000	-0.892023000
1	-5.637862000	1.614223000	-1.036050000
6	-4.626746000	-0.291077000	-0.888432000
1	-5.509000000	-0.904751000	-1.030082000
6	-3.391248000	-0.897741000	-0.696459000
1	-3.299515000	-1.976177000	-0.689627000
6	-1.011762000	1.841042000	-0.365905000
6	1.311172000	1.594973000	-0.261598000
6	1.469711000	2.980819000	-0.144456000
1	2.471864000	3.390865000	-0.086540000
6	0.350813000	3.806266000	-0.126897000
1	0.457327000	4.881923000	-0.033279000
6	-0.906555000	3.229504000	-0.258889000
1	-1.791141000	3.852586000	-0.267776000
6	3.466542000	0.682228000	0.678717000
6	2.526718000	0.748710000	-0.366847000
6	4.629412000	-0.081736000	0.534699000
6	2.788032000	0.047461000	-1.556680000
1	5.329233000	-0.129913000	1.363102000
6	4.863578000	-0.779225000	-0.649411000
6	3.943011000	-0.716989000	-1.703720000
1	2.072198000	0.118865000	-2.369025000
1	5.767110000	-1.373585000	-0.748111000
1	4.126209000	-1.253121000	-2.629380000
8	3.293257000	1.313901000	1.890938000
1	-0.552350000	-0.404965000	1.724247000
6	-1.407278000	-0.281374000	2.503787000
8	-1.671751000	-1.317744000	3.149411000
8	-1.846452000	0.882657000	2.590869000
1	2.450468000	1.793320000	1.922912000

-1434.708669

6'

25	-0.515384000	-0.970717000	-0.134503000
8	-1.540137000	-3.719733000	0.240967000
8	-0.204775000	-1.396920000	-3.038504000
7	-2.376293000	-0.128569000	-0.423959000
7	-0.025351000	1.095763000	-0.242159000
6	-1.153029000	-2.639408000	0.090548000
6	1.117569000	-1.679481000	0.230972000
8	2.083148000	-2.265586000	0.478550000
6	-0.312221000	-1.230559000	-1.897643000
6	-2.426624000	1.219397000	-0.305410000
6	-3.643307000	1.907285000	-0.387049000
1	-3.677005000	2.985193000	-0.295657000
6	-4.819669000	1.193593000	-0.601879000
1	-5.768300000	1.715991000	-0.669715000
6	-4.754978000	-0.192826000	-0.738979000
1	-5.641245000	-0.791257000	-0.917282000
6	-3.513399000	-0.812480000	-0.641627000
1	-3.423815000	-1.886744000	-0.744514000
6	-1.122668000	1.891622000	-0.130990000
6	1.200579000	1.664260000	-0.168056000
6	1.360744000	3.031581000	0.092444000
1	2.362564000	3.441902000	0.152271000
6	0.238866000	3.837500000	0.251139000
1	0.342267000	4.898160000	0.455282000
6	-1.020456000	3.263105000	0.118971000
1	-1.907383000	3.875065000	0.218251000
6	3.378408000	0.621266000	0.575846000
6	2.415139000	0.844517000	-0.424536000
6	4.550559000	-0.083602000	0.283750000
6	2.649890000	0.337721000	-1.713763000
1	5.271431000	-0.252131000	1.077648000
6	4.763678000	-0.579771000	-1.001670000
6	3.810852000	-0.374447000	-2.007960000
1	1.907312000	0.516725000	-2.484805000
1	5.674052000	-1.132051000	-1.215649000
1	3.973360000	-0.760709000	-3.009174000
8	3.220854000	1.037245000	1.881094000

1	-0.113074000	-2.145037000	2.684345000
6	-0.569088000	-1.155398000	2.874024000
8	-0.770988000	-0.806988000	4.059338000
8	-0.856577000	-0.443548000	1.848261000
1	2.338657000	1.413449000	2.027958000

-1434.729967

Mn- bpymd

1			
25	0.623888000	-0.991058000	-0.423800000
8	1.746314000	-3.490412000	-1.584978000
8	0.429948000	-2.292569000	2.199483000
7	2.440733000	-0.183885000	0.014828000
7	0.076025000	0.984063000	0.032985000
6	1.317615000	-2.519070000	-1.134955000
6	-1.040483000	-1.582083000	-0.966905000
8	-2.016570000	-2.049757000	-1.359024000
6	0.475563000	-1.785938000	1.161942000
6	2.469316000	1.165389000	0.060775000
7	3.565916000	1.900483000	0.229477000
6	4.719519000	1.237354000	0.399341000
1	5.611149000	1.841738000	0.535135000
6	4.785677000	-0.154760000	0.411762000
1	5.718877000	-0.681567000	0.569635000
6	3.599291000	-0.843582000	0.205571000
1	3.557389000	-1.926109000	0.191529000
6	1.141815000	1.824011000	-0.041998000
6	-1.169066000	1.541642000	0.078455000
6	-1.289091000	2.932741000	-0.090099000
1	-2.266782000	3.395463000	-0.077397000
6	-0.139110000	3.687767000	-0.221204000
1	-0.186094000	4.765427000	-0.344106000
7	1.092325000	3.141504000	-0.169832000
6	-3.515225000	0.829892000	-0.488752000
6	-2.341850000	0.709798000	0.345512000
6	-4.608611000	-0.030438000	-0.146975000
6	-2.317535000	-0.185639000	1.434842000
1	-5.498203000	0.024531000	-0.769916000

6	-4.552944000	-0.911215000	0.923316000
6	-3.405601000	-0.994325000	1.737911000
1	-1.431740000	-0.216169000	2.061545000
1	-5.412296000	-1.542675000	1.138416000
1	-3.373650000	-1.667287000	2.588858000
8	-3.574258000	1.627573000	-1.513251000

-1277.027228

2

25	0.452278000	-1.079632000	0.057584000
8	1.336474000	-3.911291000	-0.027336000
8	1.048423000	-0.919702000	2.956979000
7	2.308280000	-0.295872000	-0.383322000
7	0.047618000	0.979070000	0.026406000
6	0.999054000	-2.807908000	0.000702000
6	-1.220335000	-1.703361000	0.482257000
8	-2.185302000	-2.228717000	0.833941000
6	0.815586000	-0.986098000	1.830953000
6	2.430112000	1.036985000	-0.197878000
7	3.564922000	1.724517000	-0.306799000
6	4.661199000	1.036331000	-0.656923000
1	5.583710000	1.602420000	-0.742001000
6	4.630258000	-0.334040000	-0.904965000
1	5.516209000	-0.882518000	-1.201307000
6	3.411281000	-0.977903000	-0.740422000
1	3.307773000	-2.045079000	-0.893251000
6	1.161889000	1.745456000	0.107527000
6	-1.159057000	1.596293000	0.140529000
6	-1.187674000	2.957673000	0.483839000
1	-2.135518000	3.469235000	0.599634000
6	0.013117000	3.632890000	0.624016000
1	0.037261000	4.684838000	0.891694000
7	1.199443000	3.040551000	0.397871000
6	-2.599915000	0.214263000	-1.395942000
6	-2.403253000	0.864490000	-0.122426000
6	-3.858091000	-0.441334000	-1.572926000
6	-3.428460000	0.890666000	0.842238000
1	-4.025799000	-0.950812000	-2.518703000
6	-4.835183000	-0.442102000	-0.587806000

6	-4.633532000	0.228260000	0.635353000
1	-3.247355000	1.409296000	1.780793000
1	-5.772596000	-0.964220000	-0.766162000
1	-5.401239000	0.226513000	1.402767000
8	-1.698882000	0.228454000	-2.337349000
1	0.393248000	-1.320304000	-1.694207000
1	-0.192174000	-0.789764000	-1.656589000

-1278.196248

TS1

25	0.438622000	-1.089281000	0.088791000
8	1.276075000	-3.914901000	-0.218420000
8	1.236844000	-1.048715000	2.938910000
7	2.294044000	-0.274713000	-0.410028000
7	0.034622000	0.993131000	0.052807000
6	0.956389000	-2.811598000	-0.090751000
6	-1.207010000	-1.691353000	0.603357000
8	-2.167663000	-2.177709000	1.022582000
6	0.920952000	-1.059314000	1.828456000
6	2.416565000	1.055216000	-0.198859000
7	3.553387000	1.742930000	-0.287260000
6	4.651962000	1.058447000	-0.637664000
1	5.576189000	1.624310000	-0.703980000
6	4.622032000	-0.307950000	-0.907054000
1	5.510891000	-0.852867000	-1.201315000
6	3.400348000	-0.952214000	-0.765213000
1	3.294534000	-2.016986000	-0.933724000
6	1.148014000	1.763188000	0.111291000
6	-1.170726000	1.613847000	0.143490000
6	-1.205510000	2.982304000	0.452763000
1	-2.154150000	3.496466000	0.549030000
6	-0.004910000	3.660530000	0.585152000
1	0.017538000	4.717997000	0.830224000
7	1.182081000	3.064370000	0.374398000
6	-2.581152000	0.172444000	-1.362886000
6	-2.412278000	0.873726000	-0.122070000
6	-3.823915000	-0.487762000	-1.563043000
6	-3.463950000	0.934505000	0.811653000
1	-3.959088000	-1.032722000	-2.493495000

6	-4.833476000	-0.449206000	-0.609671000
6	-4.663565000	0.266391000	0.589952000
1	-3.311351000	1.486163000	1.735718000
1	-5.766221000	-0.975844000	-0.796193000
1	-5.453920000	0.295244000	1.333446000
8	-1.640788000	0.142283000	-2.288858000
1	0.171763000	-1.240348000	-1.701868000
1	-0.475044000	-0.684283000	-1.794157000

-1278.191765

TS1-H2O

25	-0.573054000	-1.064936000	0.250205000
8	-1.581062000	-3.617427000	1.343363000
8	-0.457726000	-2.105796000	-2.524192000
7	-2.466627000	-0.285835000	-0.022849000
7	-0.148119000	0.928425000	-0.289001000
6	-1.188860000	-2.620256000	0.904671000
6	1.087171000	-1.699461000	0.613789000
8	2.067332000	-2.244104000	0.896720000
6	-0.502258000	-1.691039000	-1.446237000
6	-2.539420000	1.050916000	-0.188355000
7	-3.668148000	1.749126000	-0.312857000
6	-4.815677000	1.057068000	-0.292660000
1	-5.732051000	1.631034000	-0.391023000
6	-4.843916000	-0.329338000	-0.159105000
1	-5.773098000	-0.886139000	-0.159022000
6	-3.623042000	-0.974347000	-0.021092000
1	-3.559548000	-2.049280000	0.093245000
6	-1.230699000	1.744314000	-0.254625000
6	1.068343000	1.510533000	-0.402729000
6	1.168576000	2.906845000	-0.418334000
1	2.139397000	3.381155000	-0.493757000
6	0.002939000	3.650956000	-0.336889000
1	0.026346000	4.736537000	-0.333386000
7	-1.207606000	3.073330000	-0.273381000
6	3.220559000	0.693157000	0.569192000
6	2.290048000	0.685642000	-0.509191000
6	4.431132000	-0.017324000	0.379365000
6	2.541402000	-0.046870000	-1.678894000

1	5.154669000	-0.019911000	1.190300000
6	4.676332000	-0.729055000	-0.792954000
6	3.729516000	-0.760999000	-1.829631000
1	1.797087000	-0.043448000	-2.470831000
1	5.610353000	-1.275442000	-0.898857000
1	3.920266000	-1.323451000	-2.738257000
8	2.952110000	1.303264000	1.720254000
1	-0.750482000	-0.504740000	1.833870000
1	-0.077231000	0.126894000	2.070195000
8	0.680887000	1.037021000	2.662991000
1	1.660280000	1.149147000	2.206831000
1	0.218650000	1.877608000	2.511188000

-1354.625964

3

25	0.487430000	-1.157702000	0.085365000
8	1.425787000	-3.911398000	-0.358717000
8	1.092726000	-1.137212000	2.999958000
7	2.352971000	-0.241181000	-0.354391000
7	0.034476000	1.002791000	0.042042000
6	1.065661000	-2.824041000	-0.157880000
6	-1.139892000	-1.844663000	0.406553000
8	-2.139973000	-2.388434000	0.640168000
6	0.862945000	-1.117746000	1.863190000
6	2.427113000	1.097116000	-0.186750000
7	3.542619000	1.822618000	-0.282935000
6	4.670461000	1.168213000	-0.589144000
1	5.575000000	1.764409000	-0.662923000
6	4.693472000	-0.207854000	-0.806413000
1	5.605981000	-0.731774000	-1.064678000
6	3.491729000	-0.887606000	-0.666142000
1	3.426616000	-1.959948000	-0.804348000
6	1.139097000	1.784500000	0.089372000
6	-1.168303000	1.615426000	0.146674000
6	-1.228212000	2.987964000	0.413123000
1	-2.183843000	3.488924000	0.509348000
6	-0.032946000	3.684812000	0.520759000
1	-0.021832000	4.748083000	0.740651000
7	1.155480000	3.094707000	0.328192000

6	-2.697937000	0.202819000	-1.276687000
6	-2.423590000	0.858942000	-0.057065000
6	-3.946540000	-0.389780000	-1.483839000
6	-3.413989000	0.884605000	0.939419000
1	-4.135658000	-0.879320000	-2.434035000
6	-4.915508000	-0.363372000	-0.480148000
6	-4.647038000	0.265617000	0.741747000
1	-3.199366000	1.389880000	1.876602000
1	-5.877083000	-0.838765000	-0.650237000
1	-5.394115000	0.280451000	1.529067000
8	-1.784857000	0.170936000	-2.313711000
1	0.191776000	-1.185163000	-1.547152000
1	-0.940634000	-0.247615000	-1.998958000

-1278.205108

4

25	0.607347000	-1.054582000	-0.349584000
8	1.729337000	-3.541911000	-1.438724000
8	0.396637000	-2.169759000	2.398307000
7	2.443759000	-0.184957000	-0.027074000
7	0.076410000	0.978235000	0.033124000
6	1.287904000	-2.565069000	-0.979461000
6	-0.997464000	-1.632726000	-0.898635000
8	-1.973144000	-2.083488000	-1.344941000
6	0.470417000	-1.680242000	1.344782000
6	2.467024000	1.161650000	0.063844000
7	3.566857000	1.902802000	0.221945000
6	4.733284000	1.250713000	0.307741000
1	5.623935000	1.859028000	0.433790000
6	4.811890000	-0.139604000	0.244985000
1	5.756533000	-0.663920000	0.325684000
6	3.621464000	-0.830890000	0.074297000
1	3.596860000	-1.911963000	0.014701000
6	1.141325000	1.818107000	-0.001572000
6	-1.160302000	1.543999000	0.084868000
6	-1.280969000	2.937651000	-0.030010000
1	-2.260089000	3.398954000	-0.011658000
6	-0.129060000	3.697886000	-0.128864000
1	-0.173176000	4.779226000	-0.219310000

7	1.094888000	3.145264000	-0.085438000
6	-3.467886000	0.809316000	-0.607763000
6	-2.357520000	0.717300000	0.305079000
6	-4.603692000	-0.000345000	-0.288122000
6	-2.416904000	-0.116451000	1.435192000
1	-5.452987000	0.040570000	-0.966406000
6	-4.636584000	-0.822572000	0.831549000
6	-3.541794000	-0.888724000	1.713738000
1	-1.565724000	-0.140440000	2.108805000
1	-5.523994000	-1.420872000	1.027377000
1	-3.573327000	-1.520330000	2.596210000
8	-3.438457000	1.550697000	-1.681522000
1	0.753118000	-0.549403000	-1.862341000

-1277.748876

TS2

25	-0.403848000	-1.064836000	0.000264000
8	-1.631644000	-3.542024000	1.009703000
8	0.191102000	-2.259148000	-2.649598000
7	-2.186262000	-0.231037000	-0.588602000
7	0.158077000	0.949753000	-0.376600000
6	-1.149687000	-2.575607000	0.579464000
6	1.128562000	-1.612566000	0.764935000
8	2.041331000	-2.045243000	1.337174000
6	-0.031557000	-1.748238000	-1.630417000
6	-2.213549000	1.115347000	-0.683776000
7	-3.300954000	1.844736000	-0.939840000
6	-4.447235000	1.179521000	-1.133626000
1	-5.329809000	1.779064000	-1.335854000
6	-4.515710000	-0.212214000	-1.087245000
1	-5.443127000	-0.745540000	-1.258088000
6	-3.340548000	-0.891094000	-0.801393000
1	-3.305972000	-1.972007000	-0.738294000
6	-0.905636000	1.783987000	-0.494963000
6	1.390348000	1.520642000	-0.282088000
6	1.490666000	2.917362000	-0.190155000
1	2.462298000	3.383461000	-0.086994000
6	0.335406000	3.673607000	-0.281122000
1	0.367226000	4.758056000	-0.232293000

7	-0.871905000	3.112632000	-0.463688000
6	3.591187000	0.813121000	0.716770000
6	2.608385000	0.697646000	-0.330417000
6	4.762945000	0.006949000	0.559203000
6	2.816320000	-0.154446000	-1.429096000
1	5.517643000	0.062899000	1.340324000
6	4.943433000	-0.833657000	-0.532563000
6	3.972178000	-0.921750000	-1.547613000
1	2.060748000	-0.193227000	-2.207982000
1	5.851177000	-1.429356000	-0.602793000
1	4.120294000	-1.566739000	-2.408174000
8	3.417245000	1.570772000	1.764617000
1	-0.733400000	-0.518489000	1.508086000
6	-2.012272000	0.160492000	2.523840000
8	-2.621720000	-0.809364000	2.837627000
8	-1.721687000	1.311956000	2.485248000

-1466.330996

5

25	-0.499431000	-1.065816000	0.250666000
8	-1.601012000	-3.382424000	1.736679000
8	-0.121099000	-2.745703000	-2.137968000
7	-2.323842000	-0.392207000	-0.393645000
7	0.010893000	0.823840000	-0.529419000
6	-1.180380000	-2.481501000	1.150233000
6	1.139776000	-1.512997000	0.942600000
8	2.105986000	-1.887264000	1.446478000
6	-0.248636000	-2.078028000	-1.204452000
6	-2.377054000	0.918107000	-0.716626000
7	-3.475901000	1.572577000	-1.086100000
6	-4.609901000	0.859849000	-1.155611000
1	-5.503485000	1.397553000	-1.457898000
6	-4.653568000	-0.501930000	-0.864680000
1	-5.571447000	-1.072819000	-0.933786000
6	-3.465004000	-1.102145000	-0.474462000
1	-3.411319000	-2.155197000	-0.226393000
6	-1.074840000	1.628268000	-0.660674000
6	1.241303000	1.410430000	-0.562107000
6	1.317902000	2.813463000	-0.587657000

1	2.283084000	3.301885000	-0.584752000
6	0.145122000	3.540593000	-0.661578000
1	0.158427000	4.625833000	-0.691204000
7	-1.065145000	2.951448000	-0.733799000
6	3.555302000	0.866496000	0.267007000
6	2.451812000	0.590659000	-0.622886000
6	4.701912000	0.021598000	0.111070000
6	2.532520000	-0.441880000	-1.579000000
1	5.543460000	0.195444000	0.777496000
6	4.752961000	-0.991769000	-0.835548000
6	3.667722000	-1.233830000	-1.701758000
1	1.692873000	-0.595143000	-2.249772000
1	5.648079000	-1.605421000	-0.911362000
1	3.718198000	-2.013210000	-2.455483000
8	3.508000000	1.788921000	1.180869000
1	-0.725937000	-0.185549000	1.947110000
6	-0.930193000	0.857226000	2.418744000
8	0.102900000	1.489750000	2.716825000
8	-2.140864000	1.122566000	2.575173000

-1466.349928

5'

25	-0.456190000	-1.014690000	0.078780000
8	-1.604132000	-3.580899000	0.998360000
8	0.086259000	-2.209520000	-2.565980000
7	-2.224350000	-0.218779000	-0.597040000
7	0.126821000	0.976570000	-0.397520000
6	-1.169641000	-2.572919000	0.631430000
6	1.126569000	-1.583261000	0.786660000
8	2.065379000	-2.041381000	1.278220000
6	-0.097841000	-1.727370000	-1.529340000
6	-2.254099000	1.128542000	-0.659960000
7	-3.338738000	1.856692000	-0.924710000
6	-4.474349000	1.187413000	-1.168770000
1	-5.355358000	1.786393000	-1.379070000
6	-4.534760000	-0.204967000	-1.163860000
1	-5.452830000	-0.738937000	-1.377400000
6	-3.363520000	-0.883728000	-0.857580000
1	-3.321491000	-1.965768000	-0.817490000

6	-0.947258000	1.801531000	-0.448050000
6	1.357491000	1.545219000	-0.298460000
6	1.448852000	2.939209000	-0.142510000
1	2.418053000	3.409769000	-0.041020000
6	0.285343000	3.685660000	-0.163930000
1	0.309463000	4.765900000	-0.056000000
7	-0.925618000	3.125031000	-0.342800000
6	3.601181000	0.839498000	0.601180000
6	2.568341000	0.722109000	-0.399240000
6	4.749160000	0.005827000	0.407260000
6	2.717270000	-0.149102000	-1.494750000
1	5.537310000	0.059867000	1.154660000
6	4.866910000	-0.854273000	-0.676600000
6	3.853030000	-0.937262000	-1.650710000
1	1.932100000	-0.181031000	-2.243880000
1	5.759420000	-1.468643000	-0.775010000
1	3.955369000	-1.594742000	-2.508380000
8	3.493301000	1.620518000	1.637790000
1	-2.744650000	-0.903338000	2.095210000
6	-2.013000000	-0.183239000	2.506610000
8	-0.900270000	-0.064089000	1.881500000
8	-2.317729000	0.458852000	3.537240000

-1466.371675

TS3

25	-1.383646000	-0.588682000	0.550810000
7	-1.843914000	-1.200913000	-1.543826000
15	0.611436000	0.098386000	-0.428170000
8	-0.394911000	-3.282707000	1.289665000
8	-4.189864000	-1.041731000	1.397328000
8	-0.707845000	0.610981000	3.159852000
6	-0.661620000	-1.238158000	-2.444825000
1	-0.988480000	-1.301674000	-3.491137000
1	-0.100172000	-2.150624000	-2.218123000
6	0.201106000	0.003606000	-2.229732000
6	-0.777087000	-2.227163000	0.996444000
6	-3.092220000	-0.888792000	1.058977000
6	-0.973335000	0.128257000	2.137476000
6	2.077660000	-0.978711000	-0.169352000

6	2.761245000	-1.631812000	-1.204354000
6	2.502831000	-1.169749000	1.157559000
6	3.860440000	-2.450654000	-0.918850000
6	3.604743000	-1.977048000	1.440135000
6	4.287094000	-2.621130000	0.400349000
1	2.453851000	-1.513141000	-2.238003000
1	1.972183000	-0.685198000	1.973074000
1	4.380508000	-2.951214000	-1.730432000
1	3.925887000	-2.109597000	2.469066000
1	5.139577000	-3.257079000	0.619843000
6	1.283508000	1.788300000	-0.171464000
6	2.566208000	2.124952000	-0.639674000
6	0.511221000	2.764003000	0.476155000
6	3.059187000	3.420746000	-0.473354000
6	1.008255000	4.060736000	0.642308000
6	2.280898000	4.391323000	0.169103000
1	3.186230000	1.376245000	-1.124299000
1	-0.476112000	2.517325000	0.846518000
1	4.050677000	3.670854000	-0.839443000
1	0.401058000	4.806797000	1.146504000
1	2.667388000	5.397605000	0.302288000
1	1.088009000	0.003818000	-2.868382000
1	-0.371235000	0.909041000	-2.456464000
1	-1.882976000	0.931607000	0.020958000
1	-2.420543000	-0.413257000	-1.841940000
6	-2.839618000	2.043109000	-0.722526000
8	-2.971126000	2.877784000	0.117589000
8	-3.015809000	1.590007000	-1.818068000
6	-2.646703000	-2.436322000	-1.690948000
1	-2.884839000	-2.634542000	-2.743545000
1	-2.084373000	-3.281987000	-1.288991000
1	-3.576084000	-2.334958000	-1.129945000

-1611.527205

6			
25	-0.441436000	-1.031355000	-0.025507000
8	-1.560527000	-3.685487000	0.686609000
8	0.039306000	-1.960157000	-2.781677000
7	-2.253443000	-0.205778000	-0.506645000

7	0.096622000	0.981803000	-0.339192000
6	-1.139661000	-2.647525000	0.412859000
6	1.156293000	-1.666149000	0.601457000
8	2.091846000	-2.167975000	1.050120000
6	-0.130070000	-1.594682000	-1.700476000
6	-2.288221000	1.142497000	-0.559052000
7	-3.382294000	1.874795000	-0.750174000
6	-4.536393000	1.210605000	-0.909156000
1	-5.426980000	1.812917000	-1.059818000
6	-4.602611000	-0.180790000	-0.888296000
1	-5.536624000	-0.711838000	-1.025526000
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1	-3.379724000	-1.946911000	-0.642982000
6	-0.973343000	1.811757000	-0.408646000
6	1.324620000	1.560539000	-0.287684000
6	1.434828000	2.952326000	-0.222444000
1	2.410273000	3.421972000	-0.175436000
6	0.269643000	3.706209000	-0.253597000
1	0.301266000	4.790382000	-0.206463000
7	-0.938108000	3.140027000	-0.373352000
6	3.500643000	0.721580000	0.677076000
6	2.545580000	0.726534000	-0.357803000
6	4.662437000	-0.048353000	0.552731000
6	2.790170000	-0.035155000	-1.514987000
1	5.374816000	-0.052153000	1.371618000
6	4.881599000	-0.804514000	-0.597037000
6	3.946436000	-0.799143000	-1.640506000
1	2.064089000	-0.006108000	-2.320492000
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1	4.118799000	-1.379936000	-2.540725000
8	3.351512000	1.412619000	1.857475000
1	-0.605072000	-0.462755000	1.753379000
6	-1.512055000	-0.134920000	2.416349000
8	-1.677040000	1.099340000	2.465736000
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6'

25	-0.455434000	-1.020704000	0.033197000
8	-1.588987000	-3.643451000	0.804209000
8	0.107157000	-2.051012000	-2.677138000
7	-2.238956000	-0.211607000	-0.593847000
7	0.104694000	0.990340000	-0.373770000
6	-1.160372000	-2.613253000	0.500912000
6	1.122238000	-1.626247000	0.717216000
8	2.060652000	-2.104234000	1.189661000
6	-0.087304000	-1.639205000	-1.613398000
6	-2.280276000	1.136292000	-0.605523000
7	-3.374539000	1.868309000	-0.808380000
6	-4.514640000	1.201437000	-1.039233000
1	-5.405563000	1.801883000	-1.195797000
6	-4.566534000	-0.190351000	-1.085017000
1	-5.488179000	-0.721935000	-1.288856000
6	-3.381972000	-0.873506000	-0.845506000
1	-3.333526000	-1.955941000	-0.849892000
6	-0.971139000	1.810593000	-0.416239000
6	1.326884000	1.571075000	-0.308859000
6	1.430520000	2.962762000	-0.208186000
1	2.402915000	3.438228000	-0.153933000
6	0.259451000	3.707857000	-0.199342000
1	0.283894000	4.789351000	-0.107442000
7	-0.946755000	3.138077000	-0.328155000
6	3.514032000	0.726856000	0.632012000
6	2.547057000	0.735624000	-0.392295000
6	4.671531000	-0.047871000	0.496465000
6	2.773086000	-0.035178000	-1.546782000
1	5.392749000	-0.052824000	1.307612000
6	4.873772000	-0.809356000	-0.652868000
6	3.924528000	-0.805177000	-1.683632000
1	2.037496000	-0.006974000	-2.343773000
1	5.774301000	-1.409543000	-0.742906000
1	4.082295000	-1.391525000	-2.582983000
8	3.381087000	1.418334000	1.814478000
1	-2.714491000	-1.038464000	2.088371000
6	-1.996740000	-0.306699000	2.503659000
8	-0.895754000	-0.145439000	1.865618000
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Mn-Phen

1

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7	2.150488000	-0.898366000	-0.067362000
7	0.039127000	0.742725000	0.020636000
6	0.488582000	-3.028223000	-0.857880000
6	-1.595370000	-1.621830000	-0.783432000
8	-2.647261000	-1.958430000	-1.113559000
6	-0.079926000	-1.854997000	1.337658000
6	2.411850000	0.438134000	-0.006513000
6	3.728701000	0.955694000	0.048451000
6	3.918107000	2.377015000	0.072488000
6	4.792596000	0.025520000	0.079777000
1	5.816349000	0.384143000	0.128847000
6	4.511520000	-1.328048000	0.053698000
1	5.300771000	-2.070554000	0.086444000
6	3.175373000	-1.753929000	-0.026811000
1	2.936243000	-2.810073000	-0.058059000
6	1.285306000	1.317813000	0.010607000
6	-1.038828000	1.548476000	0.080957000
6	-0.890273000	2.961382000	0.041742000
1	-1.787394000	3.568248000	0.064856000
6	0.355700000	3.540997000	0.022907000
1	0.472152000	4.620708000	0.025067000
6	1.502461000	2.711374000	0.027707000
6	2.843470000	3.220630000	0.052618000
6	-3.402339000	1.269701000	-0.728755000
6	-2.389509000	0.983856000	0.253843000
6	-4.696635000	0.724103000	-0.463958000
6	-2.680394000	0.218422000	1.396267000
1	-5.480597000	0.913705000	-1.193703000
6	-4.959547000	-0.039677000	0.667958000
6	-3.954694000	-0.300128000	1.617487000
1	-1.891331000	0.045760000	2.122756000

1	-5.960345000	-0.438574000	0.819684000
1	-4.165852000	-0.885299000	2.507095000
8	-3.149039000	1.950362000	-1.814152000
1	4.931961000	2.763660000	0.105495000
1	2.982584000	4.297446000	0.064707000

-1321.152527

2

25	0.020474000	-1.327506000	0.027852000
8	0.354616000	-4.269437000	-0.133374000
8	0.718910000	-1.303908000	2.905613000
7	2.007604000	-0.921663000	-0.406055000
7	-0.017293000	0.771621000	0.002411000
6	0.231722000	-3.122456000	-0.070947000
6	-1.724050000	-1.629398000	0.492405000
8	-2.758796000	-1.971629000	0.874686000
6	0.441479000	-1.318162000	1.786938000
6	2.328427000	0.390580000	-0.222149000
6	3.660091000	0.867716000	-0.279552000
6	3.911101000	2.261538000	-0.046547000
6	4.675047000	-0.072594000	-0.567408000
1	5.709084000	0.254362000	-0.621588000
6	4.332724000	-1.395619000	-0.776757000
1	5.082681000	-2.144412000	-1.005097000
6	2.985718000	-1.786142000	-0.677257000
1	2.702944000	-2.822787000	-0.817481000
6	1.246254000	1.294015000	0.019928000
6	-1.066146000	1.607346000	0.108872000
6	-0.859474000	2.987727000	0.375796000
1	-1.729738000	3.624814000	0.484528000
6	0.411175000	3.512089000	0.450297000
1	0.570000000	4.569719000	0.639417000
6	1.520852000	2.662677000	0.232368000
6	2.880346000	3.122172000	0.207137000
6	-2.800377000	0.501894000	-1.353216000
6	-2.439147000	1.112255000	-0.097429000
6	-4.163738000	0.093299000	-1.482335000
6	-3.406926000	1.330553000	0.899247000
1	-4.456902000	-0.380845000	-2.416048000

6	-5.091217000	0.281518000	-0.466102000
6	-4.723716000	0.906124000	0.741073000
1	-3.101507000	1.814538000	1.824256000
1	-6.115655000	-0.055361000	-0.608872000
1	-5.450621000	1.054778000	1.533639000
8	-1.944955000	0.334962000	-2.326579000
1	4.937369000	2.614130000	-0.079140000
1	3.068169000	4.177137000	0.383266000
1	-0.096654000	-1.509690000	-1.726096000
1	-0.622274000	-0.921127000	-1.670520000

-1322.321241

TS1

25	0.013448000	-1.322707000	0.077329000
8	0.337737000	-4.253802000	-0.175505000
8	0.825125000	-1.337260000	2.925119000
7	1.989293000	-0.910820000	-0.426469000
7	-0.027484000	0.773953000	0.018998000
6	0.218179000	-3.108168000	-0.066744000
6	-1.702952000	-1.619294000	0.608990000
8	-2.731430000	-1.938945000	1.031683000
6	0.505932000	-1.326675000	1.815095000
6	2.313801000	0.399454000	-0.235077000
6	3.643686000	0.879333000	-0.308247000
6	3.895003000	2.272118000	-0.068307000
6	4.655426000	-0.057001000	-0.619206000
1	5.688250000	0.271415000	-0.686517000
6	4.310331000	-1.378469000	-0.835066000
1	5.057249000	-2.124526000	-1.081783000
6	2.965175000	-1.771216000	-0.718467000
1	2.681689000	-2.807268000	-0.862395000
6	1.234433000	1.300018000	0.026672000
6	-1.076332000	1.610327000	0.112988000
6	-0.873831000	2.992086000	0.377521000
1	-1.743983000	3.630683000	0.478117000
6	0.396331000	3.516862000	0.457027000
1	0.553505000	4.574794000	0.645623000
6	1.507285000	2.669062000	0.236967000
6	2.865937000	3.130414000	0.200765000

6	-2.759835000	0.410493000	-1.329735000
6	-2.443547000	1.112455000	-0.118612000
6	-4.112204000	0.012392000	-1.510209000
6	-3.457295000	1.409571000	0.811460000
1	-4.360308000	-0.526135000	-2.421158000
6	-5.090381000	0.290269000	-0.563055000
6	-4.770046000	0.992043000	0.612951000
1	-3.193241000	1.951758000	1.716145000
1	-6.112097000	-0.039470000	-0.735219000
1	-5.532883000	1.206166000	1.355129000
8	-1.850590000	0.144679000	-2.252944000
1	4.920276000	2.626736000	-0.110482000
1	3.054537000	4.184859000	0.379261000
1	-0.256947000	-1.449568000	-1.613264000
1	-0.822204000	-0.807509000	-1.697476000

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TS1-H2O

25	0.134267000	-1.361361000	-0.184311000
8	0.605906000	-4.118863000	-1.129094000
8	-0.069333000	-2.157385000	2.661080000
7	2.161039000	-0.955371000	-0.004923000
7	0.078132000	0.702405000	0.257420000
6	0.428162000	-3.039547000	-0.746088000
6	-1.620701000	-1.691310000	-0.488316000
8	-2.688547000	-2.061940000	-0.738668000
6	0.009272000	-1.844056000	1.550078000
6	2.440271000	0.372174000	0.106927000
6	3.763832000	0.877382000	0.119761000
6	3.968536000	2.295856000	0.196253000
6	4.819451000	-0.059544000	0.053177000
1	5.847807000	0.288889000	0.062840000
6	4.521545000	-1.407547000	-0.017367000
1	5.303014000	-2.158073000	-0.058147000
6	3.177200000	-1.817844000	-0.050095000
1	2.928015000	-2.869972000	-0.121203000
6	1.326138000	1.261721000	0.219598000
6	-0.980995000	1.514625000	0.365776000
6	-0.827354000	2.923443000	0.401446000

1	-1.719677000	3.535175000	0.468895000
6	0.424511000	3.494267000	0.362753000
1	0.552309000	4.572029000	0.399923000
6	1.558075000	2.654396000	0.284049000
6	2.905193000	3.150038000	0.265122000
6	-3.219756000	1.106309000	-0.670925000
6	-2.351426000	0.954956000	0.447199000
6	-4.555998000	0.665049000	-0.517691000
6	-2.796143000	0.340720000	1.626367000
1	-5.232698000	0.777440000	-1.360871000
6	-4.988522000	0.065361000	0.664204000
6	-4.110619000	-0.113441000	1.744521000
1	-2.098832000	0.223822000	2.452050000
1	-6.017679000	-0.276856000	0.741919000
1	-4.447081000	-0.590459000	2.659902000
8	-2.790908000	1.613142000	-1.826690000
1	4.987115000	2.671655000	0.194070000
1	3.056906000	4.224106000	0.314821000
1	0.359532000	-0.944519000	-1.807087000
1	-0.100706000	-0.152566000	-2.066594000
8	-0.592785000	0.906512000	-2.690493000
1	0.039534000	1.616233000	-2.491997000
1	-1.547145000	1.218078000	-2.257800000

-1398.752309

3

25	0.065583000	-1.363419000	0.070013000
8	0.419850000	-4.244236000	-0.412908000
8	0.739791000	-1.457831000	2.964428000
7	2.047456000	-0.893881000	-0.370872000
7	-0.022430000	0.759295000	0.013167000
6	0.296183000	-3.108253000	-0.192131000
6	-1.646754000	-1.729060000	0.461190000
8	-2.712108000	-2.089128000	0.760458000
6	0.483583000	-1.393295000	1.833813000
6	2.334520000	0.428424000	-0.214373000
6	3.654663000	0.939435000	-0.280455000
6	3.872439000	2.343763000	-0.077813000

6	4.697032000	0.023269000	-0.542408000
1	5.721631000	0.377785000	-0.602276000
6	4.390122000	-1.313311000	-0.717528000
1	5.160745000	-2.047970000	-0.922734000
6	3.053352000	-1.735237000	-0.614945000
1	2.802168000	-2.783007000	-0.729258000
6	1.229929000	1.310807000	0.011398000
6	-1.076223000	1.584921000	0.116881000
6	-0.906922000	2.974368000	0.340214000
1	-1.790168000	3.594639000	0.439835000
6	0.353947000	3.526211000	0.394982000
1	0.493259000	4.590694000	0.558314000
6	1.474939000	2.692234000	0.194208000
6	2.823053000	3.184557000	0.158082000
6	-2.875406000	0.464052000	-1.253601000
6	-2.458774000	1.076306000	-0.051831000
6	-4.216760000	0.113216000	-1.434218000
6	-3.412957000	1.308266000	0.953279000
1	-4.509741000	-0.351872000	-2.370362000
6	-5.148023000	0.344836000	-0.421467000
6	-4.745314000	0.935235000	0.782860000
1	-3.093091000	1.781905000	1.877047000
1	-6.185127000	0.058578000	-0.570186000
1	-5.464029000	1.108994000	1.577665000
8	-2.000752000	0.233782000	-2.298495000
1	4.890392000	2.719317000	-0.117954000
1	2.984887000	4.247239000	0.312128000
1	-0.238664000	-1.345568000	-1.516122000
1	-1.221052000	-0.288339000	-1.967172000

-1322.334038

4			
25	0.159146000	-1.368160000	-0.293372000
8	0.729185000	-4.112769000	-1.176736000
8	-0.215797000	-2.170158000	2.543138000
7	2.157326000	-0.882256000	-0.059090000
7	0.028560000	0.746907000	0.013495000
6	0.510316000	-3.029206000	-0.802065000
6	-1.534084000	-1.650411000	-0.801226000

8	-2.582352000	-1.935379000	-1.221671000
6	-0.063944000	-1.813081000	1.444894000
6	2.404314000	0.456445000	-0.007685000
6	3.718661000	0.989220000	0.040892000
6	3.895461000	2.412592000	0.065299000
6	4.795688000	0.075738000	0.065215000
1	5.815149000	0.448022000	0.103266000
6	4.527965000	-1.280616000	0.047026000
1	5.325540000	-2.014866000	0.075536000
6	3.194642000	-1.720509000	-0.017875000
1	2.968800000	-2.780200000	-0.041182000
6	1.269133000	1.328088000	0.008393000
6	-1.048687000	1.548664000	0.088701000
6	-0.911762000	2.962243000	0.070047000
1	-1.813249000	3.562657000	0.106830000
6	0.330237000	3.551814000	0.042749000
1	0.441045000	4.632241000	0.050472000
6	1.477581000	2.726994000	0.032673000
6	2.814587000	3.247116000	0.053885000
6	-3.414412000	1.260651000	-0.733252000
6	-2.404649000	0.979466000	0.251304000
6	-4.709637000	0.715047000	-0.473041000
6	-2.700746000	0.216483000	1.390998000
1	-5.491170000	0.904455000	-1.205726000
6	-4.978095000	-0.048847000	0.658757000
6	-3.975443000	-0.307019000	1.609669000
1	-1.913277000	0.039447000	2.117723000
1	-5.979048000	-0.449189000	0.806812000
1	-4.186133000	-0.894459000	2.498245000
8	-3.162617000	1.946647000	-1.819355000
1	0.371199000	-0.981914000	-1.837237000
1	4.906366000	2.808012000	0.093631000
1	2.944823000	4.325284000	0.069949000

-1321.873083

TS2

25	-0.145927000	-1.391587000	0.052455000
8	-0.666213000	-4.080967000	1.127615000
8	0.198236000	-2.366587000	-2.727150000

7	-2.150967000	-0.957161000	-0.195243000
7	-0.045890000	0.689993000	-0.390723000
6	-0.467968000	-3.024918000	0.678871000
6	1.568225000	-1.638295000	0.537583000
8	2.620902000	-1.904578000	0.949955000
6	0.062258000	-1.953982000	-1.648950000
6	-2.416184000	0.373274000	-0.315562000
6	-3.737657000	0.886177000	-0.368741000
6	-3.933414000	2.304484000	-0.459293000
6	-4.801511000	-0.041986000	-0.329862000
1	-5.826554000	0.314264000	-0.370257000
6	-4.515647000	-1.392247000	-0.246837000
1	-5.303617000	-2.136961000	-0.225702000
6	-3.176254000	-1.811223000	-0.177087000
1	-2.935622000	-2.864827000	-0.098504000
6	-1.292749000	1.255870000	-0.396307000
6	1.022314000	1.500895000	-0.492034000
6	0.867305000	2.912161000	-0.528749000
1	1.761009000	3.521961000	-0.587219000
6	-0.382074000	3.486161000	-0.526831000
1	-0.506310000	4.563919000	-0.578317000
6	-1.519303000	2.648829000	-0.477863000
6	-2.862953000	3.151386000	-0.503362000
6	3.389092000	1.295341000	0.342614000
6	2.384159000	0.942221000	-0.624701000
6	4.690061000	0.746966000	0.118397000
6	2.691189000	0.117489000	-1.718207000
1	5.467440000	0.987368000	0.840399000
6	4.969162000	-0.078347000	-0.966582000
6	3.972656000	-0.400994000	-1.904552000
1	1.907523000	-0.111227000	-2.434724000
1	5.974841000	-0.475416000	-1.089112000
1	4.192966000	-1.036022000	-2.757301000
8	3.128398000	2.046418000	1.380172000
1	-4.949621000	2.685745000	-0.490233000
1	-3.006881000	4.226078000	-0.565784000
1	-0.360057000	-0.899517000	1.601749000
6	0.028344000	0.370138000	2.778625000
8	1.068474000	-0.014311000	3.203879000
8	-0.927703000	1.068537000	2.680776000

-1510.454497

5

25	-0.069116000	-1.264742000	-0.102571000
8	-0.698107000	-4.119769000	0.388600000
8	0.481729000	-1.847316000	-2.932770000
7	-2.021152000	-0.745434000	-0.470181000
7	0.136923000	0.821518000	-0.251621000
6	-0.468464000	-3.003078000	0.203569000
6	1.630100000	-1.659160000	0.448902000
8	2.639974000	-2.051081000	0.846743000
6	0.286559000	-1.616995000	-1.817174000
6	-2.236972000	0.599637000	-0.439011000
6	-3.531424000	1.166113000	-0.530432000
6	-3.675555000	2.591323000	-0.458421000
6	-4.621037000	0.278946000	-0.680390000
1	-5.628935000	0.676169000	-0.755256000
6	-4.385281000	-1.082662000	-0.728478000
1	-5.195427000	-1.793594000	-0.844767000
6	-3.069062000	-1.559316000	-0.614257000
1	-2.865661000	-2.623037000	-0.638552000
6	-1.086858000	1.437458000	-0.300117000
6	1.238818000	1.590312000	-0.159130000
6	1.129658000	2.998872000	-0.014352000
1	2.043136000	3.572261000	0.087225000
6	-0.096052000	3.620326000	-0.050718000
1	-0.180241000	4.700070000	0.029441000
6	-1.260588000	2.835405000	-0.219505000
6	-2.580166000	3.392590000	-0.301876000
6	3.524801000	1.163126000	0.801012000
6	2.584146000	0.996229000	-0.275424000
6	4.820804000	0.599087000	0.587638000
6	2.945981000	0.329785000	-1.458620000
1	5.549466000	0.698135000	1.389063000
6	5.153523000	-0.067483000	-0.586793000
6	4.220619000	-0.207248000	-1.630195000
1	2.213441000	0.247257000	-2.256501000
1	6.153113000	-0.482394000	-0.698664000
1	4.486184000	-0.714817000	-2.552407000

8	3.209244000	1.764091000	1.917076000
1	-4.673107000	3.014301000	-0.525950000
1	-2.685639000	4.471500000	-0.238790000
1	-0.296328000	-0.890433000	1.762256000
6	-1.190813000	-0.774577000	2.493628000
8	-1.480921000	0.410704000	2.756133000
8	-1.651780000	-1.851829000	2.929301000

-1510.477495

5'

25	-0.121543000	-1.265757000	-0.154008000
8	-0.740956000	-4.135346000	0.188831000
8	0.336797000	-1.677697000	-3.038514000
7	-2.115522000	-0.723009000	-0.492964000
7	0.028993000	0.899804000	-0.246411000
6	-0.499577000	-3.010495000	0.055669000
6	1.600404000	-1.637224000	0.300395000
8	2.652367000	-1.987318000	0.626656000
6	0.178413000	-1.507252000	-1.903487000
6	-2.350727000	0.609869000	-0.335749000
6	-3.660454000	1.153032000	-0.337149000
6	-3.836195000	2.560828000	-0.125411000
6	-4.737296000	0.263286000	-0.551003000
1	-5.753525000	0.646004000	-0.563090000
6	-4.478632000	-1.080516000	-0.744991000
1	-5.277819000	-1.792175000	-0.919210000
6	-3.150153000	-1.537665000	-0.700476000
1	-2.926928000	-2.590061000	-0.832362000
6	-1.213446000	1.469179000	-0.174868000
6	1.110793000	1.689915000	-0.145656000
6	0.973195000	3.079683000	0.117940000
1	1.873827000	3.674092000	0.215147000
6	-0.270982000	3.657811000	0.205406000
1	-0.382766000	4.723760000	0.381452000
6	-1.420844000	2.851077000	0.035551000
6	-2.756105000	3.375056000	0.064220000
6	3.467051000	1.246583000	0.645154000
6	2.459129000	1.133079000	-0.375649000
6	4.748941000	0.704968000	0.316410000

6	2.746395000	0.530550000	-1.611726000
1	5.527643000	0.764902000	1.073549000
6	5.007646000	0.103211000	-0.910681000
6	4.008921000	0.012551000	-1.896504000
1	1.961112000	0.482552000	-2.360707000
1	5.999105000	-0.299119000	-1.108282000
1	4.213795000	-0.444746000	-2.859624000
8	3.227528000	1.780544000	1.814271000
1	-4.845692000	2.960478000	-0.117839000
1	-2.886022000	4.440370000	0.230642000
1	0.329725000	-2.410203000	2.687857000
6	-0.286956000	-1.513279000	2.887971000
8	-0.625524000	-0.807482000	1.874294000
8	-0.603374000	-1.257074000	4.072724000

-1510.496596

TS3

25	-0.119411000	-1.402814000	0.103761000
8	-0.734100000	-4.034674000	1.270596000
8	0.475276000	-2.550435000	-2.568180000
7	-2.107072000	-0.982558000	-0.284459000
7	0.001507000	0.654956000	-0.415544000
6	-0.493479000	-3.004855000	0.786803000
6	1.548549000	-1.603774000	0.732620000
8	2.572899000	-1.812485000	1.238818000
6	0.234578000	-2.066305000	-1.540009000
6	-2.366684000	0.346012000	-0.427874000
6	-3.680951000	0.863904000	-0.532377000
6	-3.866415000	2.284293000	-0.632846000
6	-4.748982000	-0.059797000	-0.525837000
1	-5.770763000	0.298916000	-0.605502000
6	-4.469787000	-1.410187000	-0.421096000
1	-5.260349000	-2.152383000	-0.422689000
6	-3.135834000	-1.833256000	-0.295643000
1	-2.902724000	-2.886722000	-0.195139000
6	-1.239201000	1.226300000	-0.473503000
6	1.071312000	1.461252000	-0.502693000
6	0.936726000	2.868804000	-0.569407000
1	1.835805000	3.472704000	-0.617218000

6	-0.312205000	3.450703000	-0.598415000
1	-0.427480000	4.528696000	-0.658830000
6	-1.453100000	2.621365000	-0.573450000
6	-2.794405000	3.128990000	-0.642647000
6	3.418702000	1.142757000	0.372431000
6	2.434727000	0.878095000	-0.597227000
6	4.719784000	0.656257000	0.211976000
6	2.779676000	0.098338000	-1.713626000
1	5.455663000	0.866620000	0.981776000
6	5.043828000	-0.111215000	-0.906610000
6	4.071473000	-0.400047000	-1.872672000
1	2.022091000	-0.099655000	-2.464812000
1	6.054944000	-0.491703000	-1.018310000
1	4.319651000	-0.999326000	-2.743013000
8	3.159896000	1.864488000	1.519557000
1	-4.879760000	2.668876000	-0.697532000
1	-2.933068000	4.203719000	-0.711493000
1	-0.413804000	-0.840002000	1.615492000
6	-0.514212000	0.596494000	2.656674000
8	0.631898000	0.831819000	2.864106000
8	-1.692262000	0.717651000	2.738835000
1	2.210580000	1.858144000	1.725968000

-1510.916213

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25	-0.059358000	-1.271313000	-0.133295000
8	-0.645180000	-4.143948000	0.313277000
8	0.437317000	-1.719316000	-3.001711000
7	-2.033408000	-0.781318000	-0.428949000
7	0.098652000	0.824490000	-0.260074000
6	-0.431138000	-3.023086000	0.141518000
6	1.656855000	-1.677812000	0.336406000
8	2.686451000	-2.077390000	0.670480000
6	0.255364000	-1.551713000	-1.873901000
6	-2.271930000	0.558910000	-0.400512000
6	-3.575375000	1.104090000	-0.469149000
6	-3.741390000	2.528820000	-0.408855000
6	-4.654248000	0.199485000	-0.589932000
1	-5.669436000	0.580387000	-0.646841000

6	-4.396843000	-1.158083000	-0.635062000
1	-5.197275000	-1.882835000	-0.731363000
6	-3.070831000	-1.612839000	-0.547767000
1	-2.852099000	-2.673284000	-0.575527000
6	-1.132609000	1.418082000	-0.294656000
6	1.181623000	1.618009000	-0.201372000
6	1.064417000	3.024618000	-0.107381000
1	1.971854000	3.614599000	-0.045462000
6	-0.176413000	3.625303000	-0.122078000
1	-0.276388000	4.704801000	-0.063482000
6	-1.326903000	2.817369000	-0.236613000
6	-2.658624000	3.351353000	-0.291786000
6	3.425926000	1.047451000	0.798089000
6	2.540754000	1.026052000	-0.294221000
6	4.721844000	0.538959000	0.664398000
6	2.978875000	0.486156000	-1.515511000
1	5.381771000	0.552979000	1.526150000
6	5.137884000	0.004886000	-0.554714000
6	4.267265000	-0.025864000	-1.651846000
1	2.292663000	0.479433000	-2.356840000
1	6.144577000	-0.392243000	-0.645878000
1	4.590126000	-0.440882000	-2.601242000
8	3.074303000	1.525851000	2.041648000
1	-4.747638000	2.933325000	-0.456803000
1	-2.780800000	4.428949000	-0.241987000
1	-0.201025000	-0.938314000	1.719023000
6	-1.060560000	-0.770224000	2.488007000
8	-1.254080000	0.429973000	2.767331000
8	-1.569765000	-1.819126000	2.934156000
1	2.134885000	1.765809000	2.075953000

-1510.934009

6'

25	-0.121486000	-1.269170000	-0.182578000
8	-0.723228000	-4.148927000	0.109205000
8	0.338134000	-1.597982000	-3.080773000
7	-2.128212000	-0.737392000	-0.479933000
7	0.002675000	0.903310000	-0.251718000
6	-0.489256000	-3.021485000	-0.005306000

6	1.602429000	-1.650394000	0.243897000
8	2.660759000	-2.001032000	0.547452000
6	0.172836000	-1.464590000	-1.942716000
6	-2.373069000	0.591344000	-0.311080000
6	-3.685073000	1.124773000	-0.289536000
6	-3.868883000	2.532336000	-0.074645000
6	-4.758998000	0.228108000	-0.487351000
1	-5.778025000	0.603103000	-0.480590000
6	-4.492626000	-1.112557000	-0.691588000
1	-5.288986000	-1.829741000	-0.855508000
6	-3.160056000	-1.559348000	-0.673809000
1	-2.931192000	-2.608790000	-0.817723000
6	-1.240445000	1.461727000	-0.168002000
6	1.072008000	1.708958000	-0.178257000
6	0.936867000	3.100027000	0.048884000
1	1.834044000	3.706030000	0.110199000
6	-0.314333000	3.666958000	0.161467000
1	-0.431893000	4.733894000	0.325535000
6	-1.455180000	2.846505000	0.033344000
6	-2.795284000	3.358574000	0.088878000
6	3.402800000	1.160110000	0.623251000
6	2.429638000	1.144774000	-0.392464000
6	4.686947000	0.662311000	0.379132000
6	2.773216000	0.621361000	-1.650471000
1	5.414000000	0.671970000	1.185150000
6	5.007107000	0.144863000	-0.875586000
6	4.049826000	0.121295000	-1.898051000
1	2.023005000	0.619574000	-2.434627000
1	6.005363000	-0.244512000	-1.052611000
1	4.296215000	-0.279953000	-2.875896000
8	3.153475000	1.621079000	1.898095000
1	-4.881997000	2.921642000	-0.046669000
1	-2.931435000	4.423252000	0.252769000
1	0.357651000	-2.462745000	2.633552000
6	-0.242023000	-1.559213000	2.853385000
8	-0.593114000	-0.840519000	1.852080000
8	-0.528895000	-1.306467000	4.045668000
1	2.221435000	1.866261000	2.008350000

-1510.956037

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1

25	0.771794000	-1.007385000	-0.362750000
6	3.846946000	-0.585719000	0.060284000
7	2.575097000	1.159628000	0.086428000
7	0.259540000	1.002394000	0.036891000
7	2.571716000	-0.197437000	-0.027562000
6	4.685301000	0.531214000	0.235844000
1	5.759439000	0.536754000	0.342870000
6	3.844524000	1.628036000	0.246844000
1	4.053229000	2.680951000	0.358376000
6	1.335075000	1.825977000	0.035432000
6	1.263946000	3.209979000	-0.021803000
1	2.159464000	3.817702000	-0.043885000
6	-0.006672000	3.782930000	-0.065449000
1	-0.113059000	4.861478000	-0.118659000
6	-1.126785000	2.963132000	-0.010458000
1	-2.125924000	3.380913000	0.000436000
6	-0.980236000	1.571051000	0.071445000
6	0.569550000	-1.664371000	1.274894000
8	0.482671000	-2.078500000	2.350698000
6	1.481724000	-2.584848000	-0.911539000
8	1.937308000	-3.590977000	-1.245376000
6	-0.880019000	-1.631483000	-0.886305000
8	-1.842977000	-2.141367000	-1.260937000
1	4.098057000	-1.634450000	-0.006692000
6	-2.168896000	0.719590000	0.271951000
6	-2.254113000	-0.067353000	1.433992000
6	-3.241888000	0.743283000	-0.687156000
6	-3.367963000	-0.861868000	1.698161000
6	-4.370440000	-0.078152000	-0.376905000
6	-4.427275000	-0.858110000	0.772644000
1	-1.430935000	-0.039405000	2.142520000
8	-3.182042000	1.434631000	-1.794081000
1	-3.417166000	-1.460784000	2.602265000
1	-5.192121000	-0.088998000	-1.089465000
1	-5.306664000	-1.471646000	0.957007000

-1222.848692

2

25	0.615027000	-1.085812000	-0.012228000
6	3.656866000	-0.707103000	-0.752857000
7	2.511596000	1.056783000	-0.273644000
7	0.213034000	0.991989000	0.003534000
7	2.432388000	-0.293460000	-0.432745000
6	4.543768000	0.388694000	-0.814040000
1	5.594918000	0.369626000	-1.059308000
6	3.783217000	1.497858000	-0.505915000
1	4.042198000	2.544017000	-0.449960000
6	1.326986000	1.753583000	0.030492000
6	1.338792000	3.112352000	0.324053000
1	2.265912000	3.669834000	0.358118000
6	0.112147000	3.719772000	0.579648000
1	0.071183000	4.776148000	0.824317000
6	-1.055678000	2.968737000	0.480776000
1	-2.027610000	3.428706000	0.614880000
6	-0.991514000	1.604154000	0.167555000
6	0.961424000	-1.029495000	1.763185000
8	1.179576000	-0.981546000	2.893359000
6	1.229185000	-2.786201000	-0.124872000
8	1.635697000	-3.864445000	-0.189492000
6	-1.045010000	-1.760324000	0.375033000
8	-1.995994000	-2.334213000	0.688193000
1	0.537931000	-1.284589000	-1.787575000
1	-0.030522000	-0.748402000	-1.715055000
1	3.846968000	-1.757002000	-0.924652000
6	-2.234762000	0.836636000	-0.040089000
6	-3.187203000	0.770458000	0.990123000
6	-2.504453000	0.265829000	-1.336950000
6	-4.396337000	0.098472000	0.820780000
6	-3.759384000	-0.403980000	-1.473701000
6	-4.670413000	-0.489920000	-0.427870000
1	-2.952645000	1.234530000	1.945585000
8	-1.664882000	0.358276000	-2.333222000
1	-5.110167000	0.032084000	1.636119000
1	-3.983782000	-0.852273000	-2.438831000
1	-5.610132000	-1.016280000	-0.580760000

-1224.017252

TS1

25	0.599280000	-1.069153000	0.020327000
6	3.627394000	-0.693980000	-0.778735000
7	2.492670000	1.070623000	-0.278578000
7	0.197331000	1.004680000	0.013187000
7	2.398590000	-0.272907000	-0.488672000
6	4.533327000	0.388525000	-0.769121000
1	5.592595000	0.361008000	-0.975878000
6	3.779647000	1.497982000	-0.446402000
1	4.054628000	2.535542000	-0.336483000
6	1.307071000	1.772814000	0.009329000
6	1.309341000	3.142984000	0.246425000
1	2.230448000	3.711502000	0.246115000
6	0.078393000	3.752786000	0.475952000
1	0.030473000	4.818629000	0.673692000
6	-1.085426000	2.993280000	0.402102000
1	-2.059896000	3.454958000	0.509371000
6	-1.010691000	1.618240000	0.140138000
6	1.104277000	-1.060012000	1.757044000
8	1.431771000	-1.067680000	2.864231000
6	1.164802000	-2.765862000	-0.209657000
8	1.534326000	-3.848086000	-0.379764000
6	-1.020451000	-1.711163000	0.557393000
8	-1.954043000	-2.237386000	0.992342000
1	0.334328000	-1.174395000	-1.679339000
1	-0.343926000	-0.656729000	-1.743883000
1	3.807741000	-1.741263000	-0.975657000
6	-2.249452000	0.839837000	-0.058770000
6	-3.256938000	0.874457000	0.920863000
6	-2.463227000	0.137855000	-1.290563000
6	-4.461113000	0.195958000	0.746413000
6	-3.706165000	-0.531442000	-1.445225000
6	-4.677800000	-0.508248000	-0.450742000
1	-3.070627000	1.422529000	1.841085000
8	-1.550848000	0.105508000	-2.248777000
1	-5.218174000	0.211420000	1.524397000
1	-3.874067000	-1.073001000	-2.372580000
1	-5.613264000	-1.041060000	-0.603479000

-1224.017218

TS1-H2O

25	-0.562583000	-1.052353000	0.260943000
8	-1.543902000	-3.597358000	1.390904000
8	-0.464850000	-2.101780000	-2.507606000
7	-2.465468000	-0.294860000	-0.015831000
7	-0.145818000	0.941421000	-0.292419000
6	-1.164332000	-2.600984000	0.936433000
6	1.094830000	-1.692827000	0.615847000
8	2.068630000	-2.255875000	0.890186000
6	-0.501839000	-1.684861000	-1.429022000
6	-2.541805000	1.045619000	-0.192086000
6	-3.775666000	1.688517000	-0.350527000
1	-3.823056000	2.759386000	-0.502354000
6	-4.945914000	0.935079000	-0.334287000
1	-5.908685000	1.419955000	-0.458998000
6	-4.857007000	-0.447784000	-0.170361000
1	-5.737945000	-1.079828000	-0.164461000
6	-3.599169000	-1.020521000	-0.017990000
1	-3.492179000	-2.090843000	0.105331000
6	-1.245551000	1.745263000	-0.241742000
6	1.074287000	1.511648000	-0.402760000
6	1.228621000	2.906109000	-0.404301000
1	2.227533000	3.319790000	-0.480920000
6	0.114041000	3.726280000	-0.298455000
1	0.217787000	4.806340000	-0.280111000
6	-1.146167000	3.136501000	-0.227887000
1	-2.032845000	3.752578000	-0.149485000
6	3.222028000	0.651249000	0.559077000
6	2.289291000	0.668942000	-0.516837000
6	4.428810000	-0.061499000	0.359905000
6	2.541512000	-0.046259000	-1.696142000
1	5.152251000	-0.079491000	1.170894000
6	4.671117000	-0.759149000	-0.822233000
6	3.723685000	-0.770018000	-1.857804000
1	1.798519000	-0.025123000	-2.489307000
1	5.602137000	-1.309270000	-0.935570000
1	3.909455000	-1.321218000	-2.774536000

8	2.964910000	1.247980000	1.723441000
1	-0.730733000	-0.472819000	1.843615000
1	-0.069853000	0.175953000	2.067729000
8	0.681672000	1.110166000	2.633087000
1	1.681149000	1.172026000	2.179463000
1	0.233729000	1.942562000	2.409825000

-1322.526891

3

25	0.673137000	-1.151908000	0.045717000
6	3.708932000	-0.574069000	-0.715823000
7	2.483691000	1.142266000	-0.273365000
7	0.180083000	1.026880000	-0.007418000
7	2.467308000	-0.215227000	-0.401495000
6	4.545674000	0.560918000	-0.806301000
1	5.596171000	0.585553000	-1.054441000
6	3.735220000	1.638570000	-0.522757000
1	3.946422000	2.696168000	-0.494628000
6	1.276282000	1.808808000	0.012981000
6	1.253115000	3.175275000	0.287518000
1	2.166066000	3.755379000	0.326850000
6	0.013940000	3.762670000	0.517628000
1	-0.050965000	4.822236000	0.742088000
6	-1.138853000	2.984893000	0.428538000
1	-2.121696000	3.424446000	0.551198000
6	-1.030026000	1.618121000	0.150393000
6	1.017878000	-1.085298000	1.828352000
8	1.214221000	-1.090611000	2.972153000
6	1.348312000	-2.779310000	-0.189368000
8	1.796120000	-3.834182000	-0.389230000
6	-0.929752000	-1.894057000	0.357113000
8	-1.913676000	-2.469797000	0.586034000
1	0.366572000	-1.193270000	-1.579585000
1	-0.805180000	-0.237103000	-2.004501000
1	3.946634000	-1.617641000	-0.866059000
6	-2.267324000	0.818695000	-0.024265000
6	-3.232358000	0.797471000	0.996202000
6	-2.555147000	0.164693000	-1.241746000
6	-4.453598000	0.146768000	0.821090000

6	-3.789179000	-0.464060000	-1.426634000
6	-4.735876000	-0.474902000	-0.400958000
1	-3.010219000	1.297331000	1.934599000
8	-1.662859000	0.163466000	-2.300319000
1	-5.180579000	0.131252000	1.627194000
1	-3.985553000	-0.950653000	-2.376983000
1	-5.687557000	-0.975552000	-0.553606000

-1224.026628

4

25	0.766868000	-1.065742000	-0.293408000
6	3.857600000	-0.542943000	0.028528000
7	2.560146000	1.175646000	0.045083000
7	0.242666000	0.999516000	0.044143000
7	2.578578000	-0.181167000	-0.035149000
6	4.686371000	0.595361000	0.150856000
1	5.763209000	0.619783000	0.226596000
6	3.829929000	1.675494000	0.159229000
1	4.021256000	2.733664000	0.245478000
6	1.311563000	1.825740000	0.034453000
6	1.234740000	3.214922000	0.009278000
1	2.128147000	3.825311000	-0.019429000
6	-0.033575000	3.788327000	0.013524000
1	-0.143608000	4.867693000	-0.009756000
6	-1.148707000	2.960090000	0.070112000
1	-2.150177000	3.371986000	0.107184000
6	-0.992825000	1.567354000	0.103798000
6	0.590213000	-1.590933000	1.432485000
8	0.466560000	-2.008596000	2.512217000
6	1.499652000	-2.592694000	-0.815572000
8	1.991987000	-3.578253000	-1.198654000
6	-0.818168000	-1.690596000	-0.835244000
8	-1.777921000	-2.177876000	-1.279811000
1	0.904385000	-0.615977000	-1.826108000
1	4.127184000	-1.588136000	-0.020460000
6	-2.194421000	0.714791000	0.258653000
6	-2.347964000	-0.048882000	1.425095000
6	-3.213168000	0.728664000	-0.755626000
6	-3.486207000	-0.825855000	1.647207000

6	-4.369019000	-0.068817000	-0.489949000
6	-4.497932000	-0.824685000	0.671528000
1	-1.558166000	-0.024208000	2.170809000
8	-3.086313000	1.401721000	-1.871785000
1	-3.587506000	-1.409787000	2.557018000
1	-5.154058000	-0.081087000	-1.242932000
1	-5.395101000	-1.421640000	0.822372000

-1223.566020

TS2

25	-0.519075000	-1.061630000	-0.144731000
6	-3.562495000	-0.549774000	-0.763466000
7	-2.259594000	1.165272000	-0.724115000
7	0.031744000	0.995680000	-0.381313000
7	-2.286345000	-0.190696000	-0.633869000
6	-4.378504000	0.589302000	-0.936200000
1	-5.449207000	0.616793000	-1.072467000
6	-3.518766000	1.667329000	-0.899012000
1	-3.702791000	2.726117000	-0.993351000
6	-1.027182000	1.818236000	-0.546507000
6	-0.955425000	3.207401000	-0.541279000
1	-1.842224000	3.814128000	-0.671401000
6	0.295973000	3.784816000	-0.350934000
1	0.400776000	4.864764000	-0.332140000
6	1.406170000	2.959714000	-0.206892000
1	2.399454000	3.374806000	-0.084000000
6	1.260598000	1.567029000	-0.248297000
6	-0.090354000	-1.548490000	-1.832711000
8	0.189105000	-1.919660000	-2.897540000
6	-1.305235000	-2.617163000	0.212677000
8	-1.839722000	-3.617394000	0.470962000
6	0.983400000	-1.707610000	0.594417000
8	1.864261000	-2.226084000	1.146895000
1	-0.843704000	-0.629971000	1.402951000
1	-3.839149000	-1.593354000	-0.721129000
6	2.471227000	0.715687000	-0.197264000
6	2.823743000	-0.043693000	-1.322874000
6	3.298620000	0.727380000	0.977933000
6	3.981057000	-0.823425000	-1.345649000

6	4.479094000	-0.075727000	0.915742000
6	4.805011000	-0.830312000	-0.207141000
1	2.176306000	-0.012012000	-2.195022000
8	2.985840000	1.407157000	2.052211000
1	4.238643000	-1.404645000	-2.225875000
1	5.120695000	-0.094171000	1.794148000
1	5.711755000	-1.431905000	-0.200080000
6	-2.207493000	-0.039970000	2.405157000
8	-2.089704000	1.133796000	2.273379000
8	-2.653649000	-1.063563000	2.809784000

-1412.148859

5

25	-0.668983000	-1.076718000	0.002984000
6	-3.770958000	-0.759226000	-0.312827000
7	-2.558205000	1.014624000	-0.519669000
7	-0.238549000	0.939580000	-0.470061000
7	-2.508169000	-0.328437000	-0.303841000
6	-4.651582000	0.316940000	-0.537863000
1	-5.728733000	0.282468000	-0.600556000
6	-3.848467000	1.433555000	-0.662962000
1	-4.095491000	2.468837000	-0.840534000
6	-1.340837000	1.720638000	-0.544908000
6	-1.316905000	3.106316000	-0.628422000
1	-2.233123000	3.679719000	-0.681089000
6	-0.070101000	3.726853000	-0.618931000
1	-0.001621000	4.808518000	-0.670574000
6	1.077496000	2.945145000	-0.558924000
1	2.062733000	3.395312000	-0.574775000
6	0.978349000	1.548709000	-0.511605000
6	-0.473639000	-1.703122000	-1.658619000
8	-0.371932000	-2.101739000	-2.738272000
6	-1.326924000	-2.660993000	0.572833000
8	-1.754167000	-3.670123000	0.937005000
6	0.993691000	-1.671178000	0.495610000
8	1.957447000	-2.188822000	0.859417000
1	-0.973724000	-0.483757000	1.817256000
1	-3.987779000	-1.806413000	-0.159388000
6	2.210009000	0.732420000	-0.565027000

6	2.453154000	-0.072344000	-1.689251000
6	3.162928000	0.824372000	0.508068000
6	3.625717000	-0.817947000	-1.809200000
6	4.357021000	0.055730000	0.343288000
6	4.575881000	-0.742284000	-0.775330000
1	1.706825000	-0.104459000	-2.478831000
8	2.940289000	1.536397000	1.580418000
1	3.799699000	-1.436565000	-2.684206000
1	5.095330000	0.096716000	1.140990000
1	5.497432000	-1.316153000	-0.848014000
6	-0.544085000	0.212187000	2.639209000
8	0.322516000	-0.321435000	3.363225000
8	-1.072527000	1.343062000	2.679370000

-1412.170218

5'

25	-0.713509000	-1.083908000	0.129851000
6	-3.782198000	-0.634268000	-0.470800000
7	-2.486331000	1.083490000	-0.609618000
7	-0.166398000	0.935284000	-0.518161000
7	-2.508211000	-0.257864000	-0.383313000
6	-4.603508000	0.476062000	-0.760468000
1	-5.674496000	0.485549000	-0.896288000
6	-3.746781000	1.554903000	-0.843887000
1	-3.934175000	2.596181000	-1.056170000
6	-1.241334000	1.747007000	-0.605626000
6	-1.172382000	3.132954000	-0.682638000
1	-2.068369000	3.738405000	-0.730186000
6	0.095903000	3.710718000	-0.681564000
1	0.200190000	4.789547000	-0.735510000
6	1.217981000	2.892805000	-0.627790000
1	2.216607000	3.310767000	-0.654716000
6	1.070763000	1.499525000	-0.564184000
6	-0.503515000	-1.831001000	-1.488475000
8	-0.397712000	-2.316440000	-2.534403000
6	-1.465713000	-2.587428000	0.773842000
8	-1.958072000	-3.546217000	1.194227000
6	0.899737000	-1.687562000	0.721930000
8	1.856457000	-2.159033000	1.166131000

1	0.768190000	0.678036000	2.170944000
1	-4.049105000	-1.670825000	-0.321459000
6	2.265210000	0.629973000	-0.599695000
6	2.391522000	-0.313220000	-1.633195000
6	3.301744000	0.787163000	0.388013000
6	3.506678000	-1.143255000	-1.737214000
6	4.426985000	-0.085235000	0.250816000
6	4.523037000	-1.021104000	-0.773501000
1	1.599043000	-0.381620000	-2.372780000
8	3.222600000	1.650113000	1.365685000
1	3.585737000	-1.862708000	-2.546457000
1	5.217966000	-0.001377000	0.992841000
1	5.399994000	-1.662783000	-0.829435000
6	-0.245749000	0.619476000	2.605241000
8	-0.484990000	1.259846000	3.656185000
8	-1.104228000	-0.104884000	1.987897000

-1412.194028

TS3

25	-0.640953000	-1.215553000	0.139647000
6	-3.733761000	-0.850383000	-0.366990000
7	-2.499415000	0.883632000	-0.706656000
7	-0.182770000	0.835508000	-0.590154000
7	-2.467984000	-0.440381000	-0.381044000
6	-4.603968000	0.216690000	-0.680574000
1	-5.681042000	0.189290000	-0.749862000
6	-3.787970000	1.307781000	-0.887665000
1	-4.022227000	2.326264000	-1.155170000
6	-1.284763000	1.589924000	-0.766305000
6	-1.260466000	2.969338000	-0.974031000
1	-2.174576000	3.536041000	-1.093076000
6	-0.020121000	3.593754000	-1.009535000
1	0.044562000	4.665734000	-1.163493000
6	1.134852000	2.826464000	-0.862820000
1	2.119377000	3.276809000	-0.914175000
6	1.025980000	1.447610000	-0.668316000
6	-0.325111000	-2.031846000	-1.443532000
8	-0.109044000	-2.600387000	-2.432255000
6	-1.357287000	-2.672361000	0.872435000

8	-1.843096000	-3.604206000	1.369467000
6	0.935410000	-1.648606000	0.881653000
8	1.889012000	-1.965591000	1.462664000
1	-0.884475000	-0.465240000	1.633678000
1	-3.962648000	-1.879864000	-0.131005000
6	2.256577000	0.618214000	-0.595397000
6	2.516093000	-0.330774000	-1.598379000
6	3.202068000	0.792458000	0.430916000
6	3.687252000	-1.085634000	-1.591700000
6	4.383359000	0.043276000	0.438394000
6	4.624050000	-0.890470000	-0.568494000
1	1.786431000	-0.461249000	-2.390907000
8	3.024337000	1.676951000	1.472979000
1	3.869976000	-1.813316000	-2.376035000
1	5.090181000	0.190200000	1.249070000
1	5.541160000	-1.471951000	-0.548618000
6	-0.896451000	1.128554000	2.454831000
8	0.244513000	1.240055000	2.763919000
8	-2.046540000	1.407019000	2.360909000
1	2.100382000	1.970140000	1.524987000

-1412.607195

6			
25	-0.701614000	-1.085330000	0.021239000
6	-3.805849000	-0.734834000	-0.227463000
7	-2.583426000	1.029331000	-0.452590000
7	-0.267239000	0.932362000	-0.466165000
7	-2.540658000	-0.314341000	-0.234529000
6	-4.681840000	0.347998000	-0.443942000
1	-5.759870000	0.320678000	-0.493225000
6	-3.873573000	1.457772000	-0.582450000
1	-4.115542000	2.493859000	-0.762145000
6	-1.362515000	1.720297000	-0.516847000
6	-1.327690000	3.109210000	-0.614310000
1	-2.240341000	3.690041000	-0.638847000
6	-0.082048000	3.720134000	-0.660410000
1	-0.006424000	4.800232000	-0.726507000
6	1.064647000	2.927847000	-0.633904000
1	2.052854000	3.368615000	-0.694315000

6	0.947184000	1.539472000	-0.551422000
6	-0.563872000	-1.698641000	-1.654732000
8	-0.492888000	-2.082536000	-2.741180000
6	-1.372379000	-2.663463000	0.601561000
8	-1.808147000	-3.665408000	0.972111000
6	0.959344000	-1.722340000	0.452442000
8	1.931587000	-2.259134000	0.760648000
1	-0.927363000	-0.492949000	1.837423000
1	-4.029286000	-1.779979000	-0.069757000
6	2.176529000	0.708992000	-0.606025000
6	2.435636000	-0.075144000	-1.742873000
6	3.127084000	0.743527000	0.430253000
6	3.609429000	-0.817098000	-1.850666000
6	4.308846000	0.001857000	0.324149000
6	4.546110000	-0.774307000	-0.809511000
1	1.700827000	-0.089332000	-2.541891000
8	2.954520000	1.467038000	1.588216000
1	3.793397000	-1.419440000	-2.734463000
1	5.020666000	0.031703000	1.143129000
1	5.464135000	-1.350467000	-0.877941000
6	-0.387736000	0.219886000	2.580068000
8	0.545749000	-0.310958000	3.216874000
8	-0.886962000	1.362633000	2.641813000
1	2.071855000	1.868746000	1.629190000

-1412.630346

6'

25	-0.725082000	-1.096322000	0.098999000
6	-3.799493000	-0.622341000	-0.420199000
7	-2.504402000	1.096070000	-0.563216000
7	-0.185976000	0.944762000	-0.503942000
7	-2.522640000	-0.252823000	-0.373210000
6	-4.628327000	0.497796000	-0.647370000
1	-5.703910000	0.512740000	-0.738878000
6	-3.774055000	1.576154000	-0.734248000
1	-3.970501000	2.622459000	-0.909937000
6	-1.259979000	1.754182000	-0.589142000
6	-1.184808000	3.142701000	-0.696398000
1	-2.077701000	3.752194000	-0.743818000

6	0.078760000	3.718154000	-0.732892000
1	0.184042000	4.794862000	-0.813951000
6	1.204444000	2.897469000	-0.683321000
1	2.204179000	3.311842000	-0.745369000
6	1.045728000	1.513075000	-0.577177000
6	-0.509705000	-1.786958000	-1.545913000
8	-0.390007000	-2.232040000	-2.607276000
6	-1.477124000	-2.622341000	0.694046000
8	-1.967101000	-3.594648000	1.082263000
6	0.883247000	-1.732429000	0.663174000
8	1.843719000	-2.222033000	1.078372000
1	0.813092000	0.446285000	2.228308000
1	-4.065806000	-1.661056000	-0.285810000
6	2.243326000	0.634419000	-0.602237000
6	2.426593000	-0.255282000	-1.674983000
6	3.235644000	0.707458000	0.393361000
6	3.558005000	-1.063095000	-1.757861000
6	4.371969000	-0.105714000	0.316313000
6	4.530750000	-0.986257000	-0.752668000
1	1.667220000	-0.297167000	-2.449023000
8	3.152145000	1.538872000	1.487975000
1	3.679914000	-1.743683000	-2.594430000
1	5.113652000	-0.043109000	1.106485000
1	5.415628000	-1.614151000	-0.799829000
6	-0.218620000	0.502169000	2.616511000
8	-0.441091000	1.184005000	3.643042000
8	-1.111449000	-0.152366000	1.970245000
1	2.310518000	2.021491000	1.502931000

-1412.651509

Mn-ppy'

1			
25	-0.615693000	1.053278000	-0.038481000
6	1.190088000	-1.545410000	0.079929000
7	-0.973834000	-1.786579000	0.054398000
7	-2.387862000	-0.002256000	-0.299443000
7	0.037517000	-0.863420000	-0.032797000
6	0.898354000	-2.923975000	0.274835000

1	1.617722000	-3.720978000	0.386896000
6	-0.470695000	-3.040838000	0.244662000
1	-1.111853000	-3.905385000	0.324755000
6	-2.283586000	-1.337975000	-0.145585000
6	-3.377004000	-2.203238000	-0.192121000
1	-3.248030000	-3.270867000	-0.066073000
6	-4.633505000	-1.648146000	-0.409393000
1	-5.505881000	-2.291925000	-0.452254000
6	-4.758824000	-0.264581000	-0.574732000
1	-5.721445000	0.202026000	-0.748360000
6	-3.616587000	0.519471000	-0.507931000
1	-3.667236000	1.594565000	-0.623556000
6	-0.896339000	1.167229000	1.711582000
8	-1.088305000	1.206981000	2.851179000
6	1.010308000	1.870897000	0.182214000
8	1.971786000	2.468256000	0.400062000
6	-1.345869000	2.704550000	-0.294478000
8	-1.788638000	3.759658000	-0.444208000
6	2.517374000	-0.936690000	-0.032782000
6	2.851062000	-0.091612000	-1.155117000
6	3.489914000	-1.278023000	0.925306000
6	4.201730000	0.376187000	-1.197238000
6	4.792878000	-0.787646000	0.855770000
6	5.136607000	0.047836000	-0.222369000
8	1.994278000	0.236587000	-2.082796000
1	3.200760000	-1.928845000	1.747635000
1	4.479077000	1.018884000	-2.029621000
1	5.522410000	-1.046147000	1.617034000
1	6.147658000	0.442451000	-0.298741000

-1222.850864

2			
25	-0.593427000	1.063388000	-0.036221000
6	1.189502000	-1.562283000	0.110208000
7	-0.974428000	-1.783449000	0.094058000
7	-2.372534000	0.006782000	-0.302101000
7	0.046059000	-0.872906000	0.006203000
6	0.886800000	-2.939555000	0.311586000
1	1.600399000	-3.741832000	0.424020000

6	-0.482305000	-3.044670000	0.284206000
1	-1.132077000	-3.902536000	0.365430000
6	-2.277924000	-1.326003000	-0.126250000
6	-3.377881000	-2.184668000	-0.169252000
1	-3.256738000	-3.250778000	-0.024253000
6	-4.628627000	-1.625527000	-0.405193000
1	-5.505205000	-2.263727000	-0.445054000
6	-4.742359000	-0.243740000	-0.592548000
1	-5.699987000	0.227679000	-0.780488000
6	-3.594946000	0.533235000	-0.528725000
1	-3.638682000	1.606565000	-0.662551000
6	-0.904149000	1.087244000	1.747834000
8	-1.104676000	1.095970000	2.881905000
6	1.023012000	1.856635000	0.250082000
8	1.995951000	2.428293000	0.486035000
6	-1.333356000	2.708652000	-0.235871000
8	-1.791237000	3.760385000	-0.363275000
6	2.516144000	-0.952412000	-0.020044000
6	2.849036000	-0.170867000	-1.185680000
6	3.479589000	-1.215628000	0.970306000
6	4.182988000	0.342643000	-1.229120000
6	4.770928000	-0.696730000	0.890983000
6	5.109543000	0.091562000	-0.224106000
8	2.003046000	0.055202000	-2.155255000
1	3.192700000	-1.826677000	1.823505000
1	4.457412000	0.946032000	-2.091424000
1	5.495878000	-0.896393000	1.674123000
1	6.111722000	0.507014000	-0.306530000
1	-0.610366000	1.095631000	-1.829781000
1	0.106310000	0.795210000	-1.714398000

-1224.020084

TS1

25	-0.538174000	1.051898000	0.028757000
6	1.179741000	-1.597074000	0.177197000
7	-0.985084000	-1.784739000	0.199799000
7	-2.317726000	0.013386000	-0.350946000
7	0.046409000	-0.891201000	0.105398000
6	0.864022000	-2.971281000	0.380807000

1	1.567408000	-3.785074000	0.473983000
6	-0.507334000	-3.055966000	0.371255000
1	-1.168239000	-3.905834000	0.447264000
6	-2.268018000	-1.310175000	-0.098523000
6	-3.384573000	-2.145894000	-0.151956000
1	-3.297265000	-3.204033000	0.060970000
6	-4.605502000	-1.574792000	-0.493440000
1	-5.494175000	-2.194823000	-0.548799000
6	-4.673142000	-0.203912000	-0.764579000
1	-5.606363000	0.276051000	-1.035503000
6	-3.512705000	0.551640000	-0.674033000
1	-3.522909000	1.617362000	-0.864942000
6	-1.027473000	1.135725000	1.768658000
8	-1.347354000	1.200644000	2.875966000
6	1.055007000	1.806948000	0.463768000
8	2.017360000	2.353172000	0.796418000
6	-1.200701000	2.697610000	-0.310659000
8	-1.605360000	3.754506000	-0.547657000
6	2.493525000	-0.984308000	-0.027753000
6	2.731529000	-0.169307000	-1.184071000
6	3.536165000	-1.258539000	0.876003000
6	4.034967000	0.380089000	-1.323090000
6	4.806466000	-0.712889000	0.706198000
6	5.044628000	0.116385000	-0.403950000
8	1.808380000	0.052783000	-2.108552000
1	3.328090000	-1.896783000	1.731410000
1	4.224277000	1.014465000	-2.185231000
1	5.595585000	-0.921675000	1.421953000
1	6.028860000	0.554961000	-0.550529000
1	-0.285504000	1.022157000	-1.678552000
1	0.495569000	0.649255000	-1.671102000

-1224.019710

TS1-H₂O

25	-0.562583000	-1.052353000	0.260943000
8	-1.543902000	-3.597358000	1.390904000
8	-0.464850000	-2.101780000	-2.507606000
7	-2.465468000	-0.294860000	-0.015831000
7	-0.145818000	0.941421000	-0.292419000

6	-1.164332000	-2.600984000	0.936433000
6	1.094830000	-1.692827000	0.615847000
8	2.068630000	-2.255875000	0.890186000
6	-0.501839000	-1.684861000	-1.429022000
6	-2.541805000	1.045619000	-0.192086000
6	-3.775666000	1.688517000	-0.350527000
1	-3.823056000	2.759386000	-0.502354000
6	-4.945914000	0.935079000	-0.334287000
1	-5.908685000	1.419955000	-0.458998000
6	-4.857007000	-0.447784000	-0.170361000
1	-5.737945000	-1.079828000	-0.164461000
6	-3.599169000	-1.020521000	-0.017990000
1	-3.492179000	-2.090843000	0.105331000
6	-1.245551000	1.745263000	-0.241742000
6	1.074287000	1.511648000	-0.402760000
6	1.228621000	2.906109000	-0.404301000
1	2.227533000	3.319790000	-0.480920000
6	0.114041000	3.726280000	-0.298455000
1	0.217787000	4.806340000	-0.280111000
6	-1.146167000	3.136501000	-0.227887000
1	-2.032845000	3.752578000	-0.149485000
6	3.222028000	0.651249000	0.559077000
6	2.289291000	0.668942000	-0.516837000
6	4.428810000	-0.061499000	0.359905000
6	2.541512000	-0.046259000	-1.696142000
1	5.152251000	-0.079491000	1.170894000
6	4.671117000	-0.759149000	-0.822233000
6	3.723685000	-0.770018000	-1.857804000
1	1.798519000	-0.025123000	-2.489307000
1	5.602137000	-1.309270000	-0.935570000
1	3.909455000	-1.321218000	-2.774536000
8	2.964910000	1.247980000	1.723441000
1	-0.730733000	-0.472819000	1.843615000
1	-0.069853000	0.175953000	2.067729000
8	0.681672000	1.110166000	2.633087000
1	1.681149000	1.172026000	2.179463000
1	0.233729000	1.942562000	2.409825000

-1322.526891

3

25	-0.610573000	1.080160000	0.023220000
6	1.187118000	-1.559503000	0.137266000
7	-0.963148000	-1.789162000	0.088759000
7	-2.376034000	-0.007556000	-0.298405000
7	0.046397000	-0.869329000	0.036618000
6	0.901666000	-2.942212000	0.299084000
1	1.621004000	-3.740780000	0.400467000
6	-0.467103000	-3.053230000	0.254731000
1	-1.112037000	-3.916465000	0.310513000
6	-2.273070000	-1.338512000	-0.131789000
6	-3.361648000	-2.211147000	-0.186319000
1	-3.229901000	-3.276776000	-0.047016000
6	-4.618083000	-1.665965000	-0.426383000
1	-5.487231000	-2.313631000	-0.475309000
6	-4.743407000	-0.284468000	-0.605550000
1	-5.704574000	0.178630000	-0.797064000
6	-3.603428000	0.503857000	-0.529557000
1	-3.657574000	1.577792000	-0.657127000
6	-0.982029000	1.142678000	1.800871000
8	-1.219022000	1.244913000	2.932635000
6	0.964251000	1.885117000	0.289772000
8	1.949459000	2.470317000	0.489874000
6	-1.321453000	2.671792000	-0.344424000
8	-1.758223000	3.709506000	-0.637036000
6	2.515342000	-0.940162000	0.018237000
6	2.876717000	-0.171836000	-1.110393000
6	3.487878000	-1.195352000	1.001253000
6	4.181615000	0.318135000	-1.234491000
6	4.784726000	-0.698655000	0.881451000
6	5.130273000	0.057096000	-0.246017000
8	2.011920000	0.082550000	-2.155129000
1	3.207806000	-1.790490000	1.865769000
1	4.433688000	0.905593000	-2.111915000
1	5.517932000	-0.899720000	1.656233000
1	6.137865000	0.447944000	-0.354316000
1	-0.339997000	1.039370000	-1.566764000
1	1.097577000	0.282789000	-1.841962000

-1224.034221

4

25	-0.701224000	1.057389000	-0.303095000
6	1.181144000	-1.509305000	0.117263000
7	-0.967625000	-1.805367000	0.017883000
7	-2.449452000	-0.041660000	-0.027989000
7	0.015587000	-0.851981000	0.056124000
6	0.934179000	-2.912796000	0.083236000
1	1.675274000	-3.696392000	0.118624000
6	-0.428862000	-3.064543000	0.031747000
1	-1.047161000	-3.948787000	0.011403000
6	-2.298628000	-1.377402000	0.035572000
6	-3.372006000	-2.268321000	0.127076000
1	-3.204926000	-3.337431000	0.166690000
6	-4.655683000	-1.737640000	0.178343000
1	-5.511392000	-2.400908000	0.251478000
6	-4.826700000	-0.348796000	0.147008000
1	-5.810283000	0.103645000	0.200077000
6	-3.701502000	0.457196000	0.043338000
1	-3.784211000	1.537002000	0.015176000
6	-0.629256000	1.634881000	1.413887000
8	-0.585052000	2.083028000	2.487666000
6	0.861459000	1.753477000	-0.813334000
8	1.840262000	2.225313000	-1.232632000
6	-1.523209000	2.505014000	-0.919232000
8	-2.049399000	3.437706000	-1.381690000
6	2.463295000	-0.807404000	0.266294000
6	3.555777000	-1.099056000	-0.624855000
6	2.603437000	0.148470000	1.286919000
6	4.751706000	-0.343566000	-0.412852000
6	3.789214000	0.859840000	1.469554000
6	4.862773000	0.605494000	0.598860000
8	3.467159000	-1.983147000	-1.585715000
1	1.759770000	0.330525000	1.946386000
1	5.588601000	-0.532150000	-1.081850000
1	3.877098000	1.590963000	2.267568000
1	5.796096000	1.152329000	0.717150000
1	-0.784413000	0.583070000	-1.831438000

-1223.572450

TS2

25	0.667970000	1.134638000	0.154755000
6	-1.161311000	-1.341965000	-0.707625000
7	0.994795000	-1.598739000	-0.726190000
7	2.444173000	0.129283000	-0.251707000
7	-0.005623000	-0.676939000	-0.570484000
6	-0.887924000	-2.723959000	-0.915090000
1	-1.615301000	-3.507349000	-1.061922000
6	0.479049000	-2.850412000	-0.923414000
1	1.113690000	-3.711763000	-1.064769000
6	2.316323000	-1.167786000	-0.587683000
6	3.405741000	-2.016867000	-0.802478000
1	3.255895000	-3.055464000	-1.068955000
6	4.682270000	-1.484378000	-0.670555000
1	5.550050000	-2.115879000	-0.830418000
6	4.831715000	-0.132146000	-0.342315000
1	5.810059000	0.323180000	-0.240194000
6	3.692137000	0.634317000	-0.145219000
1	3.761680000	1.684904000	0.108004000
6	0.602509000	1.995723000	-1.434755000
8	0.554797000	2.591978000	-2.430574000
6	-0.918796000	1.739807000	0.734274000
8	-1.897981000	2.154631000	1.200404000
6	1.458286000	2.484270000	1.009397000
8	1.965653000	3.343708000	1.607505000
6	-2.460446000	-0.659329000	-0.690273000
6	-3.503900000	-1.131008000	0.182611000
6	-2.665291000	0.451120000	-1.526469000
6	-4.728215000	-0.392606000	0.143272000
6	-3.876169000	1.143391000	-1.541445000
6	-4.905652000	0.709020000	-0.688481000
8	-3.346386000	-2.155255000	0.979739000
1	-1.852104000	0.770565000	-2.172907000
1	-5.530959000	-0.719192000	0.800914000
1	-4.016391000	1.998191000	-2.196067000
1	-5.857114000	1.236903000	-0.677274000
1	0.741533000	0.383976000	1.608094000
6	0.122759000	-1.034487000	2.472091000
8	0.976827000	-1.828213000	2.243043000

8	-0.876937000	-0.602534000	2.946162000
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-1412.154635

5

25	-0.628066000	-1.087147000	0.143020000
6	1.197148000	1.378243000	-0.638045000
7	-0.965827000	1.626425000	-0.706261000
7	-2.399443000	-0.130018000	-0.306987000
7	0.036910000	0.704093000	-0.548154000
6	0.919191000	2.762498000	-0.804826000
1	1.644952000	3.553562000	-0.911061000
6	-0.448721000	2.882647000	-0.847616000
1	-1.082976000	3.745961000	-0.980623000
6	-2.284394000	1.176662000	-0.617934000
6	-3.381569000	2.007405000	-0.852723000
1	-3.244296000	3.052560000	-1.099403000
6	-4.650143000	1.447896000	-0.762808000
1	-5.524810000	2.065658000	-0.937725000
6	-4.785751000	0.088343000	-0.458265000
1	-5.758620000	-0.383938000	-0.388904000
6	-3.640601000	-0.662132000	-0.241813000
1	-3.696688000	-1.717611000	-0.008063000
6	-0.516025000	-1.955903000	-1.412898000
8	-0.463549000	-2.502720000	-2.429151000
6	0.988604000	-1.709991000	0.725402000
8	1.957449000	-2.155863000	1.162238000
6	-1.412164000	-2.516934000	0.932412000
8	-1.899969000	-3.434670000	1.436076000
6	2.493487000	0.698136000	-0.630607000
6	3.541231000	1.163049000	0.242831000
6	2.697416000	-0.401941000	-1.483872000
6	4.765290000	0.423401000	0.190817000
6	3.907425000	-1.092011000	-1.510432000
6	4.939078000	-0.667974000	-0.653313000
8	3.386548000	2.175851000	1.050669000
1	1.885934000	-0.710292000	-2.137441000
1	5.570071000	0.742321000	0.849456000
1	4.047494000	-1.936733000	-2.177831000
1	5.890263000	-1.196317000	-0.651226000

1	-0.851762000	-0.299376000	1.895579000
6	-0.533962000	0.690664000	2.411009000
8	-1.400330000	1.589832000	2.368329000
8	0.588272000	0.650947000	2.959046000

-1412.176247

5'

25	0.615618000	0.956158000	-0.199078000
6	-1.276843000	-1.611786000	-0.135623000
7	0.876014000	-1.908173000	-0.116577000
7	2.360841000	-0.166750000	-0.406529000
7	-0.108886000	-0.968580000	-0.263217000
6	-1.027836000	-2.987972000	0.132982000
1	-1.769099000	-3.758342000	0.279897000
6	0.336879000	-3.141588000	0.127018000
1	0.955219000	-4.015142000	0.265505000
6	2.206310000	-1.494682000	-0.249562000
6	3.275094000	-2.394422000	-0.244519000
1	3.108812000	-3.456844000	-0.117914000
6	4.556024000	-1.881546000	-0.416026000
1	5.409004000	-2.552334000	-0.417557000
6	4.730011000	-0.504962000	-0.596682000
1	5.712072000	-0.070150000	-0.742470000
6	3.608912000	0.312556000	-0.585203000
1	3.695738000	1.383228000	-0.723245000
6	0.451937000	1.190072000	-1.970027000
8	0.357076000	1.334685000	-3.115129000
6	-0.965643000	1.779880000	0.140585000
8	-1.930533000	2.363725000	0.392493000
6	1.453608000	2.542380000	-0.024193000
8	1.984372000	3.565229000	0.085400000
6	-2.562125000	-0.930422000	-0.332253000
6	-3.576599000	-1.004511000	0.686202000
6	-2.778303000	-0.207031000	-1.517682000
6	-4.786759000	-0.293615000	0.410562000
6	-3.974044000	0.470765000	-1.752923000
6	-4.975684000	0.422378000	-0.767598000
8	-3.403548000	-1.655872000	1.806215000
1	-1.989018000	-0.186176000	-2.264253000

1	-5.568164000	-0.321868000	1.166777000
1	-4.124607000	1.021484000	-2.676406000
1	-5.915525000	0.947179000	-0.926714000
1	0.389191000	2.318782000	2.542128000
6	0.717798000	1.293032000	2.795119000
8	0.883107000	0.480999000	1.818217000
8	0.901240000	1.003684000	3.999605000

-1412.196494

TS3

25	0.642792000	1.140648000	0.168696000
6	-1.125182000	-1.337675000	-0.776148000
7	1.024974000	-1.563293000	-0.778042000
7	2.442349000	0.175860000	-0.245692000
7	0.017351000	-0.662463000	-0.599370000
6	-0.839957000	-2.703644000	-1.038370000
1	-1.556479000	-3.488307000	-1.229149000
6	0.532279000	-2.811194000	-1.029886000
1	1.179787000	-3.657973000	-1.197941000
6	2.343294000	-1.113323000	-0.615794000
6	3.444278000	-1.940810000	-0.839174000
1	3.312843000	-2.973998000	-1.134671000
6	4.711339000	-1.392055000	-0.676487000
1	5.591075000	-2.005347000	-0.841082000
6	4.834024000	-0.047954000	-0.309888000
1	5.803678000	0.419286000	-0.181912000
6	3.680364000	0.697045000	-0.108144000
1	3.730403000	1.740792000	0.175450000
6	0.553742000	2.031542000	-1.405433000
8	0.479889000	2.643988000	-2.388775000
6	-0.959609000	1.699883000	0.751543000
8	-1.956362000	2.077815000	1.210857000
6	1.403483000	2.493034000	1.050619000
8	1.890893000	3.351110000	1.664964000
6	-2.430607000	-0.656790000	-0.727490000
6	-3.413616000	-1.022830000	0.211384000
6	-2.704817000	0.392199000	-1.622128000
6	-4.645460000	-0.360351000	0.237034000
6	-3.929262000	1.057144000	-1.597784000

6	-4.900371000	0.673875000	-0.663625000
8	-3.226707000	-2.020580000	1.142564000
1	-1.938828000	0.676571000	-2.336949000
1	-5.383683000	-0.656732000	0.975662000
1	-4.124688000	1.864729000	-2.296100000
1	-5.858079000	1.184973000	-0.630442000
1	0.719395000	0.366904000	1.611425000
6	0.205583000	-1.119331000	2.415217000
8	1.125873000	-1.834339000	2.182641000
8	-0.838659000	-0.790833000	2.877044000
1	-2.294388000	-2.287709000	1.182993000

-1412.615225

6			
25	0.611470000	1.087843000	0.147922000
6	-1.129590000	-1.401332000	-0.707921000
7	1.026807000	-1.612391000	-0.726127000
7	2.416629000	0.163642000	-0.250659000
7	0.012826000	-0.713463000	-0.567382000
6	-0.837209000	-2.770466000	-0.920385000
1	-1.549484000	-3.566907000	-1.073594000
6	0.537825000	-2.868710000	-0.924449000
1	1.188691000	-3.718109000	-1.066364000
6	2.339643000	-1.136336000	-0.595798000
6	3.455003000	-1.939752000	-0.822018000
1	3.344655000	-2.980541000	-1.098788000
6	4.710537000	-1.356903000	-0.685630000
1	5.601765000	-1.952487000	-0.853057000
6	4.809355000	-0.004778000	-0.342985000
1	5.770127000	0.484939000	-0.235959000
6	3.643263000	0.718500000	-0.138116000
1	3.671772000	1.768264000	0.124072000
6	0.512939000	1.921970000	-1.431716000
8	0.460733000	2.439917000	-2.461991000
6	-1.034099000	1.687919000	0.667652000
8	-2.030168000	2.117617000	1.056011000
6	1.347746000	2.547397000	0.936371000
8	1.809056000	3.480580000	1.434610000
6	-2.434053000	-0.719179000	-0.683332000

6	-3.400687000	-1.020955000	0.293703000
6	-2.720382000	0.266333000	-1.644743000
6	-4.634900000	-0.362736000	0.287266000
6	-3.947405000	0.926235000	-1.651478000
6	-4.905418000	0.603739000	-0.681538000
8	-3.195785000	-1.951369000	1.287598000
1	-1.963583000	0.503641000	-2.386218000
1	-5.361720000	-0.606966000	1.055577000
1	-4.154674000	1.683598000	-2.400651000
1	-5.864956000	1.112334000	-0.672136000
1	0.787383000	0.303984000	1.901583000
6	0.428011000	-0.693784000	2.380850000
8	1.270394000	-1.614144000	2.337542000
8	-0.706882000	-0.636082000	2.899630000
1	-2.252818000	-2.167466000	1.375060000

-1412.634322

6'

25	-0.614180000	-0.955958000	-0.222541000
6	1.237071000	1.638330000	-0.172749000
7	-0.908029000	1.908891000	-0.108143000
7	-2.380100000	0.148627000	-0.367418000
7	0.076861000	0.978889000	-0.261275000
6	0.988583000	3.014976000	0.070328000
1	1.725780000	3.796580000	0.177636000
6	-0.381384000	3.150846000	0.099082000
1	-1.005385000	4.019986000	0.238964000
6	-2.242046000	1.477615000	-0.213783000
6	-3.317365000	2.365410000	-0.186334000
1	-3.160648000	3.430010000	-0.065973000
6	-4.596670000	1.836539000	-0.327749000
1	-5.457427000	2.496919000	-0.311564000
6	-4.756635000	0.458404000	-0.499721000
1	-5.736267000	0.010753000	-0.620891000
6	-3.625529000	-0.346564000	-0.513991000
1	-3.704330000	-1.418375000	-0.645657000
6	-0.478862000	-1.132574000	-2.004709000
8	-0.397514000	-1.238496000	-3.154331000
6	0.982701000	-1.768186000	0.066058000

8	1.961193000	-2.339755000	0.290455000
6	-1.425545000	-2.562115000	-0.084898000
8	-1.938240000	-3.596179000	-0.007658000
6	2.525244000	0.949031000	-0.363308000
6	3.494016000	0.918010000	0.657394000
6	2.797397000	0.292713000	-1.576441000
6	4.703521000	0.242531000	0.462558000
6	4.001614000	-0.379097000	-1.775807000
6	4.954059000	-0.401698000	-0.748845000
8	3.308164000	1.514631000	1.885042000
1	2.046824000	0.317749000	-2.360156000
1	5.429775000	0.225614000	1.269189000
1	4.195616000	-0.879740000	-2.719034000
1	5.896188000	-0.923372000	-0.889622000
1	-0.346821000	-2.388622000	2.477496000
6	-0.657884000	-1.365429000	2.760575000
8	-0.837111000	-0.529752000	1.805429000
8	-0.808837000	-1.099327000	3.974348000
1	2.435124000	1.935173000	1.938737000

-1412.655960

Mn-bim

1			
25	-0.993429000	0.956560000	-0.319125000
6	-4.024296000	-0.113342000	-0.131790000
6	-2.373418000	-1.526119000	0.047350000
7	-0.094177000	-0.884554000	0.062313000
7	-2.651513000	-0.224840000	-0.094279000
6	-4.573611000	-1.365387000	-0.008174000
1	-5.597344000	-1.704191000	0.010970000
7	-3.513550000	-2.245132000	0.103067000
1	-3.578535000	-3.252120000	0.206978000
6	-0.986010000	-1.883822000	0.116353000
7	-0.358682000	-3.070959000	0.225779000
1	-0.808309000	-3.978315000	0.288880000
6	0.996622000	-2.827654000	0.253865000
1	1.714119000	-3.625283000	0.357579000
6	1.166310000	-1.458222000	0.164744000

6	-0.891813000	1.545403000	1.351653000
8	-0.838355000	1.891108000	2.454411000
6	-1.993657000	2.400728000	-0.790576000
8	-2.633350000	3.320208000	-1.069032000
6	0.531906000	1.847434000	-0.801001000
8	1.436953000	2.470287000	-1.151366000
1	-4.515731000	0.841212000	-0.244202000
6	2.406637000	-0.674315000	0.225464000
6	2.497084000	0.390568000	1.138043000
6	3.517090000	-0.999861000	-0.634471000
6	3.641628000	1.182360000	1.237312000
6	4.669312000	-0.162267000	-0.508672000
6	4.729278000	0.893660000	0.396436000
1	1.645333000	0.597949000	1.780044000
8	3.483364000	-1.985664000	-1.494341000
1	3.685625000	2.002198000	1.947886000
1	5.516473000	-0.377887000	-1.156291000
1	5.632291000	1.498319000	0.451530000

-1200.834970

2

25	0.836200000	-1.013705000	-0.096543000
6	3.918749000	-0.063900000	-0.473451000
6	2.366488000	1.434224000	-0.175872000
7	0.064929000	0.921623000	-0.018882000
7	2.562296000	0.122321000	-0.342451000
6	4.544195000	1.157899000	-0.394258000
1	5.583453000	1.439905000	-0.456328000
7	3.546256000	2.092363000	-0.204811000
1	3.670368000	3.094119000	-0.106472000
6	1.009898000	1.868446000	-0.012852000
7	0.451512000	3.092401000	0.097382000
1	0.950079000	3.975619000	0.115481000
6	-0.915793000	2.922066000	0.145152000
1	-1.593433000	3.758732000	0.209210000
6	-1.158353000	1.564016000	0.061897000
6	1.148013000	-1.034314000	1.683832000
8	1.352881000	-1.027278000	2.817966000
6	1.728335000	-2.576631000	-0.322992000

8	2.311086000	-3.562913000	-0.467156000
6	-0.730756000	-1.897181000	0.172823000
8	-1.676619000	-2.518359000	0.399607000
1	0.859638000	-0.973590000	-1.898637000
1	0.120053000	-0.764858000	-1.755525000
1	4.348288000	-1.044299000	-0.615616000
6	-2.455781000	0.873661000	0.021411000
6	-3.369089000	1.054989000	1.072003000
6	-2.800488000	0.071086000	-1.124719000
6	-4.629390000	0.451383000	1.062796000
6	-4.092061000	-0.538291000	-1.093787000
6	-4.977097000	-0.352920000	-0.035318000
1	-3.071838000	1.676649000	1.914195000
8	-1.990382000	-0.095098000	-2.139740000
1	-5.319070000	0.598114000	1.888552000
1	-4.373821000	-1.158566000	-1.942068000
1	-5.950649000	-0.838164000	-0.063279000

-1202.003541

TS1

25	0.746067000	-0.998873000	-0.033046000
6	3.834681000	-0.142454000	-0.621489000
6	2.368105000	1.402110000	-0.174703000
7	0.072900000	0.954270000	0.086456000
7	2.496160000	0.091631000	-0.412696000
6	4.516960000	1.047683000	-0.525576000
1	5.562356000	1.289077000	-0.637438000
7	3.572554000	2.013182000	-0.239694000
1	3.744412000	3.003706000	-0.106001000
6	1.038302000	1.877996000	0.071844000
7	0.504287000	3.115135000	0.179518000
1	1.018876000	3.989226000	0.173678000
6	-0.866777000	2.975284000	0.230616000
1	-1.525914000	3.827354000	0.284519000
6	-1.133628000	1.621231000	0.150798000
6	1.265145000	-1.078580000	1.694578000
8	1.603020000	-1.128798000	2.798512000
6	1.534220000	-2.573753000	-0.423381000
8	2.056680000	-3.571153000	-0.690347000

6	-0.796596000	-1.834688000	0.408085000
8	-1.727505000	-2.436721000	0.740024000
1	0.415654000	-0.916292000	-1.727058000
1	-0.394564000	-0.581846000	-1.690798000
1	4.215161000	-1.131390000	-0.828942000
6	-2.420032000	0.925321000	0.024809000
6	-3.425420000	1.096012000	0.989488000
6	-2.648832000	0.094702000	-1.120006000
6	-4.660525000	0.455222000	0.874283000
6	-3.908832000	-0.551503000	-1.206118000
6	-4.891219000	-0.374555000	-0.234208000
1	-3.220329000	1.733419000	1.846364000
8	-1.740012000	-0.064771000	-2.079300000
1	-5.424167000	0.591978000	1.634044000
1	-4.090785000	-1.194061000	-2.063936000
1	-5.844453000	-0.887511000	-0.338614000

-1202.000754

TS1-H₂O

25	-0.562583000	-1.052353000	0.260943000
8	-1.543902000	-3.597358000	1.390904000
8	-0.464850000	-2.101780000	-2.507606000
7	-2.465468000	-0.294860000	-0.015831000
7	-0.145818000	0.941421000	-0.292419000
6	-1.164332000	-2.600984000	0.936433000
6	1.094830000	-1.692827000	0.615847000
8	2.068630000	-2.255875000	0.890186000
6	-0.501839000	-1.684861000	-1.429022000
6	-2.541805000	1.045619000	-0.192086000
6	-3.775666000	1.688517000	-0.350527000
1	-3.823056000	2.759386000	-0.502354000
6	-4.945914000	0.935079000	-0.334287000
1	-5.908685000	1.419955000	-0.458998000
6	-4.857007000	-0.447784000	-0.170361000
1	-5.737945000	-1.079828000	-0.164461000
6	-3.599169000	-1.020521000	-0.017990000
1	-3.492179000	-2.090843000	0.105331000
6	-1.245551000	1.745263000	-0.241742000
6	1.074287000	1.511648000	-0.402760000

6	1.228621000	2.906109000	-0.404301000
1	2.227533000	3.319790000	-0.480920000
6	0.114041000	3.726280000	-0.298455000
1	0.217787000	4.806340000	-0.280111000
6	-1.146167000	3.136501000	-0.227887000
1	-2.032845000	3.752578000	-0.149485000
6	3.222028000	0.651249000	0.559077000
6	2.289291000	0.668942000	-0.516837000
6	4.428810000	-0.061499000	0.359905000
6	2.541512000	-0.046259000	-1.696142000
1	5.152251000	-0.079491000	1.170894000
6	4.671117000	-0.759149000	-0.822233000
6	3.723685000	-0.770018000	-1.857804000
1	1.798519000	-0.025123000	-2.489307000
1	5.602137000	-1.309270000	-0.935570000
1	3.909455000	-1.321218000	-2.774536000
8	2.964910000	1.247980000	1.723441000
1	-0.730733000	-0.472819000	1.843615000
1	-0.069853000	0.175953000	2.067729000
8	0.681672000	1.110166000	2.633087000
1	1.681149000	1.172026000	2.179463000
1	0.233729000	1.942562000	2.409825000

-1322.526891

3

25	0.866374000	-1.034206000	-0.028571000
6	3.922179000	0.005499000	-0.505653000
6	2.340798000	1.465975000	-0.211043000
7	0.049697000	0.913851000	-0.019710000
7	2.563870000	0.157967000	-0.360376000
6	4.521244000	1.243202000	-0.453896000
1	5.552665000	1.548552000	-0.535512000
7	3.505532000	2.156144000	-0.264706000
1	3.607090000	3.161829000	-0.187041000
6	0.979679000	1.874899000	-0.035970000
7	0.406687000	3.095925000	0.080340000
1	0.893699000	3.985655000	0.085301000
6	-0.954673000	2.911651000	0.155685000
1	-1.643708000	3.738473000	0.226323000

6	-1.173333000	1.550139000	0.082051000
6	1.231267000	-1.028735000	1.746493000
8	1.462531000	-1.073229000	2.884423000
6	1.760053000	-2.534685000	-0.373443000
8	2.351897000	-3.500010000	-0.644548000
6	-0.637010000	-1.954496000	0.239758000
8	-1.581045000	-2.607882000	0.438143000
1	0.559554000	-1.011666000	-1.614780000
1	-1.013137000	-0.339654000	-1.793916000
1	4.375136000	-0.965609000	-0.639384000
6	-2.467750000	0.854152000	0.040271000
6	-3.430868000	1.096395000	1.035216000
6	-2.805707000	-0.001727000	-1.030693000
6	-4.698506000	0.516374000	0.974661000
6	-4.075234000	-0.585138000	-1.092046000
6	-5.018617000	-0.326062000	-0.096627000
1	-3.167303000	1.752148000	1.860356000
8	-1.949841000	-0.255870000	-2.085175000
1	-5.425715000	0.715941000	1.755646000
1	-4.307206000	-1.239508000	-1.926765000
1	-6.000368000	-0.786942000	-0.156134000

-1202.015562

4			
25	0.982998000	-1.007081000	-0.282985000
6	4.026486000	0.135909000	-0.095791000
6	2.363096000	1.525261000	0.064660000
7	0.084913000	0.885553000	0.079257000
7	2.654331000	0.228397000	-0.061994000
6	4.566123000	1.395985000	0.013624000
1	5.587095000	1.743792000	0.030605000
7	3.498933000	2.265128000	0.113002000
1	3.551529000	3.272849000	0.206721000
6	0.977570000	1.879667000	0.121178000
7	0.354457000	3.079138000	0.202329000
1	0.806901000	3.984975000	0.248514000
6	-1.001542000	2.838995000	0.224424000
1	-1.718904000	3.639853000	0.303597000
6	-1.171259000	1.467619000	0.160480000

6	0.881700000	-1.519132000	1.447598000
8	0.788475000	-1.913277000	2.540764000
6	1.981439000	-2.389221000	-0.775704000
8	2.655512000	-3.275113000	-1.126778000
6	-0.498135000	-1.832028000	-0.822414000
8	-1.420923000	-2.386747000	-1.270542000
1	1.012207000	-0.555632000	-1.822509000
1	4.531765000	-0.812918000	-0.197656000
6	-2.414937000	0.683696000	0.230155000
6	-2.499979000	-0.368441000	1.156886000
6	-3.527812000	0.986612000	-0.633641000
6	-3.640176000	-1.166115000	1.270987000
6	-4.674812000	0.143899000	-0.495255000
6	-4.730062000	-0.898061000	0.427185000
1	-1.644653000	-0.563668000	1.797375000
8	-3.503783000	1.961594000	-1.509173000
1	-3.677813000	-1.974533000	1.995193000
1	-5.522631000	0.342760000	-1.147604000
1	-5.629332000	-1.507513000	0.491833000

-1201.552216

TS2

25	0.759435000	1.067344000	-0.066644000
6	3.746127000	-0.017466000	-0.721856000
6	2.069231000	-1.399358000	-0.821597000
7	-0.195065000	-0.778020000	-0.498070000
7	2.376476000	-0.114073000	-0.634390000
6	4.267737000	-1.264517000	-0.971267000
1	5.280835000	-1.607319000	-1.111955000
7	3.191955000	-2.128791000	-1.030264000
1	3.232094000	-3.126716000	-1.204022000
6	0.686172000	-1.756576000	-0.732091000
7	0.064792000	-2.955556000	-0.801320000
1	0.513460000	-3.852471000	-0.947529000
6	-1.280083000	-2.736291000	-0.603966000
1	-1.995587000	-3.541453000	-0.629299000
6	-1.448420000	-1.373192000	-0.430426000
6	0.455964000	1.775885000	-1.697556000
8	0.244465000	2.282991000	-2.723065000

6	1.832932000	2.387681000	0.454353000
8	2.553277000	3.222501000	0.827058000
6	-0.632522000	1.856717000	0.725896000
8	-1.472106000	2.394215000	1.325952000
1	0.974398000	0.445459000	1.430671000
1	4.259046000	0.924932000	-0.600356000
6	-2.696227000	-0.613175000	-0.269860000
6	-2.873979000	0.572728000	-1.002349000
6	-3.737529000	-1.085383000	0.610009000
6	-4.027345000	1.350870000	-0.889624000
6	-4.894965000	-0.252398000	0.715448000
6	-5.037836000	0.926256000	-0.012148000
1	-2.080998000	0.890448000	-1.672308000
8	-3.644651000	-2.203682000	1.284878000
1	-4.134648000	2.263794000	-1.467874000
1	-5.682999000	-0.578573000	1.391121000
1	-5.944551000	1.517339000	0.100093000
6	2.108867000	-0.547502000	2.418790000
8	1.632049000	-1.624370000	2.272963000
8	2.849117000	0.287138000	2.824131000

-1390.134628

5

25	-0.906534000	-1.038834000	0.094888000
6	-3.951005000	-0.081760000	-0.364652000
6	-2.321106000	1.329835000	-0.681623000
7	-0.032481000	0.738603000	-0.567068000
7	-2.580493000	0.053284000	-0.380669000
6	-4.518655000	1.132276000	-0.665451000
1	-5.547346000	1.443818000	-0.755356000
7	-3.471860000	2.012074000	-0.863080000
1	-3.548783000	2.996461000	-1.094629000
6	-0.940339000	1.706822000	-0.749962000
7	-0.334124000	2.898880000	-0.913960000
1	-0.799974000	3.789618000	-1.048597000
6	1.025704000	2.691236000	-0.836588000
1	1.729942000	3.497396000	-0.959644000
6	1.219455000	1.336803000	-0.634057000
6	-0.785661000	-1.891004000	-1.467147000

8	-0.724963000	-2.425892000	-2.490520000
6	-1.902545000	-2.376331000	0.794268000
8	-2.553532000	-3.226484000	1.228231000
6	0.611182000	-1.814390000	0.741419000
8	1.512635000	-2.361362000	1.209650000
1	-1.125273000	-0.224917000	1.832228000
1	-4.427797000	-1.025057000	-0.144738000
6	2.473794000	0.578600000	-0.568215000
6	2.585768000	-0.615125000	-1.301779000
6	3.582118000	1.057403000	0.221340000
6	3.739925000	-1.398158000	-1.270283000
6	4.738606000	0.216611000	0.247223000
6	4.816610000	-0.970207000	-0.476306000
1	1.741598000	-0.931820000	-1.908070000
8	3.547257000	2.184482000	0.884244000
1	3.799340000	-2.316758000	-1.846287000
1	5.579096000	0.543949000	0.855532000
1	5.725841000	-1.566056000	-0.427726000
6	-0.678220000	0.672658000	2.411983000
8	0.399380000	0.431577000	2.997651000
8	-1.393825000	1.696767000	2.395433000

-1390.158098

5'

25	-0.925319000	-0.898276000	-0.225678000
6	-3.866692000	0.454975000	-0.634195000
6	-2.126228000	1.736528000	-0.377217000
7	0.127293000	0.979525000	-0.322082000
7	-2.497132000	0.460622000	-0.511678000
6	-4.325347000	1.749377000	-0.573560000
1	-5.318868000	2.165191000	-0.633492000
7	-3.209818000	2.546717000	-0.409290000
1	-3.201182000	3.557563000	-0.331050000
6	-0.723446000	2.009392000	-0.250351000
7	-0.054875000	3.164986000	-0.046472000
1	-0.470920000	4.084107000	0.052828000
6	1.287602000	2.864982000	0.015362000
1	2.033712000	3.629425000	0.154923000
6	1.405832000	1.497926000	-0.172794000

6	-0.728729000	-1.209435000	-1.977410000
8	-0.611341000	-1.403434000	-3.113997000
6	-2.054573000	-2.289090000	-0.065470000
8	-2.798273000	-3.171730000	0.026701000
6	0.486911000	-1.940428000	0.220847000
8	1.338177000	-2.646994000	0.557386000
1	-1.080252000	-2.226658000	2.555117000
1	-4.423706000	-0.462054000	-0.754750000
6	2.621513000	0.681693000	-0.282856000
6	2.695060000	-0.304353000	-1.281445000
6	3.737386000	0.901695000	0.605074000
6	3.815036000	-1.122451000	-1.436632000
6	4.861108000	0.035724000	0.425654000
6	4.900254000	-0.943743000	-0.563288000
1	1.849238000	-0.427222000	-1.951055000
8	3.735326000	1.827355000	1.529330000
1	3.842333000	-1.877079000	-2.217013000
1	5.706312000	0.170550000	1.097384000
1	5.783841000	-1.571562000	-0.659327000
6	-1.198972000	-1.154654000	2.802794000
8	-1.356562000	-0.834192000	4.004084000
8	-1.165588000	-0.328148000	1.824992000

-1390.177847

TS3

25	-0.873446000	-1.101758000	0.133009000
6	-3.989499000	-0.219551000	-0.149843000
6	-2.435210000	1.216361000	-0.645697000
7	-0.132546000	0.712605000	-0.618572000
7	-2.629782000	-0.046607000	-0.257024000
6	-4.618870000	0.957781000	-0.482279000
1	-5.661874000	1.230164000	-0.522459000
7	-3.619608000	1.856164000	-0.792260000
1	-3.744616000	2.822572000	-1.071800000
6	-1.076729000	1.631678000	-0.830200000
7	-0.520796000	2.822778000	-1.152694000
1	-1.022471000	3.680680000	-1.353962000
6	0.847018000	2.657125000	-1.149256000
1	1.523266000	3.460918000	-1.394763000

6	1.084097000	1.336541000	-0.822326000
6	-0.789868000	-1.942460000	-1.462483000
8	-0.709334000	-2.521930000	-2.467251000
6	-1.759079000	-2.417303000	0.944179000
8	-2.352547000	-3.247167000	1.504130000
6	0.688379000	-1.748096000	0.717626000
8	1.662395000	-2.180129000	1.182371000
1	-0.914898000	-0.351923000	1.587807000
1	-4.422101000	-1.161050000	0.153809000
6	2.359196000	0.604314000	-0.724349000
6	2.614251000	-0.475491000	-1.586581000
6	3.315721000	0.925924000	0.256591000
6	3.795065000	-1.210551000	-1.492772000
6	4.504284000	0.193994000	0.354943000
6	4.741257000	-0.868412000	-0.517743000
1	1.865332000	-0.732934000	-2.329589000
8	3.134694000	1.947393000	1.163399000
1	3.975416000	-2.041196000	-2.167921000
1	5.222510000	0.459681000	1.124417000
1	5.664942000	-1.433272000	-0.431275000
6	-0.243443000	1.057040000	2.466361000
8	-1.080320000	1.871952000	2.251841000
8	0.746693000	0.590986000	2.926015000
1	2.237698000	2.313509000	1.083280000

-1390.599100

6			
25	0.843544000	1.052374000	0.112179000
6	3.952627000	0.254452000	-0.211698000
6	2.419623000	-1.227125000	-0.656339000
7	0.112725000	-0.745890000	-0.610840000
7	2.594916000	0.049836000	-0.299760000
6	4.597987000	-0.917909000	-0.525266000
1	5.645123000	-1.172020000	-0.573704000
7	3.611184000	-1.842336000	-0.802498000
1	3.752017000	-2.813670000	-1.058916000
6	1.062010000	-1.666470000	-0.805260000
7	0.508521000	-2.868524000	-1.064098000
1	1.012680000	-3.731949000	-1.236702000

6	-0.861373000	-2.713909000	-1.038669000
1	-1.534372000	-3.532469000	-1.239874000
6	-1.104737000	-1.384493000	-0.760680000
6	0.721534000	1.897292000	-1.455968000
8	0.643051000	2.422554000	-2.482443000
6	1.732247000	2.440222000	0.862715000
8	2.311638000	3.320869000	1.334080000
6	-0.746965000	1.740574000	0.674170000
8	-1.710972000	2.230014000	1.076535000
1	1.015091000	0.218272000	1.845482000
1	4.367110000	1.212440000	0.063840000
6	-2.379107000	-0.652517000	-0.672889000
6	-2.637006000	0.403676000	-1.563850000
6	-3.330073000	-0.947764000	0.321921000
6	-3.816527000	1.141710000	-1.483946000
6	-4.516677000	-0.211108000	0.405841000
6	-4.757008000	0.827339000	-0.494153000
1	-1.891268000	0.638790000	-2.317531000
8	-3.148557000	-1.945674000	1.253185000
1	-4.000126000	1.953702000	-2.180423000
1	-5.230565000	-0.454290000	1.186660000
1	-5.679525000	1.395429000	-0.417411000
6	0.552840000	-0.706365000	2.371587000
8	-0.550162000	-0.495543000	2.919597000
8	1.277027000	-1.723823000	2.344940000
1	-2.248771000	-2.307999000	1.192246000

-1390.619826

7'

25	-0.832504000	-0.901626000	-0.297525000
6	-3.906955000	0.212281000	-0.463223000
6	-2.275715000	1.633571000	-0.239999000
7	0.017033000	1.047685000	-0.267131000
7	-2.539577000	0.335313000	-0.412513000
6	-4.472764000	1.458490000	-0.323446000
1	-5.500302000	1.786411000	-0.313411000
7	-3.425085000	2.344445000	-0.182450000
1	-3.500380000	3.348621000	-0.061859000
6	-0.893685000	2.017562000	-0.157737000

7	-0.290605000	3.215397000	0.015649000
1	-0.757516000	4.109436000	0.124187000
6	1.070887000	3.003058000	0.011256000
1	1.777624000	3.811974000	0.111258000
6	1.257767000	1.647462000	-0.173747000
6	-0.637251000	-1.017451000	-2.075606000
8	-0.508312000	-1.081942000	-3.225039000
6	-1.826803000	-2.405550000	-0.248832000
8	-2.493761000	-3.350969000	-0.228588000
6	0.693969000	-1.828829000	0.003273000
8	1.634163000	-2.461002000	0.234334000
1	-0.697926000	-2.447180000	2.385527000
1	-4.387372000	-0.746075000	-0.593371000
6	2.502517000	0.871254000	-0.314988000
6	2.765091000	0.184889000	-1.512848000
6	3.415898000	0.747784000	0.748073000
6	3.910771000	-0.595222000	-1.660952000
6	4.567581000	-0.034373000	0.606899000
6	4.812209000	-0.701135000	-0.593763000
1	2.049531000	0.269684000	-2.325362000
8	3.224447000	1.362060000	1.967203000
1	4.097401000	-1.117739000	-2.593902000
1	5.252261000	-0.116856000	1.445355000
1	5.707550000	-1.307912000	-0.693162000
6	-0.937784000	-1.419443000	2.717643000
8	-1.067482000	-1.202506000	3.945244000
8	-1.065605000	-0.532344000	1.803278000
1	2.377382000	1.837940000	1.974503000

-1390.638925