

SUPPLEMENTARY INFORMATION

The significance of acid-base properties in the key ligand for CO₂ hydrogenation: Role of amido ligand

KUBER SINGH RAWAT^a and BISWARUP PATHAK,^{a,b,*}

^aDiscipline of Chemistry, Indian Institute of Technology Indore, Simrol, Indore 453 552, India

^bDiscipline of Metallurgy Engineering and Materials Science, Indian Institute of Technology Indore, Simrol, Indore 453 552, Madhya Pradesh, India

Email. biswarup@iiti.ac.in

Contents

S1. Figure S1: Modelled aliphatic amido Mn(I) pincer complexes

S2. Figure S2 and S3: Calculated reaction free energies

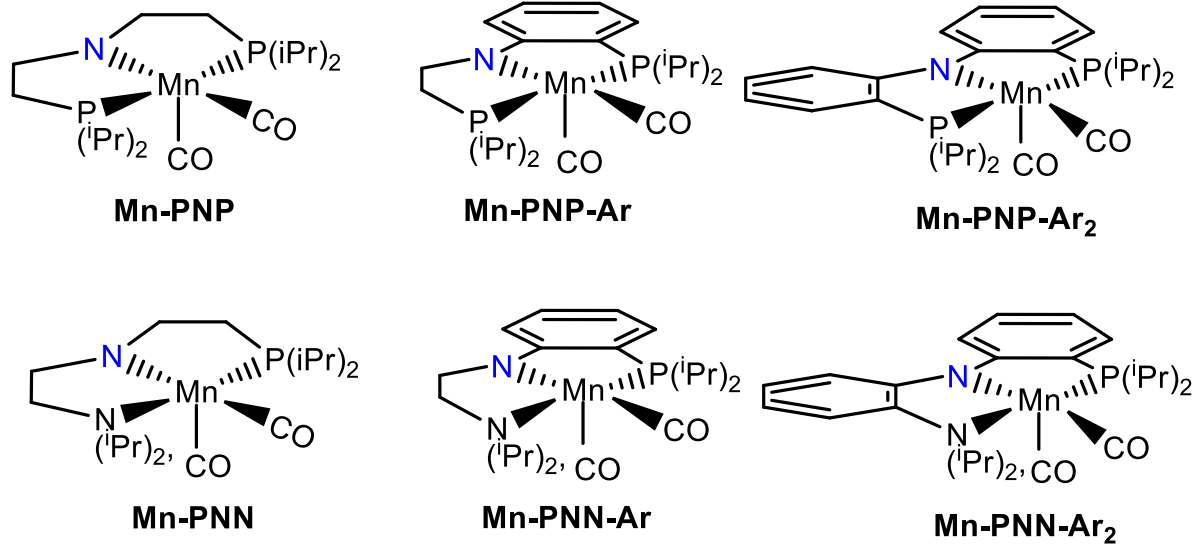
S3. Table S1: Reaction energies for heterolytic H₂ cleavage:

S4. Figure S3: Molecular orbitals

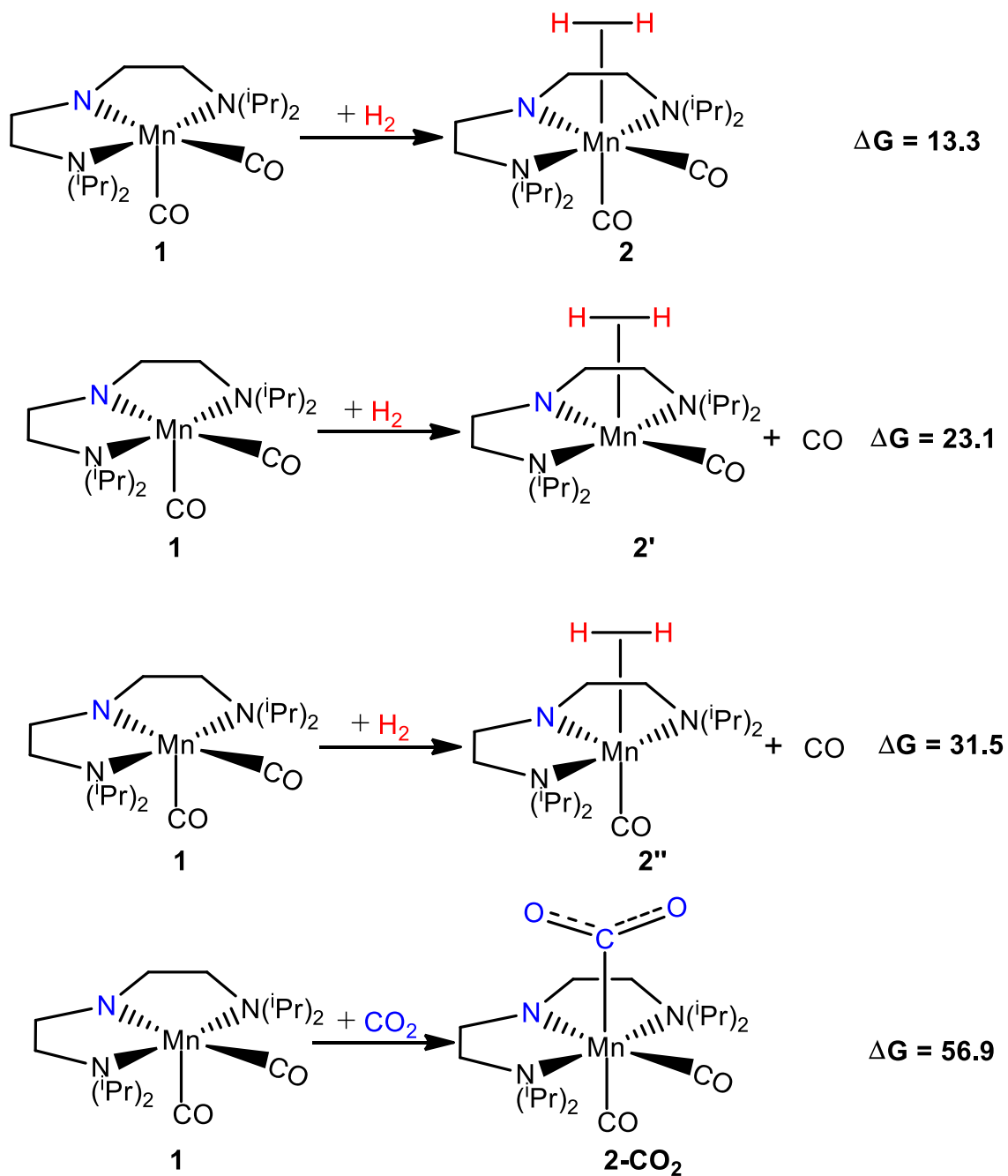
S5. Figure S4: pK_a value Calculations

S6. Reference

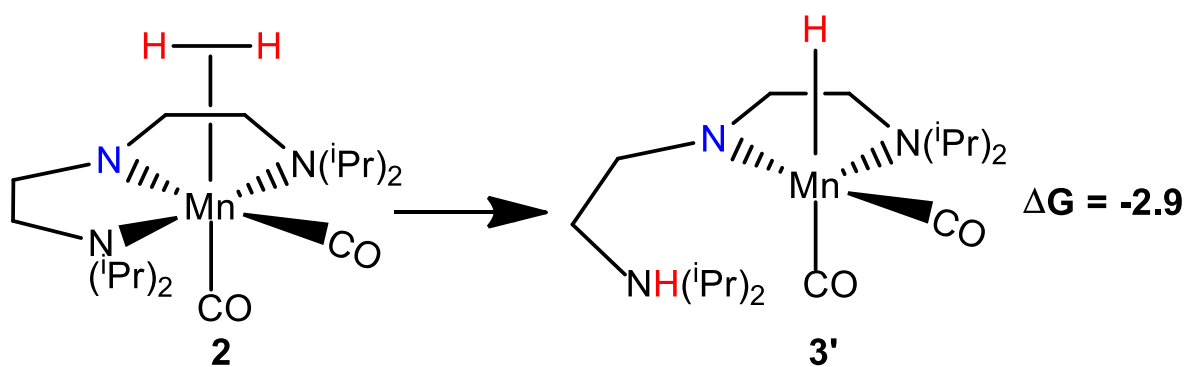
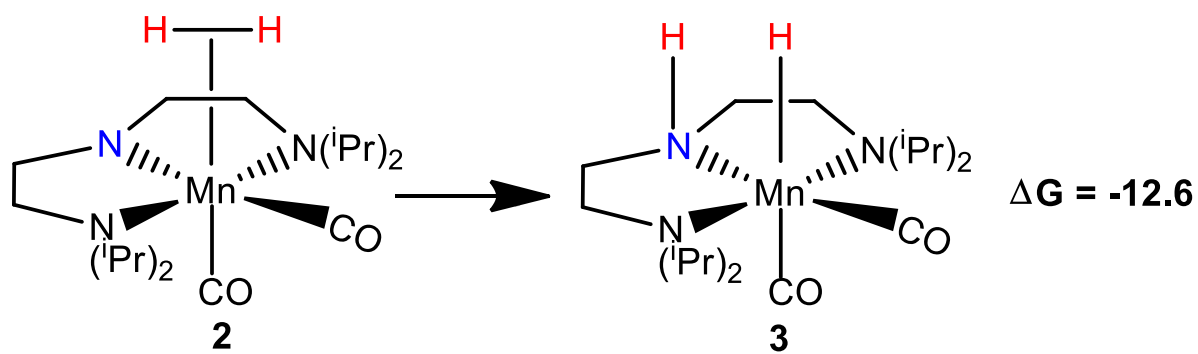
S7. Cartesian coordinates and energies



S1. Figure S1. Our modelled aliphatic amido Mn(I) pincer complexes for CO₂ hydrogenation reaction.



S2. Figure S2. The calculated reaction free energies (ΔG in kcal/mol) for the formation of different intermediates from **1** for Mn-NNN.



S2. Figure S3. The calculated reaction free energies (ΔG in kcal/mol) for heterolytic H₂ cleavage for Mn-NNN.

S3. Table S1. Reaction free energy (ΔG), free energy barrier (ΔG^\ddagger), and total free energy barrier ($\Delta\Delta G^{\ddagger H_2}$) for heterolytic H₂ cleavage. Here, all energies are in kcal/mol.

Complexes	H ₂ cleavage			
	ΔG	ΔG^\ddagger	ΔG	$\Delta\Delta G^{\ddagger H_2}$
	1→2	2→TS1	2→3	
Mn1-PNN-Ar	14.6	10.7	1.4	25.3
Mn1-PNN-Ar₂	4.3	22.0	19.1	26.3
Mn1-NNN-Ar	14.1	9.9	0.4	24.0
Mn1-NNN-Ar₂	7.2	18.5	15.2	25.7

S4. Molecular orbitals

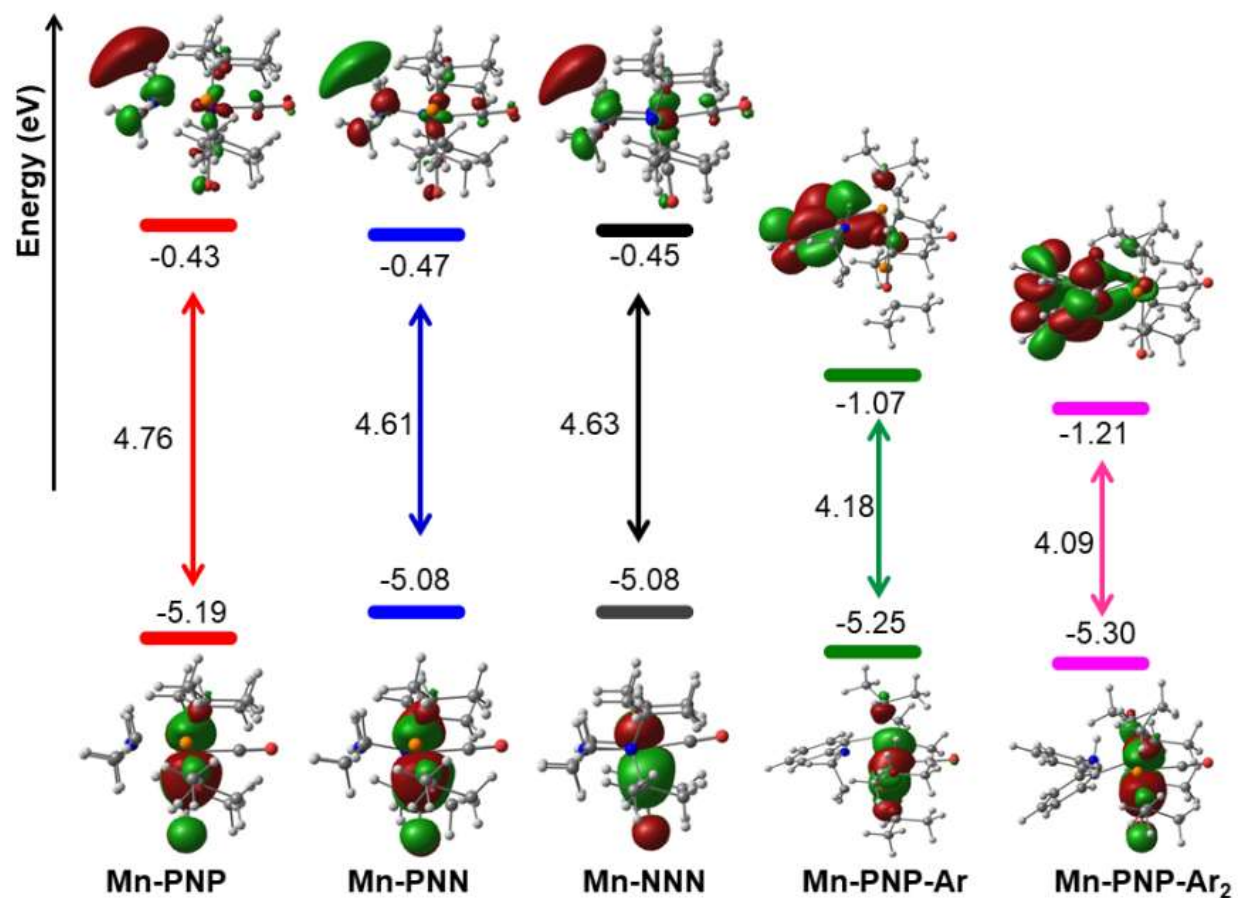


Figure S4: Molecular orbitals of the intermediates **3**.

S5. pK_a Value Calculations:

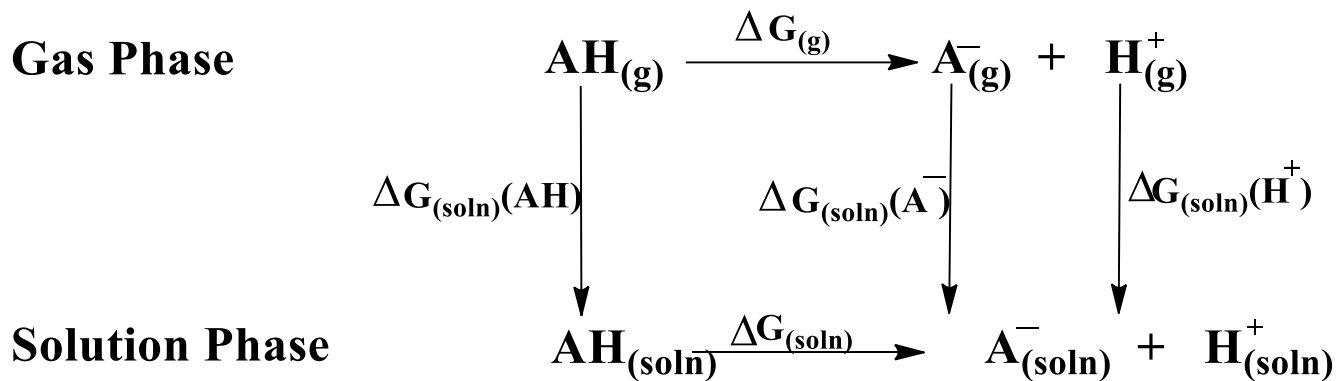


Figure S5. Thermodynamic cycle used for the calculation of pK_a value.

Where free energy of proton in gas phase and absolute solvation energy is taken as 6.3 kcal/mol¹ and -223.3 kcal/mol² respectively. The energy required to transfer a proton from gas phase to 1M solution phase in standard state is 1.89 kcal/mol.³ Direct pK_a values are calculated using above thermodynamic cycle in acetonitrile solution, computed as:

$$\text{Direct } pK_a = \frac{\Delta G_{(s)}}{2.303RT} \quad (1)$$

$$\Delta G_{(s)} = G_{(g)} + G_{(s)}(\text{A}^{-}) + \Delta G_{(s)}(\text{H}^{+}) - \Delta G_{(s)}(\text{AH}) + 1.89 \quad (2)$$

Linear correction has been taken from reference 4:

$$\text{Linear correction pKa} = (\text{Direct pKa} + 7.281)/1.194 \quad (3)$$

S6. References

Gaussian full reference (reference number 35 in the manuscript)

20. 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.

1. Tawa G J, Topol I A, Burt S K, Caldwell R A and Rashin A 1998 *J. Chem. Phys.* **109** 4852
2. Bakhouché K, Dhaouad Z, Jaidane N and Hammoutene D 2015 *Comput. Theor. Chem.* **1060** 58
3. Pratt L M, Merry S, Nguyen S C, Quan P and Thanh B T A 2006 *Tetrahedron* **62** 10821
4. Keith J A, Grice K A, Kubiak C P and Carter E A 2013 *J. Am. Chem. Soc.* **135** 15823

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

H₂

1	-4.714260000	-1.222621000	-0.059434000
1	-5.029549000	-0.597102000	-0.312102000

-1.178427

CO₂

6	0.000000000	0.000000000	0.000000000
8	0.000000000	0.000000000	1.160837000
8	0.000000000	0.000000000	-1.160837000

-188.657811

HCOOH

6	0.134348000	0.399177000	-0.000107000
8	-1.116588000	-0.088908000	0.000229000
8	1.136688000	-0.265045000	0.000084000
1	0.105571000	1.496079000	-0.000538000
1	-1.072452000	-1.059517000	-0.001325000

-189.823583

1-Mn-PNN

25	0.173784000	0.002863000	0.032401000
7	2.467498000	0.190067000	-0.321566000
15	-2.102062000	0.271360000	-0.188957000
7	0.192536000	1.829392000	-0.455802000
6	2.457515000	1.472043000	-1.094265000
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1	-1.932929000	-1.616397000	2.076109000
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6	-2.937971000	-0.574223000	-1.648563000
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6	0.964007000	2.728356000	-0.135453000
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6	2.235849000	2.045530000	-0.643586000

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1	-1.936226000	-1.466484000	1.800034000
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6	-0.046819000	-1.821472000	0.084819000
6	4.301314000	0.048189000	-2.136998000
1	5.122278000	-0.078624000	-1.430625000
1	4.183566000	1.115872000	-2.330375000
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6	4.619708000	0.396638000	1.251491000
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1	5.045042000	0.494591000	2.255415000

1	4.817861000	1.327647000	0.716325000
1	2.651786000	0.844842000	1.982095000
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1	-2.240152000	-0.669356000	-2.122431000
8	0.107140000	-2.969128000	0.199984000
1	-0.162633000	-0.017639000	-1.803390000
1	-0.153535000	0.897488000	-1.522838000

-1413.928461

3-Mn-PNN

25	-0.140442000	-0.066827000	-0.036021000
7	-2.511948000	0.210510000	-0.287657000
15	2.106218000	0.231585000	-0.206876000
7	-0.178232000	2.006249000	-0.551625000
6	-2.542683000	1.614921000	-0.790071000
1	-3.530585000	2.070643000	-0.677319000
1	-2.334621000	1.579385000	-1.861631000
6	-1.495210000	2.519710000	-0.161723000
1	-1.550291000	2.518187000	0.928206000
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1	0.917830000	2.716049000	1.071324000
6	2.253391000	2.073375000	-0.519085000
1	2.342666000	2.224077000	-1.598794000
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6	2.903378000	-1.375965000	1.991361000
1	3.387666000	-1.406169000	2.972483000
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6	2.984103000	-0.519410000	-1.687822000
6	3.141112000	-2.039569000	-1.540199000
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1	3.907576000	-2.286622000	-0.800846000
1	2.209876000	-2.522988000	-1.243295000
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6	-3.129944000	-2.163855000	-1.016547000

1	-3.194788000	-2.754555000	-1.934307000
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1	4.870244000	1.215025000	0.699963000
1	2.707408000	0.750688000	1.997215000
1	-2.757258000	0.966280000	1.604368000
1	2.226919000	-0.336364000	-2.458205000
1	-2.219905000	-0.610475000	-2.134628000
8	0.112832000	-2.971470000	0.219427000
1	-0.110340000	-0.341493000	-1.640820000
1	-0.122803000	2.021228000	-1.567522000

-1413.964414

TS2-Mn-PNN

7	-2.447892000	-0.326390000	0.194389000
7	-0.234503000	0.418893000	1.912555000

6	0.817056000	-0.207878000	2.745118000
6	-1.605583000	0.325010000	2.469967000
6	-2.450567000	-0.636993000	1.654248000
1	-3.463177000	-0.660957000	2.072431000
1	-2.026065000	-1.629207000	1.776934000
6	2.184903000	0.124979000	2.146407000
1	2.967660000	-0.466569000	2.622978000
15	2.130883000	-0.153805000	0.291515000
6	0.046465000	-0.433022000	-1.863741000
8	0.198725000	-0.459115000	-3.016321000
25	-0.120213000	-0.288775000	-0.113527000
6	-0.048431000	-2.043393000	0.162107000
8	0.047235000	-3.202784000	0.264110000
6	-3.282704000	-1.360700000	-0.571335000
1	-4.272074000	-0.914313000	-0.706884000
6	-2.723820000	-1.685182000	-1.959587000
1	-3.476000000	-2.251270000	-2.517566000
1	-2.471297000	-0.803000000	-2.537106000
1	-1.827055000	-2.298643000	-1.874787000
6	-3.511579000	-2.692644000	0.161630000
1	-4.056346000	-2.587019000	1.100056000
1	-4.115896000	-3.327835000	-0.490757000
1	-2.574457000	-3.219389000	0.349721000
6	3.140260000	-1.726235000	0.088899000
1	2.590359000	-2.435206000	0.716808000
6	3.088596000	-2.238707000	-1.357704000
1	3.530417000	-3.238084000	-1.415452000
1	2.066178000	-2.298033000	-1.731165000
1	3.659174000	-1.588992000	-2.027236000
6	4.589200000	-1.661570000	0.592486000
1	5.019542000	-2.668138000	0.595792000
1	5.215473000	-1.047156000	-0.059579000
1	4.671903000	-1.266754000	1.607719000
1	0.763097000	0.152357000	3.781194000
1	0.638687000	-1.284737000	2.751992000
1	2.409724000	1.174990000	2.338251000
1	-2.041010000	1.324642000	2.490086000
1	-1.579015000	-0.027957000	3.505889000
6	3.230169000	1.171832000	-0.484855000
1	4.243855000	0.763168000	-0.484171000

6	3.263321000	2.495686000	0.291659000
1	3.792474000	3.250312000	-0.298173000
1	2.261469000	2.881716000	0.491336000
1	3.785585000	2.402567000	1.246282000
6	2.803787000	1.407430000	-1.942769000
1	3.507327000	2.093643000	-2.424991000
1	2.781051000	0.485452000	-2.525117000
1	1.806659000	1.847120000	-1.988300000
6	-3.001840000	1.070180000	-0.031720000
1	-2.285260000	1.721697000	0.460546000
6	-4.380625000	1.339345000	0.598578000
1	-4.666258000	2.371385000	0.380254000
1	-5.161510000	0.693046000	0.190496000
1	-4.380809000	1.227873000	1.684148000
6	-3.009611000	1.477164000	-1.505019000
1	-3.213091000	2.549041000	-1.570288000
1	-2.039890000	1.291688000	-1.961968000
1	-3.787137000	0.961687000	-2.072936000
1	-0.014767000	1.407822000	1.828342000
1	-0.139737000	1.319939000	-0.492426000
6	-0.228499000	3.222956000	-0.299594000
8	-0.164349000	3.518122000	-1.429681000
8	-0.309601000	3.304092000	0.873870000

-1602.609195

4-Mn-PNN

25	-0.140442000	-0.066827000	-0.036021000
7	-2.511948000	0.210510000	-0.287657000
15	2.106218000	0.231585000	-0.206876000
7	-0.178232000	2.006249000	-0.551625000
6	-2.542683000	1.614921000	-0.790071000
1	-3.530585000	2.070643000	-0.677319000
1	-2.334621000	1.579385000	-1.861631000
6	-1.495210000	2.519710000	-0.161723000
1	-1.550291000	2.518187000	0.928206000
1	-1.652468000	3.551668000	-0.506088000
6	0.978336000	2.751286000	-0.018714000
1	0.946459000	3.805226000	-0.326204000
1	0.917830000	2.716049000	1.071324000

6	2.253391000	2.073375000	-0.519085000
1	2.342666000	2.224077000	-1.598794000
1	3.141355000	2.505390000	-0.054277000
6	3.148186000	-0.007145000	1.337130000
6	2.903378000	-1.375965000	1.991361000
1	3.387666000	-1.406169000	2.972483000
1	1.841183000	-1.570521000	2.131894000
1	3.319629000	-2.188791000	1.392031000
6	2.984103000	-0.519410000	-1.687822000
6	3.141112000	-2.039569000	-1.540199000
1	3.457589000	-2.472814000	-2.494381000
1	3.907576000	-2.286622000	-0.800846000
1	2.209876000	-2.522988000	-1.243295000
6	-3.023447000	-0.689542000	-1.401085000
6	-3.129944000	-2.163855000	-1.016547000
1	-3.194788000	-2.754555000	-1.934307000
1	-2.263870000	-2.505530000	-0.459405000
1	-4.030130000	-2.370494000	-0.434491000
6	-3.226902000	0.153457000	1.048796000
6	-2.977523000	-1.117063000	1.874980000
1	-3.160179000	-0.882928000	2.927247000
1	-3.648851000	-1.930122000	1.600480000
1	-1.952867000	-1.463513000	1.780189000
6	-0.109060000	0.248383000	1.719754000
8	-0.027553000	0.410075000	2.873985000
6	-0.026068000	-1.815640000	0.133890000
6	4.302112000	0.128089000	-2.139349000
1	5.125583000	-0.106640000	-1.464488000
1	4.235678000	1.214781000	-2.223961000
1	4.570597000	-0.259817000	-3.127822000
6	-4.335201000	-0.263819000	-2.096419000
1	-4.457415000	-0.889084000	-2.985447000
1	-4.333696000	0.773383000	-2.434077000
1	-5.213083000	-0.416458000	-1.468700000
6	-4.741925000	0.435196000	1.028420000
1	-5.072818000	0.616643000	2.054832000
1	-5.303166000	-0.422000000	0.653038000
1	-5.016728000	1.310294000	0.437656000
6	4.651748000	0.277441000	1.216225000
1	5.162887000	-0.528281000	0.684269000

1	5.095082000	0.338357000	2.215602000
1	4.870244000	1.215025000	0.699963000
1	2.707408000	0.750688000	1.997215000
1	-2.757258000	0.966280000	1.604368000
1	2.226919000	-0.336364000	-2.458205000
1	-2.219905000	-0.610475000	-2.134628000
8	0.112832000	-2.971470000	0.219427000
1	-0.110340000	-0.341493000	-1.640820000
1	-0.122803000	2.021228000	-1.567522000

-1602.621748

TS3-Mn-PNN

7	2.434916000	-0.479997000	-0.117990000
7	0.347422000	0.687328000	-1.568423000
6	-0.768230000	0.719773000	-2.521267000
6	1.634824000	0.537506000	-2.254951000
6	2.461057000	-0.548645000	-1.602922000
1	3.478697000	-0.540732000	-2.002810000
1	2.024069000	-1.506195000	-1.875293000
6	-2.062600000	1.030293000	-1.790236000
1	-2.928740000	0.847574000	-2.425673000
15	-2.116735000	0.011594000	-0.242733000
6	-0.162451000	-0.847370000	1.804913000
8	-0.478070000	-1.091137000	2.887144000
25	0.130120000	-0.417050000	0.083796000
6	-0.059577000	-2.088756000	-0.431367000
8	-0.154955000	-3.168248000	-0.830983000
6	3.300559000	-1.588719000	0.442867000
1	4.288868000	-1.157020000	0.617973000
6	2.798516000	-2.164076000	1.760979000
1	3.574514000	-2.808961000	2.179265000
1	2.565108000	-1.407848000	2.501533000
1	1.909654000	-2.774027000	1.598583000
6	3.504490000	-2.754542000	-0.522546000
1	4.002940000	-2.468191000	-1.447341000
1	4.141647000	-3.485973000	-0.023606000
1	2.566008000	-3.252792000	-0.766797000
6	-3.172897000	-1.452053000	-0.737596000
1	-2.639515000	-1.818504000	-1.621239000

6	-3.191500000	-2.586900000	0.292467000
1	-3.488657000	-3.516913000	-0.196481000
1	-2.223202000	-2.755073000	0.759259000
1	-3.910927000	-2.393474000	1.086694000
6	-4.595513000	-1.085721000	-1.156248000
1	-5.099406000	-1.973621000	-1.544809000
1	-5.180353000	-0.723735000	-0.308604000
1	-4.626471000	-0.324914000	-1.936331000
1	-0.595826000	1.486911000	-3.286849000
1	-0.845688000	-0.239782000	-3.048211000
1	-2.081992000	2.081119000	-1.497354000
1	2.169299000	1.493639000	-2.274609000
1	1.497463000	0.265146000	-3.305415000
6	-3.172529000	1.038609000	0.901966000
1	-4.023407000	1.366514000	0.296077000
6	-2.403120000	2.268055000	1.372203000
1	-3.061682000	2.913663000	1.956771000
1	-1.560416000	1.984430000	2.008944000
1	-2.018437000	2.862162000	0.545329000
6	-3.704573000	0.258630000	2.104739000
1	-4.207934000	0.950011000	2.784205000
1	-4.429649000	-0.501724000	1.822460000
1	-2.901925000	-0.225278000	2.663032000
6	2.916197000	0.868073000	0.368387000
1	2.219562000	1.582771000	-0.060512000
6	4.315950000	1.283005000	-0.102695000
1	4.522896000	2.280548000	0.287754000
1	5.096935000	0.619953000	0.271987000
1	4.407670000	1.340190000	-1.185734000
6	2.829795000	1.034103000	1.879193000
1	2.971944000	2.089137000	2.117253000
1	1.858593000	0.734476000	2.273436000
1	3.609523000	0.475120000	2.398954000
1	0.362299000	2.016592000	-1.184831000
1	0.511963000	2.582274000	0.890030000
6	0.448406000	3.474917000	0.225924000
8	0.485655000	4.582699000	0.727465000
8	0.343046000	3.217496000	-1.023491000

-1602.608019

5-Mn-PNN

7	2.371933000	-0.556706000	-0.167036000
7	0.313294000	0.578708000	-1.605151000
6	-0.807041000	0.816119000	-2.532791000
6	1.582262000	0.421414000	-2.326551000
6	2.415069000	-0.662071000	-1.658517000
1	3.440940000	-0.652291000	-2.040375000
1	1.970510000	-1.617455000	-1.922829000
6	-2.070706000	1.159204000	-1.747145000
1	-2.967638000	1.074890000	-2.362259000
15	-2.137873000	0.056064000	-0.252058000
6	-0.105382000	-0.686766000	1.788563000
8	-0.324989000	-0.809787000	2.922481000
25	0.109920000	-0.444123000	0.029774000
6	-0.104584000	-2.148968000	-0.293581000
8	-0.216483000	-3.268280000	-0.589811000
6	3.152301000	-1.703265000	0.486927000
1	4.154697000	-1.312907000	0.681270000
6	2.566411000	-2.163012000	1.825751000
1	3.291797000	-2.820109000	2.314340000
1	2.348142000	-1.347287000	2.506732000
1	1.648057000	-2.729698000	1.672102000
6	3.336339000	-2.945526000	-0.398003000
1	3.901817000	-2.749691000	-1.308972000
1	3.900006000	-3.682106000	0.179620000
1	2.381002000	-3.401241000	-0.663095000
6	-3.260046000	-1.349159000	-0.786378000
1	-2.728216000	-1.716400000	-1.672339000
6	-3.329923000	-2.504926000	0.229315000
1	-3.633992000	-3.422318000	-0.282511000
1	-2.375664000	-2.698372000	0.716859000
1	-4.068042000	-2.305667000	1.007034000
6	-4.670721000	-0.914998000	-1.210561000
1	-5.220369000	-1.781228000	-1.591789000
1	-5.236623000	-0.515935000	-0.364762000
1	-4.663571000	-0.160089000	-1.998999000
1	-0.571352000	1.639094000	-3.222836000
1	-0.973905000	-0.076329000	-3.153534000
1	-2.012169000	2.188325000	-1.388496000

1	2.126426000	1.375037000	-2.388351000
1	1.410669000	0.106097000	-3.363461000
6	-3.115734000	1.083731000	0.977646000
1	-3.974840000	1.468499000	0.416358000
6	-2.278379000	2.275661000	1.462002000
1	-2.873271000	2.893118000	2.141136000
1	-1.396269000	1.935944000	2.010199000
1	-1.948880000	2.919371000	0.645503000
6	-3.631671000	0.274640000	2.177327000
1	-4.102264000	0.953704000	2.894963000
1	-4.381057000	-0.462427000	1.890605000
1	-2.820715000	-0.241863000	2.694696000
6	2.955228000	0.785977000	0.249191000
1	2.304535000	1.514121000	-0.225766000
6	4.377548000	1.074734000	-0.264243000
1	4.652096000	2.087132000	0.041666000
1	5.121558000	0.394372000	0.156362000
1	4.450788000	1.035712000	-1.351305000
6	2.885272000	1.042514000	1.755024000
1	3.115729000	2.093939000	1.941723000
1	1.891076000	0.839413000	2.152098000
1	3.611697000	0.444403000	2.308220000
1	0.426961000	2.145824000	-1.079907000
1	0.661930000	2.647095000	0.986707000
6	0.670792000	3.505579000	0.293734000
8	0.809048000	4.642252000	0.680810000
8	0.514885000	3.170832000	-0.976112000

-1602.611814

1-Mn-NNN

25	-0.000227000	-0.019142000	0.019928000
7	2.329385000	0.245614000	-0.306627000
7	-2.328900000	0.244694000	-0.307660000
7	-0.000194000	1.752536000	-0.550292000
6	2.305342000	1.575523000	-1.002825000
1	3.288165000	2.053050000	-0.994846000
1	2.036519000	1.380492000	-2.040770000
6	1.228807000	2.496464000	-0.462678000
1	1.452579000	2.838163000	0.562818000

1	1.207498000	3.402015000	-1.090854000
6	-1.229950000	2.495712000	-0.468181000
1	-1.207626000	3.399282000	-1.099183000
1	-1.456846000	2.840685000	0.555561000
6	-2.304277000	1.572170000	-1.008247000
1	-2.032537000	1.373657000	-2.044807000
1	-3.287511000	2.048888000	-1.004390000
6	-3.061174000	0.397247000	1.012983000
6	-2.912875000	-0.781485000	1.990662000
1	-2.972450000	-0.395132000	3.010888000
1	-1.957064000	-1.285550000	1.881964000
1	-3.707424000	-1.518146000	1.872067000
6	-2.858257000	-0.787542000	-1.293828000
6	-3.170099000	-2.158283000	-0.689759000
1	-3.254487000	-2.879223000	-1.507029000
1	-4.124892000	-2.154839000	-0.160823000
1	-2.399230000	-2.513849000	-0.016011000
6	2.857959000	-0.783654000	-1.296246000
6	3.167999000	-2.156936000	-0.697047000
1	3.251492000	-2.875079000	-1.516876000
1	2.396575000	-2.513817000	-0.024645000
1	4.122753000	-2.156763000	-0.168016000
6	3.062199000	0.393480000	1.014208000
6	2.912677000	-0.787764000	1.988651000
1	2.974664000	-0.404524000	3.009918000
1	3.705407000	-1.525831000	1.866698000
1	1.955621000	-1.289456000	1.879987000
6	0.000275000	0.128153000	1.761046000
8	0.001164000	0.370917000	2.899157000
6	-0.000480000	-1.817757000	0.028829000
6	-4.071506000	-0.357548000	-2.148441000
1	-4.972208000	-0.223426000	-1.549063000
1	-3.901831000	0.554692000	-2.719595000
1	-4.273199000	-1.154763000	-2.869150000
6	4.071953000	-0.352042000	-2.149000000
1	4.272393000	-1.146575000	-2.873010000
1	3.903806000	0.562869000	-2.716309000
1	4.972821000	-0.221846000	-1.549032000
6	4.554495000	0.764284000	0.928849000
1	4.898467000	1.034833000	1.931063000

1	5.158198000	-0.081893000	0.595763000
1	4.757431000	1.612547000	0.274597000
6	-4.552904000	0.770058000	0.926976000
1	-5.157838000	-0.075761000	0.595211000
1	-4.896511000	1.042731000	1.928738000
1	-4.754452000	1.617661000	0.271411000
1	-2.541664000	1.242667000	1.467515000
1	2.544043000	1.238432000	1.471222000
1	-2.012538000	-0.914618000	-1.977162000
1	2.012280000	-0.907385000	-1.980262000
8	-0.000898000	-2.981670000	0.071410000

-1126.117318

2-Mn-NNN

25	-0.000025000	-0.070832000	-0.094396000
7	-2.353735000	0.269085000	-0.285148000
7	2.353861000	0.269196000	-0.285017000
7	0.000104000	1.886674000	-0.519865000
6	-2.351463000	1.716962000	-0.700601000
1	-3.318418000	2.185986000	-0.503141000
1	-2.187285000	1.739337000	-1.778549000
6	-1.214404000	2.510800000	-0.082431000
1	-1.322447000	2.564402000	1.021184000
1	-1.299161000	3.552890000	-0.441587000
6	1.214380000	2.510805000	-0.081827000
1	1.299152000	3.553005000	-0.440654000
1	1.322057000	2.564085000	1.021839000
6	2.351715000	1.717274000	-0.699901000
1	2.187919000	1.740094000	-1.777896000
1	3.318587000	2.186213000	-0.501875000
6	3.045881000	0.163190000	1.065000000
6	2.836704000	-1.154883000	1.822969000
1	3.057761000	-0.977965000	2.878975000
1	1.816179000	-1.516197000	1.754026000
1	3.503844000	-1.944136000	1.478775000
6	2.938105000	-0.540448000	-1.431836000
6	3.073430000	-2.036845000	-1.149780000
1	3.185208000	-2.560504000	-2.102964000
1	3.960771000	-2.257946000	-0.554299000

1	2.204685000	-2.443183000	-0.642123000
6	-2.938101000	-0.540908000	-1.431657000
6	-3.073882000	-2.037132000	-1.148922000
1	-3.185689000	-2.561229000	-2.101858000
1	-2.205302000	-2.443454000	-0.640976000
1	-3.961354000	-2.257687000	-0.553433000
6	-3.045740000	0.163680000	1.064909000
6	-2.836824000	-1.154175000	1.823359000
1	-3.057289000	-0.976708000	2.879396000
1	-3.504515000	-1.943251000	1.479817000
1	-1.816501000	-1.516007000	1.754099000
6	0.000099000	0.229043000	1.653664000
8	0.000062000	0.448047000	2.789289000
6	-0.000130000	-1.841512000	0.160312000
6	4.260970000	-0.030958000	-2.043833000
1	5.119919000	-0.228308000	-1.403979000
1	4.245890000	1.032582000	-2.280499000
1	4.423195000	-0.568793000	-2.982440000
6	-4.260739000	-0.031270000	-2.043988000
1	-4.423259000	-0.569791000	-2.982151000
1	-4.245130000	1.032072000	-2.281538000
1	-5.119763000	-0.227679000	-1.403945000
6	-4.550565000	0.496057000	1.091808000
1	-4.846370000	0.656901000	2.132108000
1	-5.150773000	-0.330918000	0.708497000
1	-4.810592000	1.396914000	0.536056000
6	4.550790000	0.495218000	1.091968000
1	5.150797000	-0.331854000	0.708548000
1	4.846642000	0.655868000	2.132285000
1	4.811053000	1.396062000	0.536308000
1	2.539692000	0.935546000	1.645622000
1	-2.539386000	0.936135000	1.645243000
1	2.181146000	-0.427624000	-2.209921000
1	-2.181058000	-0.428659000	-2.209741000
8	-0.000373000	-2.980788000	0.400076000
1	0.000008000	-0.570434000	-1.894384000
1	-0.000072000	0.202884000	-1.904904000

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TS1-Mn-NNN

25	0.003912000	0.078705000	-0.083451000
7	2.348148000	-0.258262000	-0.271059000
7	-2.352169000	-0.254719000	-0.269344000
7	-0.000603000	-1.879718000	-0.563632000
6	2.345331000	-1.680770000	-0.757128000
1	3.314326000	-2.161215000	-0.601034000
1	2.170398000	-1.653530000	-1.833212000
6	1.221841000	-2.511433000	-0.165162000
1	1.320892000	-2.603473000	0.935177000
1	1.313706000	-3.535159000	-0.569374000
6	-1.223854000	-2.508642000	-0.162939000
1	-1.317733000	-3.532354000	-0.566725000
1	-1.321171000	-2.600374000	0.937577000
6	-2.348134000	-1.677871000	-0.753681000
1	-2.174903000	-1.651563000	-1.830061000
1	-3.316722000	-2.158529000	-0.595761000
6	-3.051049000	-0.217734000	1.077863000
6	-2.874763000	1.076201000	1.886207000
1	-3.064760000	0.848699000	2.938461000
1	-1.869669000	1.480065000	1.810299000
1	-3.579457000	1.851257000	1.589129000
6	-2.939259000	0.602145000	-1.385082000
6	-3.149437000	2.072783000	-1.023742000
1	-3.266474000	2.640969000	-1.950410000
1	-4.058701000	2.220372000	-0.438466000
1	-2.311738000	2.493272000	-0.478436000
6	2.931602000	0.601740000	-1.386216000
6	3.138103000	2.072337000	-1.022615000
1	3.252387000	2.642459000	-1.948438000
1	2.299808000	2.489454000	-0.475546000
1	4.047649000	2.221506000	-0.438174000
6	3.048166000	-0.221713000	1.075505000
6	2.869323000	1.070607000	1.885833000
1	3.060854000	0.842116000	2.937597000
1	3.571732000	1.847912000	1.589214000
1	1.863084000	1.471935000	1.811370000
6	0.006623000	-0.179416000	1.681552000
8	0.008365000	-0.372300000	2.822447000
6	0.009951000	1.858275000	0.066322000

6	-4.226772000	0.079726000	-2.058727000
1	-5.104925000	0.194570000	-1.423996000
1	-4.163855000	-0.961849000	-2.371426000
1	-4.395734000	0.676155000	-2.959937000
6	4.219603000	0.083911000	-2.062491000
1	4.385677000	0.682234000	-2.962985000
1	4.159119000	-0.957327000	-2.376767000
1	5.098322000	0.200164000	-1.428806000
6	4.545086000	-0.586178000	1.076680000
1	4.848777000	-0.781614000	2.108772000
1	5.158415000	0.237738000	0.707712000
1	4.779015000	-1.477616000	0.494291000
6	-4.547101000	-0.585708000	1.080788000
1	-5.162668000	0.236220000	0.711112000
1	-4.849478000	-0.780333000	2.113417000
1	-4.779404000	-1.478547000	0.499900000
1	-2.530517000	-1.000879000	1.631278000
1	2.529899000	-1.006866000	1.628218000
1	-2.151674000	0.569552000	-2.140502000
1	2.143041000	0.568346000	-2.140604000
8	0.014560000	3.013810000	0.194965000
1	0.001983000	0.165072000	-1.890855000
1	0.000108000	-0.679212000	-1.664583000

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3-Mn-NNN

25	-0.000119000	0.103719000	-0.084818000
7	2.395611000	-0.274225000	-0.262893000
7	-2.395403000	-0.274062000	-0.262878000
7	-0.000012000	-1.939743000	-0.545612000
6	2.380664000	-1.711669000	-0.671005000
1	3.335930000	-2.204764000	-0.471357000
1	2.235664000	-1.742571000	-1.752921000
6	1.250886000	-2.518244000	-0.051413000
1	1.250932000	-2.460508000	1.038114000
1	1.358161000	-3.574559000	-0.335686000
6	-1.250966000	-2.518170000	-0.051494000
1	-1.358336000	-3.574467000	-0.335808000
1	-1.251059000	-2.460493000	1.038040000

6	-2.380602000	-1.711450000	-0.671141000
1	-2.235446000	-1.742210000	-1.753040000
1	-3.335957000	-2.204453000	-0.471677000
6	-3.092791000	-0.160952000	1.078723000
6	-2.878627000	1.166036000	1.819788000
1	-3.069543000	0.998983000	2.883280000
1	-1.861288000	1.529399000	1.714862000
1	-3.562632000	1.944012000	1.483209000
6	-2.958524000	0.528915000	-1.425378000
6	-3.118891000	2.021525000	-1.142364000
1	-3.219933000	2.542679000	-2.098222000
1	-4.019310000	2.233258000	-0.562298000
1	-2.261488000	2.437816000	-0.624945000
6	2.958715000	0.528725000	-1.425425000
6	3.118785000	2.021375000	-1.142450000
1	3.219799000	2.542528000	-2.098312000
1	2.261268000	2.437504000	-0.625086000
1	4.019124000	2.233307000	-0.562323000
6	3.092861000	-0.160872000	1.078772000
6	2.878520000	1.166242000	1.819538000
1	3.069716000	0.999532000	2.883036000
1	3.562246000	1.944308000	1.482590000
1	1.861068000	1.529311000	1.714718000
6	-0.000118000	-0.168229000	1.686913000
8	-0.000081000	-0.287178000	2.847274000
6	-0.000040000	1.858455000	0.056291000
6	-4.263621000	0.006716000	-2.064788000
1	-5.137691000	0.185195000	-1.438655000
1	-4.235167000	-1.054423000	-2.314984000
1	-4.417158000	0.551473000	-3.000853000
6	4.263962000	0.006712000	-2.064672000
1	4.417388000	0.551284000	-3.000862000
1	4.235831000	-1.054495000	-2.314605000
1	5.137955000	0.185599000	-1.438548000
6	4.597814000	-0.492942000	1.099161000
1	4.907028000	-0.629013000	2.139215000
1	5.192369000	0.324273000	0.687632000
1	4.853067000	-1.407104000	0.561317000
6	-4.597704000	-0.493230000	1.098891000
1	-5.192342000	0.323953000	0.687420000

1	-4.907001000	-0.629492000	2.138895000
1	-4.852758000	-1.407368000	0.560904000
1	-2.587459000	-0.922932000	1.674818000
1	2.587561000	-0.922792000	1.674978000
1	-2.161854000	0.430735000	-2.164794000
1	2.162114000	0.430365000	-2.164894000
8	-0.000046000	3.022588000	0.138186000
1	-0.000150000	0.364457000	-1.703682000
1	0.000051000	-2.002023000	-1.560720000

-1127.294638

TS2-Mn-NNN

7	2.300512000	-0.462026000	-0.181787000
7	0.133902000	0.388167000	-1.857387000
6	-1.087202000	-0.051888000	-2.548314000
6	1.421327000	0.020162000	-2.494278000
6	2.233599000	-0.911759000	-1.604169000
1	3.228214000	-1.034235000	-2.045588000
1	1.754068000	-1.885291000	-1.614976000
6	-2.281555000	0.516129000	-1.793216000
1	-3.196317000	0.324617000	-2.360738000
7	-2.405594000	0.032251000	-0.380307000
6	-0.216333000	-0.204150000	1.905205000
8	-0.363464000	-0.111002000	3.055703000
25	-0.034934000	-0.201701000	0.149841000
6	-0.138370000	-1.972591000	-0.050454000
8	-0.142134000	-3.136491000	-0.117299000
6	3.084847000	-1.468263000	0.673238000
1	4.083635000	-1.043320000	0.799967000
6	2.486445000	-1.659313000	2.068899000
1	3.197934000	-2.217522000	2.685156000
1	2.274337000	-0.719240000	2.567914000
1	1.558471000	-2.228603000	2.017011000
6	3.297874000	-2.854522000	0.044288000
1	3.850463000	-2.822072000	-0.895233000
1	3.891636000	-3.445754000	0.746007000
1	2.357266000	-3.383648000	-0.113409000
6	-3.068687000	-1.343550000	-0.439198000
1	-2.475023000	-1.863514000	-1.190087000

6	-2.971901000	-2.185903000	0.848943000
1	-2.813744000	-3.230375000	0.573635000
1	-2.138238000	-1.880550000	1.474272000
1	-3.884140000	-2.136747000	1.442330000
6	-4.528521000	-1.354087000	-0.933806000
1	-4.839495000	-2.396268000	-1.044535000
1	-5.208560000	-0.886162000	-0.219732000
1	-4.668109000	-0.872488000	-1.902531000
1	-1.121928000	0.314245000	-3.583972000
1	-1.093790000	-1.142096000	-2.576999000
1	-2.159810000	1.596959000	-1.772298000
1	1.972739000	0.935306000	-2.718008000
1	1.245531000	-0.482584000	-3.449851000
6	-3.248434000	1.046707000	0.376974000
1	-4.147827000	1.224355000	-0.229936000
6	-2.540966000	2.391096000	0.570593000
1	-3.259866000	3.105099000	0.980703000
1	-1.717470000	2.279211000	1.272625000
1	-2.148977000	2.822595000	-0.349172000
6	-3.700322000	0.576397000	1.764060000
1	-4.166946000	1.421132000	2.276022000
1	-4.435991000	-0.222618000	1.733420000
1	-2.851264000	0.251731000	2.364797000
6	2.961419000	0.901333000	-0.104704000
1	2.282852000	1.559260000	-0.640538000
6	4.336160000	1.002098000	-0.792718000
1	5.078687000	0.337747000	-0.343468000
1	4.291900000	0.787652000	-1.861938000
1	4.704780000	2.024907000	-0.682532000
6	3.046684000	1.432567000	1.326667000
1	3.329563000	2.487351000	1.294662000
1	2.081226000	1.360231000	1.822780000
1	3.801421000	0.908664000	1.917362000
1	0.103194000	1.402247000	-1.802405000
1	0.172048000	1.426404000	0.438537000
6	0.488678000	3.285044000	0.108081000
8	0.582156000	3.662023000	1.211840000
8	0.459777000	3.293482000	-1.072176000

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4-Mn-NNN

7	2.286817000	-0.406093000	-0.184356000
7	0.157828000	0.485738000	-1.805747000
6	-1.095013000	0.233214000	-2.536589000
6	1.412500000	0.099482000	-2.493717000
6	2.240226000	-0.833039000	-1.618650000
1	3.241233000	-0.931108000	-2.047020000
1	1.780617000	-1.815928000	-1.650334000
6	-2.229636000	0.762297000	-1.672109000
1	-3.172226000	0.727266000	-2.222901000
7	-2.351582000	0.071926000	-0.341877000
6	-0.234620000	-0.317235000	1.904142000
8	-0.412548000	-0.355455000	3.044474000
25	-0.027831000	-0.188810000	0.128333000
6	-0.097031000	-1.939073000	-0.081883000
8	-0.075655000	-3.088385000	-0.224726000
6	3.089476000	-1.418766000	0.655775000
1	4.075366000	-0.971311000	0.792609000
6	2.498215000	-1.651126000	2.047252000
1	3.229130000	-2.194459000	2.653005000
1	2.260521000	-0.726579000	2.563367000
1	1.593007000	-2.256549000	1.992897000
6	3.338800000	-2.785528000	-0.001054000
1	3.892950000	-2.720360000	-0.937473000
1	3.946934000	-3.373285000	0.690963000
1	2.415031000	-3.339428000	-0.172069000
6	-2.982344000	-1.300340000	-0.598528000
1	-2.340349000	-1.721208000	-1.370237000
6	-2.941547000	-2.289692000	0.584406000
1	-2.723172000	-3.287400000	0.200123000
1	-2.172182000	-2.039829000	1.308985000
1	-3.894651000	-2.343069000	1.108262000
6	-4.410624000	-1.271215000	-1.174256000
1	-4.705865000	-2.301187000	-1.390325000
1	-5.133385000	-0.868203000	-0.462576000
1	-4.496602000	-0.711021000	-2.105942000
1	-1.109760000	0.761276000	-3.498267000
1	-1.179421000	-0.835005000	-2.741978000
1	-2.015949000	1.810967000	-1.482134000

1	1.964694000	1.005738000	-2.752556000
1	1.189802000	-0.416217000	-3.431128000
6	-3.240434000	0.956996000	0.531565000
1	-4.119292000	1.199208000	-0.080797000
6	-2.571664000	2.274578000	0.926107000
1	-3.311363000	2.897699000	1.433909000
1	-1.750723000	2.102231000	1.621396000
1	-2.195073000	2.854273000	0.086504000
6	-3.739622000	0.295353000	1.820718000
1	-4.250410000	1.057546000	2.412942000
1	-4.453819000	-0.505010000	1.649986000
1	-2.915403000	-0.088679000	2.420625000
6	2.942366000	0.964666000	-0.080512000
1	2.278169000	1.634094000	-0.620279000
6	4.321984000	1.080242000	-0.753530000
1	4.679982000	2.103589000	-0.620449000
1	5.065419000	0.413543000	-0.309877000
1	4.287437000	0.887892000	-1.827074000
6	3.013609000	1.468414000	1.362076000
1	3.259816000	2.531247000	1.350204000
1	2.056557000	1.367413000	1.871081000
1	3.782738000	0.951307000	1.940147000
1	0.204186000	1.516974000	-1.661614000
1	0.193423000	1.749876000	0.466790000
6	0.346469000	2.891185000	0.199454000
8	0.491232000	3.599364000	1.186023000
8	0.324508000	3.120785000	-1.029174000

-1315.949984

TS3-Mn-NNN

7	2.173311000	-0.598901000	-0.199725000
7	0.181726000	0.889822000	-1.362901000
6	-1.022421000	1.059308000	-2.166845000
6	1.399551000	0.731986000	-2.163349000
6	2.188101000	-0.470931000	-1.682377000
1	3.208477000	-0.440450000	-2.072471000
1	1.709113000	-1.357183000	-2.089494000
6	-2.153466000	1.287219000	-1.199827000
1	-3.097779000	1.440746000	-1.721105000

7	-2.272741000	0.193289000	-0.187109000
6	-0.285636000	-1.306452000	1.619621000
8	-0.420516000	-1.797404000	2.654117000
25	-0.096247000	-0.475834000	0.040147000
6	-0.317056000	-2.022508000	-0.771931000
8	-0.428385000	-3.014212000	-1.352557000
6	3.005124000	-1.795439000	0.228277000
1	4.009751000	-1.415811000	0.426841000
6	2.507640000	-2.461220000	1.504225000
1	3.259176000	-3.183758000	1.828194000
1	2.340195000	-1.770121000	2.323862000
1	1.582707000	-3.006760000	1.315660000
6	3.152311000	-2.888521000	-0.835801000
1	3.639569000	-2.549876000	-1.748014000
1	3.776435000	-3.675423000	-0.411090000
1	2.193576000	-3.339425000	-1.094746000
6	-3.199539000	-0.836099000	-0.806459000
1	-2.750649000	-1.017545000	-1.784781000
6	-3.241200000	-2.188972000	-0.085287000
1	-3.279210000	-2.985550000	-0.830298000
1	-2.362939000	-2.357307000	0.531066000
1	-4.122361000	-2.283292000	0.547939000
6	-4.643299000	-0.372850000	-1.054983000
1	-5.119232000	-1.093293000	-1.722539000
1	-5.229503000	-0.348136000	-0.136994000
1	-4.722721000	0.602346000	-1.531925000
1	-0.950177000	1.930725000	-2.831599000
1	-1.208367000	0.186393000	-2.803627000
1	-1.931272000	2.213557000	-0.683531000
1	2.003149000	1.646382000	-2.123388000
1	1.160312000	0.565670000	-3.217416000
6	-2.808167000	0.828507000	1.072948000
1	-3.643740000	1.472713000	0.771374000
6	-1.746945000	1.701520000	1.747873000
1	-2.166069000	2.152734000	2.647501000
1	-0.884112000	1.106552000	2.056691000
1	-1.388735000	2.516164000	1.123968000
6	-3.357683000	-0.151614000	2.104294000
1	-3.671426000	0.426639000	2.973897000
1	-4.227747000	-0.697227000	1.752487000

1	-2.613434000	-0.870384000	2.435681000
6	2.721851000	0.668452000	0.407691000
1	2.031923000	1.431461000	0.067777000
6	4.102890000	1.111066000	-0.082595000
1	4.284784000	2.119809000	0.292623000
1	4.900479000	0.471625000	0.295528000
1	4.179650000	1.155718000	-1.167615000
6	2.683321000	0.688855000	1.932882000
1	2.883771000	1.708417000	2.266785000
1	1.710355000	0.397523000	2.328103000
1	3.445887000	0.046136000	2.374628000
1	0.326811000	2.115339000	-0.867606000
1	0.897010000	3.053711000	1.197757000
6	0.731492000	3.802771000	0.397670000
8	0.831794000	4.987694000	0.647729000
8	0.436510000	3.302307000	-0.758265000

-1315.944612

5-Mn-NNN

7	2.205470000	-0.551630000	-0.196450000
7	0.159298000	0.728708000	-1.480637000
6	-1.049135000	0.923144000	-2.276410000
6	1.378951000	0.573731000	-2.278384000
6	2.230041000	-0.548301000	-1.695108000
1	3.251225000	-0.500721000	-2.085224000
1	1.797948000	-1.489736000	-2.020867000
6	-2.180386000	1.215575000	-1.310555000
1	-3.125962000	1.345711000	-1.839459000
7	-2.307367000	0.179598000	-0.223587000
6	-0.260538000	-0.976547000	1.738901000
8	-0.424492000	-1.306025000	2.839563000
25	-0.066511000	-0.442891000	0.038609000
6	-0.211374000	-2.089457000	-0.529694000
8	-0.250153000	-3.165774000	-0.966412000
6	3.014878000	-1.733996000	0.358075000
1	4.004431000	-1.335226000	0.593559000
6	2.434481000	-2.322063000	1.645890000
1	3.166197000	-3.012967000	2.074442000
1	2.206362000	-1.573761000	2.397234000
1	1.523269000	-2.883291000	1.438185000

6	3.241444000	-2.890407000	-0.628180000
1	3.796871000	-2.598066000	-1.518993000
1	3.834596000	-3.650422000	-0.113756000
1	2.303725000	-3.358288000	-0.931369000
6	-3.091156000	-0.994742000	-0.810037000
1	-2.519092000	-1.230846000	-1.708040000
6	-3.117886000	-2.276852000	0.047912000
1	-3.024619000	-3.142665000	-0.610138000
1	-2.301250000	-2.317045000	0.761832000
1	-4.053052000	-2.382849000	0.596680000
6	-4.531273000	-0.672396000	-1.252370000
1	-4.955792000	-1.574053000	-1.701250000
1	-5.166125000	-0.400602000	-0.406596000
1	-4.597595000	0.118622000	-1.999447000
1	-0.958809000	1.781451000	-2.959858000
1	-1.257320000	0.044019000	-2.902451000
1	-1.957527000	2.167589000	-0.839647000
1	1.939499000	1.517991000	-2.329373000
1	1.144933000	0.304955000	-3.315818000
6	-3.011218000	0.867163000	0.940565000
1	-3.858394000	1.416978000	0.508371000
6	-2.095377000	1.891535000	1.624211000
1	-2.642450000	2.376969000	2.435062000
1	-1.219600000	1.403039000	2.055808000
1	-1.755176000	2.680345000	0.957178000
6	-3.578323000	-0.066135000	2.014296000
1	-3.971981000	0.552815000	2.823944000
1	-4.401459000	-0.677911000	1.654662000
1	-2.816160000	-0.717689000	2.436987000
6	2.779969000	0.761838000	0.310889000
1	2.125690000	1.515337000	-0.115664000
6	4.201070000	1.096930000	-0.176069000
1	4.457495000	2.096148000	0.183829000
1	4.953566000	0.407303000	0.212967000
1	4.280264000	1.115666000	-1.263377000
6	2.697350000	0.909232000	1.830406000
1	2.931077000	1.942620000	2.097169000
1	1.696945000	0.683872000	2.201098000
1	3.415069000	0.268950000	2.346527000
1	0.321250000	2.225507000	-0.965424000

1	0.709166000	2.817638000	1.091184000
6	0.674741000	3.647024000	0.363646000
8	0.846016000	4.796470000	0.702065000
8	0.431905000	3.268640000	-0.876259000

-1315.947479

1-Mn-PNP-Ar

25	-0.355429000	-0.367789000	-0.156379000
15	-2.508433000	0.352632000	-0.117009000
15	1.932546000	-0.552335000	0.060095000
7	0.041222000	1.560209000	-0.297577000
6	-2.300783000	1.927446000	-1.038909000
6	-1.003491000	2.570699000	-0.548821000
6	1.330752000	2.079913000	-0.242394000
6	2.441327000	1.189988000	-0.142927000
6	2.846016000	-1.575336000	-1.221843000
6	2.265146000	-2.996635000	-1.340816000
1	2.586961000	-3.437634000	-2.288896000
1	1.176059000	-3.003518000	-1.318895000
1	2.624274000	-3.643562000	-0.539143000
6	2.475935000	-1.034553000	1.805971000
6	2.447164000	-2.556853000	2.018575000
1	2.513886000	-2.773203000	3.089223000
1	3.302545000	-3.035867000	1.536585000
1	1.536632000	-3.021989000	1.643253000
6	-3.044223000	0.847579000	1.612305000
6	-3.507650000	-0.368803000	2.428568000
1	-3.600631000	-0.092087000	3.483039000
1	-2.807401000	-1.203727000	2.361557000
1	-4.487893000	-0.718818000	2.095273000
6	-3.866545000	-0.554248000	-1.020759000
6	-3.907569000	-2.050855000	-0.677354000
1	-4.624596000	-2.555678000	-1.331944000
1	-4.222190000	-2.224089000	0.353770000
1	-2.934176000	-2.521895000	-0.816507000
6	-0.518893000	-1.089480000	-1.742473000
8	-0.643037000	-1.493444000	-2.826368000
6	-0.705576000	-1.916314000	0.646027000
6	3.796766000	-0.444640000	2.317375000

1	4.653284000	-0.800852000	1.740205000
1	3.796853000	0.644756000	2.293331000
1	3.948069000	-0.757611000	3.355882000
6	-4.039278000	2.012183000	1.719005000
1	-4.178200000	2.271951000	2.773604000
1	-3.683791000	2.908518000	1.206846000
1	-5.018046000	1.753283000	1.312390000
6	-5.258000000	0.087749000	-0.930461000
1	-5.934824000	-0.402729000	-1.637101000
1	-5.686702000	-0.031800000	0.067333000
1	-5.242272000	1.153358000	-1.171033000
6	4.376547000	-1.633412000	-1.120289000
1	4.698969000	-2.105125000	-0.189499000
1	4.769248000	-2.237408000	-1.944827000
1	4.839953000	-0.650178000	-1.190531000
1	2.579077000	-1.029101000	-2.134110000
1	-3.516449000	-0.467911000	-2.056860000
1	1.662476000	-0.598584000	2.397703000
1	-2.087493000	1.184559000	2.030002000
8	-0.945726000	-2.920999000	1.181949000
6	3.747205000	1.678774000	-0.140268000
6	4.014933000	3.045801000	-0.216889000
6	2.939276000	3.929356000	-0.267532000
6	1.626898000	3.466922000	-0.273071000
1	5.036147000	3.407706000	-0.215199000
1	3.118307000	4.999364000	-0.299027000
1	0.831515000	4.197818000	-0.294496000
1	4.578026000	0.992072000	-0.053689000
1	-0.675256000	3.286787000	-1.310923000
1	-2.194508000	1.636785000	-2.087858000
1	-3.146643000	2.612943000	-0.958266000
1	-1.201354000	3.156145000	0.362250000

1851.897338

2-Mn-PNP-Ar

25	0.348364000	-0.381920000	-0.071156000
15	2.531465000	0.340167000	-0.001121000
15	-1.964928000	-0.547884000	-0.091331000
7	-0.071273000	1.651085000	0.154029000
6	2.289811000	1.999082000	0.770437000

6	1.010359000	2.624643000	0.209098000
6	-1.337568000	2.121672000	0.077650000
6	-2.447114000	1.204101000	0.026317000
6	-2.742695000	-1.448177000	1.370056000
6	-2.107436000	-2.825367000	1.631796000
1	-2.436892000	-3.191775000	2.609034000
1	-1.019197000	-2.789195000	1.639559000
1	-2.413286000	-3.560459000	0.885826000
6	-2.692573000	-1.230420000	-1.699450000
6	-2.544915000	-2.757741000	-1.783898000
1	-2.731378000	-3.085569000	-2.811130000
1	-3.275624000	-3.259317000	-1.145711000
1	-1.549544000	-3.100847000	-1.498681000
6	3.356516000	0.706280000	-1.646485000
6	3.341339000	-0.501455000	-2.598484000
1	3.649504000	-0.184102000	-3.599235000
1	2.351733000	-0.954763000	-2.680439000
1	4.035015000	-1.277974000	-2.271354000
6	3.719338000	-0.558209000	1.135856000
6	4.246082000	-1.862192000	0.517361000
1	4.746646000	-2.455677000	1.288248000
1	4.981139000	-1.660006000	-0.265212000
1	3.448979000	-2.473518000	0.091220000
6	0.388815000	-0.570040000	1.695310000
8	0.423118000	-0.644764000	2.847842000
6	0.714240000	-2.100250000	-0.368721000
6	-4.113459000	-0.793496000	-2.081198000
1	-4.862881000	-1.145705000	-1.369953000
1	-4.195852000	0.290248000	-2.159957000
1	-4.363810000	-1.219382000	-3.058668000
6	4.758073000	1.328092000	-1.574302000
1	5.049268000	1.689359000	-2.565664000
1	4.808096000	2.174659000	-0.886995000
1	5.502627000	0.591369000	-1.264966000
6	4.863885000	0.287029000	1.716034000
1	5.383495000	-0.294673000	2.484299000
1	5.599417000	0.557308000	0.957420000
1	4.506461000	1.204801000	2.186757000
6	-4.273528000	-1.565546000	1.378212000
1	-4.629223000	-2.224981000	0.583630000

1	-4.594511000	-2.001794000	2.329787000
1	-4.770584000	-0.601561000	1.278372000
1	-2.448635000	-0.783864000	2.190421000
1	3.056021000	-0.828546000	1.964230000
1	-2.015266000	-0.791201000	-2.440140000
1	2.672183000	1.461448000	-2.054782000
8	0.966051000	-3.218948000	-0.549237000
6	-3.762641000	1.676776000	0.052948000
6	-4.058749000	3.037137000	0.082888000
6	-2.993365000	3.943498000	0.055821000
6	-1.676682000	3.513384000	0.041688000
1	-5.086374000	3.379491000	0.098034000
1	-3.194850000	5.010528000	0.038880000
1	-0.893970000	4.258240000	0.002024000
1	-4.583884000	0.973323000	0.030223000
1	0.755413000	3.474036000	0.855644000
1	2.163873000	1.812940000	1.840979000
1	3.149259000	2.660993000	0.641198000
1	1.217033000	3.054170000	-0.788113000
1	0.655054000	0.062671000	-1.743168000
1	-0.113470000	-0.127602000	-1.746587000

-1853.061622

TS1-Mn-PNP-Ar

25	-0.359825000	-0.399539000	-0.022255000
15	-2.525862000	0.344586000	-0.002091000
15	1.933164000	-0.575064000	0.075664000
7	0.078721000	1.710538000	0.015435000
6	-2.280351000	2.051439000	-0.678068000
6	-1.015442000	2.683397000	-0.082881000
6	1.390854000	2.147141000	-0.028590000
6	2.448658000	1.187837000	-0.021009000
6	2.780140000	-1.469037000	-1.351706000
6	2.119965000	-2.830078000	-1.639466000
1	2.485401000	-3.211451000	-2.598005000
1	1.035174000	-2.759650000	-1.698372000
1	2.368833000	-3.568668000	-0.875472000
6	2.598292000	-1.229842000	1.715649000
6	2.468772000	-2.758832000	1.805070000

1	2.620173000	-3.075961000	2.841500000
1	3.228771000	-3.257763000	1.199320000
1	1.488910000	-3.116455000	1.486981000
6	-3.295551000	0.628278000	1.681743000
6	-3.218271000	-0.623753000	2.569332000
1	-3.522616000	-0.371159000	3.589901000
1	-2.204346000	-1.024159000	2.603215000
1	-3.883573000	-1.413147000	2.213170000
6	-3.757180000	-0.451040000	-1.166158000
6	-4.268159000	-1.792995000	-0.619765000
1	-4.807435000	-2.328286000	-1.406983000
1	-4.964140000	-1.645129000	0.209640000
1	-3.455448000	-2.434752000	-0.274926000
6	-0.415004000	-0.603844000	-1.790649000
8	-0.462122000	-0.686675000	-2.946421000
6	-0.736032000	-2.090386000	0.347937000
6	3.993924000	-0.769935000	2.157463000
1	4.779346000	-1.123421000	1.486242000
1	4.063205000	0.316004000	2.224628000
1	4.204459000	-1.178764000	3.151442000
6	-4.705021000	1.234744000	1.689993000
1	-4.966583000	1.541651000	2.707734000
1	-4.789382000	2.114436000	1.047946000
1	-5.451778000	0.505287000	1.368421000
6	-4.913541000	0.434020000	-1.655974000
1	-5.459931000	-0.095018000	-2.443615000
1	-5.624484000	0.660319000	-0.860362000
1	-4.563986000	1.377964000	-2.079190000
6	4.305773000	-1.633777000	-1.291329000
1	4.606983000	-2.283897000	-0.467286000
1	4.652149000	-2.103409000	-2.217814000
1	4.832920000	-0.685913000	-1.194178000
1	2.537708000	-0.799642000	-2.185202000
1	-3.117581000	-0.667380000	-2.028516000
1	1.869222000	-0.793389000	2.405703000
1	-2.600857000	1.367412000	2.100402000
8	-0.999345000	-3.191160000	0.609786000
6	3.777067000	1.625724000	-0.070864000
6	4.107138000	2.976364000	-0.134376000
6	3.076614000	3.916615000	-0.121077000

6	1.748476000	3.517867000	-0.056911000
1	5.144196000	3.286665000	-0.179825000
1	3.307774000	4.976435000	-0.150544000
1	0.981553000	4.279252000	-0.021560000
1	4.578679000	0.901295000	-0.052161000
1	-0.725531000	3.512230000	-0.733406000
1	-2.144427000	1.917676000	-1.755069000
1	-3.145788000	2.701344000	-0.525923000
1	-1.240069000	3.121881000	0.901516000
1	-0.095429000	0.901656000	1.077516000
1	-0.262007000	0.051035000	1.620765000

-1853.046623

3-Mn-PNP-Ar

25	-0.323923000	-0.524492000	0.017963000
15	-2.456616000	0.255696000	0.079883000
15	1.959786000	-0.575165000	0.182318000
7	0.137787000	1.505809000	0.983530000
6	-2.156661000	2.089591000	0.229785000
6	-1.078041000	2.304256000	1.289322000
6	1.271725000	2.107636000	0.327621000
6	2.329890000	1.235633000	-0.014061000
6	2.967908000	-1.402418000	-1.176575000
6	2.290683000	-2.708780000	-1.622197000
1	2.836377000	-3.130988000	-2.471897000
1	1.258638000	-2.540905000	-1.925525000
1	2.289236000	-3.454400000	-0.823071000
6	2.659397000	-1.032764000	1.866475000
6	2.502707000	-2.542028000	2.102824000
1	2.722375000	-2.781525000	3.147850000
1	3.192776000	-3.119565000	1.482487000
1	1.483947000	-2.870903000	1.885271000
6	-3.487579000	-0.182850000	1.588959000
6	-4.037872000	-1.612174000	1.464659000
1	-4.418983000	-1.949674000	2.433380000
1	-3.268200000	-2.316502000	1.141665000
1	-4.866339000	-1.658362000	0.753284000
6	-3.500977000	0.144934000	-1.469843000
6	-3.547002000	-1.284224000	-2.032795000

1	-4.022201000	-1.275138000	-3.018823000
1	-4.125465000	-1.953904000	-1.392879000
1	-2.545581000	-1.702028000	-2.140392000
6	-0.203749000	-0.108053000	-1.711369000
8	-0.143295000	0.098554000	-2.858460000
6	-0.683490000	-2.232099000	-0.185510000
6	4.057115000	-0.517920000	2.231473000
1	4.845517000	-1.058419000	1.707177000
1	4.168501000	0.546482000	2.011644000
1	4.225179000	-0.656876000	3.304837000
6	-4.571899000	0.804645000	2.041016000
1	-4.996877000	0.461753000	2.990549000
1	-4.175835000	1.808889000	2.209365000
1	-5.391364000	0.880705000	1.325219000
6	-4.902597000	0.764861000	-1.392579000
1	-5.336650000	0.819655000	-2.396168000
1	-5.572911000	0.155973000	-0.781423000
1	-4.890049000	1.776766000	-0.980558000
6	4.461919000	-1.646971000	-0.914108000
1	4.607810000	-2.424702000	-0.161521000
1	4.936450000	-1.994953000	-1.837105000
1	4.999073000	-0.758656000	-0.581779000
1	2.868319000	-0.682665000	-1.996675000
1	-2.900854000	0.744977000	-2.164192000
1	1.933672000	-0.532258000	2.518463000
1	-2.704797000	-0.205666000	2.354050000
8	-0.938956000	-3.368163000	-0.230836000
6	3.469957000	1.770753000	-0.614156000
6	3.557214000	3.131523000	-0.916155000
6	2.489976000	3.969182000	-0.615436000
6	1.350171000	3.461746000	0.012454000
1	4.444188000	3.523376000	-1.400190000
1	2.534979000	5.023306000	-0.864403000
1	0.533434000	4.133188000	0.240734000
1	4.293047000	1.123827000	-0.885456000
1	-0.844287000	3.363369000	1.414373000
1	-1.795166000	2.423049000	-0.746961000
1	-3.055728000	2.661129000	0.469602000
1	-1.439447000	1.952257000	2.257769000
1	0.448685000	1.081207000	1.849886000

1 -0.460220000 -0.978152000 1.580137000

-1853.060640

TS2-Mn-PNP-Ar

25 0.282107000 -0.294119000 0.415871000
15 2.419424000 0.441042000 0.073349000
15 -2.014654000 -0.446018000 0.278791000
7 -0.185891000 1.090712000 -1.329256000
6 2.099631000 1.994163000 -0.905250000
6 1.023147000 1.698651000 -1.945740000
6 -1.329548000 1.912062000 -1.003473000
6 -2.389087000 1.266973000 -0.327522000
6 -3.007560000 -0.603611000 1.870053000
6 -2.319798000 -1.577548000 2.841146000
1 -2.879197000 -1.608284000 3.781245000
1 -1.299007000 -1.271168000 3.062475000
1 -2.287226000 -2.593485000 2.439255000
6 -2.713814000 -1.588594000 -1.037229000
6 -2.500155000 -3.051728000 -0.621270000
1 -2.713143000 -3.715204000 -1.464845000
1 -3.167220000 -3.335222000 0.197028000
1 -1.470148000 -3.228004000 -0.303602000
6 3.529398000 -0.575689000 -1.046630000
6 3.632529000 -2.030465000 -0.562575000
1 4.114387000 -2.640981000 -1.332527000
1 2.648753000 -2.452790000 -0.363367000
1 4.233997000 -2.109365000 0.345384000
6 3.392940000 1.055200000 1.553539000
6 3.931929000 -0.110023000 2.397102000
1 4.273474000 0.264152000 3.366952000
1 4.786415000 -0.589648000 1.912960000
1 3.171292000 -0.871881000 2.580243000
6 0.096426000 0.832418000 1.779759000
8 -0.011645000 1.523700000 2.711111000
6 0.669005000 -1.691555000 1.418955000
6 -4.134875000 -1.319170000 -1.547589000
1 -4.896935000 -1.639386000 -0.837405000
1 -4.293452000 -0.261194000 -1.769089000
1 -4.295849000 -1.880705000 -2.473770000
6 4.912528000 0.004914000 -1.367694000

1	5.367026000	-0.563678000	-2.185515000
1	4.872766000	1.052166000	-1.675660000
1	5.582505000	-0.072303000	-0.508602000
6	4.478741000	2.109427000	1.291015000
1	4.843231000	2.492732000	2.249894000
1	5.335735000	1.697813000	0.757299000
1	4.100439000	2.961615000	0.722617000
6	-4.500407000	-0.949292000	1.753655000
1	-4.641750000	-1.983987000	1.434002000
1	-4.968171000	-0.847488000	2.737965000
1	-5.046402000	-0.308830000	1.061333000
1	-2.914626000	0.403365000	2.291561000
1	2.600654000	1.540149000	2.132574000
1	-2.028244000	-1.378776000	-1.864127000
1	2.939276000	-0.584056000	-1.970943000
8	0.948797000	-2.648672000	2.015918000
6	-3.537539000	1.999136000	-0.025765000
6	-3.632990000	3.355386000	-0.343748000
6	-2.565269000	3.988340000	-0.968501000
6	-1.416333000	3.268639000	-1.304284000
1	-4.526709000	3.911042000	-0.084977000
1	-2.616761000	5.045785000	-1.201476000
1	-0.599754000	3.782568000	-1.792712000
1	-4.360119000	1.527215000	0.494113000
1	0.776375000	2.591365000	-2.523737000
1	1.746289000	2.746197000	-0.193932000
1	2.996903000	2.385468000	-1.390164000
1	1.391475000	0.963862000	-2.662703000
1	-0.487268000	0.361261000	-1.969725000
1	0.478274000	-1.407904000	-0.806133000
6	0.524964000	-2.190124000	-2.490791000
8	0.867507000	-3.269310000	-2.191840000
8	0.188657000	-1.277576000	-3.161307000

-2041.709585

4-Mn-PNP-Ar

25	0.290234000	-0.336706000	0.298726000
15	2.464302000	0.414883000	0.080557000
15	-2.035226000	-0.477138000	0.222751000

7	-0.151380000	1.199257000	-1.185768000
6	2.138823000	2.074260000	-0.684982000
6	1.050798000	1.890251000	-1.737982000
6	-1.303639000	1.986258000	-0.796026000
6	-2.379091000	1.285360000	-0.208165000
6	-2.947569000	-0.764067000	1.845083000
6	-2.237525000	-1.832807000	2.692513000
1	-2.783487000	-1.970996000	3.630497000
1	-1.217085000	-1.546496000	2.940243000
1	-2.203931000	-2.798130000	2.181633000
6	-2.788178000	-1.502935000	-1.150996000
6	-2.585176000	-2.998960000	-0.864459000
1	-2.842630000	-3.580516000	-1.753905000
1	-3.223797000	-3.343375000	-0.046912000
1	-1.547448000	-3.225879000	-0.610649000
6	3.548228000	-0.479670000	-1.156323000
6	3.647705000	-1.979978000	-0.835992000
1	4.154759000	-2.491822000	-1.658727000
1	2.665957000	-2.438045000	-0.725202000
1	4.223935000	-2.159356000	0.073608000
6	3.412800000	0.809601000	1.644440000
6	3.902318000	-0.458966000	2.359192000
1	4.239152000	-0.202497000	3.367856000
1	4.750115000	-0.907375000	1.836079000
1	3.118753000	-1.213581000	2.449425000
6	0.133067000	0.594783000	1.789658000
8	0.031817000	1.193187000	2.777215000
6	0.683159000	-1.832356000	1.185850000
6	-4.225420000	-1.173003000	-1.576238000
1	-4.964940000	-1.521822000	-0.855745000
1	-4.370366000	-0.101338000	-1.730535000
1	-4.432736000	-1.673476000	-2.527385000
6	4.932031000	0.130082000	-1.416652000
1	5.370920000	-0.336790000	-2.303708000
1	4.896487000	1.207239000	-1.593821000
1	5.609914000	-0.057774000	-0.581328000
6	4.535709000	1.850136000	1.512593000
1	4.887930000	2.121561000	2.512797000
1	5.390982000	1.463620000	0.957911000
1	4.199441000	2.767645000	1.025277000

6	-4.448182000	-1.082844000	1.756872000
1	-4.616223000	-2.078397000	1.341594000
1	-4.872071000	-1.074272000	2.765581000
1	-5.012250000	-0.370100000	1.156523000
1	-2.825629000	0.200903000	2.348564000
1	2.626462000	1.254871000	2.262682000
1	-2.136868000	-1.232720000	-1.986266000
1	2.955138000	-0.383904000	-2.073515000
8	0.966104000	-2.813429000	1.726922000
6	-3.537994000	1.983458000	0.134443000
6	-3.630823000	3.362055000	-0.057541000
6	-2.549189000	4.049697000	-0.594971000
6	-1.390789000	3.365997000	-0.968520000
1	-4.532386000	3.890527000	0.228836000
1	-2.597439000	5.124112000	-0.730183000
1	-0.567235000	3.927555000	-1.386801000
1	-4.371819000	1.461533000	0.583501000
1	0.790194000	2.838442000	-2.208838000
1	1.793552000	2.733034000	0.116720000
1	3.031178000	2.520527000	-1.129493000
1	1.409411000	1.243211000	-2.539532000
1	-0.428914000	0.553191000	-1.950021000
1	0.492927000	-1.374741000	-1.204179000
6	0.413200000	-1.683278000	-2.356629000
8	0.836201000	-2.811959000	-2.549290000
8	-0.076356000	-0.796093000	-3.078720000

-2041.723227

TS3-Mn-PNP-Ar

25	-0.321902000	-0.438517000	-0.215509000
15	-2.509598000	0.272550000	-0.312314000
15	1.976564000	-0.626989000	-0.095605000
7	0.097878000	1.602474000	-0.111255000
6	-2.212107000	1.924453000	-1.073630000
6	-0.976094000	2.582530000	-0.452948000
6	1.421357000	2.048114000	-0.383905000
6	2.474263000	1.100506000	-0.440776000
6	2.817092000	-1.724914000	-1.373031000
6	2.063696000	-3.055043000	-1.553536000

1	2.537209000	-3.629113000	-2.355484000
1	1.019051000	-2.908634000	-1.819847000
1	2.097484000	-3.663165000	-0.647117000
6	2.655509000	-0.993447000	1.622869000
6	2.333703000	-2.434755000	2.044956000
1	2.555220000	-2.560485000	3.108407000
1	2.941375000	-3.157176000	1.494618000
1	1.282586000	-2.685735000	1.893259000
6	-3.372763000	0.621328000	1.312107000
6	-3.455326000	-0.625459000	2.209267000
1	-3.712615000	-0.325568000	3.228587000
1	-2.512552000	-1.170862000	2.256733000
1	-4.225769000	-1.315216000	1.860932000
6	-3.658850000	-0.594033000	-1.508816000
6	-4.213240000	-1.906830000	-0.935229000
1	-4.682731000	-2.484322000	-1.736907000
1	-4.978760000	-1.714246000	-0.180528000
1	-3.436841000	-2.528501000	-0.486452000
6	-0.300518000	-0.659673000	-1.955120000
8	-0.288881000	-0.761985000	-3.109934000
6	-0.712211000	-2.154336000	0.084102000
6	4.119095000	-0.629787000	1.907662000
1	4.821020000	-1.270438000	1.374031000
1	4.337414000	0.409067000	1.658551000
1	4.306801000	-0.757629000	2.978592000
6	-4.736253000	1.319438000	1.212767000
1	-5.044136000	1.654572000	2.208009000
1	-4.715497000	2.195238000	0.561189000
1	-5.505136000	0.635839000	0.846531000
6	-4.779489000	0.270595000	-2.106618000
1	-5.286814000	-0.297262000	-2.893033000
1	-5.529311000	0.540609000	-1.362005000
1	-4.401986000	1.189176000	-2.559709000
6	4.315020000	-2.011314000	-1.183961000
1	4.485398000	-2.668359000	-0.328609000
1	4.690645000	-2.529687000	-2.071491000
1	4.919104000	-1.115464000	-1.050134000
1	2.687188000	-1.134017000	-2.286484000
1	-2.968024000	-0.849756000	-2.319267000
1	2.045551000	-0.322377000	2.232909000

1	-2.669803000	1.323343000	1.776137000
8	-0.983322000	-3.262835000	0.280470000
6	3.780806000	1.520372000	-0.708891000
6	4.084814000	2.863671000	-0.910223000
6	3.063683000	3.804338000	-0.803247000
6	1.757381000	3.407711000	-0.534024000
1	5.101317000	3.168683000	-1.128334000
1	3.281368000	4.860248000	-0.921615000
1	1.001390000	4.172841000	-0.426845000
1	4.578738000	0.793115000	-0.763751000
1	-0.609142000	3.318668000	-1.168476000
1	-2.021471000	1.717267000	-2.130459000
1	-3.075635000	2.590892000	-1.014898000
1	-1.265676000	3.136800000	0.449090000
1	0.064838000	1.645965000	1.271275000
1	-0.359621000	-0.300699000	1.872334000
6	-0.267796000	0.414591000	2.750997000
8	-0.411701000	-0.038415000	3.863987000
8	-0.016710000	1.634514000	2.408091000

-2041.715724

5-Mn-PNP-Ar

25	0.327633000	-0.590984000	0.126709000
15	2.510733000	0.028928000	0.437800000
15	-1.970886000	-0.702699000	-0.091651000
7	-0.058031000	1.194225000	0.936653000
6	2.272935000	1.160884000	1.866767000
6	0.983491000	1.963522000	1.665974000
6	-1.371571000	1.635788000	1.186288000
6	-2.468562000	0.833191000	0.769007000
6	-2.818178000	-2.137699000	0.778736000
6	-2.216032000	-3.495419000	0.371880000
1	-2.525846000	-4.253921000	1.096833000
1	-1.127538000	-3.481087000	0.347974000
1	-2.571297000	-3.814450000	-0.609019000
6	-2.606310000	-0.541088000	-1.860985000
6	-2.511604000	-1.873832000	-2.620894000
1	-2.634938000	-1.687982000	-3.691892000
1	-3.307242000	-2.557309000	-2.315863000

1	-1.554714000	-2.376195000	-2.478240000
6	3.242652000	1.100440000	-0.912284000
6	3.114611000	0.444336000	-2.296113000
1	3.348999000	1.174116000	-3.076147000
1	2.105991000	0.069231000	-2.477209000
1	3.802342000	-0.396286000	-2.408248000
6	3.744516000	-1.247112000	1.022189000
6	4.224630000	-2.146424000	-0.126979000
1	4.770033000	-3.002313000	0.281226000
1	4.907746000	-1.610183000	-0.789735000
1	3.397650000	-2.531764000	-0.725998000
6	0.412021000	-1.734152000	1.446777000
8	0.481229000	-2.435568000	2.370329000
6	0.692708000	-1.865689000	-1.066550000
6	-3.981588000	0.108641000	-2.060924000
1	-4.783864000	-0.483198000	-1.615550000
1	-4.022894000	1.114431000	-1.643661000
1	-4.185131000	0.184339000	-3.133944000
6	4.666234000	1.618952000	-0.668203000
1	4.905989000	2.385129000	-1.412010000
1	4.784589000	2.068877000	0.319876000
1	5.403950000	0.820361000	-0.772258000
6	4.922627000	-0.716971000	1.854715000
1	5.470956000	-1.564953000	2.277261000
1	5.625038000	-0.140597000	1.251467000
1	4.595383000	-0.091138000	2.687561000
6	-4.350485000	-2.199975000	0.709685000
1	-4.699734000	-2.358463000	-0.312816000
1	-4.700243000	-3.047745000	1.307486000
1	-4.829141000	-1.305693000	1.106198000
1	-2.524954000	-1.940072000	1.816312000
1	3.120021000	-1.856706000	1.684168000
1	-1.860069000	0.136179000	-2.288708000
1	2.565416000	1.961676000	-0.888418000
8	0.944376000	-2.698722000	-1.835698000
6	-3.779088000	1.254823000	1.004023000
6	-4.051780000	2.462973000	1.642349000
6	-2.984189000	3.269693000	2.027401000
6	-1.669984000	2.873298000	1.799687000
1	-5.075261000	2.771510000	1.818563000

1	-3.170319000	4.226502000	2.503611000
1	-0.876442000	3.547357000	2.088713000
1	-4.607851000	0.643793000	0.675930000
1	0.614295000	2.251303000	2.654732000
1	2.166744000	0.506360000	2.736510000
1	3.123837000	1.822581000	2.044747000
1	1.213156000	2.900167000	1.138446000
1	0.070766000	2.152771000	-0.620996000
1	0.014971000	1.184692000	-2.522529000
6	0.166087000	2.277946000	-2.540282000
8	0.300739000	2.897181000	-3.564262000
8	0.194713000	2.840047000	-1.335928000

-2041.717737

1-Mn-PNP-Ar₂

25	-0.023544000	-0.755831000	0.127925000
15	2.271038000	-0.414187000	0.081940000
15	-2.262933000	-0.465235000	-0.232334000
7	-0.074977000	1.252304000	-0.015639000
6	2.333658000	1.366230000	-0.338010000
6	1.052605000	1.980516000	-0.403028000
6	-1.214812000	1.921127000	0.461094000
6	-2.453415000	1.231411000	0.402960000
6	-3.579655000	-1.506934000	0.598002000
6	-3.128845000	-2.971872000	0.717909000
1	-3.885657000	-3.542489000	1.264748000
1	-2.184210000	-3.062739000	1.253564000
1	-3.004743000	-3.437736000	-0.262748000
6	-2.549295000	-0.345957000	-2.085505000
6	-2.495458000	-1.730692000	-2.747589000
1	-2.490121000	-1.620613000	-3.836239000
1	-3.366692000	-2.335849000	-2.484488000
1	-1.599845000	-2.284983000	-2.459967000
6	3.127230000	-1.344632000	-1.321108000
6	3.455896000	-2.788644000	-0.906127000
1	3.677805000	-3.379803000	-1.799508000
1	2.637395000	-3.278409000	-0.379754000
1	4.341602000	-2.815526000	-0.267502000
6	3.205272000	-0.617209000	1.697218000
6	3.020012000	-2.012951000	2.317839000

1	3.258148000	-1.966922000	3.384554000
1	3.688713000	-2.744906000	1.863472000
1	1.998166000	-2.377938000	2.217215000
6	-0.219085000	-1.076048000	1.839397000
8	-0.378951000	-1.231711000	2.978401000
6	0.042489000	-2.498752000	-0.238987000
6	-3.763737000	0.471985000	-2.543068000
1	-4.702119000	-0.054217000	-2.363938000
1	-3.811229000	1.440823000	-2.041941000
1	-3.689771000	0.654593000	-3.620145000
6	4.341432000	-0.696004000	-1.999177000
1	4.689440000	-1.352870000	-2.803398000
1	4.099303000	0.269560000	-2.442356000
1	5.174414000	-0.559795000	-1.305177000
6	4.685548000	-0.215420000	1.683499000
1	5.097949000	-0.316276000	2.692727000
1	5.270225000	-0.863586000	1.026170000
1	4.832114000	0.819282000	1.373325000
6	-4.994265000	-1.426377000	0.002145000
1	-5.040324000	-1.916874000	-0.972506000
1	-5.693268000	-1.947784000	0.663241000
1	-5.352684000	-0.404227000	-0.120428000
1	-3.601872000	-1.077277000	1.605741000
1	2.657154000	0.099634000	2.320133000
1	-1.647431000	0.205189000	-2.379354000
1	2.316802000	-1.385228000	-2.058489000
8	0.092386000	-3.632037000	-0.488845000
6	3.481458000	2.102217000	-0.653691000
6	3.401769000	3.417424000	-1.101930000
6	2.139031000	3.990982000	-1.268819000
6	0.989586000	3.290606000	-0.933193000
1	4.301071000	3.970348000	-1.345634000
1	2.047759000	4.995637000	-1.668523000
1	0.024558000	3.755365000	-1.084596000
6	-3.619610000	1.803199000	0.908435000
6	-3.596889000	3.063372000	1.505439000
6	-2.377949000	3.734509000	1.604777000
6	-1.207632000	3.180241000	1.095971000
1	-4.505118000	3.499402000	1.904135000
1	-2.330392000	4.698458000	2.100523000

1	-0.275450000	3.714120000	1.220980000
1	-4.554984000	1.259625000	0.860103000
1	4.455639000	1.641018000	-0.569877000

-2004.343682

2-Mn-PNP-Ar₂

25	-0.006182000	-0.791133000	-0.099638000
15	2.286887000	-0.449708000	0.030652000
15	-2.288100000	-0.435711000	-0.280523000
7	-0.022558000	1.301937000	-0.079947000
6	2.378279000	1.321442000	-0.419467000
6	1.115074000	1.985943000	-0.457225000
6	-1.143653000	1.951048000	0.409485000
6	-2.391302000	1.265259000	0.373855000
6	-3.460915000	-1.460099000	0.781418000
6	-3.000260000	-2.922161000	0.887432000
1	-3.684380000	-3.471491000	1.541476000
1	-1.999396000	-3.003814000	1.306918000
1	-3.000366000	-3.419320000	-0.085812000
6	-2.921596000	-0.352310000	-2.051663000
6	-2.928422000	-1.744579000	-2.701372000
1	-3.123411000	-1.653461000	-3.774119000
1	-3.711489000	-2.379062000	-2.279268000
1	-1.973790000	-2.262284000	-2.576400000
6	3.284182000	-1.445816000	-1.229426000
6	3.536075000	-2.876686000	-0.723718000
1	3.822471000	-3.511986000	-1.566942000
1	2.660345000	-3.323763000	-0.253961000
1	4.359276000	-2.896594000	-0.006439000
6	3.076032000	-0.583132000	1.732041000
6	2.873779000	-1.956854000	2.395916000
1	2.997595000	-1.854754000	3.478015000
1	3.610917000	-2.681469000	2.048426000
1	1.882061000	-2.369506000	2.211662000
6	-0.207060000	-0.879861000	1.671298000
8	-0.358145000	-0.915610000	2.814672000
6	0.041380000	-2.568212000	-0.268570000
6	-4.230260000	0.409802000	-2.298100000
1	-5.104951000	-0.152758000	-1.971862000

1	-4.233618000	1.378229000	-1.794680000
1	-4.339874000	0.591384000	-3.372277000
6	4.578406000	-0.848690000	-1.799375000
1	5.007575000	-1.559229000	-2.513755000
1	4.400673000	0.085236000	-2.331679000
1	5.329147000	-0.671394000	-1.026153000
6	4.541797000	-0.141791000	1.831567000
1	4.856067000	-0.165352000	2.880083000
1	5.201257000	-0.815904000	1.279308000
1	4.695106000	0.873951000	1.466432000
6	-4.953990000	-1.411720000	0.419325000
1	-5.152210000	-1.932967000	-0.519636000
1	-5.525533000	-1.921836000	1.200841000
1	-5.349028000	-0.400552000	0.331959000
1	-3.329591000	-0.993534000	1.763759000
1	2.462389000	0.143959000	2.277075000
1	-2.119988000	0.235579000	-2.514823000
1	2.567745000	-1.511077000	-2.054832000
8	0.088359000	-3.720357000	-0.384431000
6	3.551292000	2.026850000	-0.720586000
6	3.519693000	3.352074000	-1.139759000
6	2.276362000	3.976595000	-1.286061000
6	1.105307000	3.315028000	-0.957353000
1	4.438120000	3.876589000	-1.374664000
1	2.220983000	4.991813000	-1.665713000
1	0.157430000	3.818116000	-1.094442000
6	-3.547150000	1.855507000	0.892424000
6	-3.514643000	3.117010000	1.479319000
6	-2.287136000	3.780611000	1.564042000
6	-1.129728000	3.217027000	1.047957000
1	-4.417110000	3.560901000	1.882150000
1	-2.227346000	4.745701000	2.056788000
1	-0.191786000	3.742152000	1.166453000
1	-4.488009000	1.322027000	0.855856000
1	4.509638000	1.534148000	-0.638599000
1	-0.238382000	-0.617743000	-1.824547000
1	0.551131000	-0.589850000	-1.750300000

-2005.511787

TS1-Mn-PNP-Ar

25	-0.033353000	-0.763145000	0.013926000
15	2.248599000	-0.497321000	0.045581000
15	-2.297249000	-0.427254000	-0.266095000
7	-0.000982000	1.394644000	-0.218994000
6	2.432660000	1.310755000	-0.279152000
6	1.232607000	2.049329000	-0.421191000
6	-1.154604000	2.038089000	0.261465000
6	-2.393785000	1.343294000	0.216287000
6	-3.496269000	-1.332380000	0.870116000
6	-3.046825000	-2.786593000	1.092164000
1	-3.713618000	-3.265167000	1.815968000
1	-2.030763000	-2.844995000	1.478343000
1	-3.089225000	-3.366654000	0.166936000
6	-2.900153000	-0.507587000	-2.044251000
6	-2.914600000	-1.958391000	-2.546926000
1	-3.099168000	-1.975263000	-3.625400000
1	-3.706501000	-2.542140000	-2.070940000
1	-1.962594000	-2.458981000	-2.359985000
6	3.142594000	-1.388719000	-1.361108000
6	3.389360000	-2.866426000	-1.011642000
1	3.648979000	-3.412399000	-1.923673000
1	2.518080000	-3.351995000	-0.573264000
1	4.227810000	-2.971843000	-0.319462000
6	3.133096000	-0.816008000	1.675774000
6	2.812611000	-2.213900000	2.236361000
1	3.023966000	-2.230140000	3.309672000
1	3.428833000	-2.982902000	1.768706000
1	1.766963000	-2.486260000	2.095381000
6	-0.212535000	-0.836767000	1.792517000
8	-0.353992000	-0.841566000	2.942104000
6	-0.028971000	-2.514764000	-0.247149000
6	-4.194103000	0.241189000	-2.387804000
1	-5.080442000	-0.265904000	-2.006342000
1	-4.188025000	1.262550000	-2.001681000
1	-4.294412000	0.298480000	-3.476759000
6	4.414017000	-0.763989000	-1.951115000
1	4.763906000	-1.393824000	-2.775894000
1	4.236332000	0.233625000	-2.352441000
1	5.224551000	-0.705268000	-1.220835000

6	4.643621000	-0.551162000	1.727999000
1	5.008083000	-0.741798000	2.742705000
1	5.191201000	-1.215943000	1.055993000
1	4.896182000	0.479463000	1.480780000
6	-4.987398000	-1.305389000	0.498095000
1	-5.182540000	-1.901611000	-0.395666000
1	-5.566346000	-1.746083000	1.315669000
1	-5.377452000	-0.303449000	0.324130000
1	-3.361874000	-0.790196000	1.812481000
1	2.631202000	-0.080012000	2.314776000
1	-2.075661000	0.008326000	-2.547722000
1	2.365466000	-1.352209000	-2.130492000
8	-0.020977000	-3.656344000	-0.458095000
6	3.659205000	1.966210000	-0.466628000
6	3.724790000	3.305583000	-0.830618000
6	2.538018000	4.003094000	-1.061186000
6	1.312414000	3.381633000	-0.872107000
1	4.685793000	3.788281000	-0.963865000
1	2.566139000	5.032356000	-1.401738000
1	0.402683000	3.925265000	-1.087328000
6	-3.556308000	1.967845000	0.676190000
6	-3.529647000	3.243652000	1.232818000
6	-2.301929000	3.890620000	1.356186000
6	-1.134932000	3.302340000	0.882290000
1	-4.441537000	3.705738000	1.591564000
1	-2.243112000	4.861590000	1.836030000
1	-0.196889000	3.818585000	1.024716000
1	-4.499819000	1.441365000	0.629434000
1	4.582279000	1.419481000	-0.344722000
1	0.089152000	-0.444270000	-1.637025000
1	-0.075025000	0.512876000	-1.151898000

-2005.489376

3-Mn-PNP-Ar

25	0.064350000	-0.826711000	-0.023689000
15	-2.192686000	-0.547775000	-0.036962000
15	2.294342000	-0.406147000	0.311389000
7	0.036057000	1.397637000	0.499648000
6	-2.419026000	1.274921000	0.273657000

6	-1.274206000	2.026633000	0.581418000
6	1.119536000	2.053633000	-0.206213000
6	2.357593000	1.372454000	-0.218439000
6	3.579480000	-1.245287000	-0.783486000
6	3.183027000	-2.705489000	-1.054195000
1	3.903772000	-3.156241000	-1.743632000
1	2.192632000	-2.773453000	-1.501589000
1	3.179945000	-3.300890000	-0.137631000
6	2.863701000	-0.422279000	2.101355000
6	2.908542000	-1.868087000	2.615356000
1	3.039107000	-1.875869000	3.701873000
1	3.743256000	-2.423829000	2.180325000
1	1.980827000	-2.393261000	2.378153000
6	-3.124276000	-1.377050000	1.385111000
6	-3.288182000	-2.882028000	1.112692000
1	-3.581627000	-3.385840000	2.038872000
1	-2.367983000	-3.347200000	0.759411000
1	-4.074347000	-3.070533000	0.377662000
6	-3.099021000	-0.890882000	-1.657642000
6	-2.681304000	-2.257613000	-2.232339000
1	-2.999536000	-2.322144000	-3.277468000
1	-3.154116000	-3.080173000	-1.692804000
1	-1.603613000	-2.405954000	-2.195768000
6	0.261066000	-0.656453000	-1.792900000
8	0.409335000	-0.595077000	-2.946818000
6	0.083421000	-2.584041000	0.019521000
6	4.115820000	0.381118000	2.472499000
1	5.033079000	-0.114416000	2.154724000
1	4.099618000	1.383869000	2.038659000
1	4.164991000	0.489491000	3.561191000
6	-4.443161000	-0.770625000	1.881290000
1	-4.803826000	-1.361413000	2.730172000
1	-4.320997000	0.256126000	2.227166000
1	-5.225425000	-0.787105000	1.119515000
6	-4.628031000	-0.760003000	-1.694367000
1	-4.979872000	-0.953314000	-2.713174000
1	-5.108865000	-1.492151000	-1.042569000
1	-4.980203000	0.232665000	-1.417727000
6	5.049965000	-1.169068000	-0.344989000
1	5.228736000	-1.776975000	0.544417000

1	5.683492000	-1.567375000	-1.143825000
1	5.388360000	-0.155735000	-0.128940000
1	3.466319000	-0.693826000	-1.723048000
1	-2.665781000	-0.116718000	-2.301838000
1	2.001979000	0.058946000	2.578461000
1	-2.377994000	-1.265179000	2.176752000
8	0.083380000	-3.745033000	0.118573000
6	-3.662264000	1.924883000	0.338305000
6	-3.771294000	3.254980000	0.729903000
6	-2.631240000	3.960833000	1.109113000
6	-1.388453000	3.342305000	1.040950000
1	-4.746069000	3.727662000	0.767360000
1	-2.707359000	4.984085000	1.458144000
1	-0.497409000	3.881504000	1.338635000
6	3.448572000	1.980093000	-0.841877000
6	3.317728000	3.203980000	-1.500026000
6	2.072500000	3.817859000	-1.554226000
6	0.974604000	3.249233000	-0.905513000
1	4.174267000	3.650087000	-1.991750000
1	1.942480000	4.745182000	-2.100325000
1	0.014236000	3.740384000	-0.963363000
1	4.407483000	1.480065000	-0.860242000
1	-4.565982000	1.381998000	0.107597000
1	-0.094221000	-0.992900000	1.600442000
1	0.332372000	1.190342000	1.450660000

-2005.496439

TS2-Mn-PNP-Ar2

25	0.094407000	-0.778912000	-0.270387000
15	-2.169046000	-0.475103000	-0.391849000
15	2.344842000	-0.378516000	0.071532000
7	0.068671000	1.373904000	0.397340000
6	-2.390679000	1.293785000	0.133557000
6	-1.243094000	1.998949000	0.524527000
6	1.132194000	2.085795000	-0.294237000
6	2.376486000	1.422206000	-0.372272000
6	3.598189000	-1.158873000	-1.099666000
6	3.207946000	-2.609336000	-1.425538000
1	3.922197000	-3.024209000	-2.143423000

1	2.213186000	-2.668873000	-1.863363000
1	3.223266000	-3.243134000	-0.535333000
6	2.962235000	-0.475016000	1.840104000
6	2.996087000	-1.940625000	2.297313000
1	3.150887000	-1.991731000	3.379268000
1	3.813133000	-2.489391000	1.821436000
1	2.058026000	-2.448958000	2.063702000
6	-3.200167000	-1.494429000	0.818911000
6	-3.383516000	-2.928999000	0.294179000
1	-3.711027000	-3.570854000	1.117388000
1	-2.463312000	-3.352660000	-0.108205000
1	-4.152941000	-2.973223000	-0.480074000
6	-2.939181000	-0.566151000	-2.110293000
6	-2.577247000	-1.886963000	-2.816571000
1	-2.730115000	-1.771916000	-3.893745000
1	-3.212425000	-2.707284000	-2.479553000
1	-1.539561000	-2.173462000	-2.652586000
6	0.343756000	-0.508803000	-2.015217000
8	0.527563000	-0.370340000	-3.155107000
6	0.098243000	-2.541898000	-0.354817000
6	4.239754000	0.291697000	2.205440000
1	5.140546000	-0.212646000	1.856882000
1	4.234769000	1.306775000	1.801191000
1	4.310085000	0.368865000	3.295427000
6	-4.531444000	-0.936422000	1.338415000
1	-4.954655000	-1.650611000	2.052602000
1	-4.404804000	0.011214000	1.862322000
1	-5.266942000	-0.798174000	0.542652000
6	-4.442079000	-0.289271000	-2.254131000
1	-4.719280000	-0.359994000	-3.311042000
1	-5.041097000	-1.024968000	-1.712957000
1	-4.723242000	0.706923000	-1.914276000
6	5.079141000	-1.090435000	-0.697082000
1	5.286812000	-1.745391000	0.151832000
1	5.693721000	-1.437150000	-1.533677000
1	5.413209000	-0.087091000	-0.434007000
1	3.455322000	-0.565477000	-2.009075000
1	-2.389576000	0.236640000	-2.615449000
1	2.134160000	0.012201000	2.361685000
1	-2.509415000	-1.546526000	1.662124000

8	0.084226000	-3.703829000	-0.338256000
6	-3.631337000	1.938772000	0.266702000
6	-3.733229000	3.216452000	0.806020000
6	-2.589049000	3.870913000	1.258935000
6	-1.349593000	3.257881000	1.121901000
1	-4.705655000	3.686458000	0.897771000
1	-2.660253000	4.849505000	1.719164000
1	-0.454560000	3.754877000	1.476073000
6	3.446802000	2.075615000	-0.984977000
6	3.288175000	3.335720000	-1.564004000
6	2.037615000	3.940976000	-1.547367000
6	0.960182000	3.321836000	-0.910465000
1	4.128036000	3.819549000	-2.048680000
1	1.887571000	4.900429000	-2.029004000
1	-0.005243000	3.806998000	-0.910846000
1	4.409333000	1.587163000	-1.056357000
1	-4.536140000	1.429622000	-0.027326000
1	-0.124023000	-1.065193000	1.378762000
1	0.372609000	1.184023000	1.352905000
6	-0.406893000	-0.722032000	3.166771000
8	-0.750325000	-1.787404000	3.516975000
8	-0.125988000	0.423992000	3.225394000

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4-Mn-PNP-Ar₂

25	0.075250000	-0.738418000	-0.171139000
15	-2.213285000	-0.489857000	-0.336879000
15	2.362230000	-0.368193000	0.092654000
7	0.035444000	1.347174000	0.364738000
6	-2.427325000	1.301357000	0.064295000
6	-1.272682000	1.997549000	0.447367000
6	1.110027000	2.059663000	-0.317852000
6	2.369416000	1.422846000	-0.352411000
6	3.520384000	-1.163117000	-1.163676000
6	3.100006000	-2.608857000	-1.475209000
1	3.787206000	-3.031389000	-2.214233000
1	2.094040000	-2.662817000	-1.887431000
1	3.136368000	-3.242904000	-0.586363000
6	3.059009000	-0.514255000	1.823527000

6	3.101423000	-1.991130000	2.244678000
1	3.324260000	-2.062773000	3.312840000
1	3.876772000	-2.543109000	1.706746000
1	2.144254000	-2.488353000	2.070717000
6	-3.218085000	-1.431703000	0.951080000
6	-3.379017000	-2.906266000	0.542832000
1	-3.698400000	-3.480640000	1.416893000
1	-2.452539000	-3.350812000	0.179138000
1	-4.145732000	-3.026232000	-0.226122000
6	-2.945009000	-0.735208000	-2.051133000
6	-2.558450000	-2.101408000	-2.647351000
1	-2.737021000	-2.082973000	-3.726268000
1	-3.161264000	-2.906694000	-2.226665000
1	-1.509738000	-2.347153000	-2.487285000
6	0.292528000	-0.561979000	-1.918549000
8	0.454180000	-0.444216000	-3.058710000
6	0.089394000	-2.520637000	-0.236093000
6	4.367490000	0.228077000	2.125033000
1	5.239284000	-0.271187000	1.703001000
1	4.345237000	1.256830000	1.758089000
1	4.505616000	0.268151000	3.210088000
6	-4.560196000	-0.846046000	1.409029000
1	-4.979208000	-1.503161000	2.177670000
1	-4.447841000	0.142667000	1.853584000
1	-5.289508000	-0.784646000	0.598145000
6	-4.452320000	-0.495118000	-2.212146000
1	-4.726890000	-0.638791000	-3.261979000
1	-5.037177000	-1.204338000	-1.622983000
1	-4.749962000	0.516065000	-1.937069000
6	5.023787000	-1.115587000	-0.848925000
1	5.274547000	-1.784237000	-0.023001000
1	5.580814000	-1.457531000	-1.726400000
1	5.385873000	-0.120209000	-0.595047000
1	3.332104000	-0.559417000	-2.057662000
1	-2.409545000	0.036969000	-2.615294000
1	2.271206000	-0.023330000	2.399832000
1	-2.539496000	-1.406588000	1.806913000
8	0.081831000	-3.676409000	-0.237029000
6	-3.662096000	1.965037000	0.150993000
6	-3.751896000	3.260275000	0.647219000

6	-2.605108000	3.905228000	1.108286000
6	-1.372604000	3.271166000	1.013913000
1	-4.717144000	3.749456000	0.706703000
1	-2.669583000	4.894618000	1.545665000
1	-0.479691000	3.761915000	1.380666000
6	3.451232000	2.092453000	-0.928137000
6	3.291223000	3.344560000	-1.520373000
6	2.027078000	3.920903000	-1.558558000
6	0.939792000	3.285519000	-0.957273000
1	4.139398000	3.843753000	-1.973644000
1	1.874619000	4.872333000	-2.055014000
1	-0.032827000	3.753136000	-1.000386000
1	4.424878000	1.622472000	-0.955441000
1	-4.569720000	1.458018000	-0.140451000
1	-0.083383000	-0.967448000	1.647253000
1	0.301503000	1.211886000	1.369522000
6	-0.251829000	-0.603009000	2.773262000
8	-0.729737000	-1.487381000	3.466958000
8	0.108490000	0.570203000	2.976407000

-2194.159462

TS3-Mn-PNP-Ar₂

25	0.041240000	-0.722999000	-0.159792000
15	-2.256762000	-0.516711000	-0.280369000
15	2.344202000	-0.351278000	0.071452000
7	-0.032194000	1.352632000	0.307137000
6	-2.484328000	1.288442000	0.012200000
6	-1.319313000	2.000612000	0.354924000
6	1.056168000	2.063957000	-0.304290000
6	2.336812000	1.450950000	-0.299726000
6	3.411343000	-1.117152000	-1.284834000
6	2.967940000	-2.555240000	-1.603682000
1	3.658757000	-2.989769000	-2.332335000
1	1.967566000	-2.593160000	-2.032325000
1	2.979773000	-3.191796000	-0.716037000
6	3.150633000	-0.600345000	1.747094000
6	3.137206000	-2.088816000	2.127610000
1	3.412604000	-2.200509000	3.179939000
1	3.853159000	-2.664283000	1.535172000

1	2.148124000	-2.532423000	1.995445000
6	-3.191933000	-1.376346000	1.121374000
6	-3.288967000	-2.891806000	0.879368000
1	-3.600418000	-3.380757000	1.806767000
1	-2.339872000	-3.334113000	0.575942000
1	-4.037576000	-3.126776000	0.120508000
6	-3.016414000	-0.915186000	-1.957637000
6	-2.543993000	-2.280328000	-2.489104000
1	-2.854483000	-2.382898000	-3.532799000
1	-2.986476000	-3.106024000	-1.931696000
1	-1.460471000	-2.389936000	-2.451129000
6	0.210889000	-0.583525000	-1.912559000
8	0.332120000	-0.470268000	-3.057661000
6	0.084604000	-2.510167000	-0.200855000
6	4.515497000	0.059328000	1.987186000
1	5.334791000	-0.492992000	1.529637000
1	4.540096000	1.088313000	1.622796000
1	4.702862000	0.089046000	3.065141000
6	-4.546307000	-0.801263000	1.558765000
1	-4.911639000	-1.387016000	2.408320000
1	-4.464079000	0.234219000	1.888331000
1	-5.302154000	-0.857597000	0.773856000
6	-4.539428000	-0.789049000	-2.105567000
1	-4.809156000	-0.971108000	-3.150644000
1	-5.065706000	-1.530714000	-1.502804000
1	-4.910627000	0.200998000	-1.846164000
6	4.936406000	-1.081224000	-1.097391000
1	5.255430000	-1.775801000	-0.317896000
1	5.412958000	-1.397916000	-2.030161000
1	5.325866000	-0.095382000	-0.850818000
1	3.154746000	-0.486219000	-2.142171000
1	-2.544250000	-0.145610000	-2.578550000
1	2.447347000	-0.080810000	2.397899000
1	-2.500095000	-1.227259000	1.955582000
8	0.088407000	-3.666721000	-0.201253000
6	-3.724074000	1.947356000	0.061195000
6	-3.825912000	3.265831000	0.485396000
6	-2.680823000	3.932995000	0.921712000
6	-1.445838000	3.302710000	0.866280000
1	-4.792663000	3.754692000	0.512698000

1	-2.750918000	4.941499000	1.313225000
1	-0.562861000	3.819494000	1.219757000
6	3.438544000	2.150026000	-0.800611000
6	3.300197000	3.411209000	-1.374957000
6	2.026865000	3.961003000	-1.480382000
6	0.920453000	3.299082000	-0.954335000
1	4.165406000	3.932658000	-1.766457000
1	1.883198000	4.913366000	-1.978781000
1	-0.053803000	3.752806000	-1.059244000
1	4.418022000	1.693442000	-0.781624000
1	-4.626996000	1.419743000	-0.207460000
1	-0.230279000	-0.896564000	1.698424000
1	0.167174000	1.159541000	1.552830000
6	-0.011054000	-0.461394000	2.739955000
8	-0.035043000	-1.246704000	3.659941000
8	0.190564000	0.805449000	2.730555000

-2194.153795

5-Mn-PNP-Ar₂

25	0.103704000	-0.869755000	-0.156035000
15	-2.190831000	-0.710590000	-0.294064000
15	2.346165000	-0.436119000	0.166536000
7	0.026673000	1.156541000	-0.404947000
6	-2.416420000	1.099492000	-0.457790000
6	-1.209533000	1.843666000	-0.446355000
6	1.179077000	1.761933000	-0.960887000
6	2.444923000	1.208482000	-0.632412000
6	3.622961000	-1.498079000	-0.718649000
6	3.235408000	-2.985711000	-0.678232000
1	3.959659000	-3.563118000	-1.260701000
1	2.248546000	-3.161609000	-1.102610000
1	3.239427000	-3.378973000	0.340547000
6	2.799883000	-0.248387000	1.978140000
6	2.966443000	-1.615302000	2.661649000
1	3.040480000	-1.471213000	3.743615000
1	3.874829000	-2.126329000	2.337180000
1	2.118686000	-2.276435000	2.471564000
6	-3.028750000	-1.200189000	1.326548000
6	-3.237184000	-2.721760000	1.405449000
1	-3.465379000	-3.001092000	2.437962000

1	-2.360443000	-3.288360000	1.094569000
1	-4.083686000	-3.030805000	0.788143000
6	-3.034883000	-1.505079000	-1.769950000
6	-2.671024000	-2.993532000	-1.914742000
1	-2.898016000	-3.320238000	-2.933593000
1	-3.250144000	-3.616710000	-1.232211000
1	-1.613728000	-3.180046000	-1.730075000
6	0.336012000	-1.431667000	-1.801163000
8	0.500114000	-1.745143000	-2.905042000
6	0.140906000	-2.530660000	0.496321000
6	3.962890000	0.704506000	2.281869000
1	4.923575000	0.297223000	1.962512000
1	3.823030000	1.675108000	1.802484000
1	4.016923000	0.871152000	3.362397000
6	-4.308881000	-0.463029000	1.740714000
1	-4.624724000	-0.829465000	2.722649000
1	-4.162512000	0.613733000	1.823627000
1	-5.129483000	-0.645244000	1.042935000
6	-4.550583000	-1.300035000	-1.894409000
1	-4.904446000	-1.785751000	-2.809262000
1	-5.089203000	-1.750381000	-1.057308000
1	-4.824445000	-0.247468000	-1.959543000
6	5.089916000	-1.326918000	-0.292090000
1	5.261869000	-1.721949000	0.710541000
1	5.727766000	-1.892221000	-0.978513000
1	5.430491000	-0.292887000	-0.308293000
1	3.518885000	-1.150257000	-1.752082000
1	-2.544159000	-0.962194000	-2.586391000
1	1.890071000	0.204776000	2.381157000
1	-2.243298000	-0.935227000	2.044774000
8	0.166329000	-3.606892000	0.928018000
6	-3.650159000	1.764578000	-0.465588000
6	-3.728068000	3.151064000	-0.411130000
6	-2.545083000	3.884020000	-0.302658000
6	-1.312980000	3.246400000	-0.313611000
1	-4.691170000	3.647026000	-0.413746000
1	-2.580767000	4.962765000	-0.196472000
1	-0.416394000	3.838102000	-0.191372000
6	3.617897000	1.809872000	-1.093133000
6	3.580257000	2.916720000	-1.937718000

6	2.339211000	3.393893000	-2.354992000
6	1.160298000	2.828196000	-1.880938000
1	4.498797000	3.371092000	-2.289275000
1	2.281827000	4.214076000	-3.062590000
1	0.217036000	3.210891000	-2.243491000
1	4.578497000	1.400103000	-0.812819000
1	-4.566833000	1.192896000	-0.482949000
1	-1.861994000	1.699032000	2.223014000
1	0.124801000	1.565225000	1.431685000
6	-1.042247000	1.848169000	2.943157000
8	-1.219786000	2.055516000	4.114906000
8	0.176417000	1.780224000	2.397865000

-2194.161465

1-Mn-PNN-Ar

25	-0.538970000	-0.350558000	-0.196747000
7	-2.637661000	0.426127000	-0.103364000
15	1.746954000	-0.535159000	0.056843000
7	-0.124117000	1.549123000	-0.225505000
6	-2.430228000	1.673494000	-0.900449000
6	-1.230365000	2.470366000	-0.429865000
6	1.144775000	2.092152000	-0.219093000
6	2.260969000	1.208992000	-0.149549000
6	2.698358000	-1.568186000	-1.190169000
6	2.110044000	-2.983926000	-1.331018000
1	2.511592000	-3.449418000	-2.236120000
1	1.024234000	-2.977503000	-1.412317000
1	2.382380000	-3.618212000	-0.486182000
6	2.267330000	-0.989302000	1.818920000
6	2.276815000	-2.507561000	2.061160000
1	2.354082000	-2.698945000	3.135947000
1	3.141675000	-2.975927000	1.586070000
1	1.377047000	-3.002845000	1.700577000
6	-2.850971000	0.762867000	1.366873000
6	-3.178832000	-0.448868000	2.241140000
1	-3.077637000	-0.153178000	3.288461000
1	-2.503381000	-1.281906000	2.063113000
1	-4.205145000	-0.790566000	2.098068000
6	-3.719884000	-0.368372000	-0.820983000

6	-3.723601000	-1.880638000	-0.585560000
1	-4.493507000	-2.316893000	-1.228381000
1	-3.955039000	-2.160943000	0.439706000
1	-2.771986000	-2.324569000	-0.861726000
6	-0.590555000	-0.976067000	-1.828167000
8	-0.626156000	-1.326126000	-2.936859000
6	-0.810381000	-1.977482000	0.470697000
6	3.566037000	-0.356007000	2.336859000
1	4.438510000	-0.698762000	1.775573000
1	3.538887000	0.732376000	2.294254000
1	3.712476000	-0.648309000	3.382013000
6	-3.842966000	1.898720000	1.691913000
1	-3.698264000	2.174285000	2.740050000
1	-3.679276000	2.798945000	1.100199000
1	-4.882436000	1.594773000	1.574137000
6	-5.146389000	0.185638000	-0.660485000
1	-5.785114000	-0.272878000	-1.419523000
1	-5.568305000	-0.064701000	0.314570000
1	-5.201551000	1.266306000	-0.794875000
6	4.223330000	-1.642395000	-1.025405000
1	4.504306000	-2.123368000	-0.086306000
1	4.642722000	-2.244894000	-1.837696000
1	4.700664000	-0.664606000	-1.069855000
1	2.476633000	-1.021863000	-2.114343000
1	-3.443710000	-0.241805000	-1.870159000
1	1.434686000	-0.563723000	2.391373000
1	-1.866561000	1.119184000	1.683125000
8	-0.923197000	-3.049401000	0.910380000
6	3.561046000	1.711573000	-0.173392000
6	3.808332000	3.082464000	-0.262676000
6	2.722726000	3.956687000	-0.300238000
6	1.415581000	3.481587000	-0.272300000
1	4.825069000	3.456106000	-0.284571000
1	2.892729000	5.027549000	-0.348117000
1	0.603331000	4.195681000	-0.288546000
1	4.403046000	1.037118000	-0.099681000
1	-1.014366000	3.208788000	-1.213694000
1	-2.231366000	1.350104000	-1.922645000
1	-3.324690000	2.303916000	-0.923049000
1	-1.451539000	3.045060000	0.481222000

-1565.244034

2-Mn-PNN-Ar

25	-0.510379000	-0.411242000	0.009278000
7	-2.706135000	0.381055000	-0.067880000
15	1.809380000	-0.502481000	0.102867000
7	-0.141417000	1.583458000	-0.218076000
6	-2.457531000	1.620590000	-0.872928000
6	-1.289437000	2.448244000	-0.371451000
6	1.094463000	2.127981000	-0.170253000
6	2.238437000	1.265394000	-0.056197000
6	2.668474000	-1.405703000	-1.308147000
6	2.122510000	-2.826943000	-1.533133000
1	2.475246000	-3.195390000	-2.501400000
1	1.034244000	-2.862429000	-1.542427000
1	2.475333000	-3.521585000	-0.769825000
6	2.502948000	-1.102114000	1.757201000
6	2.520146000	-2.636063000	1.859629000
1	2.682896000	-2.926510000	2.902165000
1	3.338582000	-3.061041000	1.274305000
1	1.589214000	-3.095496000	1.528524000
6	-3.106163000	0.753819000	1.349243000
6	-3.382625000	-0.462750000	2.233631000
1	-3.345325000	-0.154093000	3.281427000
1	-2.646384000	-1.251595000	2.083562000
1	-4.375414000	-0.877743000	2.051686000
6	-3.680067000	-0.464631000	-0.879870000
6	-3.709034000	-1.962006000	-0.569184000
1	-4.369075000	-2.441150000	-1.297924000
1	-4.094859000	-2.194184000	0.421258000
1	-2.725568000	-2.406428000	-0.675715000
6	-0.521148000	-0.765818000	-1.726265000
8	-0.523328000	-0.980061000	-2.862542000
6	-0.716645000	-2.130752000	0.429424000
6	3.847067000	-0.514876000	2.207443000
1	4.663977000	-0.801334000	1.541652000
1	3.817952000	0.572726000	2.267535000
1	4.086562000	-0.899629000	3.204488000
6	-4.229268000	1.793957000	1.534945000

1	-4.218982000	2.101898000	2.584374000
1	-4.077839000	2.693707000	0.938264000
1	-5.220673000	1.398246000	1.321186000
6	-5.122636000	0.067815000	-0.946309000
1	-5.633096000	-0.420000000	-1.780624000
1	-5.681275000	-0.171512000	-0.039341000
1	-5.176874000	1.143636000	-1.113093000
6	4.203333000	-1.424901000	-1.281018000
1	4.584127000	-2.003089000	-0.436161000
1	4.573284000	-1.901797000	-2.194471000
1	4.632627000	-0.425049000	-1.239169000
1	2.349915000	-0.789364000	-2.156714000
1	-3.267052000	-0.388393000	-1.887633000
1	1.737915000	-0.731831000	2.447488000
1	-2.208559000	1.232164000	1.737898000
8	-0.777346000	-3.255497000	0.715102000
6	3.528843000	1.802346000	-0.065083000
6	3.754530000	3.174325000	-0.158356000
6	2.647315000	4.027293000	-0.223400000
6	1.353000000	3.532141000	-0.221780000
1	4.763815000	3.567806000	-0.160285000
1	2.797983000	5.101646000	-0.270561000
1	0.526987000	4.230119000	-0.259287000
1	4.384852000	1.146635000	0.019289000
1	-1.123179000	3.233055000	-1.123886000
1	-2.213373000	1.288889000	-1.881888000
1	-3.353945000	2.242711000	-0.946832000
1	-1.542361000	2.977096000	0.563279000
1	-0.556600000	-0.336506000	1.890555000
1	-0.327129000	0.372858000	1.695687000

-1566.401872

TS1-Mn-PNN-Ar

25	-0.515283000	-0.412609000	-0.044377000
7	-2.681402000	0.396515000	-0.003883000
15	1.781398000	-0.542872000	0.090545000
7	-0.133754000	1.658628000	0.040957000
6	-2.439522000	1.674023000	-0.745354000
6	-1.283492000	2.512157000	-0.208342000

6	1.152937000	2.154645000	-0.024833000
6	2.245041000	1.239463000	0.008728000
6	2.698548000	-1.398842000	-1.318085000
6	2.092850000	-2.778918000	-1.632168000
1	1.010929000	-2.741991000	-1.743623000
1	2.327562000	-3.509726000	-0.856432000
1	2.513194000	-3.149342000	-2.572370000
6	2.435194000	-1.179340000	1.742731000
6	2.382876000	-2.713339000	1.825964000
1	2.532412000	-3.024122000	2.864613000
1	3.177620000	-3.172088000	1.233333000
1	1.428546000	-3.120342000	1.491355000
6	-3.156418000	0.713634000	1.403779000
6	-3.093703000	-0.451610000	2.401424000
1	-3.064575000	-0.029962000	3.410354000
1	-2.196040000	-1.048163000	2.263370000
1	-3.965853000	-1.101586000	2.348102000
6	-3.586565000	-0.473964000	-0.870922000
6	-4.047597000	-1.769359000	-0.201725000
1	-4.406579000	-2.446588000	-0.980880000
1	-4.877840000	-1.598318000	0.485942000
1	-3.247479000	-2.272827000	0.331735000
6	-0.479400000	-0.606739000	-1.818492000
8	-0.407036000	-0.706038000	-2.971668000
6	-0.786500000	-2.135511000	0.265140000
6	3.795897000	-0.649571000	2.214015000
1	4.610858000	-0.959571000	1.556902000
1	3.807804000	0.438182000	2.285760000
1	4.007659000	-1.051280000	3.210536000
6	-4.529061000	1.399898000	1.513252000
1	-4.645058000	1.778588000	2.532487000
1	-4.643223000	2.247415000	0.835849000
1	-5.345524000	0.698928000	1.332205000
6	-4.810072000	0.215193000	-1.511224000
1	-5.276940000	-0.506159000	-2.187496000
1	-5.561823000	0.509308000	-0.779369000
1	-4.549716000	1.088054000	-2.110084000
6	4.226581000	-1.513447000	-1.211798000
1	4.524856000	-2.165267000	-0.388154000
1	4.616503000	-1.957096000	-2.133678000

1	4.718108000	-0.550319000	-1.084878000
1	2.460699000	-0.733248000	-2.155701000
1	-2.929216000	-0.758756000	-1.692495000
1	1.670018000	-0.783552000	2.417691000
1	-2.414451000	1.432591000	1.750963000
8	-0.915117000	-3.270083000	0.482743000
6	3.553099000	1.736063000	-0.034088000
6	3.818218000	3.099665000	-0.130878000
6	2.747374000	3.994229000	-0.166236000
6	1.437944000	3.537190000	-0.104041000
1	4.840532000	3.456199000	-0.171944000
1	2.933293000	5.061124000	-0.232755000
1	0.628255000	4.255298000	-0.107772000
1	4.388888000	1.052342000	0.009948000
1	-1.057112000	3.255613000	-0.980535000
1	-2.203954000	1.393304000	-1.771816000
1	-3.334962000	2.301429000	-0.777983000
1	-1.576561000	3.076623000	0.688478000
1	-0.410847000	-0.001184000	1.614219000
1	-0.290930000	0.884626000	1.086165000

-1566.384861

3-Mn-PNN-Ar

25	-0.477464000	-0.472066000	0.009501000
7	-2.647626000	0.369352000	0.033263000
15	1.783867000	-0.555028000	0.157206000
7	-0.050991000	1.517494000	0.868245000
6	-2.305868000	1.819686000	-0.064656000
6	-1.314678000	2.280607000	0.987524000
6	1.126113000	2.125068000	0.281725000
6	2.181350000	1.245743000	-0.038225000
6	2.804741000	-1.402744000	-1.179990000
6	2.126000000	-2.707175000	-1.628781000
1	2.684517000	-3.138464000	-2.465463000
1	1.101292000	-2.536199000	-1.953318000
1	2.104341000	-3.446939000	-0.824893000
6	2.459680000	-0.999587000	1.855912000
6	2.288349000	-2.503302000	2.116610000
1	2.505877000	-2.725597000	3.165980000

1	2.973717000	-3.098214000	1.507563000
1	1.267857000	-2.829192000	1.905816000
6	-3.275147000	0.054850000	1.380481000
6	-3.717095000	-1.400664000	1.512278000
1	-3.882177000	-1.617613000	2.571000000
1	-2.950125000	-2.078208000	1.144682000
1	-4.654964000	-1.596755000	0.989791000
6	-3.451688000	0.036545000	-1.214838000
6	-3.481307000	-1.438190000	-1.627910000
1	-3.884426000	-1.492031000	-2.643479000
1	-4.117102000	-2.051186000	-0.991799000
1	-2.482582000	-1.863266000	-1.639747000
6	-0.325119000	-0.153673000	-1.744819000
8	-0.196250000	-0.050457000	-2.900568000
6	-0.733494000	-2.203457000	-0.079821000
6	3.857287000	-0.492255000	2.232501000
1	4.648260000	-1.046964000	1.727234000
1	3.982263000	0.567947000	2.000928000
1	4.008338000	-0.618416000	3.309986000
6	-4.395099000	0.990195000	1.878626000
1	-4.584266000	0.749710000	2.928742000
1	-4.125076000	2.046861000	1.838670000
1	-5.333276000	0.859774000	1.340659000
6	-4.881932000	0.604374000	-1.255338000
1	-5.253780000	0.534755000	-2.281025000
1	-5.561000000	0.028709000	-0.623541000
1	-4.938247000	1.652547000	-0.958117000
6	4.291501000	-1.660349000	-0.889116000
1	4.415418000	-2.431661000	-0.126173000
1	4.777421000	-2.023420000	-1.800286000
1	4.833917000	-0.775269000	-0.557051000
1	2.727363000	-0.687955000	-2.006829000
1	-2.884617000	0.542741000	-1.998169000
1	1.729231000	-0.481370000	2.488063000
1	-2.436205000	0.164831000	2.065681000
8	-0.866978000	-3.361531000	-0.028200000
6	3.355682000	1.772323000	-0.578634000
6	3.484801000	3.139412000	-0.827500000
6	2.430652000	3.993361000	-0.524094000
6	1.255662000	3.490227000	0.037908000

1	4.397594000	3.527266000	-1.264602000
1	2.514129000	5.056383000	-0.719414000
1	0.455545000	4.178152000	0.274614000
1	4.174273000	1.115106000	-0.838050000
1	-1.165539000	3.355421000	0.883318000
1	-1.849610000	1.972754000	-1.043364000
1	-3.193977000	2.458843000	-0.018138000
1	-1.701965000	2.122333000	1.993386000
1	-0.604717000	-0.901280000	1.571813000
1	0.194694000	1.174935000	1.790464000

-1566.399571

1-Mn-PNN-Ar₂

25	-0.091615000	-0.764468000	-0.245532000
7	-2.380821000	-0.418326000	-0.082376000
15	2.098370000	-0.390154000	0.245245000
7	-0.117804000	1.193891000	-0.097811000
6	-2.474649000	0.999428000	0.339803000
6	-1.288645000	1.775434000	0.350239000
6	0.993381000	1.949064000	-0.487422000
6	2.256951000	1.317751000	-0.377431000
6	3.531534000	-1.345588000	-0.494194000
6	3.191007000	-2.833311000	-0.669896000
1	4.028210000	-3.341225000	-1.158167000
1	2.304800000	-2.975766000	-1.287223000
1	3.014817000	-3.325857000	0.289171000
6	2.247028000	-0.257199000	2.113762000
6	2.214436000	-1.641611000	2.778002000
1	2.135851000	-1.528186000	3.863474000
1	3.127079000	-2.207417000	2.573842000
1	1.364879000	-2.237781000	2.439360000
6	-2.787362000	-1.377333000	1.055463000
6	-3.064281000	-2.807849000	0.584158000
1	-3.069254000	-3.459525000	1.460807000
1	-2.319500000	-3.190713000	-0.101080000
1	-4.046797000	-2.883281000	0.114255000
6	-3.026481000	-0.553116000	-1.468638000
6	-2.729517000	-1.852803000	-2.239844000
1	-2.761030000	-1.618457000	-3.306975000

1	-3.477406000	-2.623642000	-2.054804000
1	-1.748462000	-2.259108000	-2.018592000
6	0.287758000	-1.006451000	-1.935099000
8	0.576171000	-1.108375000	-3.054874000
6	-0.001079000	-2.522627000	0.070447000
6	3.381705000	0.621827000	2.655808000
1	4.354864000	0.138833000	2.560930000
1	3.424830000	1.587357000	2.147947000
1	3.211455000	0.810629000	3.720767000
6	-3.939031000	-0.981687000	1.998733000
1	-4.020180000	-1.770760000	2.751764000
1	-3.759519000	-0.046903000	2.524698000
1	-4.900903000	-0.923383000	1.484989000
6	-4.542388000	-0.301859000	-1.552754000
1	-4.865213000	-0.503162000	-2.577547000
1	-5.097321000	-0.978047000	-0.898089000
1	-4.820177000	0.723699000	-1.322977000
6	4.887323000	-1.183635000	0.211468000
1	4.887673000	-1.680209000	1.184095000
1	5.666017000	-1.654961000	-0.395968000
1	5.171948000	-0.142798000	0.366034000
1	3.604384000	-0.898450000	-1.491913000
1	-2.519714000	0.251910000	-2.005742000
1	1.300121000	0.249130000	2.338097000
1	-1.892372000	-1.402401000	1.686964000
8	0.130658000	-3.653012000	0.301663000
6	-3.676766000	1.606281000	0.714849000
6	-3.736870000	2.916483000	1.182908000
6	-2.553181000	3.642266000	1.300412000
6	-1.353659000	3.080603000	0.894488000
1	-4.688443000	3.344263000	1.474725000
1	-2.561727000	4.646932000	1.709774000
1	-0.439738000	3.647822000	1.003738000
6	3.417814000	1.956489000	-0.808605000
6	3.358803000	3.233298000	-1.367482000
6	2.115800000	3.853376000	-1.503822000
6	0.948920000	3.228846000	-1.074252000
1	4.262442000	3.725324000	-1.707100000
1	2.049158000	4.832426000	-1.966524000
1	-0.003438000	3.718606000	-1.226783000

1	4.376306000	1.458993000	-0.728625000
1	-4.594393000	1.045828000	0.672680000

-1717.676580

2-Mn-PNN-Ar₂

25	0.083365000	-0.923381000	-0.036719000
7	2.491515000	-0.428048000	0.006827000
15	-2.133466000	-0.355826000	-0.267227000
7	0.216514000	1.108265000	0.140110000
6	2.463796000	0.887022000	-0.662419000
6	1.297898000	1.683698000	-0.492051000
6	-0.837056000	1.841487000	0.652564000
6	-2.128737000	1.254847000	0.600504000
6	-3.529872000	-1.338082000	0.519298000
6	-3.269765000	-2.851140000	0.476587000
1	-4.098326000	-3.374017000	0.964112000
1	-2.352891000	-3.123276000	0.996613000
1	-3.199288000	-3.223616000	-0.548483000
6	-2.525824000	0.050502000	-2.061288000
6	-2.617569000	-1.229418000	-2.904371000
1	-2.659123000	-0.973292000	-3.967160000
1	-3.519436000	-1.800473000	-2.669037000
1	-1.756328000	-1.883157000	-2.748294000
6	3.420726000	-1.392685000	-0.714775000
6	2.955770000	-2.851319000	-0.691731000
1	3.714573000	-3.466906000	-1.183136000
1	2.028688000	-2.975668000	-1.242992000
1	2.814242000	-3.239736000	0.314876000
6	2.737572000	-0.207182000	1.503659000
6	2.786379000	-1.511433000	2.300938000
1	2.681166000	-1.275172000	3.362573000
1	3.732910000	-2.038203000	2.174227000
1	1.977259000	-2.185554000	2.026538000
6	-0.252859000	-1.160881000	1.694857000
8	-0.535563000	-1.320308000	2.802506000
6	-0.086253000	-2.687984000	-0.272543000
6	-3.691319000	1.011402000	-2.330683000
1	-4.660744000	0.527631000	-2.210913000
1	-3.656655000	1.884973000	-1.676528000
1	-3.628444000	1.366019000	-3.364668000

6	4.913790000	-1.346739000	-0.326710000
1	5.482305000	-1.875149000	-1.096766000
1	5.316578000	-0.340146000	-0.250004000
1	5.101058000	-1.855622000	0.619811000
6	3.925375000	0.694235000	1.886451000
1	3.778670000	1.014318000	2.922158000
1	4.886505000	0.182924000	1.837196000
1	3.972169000	1.591354000	1.268699000
6	-4.945594000	-1.030145000	0.005365000
1	-5.090143000	-1.416851000	-1.005768000
1	-5.676222000	-1.525977000	0.651660000
1	-5.180485000	0.033513000	-0.006511000
1	-3.464785000	-1.016838000	1.564492000
1	1.842101000	0.334458000	1.807339000
1	-1.605051000	0.576362000	-2.337717000
1	3.347460000	-1.079146000	-1.757102000
8	-0.249047000	-3.827983000	-0.400827000
6	3.519959000	1.388337000	-1.424534000
6	3.471631000	2.651776000	-2.016288000
6	2.338571000	3.440641000	-1.838406000
6	1.269815000	2.961855000	-1.093095000
1	4.310013000	3.002866000	-2.606076000
1	2.272878000	4.420532000	-2.299357000
1	0.372243000	3.559430000	-1.004988000
6	-3.222897000	1.889830000	1.191388000
6	-3.074190000	3.118763000	1.831017000
6	-1.806953000	3.709023000	1.877830000
6	-0.706090000	3.089362000	1.302117000
1	-3.926621000	3.602886000	2.292486000
1	-1.672978000	4.657250000	2.388129000
1	0.272854000	3.545454000	1.381647000
1	-4.201905000	1.428194000	1.164127000
1	4.413075000	0.802229000	-1.573620000
1	0.446018000	-1.088671000	-1.818685000
1	0.387365000	-0.320841000	-1.766553000

-1718.850941

TS1-Mn-PNN-Ar₂

25	0.057827000	-0.932922000	0.074372000
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7	-2.557765000	-0.543300000	0.006784000
15	2.235496000	-0.243753000	0.257516000
7	-0.311232000	1.183899000	0.199392000
6	-2.692625000	0.815908000	0.535447000
6	-1.581429000	1.684810000	0.559007000
6	0.705141000	1.976455000	-0.355734000
6	2.034309000	1.477510000	-0.355028000
6	3.569032000	-1.015531000	-0.824808000
6	3.367140000	-2.534023000	-0.961508000
1	4.130051000	-2.938730000	-1.633416000
1	2.391689000	-2.783444000	-1.375239000
1	3.465701000	-3.044340000	-0.000556000
6	2.834997000	-0.093503000	2.029722000
6	3.070714000	-1.483214000	2.639015000
1	3.250993000	-1.390205000	3.714185000
1	3.945045000	-1.972245000	2.201512000
1	2.207031000	-2.136024000	2.496626000
6	-3.366929000	-1.530627000	0.836132000
6	-2.634497000	-2.852578000	1.069581000
1	-3.255777000	-3.500319000	1.695163000
1	-1.697625000	-2.677525000	1.592782000
1	-2.424560000	-3.385189000	0.142785000
6	-2.757440000	-0.525028000	-1.502393000
6	-2.610061000	-1.911511000	-2.135332000
1	-2.457603000	-1.792988000	-3.210435000
1	-3.500034000	-2.525101000	-1.994731000
1	-1.752817000	-2.447218000	-1.732410000
6	0.317697000	-1.091952000	-1.691785000
8	0.573786000	-1.159998000	-2.818545000
6	0.393052000	-2.648126000	0.396621000
6	3.994061000	0.873650000	2.303128000
1	4.955291000	0.466725000	1.989622000
1	3.847980000	1.836040000	1.807788000
1	4.054501000	1.060258000	3.380274000
6	-4.813535000	-1.831305000	0.391888000
1	-5.309057000	-2.374752000	1.200829000
1	-5.405977000	-0.943320000	0.183803000
1	-4.846480000	-2.468817000	-0.491945000
6	-4.028495000	0.162763000	-2.033842000
1	-3.914147000	0.285526000	-3.114835000

1	-4.931502000	-0.423767000	-1.865945000
1	-4.170513000	1.154946000	-1.604824000
6	5.029305000	-0.720244000	-0.446832000
1	5.307413000	-1.229948000	0.477941000
1	5.684132000	-1.099601000	-1.237225000
1	5.244141000	0.340428000	-0.322155000
1	3.361717000	-0.558878000	-1.798295000
1	-1.919082000	0.086394000	-1.842315000
1	1.937215000	0.323895000	2.496706000
1	-3.425946000	-1.050117000	1.813790000
8	0.644727000	-3.754131000	0.633609000
6	-3.914278000	1.299700000	1.028063000
6	-4.052801000	2.581582000	1.546643000
6	-2.943948000	3.423113000	1.594441000
6	-1.724149000	2.967316000	1.119080000
1	-5.016897000	2.911844000	1.915426000
1	-3.019947000	4.416927000	2.020934000
1	-0.848618000	3.596638000	1.208548000
6	3.060246000	2.238265000	-0.922178000
6	2.806621000	3.468569000	-1.522785000
6	1.492572000	3.931250000	-1.574385000
6	0.456884000	3.201216000	-1.002949000
1	3.614483000	4.039852000	-1.964071000
1	1.264248000	4.865901000	-2.075107000
1	-0.556268000	3.570020000	-1.083862000
1	4.073180000	1.858696000	-0.920755000
1	-4.786738000	0.666048000	1.007510000
1	-0.125714000	-0.539103000	1.740395000
1	-0.082241000	0.422891000	1.180459000

-1718.815943

3-Mn-PNN-Ar₂

25	0.034209000	-0.849484000	0.023697000
7	-2.415797000	-0.578766000	-0.059429000
15	2.214855000	-0.275792000	0.299889000
7	-0.187847000	1.211369000	0.543310000
6	-2.625505000	0.825642000	0.324596000
6	-1.556061000	1.668858000	0.660415000
6	0.777001000	2.017500000	-0.191235000

6	2.086275000	1.496112000	-0.235012000
6	3.558868000	-0.978712000	-0.817980000
6	3.327764000	-2.476145000	-1.075044000
1	4.078195000	-2.841452000	-1.783063000
1	2.341919000	-2.663049000	-1.497386000
1	3.417888000	-3.064396000	-0.158748000
6	2.811039000	-0.233627000	2.080266000
6	3.056239000	-1.662355000	2.587378000
1	3.235382000	-1.647983000	3.666834000
1	3.933458000	-2.111294000	2.114780000
1	2.193921000	-2.304199000	2.394994000
6	-2.929697000	-1.507655000	1.057019000
6	-2.899870000	-2.987135000	0.672245000
1	-2.971792000	-3.575524000	1.590157000
1	-1.982857000	-3.272039000	0.171929000
1	-3.749645000	-3.258754000	0.042427000
6	-2.880776000	-0.795168000	-1.504361000
6	-2.407597000	-2.106968000	-2.157818000
1	-2.342843000	-1.935017000	-3.235184000
1	-3.114925000	-2.920609000	-1.999158000
1	-1.428790000	-2.420145000	-1.812599000
6	0.280183000	-0.665263000	-1.745556000
8	0.529788000	-0.608858000	-2.882097000
6	0.296465000	-2.586661000	0.116388000
6	3.956827000	0.724738000	2.427086000
1	4.920367000	0.361817000	2.069413000
1	3.791121000	1.722403000	2.013355000
1	4.028528000	0.822196000	3.515497000
6	-4.298648000	-1.221994000	1.706242000
1	-4.456460000	-1.988249000	2.470368000
1	-4.341599000	-0.257524000	2.209385000
1	-5.130935000	-1.291718000	1.002676000
6	-4.386591000	-0.665548000	-1.814860000
1	-4.539635000	-0.951823000	-2.858691000
1	-4.983868000	-1.344930000	-1.203476000
1	-4.770743000	0.346108000	-1.707496000
6	5.019539000	-0.729281000	-0.412820000
1	5.287191000	-1.301378000	0.478064000
1	5.676559000	-1.062702000	-1.222284000
1	5.245659000	0.318880000	-0.216211000

1	3.362828000	-0.450611000	-1.757301000
1	-2.364330000	0.017122000	-2.019891000
1	1.904487000	0.129244000	2.578504000
1	-2.174139000	-1.357651000	1.827554000
8	0.517107000	-3.719980000	0.277838000
6	-3.913957000	1.383581000	0.438432000
6	-4.136377000	2.672200000	0.904877000
6	-3.063224000	3.458537000	1.314470000
6	-1.782380000	2.944617000	1.193214000
1	-5.151821000	3.044398000	0.977291000
1	-3.219985000	4.450491000	1.721352000
1	-0.928271000	3.535233000	1.502105000
6	3.077584000	2.227592000	-0.889103000
6	2.776669000	3.427924000	-1.535963000
6	1.465959000	3.889658000	-1.545484000
6	0.463023000	3.190154000	-0.869580000
1	3.556388000	3.975796000	-2.052088000
1	1.210290000	4.798086000	-2.078796000
1	-0.551706000	3.560879000	-0.891609000
1	4.088757000	1.846708000	-0.938790000
1	-4.773105000	0.785526000	0.195507000
1	-0.115682000	-1.076009000	1.626292000
1	0.155968000	1.095027000	1.493583000

3-sol -1718.820456

1-Mn-NNN-Ar

25	-0.414558000	-0.381860000	-0.223376000
7	-2.480156000	0.512170000	-0.117513000
7	1.917078000	-0.552816000	0.097565000
7	0.070816000	1.451463000	-0.258716000
6	-2.204878000	1.730747000	-0.943069000
6	-0.947605000	2.454021000	-0.500937000
6	1.383141000	1.843742000	-0.248497000
6	2.376560000	0.841486000	-0.106893000
6	2.558920000	-1.475872000	-0.948156000
6	1.891868000	-2.851519000	-1.136615000
1	2.105726000	-3.179729000	-2.157215000
1	0.815611000	-2.823966000	-1.019780000
1	2.297642000	-3.605858000	-0.463461000
6	2.020107000	-0.915716000	1.594191000

6	1.996274000	-2.418560000	1.888118000
1	1.843550000	-2.548463000	2.962301000
1	2.948056000	-2.889894000	1.635666000
1	1.201323000	-2.949309000	1.381258000
6	-2.661725000	0.898929000	1.347670000
6	-3.061686000	-0.266009000	2.253912000
1	-2.950707000	0.055394000	3.292702000
1	-2.431888000	-1.139249000	2.107412000
1	-4.104277000	-0.555485000	2.113807000
6	-3.626047000	-0.216022000	-0.810109000
6	-3.728529000	-1.721820000	-0.558001000
1	-4.568599000	-2.102115000	-1.145989000
1	-3.913208000	-1.977398000	0.482778000
1	-2.834853000	-2.242009000	-0.889815000
6	-0.578598000	-0.995060000	-1.853589000
8	-0.697598000	-1.328249000	-2.960942000
6	-0.853724000	-1.971756000	0.468218000
6	3.186953000	-0.301942000	2.388884000
1	4.158826000	-0.664419000	2.047707000
1	3.192978000	0.785656000	2.362251000
1	3.070328000	-0.608079000	3.432352000
6	-3.574096000	2.105482000	1.652307000
1	-3.391170000	2.401359000	2.688882000
1	-3.364681000	2.976125000	1.031948000
1	-4.633231000	1.866948000	1.563292000
6	-5.008703000	0.435684000	-0.633802000
1	-5.687499000	0.016412000	-1.380578000
1	-5.433468000	0.222320000	0.348774000
1	-4.991147000	1.516087000	-0.777261000
6	4.080621000	-1.735171000	-0.847533000
1	4.382561000	-1.998308000	0.167342000
1	4.327045000	-2.586060000	-1.487122000
1	4.685767000	-0.899793000	-1.189901000
1	2.373119000	-0.911431000	-1.864080000
1	-3.360346000	-0.118044000	-1.864749000
1	1.107339000	-0.483717000	2.017697000
1	-1.654163000	1.196983000	1.647467000
8	-1.143745000	-3.002593000	0.921217000
6	3.716856000	1.222866000	-0.094793000
6	4.114563000	2.553816000	-0.236849000

6	3.141631000	3.539782000	-0.363281000
6	1.796842000	3.193028000	-0.360196000
1	5.168178000	2.806103000	-0.223149000
1	3.425476000	4.582818000	-0.457003000
1	1.054353000	3.975010000	-0.442236000
1	4.484389000	0.488963000	0.074515000
1	-0.671881000	3.142766000	-1.310897000
1	-2.043051000	1.376666000	-1.961310000
1	-3.058601000	2.414370000	-0.965613000
1	-1.121444000	3.076025000	0.388962000

-1278.572432

2-Mn-NNN-Ar

25	-0.389125000	-0.442199000	-0.007541000
7	-2.521640000	0.489986000	0.010810000
7	1.982210000	-0.553860000	0.126392000
7	0.126943000	1.429418000	0.501328000
6	-2.118170000	1.919531000	-0.203663000
6	-0.966631000	2.357083000	0.688408000
6	1.364580000	1.852070000	0.146830000
6	2.331816000	0.853176000	-0.191554000
6	2.676787000	-1.517722000	-0.838335000
6	1.885724000	-2.787232000	-1.166189000
1	2.490612000	-3.401806000	-1.838954000
1	0.955900000	-2.561824000	-1.678545000
1	1.661600000	-3.385848000	-0.285440000
6	2.246821000	-0.767518000	1.624133000
6	1.885877000	-2.173878000	2.105500000
1	1.867711000	-2.176192000	3.198523000
1	2.623463000	-2.913356000	1.791718000
1	0.910016000	-2.499059000	1.751251000
6	-3.116226000	0.327374000	1.402395000
6	-3.590649000	-1.096096000	1.695352000
1	-3.718184000	-1.208155000	2.775038000
1	-2.875854000	-1.845086000	1.359910000
1	-4.555833000	-1.306521000	1.231170000
6	-3.407710000	0.118586000	-1.176114000
6	-3.531285000	-1.371789000	-1.501046000
1	-4.130706000	-1.464294000	-2.411109000
1	-4.027033000	-1.949157000	-0.723947000

1	-2.562784000	-1.817577000	-1.702150000
6	-0.265725000	-0.259273000	-1.772705000
8	-0.185459000	-0.144907000	-2.919221000
6	-0.843495000	-2.168742000	-0.119919000
6	3.632948000	-0.372696000	2.170460000
1	4.392640000	-1.134901000	2.002349000
1	3.982223000	0.573595000	1.758394000
1	3.534594000	-0.244975000	3.252562000
6	-4.193652000	1.333526000	1.857099000
1	-4.331186000	1.195473000	2.933320000
1	-3.898311000	2.372043000	1.706555000
1	-5.160510000	1.175778000	1.382744000
6	-4.807355000	0.757602000	-1.175326000
1	-5.227871000	0.669648000	-2.180268000
1	-5.484594000	0.240851000	-0.492781000
1	-4.794277000	1.816719000	-0.918178000
6	4.116813000	-1.947934000	-0.483345000
1	4.125658000	-2.717695000	0.290482000
1	4.566787000	-2.385531000	-1.378464000
1	4.758305000	-1.135577000	-0.155743000
1	2.721665000	-0.943786000	-1.764454000
1	-2.863876000	0.552284000	-2.017087000
1	1.552534000	-0.062745000	2.081072000
1	-2.266879000	0.515784000	2.055351000
8	-1.146778000	-3.288677000	-0.123124000
6	3.551101000	1.238889000	-0.738478000
6	3.902284000	2.583166000	-0.902358000
6	3.015978000	3.562104000	-0.462509000
6	1.779154000	3.208621000	0.061746000
1	4.858054000	2.844640000	-1.340031000
1	3.279901000	4.612376000	-0.537267000
1	1.107730000	3.994385000	0.381404000
1	4.271290000	0.497145000	-1.045955000
1	-0.723627000	3.383913000	0.399012000
1	-1.766116000	1.990980000	-1.232847000
1	-2.970238000	2.597019000	-0.100821000
1	-1.278181000	2.406526000	1.742449000
1	-0.658936000	-0.963044000	1.790339000
1	-0.386162000	-0.250279000	1.855662000

-1279.731102

TS1-Mn-NN-Ar

25	-0.393600000	-0.531965000	0.001954000
7	-2.517019000	0.450789000	0.037385000
7	2.067134000	-0.523026000	0.136202000
7	0.155081000	1.335347000	0.846218000
6	-2.088179000	1.890080000	0.056082000
6	-1.012472000	2.178451000	1.093298000
6	1.336605000	1.828472000	0.293856000
6	2.313745000	0.896347000	-0.150117000
6	2.737513000	-1.443952000	-0.869975000
6	1.968350000	-2.740645000	-1.139885000
1	2.573258000	-3.372944000	-1.796560000
1	1.027793000	-2.542523000	-1.645414000
1	1.760088000	-3.305015000	-0.234073000
6	2.379892000	-0.734789000	1.620283000
6	1.974333000	-2.115869000	2.117871000
1	2.111299000	-2.155915000	3.201606000
1	2.606513000	-2.891992000	1.683151000
1	0.932551000	-2.333498000	1.892306000
6	-3.212203000	0.116481000	1.352635000
6	-3.768639000	-1.304160000	1.415428000
1	-3.998133000	-1.531090000	2.460324000
1	-3.052453000	-2.039346000	1.060896000
1	-4.696146000	-1.407551000	0.850646000
6	-3.337207000	0.261153000	-1.237105000
6	-3.494736000	-1.182714000	-1.719776000
1	-2.545542000	-1.706498000	-1.723577000
1	-3.866266000	-1.150245000	-2.748667000
1	-4.205830000	-1.761878000	-1.133668000
6	-0.227035000	-0.263182000	-1.767096000
8	-0.089391000	-0.126843000	-2.909466000
6	-0.833518000	-2.247416000	-0.144254000
6	3.803600000	-0.387335000	2.092120000
1	4.521076000	-1.187692000	1.912836000
1	4.176263000	0.534037000	1.639399000
1	3.753725000	-0.228153000	3.173096000
6	-4.279108000	1.104729000	1.874078000
1	-4.356017000	0.970364000	2.956534000

1	-4.029044000	2.150992000	1.702017000
1	-5.266821000	0.916265000	1.452673000
6	-4.712214000	0.953087000	-1.251143000
1	-5.027880000	1.069427000	-2.291293000
1	-5.469249000	0.352216000	-0.743063000
1	-4.701719000	1.945413000	-0.802763000
6	4.214065000	-1.802078000	-0.593017000
1	4.295722000	-2.612146000	0.135844000
1	4.660825000	-2.154864000	-1.526444000
1	4.810985000	-0.966842000	-0.235115000
1	2.699660000	-0.883688000	-1.804152000
1	-2.720373000	0.753433000	-1.990994000
1	1.737510000	0.026083000	2.060136000
1	-2.390113000	0.148098000	2.063020000
8	-1.130060000	-3.368141000	-0.092026000
6	3.447337000	1.374127000	-0.807334000
6	3.655521000	2.737749000	-1.024374000
6	2.722277000	3.649206000	-0.551066000
6	1.579282000	3.197715000	0.103404000
1	4.542017000	3.070537000	-1.550783000
1	2.865598000	4.713529000	-0.701179000
1	0.851775000	3.923824000	0.438512000
1	4.192255000	0.686910000	-1.174754000
1	-0.772478000	3.240480000	1.064607000
1	-1.664632000	2.103888000	-0.926736000
1	-2.938753000	2.559148000	0.202934000
1	-1.382143000	1.972974000	2.101869000
1	-0.414971000	-0.646633000	1.706468000
1	0.035621000	0.365389000	1.511327000

-1279.715286

3-Mn-NNN-Ar

25	-0.407236000	-0.547741000	0.008474000
7	-2.513351000	0.382763000	0.085025000
7	2.131554000	-0.492494000	0.178729000
7	0.135361000	1.217601000	1.085081000
6	-2.089944000	1.807878000	0.254464000
6	-1.086673000	1.992840000	1.377403000
6	1.246372000	1.817499000	0.400430000

6	2.270914000	0.947231000	-0.042280000
6	2.830387000	-1.292648000	-0.912339000
6	2.112252000	-2.586035000	-1.309737000
1	2.687539000	-3.061866000	-2.109500000
1	1.117307000	-2.378102000	-1.690059000
1	2.026689000	-3.298897000	-0.492749000
6	2.446875000	-0.860364000	1.619131000
6	2.222316000	-2.340376000	1.922382000
1	2.262713000	-2.478303000	3.006262000
1	2.990301000	-2.978053000	1.484005000
1	1.238945000	-2.654837000	1.577091000
6	-3.220794000	-0.114453000	1.338877000
6	-3.806691000	-1.517295000	1.191359000
1	-4.034014000	-1.900374000	2.189705000
1	-3.101547000	-2.199877000	0.724707000
1	-4.738841000	-1.518971000	0.623280000
6	-3.284500000	0.321132000	-1.227764000
6	-3.392172000	-1.057918000	-1.884893000
1	-3.732664000	-0.910161000	-2.913991000
1	-4.109316000	-1.713610000	-1.394865000
1	-2.427530000	-1.554743000	-1.918287000
6	-0.188803000	-0.035251000	-1.704379000
8	-0.035564000	0.177930000	-2.839707000
6	-0.816367000	-2.227684000	-0.288810000
6	3.800577000	-0.375202000	2.169516000
1	4.633579000	-1.007136000	1.864431000
1	4.015635000	0.653349000	1.873948000
1	3.753210000	-0.402645000	3.261961000
6	-4.268255000	0.819654000	1.976913000
1	-4.548496000	0.389322000	2.942489000
1	-3.888712000	1.822996000	2.176752000
1	-5.178421000	0.911910000	1.385199000
6	-4.669498000	0.992015000	-1.213168000
1	-5.005920000	1.115079000	-2.246048000
1	-5.410973000	0.376037000	-0.700953000
1	-4.662202000	1.980578000	-0.752065000
6	4.325069000	-1.605332000	-0.691899000
1	4.464630000	-2.426643000	0.012932000
1	4.751922000	-1.923044000	-1.646892000
1	4.905829000	-0.757444000	-0.334694000

1	2.752041000	-0.642707000	-1.784249000
1	-2.652627000	0.909838000	-1.894846000
1	1.685923000	-0.339709000	2.199377000
1	-2.402118000	-0.215028000	2.049517000
8	-1.076646000	-3.361807000	-0.373125000
6	3.342981000	1.518300000	-0.734113000
6	3.399145000	2.883925000	-1.014630000
6	2.376105000	3.719485000	-0.591826000
6	1.307069000	3.180708000	0.121931000
1	4.242389000	3.279461000	-1.568641000
1	2.398207000	4.780373000	-0.811660000
1	0.507471000	3.835332000	0.439484000
1	4.151000000	0.899804000	-1.090203000
1	-0.889316000	3.055432000	1.532436000
1	-1.612368000	2.112065000	-0.677764000
1	-2.941399000	2.475148000	0.415328000
1	-1.478434000	1.611692000	2.319046000
1	-0.561298000	-1.171212000	1.506884000
1	0.456311000	0.805726000	1.952168000

-1279.730503

1-Mn-NNN-Ar₂

25	0.022927000	-0.787117000	-0.205954000
7	-2.269030000	-0.319892000	-0.078547000
7	2.244923000	-0.393474000	0.312186000
7	0.072846000	1.128030000	-0.043289000
6	-2.288193000	1.111606000	0.316066000
6	-1.058344000	1.813846000	0.331780000
6	1.255992000	1.721181000	-0.457082000
6	2.418157000	0.920249000	-0.342717000
6	3.304351000	-1.381056000	-0.172390000
6	2.840318000	-2.835627000	-0.263060000
1	3.684566000	-3.439067000	-0.608261000
1	2.037814000	-2.953434000	-0.985580000
1	2.513774000	-3.240803000	0.692586000
6	2.130863000	-0.165811000	1.830084000
6	1.879431000	-1.449127000	2.621376000
1	1.645717000	-1.174541000	3.653277000
1	2.752260000	-2.102229000	2.647917000
1	1.037013000	-2.014244000	2.225264000

6	-2.765192000	-1.236287000	1.062887000
6	-3.221890000	-2.622550000	0.597025000
1	-3.322730000	-3.257456000	1.480149000
1	-2.529022000	-3.112557000	-0.073555000
1	-4.200858000	-2.573186000	0.116413000
6	-2.893388000	-0.429628000	-1.477914000
6	-2.690850000	-1.764942000	-2.217667000
1	-2.660810000	-1.548392000	-3.288457000
1	-3.513919000	-2.458814000	-2.049517000
1	-1.761369000	-2.258608000	-1.955188000
6	0.323958000	-1.052172000	-1.913018000
8	0.575120000	-1.174577000	-3.037406000
6	-0.088132000	-2.555271000	0.089290000
6	3.247388000	0.661778000	2.492179000
1	4.129978000	0.070161000	2.733255000
1	3.548407000	1.511160000	1.878607000
1	2.853467000	1.058869000	3.431970000
6	-3.840322000	-0.712092000	2.032863000
1	-3.966684000	-1.473397000	2.807893000
1	-3.556308000	0.213413000	2.528448000
1	-4.810871000	-0.576300000	1.550530000
6	-4.380051000	-0.049419000	-1.603159000
1	-4.704820000	-0.269516000	-2.623414000
1	-5.003803000	-0.639379000	-0.927330000
1	-4.566172000	1.006792000	-1.425773000
6	4.656297000	-1.348673000	0.567472000
1	4.599298000	-1.862928000	1.528560000
1	5.390054000	-1.881771000	-0.042544000
1	5.038189000	-0.346975000	0.745245000
1	3.478908000	-1.065672000	-1.201338000
1	-2.308348000	0.319133000	-2.016664000
1	1.227783000	0.441816000	1.908136000
1	-1.869223000	-1.371853000	1.676148000
8	-0.182427000	-3.693477000	0.290413000
6	-3.456952000	1.801957000	0.648057000
6	-3.442679000	3.131850000	1.063367000
6	-2.220584000	3.793596000	1.167512000
6	-1.049308000	3.145512000	0.809706000
1	-4.370949000	3.627177000	1.321523000
1	-2.177880000	4.815308000	1.529794000

1	-0.103070000	3.658802000	0.910786000
6	3.625697000	1.393478000	-0.852126000
6	3.712698000	2.640707000	-1.475426000
6	2.571719000	3.426915000	-1.594671000
6	1.357466000	2.971437000	-1.093367000
1	4.664449000	2.978590000	-1.867837000
1	2.616537000	4.386873000	-2.097419000
1	0.464040000	3.562800000	-1.240511000
1	4.525649000	0.802788000	-0.784373000
1	-4.407642000	1.298409000	0.611206000

-1431.011957

2-Mn-NNN-Ar₂

25	-0.006659000	-0.948807000	-0.060424000
7	2.396201000	-0.333126000	0.002204000
7	-2.310157000	-0.321114000	-0.312525000
7	0.020342000	1.035564000	0.055966000
6	2.310557000	1.006510000	-0.616471000
6	1.086935000	1.716272000	-0.472220000
6	-1.094721000	1.625597000	0.606111000
6	-2.312834000	0.904845000	0.518683000
6	-3.380893000	-1.298143000	0.167006000
6	-3.002569000	-2.774506000	0.032640000
1	-3.860353000	-3.379954000	0.338170000
1	-2.175780000	-3.031536000	0.687395000
1	-2.743600000	-3.058180000	-0.985359000
6	-2.351038000	0.093824000	-1.788245000
6	-2.311669000	-1.099692000	-2.743546000
1	-2.072319000	-0.736724000	-3.746299000
1	-3.272291000	-1.612118000	-2.802894000
1	-1.554637000	-1.828307000	-2.457574000
6	3.390732000	-1.211802000	-0.746103000
6	2.994733000	-2.687975000	-0.815236000
1	3.789873000	-3.240347000	-1.323897000
1	2.084992000	-2.825058000	-1.392216000
1	2.853525000	-3.137181000	0.165684000
6	2.607784000	-0.160626000	1.510030000
6	2.693194000	-1.494016000	2.254859000
1	2.560039000	-1.306907000	3.323121000
1	3.661363000	-1.978933000	2.125737000

1	1.916701000	-2.188141000	1.938212000
6	-0.359361000	-1.189540000	1.674915000
8	-0.636830000	-1.366121000	2.778538000
6	-0.001073000	-2.736058000	-0.253657000
6	-3.453539000	1.082052000	-2.211346000
1	-4.418818000	0.605187000	-2.376438000
1	-3.576576000	1.888688000	-1.488262000
1	-3.146056000	1.534016000	-3.158777000
6	4.869588000	-1.120090000	-0.315207000
1	5.480435000	-1.576146000	-1.098892000
1	5.222194000	-0.102397000	-0.171114000
1	5.058224000	-1.674376000	0.605286000
6	3.748734000	0.771929000	1.956196000
1	3.564630000	1.043657000	2.999643000
1	4.730806000	0.302088000	1.911129000
1	3.772102000	1.694210000	1.375413000
6	-4.799791000	-1.102782000	-0.404346000
1	-4.883610000	-1.493479000	-1.419745000
1	-5.496185000	-1.669745000	0.218967000
1	-5.131823000	-0.068334000	-0.413707000
1	-3.429686000	-1.104032000	1.238739000
1	1.686292000	0.333628000	1.817635000
1	-1.416165000	0.642507000	-1.899829000
1	3.329912000	-0.842200000	-1.770467000
8	0.013475000	-3.891022000	-0.328544000
6	3.368770000	1.614614000	-1.294537000
6	3.267572000	2.904703000	-1.817120000
6	2.078718000	3.612582000	-1.652842000
6	1.006638000	3.027406000	-0.995157000
1	4.109269000	3.341409000	-2.341243000
1	1.975742000	4.613823000	-2.057799000
1	0.068945000	3.562249000	-0.917810000
6	-3.436185000	1.389620000	1.189339000
6	-3.393032000	2.574143000	1.926937000
6	-2.203714000	3.296434000	1.993432000
6	-1.070724000	2.826553000	1.343445000
1	-4.282213000	2.918615000	2.441407000
1	-2.149647000	4.212180000	2.572380000
1	-0.132186000	3.357841000	1.439349000
1	-4.374349000	0.858532000	1.152655000

1	4.305317000	1.095410000	-1.426025000
1	0.428355000	-0.355171000	-1.819594000
1	0.409334000	-1.117835000	-1.877189000

-1432.181543

TS1-Mn-NN-Ar2

25	-0.127619000	-0.986573000	-0.068419000
7	2.451948000	-0.419947000	-0.008172000
7	-2.410608000	-0.198475000	-0.298566000
7	0.064278000	1.079493000	-0.305050000
6	2.478019000	0.946008000	-0.538567000
6	1.290382000	1.698298000	-0.616977000
6	-0.981835000	1.720227000	0.365134000
6	-2.243811000	1.078950000	0.419357000
6	-3.460309000	-1.077927000	0.382117000
6	-3.171800000	-2.580402000	0.318267000
1	-4.011605000	-3.110192000	0.776376000
1	-2.279502000	-2.836968000	0.880426000
1	-3.060454000	-2.951965000	-0.698106000
6	-2.615163000	0.091496000	-1.789283000
6	-2.678262000	-1.179753000	-2.631952000
1	-2.598462000	-0.902501000	-3.686312000
1	-3.621011000	-1.713628000	-2.504859000
1	-1.851863000	-1.846797000	-2.392332000
6	3.353758000	-1.327100000	-0.838244000
6	2.737166000	-2.700221000	-1.100690000
1	3.416215000	-3.282832000	-1.730251000
1	1.793815000	-2.595338000	-1.630174000
1	2.565911000	-3.264265000	-0.184591000
6	2.642994000	-0.388768000	1.501906000
6	2.585363000	-1.784616000	2.127918000
1	2.422622000	-1.682218000	3.203178000
1	3.513496000	-2.338790000	1.987186000
1	1.766306000	-2.373604000	1.719793000
6	-0.410338000	-1.120193000	1.717186000
8	-0.667264000	-1.226109000	2.837617000
6	-0.235375000	-2.746905000	-0.322519000
6	-3.751635000	1.060318000	-2.166385000
1	-4.728071000	0.580906000	-2.215017000
1	-3.809515000	1.911021000	-1.486108000

1	-3.532242000	1.453085000	-3.163350000
6	4.812965000	-1.512860000	-0.374817000
1	5.361806000	-2.007947000	-1.180243000
1	5.328793000	-0.581461000	-0.153392000
1	4.885041000	-2.152683000	0.505171000
6	3.856387000	0.385496000	2.048937000
1	3.929850000	1.388020000	1.626787000
1	3.721163000	0.494487000	3.128980000
1	4.801523000	-0.132739000	1.889540000
6	-4.928918000	-0.854280000	-0.033041000
1	-5.146616000	-1.315103000	-0.997821000
1	-5.566146000	-1.340608000	0.710005000
1	-5.222804000	0.190569000	-0.087112000
1	-3.367993000	-0.804120000	1.433285000
1	1.761945000	0.161611000	1.837289000
1	-1.698097000	0.608850000	-2.065844000
1	3.388266000	-0.828371000	-1.807832000
8	-0.280645000	-3.886604000	-0.520074000
6	3.664899000	1.551395000	-0.981294000
6	3.692061000	2.843496000	-1.492003000
6	2.507707000	3.573327000	-1.581854000
6	1.321491000	2.994903000	-1.159186000
1	4.631884000	3.271452000	-1.820949000
1	2.504474000	4.574334000	-1.998006000
1	0.387772000	3.532287000	-1.267528000
6	-3.258229000	1.673167000	1.172891000
6	-3.058867000	2.857053000	1.881736000
6	-1.811911000	3.469370000	1.844749000
6	-0.787366000	2.904345000	1.095480000
1	-3.870837000	3.279171000	2.461631000
1	-1.624166000	4.375943000	2.409083000
1	0.191978000	3.361979000	1.105968000
1	-4.230384000	1.211498000	1.233920000
1	4.595912000	1.009507000	-0.925662000
1	-0.077176000	0.274286000	-1.233545000
1	0.066359000	-0.727286000	-1.720134000

-1432.152045

3-Mn-NNN-Ar₂

25	-0.111497000	-1.033295000	-0.166787000
7	2.457940000	-0.437645000	-0.009188000
7	-2.515327000	-0.122829000	-0.304535000
7	0.001602000	1.034583000	-0.531343000
6	2.476781000	0.916692000	-0.548894000
6	1.296060000	1.637853000	-0.766788000
6	-0.942294000	1.683569000	0.339547000
6	-2.232333000	1.113055000	0.426666000
6	-3.531256000	-0.985421000	0.432980000
6	-3.258200000	-2.489765000	0.345627000
1	-4.046849000	-3.014185000	0.892903000
1	-2.309792000	-2.739452000	0.810510000
1	-3.251911000	-2.868153000	-0.673817000
6	-2.772313000	0.147552000	-1.776514000
6	-2.921486000	-1.132148000	-2.595245000
1	-2.879577000	-0.871161000	-3.655973000
1	-3.874896000	-1.631164000	-2.419064000
1	-2.100150000	-1.813895000	-2.377726000
6	3.383321000	-1.340851000	-0.823942000
6	2.785217000	-2.724589000	-1.078970000
1	3.473205000	-3.298453000	-1.707213000
1	1.837513000	-2.633090000	-1.601844000
1	2.626523000	-3.286088000	-0.159029000
6	2.625409000	-0.402312000	1.503335000
6	2.559972000	-1.798832000	2.126264000
1	2.385179000	-1.696457000	3.199612000
1	3.489682000	-2.352878000	1.994895000
1	1.743044000	-2.382439000	1.707291000
6	-0.395034000	-1.028154000	1.621172000
8	-0.666462000	-1.126617000	2.745978000
6	-0.217570000	-2.791444000	-0.314129000
6	-3.878955000	1.166411000	-2.105622000
1	-4.877064000	0.732219000	-2.073482000
1	-3.850149000	2.028953000	-1.437072000
1	-3.713930000	1.531279000	-3.123376000
6	4.839477000	-1.510652000	-0.343468000
1	5.393252000	-2.027814000	-1.131361000
1	5.359037000	-0.576025000	-0.144015000
1	4.903953000	-2.127411000	0.553251000
6	3.826993000	0.375302000	2.071941000

1	3.686766000	0.454141000	3.153933000
1	4.780717000	-0.123394000	1.902387000
1	3.887077000	1.390500000	1.678444000
6	-5.017570000	-0.727089000	0.115166000
1	-5.306166000	-1.159455000	-0.844227000
1	-5.619865000	-1.216160000	0.885173000
1	-5.287857000	0.327013000	0.102882000
1	-3.368109000	-0.723608000	1.478354000
1	1.736613000	0.142084000	1.825492000
1	-1.848306000	0.604200000	-2.134958000
1	3.421559000	-0.848488000	-1.797287000
8	-0.284547000	-3.940424000	-0.473888000
6	3.680003000	1.553096000	-0.908836000
6	3.712815000	2.823318000	-1.467614000
6	2.525234000	3.516982000	-1.691878000
6	1.327430000	2.913518000	-1.343169000
1	4.666505000	3.266452000	-1.730482000
1	2.531911000	4.503566000	-2.139655000
1	0.386520000	3.422153000	-1.519898000
6	-3.145821000	1.722801000	1.291057000
6	-2.794828000	2.816724000	2.082457000
6	-1.506964000	3.330159000	2.020502000
6	-0.586210000	2.764689000	1.141134000
1	-3.530385000	3.248843000	2.750683000
1	-1.211226000	4.163637000	2.646677000
1	0.421514000	3.153886000	1.094568000
1	-4.147295000	1.333331000	1.383787000
1	4.616211000	1.041680000	-0.754617000
1	-0.411986000	0.920876000	-1.452210000
1	0.047472000	-1.127881000	-1.791781000

-1432.157373