

## Supporting Information

### Theoretical Insights into CO<sub>2</sub> Hydrogenation to Methanol by Mn-PNP Complex

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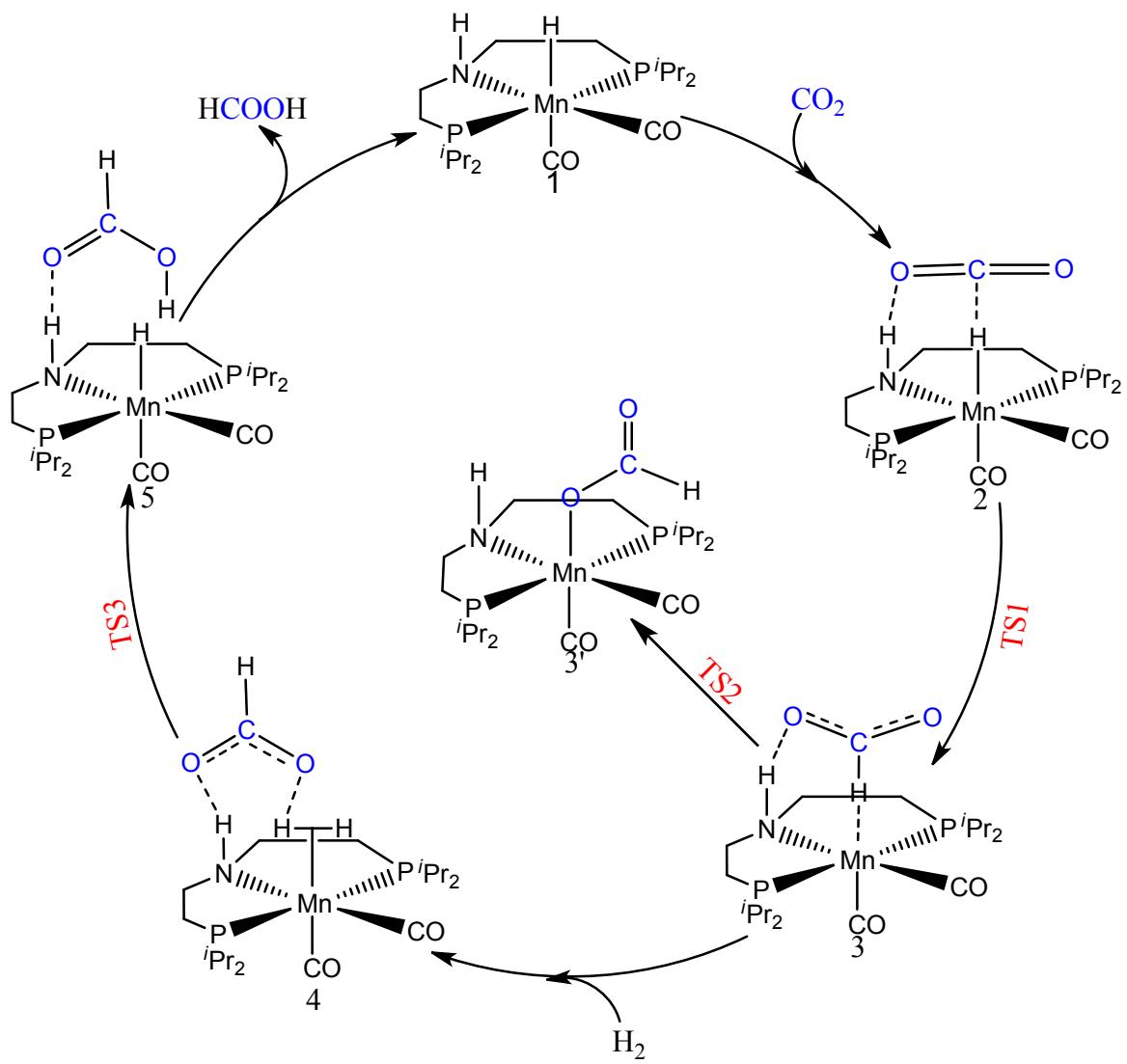
15. Cartesian coordinates and energies (in Hartree) in solvent phase for all the species

16. References

## **1. Gaussian full references**

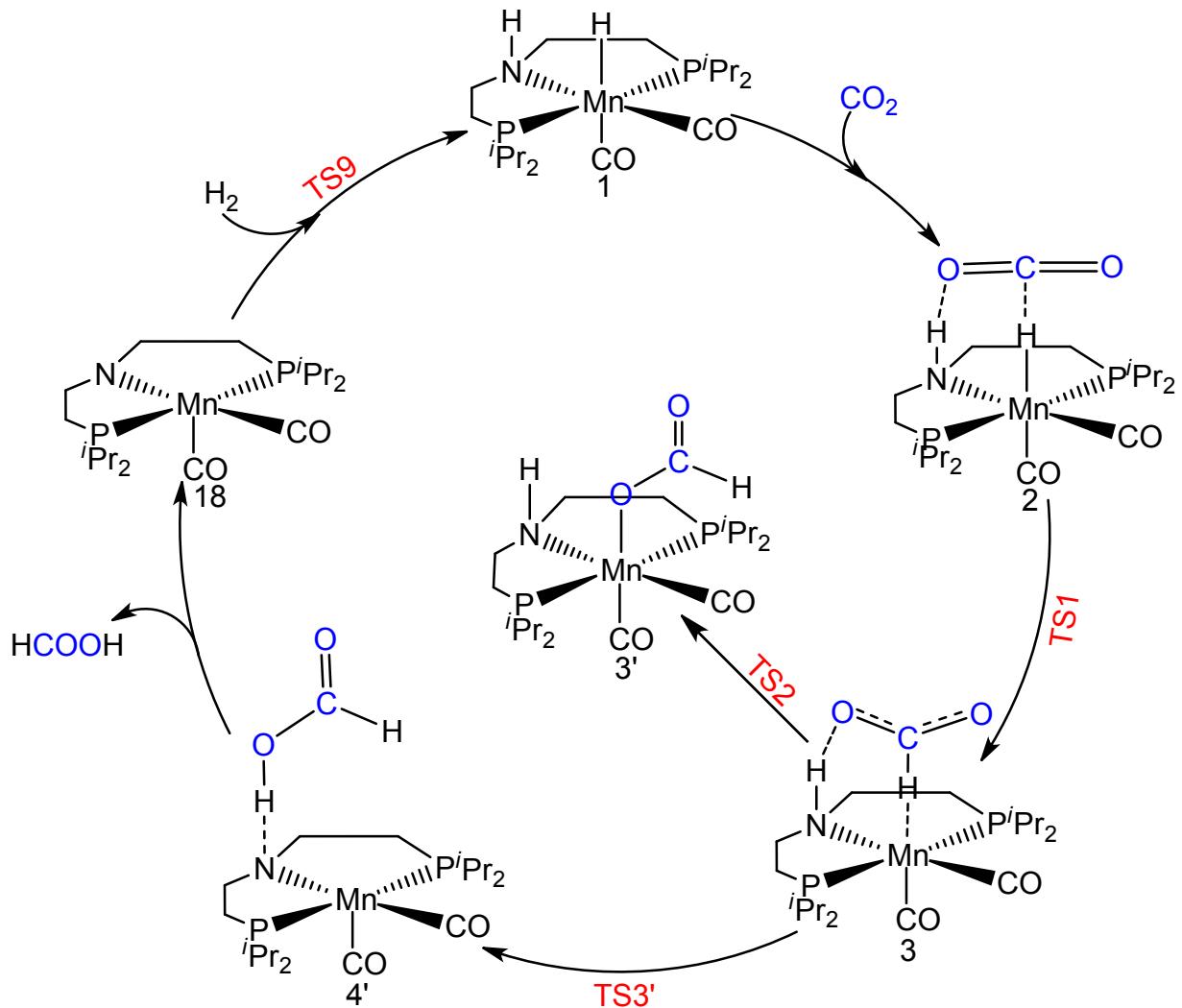
Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

## **2. Scheme of ligand assisted CO<sub>2</sub> hydrogenation to HCOOH by Mn-PNP catalyst**



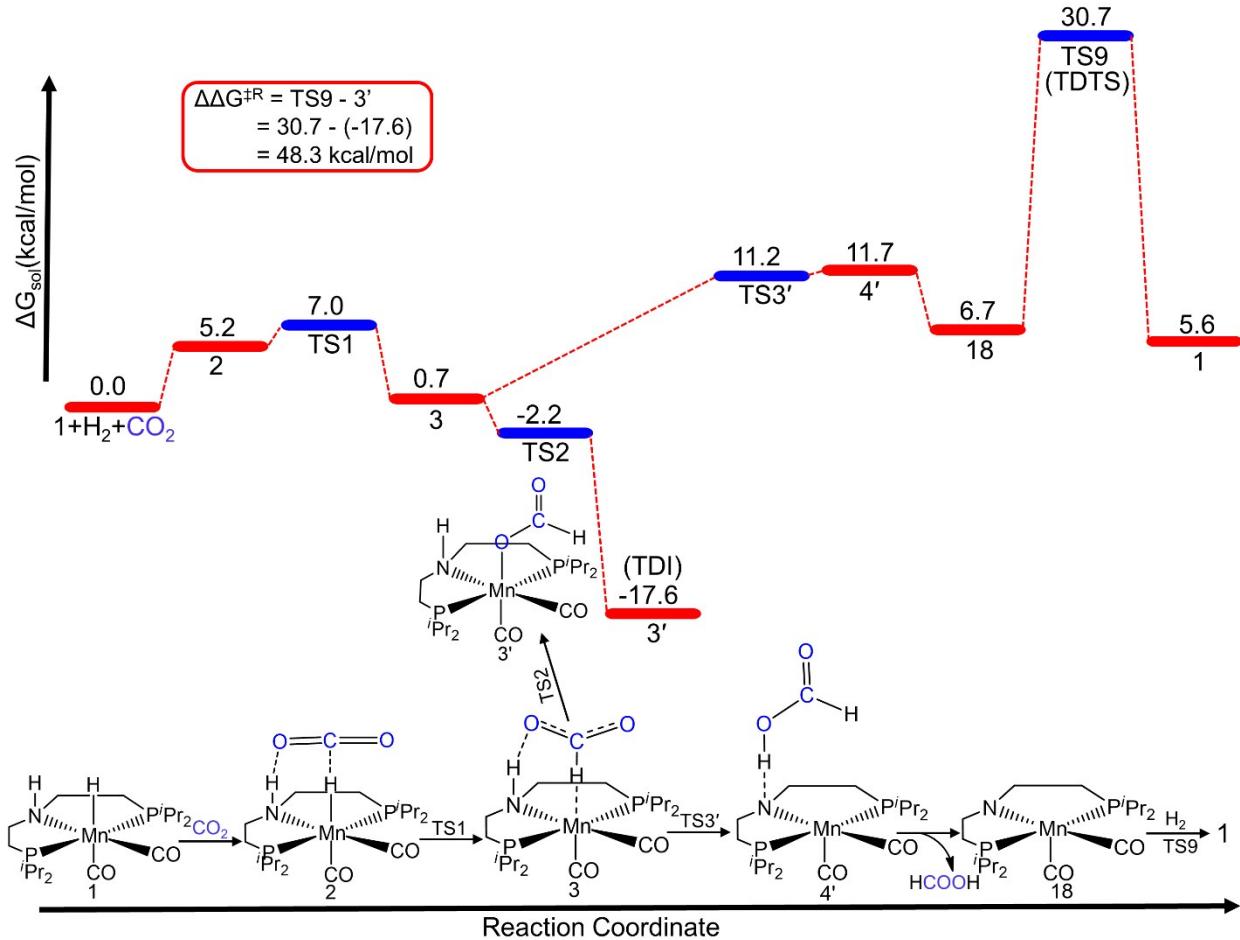
**Scheme S1:** Ligand assisted  $\text{CO}_2$  hydrogenation to  $\text{HCOOH}$  catalyzed by Mn-PNP catalyst.

### 3. Scheme of ligand participated $\text{CO}_2$ hydrogenation to $\text{HCOOH}$ by Mn-PNP catalyst



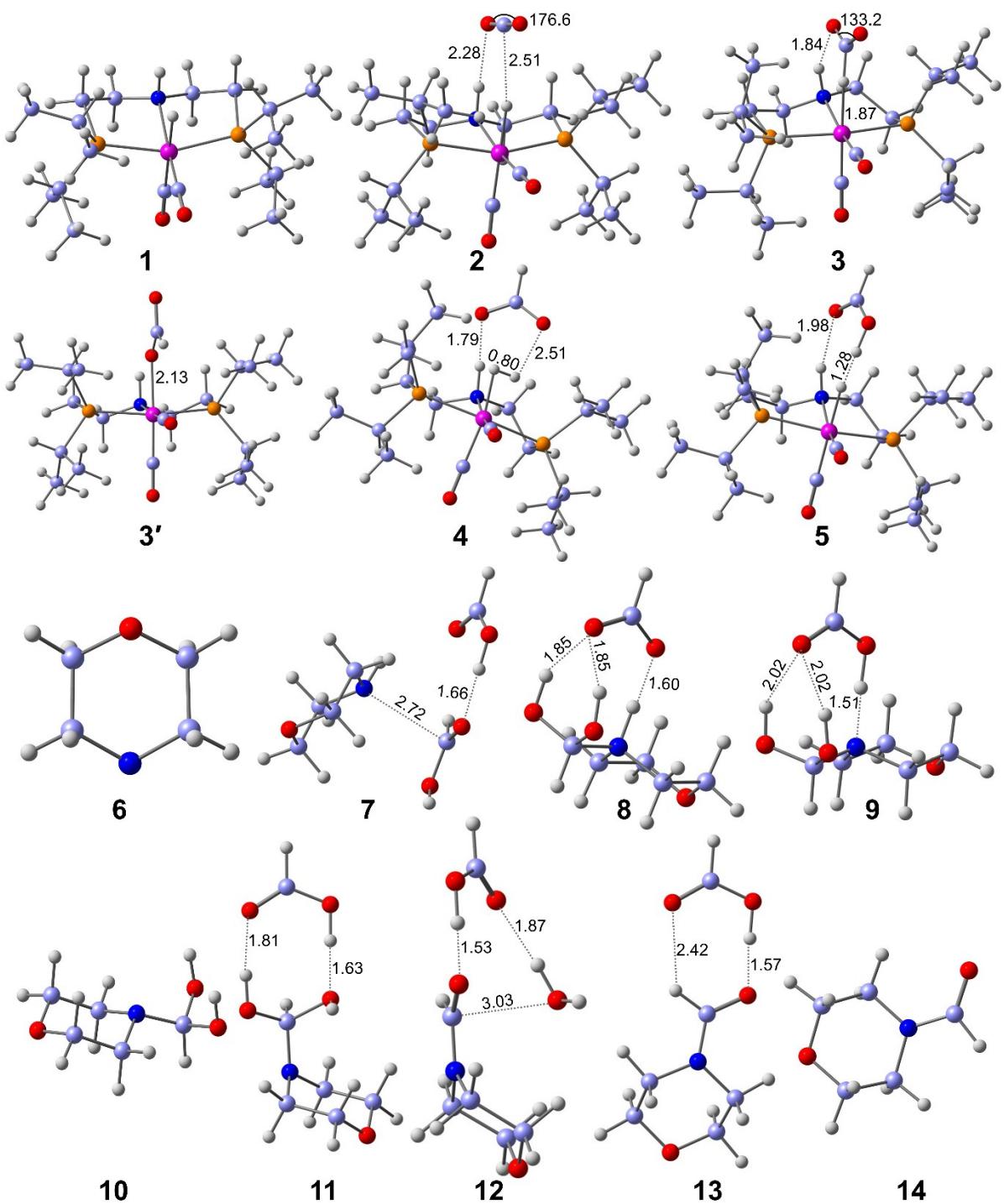
**Scheme S2:** Ligand participated  $\text{CO}_2$  hydrogenation to  $\text{HCOOH}$  catalyzed by Mn-PNP.

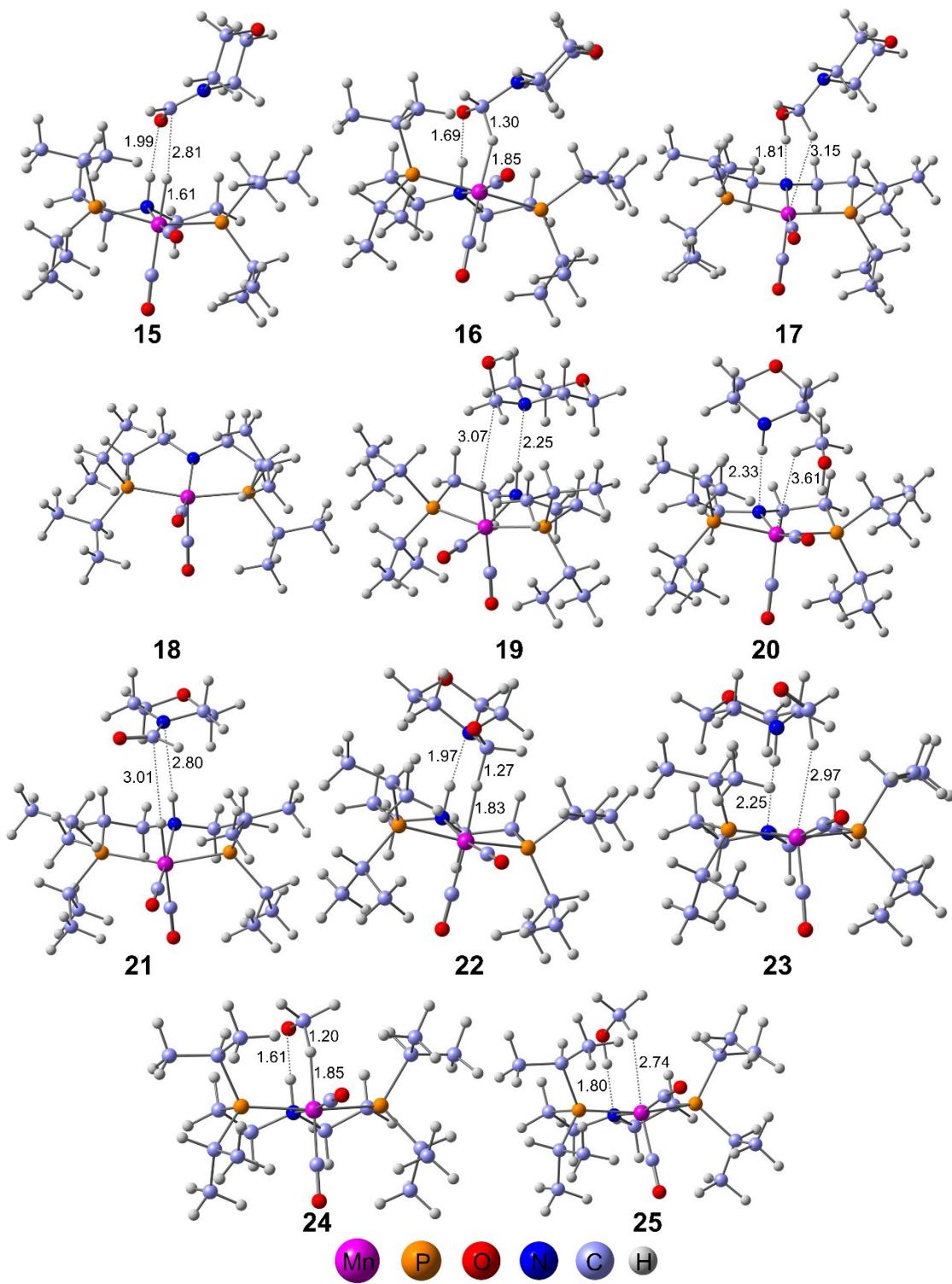
**4. Reaction free energy profile of ligand participated CO<sub>2</sub> hydrogenation to HCOOH by Mn-PNP catalyst**



**Figure S1:** Reaction free energy profile diagram of CO<sub>2</sub> hydrogenation to HCOOH *via* ligand participated mechanism catalysed by **Mn-PNP** complex.  $\Delta\Delta G^{\ddagger R}$  and  $\Delta G_{\text{rxn}}$  denote the total free energy barrier and total reaction free energy of the catalytic cycle, respectively.

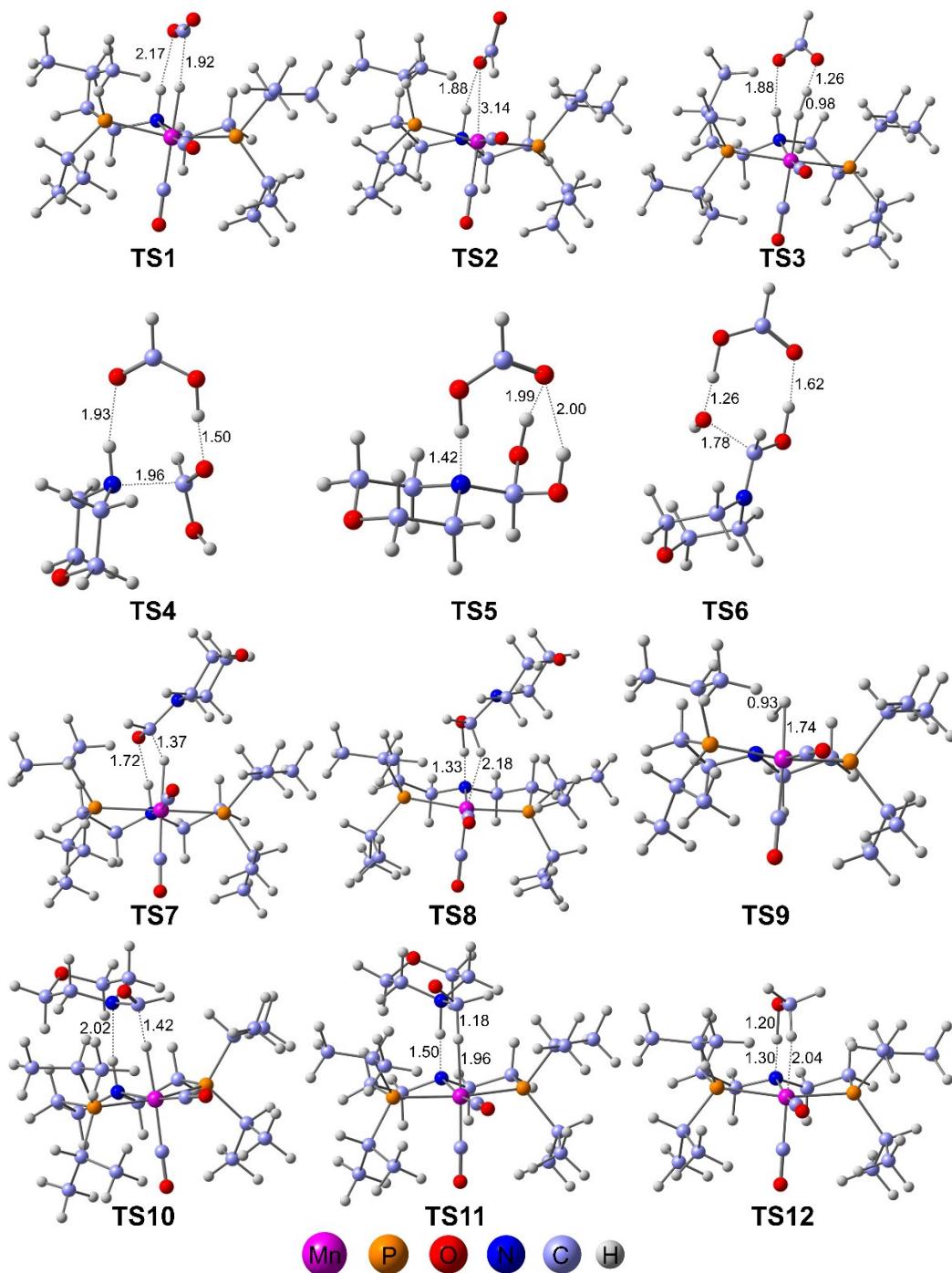
**5. Intermediates of CO<sub>2</sub> hydrogenation reaction to methanol catalyzed by Mn-PNP**





**Figure S2:** Optimized geometries of intermediates for  $\text{CO}_2$  hydrogenation to methanol catalyzed by **Mn-PNP** complex. Bond lengths and bond angles are in Å and °, respectively.

## 6. Transition states of CO<sub>2</sub> hydrogenation reaction to methanol catalyzed by Mn-PNP



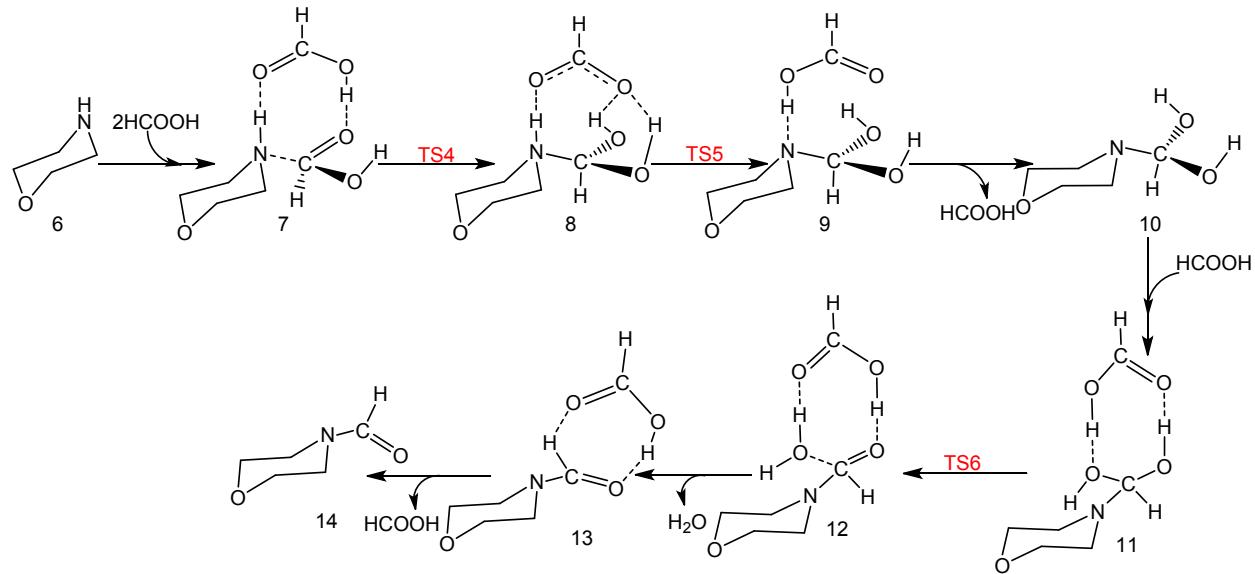
**Figure S3:** Optimized geometries of transition states for CO<sub>2</sub> hydrogenation to methanol catalyzed by **Mn-PNP** complex. Bond lengths and bond angles are in Å and °, respectively.

**7. Table of ligand assisted reaction free energy for CO<sub>2</sub> hydrogenation reaction to HCOOH by PNP based Mn(I), Fe(II) and Ru(II) complexes**

**Table S1:** Ligand assisted reaction free energy for CO<sub>2</sub> hydrogenation reaction to HCOOH by PNP based Mn(I), Fe(II) and Ru(II) complexes. ΔΔG<sup>‡</sup> represents the total reaction free energy barriers for reaction. All free energies are in kcal/mol.

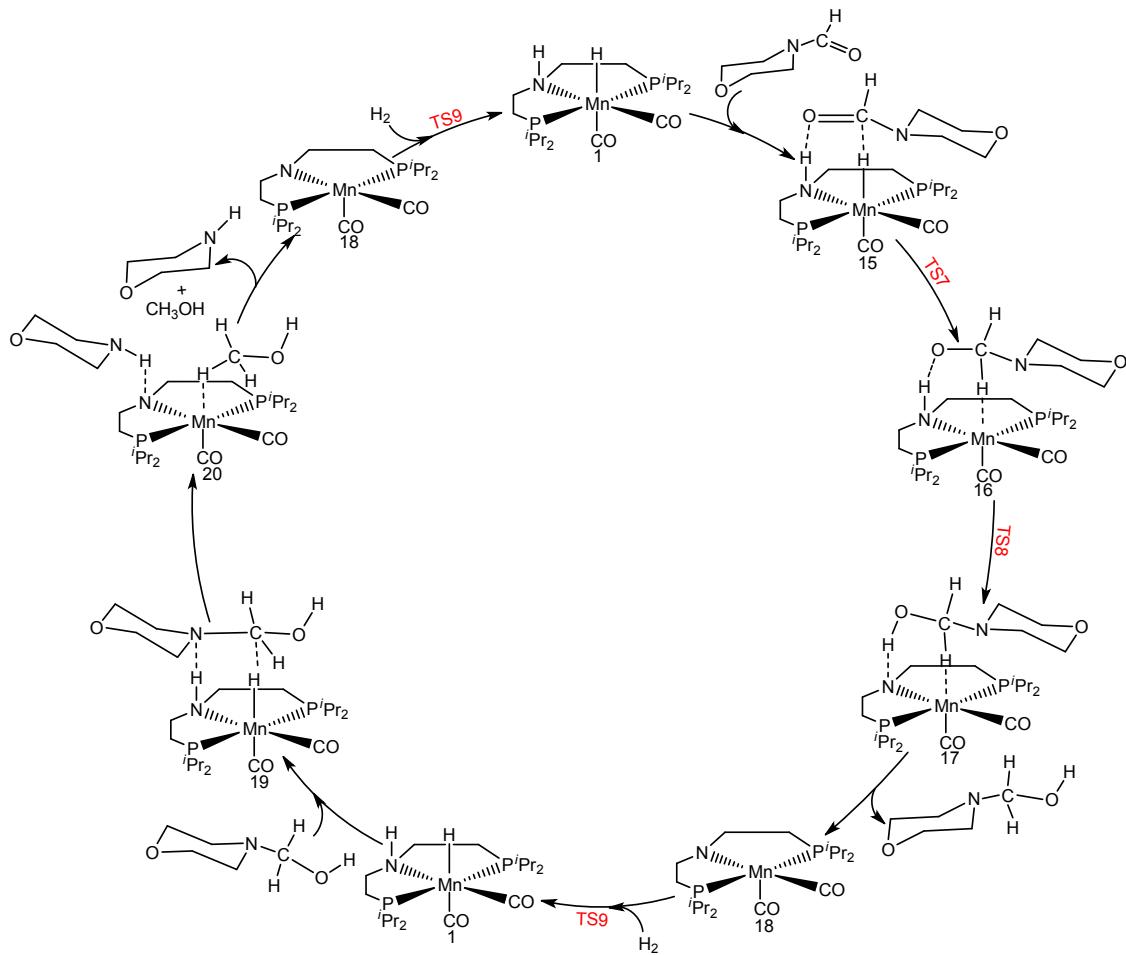
Complexes	Relative Free Energies (kcal/mol)										ΔΔG <sup>‡</sup>
	1+H <sub>2</sub> + CO <sub>2</sub>	2	TS1	3	TS2	3'	4	TS3	5	1+ HCOOH	
Mn-PNP	0.0	5.2	7.0	0.7	-2.2	-17.6	4.0	8.3	8.1	5.6	30.2
Fe-PNP	0.0	3.8	5.3	-9.5	-5.1	-17.6	2.3	4.7	4.9	5.6	28.5
Ru-PNP	0.0	4.1	4.5	-9.3	-6.8	-14.4	-1.5	5.6	5.6	5.6	24.5

**8. Scheme of HCOOH to N-formylmorpholine (amidation)**



**Scheme S3:** HCOOH to N-formylmorpholine (amidation)

**9. Scheme of Mn-PNP catalyzed N-formylmorpholine hydrogenation to methanol by C=O bond hydrogenation followed by C–N bond hydrogenation**



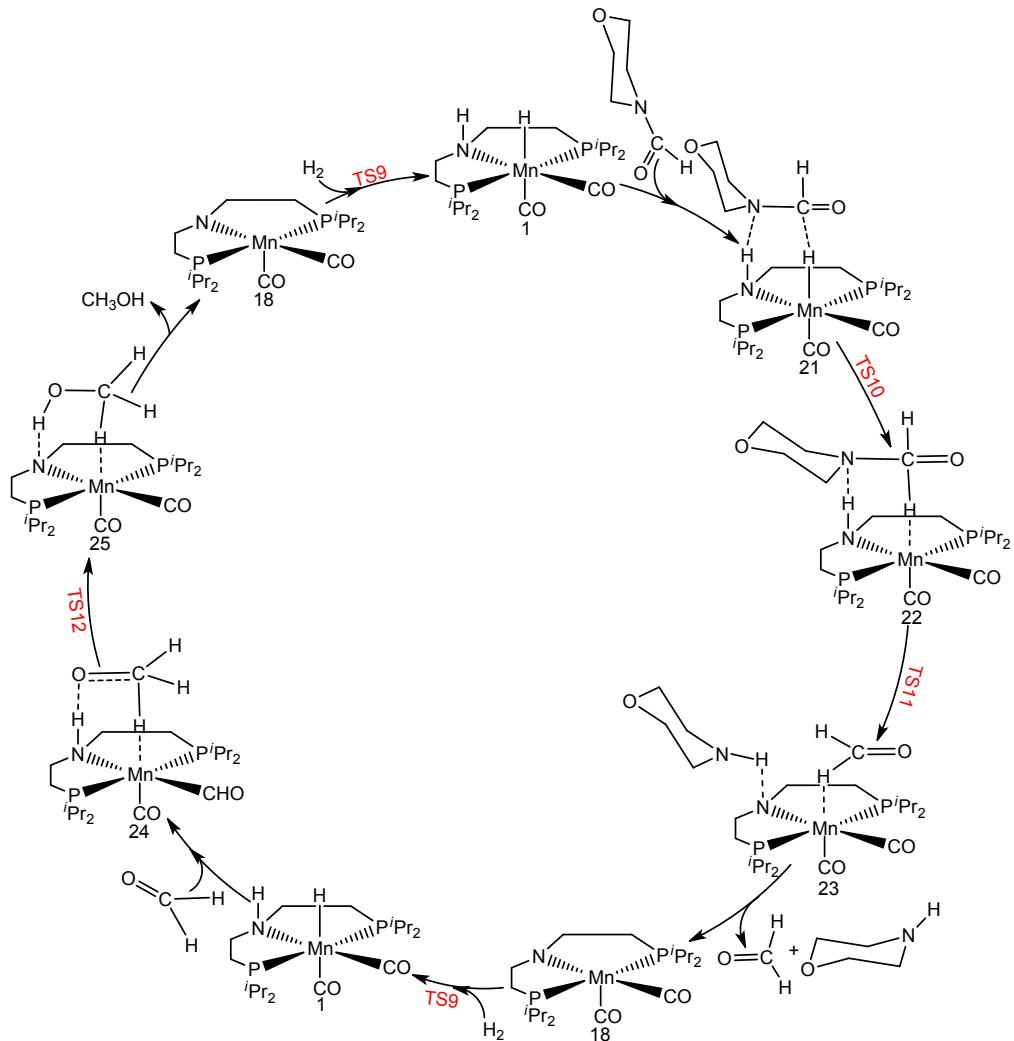
**Scheme S4:** N-formylmorpholine hydrogenation reaction to methanol *via* C=O bond hydrogenation followed by C–N bond hydrogenation catalyzed by **Mn-PNP** complex.

**10. Table of N-formylmorpholine hydrogenation to methanol via C=O bond hydrogenation followed by C–N bond hydrogenation reaction by PNP based Mn(I), Fe(II) and Ru(II) complexes.**

**Table S2:** N-formylmorpholine hydrogenation to methanol via C=O bond hydrogenation followed by C–N bond hydrogenation reaction by PNP based Mn(I), Fe(II) and Ru(II) complexes.  $\Delta\Delta G^{\ddagger R}$  represents the total reaction free energy barriers for reaction. All free energies are in kcal/mol.

Complexes	Relative Free Energies (kcal/mol)														$\Delta\Delta G^{\ddagger R}$
	1	15	TS7	16	TS8	17	18	TS9	1	19	20	18	TS9	1	
Mn-PNP	0.0	5.7	21.0	21.1	23.1	20.7	14.2	38.2	13.1	16.7	16.9	1.5	25.5	0.4	38.2
Fe-PNP	0.0	5.0	17.4	17.9	17.5	17.7	18.4	37.6	13.0	16.1	14.5	5.8	25.0	0.4	37.6
Ru-PNP	0.0	4.3	16.4	17.3	22.9	18.5	18.4	38.8	13.0	16.1	15.0	5.8	26.2	0.4	38.8

**11. Scheme of Mn-PNP catalyzed N-formylmorpholine hydrogenation to methanol by C–N bond hydrogenation followed by C=O bond hydrogenation**



**Scheme S5:** N-formylmorpholine hydrogenation to methanol *via* C–N bond hydrogenation followed by C=O bond hydrogenation catalysed by **Mn-PNP** complex.

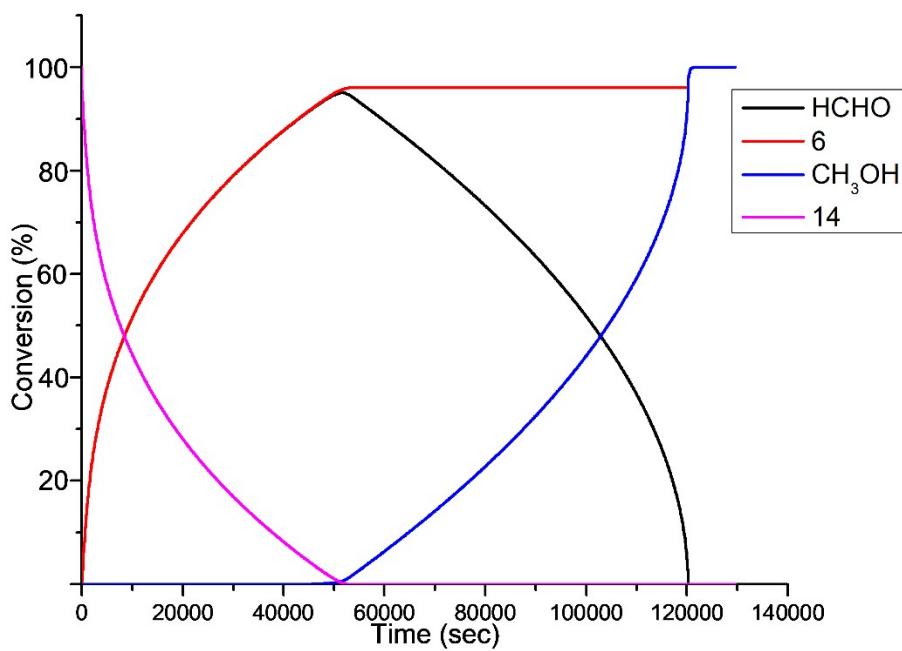
**12. Table of N-formylmorpholine hydrogenation to methanol via C–N bond hydrogenation followed by C=O bond hydrogenation reaction by PNP based Mn(I), Fe(II) and Ru(II) complexes**

**Table S3:** N-formylmorpholine hydrogenation to methanol via C–N bond hydrogenation followed by C=O bond hydrogenation reaction by PNP based Mn(I), Fe(II) and Ru(II) complexes.  $\Delta\Delta G^{\ddagger R}$  represents the total reaction free energy barriers for reaction. All free energies are in kcal/mol.

Complexes	Relative Free Energies (kcal/mol)															$\Delta\Delta G^{\ddagger R}$
	1	21	TS10	22	TS11	23	18	TS9	1	24	TS12	25	18	TS9	1	
Mn-PNP	0.0	9.3	26.7	24.7	36.0	29.3	14.4	38.4	13.3	9.2	8.8	8.1	1.5	25.0	0.4	38.4
Fe-PNP	0.0	7.9	21.1	23.1	31.1	26.1	18.7	37.9	13.3	7.1	-	2.5	5.8	25.0	0.4	37.9
Ru-PNP	0.0	8.7	23.7	23.5	30.5	29.0	18.7	39.0	13.3	6.3	12.1	3.9	5.8	26.2	0.4	39.0

**13. Microkinetic model**

**Text S1:** We have used Complex Pathway Simulator (COPASI) software (version 4.22)<sup>1</sup> for Microkinetic modeling with Livermore Solver for Ordinary Differential Equations (LSODA) algorithm.<sup>2</sup> However, the microkinetic modelling part has been simplified. Here, we have just considered the main important steps of the overall reaction. In case of dimerization reactions which are proceeding without barrier, the rate constants have been calculated by diffusion-controlled method.<sup>3</sup> Therefore, rate constant is given by  $k=8k_B T/3\eta$ , where  $k_B$  is the Boltzmann constant,  $T$  is the temperature, and  $\eta$  is the solvent's viscosity.<sup>4</sup> Diffusion controlled rate constant has been find out at 298.15 K whereas all the other rate constants have been found out at 383.15 K. Here all the factors have been considered as described in the experiment.<sup>5</sup> The initial concentration of morpholine has been considered 1.0 M, whereas Mn-PNP catalyst is 0.005 M and concentration of gaseous molecules have been varied to understand the gaseous concentration effect towards product formation. The concentration of the gaseous molecules ( $H_2$  and  $CO_2$ ) have been considered to remain fixed during the reaction. Furthermore, we have followed reaction time effect towards product formation. For first step i.e.,  $CO_2$  hydrogenation to methanol followed by amide formation in the presence of amine simulations have been carried out up to 24 hours (86400 Sec) and for second step amide hydrogenation to methanol and amine simulations were carried out for a total time 36 hour (129600 Sec). The elementary steps of the reaction mechanisms which are considered in the microkinetic model are given below with reaction free energy and rate constant.



**Figure S4:** Amide conversion to methanol over time. Simulations on the based-on scheme S5.

Change of concentration of reactant amide (14), intermediate (HCHO) and products CH<sub>3</sub>OH and amine (6).

**14. Table of reaction mechanisms elementary step's reaction free energy barrier and rate constant**

Table S3: Reaction mechanisms elementary step's gibbs free energy and rate constant.  $\Delta\Delta G^{\ddagger R}$  represents the total reaction free energy barriers for reaction. All free energies are in kcal/mol and rate constants are in  $M^{-1}S^{-1}$

Steps	Reaction free energy barrier ( $\Delta\Delta G^{\ddagger R}$ ) in kcal/mol	Rate constant (At 383.15 K) (k) in $M^{-1}S^{-1}$
$1 + CO_2 = 3'$	7.0	8.11E+08
$3' = 1 + CO_2$	24.6	7.40E-02
$3' + H_2 = 1 + HCOOH$	25.9	1.34E-02
$1 + HCOOH = 3' + H_2$	2.7	2.30E+11
$6 + 2HCOOH = 9$	13.8	1.07E+05
$9 = 6 + 2HCOOH$	3.5	8.05E+10
$9 = 14 + HCOOH + H_2O$	8.3	1.47E+08
$14 + HCOOH + H_2O = 9$	29	2.29E-04
$1 + 14 \rightarrow 21$		1.65E+10
$21 = 22$	17.4	9.47E+02
$22 = 21$	2.0	5.77E+11
$22 = 18 + HCHO + 6$	11.3	2.86E+06
$18 + HCHO + 6 = 22$	21.6	3.81E+00
$18 + H_2 = 1$	24.0	1.63E-01
$1 = 18 + H_2$	25.1	3.84E-02
$1 + HCHO = 18 + CH_3OH$	2.9	1.77E+11
$18 + CH_3OH = 1 + HCHO$	14.7	3.29E+04
$18 + H_2 = 1$	24.0	1.63E-01
$1 = 18 + H_2$	25.1	3.84E-02

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

**H<sub>2</sub>**

1	0.0000000000	0.0000000000	0.371915000
1	0.0000000000	0.0000000000	-0.371915000

-1.180458

**CO<sub>2</sub>**

6	0.0000000000	0.0000000000	0.0000000000
8	0.0000000000	0.0000000000	1.169170000
8	0.0000000000	0.0000000000	-1.169170000

-188.602354

**HCOOH**

6	0.130016000	0.402410000	-0.000197000
1	0.104426000	1.499614000	0.000402000
8	-1.117883000	-0.090548000	0.000045000
1	-1.076069000	-1.064877000	-0.000019000
8	1.141827000	-0.265602000	0.000054000

-189.773882

**H<sub>2</sub>O**

8	0.000000000	0.000000000	0.117627000
1	0.000000000	0.767285000	-0.470507000
1	0.000000000	-0.767285000	-0.470507000

-76.437760

**CH<sub>3</sub>OH**

8	-0.753339000	-0.123168000	0.000009000
1	-1.153210000	0.756524000	0.000005000
6	0.672138000	0.020112000	0.000016000
1	1.028275000	0.545988000	0.895267000
1	1.090942000	-0.988822000	-0.002967000
1	1.027878000	0.550983000	-0.892469000

-115.713041

**1-Mn-PNP**

25	-0.000002000	0.052204000	0.065363000
15	-2.243903000	0.070064000	-0.325678000
15	2.243916000	0.070065000	-0.325646000
8	-0.000193000	-2.110900000	2.071588000

8	-0.000172000	2.114543000	2.148968000
7	0.000038000	-1.229164000	-1.701616000
6	-1.239554000	-2.030762000	-1.818316000
1	-1.265430000	-2.720412000	-0.969273000
1	-1.234356000	-2.626909000	-2.742588000
6	1.239630000	-2.030757000	-1.818327000
1	1.234446000	-2.626887000	-2.742611000
1	1.265508000	-2.720419000	-0.969295000
6	-3.038396000	1.638800000	-0.992568000
1	-2.379522000	1.855122000	-1.843705000
6	3.459858000	-0.577849000	0.958948000
1	4.463541000	-0.289676000	0.624081000
6	2.437260000	-1.081340000	-1.791265000
1	2.432419000	-0.463486000	-2.697381000
1	3.382569000	-1.630047000	-1.781112000
6	3.038414000	1.638808000	-0.992507000
1	2.379502000	1.855188000	-1.843601000
6	-2.437201000	-1.081361000	-1.791286000
1	-3.382503000	-1.630080000	-1.781141000
1	-2.432355000	-0.463516000	-2.697409000
6	-3.183970000	0.074136000	2.325906000
1	-2.193263000	-0.208862000	2.694408000
1	-3.929217000	-0.262390000	3.056704000
1	-3.223247000	1.165498000	2.286996000
6	-3.420765000	-2.111066000	1.086137000
1	-3.701882000	-2.617444000	0.158456000
1	-4.129889000	-2.429666000	1.859647000
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6	-3.459847000	-0.577857000	0.958908000
1	-4.463533000	-0.289701000	0.624031000
6	-0.000012000	-1.281115000	1.232544000
6	0.000006000	1.275029000	1.323778000
6	-2.943659000	2.823089000	-0.018320000
1	-3.635181000	2.703315000	0.822254000
1	-3.220134000	3.749891000	-0.535238000
1	-1.933847000	2.942864000	0.381027000
6	-4.475788000	1.467886000	-1.510872000
1	-4.574974000	0.633311000	-2.212125000
1	-4.790418000	2.379490000	-2.033325000
1	-5.181665000	1.305861000	-0.689006000
6	4.475773000	1.467876000	-1.510893000
1	5.181689000	1.305792000	-0.689072000
1	4.790403000	2.379493000	-2.033324000
1	4.574895000	0.633328000	-2.212189000
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1	2.429085000	-2.462169000	1.382784000

1	4.129925000	-2.429645000	1.859696000
1	3.701958000	-2.617429000	0.158496000
6	3.183966000	0.074144000	2.325942000
1	3.223223000	1.165508000	2.287026000
1	3.929220000	-0.262364000	3.056743000
1	2.193264000	-0.208869000	2.694443000
6	2.943763000	2.823050000	-0.018194000
1	1.933971000	2.942851000	0.381192000
1	3.220266000	3.749866000	-0.535072000
1	3.635306000	2.703196000	0.822352000
1	0.000035000	-0.558714000	-2.470515000
1	0.000018000	1.280314000	-0.987200000

-1700.378899

## 2-Mn-PNP

25	-0.002040000	-0.386739000	-0.133202000
15	2.240187000	-0.090204000	0.128333000
15	-2.242885000	-0.084486000	0.133721000
8	-0.006361000	-3.334930000	-0.046860000
8	-0.005335000	-0.385690000	-3.063685000
7	0.001149000	-0.062982000	2.023624000
6	1.240931000	-0.559253000	2.664307000
1	1.262912000	-1.646069000	2.538701000
1	1.238582000	-0.339471000	3.741996000
6	-1.238355000	-0.555494000	2.667538000
1	-1.232825000	-0.335322000	3.745145000
1	-1.263612000	-1.642298000	2.542497000
6	3.001783000	1.521003000	-0.478142000
1	2.403982000	2.251435000	0.081500000
6	-3.485089000	-1.414553000	-0.342780000
1	-4.482270000	-0.966813000	-0.256356000
6	-2.440175000	0.102409000	1.986812000
1	-2.446618000	1.175203000	2.212813000
1	-3.382334000	-0.309368000	2.357682000
6	-3.002329000	1.528067000	-0.471275000
1	-2.395558000	2.258355000	0.078893000
6	2.442717000	0.096001000	1.980858000
1	3.384855000	-0.318102000	2.349232000
1	2.451557000	1.168756000	2.206622000
6	3.255269000	-1.860188000	-1.809240000
1	2.265035000	-2.310493000	-1.931459000
1	4.006168000	-2.607304000	-2.093169000
1	3.331092000	-1.028061000	-2.514012000
6	3.418693000	-2.643915000	0.584890000
1	3.655919000	-2.391922000	1.622674000

1	4.152814000	-3.388887000	0.255170000
1	2.434159000	-3.117133000	0.562862000
6	3.478611000	-1.422906000	-0.350447000
1	4.476945000	-0.978189000	-0.261923000
6	-0.004343000	-2.155227000	-0.031071000
6	-0.004031000	-0.400335000	-1.887026000
6	2.759518000	1.782260000	-1.971293000
1	3.358607000	1.116143000	-2.600609000
1	3.048290000	2.810955000	-2.218254000
1	1.707630000	1.649634000	-2.231582000
6	4.478968000	1.721984000	-0.105881000
1	4.675178000	1.520668000	0.952360000
1	4.773968000	2.758605000	-0.308698000
1	5.132805000	1.076286000	-0.701777000
6	-4.475240000	1.736704000	-0.086486000
1	-5.137104000	1.090809000	-0.673219000
1	-4.767973000	2.773526000	-0.291621000
1	-4.662703000	1.541307000	0.974428000
6	-3.429256000	-2.633690000	0.595290000
1	-2.445213000	-3.108160000	0.576731000
1	-4.163406000	-3.378504000	0.265285000
1	-3.668832000	-2.379217000	1.631916000
6	-3.261678000	-1.855927000	-1.800409000
1	-3.332717000	-1.025066000	-2.507121000
1	-4.015482000	-2.600365000	-2.083675000
1	-2.273264000	-2.310744000	-1.920343000
6	-2.772815000	1.782272000	-1.967660000
1	-1.724212000	1.643197000	-2.237726000
1	-3.058297000	2.811596000	-2.215752000
1	-3.381705000	1.117129000	-2.588582000
1	0.003452000	0.953407000	2.108401000
1	-0.001127000	1.218700000	-0.247947000
6	0.020820000	3.573570000	0.632191000
8	-0.048134000	4.012579000	-0.448452000
8	0.091172000	3.197888000	1.740461000

-1888.973033

### TS1-Mn-PNP

25	-0.000112000	-0.302376000	-0.161244000
15	2.257498000	-0.073322000	0.159251000
15	-2.257577000	-0.072962000	0.159260000
8	-0.000227000	-3.237467000	-0.397247000
8	-0.000317000	-0.039845000	-3.081417000
7	-0.000035000	-0.205135000	2.077454000
6	1.242512000	-0.764236000	2.655193000

1	1.256654000	-1.836065000	2.435151000
1	1.254973000	-0.642333000	3.748132000
6	-1.242813000	-0.763519000	2.655397000
1	-1.255205000	-0.641172000	3.748288000
1	-1.257376000	-1.835440000	2.435817000
6	3.059526000	1.564494000	-0.297756000
1	2.505763000	2.256562000	0.348437000
6	-3.459323000	-1.392895000	-0.432224000
1	-4.467163000	-0.980027000	-0.309311000
6	-2.445414000	-0.056794000	2.023234000
1	-2.457912000	0.992598000	2.339912000
1	-3.386243000	-0.504980000	2.353966000
6	-3.059166000	1.564943000	-0.298184000
1	-2.506251000	2.256685000	0.349105000
6	2.445356000	-0.057763000	2.023218000
1	3.386030000	-0.506331000	2.353858000
1	2.458240000	0.991556000	2.340148000
6	3.219895000	-1.696660000	-1.922361000
1	2.217805000	-2.108550000	-2.075081000
1	3.949563000	-2.435452000	-2.274362000
1	3.314377000	-0.808408000	-2.552397000
6	3.373295000	-2.686142000	0.397058000
1	3.601606000	-2.522539000	1.454052000
1	4.103178000	-3.409447000	0.014330000
1	2.384753000	-3.145793000	0.325573000
6	3.458803000	-1.393325000	-0.433136000
1	4.466761000	-0.980488000	-0.311157000
6	-0.000143000	-2.068170000	-0.257797000
6	-0.000254000	-0.151962000	-1.912333000
6	2.792199000	1.981755000	-1.751287000
1	3.333790000	1.346563000	-2.459400000
1	3.135099000	3.011517000	-1.906840000
1	1.727207000	1.937682000	-1.988119000
6	4.551333000	1.677909000	0.055268000
1	4.764202000	1.369019000	1.084189000
1	4.876063000	2.719438000	-0.053680000
1	5.169499000	1.073221000	-0.616762000
6	-4.551455000	1.678097000	0.052882000
1	-5.168695000	1.074703000	-0.621165000
1	-4.875815000	2.719877000	-0.054720000
1	-4.765961000	1.367391000	1.080922000
6	-3.373281000	-2.685670000	0.398003000
1	-2.384947000	-3.145602000	0.325548000
1	-4.103769000	-3.408789000	0.016081000
1	-3.600454000	-2.521932000	1.455223000
6	-3.221530000	-1.696278000	-1.921603000

1	-3.316658000	-0.808087000	-2.551650000
1	-3.951328000	-2.435237000	-2.272983000
1	-2.219485000	-2.108059000	-2.075051000
6	-2.789717000	1.983076000	-1.751071000
1	-1.724160000	1.940991000	-1.985706000
1	-3.134162000	3.012277000	-1.906976000
1	-3.328706000	1.347146000	-2.460503000
1	0.000245000	0.800470000	2.255560000
1	-0.000549000	1.384170000	-0.089025000
6	0.000346000	3.162720000	0.628050000
8	0.001766000	3.757336000	-0.390611000
8	-0.000939000	2.916846000	1.787846000

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### 3-Mn-PNP

15	-2.271838000	-0.284917000	0.145877000
7	-0.077926000	0.534254000	1.931409000
6	1.064509000	0.051731000	2.752648000
6	-1.402553000	0.449349000	2.633894000
6	-2.345120000	-0.561352000	1.978873000
1	-3.353562000	-0.482555000	2.395495000
1	-1.989133000	-1.579503000	2.159259000
6	2.382356000	0.452788000	2.085520000
1	3.229779000	-0.010842000	2.597516000
15	2.332204000	-0.010168000	0.279416000
6	0.149206000	-0.402445000	-1.854369000
8	0.246735000	-0.518100000	-3.010047000
25	0.029654000	-0.171341000	-0.091243000
6	0.075957000	-1.894848000	0.241142000
8	0.090080000	-3.040135000	0.478141000
6	-3.299298000	-1.640116000	-0.657223000
1	-4.300041000	-1.209517000	-0.778546000
6	-2.754412000	-1.988727000	-2.053173000
1	-3.450596000	-2.667459000	-2.558992000
1	-2.626409000	-1.105060000	-2.683281000
1	-1.784976000	-2.491612000	-1.983062000
6	-3.434548000	-2.904996000	0.207993000
1	-3.926400000	-2.702460000	1.163618000
1	-4.043264000	-3.641494000	-0.328968000
1	-2.461499000	-3.363011000	0.408718000
6	3.258446000	-1.646447000	0.257354000
1	2.746341000	-2.196500000	1.057942000
6	3.073644000	-2.444021000	-1.046625000
1	3.414270000	-3.474109000	-0.893091000
1	2.031968000	-2.479789000	-1.369958000

1	3.662542000	-2.022064000	-1.864686000
6	4.746975000	-1.539056000	0.628468000
1	5.162643000	-2.544926000	0.757187000
1	5.323053000	-1.045842000	-0.160751000
1	4.913880000	-0.992481000	1.561501000
1	1.016209000	0.480519000	3.762169000
1	0.983405000	-1.035444000	2.846806000
1	2.513048000	1.537112000	2.154767000
1	-1.847954000	1.448405000	2.603753000
1	-1.248085000	0.195251000	3.687391000
6	3.483686000	1.228707000	-0.533539000
1	4.410887000	1.177443000	0.051257000
6	2.946273000	2.667194000	-0.472030000
1	3.746250000	3.359170000	-0.758380000
1	2.123320000	2.805819000	-1.177355000
1	2.593194000	2.961882000	0.519562000
6	3.790260000	0.852041000	-1.993539000
1	4.393136000	1.643187000	-2.453469000
1	4.352479000	-0.079476000	-2.079615000
1	2.869847000	0.752917000	-2.578933000
6	-3.255278000	1.281608000	-0.161882000
1	-2.650451000	2.063710000	0.309436000
6	-4.650686000	1.303198000	0.479617000
1	-5.132508000	2.264011000	0.264211000
1	-5.299916000	0.516357000	0.080953000
1	-4.609657000	1.193385000	1.566944000
6	-3.319337000	1.569129000	-1.672297000
1	-3.751236000	2.561744000	-1.839117000
1	-2.326214000	1.560215000	-2.129896000
1	-3.954492000	0.841470000	-2.189413000
1	0.058452000	1.545616000	1.760399000
1	-0.038383000	1.648924000	-0.495751000
6	-0.277633000	2.788294000	-0.310892000
8	-0.461645000	3.402337000	-1.366883000
8	-0.280914000	3.131502000	0.890858000

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### TS2-Mn-PNP

25	0.000031000	-0.263286000	-0.122834000
15	2.303515000	-0.073699000	0.186199000
15	-2.303434000	-0.074024000	0.186221000
8	0.000302000	-3.146182000	-0.576186000
8	-0.000079000	0.114088000	-3.047323000
7	0.000049000	-0.347231000	1.999583000
6	1.237119000	-0.910310000	2.596693000

1	1.277729000	-1.975302000	2.348236000
1	1.204725000	-0.822678000	3.690857000
6	-1.236917000	-0.910557000	2.596689000
1	-1.204531000	-0.822935000	3.690854000
1	-1.277322000	-1.975554000	2.348218000
6	3.102071000	1.582372000	-0.190905000
1	2.491994000	2.260008000	0.417363000
6	-3.446304000	-1.387478000	-0.508235000
1	-4.461369000	-0.986631000	-0.406787000
6	-2.452002000	-0.165282000	2.041430000
1	-2.446602000	0.866568000	2.408354000
1	-3.386389000	-0.628553000	2.367273000
6	-3.102093000	1.582041000	-0.190742000
1	-2.492364000	2.259584000	0.417977000
6	2.452052000	-0.164805000	2.041414000
1	3.386538000	-0.627839000	2.367312000
1	2.446407000	0.867068000	2.408271000
6	3.149855000	-1.622671000	-1.999406000
1	2.148804000	-2.041226000	-2.135351000
1	3.873258000	-2.335381000	-2.410872000
1	3.210860000	-0.705791000	-2.589900000
6	3.376536000	-2.709308000	0.276011000
1	3.647607000	-2.589168000	1.328220000
1	4.083205000	-3.422175000	-0.163881000
1	2.382196000	-3.159638000	0.224294000
6	3.446541000	-1.387070000	-0.508153000
1	4.461549000	-0.986050000	-0.406797000
6	0.000179000	-1.991827000	-0.391246000
6	-0.000038000	-0.010063000	-1.888661000
6	2.967388000	2.010991000	-1.660503000
1	3.600002000	1.405056000	-2.316622000
1	3.292169000	3.052344000	-1.762978000
1	1.938008000	1.947507000	-2.021604000
6	4.559965000	1.690943000	0.287425000
1	4.682259000	1.405041000	1.336736000
1	4.895315000	2.729385000	0.186607000
1	5.230198000	1.071156000	-0.317324000
6	-4.560189000	1.690198000	0.287050000
1	-5.230093000	1.070571000	-0.318230000
1	-4.895651000	2.728634000	0.186554000
1	-4.682844000	1.403817000	1.336191000
6	-3.376068000	-2.709805000	0.275765000
1	-2.381641000	-3.159941000	0.224054000
1	-4.082568000	-3.422760000	-0.164256000
1	-3.647230000	-2.589851000	1.327970000
6	-3.149648000	-1.622871000	-1.999520000

1	-3.210754000	-0.705918000	-2.589891000
1	-3.873003000	-2.335591000	-2.411054000
1	-2.148560000	-2.041319000	-2.135553000
6	-2.966867000	2.011143000	-1.660145000
1	-1.937228000	1.948474000	-2.020640000
1	-3.292277000	3.052310000	-1.762510000
1	-3.598682000	1.404979000	-2.316821000
1	-0.000053000	0.673258000	2.154222000
1	0.001724000	2.233971000	-0.531635000
6	-0.000200000	2.959936000	0.331828000
8	-0.001667000	4.167255000	0.021679000
8	-0.000555000	2.436054000	1.486816000

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### 3'-Mn-PNP

25	0.000021000	-0.139215000	0.117603000
15	-2.309646000	-0.081532000	-0.212005000
15	2.309656000	-0.081153000	-0.212093000
8	0.000221000	-2.969257000	0.886181000
8	0.000030000	0.614756000	2.963372000
7	-0.000032000	-0.581494000	-2.031895000
6	-1.239323000	-1.247443000	-2.497869000
1	-1.256445000	-2.253316000	-2.067345000
1	-1.236118000	-1.349642000	-3.591909000
6	1.239568000	-1.246605000	-2.498220000
1	1.236273000	-1.348488000	-3.592288000
1	1.257317000	-2.252584000	-2.067987000
6	-3.173100000	1.576305000	-0.068861000
1	-2.530777000	2.210929000	-0.689866000
6	3.433497000	-1.311804000	0.650170000
1	4.453981000	-0.927697000	0.535533000
6	2.449813000	-0.429640000	-2.041702000
1	2.441556000	0.543126000	-2.546999000
1	3.386109000	-0.925766000	-2.308398000
6	3.173065000	1.576617000	-0.067898000
1	2.530362000	2.211778000	-0.687948000
6	-2.449941000	-0.430995000	-2.041431000
1	-3.385987000	-0.927750000	-2.307825000
1	-2.442307000	0.541563000	-2.547129000
6	-3.097261000	-1.378966000	2.152802000
1	-2.099209000	-1.796883000	2.311962000
1	-3.819980000	-2.026383000	2.662820000
1	-3.126650000	-0.399515000	2.636106000
6	-3.383416000	-2.716003000	0.022947000
1	-3.714561000	-2.720616000	-1.019284000

1	-4.051246000	-3.383179000	0.580196000
1	-2.378995000	-3.145013000	0.068870000
6	-3.433326000	-1.311581000	0.651255000
1	-4.453768000	-0.927305000	0.536885000
6	0.000123000	-1.838651000	0.574154000
6	0.000064000	0.333411000	1.828040000
6	-3.152764000	2.134418000	1.362846000
1	-3.852497000	1.596542000	2.010849000
1	-3.461378000	3.185823000	1.350754000
1	-2.159240000	2.080837000	1.814742000
6	-4.595561000	1.603691000	-0.651449000
1	-4.634538000	1.239545000	-1.682344000
1	-4.969326000	2.634457000	-0.649810000
1	-5.290102000	1.005346000	-0.052089000
6	4.595201000	1.604744000	-0.651201000
1	5.289948000	1.005390000	-0.053088000
1	4.969109000	2.635453000	-0.648180000
1	4.633603000	1.242169000	-1.682669000
6	3.382974000	-2.715918000	0.021232000
1	2.378510000	-3.144795000	0.067592000
1	4.051031000	-3.383464000	0.577763000
1	3.713481000	-2.720132000	-1.021201000
6	3.098013000	-1.379907000	2.151821000
1	3.128444000	-0.400828000	2.635786000
1	3.820398000	-2.028258000	2.661130000
1	2.099684000	-1.797104000	2.311115000
6	3.153478000	2.133367000	1.364375000
1	2.160455000	2.078577000	1.817185000
1	3.461264000	3.185023000	1.353024000
1	3.854267000	1.595430000	2.011189000
1	-0.000407000	0.376978000	-2.391700000
1	0.002705000	2.904018000	0.981605000
6	0.000260000	2.948523000	-0.126929000
8	-0.001411000	4.060194000	-0.682235000
8	-0.000540000	1.813740000	-0.726929000

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#### 4-Mn-PNP

15	2.270947000	-0.315500000	-0.105241000
7	0.055421000	1.154572000	-1.429140000
6	-1.009785000	0.897712000	-2.430308000
6	1.402888000	1.427070000	-2.016275000
6	2.350701000	0.237114000	-1.872600000
1	3.362456000	0.499352000	-2.195625000
1	2.009873000	-0.598897000	-2.490240000

6	-2.367683000	0.975518000	-1.724873000
1	-3.171971000	0.646399000	-2.387968000
15	-2.316047000	-0.050034000	-0.165871000
6	-0.152471000	-1.296131000	1.649442000
8	-0.254253000	-1.923715000	2.625627000
25	-0.030247000	-0.299569000	0.174382000
6	-0.063160000	-1.732146000	-0.874387000
8	-0.074059000	-2.678828000	-1.554383000
6	3.288712000	-1.892730000	0.031110000
1	4.280006000	-1.558963000	0.359292000
6	2.722885000	-2.835431000	1.106899000
1	3.412537000	-3.673949000	1.256499000
1	2.582981000	-2.338558000	2.070502000
1	1.756892000	-3.246151000	0.798576000
6	3.462073000	-2.634551000	-1.305790000
1	3.968863000	-2.022263000	-2.056937000
1	4.072206000	-3.530122000	-1.141424000
1	2.501103000	-2.959982000	-1.715667000
6	-3.269514000	-1.589462000	-0.673296000
1	-2.797900000	-1.832839000	-1.634978000
6	-3.062452000	-2.795421000	0.259732000
1	-3.520042000	-3.683109000	-0.191574000
1	-2.006208000	-3.013825000	0.425998000
1	-3.530570000	-2.643782000	1.235621000
6	-4.765324000	-1.336806000	-0.929297000
1	-5.209451000	-2.223961000	-1.394685000
1	-5.308234000	-1.149720000	0.002130000
1	-4.943273000	-0.490144000	-1.599112000
1	-0.968954000	1.650782000	-3.228825000
1	-0.849792000	-0.083302000	-2.887915000
1	-2.566746000	2.013252000	-1.442878000
1	1.802528000	2.292638000	-1.478738000
1	1.304860000	1.710263000	-3.070693000
6	-3.413967000	0.869975000	1.041793000
1	-4.343896000	1.067574000	0.493381000
6	-2.798245000	2.215120000	1.460944000
1	-3.547829000	2.796745000	2.009541000
1	-1.949761000	2.061594000	2.137191000
1	-2.445310000	2.818067000	0.621237000
6	-3.732258000	0.025124000	2.287557000
1	-4.310156000	0.628046000	2.996998000
1	-4.321250000	-0.864522000	2.056772000
1	-2.814518000	-0.294171000	2.793911000
6	3.244547000	0.955480000	0.861838000
1	2.638219000	1.862513000	0.762605000
6	4.652390000	1.241988000	0.317676000

1	5.125368000	2.016490000	0.932733000
1	5.300020000	0.358866000	0.351565000
1	4.632090000	1.610671000	-0.711975000
6	3.283907000	0.566670000	2.350339000
1	3.719713000	1.385975000	2.932590000
1	2.283802000	0.367691000	2.749513000
1	3.903090000	-0.321771000	2.518969000
1	-0.209816000	2.063520000	-0.997637000
1	0.051737000	5.219718000	0.577446000
6	0.185907000	4.167343000	0.230739000
8	-0.634095000	3.764809000	-0.649153000
8	1.122821000	3.508364000	0.749535000
1	-0.336859000	1.069768000	1.183370000
1	0.450698000	1.116691000	1.071068000

-1890.155375

### TS3-Mn-PNP

15	2.250070000	-0.332450000	-0.127281000
7	0.063878000	0.963085000	-1.655829000
6	-1.022924000	0.608238000	-2.602416000
6	1.407204000	1.126373000	-2.292791000
6	2.358858000	-0.024115000	-1.957609000
1	3.372543000	0.196437000	-2.306278000
1	2.028787000	-0.941423000	-2.453165000
6	-2.373594000	0.758181000	-1.893106000
1	-3.177518000	0.337341000	-2.503567000
15	-2.301768000	-0.057711000	-0.208949000
6	-0.161638000	-1.100380000	1.725045000
8	-0.2622515000	-1.552537000	2.799680000
25	-0.035781000	-0.340078000	0.132584000
6	-0.086537000	-1.874240000	-0.736759000
8	-0.118166000	-2.909656000	-1.288635000
6	3.302470000	-1.853549000	0.227708000
1	4.299172000	-1.472935000	0.478538000
6	2.757095000	-2.616885000	1.446943000
1	3.456446000	-3.413607000	1.726437000
1	2.615667000	-1.969923000	2.316524000
1	1.791425000	-3.077858000	1.217683000
6	3.444725000	-2.795424000	-0.980218000
1	3.941224000	-2.312579000	-1.826747000
1	4.049845000	-3.662974000	-0.691864000
1	2.471704000	-3.167532000	-1.315477000
6	-3.315528000	-1.617293000	-0.493141000
1	-2.872155000	-1.997500000	-1.423461000
6	-3.106331000	-2.694432000	0.585520000

1	-3.585507000	-3.627189000	0.265995000
1	-2.048531000	-2.901360000	0.757535000
1	-3.551804000	-2.407141000	1.541797000
6	-4.811507000	-1.366301000	-0.743011000
1	-5.290037000	-2.295314000	-1.073857000
1	-5.321756000	-1.042581000	0.169926000
1	-4.989638000	-0.610804000	-1.514800000
1	-0.994592000	1.264653000	-3.483719000
1	-0.865042000	-0.418289000	-2.946007000
1	-2.593381000	1.820630000	-1.751823000
1	1.821620000	2.071174000	-1.927256000
1	1.299131000	1.225922000	-3.379155000
6	-3.371561000	1.046208000	0.867053000
1	-4.329019000	1.140072000	0.338821000
6	-2.767292000	2.448905000	1.036848000
1	-3.497025000	3.096601000	1.536703000
1	-1.869003000	2.411999000	1.657296000
1	-2.493324000	2.922171000	0.090819000
6	-3.616022000	0.412557000	2.247431000
1	-4.168267000	1.115490000	2.881888000
1	-4.201350000	-0.507835000	2.192116000
1	-2.667864000	0.185399000	2.747167000
6	3.200335000	1.082567000	0.649875000
1	2.609675000	1.961969000	0.373306000
6	4.634478000	1.280199000	0.136563000
1	5.070345000	2.170200000	0.606037000
1	5.280989000	0.431963000	0.386078000
1	4.672185000	1.428948000	-0.946666000
6	3.155993000	0.961635000	2.181983000
1	3.557924000	1.872470000	2.639601000
1	2.131494000	0.824916000	2.541080000
1	3.763314000	0.119828000	2.533798000
1	-0.165406000	1.896946000	-1.291464000
1	0.554892000	5.089263000	0.460017000
6	0.340578000	4.028798000	0.234406000
8	-0.168013000	3.720872000	-0.853922000
8	0.673165000	3.223075000	1.188957000
1	-0.011429000	1.105431000	1.068039000
1	0.318506000	2.029523000	1.017162000

-1890.148414

### 5-Mn-PNP

15	2.222159000	-0.375606000	-0.129965000
7	0.073359000	0.909612000	-1.720863000
6	-1.022364000	0.536076000	-2.646024000

6	1.419422000	1.020156000	-2.358123000
6	2.340342000	-0.140273000	-1.972744000
1	3.359617000	0.035958000	-2.330776000
1	1.982787000	-1.067453000	-2.428912000
6	-2.367396000	0.718762000	-1.933540000
1	-3.176616000	0.283314000	-2.526919000
15	-2.300151000	-0.041925000	-0.220040000
6	-0.184788000	-1.042747000	1.758856000
8	-0.283518000	-1.427661000	2.863124000
25	-0.055265000	-0.369998000	0.137545000
6	-0.131865000	-1.932731000	-0.687882000
8	-0.185702000	-2.993881000	-1.193665000
6	3.272766000	-1.885731000	0.277622000
1	4.278483000	-1.505465000	0.490220000
6	2.740098000	-2.580933000	1.542558000
1	3.429735000	-3.377642000	1.845987000
1	2.626529000	-1.891919000	2.383719000
1	1.760836000	-3.030502000	1.352717000
6	3.379714000	-2.889233000	-0.883354000
1	3.870148000	-2.457672000	-1.760683000
1	3.974657000	-3.752347000	-0.561744000
1	2.394912000	-3.259510000	-1.184305000
6	-3.362730000	-1.579615000	-0.449572000
1	-2.934567000	-2.001281000	-1.369297000
6	-3.171793000	-2.625797000	0.662494000
1	-3.668485000	-3.560092000	0.375243000
1	-2.116580000	-2.842942000	0.838148000
1	-3.609621000	-2.298986000	1.609855000
6	-4.853887000	-1.300782000	-0.697991000
1	-5.356892000	-2.226249000	-1.001980000
1	-5.350751000	-0.941953000	0.209322000
1	-5.019830000	-0.560841000	-1.487552000
1	-0.996119000	1.159265000	-3.551928000
1	-0.874775000	-0.504109000	-2.950920000
1	-2.581719000	1.787033000	-1.830878000
1	1.855871000	1.967974000	-2.027501000
1	1.317165000	1.079493000	-3.448377000
6	-3.351020000	1.126963000	0.807878000
1	-4.308305000	1.217242000	0.278698000
6	-2.721894000	2.523839000	0.920564000
1	-3.433153000	3.203941000	1.404011000
1	-1.818361000	2.488856000	1.532819000
1	-2.452081000	2.958410000	-0.045780000
6	-3.603476000	0.555838000	2.213896000
1	-4.146950000	1.290562000	2.819513000
1	-4.199566000	-0.359148000	2.195590000

1	-2.657829000	0.336511000	2.721871000
6	3.200138000	1.058663000	0.580291000
1	2.612582000	1.930846000	0.275202000
6	4.628036000	1.231404000	0.040156000
1	5.076926000	2.133180000	0.473856000
1	5.272430000	0.387175000	0.308118000
1	4.651480000	1.344181000	-1.047788000
6	3.181537000	0.998938000	2.116306000
1	3.588884000	1.927162000	2.532644000
1	2.164056000	0.871053000	2.497699000
1	3.797801000	0.172465000	2.488126000
1	-0.135812000	1.845394000	-1.365772000
1	0.745113000	5.112075000	0.486771000
6	0.491635000	4.071046000	0.237427000
8	0.086840000	3.745025000	-0.872621000
8	0.682994000	3.266205000	1.260932000
1	0.010959000	1.069572000	0.972391000
1	0.405262000	2.281517000	1.051015000

-1890.148836

### TS3'-Mn-PNP

15	-2.245673000	-0.445135000	0.169420000
7	-0.100070000	0.620726000	1.665141000
6	1.095992000	0.810161000	2.521343000
6	-1.310172000	0.541678000	2.532262000
6	-2.338025000	-0.472042000	2.010914000
1	-3.338417000	-0.288476000	2.415267000
1	-2.031224000	-1.479687000	2.306743000
6	2.321725000	1.148838000	1.675950000
1	3.243742000	1.073353000	2.258531000
15	2.324420000	0.027426000	0.195467000
6	0.125047000	-0.648083000	-1.800418000
8	0.187338000	-0.795548000	-2.959872000
25	0.045585000	-0.386102000	-0.038546000
6	0.130343000	-2.092377000	0.317653000
8	0.153591000	-3.220657000	0.637726000
6	-3.308524000	-1.843452000	-0.490918000
1	-4.307209000	-1.416717000	-0.637942000
6	-2.782709000	-2.329904000	-1.853199000
1	-3.485957000	-3.053553000	-2.280963000
1	-2.659124000	-1.514924000	-2.571079000
1	-1.813240000	-2.824756000	-1.741563000
6	-3.433453000	-3.017704000	0.495047000
1	-3.914442000	-2.721607000	1.431632000
1	-4.045843000	-3.805470000	0.041285000

1	-2.455976000	-3.450510000	0.729724000
6	3.399650000	-1.411899000	0.736466000
1	2.883782000	-1.728899000	1.653374000
6	3.382598000	-2.600170000	-0.245066000
1	3.700554000	-3.509079000	0.277708000
1	2.393476000	-2.783950000	-0.667187000
1	4.076833000	-2.441742000	-1.073864000
6	4.844476000	-1.026886000	1.095825000
1	5.365783000	-1.902149000	1.500715000
1	5.399268000	-0.695117000	0.211737000
1	4.899023000	-0.234917000	1.848084000
1	0.921953000	1.621951000	3.244727000
1	1.275910000	-0.102671000	3.109732000
1	2.243926000	2.176533000	1.310684000
1	-1.773409000	1.537344000	2.614545000
1	-1.021874000	0.253763000	3.551236000
6	3.294523000	0.995499000	-1.084652000
1	4.202346000	1.345108000	-0.575898000
6	2.488440000	2.221345000	-1.545592000
1	3.082739000	2.808402000	-2.254540000
1	1.568863000	1.914792000	-2.054756000
1	2.217171000	2.884810000	-0.720519000
6	3.699398000	0.141873000	-2.298288000
1	4.166055000	0.783329000	-3.054737000
1	4.422144000	-0.633886000	-2.038843000
1	2.829897000	-0.337362000	-2.759203000
6	-3.135565000	1.125895000	-0.329267000
1	-2.544611000	1.903814000	0.166266000
6	-4.582169000	1.247781000	0.176531000
1	-4.975113000	2.236851000	-0.086279000
1	-5.239099000	0.503047000	-0.284963000
1	-4.655312000	1.141785000	1.262645000
6	-3.054603000	1.345607000	-1.849575000
1	-3.413803000	2.349503000	-2.101152000
1	-2.032437000	1.245764000	-2.227527000
1	-3.684008000	0.626814000	-2.385564000
1	-0.234319000	2.046921000	1.138887000
1	-0.462077000	2.627604000	-0.971893000
6	-0.466213000	3.466575000	-0.253033000
8	-0.585842000	4.622541000	-0.637012000
8	-0.336448000	3.118748000	1.006335000

-1888.963352

**4'-Mn-PNP**  
 15    2.244346000    -0.459254000    -0.207814000

7	0.061498000	0.473242000	-1.709268000
6	-1.131597000	0.758521000	-2.539394000
6	1.251454000	0.381907000	-2.594877000
6	2.295334000	-0.597289000	-2.045853000
1	3.284559000	-0.437799000	-2.485235000
1	1.979814000	-1.619525000	-2.274772000
6	-2.318519000	1.151325000	-1.664080000
1	-3.256811000	1.132314000	-2.224376000
15	-2.335778000	0.015158000	-0.195730000
6	-0.061779000	-0.346398000	1.819511000
8	-0.075571000	-0.296813000	2.989883000
25	-0.046530000	-0.381559000	0.039850000
6	-0.120640000	-2.127212000	0.006050000
8	-0.125516000	-3.296052000	-0.098672000
6	3.310813000	-1.823724000	0.514228000
1	4.319333000	-1.402796000	0.598217000
6	2.822940000	-2.197569000	1.925772000
1	3.526625000	-2.901978000	2.383873000
1	2.740171000	-1.327825000	2.582740000
1	1.840709000	-2.676858000	1.885323000
6	3.391552000	-3.066391000	-0.389044000
1	3.848454000	-2.841855000	-1.357245000
1	4.008774000	-3.828217000	0.101179000
1	2.403527000	-3.502384000	-0.564662000
6	-3.409876000	-1.409288000	-0.789046000
1	-2.866759000	-1.718877000	-1.692937000
6	-3.451261000	-2.615906000	0.168374000
1	-3.780086000	-3.504024000	-0.383212000
1	-2.482621000	-2.839712000	0.614575000
1	-4.166832000	-2.455638000	0.978733000
6	-4.838886000	-1.002946000	-1.187897000
1	-5.354410000	-1.866267000	-1.624663000
1	-5.417705000	-0.684138000	-0.314306000
1	-4.865493000	-0.197404000	-1.926456000
1	-0.916865000	1.574174000	-3.247571000
1	-1.377227000	-0.126339000	-3.147858000
1	-2.176515000	2.169091000	-1.290937000
1	1.699772000	1.379671000	-2.730675000
1	0.945820000	0.047677000	-3.595491000
6	-3.332123000	0.960202000	1.081008000
1	-4.253827000	1.275155000	0.574975000
6	-2.572647000	2.217295000	1.537645000
1	-3.190147000	2.782110000	2.244899000
1	-1.643936000	1.947807000	2.049164000
1	-2.327036000	2.890212000	0.711916000
6	-3.700899000	0.093411000	2.297309000

1	-4.187469000	0.716743000	3.056288000
1	-4.394893000	-0.708724000	2.039865000
1	-2.811739000	-0.353304000	2.754004000
6	3.175085000	1.125263000	0.174961000
1	2.574681000	1.888197000	-0.331868000
6	4.598808000	1.197074000	-0.400183000
1	5.023335000	2.185998000	-0.191520000
1	5.261275000	0.455188000	0.058014000
1	4.619927000	1.051939000	-1.483686000
6	3.173834000	1.424546000	1.683773000
1	3.554220000	2.436306000	1.862350000
1	2.173937000	1.357641000	2.121457000
1	3.824900000	0.728760000	2.224038000
1	0.253985000	2.036221000	-1.136468000
1	0.399768000	2.554132000	0.965070000
6	0.456132000	3.399517000	0.257109000
8	0.589085000	4.549821000	0.638185000
8	0.370084000	3.060297000	-1.018537000

-1888.962569

<b>6</b>			
6	1.185061000	-0.747559000	0.201056000
6	1.210438000	0.723326000	-0.222562000
6	-1.210439000	0.723325000	-0.222561000
6	-1.185061000	-0.747560000	0.201055000
1	2.092109000	1.219875000	0.196842000
1	1.227645000	-0.823044000	1.301081000
1	2.030760000	-1.299660000	-0.219995000
1	-2.092109000	1.219874000	0.196844000
1	-1.281578000	0.779537000	-1.316487000
1	-1.227646000	-0.823047000	1.301081000
1	-2.030758000	-1.299663000	-0.219997000
1	1.281576000	0.779537000	-1.316487000
8	0.000001000	-1.397868000	-0.274950000
7	-0.000001000	1.452480000	0.190040000
1	0.000000000	1.552978000	1.204507000

-287.729062

<b>7</b>			
6	3.179262000	-1.123024000	0.228829000
1	3.913461000	-1.939873000	0.194953000
8	3.083881000	-0.514654000	-0.945264000
1	2.410922000	0.231564000	-0.907625000
8	2.544291000	-0.834269000	1.230893000

8	-0.116726000	2.658752000	0.380383000
1	-0.417149000	2.989598000	-0.485765000
6	0.828699000	1.739913000	0.197242000
1	1.208477000	1.342487000	1.138786000
8	1.281595000	1.444195000	-0.904323000
6	-0.679847000	-1.243443000	-0.629612000
6	-1.809633000	-0.587917000	1.409034000
6	-2.898371000	0.066752000	0.563229000
8	-3.032456000	-0.594523000	-0.701782000
6	-1.797804000	-0.581383000	-1.430087000
1	0.262628000	-1.155915000	-1.179777000
1	-1.686454000	-0.031891000	2.344839000
1	-2.654178000	1.127937000	0.400422000
1	-1.519887000	0.456988000	-1.667622000
7	-0.551028000	-0.558078000	0.658987000
1	-3.872763000	-0.004198000	1.053502000
1	-2.123639000	-1.617196000	1.659312000
1	-0.911247000	-2.316787000	-0.510209000
1	-1.983667000	-1.119666000	-2.363104000
1	0.212184000	-0.957891000	1.198322000

-667.262756

#### TS4

6	-3.398996000	-0.946742000	-0.031589000
1	-4.379870000	-1.441400000	0.014549000
8	-3.440653000	0.272600000	0.452176000
1	-2.520000000	0.755360000	0.414692000
8	-2.410289000	-1.511236000	-0.492769000
8	0.668467000	2.202784000	-0.571211000
1	0.753829000	2.642987000	0.291061000
6	-0.425023000	1.382840000	-0.503855000
1	-0.750105000	1.117743000	-1.516613000
8	-1.245643000	1.536592000	0.445275000
6	0.729842000	-0.657057000	1.165335000
6	1.305012000	-0.870124000	-1.226265000
6	2.694998000	-0.345712000	-0.879905000
8	3.062271000	-0.720926000	0.452590000
6	2.152897000	-0.159244000	1.402886000
1	0.024755000	-0.132647000	1.818404000
1	0.997724000	-0.507430000	-2.213200000
1	2.727066000	0.746966000	-0.980477000
1	2.197223000	0.937598000	1.350797000
7	0.310173000	-0.416529000	-0.230926000
1	3.437621000	-0.788177000	-1.547665000
1	1.322595000	-1.967575000	-1.254152000

1	0.674838000	-1.731320000	1.383683000
1	2.495877000	-0.471917000	2.391837000
1	-0.578362000	-0.906757000	-0.384567000

-667.254804

**8**

6	2.239492000	0.522314000	-1.175324000
6	1.153634000	-0.547526000	-1.232342000
6	1.154090000	-0.547956000	1.232241000
6	2.239934000	0.521897000	1.175186000
1	0.506282000	-0.405413000	-2.097609000
1	1.786047000	1.524006000	-1.210897000
1	2.906783000	0.408705000	-2.031814000
1	0.507066000	-0.406160000	2.097802000
1	1.595397000	-1.548128000	1.268391000
1	1.786498000	1.523575000	1.211285000
1	2.907549000	0.407987000	2.031383000
1	1.594956000	-1.547673000	-1.269047000
8	3.038788000	0.387208000	-0.000245000
7	0.302261000	-0.465458000	0.000125000
1	-0.195124000	0.491162000	0.000398000
6	-0.828240000	-1.529639000	0.000117000
1	-0.332314000	-2.502911000	0.000330000
8	-1.557827000	-1.386304000	-1.161732000
1	-2.146912000	-0.604504000	-1.034015000
8	-1.558172000	-1.385962000	1.161716000
8	-2.853288000	0.752319000	-0.000402000
1	-2.147238000	-0.604235000	1.033613000
6	-2.180588000	1.828565000	0.000196000
1	-2.748892000	2.778139000	0.000310000
8	-0.920231000	1.914954000	0.000483000

-667.263618

**TS5**

6	-2.200472000	0.496321000	1.174495000
6	-1.103613000	-0.562359000	1.217420000
6	-1.103381000	-0.562287000	-1.217551000
6	-2.200081000	0.496540000	-1.174810000
1	-0.473000000	-0.416818000	2.095654000
1	-1.759347000	1.503696000	1.217044000
1	-2.868082000	0.371440000	2.029808000
1	-0.472586000	-0.416962000	-2.095687000
1	-1.552760000	-1.563756000	-1.269162000
1	-1.758812000	1.503868000	-1.216948000

1	-2.867416000	0.371954000	-2.030379000
1	-1.552800000	-1.563909000	1.269070000
8	-3.003630000	0.367913000	-0.000302000
7	-0.249500000	-0.462620000	0.000009000
1	0.363917000	0.819519000	0.000469000
6	0.813607000	-1.526436000	0.000027000
1	0.333746000	-2.511541000	-0.000131000
8	1.572099000	-1.431859000	1.166105000
1	2.131592000	-0.634408000	1.090556000
8	1.572339000	-1.431650000	-1.165832000
8	2.813151000	0.891033000	-0.000687000
1	2.131628000	-0.634052000	-1.090033000
6	2.078376000	1.890624000	0.000030000
1	2.505678000	2.904213000	-0.000008000
8	0.780806000	1.868398000	0.000967000

-667.261204

<b>9</b>			
6	-2.195620000	0.510229000	1.174707000
6	-1.111891000	-0.561926000	1.214899000
6	-1.111505000	-0.561401000	-1.215072000
6	-2.195227000	0.510756000	-1.174766000
1	-0.482092000	-0.425503000	2.095333000
1	-1.741904000	1.512184000	1.218837000
1	-2.865271000	0.393090000	2.029641000
1	-0.481406000	-0.424608000	-2.095238000
1	-1.575927000	-1.557039000	-1.268146000
1	-1.741483000	1.512724000	-1.218296000
1	-2.864592000	0.394003000	-2.029978000
1	-1.576320000	-1.557590000	1.267397000
8	-3.000831000	0.394918000	-0.000192000
7	-0.256922000	-0.469611000	0.000063000
1	0.402427000	0.892152000	0.000414000
6	0.789239000	-1.541148000	-0.000063000
1	0.305230000	-2.524996000	-0.000190000
8	1.552443000	-1.458213000	1.166160000
1	2.109621000	-0.659685000	1.099245000
8	1.552333000	-1.457919000	-1.166346000
8	2.824198000	0.877907000	-0.000184000
1	2.109595000	-0.659479000	-1.099263000
6	2.114657000	1.890279000	0.000235000
1	2.553078000	2.898010000	0.000402000
8	0.810555000	1.894967000	0.000531000

-667.260425

**10**

6	1.829387000	-1.176113000	-0.261786000
6	0.416406000	-1.202183000	0.311644000
6	0.416403000	1.202223000	0.311572000
6	1.829385000	1.176109000	-0.261859000
1	-0.099223000	-2.097059000	-0.040428000
1	1.785658000	-1.226909000	-1.361060000
1	2.404908000	-2.027775000	0.109340000
1	-0.099217000	2.097078000	-0.040560000
1	0.471492000	1.249829000	1.414062000
1	1.785650000	1.226831000	-1.361137000
1	2.404909000	2.027795000	0.109207000
1	0.471493000	-1.249716000	1.414138000
8	2.536553000	0.000011000	0.138690000
7	-0.319703000	0.000006000	-0.124279000
6	-1.710552000	-0.000020000	0.309699000
1	-1.825353000	-0.000087000	1.403413000
8	-2.355975000	-1.167627000	-0.135975000
1	-2.172281000	-1.270152000	-1.083916000
8	-2.356037000	1.167608000	-0.135827000
1	-2.172616000	1.270108000	-1.083821000

-477.479284

**11**

6	2.492932000	-1.356172000	0.365753000
6	1.847068000	-0.416616000	1.386993000
6	1.821617000	1.328971000	-0.311861000
6	2.500784000	0.349686000	-1.276025000
1	1.206968000	-0.982892000	2.070776000
1	1.721081000	-1.922315000	-0.175439000
1	3.171946000	-2.056947000	0.859249000
1	1.158258000	2.005787000	-0.854026000
1	2.597914000	1.934343000	0.172842000
1	1.757619000	-0.174787000	-1.897662000
1	3.186204000	0.883212000	-1.940622000
1	2.640596000	0.055914000	1.980324000
8	3.289309000	-0.610911000	-0.566522000
7	1.065711000	0.648932000	0.749818000
6	-0.314864000	0.399776000	0.568172000
1	-0.727013000	-0.020406000	1.492485000
8	-0.639932000	-0.675459000	-0.410727000
1	-0.416933000	-0.349136000	-1.297674000
8	-0.952503000	1.565182000	0.164892000
1	-1.913307000	1.370239000	0.102466000

6	-3.976607000	-0.390244000	-0.130689000
1	-5.033066000	-0.687294000	-0.129364000
8	-3.179571000	-1.415001000	-0.362628000
1	-2.209041000	-1.131725000	-0.379572000
8	-3.620650000	0.766324000	0.066664000

-667.249144

### TS6

6	2.502131000	-1.337521000	0.344289000
6	1.779197000	-0.470095000	1.376683000
6	1.788795000	1.363717000	-0.255138000
6	2.530316000	0.436090000	-1.222117000
1	1.114510000	-1.082293000	1.991515000
1	1.768702000	-1.895770000	-0.254647000
1	3.176581000	-2.040815000	0.839013000
1	1.129504000	2.044265000	-0.794954000
1	2.517417000	1.959853000	0.306239000
1	1.816757000	-0.082332000	-1.881041000
1	3.223965000	1.010212000	-1.841687000
1	2.516412000	0.008163000	2.032239000
8	3.315568000	-0.525950000	-0.512168000
7	1.005441000	0.585525000	0.714311000
6	-0.340114000	0.446699000	0.603120000
1	-0.799374000	-0.067516000	1.447457000
8	-0.739431000	-0.879620000	-0.520113000
1	-0.538387000	-0.549586000	-1.410283000
8	-0.988576000	1.504104000	0.098765000
1	-1.972636000	1.295515000	0.094229000
6	-3.878805000	-0.352256000	-0.099110000
1	-4.950788000	-0.598795000	-0.063375000
8	-3.116354000	-1.354687000	-0.378987000
1	-1.979688000	-1.106449000	-0.457531000
8	-3.514978000	0.817036000	0.125790000

-667.247160

### 12

6	2.573317000	-1.205169000	0.449508000
6	1.712301000	-0.367919000	1.397163000
6	1.808013000	1.461159000	-0.257884000
6	2.673661000	0.551610000	-1.132445000
1	1.006409000	-1.004024000	1.936301000
1	1.921713000	-1.799823000	-0.206090000
1	3.225712000	-1.872459000	1.017510000
1	1.161641000	2.094098000	-0.866764000

1	2.444765000	2.094825000	0.369971000
1	2.036907000	-0.003778000	-1.837369000
1	3.396167000	1.145097000	-1.697413000
1	2.347590000	0.152688000	2.122621000
8	3.428131000	-0.364023000	-0.333698000
7	0.973982000	0.630702000	0.617370000
6	-0.357911000	0.645797000	0.565877000
1	-0.845822000	-0.072009000	1.235623000
8	-0.685750000	-2.026483000	-0.822660000
1	-0.527419000	-1.623736000	-1.686058000
8	-1.031235000	1.406177000	-0.166702000
1	-2.543545000	1.180295000	-0.136387000
6	-3.951945000	-0.162096000	0.035065000
1	-5.046421000	-0.253303000	0.070998000
8	-3.214364000	-1.137706000	0.134641000
1	-1.563886000	-1.702812000	-0.545325000
8	-3.568818000	1.085752000	-0.116945000

-667.287281

**13**

6	-2.667501000	1.309141000	-0.426730000
6	-1.519463000	1.253824000	0.582114000
6	-1.654649000	-1.210595000	0.479753000
6	-2.800665000	-1.049370000	-0.520578000
1	-0.827103000	2.084534000	0.425040000
1	-2.265087000	1.358324000	-1.450139000
1	-3.289624000	2.188532000	-0.245373000
1	-1.047830000	-2.085891000	0.245535000
1	-2.055267000	-1.313409000	1.495344000
1	-2.405764000	-1.062088000	-1.547888000
1	-3.520330000	-1.863069000	-0.406402000
1	-1.918703000	1.315384000	1.601559000
8	-3.517374000	0.167625000	-0.291684000
7	-0.803547000	-0.017035000	0.432056000
6	0.517863000	-0.079387000	0.244580000
1	1.031196000	0.890705000	0.217344000
8	1.162042000	-1.142936000	0.108245000
1	2.708467000	-0.971154000	-0.085670000
6	4.116548000	0.358056000	-0.211417000
1	5.205461000	0.436712000	-0.344791000
8	3.392191000	1.334559000	-0.082354000
8	3.720217000	-0.902916000	-0.211117000

-590.855963

**14**

6	-1.603417000	0.984469000	-0.385059000
6	-0.342216000	1.325569000	0.410369000
6	0.145281000	-1.088183000	0.528162000
6	-1.138245000	-1.331345000	-0.266668000
1	0.081631000	2.273537000	0.067695000
1	-1.382804000	1.005565000	-1.463621000
1	-2.398053000	1.702778000	-0.169446000
1	0.916279000	-1.811853000	0.259004000
1	-0.061004000	-1.170066000	1.603046000
1	-0.909723000	-1.372205000	-1.342681000
1	-1.601215000	-2.273827000	0.034861000
1	-0.593072000	1.418925000	1.474822000
8	-2.103412000	-0.303766000	-0.016990000
7	0.643929000	0.257935000	0.241333000
6	1.915045000	0.488988000	-0.154493000
1	2.117274000	1.558559000	-0.335362000
8	2.786475000	-0.372977000	-0.309450000

-401.081679

**15-Mn-PNP**

25	-1.178662000	0.440920000	-0.149316000
15	-2.177928000	-1.582421000	0.145376000
15	0.387022000	2.080045000	0.015038000
8	-3.522763000	2.178555000	0.295440000
8	-1.533281000	0.569668000	-3.056494000
7	-0.674731000	0.149829000	1.954042000
6	-1.729312000	-0.583258000	2.686844000
1	-2.631844000	0.035827000	2.685243000
1	-1.432582000	-0.750922000	3.733174000
6	-0.259093000	1.407094000	2.613181000
1	0.048164000	1.218411000	3.652762000
1	-1.121449000	2.081027000	2.631086000
6	-1.343054000	-3.098439000	-0.601543000
1	-0.396649000	-3.108695000	-0.046296000
6	-0.044045000	3.886339000	-0.295414000
1	0.902766000	4.437489000	-0.345352000
6	0.896963000	2.009839000	1.813232000
1	1.762192000	1.340721000	1.881334000
1	1.199079000	2.981654000	2.212637000
6	2.042054000	1.826867000	-0.836524000
1	2.306214000	0.837414000	-0.448334000
6	-1.973612000	-1.918072000	1.978589000
1	-2.831322000	-2.446120000	2.404797000
1	-1.095468000	-2.561313000	2.107495000

6	-4.388989000	-1.584400000	-1.602085000
1	-4.146559000	-0.551000000	-1.871479000
1	-5.465602000	-1.730837000	-1.750528000
1	-3.866255000	-2.245210000	-2.298860000
6	-4.886048000	-1.020193000	0.808389000
1	-4.676101000	-1.219299000	1.863687000
1	-5.942950000	-1.257454000	0.636147000
1	-4.750576000	0.048484000	0.629928000
6	-4.015896000	-1.865005000	-0.137364000
1	-4.207812000	-2.921743000	0.083942000
6	-2.586384000	1.471066000	0.169374000
6	-1.400414000	0.527444000	-1.886812000
6	-0.992143000	-2.931738000	-2.087551000
1	-1.885662000	-2.918772000	-2.719487000
1	-0.370854000	-3.773953000	-2.416501000
1	-0.439006000	-2.005408000	-2.257613000
6	-2.064216000	-4.429661000	-0.338716000
1	-2.329866000	-4.558903000	0.716050000
1	-1.415245000	-5.266323000	-0.624251000
1	-2.980606000	-4.510300000	-0.933392000
6	3.142792000	2.823221000	-0.439730000
1	2.944071000	3.823398000	-0.839391000
1	4.104500000	2.495849000	-0.854058000
1	3.260646000	2.909386000	0.645145000
6	-0.889951000	4.494149000	0.837615000
1	-1.837067000	3.961905000	0.958803000
1	-1.125241000	5.537759000	0.595961000
1	-0.368421000	4.492173000	1.799022000
6	-0.777424000	4.032094000	-1.640784000
1	-0.202841000	3.629169000	-2.478428000
1	-0.973765000	5.091237000	-1.846748000
1	-1.736504000	3.506100000	-1.614371000
6	1.929747000	1.706886000	-2.363167000
1	1.152994000	0.996732000	-2.655377000
1	2.884719000	1.362501000	-2.778996000
1	1.708000000	2.673575000	-2.827351000
1	0.150725000	-0.456724000	1.942664000
1	0.111914000	-0.468370000	-0.458001000
6	3.687680000	-1.675955000	-1.057618000
6	4.398413000	-0.582297000	1.038494000
6	5.749483000	-1.280365000	0.878031000
8	6.053014000	-1.502873000	-0.502715000
6	5.068311000	-2.329002000	-1.129876000
1	2.921057000	-2.343254000	-1.460557000
1	4.117802000	-0.502282000	2.089915000
1	5.741516000	-2.240280000	1.416759000

1	5.042747000	-3.315972000	-0.642472000
7	3.372704000	-1.354880000	0.335221000
1	6.551160000	-0.654785000	1.277616000
1	4.448199000	0.424752000	0.606849000
1	3.686081000	-0.750605000	-1.647243000
1	5.378532000	-2.452926000	-2.170158000
6	2.215319000	-1.723805000	0.917670000
8	1.878538000	-1.444619000	2.078587000
1	1.566358000	-2.308847000	0.252103000

-2101.451484

#### TS7-Mn-PNP

25	-0.634686000	0.461636000	-0.153595000
15	-2.496663000	-0.933794000	0.133703000
15	1.221396000	1.825467000	0.125844000
8	-2.357548000	2.801139000	-0.537475000
8	-0.325551000	0.008067000	-3.043167000
7	-0.662084000	0.444263000	1.977531000
6	-2.018433000	0.293459000	2.562135000
1	-2.592767000	1.195085000	2.325817000
1	-1.954020000	0.215161000	3.657051000
6	0.089325000	1.540260000	2.632740000
1	0.212309000	1.327413000	3.704358000
1	-0.503366000	2.455955000	2.546050000
6	-2.425140000	-2.775699000	-0.246615000
1	-1.620735000	-3.106358000	0.417397000
6	1.163112000	3.670158000	-0.258634000
1	2.205796000	4.004506000	-0.198164000
6	1.456590000	1.710626000	1.970381000
1	2.060066000	0.815717000	2.154432000
1	1.996132000	2.566030000	2.386647000
6	2.896483000	1.308743000	-0.538652000
1	2.908736000	0.249363000	-0.283421000
6	-2.687446000	-0.954856000	1.986719000
1	-3.727505000	-1.036136000	2.311966000
1	-2.148146000	-1.840570000	2.336495000
6	-4.021041000	0.014915000	-2.045180000
1	-3.434693000	0.931846000	-2.144356000
1	-5.014022000	0.201496000	-2.470833000
1	-3.537702000	-0.755278000	-2.651876000
6	-4.868530000	0.690555000	0.251253000
1	-5.068702000	0.373594000	1.278554000
1	-5.835761000	0.914736000	-0.214281000
1	-4.296893000	1.619872000	0.282303000
6	-4.161086000	-0.402409000	-0.569863000

1	-4.792168000	-1.295865000	-0.527213000
6	-1.677427000	1.858760000	-0.371758000
6	-0.452275000	0.197255000	-1.893824000
6	-2.008543000	-3.073610000	-1.694999000
1	-2.806632000	-2.822731000	-2.401534000
1	-1.797999000	-4.143692000	-1.807042000
1	-1.112619000	-2.519170000	-1.987053000
6	-3.685869000	-3.564319000	0.146647000
1	-4.018879000	-3.337782000	1.164581000
1	-3.470593000	-4.638279000	0.098000000
1	-4.518392000	-3.369482000	-0.537203000
6	4.101744000	1.971549000	0.147025000
1	4.149588000	3.045951000	-0.058961000
1	5.025946000	1.523818000	-0.237090000
1	4.095992000	1.832658000	1.232132000
6	0.355313000	4.487324000	0.764968000
1	-0.693538000	4.181059000	0.790648000
1	0.381558000	5.545721000	0.479884000
1	0.765033000	4.412510000	1.776041000
6	0.651826000	3.941640000	-1.686702000
1	1.186936000	3.369767000	-2.446718000
1	0.779024000	5.005498000	-1.920023000
1	-0.410078000	3.705946000	-1.777479000
6	3.009109000	1.407343000	-2.068213000
1	2.140795000	0.982314000	-2.578862000
1	3.896959000	0.856779000	-2.400251000
1	3.129302000	2.445140000	-2.393562000
1	-0.159341000	-0.456824000	2.159173000
1	0.498323000	-0.918970000	0.125079000
6	2.466167000	-2.365067000	-1.039311000
6	3.213422000	-1.919852000	1.265259000
6	4.521451000	-2.621805000	0.914624000
8	4.837622000	-2.460156000	-0.473741000
6	3.815087000	-3.031901000	-1.295913000
1	1.683330000	-2.903872000	-1.585808000
1	2.924187000	-2.137771000	2.296109000
1	4.450116000	-3.694993000	1.151961000
1	3.744282000	-4.112589000	-1.095091000
7	2.155297000	-2.398121000	0.384189000
1	5.353644000	-2.188572000	1.475586000
1	3.366473000	-0.832775000	1.188658000
1	2.482418000	-1.335610000	-1.430407000
1	4.127329000	-2.883163000	-2.332857000
6	0.798269000	-2.114175000	0.734576000
8	0.486849000	-2.046380000	1.990636000
1	0.170336000	-2.721142000	0.065782000

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**16-Mn-PNP**

25	-0.625496000	0.458430000	-0.151858000
15	-2.508240000	-0.917455000	0.134052000
15	1.244275000	1.813333000	0.125773000
8	-2.325066000	2.811630000	-0.533022000
8	-0.330772000	0.014464000	-3.046322000
7	-0.651505000	0.439284000	1.971301000
6	-2.007945000	0.303094000	2.560332000
1	-2.573454000	1.211793000	2.329481000
1	-1.939360000	0.221497000	3.654660000
6	0.113616000	1.522344000	2.632760000
1	0.238148000	1.298032000	3.701767000
1	-0.469681000	2.445088000	2.557438000
6	-2.458471000	-2.758690000	-0.250763000
1	-1.655886000	-3.099745000	0.410048000
6	1.191830000	3.659795000	-0.248689000
1	2.236508000	3.987456000	-0.187299000
6	1.480912000	1.685693000	1.968734000
1	2.077422000	0.785004000	2.146258000
1	2.028068000	2.534357000	2.388770000
6	2.914057000	1.291301000	-0.548155000
1	2.924609000	0.230462000	-0.298783000
6	-2.694362000	-0.936507000	1.986611000
1	-3.734458000	-1.004512000	2.314603000
1	-2.164238000	-1.828702000	2.333494000
6	-4.022398000	0.056802000	-2.042572000
1	-3.427223000	0.968017000	-2.141370000
1	-5.014026000	0.254583000	-2.466180000
1	-3.548389000	-0.717219000	-2.651675000
6	-4.859173000	0.736424000	0.257209000
1	-5.062746000	0.418266000	1.283400000
1	-5.823759000	0.973599000	-0.207246000
1	-4.276597000	1.658753000	0.291287000
6	-4.165311000	-0.362095000	-0.567997000
1	-4.806421000	-1.248465000	-0.527014000
6	-1.652914000	1.863686000	-0.373201000
6	-0.449354000	0.196763000	-1.896054000
6	-2.050499000	-3.058398000	-1.701245000
1	-2.846365000	-2.793384000	-2.405041000
1	-1.856822000	-4.131267000	-1.816465000
1	-1.146399000	-2.517870000	-1.994183000
6	-3.728219000	-3.531729000	0.144669000
1	-4.056635000	-3.301936000	1.163329000

1	-3.525718000	-4.608079000	0.095026000
1	-4.559548000	-3.326735000	-0.537640000
6	4.123968000	1.945440000	0.137761000
1	4.175490000	3.020932000	-0.061402000
1	5.044892000	1.496338000	-0.252396000
1	4.121106000	1.799037000	1.221883000
6	0.390747000	4.475381000	0.781476000
1	-0.659698000	4.174905000	0.808608000
1	0.422045000	5.534984000	0.501655000
1	0.802994000	4.393218000	1.790901000
6	0.681303000	3.943706000	-1.674685000
1	1.209642000	3.370968000	-2.438699000
1	0.819276000	5.007475000	-1.901894000
1	-0.383087000	3.720056000	-1.765903000
6	3.021284000	1.397265000	-2.077564000
1	2.149591000	0.977825000	-2.587171000
1	3.905612000	0.844567000	-2.415140000
1	3.144438000	2.436055000	-2.398454000
1	-0.159408000	-0.475341000	2.149362000
1	0.521803000	-0.959311000	0.143073000
6	2.448546000	-2.390721000	-1.038318000
6	3.181870000	-1.942610000	1.262591000
6	4.495241000	-2.638732000	0.921930000
8	4.818800000	-2.478259000	-0.465222000
6	3.800941000	-3.051443000	-1.292314000
1	1.670940000	-2.928879000	-1.593513000
1	2.891246000	-2.152906000	2.294702000
1	4.427625000	-3.711847000	1.160867000
1	3.733133000	-4.132895000	-1.094343000
7	2.128962000	-2.434985000	0.383020000
1	5.322627000	-2.200584000	1.486361000
1	3.331587000	-0.855062000	1.178696000
1	2.465048000	-1.358944000	-1.426046000
1	4.116753000	-2.899196000	-2.327767000
6	0.764641000	-2.098501000	0.715358000
8	0.449718000	-2.043564000	1.982676000
1	0.140678000	-2.723185000	0.056642000

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#### TS8-Mn-PNP

25	-0.788433000	0.463005000	-0.143474000
15	-2.413400000	-1.193613000	0.154376000
15	0.959202000	1.980164000	0.090760000
8	-2.761380000	2.601520000	-0.316108000
8	-0.663680000	0.238705000	-3.081935000

7	-0.603192000	0.255597000	1.884141000
6	-1.833754000	-0.118351000	2.615436000
1	-2.550573000	0.715205000	2.588698000
1	-1.601600000	-0.306328000	3.675849000
6	0.099441000	1.323810000	2.620752000
1	0.359837000	0.974816000	3.633075000
1	-0.563282000	2.191882000	2.746785000
6	-2.074250000	-2.960267000	-0.398762000
1	-1.216128000	-3.222364000	0.229493000
6	0.702673000	3.829873000	-0.122368000
1	1.709389000	4.263618000	-0.081679000
6	1.376883000	1.728177000	1.883436000
1	2.090563000	0.900175000	1.924165000
1	1.854386000	2.602193000	2.335632000
6	2.584700000	1.626175000	-0.776366000
1	2.691267000	0.554652000	-0.589893000
6	-2.452163000	-1.378666000	2.004934000
1	-3.456797000	-1.567797000	2.391195000
1	-1.826506000	-2.242622000	2.245666000
6	-4.233873000	-0.385784000	-1.840799000
1	-3.754365000	0.589859000	-1.958551000
1	-5.277247000	-0.290257000	-2.163032000
1	-3.738142000	-1.084633000	-2.519622000
6	-4.920934000	0.130605000	0.547645000
1	-4.982685000	-0.231770000	1.577306000
1	-5.947605000	0.258437000	0.184520000
1	-4.450875000	1.115419000	0.557950000
6	-4.184311000	-0.8555852000	-0.376321000
1	-4.702277000	-1.818292000	-0.303282000
6	-1.975760000	1.732702000	-0.256900000
6	-0.702590000	0.320505000	-1.914879000
6	-1.635613000	-3.071454000	-1.866265000
1	-2.456549000	-2.841998000	-2.552912000
1	-1.310529000	-4.097288000	-2.075597000
1	-0.804861000	-2.399921000	-2.096530000
6	-3.201134000	-3.953548000	-0.070413000
1	-3.552869000	-3.858082000	0.962107000
1	-2.833270000	-4.977574000	-0.203793000
1	-4.059379000	-3.826391000	-0.738203000
6	3.802653000	2.339057000	-0.167337000
1	3.757791000	3.421514000	-0.327038000
1	4.715834000	1.973958000	-0.651950000
1	3.904563000	2.157652000	0.906348000
6	-0.124315000	4.451977000	1.016949000
1	-1.126895000	4.019689000	1.070474000
1	-0.236947000	5.526880000	0.833357000

1	0.355062000	4.334664000	1.992441000
6	0.081138000	4.170058000	-1.490258000
1	0.631827000	3.735712000	-2.326319000
1	0.076425000	5.258153000	-1.624462000
1	-0.952445000	3.823181000	-1.552573000
6	2.543341000	1.817807000	-2.300644000
1	1.653407000	1.376429000	-2.755005000
1	3.422344000	1.338317000	-2.746919000
1	2.580736000	2.877618000	-2.571366000
1	0.153721000	-0.842587000	1.922739000
1	0.876295000	-0.938486000	-0.023192000
6	2.979588000	-2.299220000	-1.050046000
6	3.517951000	-1.478295000	1.166427000
6	4.901487000	-2.104122000	1.023679000
8	5.312216000	-2.134676000	-0.349260000
6	4.387505000	-2.882950000	-1.144627000
1	2.280909000	-2.941944000	-1.598909000
1	3.188255000	-1.514699000	2.207450000
1	4.894638000	-3.127890000	1.429511000
1	4.377554000	-3.932129000	-0.809578000
7	2.568171000	-2.228232000	0.348973000
1	5.651137000	-1.513468000	1.557051000
1	3.589559000	-0.419272000	0.868736000
1	2.966746000	-1.307012000	-1.538136000
1	4.756494000	-2.841037000	-2.172920000
6	1.153122000	-1.923489000	0.526628000
8	0.770471000	-1.841551000	1.833193000
1	0.620296000	-2.695635000	-0.047617000

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### 17-Mn-PNP

25	-1.142232000	0.436059000	-0.078614000
15	-2.216225000	-1.598818000	0.187155000
15	0.396280000	2.171896000	0.036792000
8	-3.500265000	2.134499000	0.119437000
8	-1.364480000	0.483186000	-3.024186000
7	-0.579451000	0.085741000	1.763870000
6	-1.447329000	-0.703084000	2.661787000
1	-2.310700000	-0.093940000	2.976831000
1	-0.901411000	-0.965896000	3.582352000
6	0.089153000	1.131706000	2.555132000
1	0.585266000	0.685621000	3.432911000
1	-0.653767000	1.845608000	2.947464000
6	-1.421781000	-3.088355000	-0.651793000
1	-0.490395000	-3.173244000	-0.080179000

6	-0.164880000	3.961670000	0.045926000
1	0.751261000	4.564847000	0.022235000
6	1.131762000	1.860280000	1.711227000
1	1.990396000	1.200446000	1.557005000
1	1.496755000	2.772162000	2.192572000
6	1.914916000	2.122303000	-1.073810000
1	2.203587000	1.066778000	-0.997373000
6	-1.924656000	-1.989425000	1.981652000
1	-2.814609000	-2.402150000	2.464625000
1	-1.136862000	-2.746015000	2.028486000
6	-4.452406000	-1.436166000	-1.509744000
1	-4.173868000	-0.405477000	-1.753074000
1	-5.536836000	-1.533187000	-1.636969000
1	-3.973216000	-2.096718000	-2.237865000
6	-4.867901000	-0.940330000	0.941025000
1	-4.613744000	-1.170153000	1.979892000
1	-5.935865000	-1.150827000	0.810020000
1	-4.718360000	0.129110000	0.782740000
6	-4.062059000	-1.782313000	-0.063677000
1	-4.289224000	-2.837916000	0.124931000
6	-2.555988000	1.443757000	0.009872000
6	-1.249690000	0.444056000	-1.857641000
6	-1.039989000	-2.858309000	-2.120832000
1	-1.913926000	-2.681187000	-2.755015000
1	-0.525011000	-3.746159000	-2.506528000
1	-0.367724000	-2.004669000	-2.230432000
6	-2.210732000	-4.394574000	-0.469569000
1	-2.489287000	-4.570558000	0.574893000
1	-1.597627000	-5.242116000	-0.797572000
1	-3.125014000	-4.398478000	-1.072940000
6	3.090507000	2.978067000	-0.571819000
1	2.858707000	4.047228000	-0.625108000
1	3.966012000	2.801037000	-1.207707000
1	3.378777000	2.743882000	0.456643000
6	-0.935995000	4.308669000	1.332682000
1	-1.822366000	3.678565000	1.448952000
1	-1.273525000	5.350485000	1.282604000
1	-0.319745000	4.205966000	2.229899000
6	-1.012575000	4.298859000	-1.194934000
1	-0.510473000	4.052303000	-2.132196000
1	-1.229239000	5.373563000	-1.205605000
1	-1.966964000	3.766954000	-1.175432000
6	1.630721000	2.414523000	-2.556074000
1	0.763601000	1.869582000	-2.934178000
1	2.501019000	2.121329000	-3.154713000
1	1.468308000	3.483671000	-2.725396000

1	0.692982000	-1.156270000	1.444761000
1	1.652221000	-0.966079000	-0.438243000
6	4.084255000	-2.089748000	-1.038894000
6	3.968329000	-0.777455000	0.968036000
6	5.472725000	-0.947071000	1.144156000
8	6.123447000	-1.107993000	-0.121019000
6	5.590423000	-2.229266000	-0.832714000
1	3.700819000	-2.986638000	-1.539041000
1	3.483924000	-0.698415000	1.945064000
1	5.679199000	-1.821174000	1.781418000
1	5.804495000	-3.155823000	-0.277239000
7	3.418226000	-1.934848000	0.257082000
1	5.910330000	-0.058648000	1.607099000
1	3.782099000	0.159554000	0.410159000
1	3.889818000	-1.223336000	-1.701170000
1	6.110239000	-2.263068000	-1.793799000
6	1.968073000	-1.877191000	0.111675000
8	1.336086000	-1.920370000	1.366196000
1	1.675860000	-2.742621000	-0.499752000

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### 18-Mn-PNP

25	0.000032000	0.142964000	-0.214501000
15	-2.262928000	-0.139192000	-0.242162000
15	2.262924000	-0.138544000	-0.242752000
8	-0.000048000	1.181158000	2.543690000
8	-0.000007000	2.779774000	-1.478145000
7	0.000196000	-1.364695000	-1.370279000
6	-1.190163000	-2.072466000	-1.873812000
1	-1.286265000	-3.044718000	-1.362105000
1	-1.060564000	-2.313056000	-2.941625000
6	1.190715000	-2.070421000	-1.876295000
1	1.060182000	-2.309034000	-2.944443000
1	1.288214000	-3.043600000	-1.366602000
6	-3.393498000	1.300675000	-0.638184000
1	-3.037627000	1.581931000	-1.639043000
6	3.070824000	-1.094048000	1.158916000
1	4.043728000	-1.424986000	0.772261000
6	2.475043000	-1.252720000	-1.705288000
1	2.615403000	-0.595728000	-2.570606000
1	3.359713000	-1.892584000	-1.622479000
6	3.392915000	1.302334000	-0.636784000
1	3.037268000	1.584525000	-1.637458000
6	-2.474987000	-1.255529000	-1.703109000
1	-3.359148000	-1.895921000	-1.618952000

1	-2.616305000	-0.599837000	-2.569260000
6	-3.305629000	-0.246743000	2.423133000
1	-2.377058000	0.203053000	2.786330000
1	-3.701157000	-0.886432000	3.221121000
1	-4.031080000	0.553015000	2.258187000
6	-2.225116000	-2.334048000	1.498138000
1	-2.105371000	-3.001763000	0.641063000
1	-2.706774000	-2.904153000	2.300987000
1	-1.226324000	-2.041276000	1.838605000
6	-3.070258000	-1.093002000	1.160999000
1	-4.042637000	-1.425835000	0.774647000
6	0.000088000	0.776828000	1.439579000
6	-0.000056000	1.747658000	-0.914327000
6	-3.177566000	2.518004000	0.277601000
1	-3.576027000	2.350664000	1.281468000
1	-3.698287000	3.386750000	-0.141854000
1	-2.118840000	2.771221000	0.371786000
6	-4.878838000	0.918768000	-0.742847000
1	-5.042081000	0.081796000	-1.429697000
1	-5.457783000	1.772745000	-1.113891000
1	-5.290804000	0.641930000	0.233305000
6	4.878527000	0.921410000	-0.741273000
1	5.290278000	0.643883000	0.234778000
1	5.457105000	1.776104000	-1.111236000
1	5.042577000	0.085218000	-1.428887000
6	2.227180000	-2.336791000	1.493486000
1	1.227828000	-2.046045000	1.833998000
1	2.709263000	-2.907657000	2.295538000
1	2.108764000	-3.003136000	0.635174000
6	3.304748000	-0.249766000	2.422639000
1	4.029195000	0.551229000	2.259307000
1	3.700887000	-0.890369000	3.219587000
1	2.375504000	0.198200000	2.786388000
6	3.175925000	2.518510000	0.280264000
1	2.117029000	2.771176000	0.374082000
1	3.696547000	3.387958000	-0.137851000
1	3.573825000	2.350149000	1.284182000

-1699.196620

#### TS9-Mn-PNP

25	0.000044000	0.091451000	-0.001111000
15	-2.285278000	0.041177000	-0.322708000
15	2.285337000	0.041266000	-0.322766000
8	-0.000113000	-2.013117000	2.050297000
8	-0.000068000	2.231862000	2.019426000

7	0.000006000	-1.214719000	-1.690743000
6	-1.209891000	-2.009931000	-1.809808000
1	-1.283616000	-2.754425000	-0.992097000
1	-1.204357000	-2.583603000	-2.754105000
6	1.210037000	-2.009668000	-1.810191000
1	1.204462000	-2.583117000	-2.754625000
1	1.284007000	-2.754345000	-0.992672000
6	-3.099619000	1.605501000	-0.975454000
1	-2.449282000	1.844444000	-1.827858000
6	3.442540000	-0.610737000	1.004302000
1	4.454183000	-0.320444000	0.696341000
6	2.443327000	-1.102109000	-1.786070000
1	2.442959000	-0.468530000	-2.680437000
1	3.377170000	-1.671276000	-1.781637000
6	3.099672000	1.605708000	-0.975270000
1	2.449963000	1.844053000	-1.828326000
6	-2.443312000	-1.102552000	-1.785719000
1	-3.377092000	-1.671810000	-1.781079000
1	-2.443081000	-0.469161000	-2.680216000
6	-3.132755000	0.042935000	2.364293000
1	-2.143040000	-0.253635000	2.724047000
1	-3.872572000	-0.281077000	3.105781000
1	-3.157361000	1.134525000	2.323073000
6	-3.405746000	-2.144424000	1.123665000
1	-3.701783000	-2.642666000	0.196740000
1	-4.105102000	-2.461371000	1.906419000
1	-2.412135000	-2.504099000	1.402803000
6	-3.442405000	-0.610289000	1.004710000
1	-4.454016000	-0.319628000	0.696972000
6	-0.000017000	-1.165463000	1.241194000
6	0.000009000	1.391243000	1.201621000
6	-3.041649000	2.787954000	0.004022000
1	-3.721473000	2.639384000	0.849411000
1	-3.357844000	3.704207000	-0.508386000
1	-2.035599000	2.950017000	0.397220000
6	-4.531269000	1.398731000	-1.498701000
1	-4.603695000	0.571254000	-2.210894000
1	-4.870721000	2.308001000	-2.009060000
1	-5.232457000	1.205420000	-0.679622000
6	4.531808000	1.399261000	-1.497306000
1	5.232455000	1.206772000	-0.677574000
1	4.871246000	2.308357000	-2.007983000
1	4.605116000	0.571354000	-2.208914000
6	3.405390000	-2.144867000	1.123120000
1	2.411691000	-2.504278000	1.402270000
1	4.104683000	-2.462098000	1.905816000

1	3.701246000	-2.643099000	0.196132000
6	3.133424000	0.042506000	2.363990000
1	3.157998000	1.134098000	2.322717000
1	3.873526000	-0.281471000	3.105209000
1	2.143841000	-0.254068000	2.724117000
6	3.040427000	2.788529000	0.003667000
1	2.033868000	2.950704000	0.395502000
1	3.357260000	3.704589000	-0.508695000
1	3.719156000	2.640311000	0.849995000
1	-0.000043000	0.280138000	-1.724135000
1	0.000036000	1.142760000	-1.381348000

-1700.338902

### 19-Mn-PNP

25	-1.171036000	-0.325980000	0.012285000
15	-1.523211000	1.917639000	-0.024951000
15	-0.105484000	-2.332622000	0.064011000
8	-3.081701000	-0.994476000	-2.134050000
8	-3.128837000	-0.922710000	2.109633000
7	0.510640000	0.192440000	-1.285676000
6	0.234366000	1.401507000	-2.093442000
1	-0.575645000	1.161429000	-2.788333000
1	1.114850000	1.683784000	-2.689798000
6	0.939075000	-0.964297000	-2.103228000
1	1.800943000	-0.698955000	-2.734196000
1	0.109711000	-1.231309000	-2.765157000
6	-1.203770000	2.926916000	1.529355000
1	-0.222696000	2.542268000	1.831947000
6	-0.975868000	-3.921636000	-0.447271000
1	-0.322221000	-4.753032000	-0.156932000
6	1.288199000	-2.124454000	-1.171027000
1	2.188409000	-1.877166000	-0.601067000
1	1.505255000	-3.036942000	-1.731705000
6	0.858940000	-2.781932000	1.614678000
1	1.502148000	-1.897543000	1.712691000
6	-0.170784000	2.540400000	-1.158150000
1	-0.457505000	3.435492000	-1.716246000
1	0.681215000	2.814651000	-0.526742000
6	-4.338704000	1.929863000	-0.120353000
1	-4.367234000	0.881101000	-0.429631000
1	-5.259639000	2.412869000	-0.468762000
1	-4.341497000	1.952519000	0.971904000
6	-3.172873000	2.563258000	-2.264698000
1	-2.380856000	3.144057000	-2.745831000
1	-4.131127000	2.966579000	-2.613685000

1	-3.103595000	1.529533000	-2.613715000
6	-3.115249000	2.640089000	-0.728775000
1	-3.139200000	3.697667000	-0.439134000
6	-2.279974000	-0.720187000	-1.312134000
6	-2.355446000	-0.688900000	1.252865000
6	-2.191128000	2.610450000	2.663710000
1	-3.178986000	3.037074000	2.460329000
1	-1.832419000	3.056044000	3.599256000
1	-2.306192000	1.535361000	2.820811000
6	-1.091897000	4.444467000	1.309397000
1	-0.365259000	4.705407000	0.533892000
1	-0.770933000	4.928210000	2.239902000
1	-2.056445000	4.883388000	1.031437000
6	1.753182000	-4.026416000	1.495638000
1	1.158030000	-4.945437000	1.466397000
1	2.411093000	-4.093702000	2.370625000
1	2.388453000	-4.006407000	0.604221000
6	-1.209204000	-4.005096000	-1.966262000
1	-1.840563000	-3.185982000	-2.320065000
1	-1.722472000	-4.945012000	-2.202646000
1	-0.276880000	-3.992458000	-2.537840000
6	-2.315405000	-4.053748000	0.299178000
1	-2.196922000	-4.029543000	1.385333000
1	-2.797718000	-5.002669000	0.035503000
1	-2.990538000	-3.238369000	0.021252000
6	-0.018394000	-2.847755000	2.873191000
1	-0.657915000	-1.966529000	2.960740000
1	0.617322000	-2.902527000	3.765212000
1	-0.653966000	-3.739543000	2.873327000
1	1.293289000	0.421310000	-0.660212000
1	-0.188256000	0.037171000	1.231427000
1	3.986964000	1.031460000	3.080589000
1	2.112525000	0.324797000	2.036851000
6	3.756298000	2.199965000	-0.228938000
6	4.208158000	-0.077377000	0.426454000
6	4.717045000	-0.354235000	-0.986333000
8	5.249388000	0.830431000	-1.583098000
6	4.262928000	1.865399000	-1.627990000
1	2.974768000	2.964826000	-0.293454000
1	3.760135000	-0.985051000	0.846493000
1	3.904522000	-0.748350000	-1.614253000
1	3.425050000	1.548402000	-2.268365000
7	3.196858000	0.991253000	0.399451000
1	5.527933000	-1.086540000	-0.963398000
1	5.069630000	0.200014000	1.056867000
1	4.584568000	2.610847000	0.369086000

1	4.742956000	2.735734000	-2.082240000
6	2.593671000	1.244850000	1.691203000
8	3.481726000	1.760702000	2.697451000
1	1.827136000	2.011130000	1.565975000

-2102.614448

### 20-Mn-PNP

25	-0.178541000	0.921544000	-0.146477000
15	2.135767000	1.054366000	-0.254650000
15	-2.391343000	0.228995000	-0.269853000
8	-0.310588000	1.588051000	2.720762000
7	0.026891000	-0.131241000	-1.736823000
6	1.200118000	0.004891000	-2.615661000
1	1.091777000	0.896978000	-3.255178000
1	1.267058000	-0.857281000	-3.298855000
6	-1.097689000	-0.644117000	-2.529891000
1	-0.781849000	-1.536788000	-3.095231000
1	-1.404732000	0.099851000	-3.284346000
6	3.152229000	0.100523000	1.010345000
1	2.646097000	-0.873780000	0.984857000
6	-3.742796000	1.416441000	-0.802081000
1	-4.675571000	0.838521000	-0.789268000
6	-2.281036000	-1.015512000	-1.639894000
1	-2.088800000	-1.980039000	-1.160693000
1	-3.214561000	-1.107321000	-2.203565000
6	-3.128206000	-0.798915000	1.121714000
1	-2.309318000	-1.503541000	1.312692000
6	2.488659000	0.088240000	-1.800237000
1	3.322484000	0.501304000	-2.374601000
1	2.779903000	-0.915426000	-1.484601000
6	2.625817000	3.684425000	0.649956000
1	1.555393000	3.906844000	0.642638000
1	3.165984000	4.628070000	0.509403000
1	2.881412000	3.299755000	1.639415000
6	2.682140000	3.320818000	-1.854811000
1	3.015007000	2.687426000	-2.681586000
1	3.198953000	4.283118000	-1.948521000
1	1.611674000	3.506369000	-1.975593000
6	2.994833000	2.705308000	-0.478827000
1	4.071197000	2.498931000	-0.430561000
6	-0.248844000	1.296525000	1.578678000
6	3.071664000	0.637643000	2.448089000
1	3.662808000	1.551239000	2.566676000
1	3.486980000	-0.108631000	3.135345000
1	2.050884000	0.847131000	2.767057000

6	4.624167000	-0.093081000	0.603451000
1	4.741145000	-0.509551000	-0.400944000
1	5.106680000	-0.783991000	1.305066000
1	5.176994000	0.852032000	0.645181000
6	-4.373765000	-1.605579000	0.716211000
1	-5.223380000	-0.946393000	0.507603000
1	-4.666263000	-2.263846000	1.542810000
1	-4.205502000	-2.233660000	-0.162716000
6	-3.506177000	1.915504000	-2.239256000
1	-2.539292000	2.418482000	-2.333170000
1	-4.285321000	2.638841000	-2.506448000
1	-3.544593000	1.105675000	-2.972466000
6	-3.882439000	2.606198000	0.164571000
1	-4.085463000	2.295435000	1.190731000
1	-4.714169000	3.242843000	-0.159750000
1	-2.977606000	3.218998000	0.170610000
6	-3.392988000	-0.030676000	2.427685000
1	-2.576762000	0.638816000	2.702084000
1	-3.529624000	-0.746854000	3.246354000
1	-4.312665000	0.558020000	2.358433000
1	0.781642000	-1.960158000	-0.511869000
1	0.648474000	-1.383203000	2.512771000
1	0.017215000	0.148804000	4.124261000
1	-0.968542000	-1.798051000	3.141114000
6	2.167092000	-3.497853000	-0.506151000
6	-0.036705000	-3.565645000	0.463093000
6	-0.500522000	-4.437217000	-0.708301000
8	0.587935000	-5.200994000	-1.242526000
6	1.662913000	-4.353586000	-1.669633000
1	2.969568000	-2.835278000	-0.847146000
1	-0.863892000	-2.942393000	0.815844000
1	-0.923397000	-3.805113000	-1.506860000
1	1.315550000	-3.703163000	-2.490414000
7	1.099452000	-2.705611000	0.115284000
1	-1.261362000	-5.158708000	-0.394526000
1	0.262474000	-4.216735000	1.295218000
1	2.593935000	-4.157947000	0.261094000
1	2.444902000	-5.016744000	-2.052305000
6	0.088246000	-1.669313000	3.410999000
8	0.244372000	-0.726097000	4.474187000
1	0.472948000	-2.628405000	3.767405000
6	-0.482658000	2.593339000	-0.533773000
8	-0.681473000	3.705077000	-0.857532000

-2102.614179

**21-Mn-PNP**

25	-1.181057000	0.160331000	0.023870000
15	-0.395441000	2.304773000	-0.073164000
15	-1.149204000	-2.115392000	0.051145000
8	-3.312567000	0.464033000	-1.992727000
8	-3.075160000	0.546794000	2.226153000
7	0.527553000	-0.176682000	-1.436730000
6	0.786033000	1.027567000	-2.250697000
1	-0.090054000	1.189362000	-2.885521000
1	1.656021000	0.881778000	-2.909067000
6	0.323145000	-1.419423000	-2.208309000
1	1.166490000	-1.609948000	-2.889382000
1	-0.574005000	-1.281832000	-2.819511000
6	0.494284000	3.014467000	1.417855000
1	1.259462000	2.249293000	1.588486000
6	-2.669157000	-3.114524000	-0.436001000
1	-2.466818000	-4.158764000	-0.169864000
6	0.141011000	-2.582477000	-1.229559000
1	1.080456000	-2.765283000	-0.696036000
1	-0.106682000	-3.507375000	-1.756524000
6	-0.461125000	-2.974266000	1.575698000
1	0.532325000	-2.511024000	1.633794000
6	1.008340000	2.216498000	-1.313293000
1	1.130454000	3.144582000	-1.877970000
1	1.930863000	2.066551000	-0.740461000
6	-2.837210000	3.683983000	0.051277000
1	-3.383161000	2.758551000	-0.156195000
1	-3.457824000	4.527809000	-0.273642000
1	-2.711895000	3.758328000	1.134333000
6	-1.730094000	3.628730000	-2.218101000
1	-0.804514000	3.733975000	-2.791366000
1	-2.396630000	4.444889000	-2.521893000
1	-2.207701000	2.688379000	-2.505059000
6	-1.494015000	3.699352000	-0.699329000
1	-0.974529000	4.639805000	-0.479456000
6	-2.428835000	0.337842000	-1.220974000
6	-2.324254000	0.393164000	1.332708000
6	-0.383144000	3.064412000	2.677555000
1	-1.140172000	3.853629000	2.615414000
1	0.243018000	3.282932000	3.551058000
1	-0.889995000	2.112549000	2.852205000
6	1.194762000	4.361566000	1.178594000
1	1.831051000	4.353874000	0.287735000
1	1.833628000	4.599016000	2.038016000
1	0.474785000	5.180695000	1.073503000
6	-0.287945000	-4.495615000	1.448491000

1	-1.254974000	-5.010176000	1.453663000
1	0.286432000	-4.874712000	2.302369000
1	0.244101000	-4.784345000	0.535988000
6	-2.952373000	-3.052312000	-1.947188000
1	-3.124761000	-2.025583000	-2.279150000
1	-3.857511000	-3.629631000	-2.170907000
1	-2.141021000	-3.476050000	-2.545855000
6	-3.894913000	-2.623397000	0.354226000
1	-3.745160000	-2.674751000	1.435631000
1	-4.769714000	-3.236628000	0.107036000
1	-4.123516000	-1.583581000	0.100166000
6	-1.209701000	-2.600970000	2.863064000
1	-1.320100000	-1.518407000	2.957532000
1	-0.653778000	-2.968811000	3.733853000
1	-2.204660000	-3.056501000	2.896691000
1	1.322536000	-0.310746000	-0.810360000
1	-0.021623000	-0.013546000	1.173332000
6	4.577377000	0.450381000	0.247582000
6	3.871385000	-1.914201000	0.372275000
6	4.037368000	-1.989886000	-1.144064000
8	5.044320000	-1.083282000	-1.594451000
6	4.710588000	0.267362000	-1.261957000
1	4.222568000	1.453981000	0.489289000
1	3.041213000	-2.546005000	0.700816000
1	3.085784000	-1.761370000	-1.645743000
1	3.771812000	0.550257000	-1.763370000
7	3.619186000	-0.526295000	0.775496000
1	4.355363000	-2.991828000	-1.440901000
1	4.790001000	-2.275329000	0.854694000
1	5.553711000	0.302493000	0.729482000
1	5.515880000	0.894634000	-1.650420000
6	2.891138000	-0.239433000	1.888166000
8	2.882169000	0.851136000	2.460455000
1	2.275684000	-1.085648000	2.232176000

-2101.445708

#### TS10-Mn-PNP

25	-0.093744000	0.864216000	0.085795000
15	2.210647000	0.804108000	-0.093654000
15	-2.365532000	0.453931000	-0.046656000
8	-0.271607000	3.275135000	-1.576484000
8	-0.170353000	2.439748000	2.566389000
7	-0.015111000	-0.545830000	-1.532669000
6	1.205011000	-0.423136000	-2.368444000
1	1.127911000	0.511631000	-2.932062000

1	1.255544000	-1.246746000	-3.095320000
6	-1.244895000	-0.573511000	-2.363177000
1	-1.190651000	-1.385907000	-3.101982000
1	-1.290548000	0.372712000	-2.910914000
6	3.220457000	0.063321000	1.294366000
1	2.626780000	-0.814621000	1.574734000
6	-3.551384000	1.858315000	-0.453267000
1	-4.555000000	1.473698000	-0.242021000
6	-2.480704000	-0.740995000	-1.478340000
1	-2.504816000	-1.751369000	-1.060025000
1	-3.396705000	-0.619325000	-2.061864000
6	-3.238169000	-0.502011000	1.316086000
1	-2.671297000	-1.438227000	1.327915000
6	2.449333000	-0.419748000	-1.481802000
1	3.350469000	-0.230396000	-2.070208000
1	2.571558000	-1.402433000	-1.021280000
6	2.738886000	3.563518000	0.232785000
1	1.728201000	3.880440000	-0.035121000
1	3.417435000	4.401580000	0.034228000
1	2.752073000	3.369753000	1.307126000
6	3.083277000	2.657486000	-2.102592000
1	3.490370000	1.856294000	-2.725214000
1	3.663073000	3.563191000	-2.316562000
1	2.052784000	2.847546000	-2.412845000
6	3.173918000	2.341880000	-0.599353000
1	4.221982000	2.118966000	-0.364859000
6	-0.208016000	2.298130000	-0.927633000
6	-0.142183000	1.814921000	1.576031000
6	3.278093000	0.970603000	2.534538000
1	3.933222000	1.833809000	2.374070000
1	3.687937000	0.401765000	3.377143000
1	2.289898000	1.334317000	2.828158000
6	4.631988000	-0.390573000	0.886138000
1	4.625266000	-1.093907000	0.048159000
1	5.108237000	-0.896902000	1.734359000
1	5.272043000	0.455605000	0.611672000
6	-4.705014000	-0.856405000	1.023164000
1	-5.355828000	0.020132000	1.104291000
1	-5.055842000	-1.590330000	1.758076000
1	-4.840877000	-1.291649000	0.027729000
6	-3.522716000	2.281075000	-1.933205000
1	-2.545483000	2.665833000	-2.232082000
1	-4.253036000	3.084066000	-2.087996000
1	-3.793154000	1.463255000	-2.606732000
6	-3.288520000	3.065168000	0.465471000
1	-3.319624000	2.799048000	1.524932000

1	-4.049978000	3.834307000	0.291125000
1	-2.309378000	3.507293000	0.262941000
6	-3.076794000	0.141791000	2.700992000
1	-2.030102000	0.359769000	2.927404000
1	-3.456947000	-0.540806000	3.469842000
1	-3.646089000	1.073169000	2.780739000
1	0.044173000	-1.437478000	-1.006384000
1	0.092352000	-0.607246000	1.076887000
6	1.450383000	-3.506946000	0.344290000
6	-0.940272000	-3.721280000	0.389845000
6	-0.885056000	-4.429798000	-0.960862000
8	0.358708000	-5.109697000	-1.140054000
6	1.465987000	-4.211243000	-1.008022000
1	2.286905000	-2.811325000	0.423579000
1	-1.888903000	-3.185057000	0.477623000
1	-1.027405000	-3.698233000	-1.773200000
1	1.436597000	-3.471403000	-1.824434000
7	0.184382000	-2.779619000	0.496386000
1	-1.668837000	-5.188354000	-1.031635000
1	-0.905277000	-4.470497000	1.199132000
1	1.575750000	-4.248555000	1.148655000
1	2.369262000	-4.816775000	-1.117795000
6	0.129151000	-1.900470000	1.671612000
8	1.072325000	-1.933514000	2.521766000
1	-0.911193000	-1.842388000	2.029110000

-2101.417977

## 22-Mn-PNP

25	0.090854000	-0.843418000	0.089081000
15	-2.219096000	-0.800111000	-0.095245000
15	2.375448000	-0.446127000	-0.048156000
8	0.263979000	-3.253258000	-1.567344000
8	0.170861000	-2.425960000	2.568773000
7	0.014935000	0.538776000	-1.530986000
6	-1.202216000	0.409489000	-2.371991000
1	-1.121764000	-0.527975000	-2.930825000
1	-1.248751000	1.229420000	-3.102785000
6	1.244648000	0.566056000	-2.363323000
1	1.185235000	1.375370000	-3.104642000
1	1.294230000	-0.381644000	-2.908138000
6	-3.221626000	-0.054734000	1.294460000
1	-2.616298000	0.811720000	1.591002000
6	3.544024000	-1.863220000	-0.457848000
1	4.550043000	-1.487323000	-0.242694000
6	2.480727000	0.744409000	-1.481795000

1	2.496434000	1.755040000	-1.063653000
1	3.396881000	0.628620000	-2.066120000
6	3.263997000	0.503611000	1.307972000
1	2.692679000	1.436635000	1.339930000
6	-2.452054000	0.411430000	-1.493274000
1	-3.349435000	0.216039000	-2.085230000
1	-2.577934000	1.397680000	-1.042374000
6	-2.727387000	-3.563794000	0.246730000
1	-1.720022000	-3.882631000	-0.030916000
1	-3.407716000	-4.402870000	0.059509000
1	-2.729214000	-3.365286000	1.320133000
6	-3.093695000	-2.668805000	-2.090019000
1	-3.509086000	-1.872241000	-2.712873000
1	-3.672048000	-3.577495000	-2.294434000
1	-2.065310000	-2.856978000	-2.408487000
6	-3.173250000	-2.347291000	-0.587351000
1	-4.220083000	-2.126986000	-0.344677000
6	0.204759000	-2.281602000	-0.913201000
6	0.140512000	-1.796156000	1.583906000
6	-3.299964000	-0.974584000	2.524271000
1	-3.963171000	-1.829062000	2.350761000
1	-3.709950000	-0.408597000	3.368575000
1	-2.318241000	-1.351160000	2.823662000
6	-4.624058000	0.421218000	0.880174000
1	-4.601095000	1.140706000	0.056429000
1	-5.103378000	0.916420000	1.733095000
1	-5.270403000	-0.412367000	0.582409000
6	4.723202000	0.868022000	0.989670000
1	5.379568000	-0.006582000	1.040966000
1	5.086143000	1.590302000	1.730105000
1	4.835572000	1.322099000	-0.000111000
6	3.515674000	-2.279293000	-1.939627000
1	2.536368000	-2.655039000	-2.243144000
1	4.239778000	-3.087562000	-2.095360000
1	3.794892000	-1.460812000	-2.608615000
6	3.270639000	-3.070986000	0.456703000
1	3.296310000	-2.807856000	1.516901000
1	4.030892000	-3.841698000	0.284749000
1	2.292135000	-3.510724000	0.247247000
6	3.132192000	-0.155555000	2.688939000
1	2.092204000	-0.388058000	2.931763000
1	3.516173000	0.524849000	3.457623000
1	3.714339000	-1.080306000	2.751311000
1	-0.045304000	1.439822000	-1.011457000
1	-0.135433000	0.665613000	1.091434000
6	-1.450364000	3.462244000	0.337223000

6	0.925793000	3.705783000	0.398683000
6	0.869490000	4.463693000	-0.925372000
8	-0.383871000	5.129552000	-1.092338000
6	-1.478559000	4.211349000	-0.990529000
1	-2.282948000	2.760020000	0.398151000
1	1.885124000	3.185848000	0.471467000
1	1.030055000	3.763130000	-1.761751000
1	-1.438986000	3.499495000	-1.831423000
7	-0.178934000	2.739233000	0.456980000
1	1.640865000	5.237455000	-0.963284000
1	0.872851000	4.423061000	1.236433000
1	-1.579298000	4.175912000	1.165631000
1	-2.389860000	4.808466000	-1.080439000
6	-0.121396000	1.817988000	1.634661000
8	-1.051195000	1.907273000	2.523310000
1	0.923584000	1.813989000	1.992623000

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#### TS11-Mn-PNP

25	0.152720000	-0.822787000	0.061846000
15	-2.156372000	-0.928475000	-0.105391000
15	2.405577000	-0.294463000	-0.042707000
8	0.457357000	-3.047881000	-1.801187000
8	0.351148000	-2.603019000	2.404852000
7	-0.029415000	0.661885000	-1.366123000
6	-1.198741000	0.506828000	-2.252925000
1	-1.047534000	-0.355504000	-2.922016000
1	-1.306904000	1.388267000	-2.908153000
6	1.160636000	0.843865000	-2.220394000
1	1.042276000	1.732807000	-2.863475000
1	1.262092000	-0.016268000	-2.902608000
6	-3.184207000	-0.305225000	1.329665000
1	-2.652055000	0.603399000	1.640553000
6	3.652149000	-1.622829000	-0.512073000
1	4.632641000	-1.217958000	-0.239134000
6	2.443620000	0.983424000	-1.397202000
1	2.489149000	1.964769000	-0.919859000
1	3.332067000	0.903927000	-2.028313000
6	3.218253000	0.616456000	1.386775000
1	2.581371000	1.502318000	1.482308000
6	-2.489049000	0.307285000	-1.457565000
1	-3.318399000	0.014938000	-2.105856000
1	-2.782978000	1.240560000	-0.976427000
6	-2.414407000	-3.734864000	0.158746000
1	-1.398939000	-3.959722000	-0.176330000

1	-3.032021000	-4.621810000	-0.025318000
1	-2.378629000	-3.569770000	1.237467000
6	-2.964381000	-2.802781000	-2.127237000
1	-3.489572000	-2.034577000	-2.700643000
1	-3.459071000	-3.759284000	-2.333747000
1	-1.940653000	-2.874742000	-2.503404000
6	-2.999166000	-2.535202000	-0.611827000
1	-4.048669000	-2.415612000	-0.316310000
6	0.343085000	-2.160546000	-1.042048000
6	0.271746000	-1.884429000	1.483927000
6	-3.152829000	-1.262152000	2.532807000
1	-3.736273000	-2.169730000	2.343958000
1	-3.596426000	-0.762490000	3.401689000
1	-2.134070000	-1.554105000	2.800533000
6	-4.632438000	0.058876000	0.961597000
1	-4.694896000	0.790489000	0.150240000
1	-5.127988000	0.496952000	1.836316000
1	-5.213533000	-0.822151000	0.666368000
6	4.648593000	1.106609000	1.107067000
1	5.363947000	0.278046000	1.092247000
1	4.960538000	1.791074000	1.904571000
1	4.730037000	1.644775000	0.157130000
6	3.682741000	-1.933480000	-2.019351000
1	2.717687000	-2.291057000	-2.384676000
1	4.418962000	-2.724592000	-2.204749000
1	3.979094000	-1.068087000	-2.618073000
6	3.413135000	-2.906197000	0.305039000
1	3.362923000	-2.717660000	1.380190000
1	4.232147000	-3.612335000	0.125793000
1	2.479693000	-3.392431000	0.010103000
6	3.133695000	-0.147003000	2.716865000
1	2.112532000	-0.466473000	2.939761000
1	3.472347000	0.500866000	3.533575000
1	3.777137000	-1.032604000	2.714867000
1	-0.224125000	1.840390000	-0.451441000
1	-0.139084000	0.671346000	1.290315000
6	-1.683838000	3.289717000	0.344276000
6	0.690219000	3.678833000	0.335262000
6	0.532790000	4.472972000	-0.959182000
8	-0.761428000	5.068661000	-1.045155000
6	-1.792136000	4.080778000	-0.954300000
1	-2.464729000	2.535320000	0.417640000
1	1.675423000	3.212650000	0.373426000
1	0.701995000	3.817292000	-1.827538000
1	-1.738878000	3.407482000	-1.823477000
7	-0.356377000	2.628867000	0.421404000

1	1.259860000	5.287735000	-0.992257000
1	0.594597000	4.340763000	1.203565000
1	-1.793722000	3.948095000	1.209573000
1	-2.743435000	4.616758000	-0.988604000
6	-0.225031000	1.747531000	1.756544000
8	-1.184622000	1.885800000	2.603890000
1	0.802271000	1.967138000	2.102601000

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### 23-Mn-PNP

25	0.009722000	0.994374000	-0.046854000
15	2.293350000	0.628090000	-0.179261000
15	-2.285433000	0.747475000	-0.078505000
8	0.037405000	3.692110000	-1.144392000
8	0.122449000	2.038263000	2.714078000
7	-0.062383000	-0.168874000	-1.585629000
6	1.115485000	-0.395805000	-2.434858000
1	1.248019000	0.444037000	-3.138308000
1	0.969225000	-1.294584000	-3.057147000
6	-1.270478000	-0.261254000	-2.419190000
1	-1.217767000	-1.147897000	-3.072736000
1	-1.338338000	0.611082000	-3.091608000
6	3.139866000	-0.322697000	1.205351000
1	2.414201000	-1.115709000	1.423544000
6	-3.415945000	2.218695000	-0.343423000
1	-4.439135000	1.853919000	-0.190783000
6	-2.524488000	-0.358444000	-1.551839000
1	-2.621865000	-1.379148000	-1.174807000
1	-3.438248000	-0.131566000	-2.107470000
6	-3.082386000	-0.275647000	1.286734000
1	-2.433280000	-1.160813000	1.291802000
6	2.373126000	-0.576018000	-1.589184000
1	3.290673000	-0.487325000	-2.177670000
1	2.367462000	-1.572742000	-1.143035000
6	3.274134000	3.233676000	0.319767000
1	2.292691000	3.693152000	0.178147000
1	4.034370000	3.991540000	0.096616000
1	3.369118000	2.967080000	1.374015000
6	3.288402000	2.462861000	-2.088463000
1	3.540475000	1.665165000	-2.792127000
1	3.952025000	3.309903000	-2.297843000
1	2.263441000	2.786887000	-2.290795000
6	3.459973000	2.028891000	-0.621369000
1	4.476054000	1.634382000	-0.494525000
6	0.028627000	2.621473000	-0.659021000

6	0.075161000	1.592705000	1.628305000
6	3.326106000	0.484573000	2.500227000
1	4.130701000	1.220178000	2.398911000
1	3.608260000	-0.198107000	3.309826000
1	2.416837000	1.005415000	2.805652000
6	4.469052000	-0.978897000	0.791310000
1	4.368996000	-1.634255000	-0.078527000
1	4.845389000	-1.588742000	1.621192000
1	5.234328000	-0.228415000	0.564386000
6	-4.517644000	-0.731933000	0.971983000
1	-5.216190000	0.111198000	0.989533000
1	-4.848919000	-1.446044000	1.735097000
1	-4.606066000	-1.223873000	-0.000845000
6	-3.312557000	2.770609000	-1.777500000
1	-2.299804000	3.115273000	-2.003005000
1	-3.985761000	3.629515000	-1.882531000
1	-3.600990000	2.034346000	-2.532730000
6	-3.125838000	3.330824000	0.681464000
1	-3.191504000	2.981610000	1.714195000
1	-3.851213000	4.143212000	0.556424000
1	-2.125821000	3.747882000	0.532746000
6	-3.015042000	0.354303000	2.686350000
1	-2.014631000	0.706954000	2.941450000
1	-3.309804000	-0.392235000	3.433108000
1	-3.709120000	1.195592000	2.778218000
1	-0.234483000	-1.994813000	-0.283937000
1	-0.104924000	-1.019256000	2.137558000
6	0.945160000	-3.627059000	0.167439000
6	-1.455383000	-3.645495000	0.023657000
6	-1.351853000	-4.307576000	-1.352770000
8	-0.154273000	-5.086050000	-1.451492000
6	1.015336000	-4.294356000	-1.207390000
1	1.820129000	-2.994728000	0.337445000
1	-2.359668000	-3.033192000	0.083216000
1	-1.357569000	-3.535562000	-2.140410000
1	1.109534000	-3.528145000	-1.994153000
7	-0.273761000	-2.826557000	0.320910000
1	-2.184620000	-4.994641000	-1.528849000
1	-1.534433000	-4.421977000	0.794913000
1	0.949718000	-4.393691000	0.951363000
1	1.869212000	-4.974389000	-1.276302000
6	-0.046584000	-2.029014000	2.578492000
8	1.007535000	-2.483836000	3.014657000
1	-1.013816000	-2.531646000	2.752436000

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**24-Mn-PNP**

8	-0.095527000	-2.806759000	1.731438000
6	-0.019867000	-2.832589000	0.398030000
1	-0.881464000	-3.279081000	-0.134448000
1	0.902526000	-3.266482000	-0.033201000
25	0.004845000	0.096505000	-0.131140000
15	-2.298506000	-0.057467000	0.137522000
15	2.304739000	-0.076896000	0.146130000
8	0.010458000	3.019050000	-0.163367000
8	0.008321000	0.112005000	-3.075051000
7	-0.003978000	-0.160508000	1.965066000
6	-1.223899000	0.348186000	2.641439000
1	-1.228313000	1.440842000	2.566441000
1	-1.201254000	0.087331000	3.709177000
6	1.225578000	0.305277000	2.653701000
1	1.193185000	0.024652000	3.716167000
1	1.254994000	1.398689000	2.600577000
6	-3.174273000	-1.594350000	-0.492315000
1	-2.695525000	-2.375860000	0.107889000
6	3.419308000	1.368282000	-0.293640000
1	4.443137000	0.983333000	-0.236282000
6	2.457634000	-0.308769000	1.987188000
1	2.465598000	-1.388306000	2.169241000
1	3.383060000	0.107469000	2.393742000
6	3.181518000	-1.603599000	-0.510604000
1	2.717427000	-2.395215000	0.087987000
6	-2.464968000	-0.253654000	1.981181000
1	-3.384585000	0.185501000	2.376167000
1	-2.489161000	-1.329995000	2.179145000
6	-3.111706000	1.836100000	-1.782402000
1	-2.110160000	2.268271000	-1.864202000
1	-3.834746000	2.604346000	-2.080022000
1	-3.182206000	1.016196000	-2.501961000
6	-3.308287000	2.568169000	0.636164000
1	-3.596263000	2.294409000	1.654932000
1	-3.991863000	3.358702000	0.305001000
1	-2.303193000	2.994042000	0.664415000
6	-3.403755000	1.382718000	-0.341046000
1	-4.428540000	0.998410000	-0.296561000
6	0.008738000	1.847191000	-0.132895000
6	0.007250000	0.086258000	-1.905963000
6	-2.881319000	-1.898021000	-1.968833000
1	-3.330731000	-1.153973000	-2.634225000
1	-3.305634000	-2.873478000	-2.233459000
1	-1.807369000	-1.930497000	-2.168906000

6	-4.682240000	-1.633529000	-0.194151000
1	-4.907737000	-1.393375000	0.850136000
1	-5.065862000	-2.640559000	-0.394800000
1	-5.238257000	-0.939551000	-0.833168000
6	4.693862000	-1.636650000	-0.235696000
1	5.235981000	-0.934708000	-0.877939000
1	5.079831000	-2.639973000	-0.449824000
1	4.933794000	-1.402956000	0.806890000
6	3.307610000	2.539639000	0.698444000
1	2.301551000	2.963339000	0.719830000
1	3.993924000	3.336120000	0.387781000
1	3.583205000	2.251582000	1.716740000
6	3.152474000	1.839446000	-1.734284000
1	3.240942000	1.028810000	-2.462454000
1	3.877822000	2.614239000	-2.008339000
1	2.150724000	2.268226000	-1.830908000
6	2.866624000	-1.896793000	-1.984616000
1	1.789760000	-1.945484000	-2.163652000
1	3.302089000	-2.862215000	-2.267278000
1	3.289702000	-1.138434000	-2.651005000
1	-0.028207000	-1.229751000	2.032368000
1	-0.002658000	-1.752467000	-0.116121000

-1814.897470

#### TS12-Mn-PNP

8	-0.125951000	-2.685731000	1.795774000
6	-0.014361000	-2.889773000	0.440388000
1	-0.860980000	-3.440240000	0.001230000
1	0.915443000	-3.397128000	0.138024000
25	0.005438000	0.122183000	-0.119718000
15	-2.298888000	-0.040909000	0.134176000
15	2.305273000	-0.085427000	0.156408000
8	0.015442000	3.035706000	-0.188753000
8	0.005102000	0.141449000	-3.067857000
7	-0.016334000	-0.193643000	1.909954000
6	-1.213252000	0.289002000	2.632048000
1	-1.224956000	1.388253000	2.639771000
1	-1.179103000	-0.038830000	3.683003000
6	1.202586000	0.189407000	2.653861000
1	1.140863000	-0.173630000	3.691979000
1	1.279163000	1.284835000	2.702470000
6	-3.156846000	-1.580386000	-0.520470000
1	-2.682350000	-2.362008000	0.083296000
6	3.446580000	1.363960000	-0.181684000
1	4.462526000	0.977370000	-0.045730000

6	2.441299000	-0.407021000	1.981471000
1	2.436898000	-1.493220000	2.116761000
1	3.368472000	-0.016284000	2.410448000
6	3.167894000	-1.587183000	-0.585998000
1	2.759626000	-2.399899000	0.024952000
6	-2.479695000	-0.258928000	1.971184000
1	-3.384939000	0.208166000	2.367656000
1	-2.544654000	-1.335637000	2.155036000
6	-3.125225000	1.851711000	-1.782808000
1	-2.121762000	2.277467000	-1.874344000
1	-3.846297000	2.624944000	-2.072307000
1	-3.208517000	1.032956000	-2.502334000
6	-3.295608000	2.582959000	0.638446000
1	-3.575135000	2.308948000	1.659376000
1	-3.978120000	3.377342000	0.314172000
1	-2.287845000	3.002881000	0.659138000
6	-3.405394000	1.398798000	-0.339169000
1	-4.430700000	1.016706000	-0.284615000
6	0.013343000	1.863271000	-0.155120000
6	0.007344000	0.100199000	-1.898230000
6	-2.846376000	-1.881038000	-1.993507000
1	-3.280724000	-1.132094000	-2.663235000
1	-3.273619000	-2.852903000	-2.266717000
1	-1.770308000	-1.920638000	-2.178782000
6	-4.668032000	-1.625281000	-0.239610000
1	-4.905552000	-1.388994000	0.802903000
1	-5.047689000	-2.632185000	-0.448430000
1	-5.217451000	-0.929421000	-0.882353000
6	4.694536000	-1.594284000	-0.407941000
1	5.179778000	-0.863183000	-1.063339000
1	5.087229000	-2.582721000	-0.673085000
1	4.994185000	-1.383017000	0.623984000
6	3.257919000	2.520049000	0.815953000
1	2.258842000	2.955383000	0.757520000
1	3.978330000	3.312711000	0.581596000
1	3.439404000	2.210301000	1.848823000
6	3.294841000	1.848594000	-1.633584000
1	3.496111000	1.054327000	-2.357802000
1	4.003118000	2.662157000	-1.828273000
1	2.285873000	2.228397000	-1.822124000
6	2.765829000	-1.863358000	-2.041812000
1	1.683952000	-1.972032000	-2.143584000
1	3.234389000	-2.794393000	-2.381296000
1	3.088806000	-1.065370000	-2.717295000
1	-0.073390000	-1.495127000	1.932928000
1	0.002671000	-1.913821000	-0.158731000

-1814.898095

**25-Mn-PNP**

8	0.009103000	2.992255000	1.630619000
6	0.000980000	3.353230000	0.258383000
1	0.888741000	3.948233000	0.007422000
1	-0.890769000	3.946222000	0.016700000
25	-0.000296000	-0.251133000	-0.070348000
15	2.293732000	0.022847000	0.151839000
15	-2.294090000	0.024844000	0.152043000
8	-0.001762000	-3.154161000	-0.328066000
8	0.000441000	-0.165001000	-3.020874000
7	0.000178000	0.199061000	1.828315000
6	1.198841000	-0.027107000	2.659510000
1	1.290831000	-1.098618000	2.900464000
1	1.099061000	0.500835000	3.621391000
6	-1.198994000	-0.023195000	2.659741000
1	-1.098069000	0.505976000	3.620832000
1	-1.293368000	-1.094143000	2.902343000
6	3.114719000	1.508428000	-0.672063000
1	2.637475000	2.339034000	-0.138130000
6	-3.463657000	-1.416456000	-0.092560000
1	-4.470375000	-1.021562000	0.085085000
6	-2.455405000	0.474819000	1.945824000
1	-2.497599000	1.566994000	2.001890000
1	-3.370879000	0.079706000	2.395831000
6	-3.115483000	1.508837000	-0.674392000
1	-2.638515000	2.340625000	-0.142094000
6	2.456335000	0.469339000	1.946365000
1	3.370970000	0.071349000	2.395509000
1	2.500801000	1.561296000	2.004270000
6	3.382453000	-1.948239000	-1.537379000
1	2.371990000	-2.295440000	-1.774294000
1	4.068122000	-2.794420000	-1.661402000
1	3.659119000	-1.187576000	-2.272193000
6	3.210947000	-2.541890000	0.924955000
1	3.322865000	-2.197559000	1.956869000
1	3.942482000	-3.342712000	0.764962000
1	2.214970000	-2.976332000	0.815099000
6	3.462538000	-1.418493000	-0.096395000
1	4.469560000	-1.024320000	0.081210000
6	-0.001138000	-1.982802000	-0.237976000
6	0.000073000	-0.148751000	-1.848428000
6	2.788428000	1.679126000	-2.162081000
1	3.184773000	0.859576000	-2.769057000

1	3.240321000	2.608532000	-2.528176000
1	1.712692000	1.736804000	-2.336084000
6	4.628735000	1.590098000	-0.414888000
1	4.880239000	1.456663000	0.642413000
1	5.001040000	2.573523000	-0.724422000
1	5.173624000	0.836452000	-0.993614000
6	-4.629521000	1.590676000	-0.417423000
1	-5.174244000	0.835833000	-0.994744000
1	-5.002010000	2.573440000	-0.728831000
1	-4.881070000	1.459206000	0.640115000
6	-3.211755000	-2.538036000	0.930718000
1	-2.215630000	-2.972332000	0.821683000
1	-3.943019000	-3.339368000	0.772071000
1	-3.323872000	-2.191903000	1.962010000
6	-3.384983000	-1.948826000	-1.532653000
1	-3.662663000	-1.189571000	-2.268535000
1	-4.070589000	-2.795394000	-1.654362000
1	-2.374698000	-2.296148000	-1.770040000
6	-2.789180000	1.676871000	-2.164729000
1	-1.713474000	1.735307000	-2.338665000
1	-3.241961000	2.605076000	-2.532773000
1	-3.184566000	0.855693000	-2.770132000
1	0.004667000	1.994480000	1.688226000
1	-0.001323000	2.465566000	-0.397201000

-1814.899279

### 1-Fe-PNP

26	0.000003000	-0.034788000	-0.055855000
15	2.210781000	0.130945000	-0.208354000
15	-2.210802000	0.130836000	-0.208273000
8	0.000138000	-2.520957000	1.418097000
7	-0.000066000	1.826859000	-1.102013000
6	1.227945000	2.621110000	-0.864309000
1	1.192210000	2.950335000	0.177379000
1	1.244033000	3.513981000	-1.506415000
6	-1.228144000	2.621025000	-0.864363000
1	-1.244288000	3.513883000	-1.506487000
1	-1.192472000	2.950267000	0.177321000
6	3.126889000	-1.071623000	-1.327349000
1	2.694323000	-0.815306000	-2.303756000
6	-3.297571000	0.325011000	1.312426000
1	-4.324378000	0.448267000	0.945909000
6	-2.457670000	1.749089000	-1.112387000
1	-2.548924000	1.526465000	-2.181944000
1	-3.373924000	2.263377000	-0.806507000

6	-3.126829000	-1.071801000	-1.327244000
1	-2.694025000	-0.815630000	-2.303582000
6	2.457572000	1.749297000	-1.112315000
1	3.373749000	2.263636000	-0.806286000
1	2.548946000	1.526798000	-2.181886000
6	3.231117000	-0.924202000	2.205843000
1	2.206880000	-1.101822000	2.548782000
1	3.864804000	-0.784951000	3.089849000
1	3.575934000	-1.825307000	1.691789000
6	2.923442000	1.578736000	2.120162000
1	3.072989000	2.502027000	1.551443000
1	3.554609000	1.640553000	3.014860000
1	1.876127000	1.537633000	2.435332000
6	3.297593000	0.325084000	1.312331000
1	4.324335000	0.448650000	0.945732000
6	0.000099000	-1.513015000	0.814389000
6	2.771623000	-2.541224000	-1.053039000
1	3.177592000	-2.890936000	-0.098755000
1	3.195323000	-3.176366000	-1.840573000
1	1.688525000	-2.684075000	-1.038699000
6	4.647308000	-0.860002000	-1.395644000
1	4.915223000	0.185407000	-1.583885000
1	5.071418000	-1.464232000	-2.206586000
1	5.134785000	-1.173725000	-0.466096000
6	-4.647213000	-0.860019000	-1.395838000
1	-5.134897000	-1.173686000	-0.466380000
1	-5.071230000	-1.464222000	-2.206850000
1	-4.914988000	0.185413000	-1.584146000
6	-2.923624000	1.578910000	2.119981000
1	-1.876247000	1.538137000	2.434999000
1	-3.554651000	1.640717000	3.014778000
1	-3.073519000	2.502056000	1.551119000
6	-3.230718000	-0.924089000	2.206182000
1	-3.575130000	-1.825428000	1.692272000
1	-3.864548000	-0.784906000	3.090097000
1	-2.206453000	-1.101266000	2.549260000
6	-2.771834000	-2.541423000	-1.052698000
1	-1.688761000	-2.684385000	-1.037614000
1	-3.195039000	-3.176530000	-1.840525000
1	-3.178542000	-2.891096000	-0.098713000
1	-0.000040000	1.534295000	-2.079066000
1	-0.000195000	-0.743505000	-1.464701000
1	0.000102000	0.817704000	1.252698000

-1607.127269

**2-Fe-PNP**

26	-0.022250000	-0.330213000	-0.067550000
15	2.188085000	-0.262350000	0.133272000
15	-2.227169000	-0.187365000	0.148182000
8	-0.039477000	-0.822224000	-2.914349000
7	-0.008782000	-0.022271000	2.043880000
6	1.212354000	-0.553183000	2.693280000
1	1.163589000	-1.642552000	2.619245000
1	1.235351000	-0.280953000	3.758720000
6	-1.245539000	-0.503255000	2.701907000
1	-1.251060000	-0.228839000	3.767020000
1	-1.240473000	-1.593805000	2.629344000
6	3.093689000	1.222518000	-0.582596000
1	2.673582000	2.034615000	0.025363000
6	-3.364735000	-1.636952000	-0.219687000
1	-4.380042000	-1.305984000	0.031354000
6	-2.461959000	0.078805000	1.982939000
1	-2.519636000	1.158823000	2.161604000
1	-3.390616000	-0.364974000	2.354536000
6	-3.082772000	1.325896000	-0.570085000
1	-2.610841000	2.125738000	0.016296000
6	2.446335000	-0.017271000	1.968173000
1	3.358927000	-0.500803000	2.330094000
1	2.548210000	1.058198000	2.153268000
6	3.210082000	-2.110295000	-1.747076000
1	2.187073000	-2.359887000	-2.045864000
1	3.842529000	-2.983925000	-1.945275000
1	3.560488000	-1.297345000	-2.388804000
6	2.885494000	-2.960923000	0.608551000
1	3.026657000	-2.772542000	1.677465000
1	3.514870000	-3.818180000	0.340980000
1	1.838007000	-3.233131000	0.446430000
6	3.271321000	-1.748505000	-0.254311000
1	4.298255000	-1.458396000	0.000585000
6	-0.032582000	-0.615850000	-1.757806000
6	2.710795000	1.510683000	-2.041918000
1	3.112074000	0.757203000	-2.726647000
1	3.119177000	2.481844000	-2.346577000
1	1.625350000	1.539290000	-2.158499000
6	4.617268000	1.208496000	-0.385851000
1	4.901644000	1.010571000	0.653364000
1	5.038223000	2.181113000	-0.667607000
1	5.093043000	0.450997000	-1.018311000
6	-4.600952000	1.379241000	-0.339902000
1	-5.122729000	0.635968000	-0.952893000
1	-4.986890000	2.365817000	-0.623434000

1	-4.870260000	1.204570000	0.707482000
6	-3.022834000	-2.851755000	0.658492000
1	-1.982399000	-3.156660000	0.508719000
1	-3.674511000	-3.692935000	0.393305000
1	-3.168685000	-2.649223000	1.724201000
6	-3.317128000	-2.019935000	-1.707850000
1	-3.632736000	-1.201338000	-2.360200000
1	-3.985079000	-2.869027000	-1.895831000
1	-2.305025000	-2.315520000	-2.002268000
6	-2.722030000	1.578271000	-2.041509000
1	-1.639775000	1.552995000	-2.185725000
1	-3.090211000	2.564661000	-2.348631000
1	-3.176563000	0.838043000	-2.707095000
1	0.013819000	0.994129000	2.129559000
1	-0.002822000	1.226962000	-0.231415000
1	-0.043452000	-1.861952000	0.248420000
6	0.217936000	3.499940000	0.563314000
8	0.089668000	3.932048000	-0.515431000
8	0.357399000	3.162430000	1.678113000

-1795.723538

### TS1-Fe-PNP

26	0.000052000	-0.270989000	-0.074484000
15	2.210888000	-0.221893000	0.143606000
15	-2.210801000	-0.222016000	0.143514000
8	0.000147000	-0.397807000	-2.961217000
7	0.000022000	-0.246864000	2.053701000
6	1.227462000	-0.836583000	2.640546000
1	1.193550000	-1.910185000	2.437852000
1	1.241740000	-0.694079000	3.730848000
6	-1.227459000	-0.836556000	2.640473000
1	-1.241790000	-0.694105000	3.730781000
1	-1.193539000	-1.910147000	2.437723000
6	3.112524000	1.341034000	-0.382576000
1	2.700285000	2.070349000	0.327763000
6	-3.285747000	-1.651613000	-0.428180000
1	-4.315823000	-1.395467000	-0.150689000
6	-2.458640000	-0.203200000	1.993987000
1	-2.547310000	0.842926000	2.308355000
1	-3.375260000	-0.716734000	2.300039000
6	-3.112574000	1.340727000	-0.382919000
1	-2.700357000	2.070199000	0.327270000
6	2.458695000	-0.203284000	1.994105000
1	3.375268000	-0.716940000	2.300086000
1	2.547489000	0.842791000	2.308602000

6	3.209580000	-1.830546000	-1.952980000
1	2.186085000	-2.055831000	-2.268853000
1	3.850038000	-2.665182000	-2.261974000
1	3.542176000	-0.941155000	-2.494887000
6	2.908219000	-2.959538000	0.286256000
1	3.071323000	-2.905967000	1.367289000
1	3.527542000	-3.779217000	-0.097270000
1	1.856563000	-3.207576000	0.111538000
6	3.285994000	-1.651349000	-0.428238000
1	4.316051000	-1.395084000	-0.150780000
6	0.000116000	-0.338289000	-1.789259000
6	2.719424000	1.816722000	-1.790174000
1	3.098185000	1.148039000	-2.569311000
1	3.145548000	2.810309000	-1.974512000
1	1.633806000	1.884778000	-1.890006000
6	4.637540000	1.297547000	-0.200703000
1	4.928182000	0.967148000	0.802474000
1	5.059391000	2.297323000	-0.358055000
1	5.106731000	0.626732000	-0.928822000
6	-4.637601000	1.297208000	-0.200990000
1	-5.106799000	0.626334000	-0.929050000
1	-5.059489000	2.296956000	-0.358404000
1	-4.928236000	0.966878000	0.802212000
6	-2.907775000	-2.959698000	0.286407000
1	-1.856125000	-3.207683000	0.111559000
1	-3.527103000	-3.779449000	-0.096949000
1	-3.070706000	-2.906048000	1.367469000
6	-3.209366000	-1.830811000	-1.952946000
1	-3.542424000	-0.941589000	-2.494866000
1	-3.849459000	-2.665749000	-2.261869000
1	-2.185792000	-2.055643000	-2.268897000
6	-2.719487000	1.816193000	-1.790591000
1	-1.633866000	1.884260000	-1.890466000
1	-3.145649000	2.809735000	-1.975079000
1	-3.098240000	1.147358000	-2.569601000
1	0.000003000	0.750771000	2.272728000
1	-0.000084000	1.307966000	-0.039857000
1	0.000111000	-1.817237000	0.032617000
6	-0.000456000	3.164657000	0.713082000
8	0.000379000	3.733453000	-0.317170000
8	-0.001464000	2.890211000	1.862770000

-1795.721115

**3-Fe-PNP**  
 26 -0.009386000 -0.176584000 -0.062584000

15	2.233818000	-0.209394000	0.153417000
15	-2.253287000	-0.178068000	0.161723000
8	-0.016774000	-0.382300000	-2.952750000
7	-0.005259000	-0.189773000	2.043249000
6	1.215169000	-0.787597000	2.645297000
1	1.166448000	-1.866061000	2.474391000
1	1.223918000	-0.618301000	3.730497000
6	-1.233174000	-0.763807000	2.652448000
1	-1.235168000	-0.589793000	3.736919000
1	-1.202915000	-1.843710000	2.486231000
6	3.171607000	1.314649000	-0.405942000
1	2.823550000	2.066013000	0.315158000
6	-3.248659000	-1.651163000	-0.415970000
1	-4.283523000	-1.449336000	-0.113255000
6	-2.477210000	-0.151017000	2.010017000
1	-2.574940000	0.896731000	2.313265000
1	-3.384512000	-0.674569000	2.325955000
6	-3.164155000	1.364293000	-0.395218000
1	-2.806947000	2.106698000	0.330648000
6	2.465445000	-0.190432000	2.000468000
1	3.366737000	-0.726829000	2.311886000
1	2.576270000	0.855566000	2.304660000
6	3.136191000	-1.858489000	-1.955851000
1	2.107923000	-2.018067000	-2.294359000
1	3.728672000	-2.729244000	-2.258908000
1	3.536626000	-0.988386000	-2.482079000
6	2.720207000	-2.985149000	0.270274000
1	2.863348000	-2.949236000	1.354277000
1	3.294425000	-3.839148000	-0.106718000
1	1.660316000	-3.169083000	0.068330000
6	3.199381000	-1.701419000	-0.428355000
1	4.239098000	-1.516763000	-0.131588000
6	-0.012970000	-0.255769000	-1.794555000
6	2.746498000	1.798438000	-1.802466000
1	3.020226000	1.087075000	-2.587107000
1	3.248143000	2.746948000	-2.025484000
1	1.668901000	1.972171000	-1.852780000
6	4.697973000	1.190527000	-0.278637000
1	5.006340000	0.851189000	0.715910000
1	5.161847000	2.167278000	-0.456557000
1	5.105522000	0.493606000	-1.018842000
6	-4.692842000	1.266145000	-0.271307000
1	-5.111311000	0.577167000	-1.012805000
1	-5.139185000	2.251063000	-0.449167000
1	-5.008859000	0.931724000	0.722455000
6	-2.786295000	-2.943105000	0.278630000

1	-1.730820000	-3.144191000	0.069813000
1	-3.376891000	-3.787345000	-0.094949000
1	-2.921690000	-2.905138000	1.363610000
6	-3.196101000	-1.805700000	-1.944093000
1	-3.584888000	-0.927647000	-2.465984000
1	-3.804776000	-2.665553000	-2.246055000
1	-2.172451000	-1.981428000	-2.288591000
6	-2.729803000	1.849609000	-1.788757000
1	-1.649725000	2.009504000	-1.840125000
1	-3.219734000	2.805101000	-2.007990000
1	-3.011093000	1.145807000	-2.577504000
1	0.010235000	0.828796000	2.240415000
1	-0.116992000	1.720411000	0.068193000
1	-0.017220000	-1.658747000	-0.095495000
6	0.059056000	2.734386000	0.621792000
8	0.142358000	3.693803000	-0.157883000
8	0.111425000	2.653605000	1.871182000

-1795.744694

### TS2-Fe-PNP

26	0.015946000	-0.175100000	0.063375000
15	-2.232849000	-0.257307000	-0.163575000
15	2.268895000	-0.181584000	-0.142078000
8	-0.006345000	-0.059865000	2.958727000
7	0.028307000	-0.410284000	-2.007140000
6	-1.170127000	-1.089163000	-2.564232000
1	-1.100318000	-2.143964000	-2.284953000
1	-1.163627000	-1.029686000	-3.660909000
6	1.275286000	-0.967137000	-2.588736000
1	1.267903000	-0.852992000	-3.680852000
1	1.287670000	-2.036919000	-2.365761000
6	-3.187956000	1.314258000	0.197701000
1	-2.798370000	1.977325000	-0.583740000
6	3.211250000	-1.637599000	0.559149000
1	4.274065000	-1.416091000	0.405883000
6	2.495070000	-0.271498000	-1.986767000
1	2.552150000	0.760486000	-2.350304000
1	3.421869000	-0.775928000	-2.274421000
6	3.221779000	1.374429000	0.298875000
1	2.762495000	2.108236000	-0.376450000
6	-2.442647000	-0.457355000	-2.001623000
1	-3.323687000	-1.053726000	-2.255737000
1	-2.578628000	0.544590000	-2.419968000
6	-3.146135000	-1.663615000	2.111152000
1	-2.120392000	-1.761005000	2.479065000

1	-3.725949000	-2.506093000	2.504976000
1	-3.572006000	-0.747433000	2.527641000
6	-2.672703000	-3.031534000	0.037170000
1	-2.796139000	-3.122131000	-1.045946000
1	-3.238580000	-3.848014000	0.500017000
1	-1.613496000	-3.170302000	0.276073000
6	-3.186332000	-1.685259000	0.575139000
1	-4.223419000	-1.553366000	0.242939000
6	0.002469000	-0.055535000	1.794027000
6	-2.825355000	1.943278000	1.552531000
1	-3.140171000	1.322453000	2.396257000
1	-3.327502000	2.912550000	1.648623000
1	-1.750097000	2.116152000	1.641600000
6	-4.706784000	1.167292000	0.020388000
1	-4.970529000	0.723715000	-0.945601000
1	-5.179791000	2.154576000	0.072805000
1	-5.146191000	0.549756000	0.811351000
6	4.722373000	1.294843000	-0.024695000
1	5.243589000	0.620800000	0.663117000
1	5.173531000	2.287675000	0.084100000
1	4.911742000	0.954222000	-1.047512000
6	2.873897000	-2.940551000	-0.185708000
1	1.801874000	-3.156893000	-0.130097000
1	3.411343000	-3.773493000	0.281484000
1	3.169822000	-2.910332000	-1.238033000
6	2.938374000	-1.801969000	2.063568000
1	3.164958000	-0.901151000	2.638450000
1	3.556502000	-2.615073000	2.460611000
1	1.889072000	-2.058418000	2.236751000
6	2.982328000	1.858830000	1.737833000
1	1.918497000	1.932518000	1.978335000
1	3.421983000	2.854779000	1.861974000
1	3.454774000	1.199531000	2.472012000
1	-0.035664000	0.595487000	-2.230046000
1	0.368065000	2.269551000	0.265815000
1	0.055910000	-1.626979000	0.296922000
6	-0.058697000	2.933997000	-0.538061000
8	-0.059798000	4.156980000	-0.288177000
8	-0.485512000	2.336543000	-1.572513000

-1795.737817

### 3'-Fe-PNP

26	0.000013000	-0.082810000	0.028728000
15	-2.241910000	-0.226307000	-0.146403000
15	2.241906000	-0.226340000	-0.146429000

8	0.000134000	0.569707000	2.848929000
7	-0.000082000	-0.752612000	-1.974647000
6	-1.227107000	-1.480200000	-2.383372000
1	-1.192154000	-2.463106000	-1.907386000
1	-1.238874000	-1.632135000	-3.471559000
6	1.226946000	-1.480217000	-2.383349000
1	1.238687000	-1.632175000	-3.471532000
1	1.191976000	-2.463117000	-1.907351000
6	-3.226236000	1.362522000	-0.045383000
1	-2.682759000	1.988171000	-0.765022000
6	3.172085000	-1.516808000	0.843710000
1	4.239071000	-1.306878000	0.698937000
6	2.462068000	-0.702545000	-1.934372000
1	2.538719000	0.231251000	-2.503043000
1	3.377485000	-1.273747000	-2.113903000
6	3.226254000	1.362483000	-0.045447000
1	2.682730000	1.988151000	-0.765035000
6	-2.462179000	-0.702504000	-1.934341000
1	-3.377617000	-1.273686000	-2.113830000
1	-2.538833000	0.231294000	-2.503009000
6	-2.835061000	-1.415583000	2.341857000
1	-1.787475000	-1.680614000	2.514371000
1	-3.460976000	-2.116124000	2.906774000
1	-3.000108000	-0.416283000	2.750713000
6	-2.882730000	-2.942156000	0.342468000
1	-3.206905000	-3.101564000	-0.689888000
1	-3.419073000	-3.664065000	0.969156000
1	-1.812806000	-3.165885000	0.411097000
6	-3.172091000	-1.516758000	0.843751000
1	-4.239076000	-1.306769000	0.699043000
6	0.000009000	0.344503000	1.702454000
6	-3.133314000	2.045748000	1.328365000
1	-3.729374000	1.518279000	2.079850000
1	-3.526971000	3.066089000	1.257229000
1	-2.103991000	2.107295000	1.689737000
6	-4.688555000	1.241462000	-0.504966000
1	-4.780644000	0.790387000	-1.497694000
1	-5.142561000	2.238444000	-0.549983000
1	-5.281390000	0.644778000	0.196799000
6	4.688541000	1.241430000	-0.505138000
1	5.281426000	0.644730000	0.196570000
1	5.142545000	2.238411000	-0.550166000
1	4.780558000	0.790377000	-1.497884000
6	2.882635000	-2.942214000	0.342501000
1	1.812695000	-3.165868000	0.411132000
1	3.418924000	-3.664125000	0.969233000

1	3.206810000	-3.101704000	-0.689842000
6	2.835150000	-1.415565000	2.341832000
1	3.000305000	-0.416267000	2.750648000
1	3.461039000	-2.116142000	2.906733000
1	1.787552000	-1.680505000	2.514413000
6	3.133432000	2.045693000	1.328316000
1	2.104132000	2.107253000	1.689752000
1	3.527103000	3.066027000	1.257169000
1	3.729528000	1.518202000	2.079756000
1	-0.000072000	0.158866000	-2.441284000
1	-0.000086000	2.924842000	0.704775000
1	0.000003000	-1.526818000	0.486830000
6	0.000074000	2.910200000	-0.405644000
8	-0.000034000	3.994694000	-1.015612000
8	0.000054000	1.746703000	-0.942526000

-1795.757625

#### 4-Fe-PNP

15	-2.125868000	-0.467008000	0.310793000
7	-0.022604000	1.287943000	1.393838000
6	1.050256000	1.047290000	2.388058000
6	-1.362574000	1.511932000	2.007503000
6	-2.192088000	0.230073000	2.025385000
1	-3.216517000	0.424803000	2.358549000
1	-1.749579000	-0.507493000	2.700574000
6	2.394489000	1.043187000	1.657946000
1	3.209364000	0.744480000	2.322879000
15	2.249798000	-0.096028000	0.197765000
6	0.089926000	-1.324457000	-1.438236000
8	0.121783000	-2.133247000	-2.272611000
26	0.035010000	-0.134362000	-0.164278000
6	-2.817639000	-2.197237000	0.488406000
1	-3.759797000	-2.061734000	1.035923000
6	-3.126160000	-2.863213000	-0.863859000
1	-3.508892000	-3.875355000	-0.689501000
1	-3.882084000	-2.322299000	-1.436631000
1	-2.226745000	-2.950404000	-1.480341000
6	-1.894202000	-3.099419000	1.324311000
1	-1.638585000	-2.663868000	2.294184000
1	-2.395532000	-4.056374000	1.509666000
1	-0.959825000	-3.300588000	0.792320000
6	3.001947000	-1.678845000	0.870226000
1	2.525041000	-1.734367000	1.858554000
6	2.595394000	-2.944237000	0.099140000
1	3.003841000	-3.825981000	0.606228000

1	1.509451000	-3.050743000	0.057498000
1	2.978080000	-2.945975000	-0.925519000
6	4.525003000	-1.602532000	1.072460000
1	4.862129000	-2.478979000	1.637302000
1	5.059796000	-1.603054000	0.117642000
1	4.833135000	-0.712940000	1.630912000
1	1.041742000	1.835348000	3.153498000
1	0.864495000	0.089673000	2.884222000
1	2.611731000	2.048793000	1.287394000
1	-1.852725000	2.274439000	1.395797000
1	-1.251772000	1.916399000	3.021284000
6	3.445618000	0.585620000	-1.070808000
1	4.399243000	0.724061000	-0.545418000
6	2.968207000	1.948150000	-1.602404000
1	3.767458000	2.404935000	-2.197053000
1	2.100500000	1.823914000	-2.259526000
1	2.680821000	2.651618000	-0.816752000
6	3.648653000	-0.394299000	-2.239039000
1	4.305513000	0.060798000	-2.989095000
1	4.106404000	-1.336389000	-1.928801000
1	2.695404000	-0.622418000	-2.728508000
6	-3.389040000	0.550075000	-0.624748000
1	-3.089750000	1.568367000	-0.348153000
6	-4.845621000	0.317868000	-0.193110000
1	-5.492988000	1.059490000	-0.675300000
1	-5.205000000	-0.672655000	-0.490500000
1	-4.983010000	0.416802000	0.888197000
6	-3.222884000	0.447292000	-2.151187000
1	-3.846562000	1.207132000	-2.635497000
1	-2.187827000	0.621085000	-2.457503000
1	-3.530577000	-0.528288000	-2.538438000
1	0.209642000	2.188238000	0.921481000
1	-0.325965000	4.997987000	-1.172723000
6	-0.439655000	4.054568000	-0.586030000
8	0.532199000	3.759739000	0.175172000
8	-1.501471000	3.401669000	-0.752277000
1	0.286621000	1.141545000	-1.224953000
1	-0.506666000	1.178854000	-1.086842000
1	0.151116000	-1.221683000	0.852615000

-1796.913756

### TS3-Fe-PNP

15	-2.132626000	-0.427119000	0.317330000
7	0.024879000	1.204629000	1.497725000
6	1.049998000	0.834754000	2.503920000

6	-1.317636000	1.488997000	2.078353000
6	-2.218212000	0.256187000	2.043137000
1	-3.238407000	0.508099000	2.351018000
1	-1.839172000	-0.510420000	2.723947000
6	2.414501000	0.800342000	1.811403000
1	3.177509000	0.367655000	2.464813000
15	2.241436000	-0.169245000	0.224423000
6	0.053219000	-1.248087000	-1.474192000
8	0.054913000	-1.949922000	-2.409380000
26	0.035978000	-0.182340000	-0.116556000
6	-2.918418000	-2.122799000	0.468027000
1	-3.882923000	-1.951200000	0.963945000
6	-3.176298000	-2.771270000	-0.903414000
1	-3.604438000	-3.770344000	-0.760330000
1	-3.878423000	-2.199670000	-1.514118000
1	-2.246090000	-2.884573000	-1.468435000
6	-2.082636000	-3.069014000	1.345844000
1	-1.878952000	-2.658334000	2.338825000
1	-2.626360000	-4.011685000	1.480822000
1	-1.121258000	-3.287649000	0.872811000
6	3.038429000	-1.802349000	0.705480000
1	2.597886000	-1.966113000	1.698488000
6	2.608119000	-2.982895000	-0.178580000
1	3.037942000	-3.911995000	0.214692000
1	1.520832000	-3.086004000	-0.190391000
1	2.951095000	-2.871788000	-1.211666000
6	4.566648000	-1.734744000	0.859186000
1	4.932628000	-2.661288000	1.316572000
1	5.063620000	-1.629630000	-0.110531000
1	4.888938000	-0.903066000	1.494318000
1	1.060971000	1.563230000	3.327427000
1	0.790970000	-0.144879000	2.913710000
1	2.728965000	1.820276000	1.569401000
1	-1.758877000	2.290312000	1.478151000
1	-1.217493000	1.872685000	3.101841000
6	3.424412000	0.668452000	-0.965037000
1	4.401170000	0.717475000	-0.466658000
6	2.958597000	2.098108000	-1.287498000
1	3.706459000	2.591531000	-1.919484000
1	2.008295000	2.080576000	-1.828900000
1	2.812140000	2.715006000	-0.397037000
6	3.560902000	-0.144932000	-2.264168000
1	4.209689000	0.388261000	-2.968884000
1	3.996074000	-1.133916000	-2.100111000
1	2.584977000	-0.277652000	-2.744284000
6	-3.365096000	0.641639000	-0.614522000

1	-3.060365000	1.649586000	-0.304398000
6	-4.837508000	0.435676000	-0.225655000
1	-5.457078000	1.205623000	-0.700664000
1	-5.211607000	-0.537152000	-0.560949000
1	-4.998276000	0.504121000	0.855071000
6	-3.159835000	0.571002000	-2.137869000
1	-3.748165000	1.357160000	-2.625412000
1	-2.109832000	0.718089000	-2.402223000
1	-3.485048000	-0.388189000	-2.551700000
1	0.331498000	2.092642000	1.079934000
1	-0.762298000	4.994628000	-0.838456000
6	-0.422717000	3.985730000	-0.542601000
8	0.404705000	3.851345000	0.368994000
8	-0.979895000	3.036020000	-1.227205000
1	0.023637000	1.057196000	-1.160929000
1	-0.472165000	1.941709000	-1.075773000
1	0.133600000	-1.324743000	0.885479000

-1796.902605

### 5-Fe-PNP

15	-2.126862000	-0.450518000	0.314753000
7	0.023615000	1.150215000	1.542564000
6	1.037088000	0.743203000	2.545644000
6	-1.320236000	1.430089000	2.120601000
6	-2.226882000	0.203012000	2.052673000
1	-3.248338000	0.454928000	2.356882000
1	-1.857324000	-0.577351000	2.722772000
6	2.406647000	0.706434000	1.864023000
1	3.152861000	0.231926000	2.507933000
15	2.234898000	-0.196689000	0.234941000
6	0.055039000	-1.188391000	-1.522142000
8	0.058774000	-1.817108000	-2.511189000
26	0.035918000	-0.207235000	-0.109498000
6	-2.933120000	-2.140690000	0.427191000
1	-3.913643000	-1.967494000	0.889674000
6	-3.144292000	-2.769123000	-0.961528000
1	-3.587351000	-3.765861000	-0.850347000
1	-3.815903000	-2.181634000	-1.591592000
1	-2.193340000	-2.882723000	-1.491088000
6	-2.139986000	-3.105621000	1.323516000
1	-1.980929000	-2.713793000	2.332266000
1	-2.691984000	-4.048676000	1.417294000
1	-1.158862000	-3.318379000	0.890488000
6	3.046877000	-1.843620000	0.642338000
1	2.599022000	-2.059457000	1.622005000

6	2.630114000	-2.979907000	-0.303698000
1	3.051285000	-3.928568000	0.050698000
1	1.542777000	-3.076445000	-0.338618000
1	2.990346000	-2.819433000	-1.324342000
6	4.573273000	-1.774795000	0.811787000
1	4.942093000	-2.720779000	1.225451000
1	5.078134000	-1.618432000	-0.146939000
1	4.884835000	-0.973738000	1.490346000
1	1.051165000	1.448943000	3.389158000
1	0.760793000	-0.243856000	2.924733000
1	2.747851000	1.727576000	1.667536000
1	-1.754719000	2.247809000	1.537632000
1	-1.224757000	1.790954000	3.153140000
6	3.425764000	0.700073000	-0.905843000
1	4.398954000	0.732888000	-0.399048000
6	2.953730000	2.139505000	-1.169595000
1	3.690827000	2.658690000	-1.793733000
1	1.994910000	2.136704000	-1.696276000
1	2.822107000	2.723735000	-0.254566000
6	3.575965000	-0.053427000	-2.239163000
1	4.222764000	0.515503000	-2.917451000
1	4.019501000	-1.044545000	-2.115807000
1	2.603255000	-0.175120000	-2.728616000
6	-3.360890000	0.639179000	-0.597966000
1	-3.068777000	1.639862000	-0.252211000
6	-4.836650000	0.416304000	-0.231295000
1	-5.454518000	1.201687000	-0.682878000
1	-5.204160000	-0.544217000	-0.607112000
1	-5.007683000	0.442611000	0.849793000
6	-3.142510000	0.616241000	-2.120660000
1	-3.724985000	1.417429000	-2.590810000
1	-2.088663000	0.765365000	-2.369006000
1	-3.466329000	-0.329839000	-2.565135000
1	0.339397000	2.038784000	1.143734000
1	-0.736278000	5.098174000	-0.794025000
6	-0.409361000	4.086901000	-0.507647000
8	0.314216000	3.887939000	0.462835000
8	-0.893325000	3.170752000	-1.317129000
1	-0.030683000	1.053058000	-1.074388000
1	-0.521946000	2.205270000	-1.111391000
1	0.137839000	-1.381715000	0.881853000

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**15-Fe-PNP**  
 26 -1.088881000 0.482093000 -0.093486000

15	-2.412482000	-1.280167000	0.152546000
15	0.422764000	2.095944000	0.064391000
8	-1.667470000	0.886018000	-2.895345000
7	-0.695779000	0.198287000	1.986346000
6	-1.839570000	-0.410145000	2.701159000
1	-2.647633000	0.326501000	2.704962000
1	-1.570722000	-0.632648000	3.744779000
6	-0.221818000	1.432343000	2.652575000
1	0.082952000	1.219610000	3.688170000
1	-1.062285000	2.131051000	2.679861000
6	-1.887419000	-2.902856000	-0.642034000
1	-0.961344000	-3.115072000	-0.090867000
6	-0.020849000	3.904910000	-0.192913000
1	0.907764000	4.477170000	-0.073063000
6	0.943010000	2.017180000	1.855596000
1	1.805229000	1.344137000	1.921617000
1	1.249561000	2.990251000	2.251279000
6	2.065804000	1.840081000	-0.806623000
1	2.362234000	0.885101000	-0.357757000
6	-2.271268000	-1.682573000	1.972101000
1	-3.204276000	-2.079737000	2.384141000
1	-1.503528000	-2.455864000	2.088423000
6	-4.620441000	-0.922063000	-1.582737000
1	-4.180420000	0.017998000	-1.930674000
1	-5.708263000	-0.849373000	-1.701207000
1	-4.270565000	-1.721990000	-2.240917000
6	-4.905364000	-0.110726000	0.792752000
1	-4.768988000	-0.328892000	1.856737000
1	-5.984463000	-0.060987000	0.603104000
1	-4.468065000	0.871537000	0.590256000
6	-4.271062000	-1.182130000	-0.108189000
1	-4.674900000	-2.159342000	0.185215000
6	-1.431350000	0.723651000	-1.754753000
6	-1.500712000	-2.749034000	-2.121102000
1	-2.371080000	-2.551977000	-2.754987000
1	-1.036157000	-3.675404000	-2.480914000
1	-0.789669000	-1.929403000	-2.250322000
6	-2.858066000	-4.073632000	-0.423981000
1	-3.137667000	-4.189796000	0.628794000
1	-2.392978000	-5.011263000	-0.751394000
1	-3.776481000	-3.943618000	-1.006815000
6	3.142989000	2.889796000	-0.495754000
1	2.912094000	3.851288000	-0.967508000
1	4.111375000	2.557679000	-0.890037000
1	3.262174000	3.059576000	0.579470000
6	-1.028938000	4.388863000	0.862784000

1	-1.931348000	3.769106000	0.845471000
1	-1.316519000	5.425630000	0.650666000
1	-0.616352000	4.364992000	1.876119000
6	-0.578839000	4.144445000	-1.606091000
1	0.130550000	3.870401000	-2.391020000
1	-0.822628000	5.205866000	-1.735292000
1	-1.493948000	3.565299000	-1.764398000
6	1.930851000	1.602623000	-2.317729000
1	1.177176000	0.841577000	-2.532801000
1	2.890833000	1.263653000	-2.726577000
1	1.659514000	2.518600000	-2.851575000
1	0.076985000	-0.473351000	2.022778000
1	0.086400000	-0.500308000	-0.404528000
6	3.329907000	-1.859420000	-1.074763000
6	4.222544000	-0.841805000	0.987949000
6	5.523624000	-1.605051000	0.735710000
8	5.730970000	-1.819488000	-0.664072000
6	4.667024000	-2.581352000	-1.242427000
1	2.505561000	-2.477636000	-1.440063000
1	4.010114000	-0.764411000	2.055487000
1	5.498365000	-2.572447000	1.260591000
1	4.618813000	-3.574381000	-0.769281000
7	3.118446000	-1.550052000	0.339086000
1	6.379854000	-1.028374000	1.093661000
1	4.300492000	0.168741000	0.567200000
1	3.340504000	-0.924237000	-1.648066000
1	4.907238000	-2.701882000	-2.301496000
6	1.981496000	-1.873923000	0.986477000
8	1.729699000	-1.595139000	2.169421000
1	1.268458000	-2.424194000	0.358496000
1	-2.230859000	1.445873000	0.374757000

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### TS7-Fe-PNP

26	-0.543006000	0.365140000	-0.071028000
15	-2.547245000	-0.610034000	0.114548000
15	1.220471000	1.728488000	0.113598000
8	-0.435138000	0.225275000	-2.959583000
7	-0.592549000	0.415962000	2.030305000
6	-1.959966000	0.371346000	2.610156000
1	-2.419913000	1.347052000	2.432708000
1	-1.905693000	0.217245000	3.697686000
6	0.188736000	1.507329000	2.666437000
1	0.358349000	1.280950000	3.728706000
1	-0.421495000	2.412700000	2.618736000

6	-2.815198000	-2.389119000	-0.436489000
1	-2.215564000	-2.939691000	0.298486000
6	0.951759000	3.522604000	-0.388762000
1	1.945556000	3.985146000	-0.422321000
6	1.519038000	1.734794000	1.951958000
1	2.205584000	0.908348000	2.162468000
1	1.997801000	2.653609000	2.304715000
6	2.927686000	1.330514000	-0.568706000
1	3.084946000	0.300286000	-0.238801000
6	-2.778814000	-0.738912000	1.955540000
1	-3.829278000	-0.689801000	2.258742000
1	-2.375197000	-1.711403000	2.253670000
6	-3.913473000	0.649840000	-2.002097000
1	-3.056429000	1.306935000	-2.180437000
1	-4.816279000	1.161728000	-2.355680000
1	-3.782511000	-0.249108000	-2.610991000
6	-4.291545000	1.626368000	0.294596000
1	-4.516355000	1.429375000	1.347219000
1	-5.151386000	2.157871000	-0.130121000
1	-3.420964000	2.287764000	0.243930000
6	-4.046006000	0.335018000	-0.502910000
1	-4.908631000	-0.323869000	-0.350886000
6	-0.478827000	0.275450000	-1.789758000
6	-2.227306000	-2.679823000	-1.826070000
1	-2.782586000	-2.167730000	-2.618086000
1	-2.275941000	-3.755755000	-2.031510000
1	-1.182715000	-2.366082000	-1.893383000
6	-4.264527000	-2.887688000	-0.320408000
1	-4.700334000	-2.670718000	0.660544000
1	-4.293947000	-3.974010000	-0.465884000
1	-4.906166000	-2.437774000	-1.085660000
6	4.066022000	2.187468000	0.010057000
1	3.976880000	3.238221000	-0.286777000
1	5.026689000	1.820844000	-0.371184000
1	4.107724000	2.144787000	1.102443000
6	0.091715000	4.300305000	0.620420000
1	-0.894031000	3.835144000	0.726685000
1	-0.057695000	5.324666000	0.259063000
1	0.556480000	4.366786000	1.608568000
6	0.311648000	3.608179000	-1.786413000
1	0.881836000	3.075739000	-2.550810000
1	0.236874000	4.658324000	-2.093224000
1	-0.694919000	3.180412000	-1.763005000
6	2.973951000	1.325231000	-2.105388000
1	2.157229000	0.745702000	-2.543740000
1	3.918932000	0.881259000	-2.439239000

1	2.928235000	2.341842000	-2.508919000
1	-0.147722000	-0.495963000	2.247981000
1	0.271770000	-1.069945000	0.173815000
6	2.110311000	-2.426095000	-0.996416000
6	2.893756000	-2.025916000	1.287721000
6	4.279632000	-2.465713000	0.831802000
8	4.491869000	-2.170471000	-0.553134000
6	3.527362000	-2.849647000	-1.363460000
1	1.389030000	-3.024295000	-1.564704000
1	2.714735000	-2.341897000	2.317990000
1	4.407646000	-3.546648000	1.000656000
1	3.645754000	-3.938028000	-1.242213000
7	1.868090000	-2.618305000	0.432689000
1	5.052290000	-1.928151000	1.387569000
1	2.829216000	-0.928105000	1.265613000
1	1.947318000	-1.370885000	-1.269298000
1	3.746470000	-2.583732000	-2.400765000
6	0.526308000	-2.375127000	0.838850000
8	0.242208000	-2.275398000	2.082416000
1	-0.155406000	-2.917495000	0.166277000
1	-1.330276000	1.660638000	-0.104587000

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### 16-Fe-PNP

26	-0.529604000	0.335131000	-0.064130000
15	-2.546605000	-0.639856000	0.119176000
15	1.211316000	1.744243000	0.106704000
8	-0.419796000	0.176836000	-2.955644000
7	-0.600173000	0.421661000	2.017294000
6	-1.968293000	0.386429000	2.597813000
1	-2.429958000	1.360874000	2.416753000
1	-1.911099000	0.240770000	3.686189000
6	0.186545000	1.504170000	2.662826000
1	0.367637000	1.256818000	3.718286000
1	-0.423045000	2.411188000	2.642169000
6	-2.814255000	-2.423563000	-0.411314000
1	-2.213952000	-2.966910000	0.328562000
6	0.874228000	3.524143000	-0.397151000
1	1.851636000	4.019586000	-0.436892000
6	1.511505000	1.747205000	1.942936000
1	2.204262000	0.923159000	2.142006000
1	1.985086000	2.667441000	2.298880000
6	2.922324000	1.391761000	-0.587835000
1	3.109350000	0.365840000	-0.259345000
6	-2.790254000	-0.731253000	1.958784000

1	-3.842579000	-0.670176000	2.252644000
1	-2.394157000	-1.700251000	2.276985000
6	-3.869378000	0.615919000	-2.031151000
1	-3.011070000	1.272395000	-2.204480000
1	-4.767618000	1.124599000	-2.400095000
1	-3.730850000	-0.288015000	-2.630458000
6	-4.266260000	1.617020000	0.251561000
1	-4.507122000	1.432819000	1.302661000
1	-5.115317000	2.151529000	-0.190244000
1	-3.390712000	2.272360000	0.205756000
6	-4.022670000	0.315795000	-0.531066000
1	-4.892829000	-0.334256000	-0.383582000
6	-0.456630000	0.222505000	-1.788257000
6	-2.227862000	-2.730400000	-1.798158000
1	-2.777945000	-2.221288000	-2.595531000
1	-2.285986000	-3.807644000	-1.992998000
1	-1.179580000	-2.429660000	-1.867801000
6	-4.265789000	-2.914383000	-0.289137000
1	-4.700375000	-2.685465000	0.689566000
1	-4.298598000	-4.001982000	-0.422709000
1	-4.905695000	-2.470669000	-1.059383000
6	4.036304000	2.281729000	-0.011282000
1	3.915317000	3.329389000	-0.307446000
1	5.005770000	1.943553000	-0.395954000
1	4.082457000	2.239189000	1.080744000
6	-0.004251000	4.272004000	0.618865000
1	-0.972304000	3.773527000	0.736574000
1	-0.193633000	5.289160000	0.256463000
1	0.467996000	4.357426000	1.601865000
6	0.224483000	3.588328000	-1.791669000
1	0.802961000	3.067546000	-2.557776000
1	0.123589000	4.635452000	-2.100593000
1	-0.772209000	3.138371000	-1.763526000
6	2.960976000	1.390816000	-2.124612000
1	2.165757000	0.780604000	-2.560764000
1	3.920504000	0.982919000	-2.462439000
1	2.876287000	2.405336000	-2.527062000
1	-0.162543000	-0.510685000	2.242252000
1	0.365257000	-1.151916000	0.273977000
6	2.129954000	-2.438115000	-0.971821000
6	2.930494000	-1.982749000	1.272778000
6	4.309951000	-2.455070000	0.830898000
8	4.522000000	-2.213655000	-0.565668000
6	3.535271000	-2.893023000	-1.348779000
1	1.392242000	-3.026125000	-1.531063000
1	2.757676000	-2.239978000	2.320376000

1	4.424638000	-3.530801000	1.038772000
1	3.634364000	-3.980467000	-1.203449000
7	1.895591000	-2.614766000	0.459589000
1	5.092939000	-1.907510000	1.362439000
1	2.882478000	-0.884742000	1.195340000
1	1.994031000	-1.381395000	-1.265447000
1	3.748298000	-2.655257000	-2.394448000
6	0.535091000	-2.244643000	0.848631000
8	0.281240000	-2.151402000	2.132804000
1	-0.138226000	-2.884006000	0.248909000
1	-1.318470000	1.597884000	-0.172775000

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#### TS8-Fe-PNP

26	0.562915000	-0.349640000	-0.068505000
15	2.402931000	0.919565000	0.118766000
15	-0.940032000	-2.012245000	0.120213000
8	0.402117000	-0.174871000	-2.960775000
7	0.623990000	-0.419930000	1.949696000
6	1.925153000	-0.146753000	2.596674000
1	2.568173000	-1.035454000	2.520668000
1	1.780001000	0.045224000	3.672810000
6	-0.004349000	-1.553458000	2.657028000
1	-0.252409000	-1.260219000	3.690735000
1	0.713025000	-2.381856000	2.735519000
6	2.405644000	2.715125000	-0.442944000
1	1.796578000	3.195432000	0.332254000
6	-0.274106000	-3.713429000	-0.308805000
1	-1.097434000	-4.416118000	-0.141474000
6	-1.272015000	-2.030900000	1.945348000
1	-2.086614000	-1.318705000	2.115064000
1	-1.598782000	-3.010670000	2.310149000
6	-2.673610000	-1.987953000	-0.627716000
1	-3.221985000	-1.347339000	0.071682000
6	2.615346000	1.060280000	1.957634000
1	3.666333000	1.134498000	2.254970000
1	2.108949000	1.979993000	2.266709000
6	3.952348000	-0.041738000	-2.027748000
1	3.166263000	-0.759553000	-2.281136000
1	4.908887000	-0.446340000	-2.378533000
1	3.760395000	0.881519000	-2.581787000
6	4.369216000	-1.117854000	0.222575000
1	4.517704000	-0.964813000	1.295262000
1	5.304825000	-1.517159000	-0.186450000
1	3.589033000	-1.872955000	0.088083000

6	4.008563000	0.185148000	-0.508873000
1	4.788124000	0.923038000	-0.285722000
6	0.438813000	-0.209757000	-1.792305000
6	1.683156000	2.925041000	-1.782972000
1	0.666271000	2.525576000	-1.755629000
1	2.209041000	2.444435000	-2.613476000
1	1.622273000	3.997073000	-2.004110000
6	3.788533000	3.385217000	-0.429407000
1	4.307900000	3.244549000	0.524548000
1	3.676751000	4.463539000	-0.591902000
1	4.429499000	2.997876000	-1.228398000
6	-3.390740000	-3.347619000	-0.649858000
1	-2.951933000	-4.025478000	-1.389329000
1	-4.441060000	-3.198083000	-0.926102000
1	-3.371799000	-3.844039000	0.325971000
6	0.893761000	-4.144113000	0.592308000
1	1.710125000	-3.416454000	0.560618000
1	1.282295000	-5.109062000	0.245640000
1	0.582277000	-4.269649000	1.632869000
6	0.131066000	-3.763602000	-1.791334000
1	-0.698568000	-3.515943000	-2.459815000
1	0.474389000	-4.772296000	-2.049009000
1	0.947605000	-3.062240000	-1.989516000
6	-2.719080000	-1.304500000	-2.002885000
1	-2.318794000	-0.288929000	-1.957868000
1	-3.757126000	-1.242688000	-2.350006000
1	-2.147115000	-1.855716000	-2.755336000
1	-0.117115000	0.713795000	2.213190000
1	-0.561702000	1.258978000	0.283477000
6	-2.398809000	2.852441000	-0.696569000
6	-3.188111000	1.400063000	1.048239000
6	-4.613836000	1.830397000	0.729932000
8	-4.749064000	2.202933000	-0.646342000
6	-3.841812000	3.257902000	-0.979223000
1	-1.731850000	3.694499000	-0.914919000
1	-3.090465000	1.165529000	2.111007000
1	-4.903030000	2.677431000	1.371857000
1	-4.096748000	4.161330000	-0.402976000
7	-2.247848000	2.466587000	0.708477000
1	-5.311110000	1.005163000	0.897720000
1	-2.948321000	0.488371000	0.476260000
1	-2.119395000	2.018993000	-1.369495000
1	-3.981893000	3.465249000	-2.043357000
6	-0.867834000	2.108069000	1.009353000
8	-0.660307000	1.712822000	2.299905000
1	-0.246664000	2.966066000	0.708619000

1 1.517146000 -1.437285000 -0.313115000

-2008.181083

**17-Fe-PNP**

26	0.762843000	0.387473000	0.088544000
15	2.431931000	-1.090308000	-0.159864000
15	-0.717671000	2.061054000	-0.074124000
8	0.800523000	0.368846000	2.991452000
7	0.619474000	0.266893000	-1.870673000
6	1.785508000	-0.178169000	-2.656054000
1	2.500971000	0.652520000	-2.772343000
1	1.472339000	-0.459137000	-3.676111000
6	-0.061339000	1.323843000	-2.634872000
1	-0.432118000	0.921038000	-3.593204000
1	0.653124000	2.121445000	-2.896674000
6	2.270347000	-2.841191000	0.505163000
1	1.487061000	-3.246774000	-0.147853000
6	-0.038677000	3.790966000	0.172797000
1	-0.902912000	4.466974000	0.186933000
6	-1.232430000	1.917361000	-1.851962000
1	-2.078675000	1.222711000	-1.864908000
1	-1.572833000	2.865304000	-2.280269000
6	-2.361990000	2.030737000	0.834003000
1	-2.697938000	1.002764000	0.654495000
6	2.471394000	-1.375108000	-1.993654000
1	3.487054000	-1.529232000	-2.371187000
1	1.894453000	-2.284676000	-2.184897000
6	4.268925000	-0.182787000	1.776207000
1	3.575729000	0.618426000	2.051210000
1	5.286569000	0.152960000	2.007531000
1	4.055299000	-1.049098000	2.408324000
6	4.564909000	0.709430000	-0.570716000
1	4.580871000	0.484294000	-1.641002000
1	5.573922000	1.029579000	-0.285326000
1	3.880460000	1.547517000	-0.406873000
6	4.154933000	-0.505873000	0.278099000
1	4.829801000	-1.335508000	0.035832000
6	0.757890000	0.343611000	1.820648000
6	1.744347000	-2.907296000	1.947339000
1	2.458880000	-2.493800000	2.665466000
1	1.564829000	-3.952726000	2.224775000
1	0.804375000	-2.361351000	2.058349000
6	3.531676000	-3.700302000	0.320536000
1	3.913147000	-3.662660000	-0.705424000
1	3.303574000	-4.747146000	0.552742000

1	4.333948000	-3.381926000	0.995005000
6	-3.415818000	2.990056000	0.256010000
1	-3.124194000	4.036874000	0.395299000
1	-4.368879000	2.843881000	0.778159000
1	-3.594929000	2.825369000	-0.810147000
6	0.888137000	4.201646000	-0.983722000
1	1.721195000	3.496723000	-1.079470000
1	1.307007000	5.194654000	-0.782686000
1	0.364550000	4.251869000	-1.942207000
6	0.715271000	3.904237000	1.510408000
1	0.103205000	3.629893000	2.371932000
1	1.052804000	4.937337000	1.654643000
1	1.593625000	3.251815000	1.504416000
6	-2.237908000	2.213737000	2.355445000
1	-1.476493000	1.565834000	2.795763000
1	-3.197736000	1.975037000	2.828089000
1	-1.999070000	3.250978000	2.611368000
1	-0.295903000	-1.113399000	-1.897609000
1	-0.932380000	-1.094955000	0.056913000
6	-3.076512000	-2.370874000	1.040357000
6	-3.465180000	-1.329607000	-1.091273000
6	-4.934739000	-1.719950000	-0.988821000
8	-5.354202000	-1.794699000	0.378822000
6	-4.557512000	-2.733119000	1.108351000
1	-2.488673000	-3.135602000	1.561434000
1	-3.148366000	-1.315847000	-2.136919000
1	-5.099927000	-2.691780000	-1.479949000
1	-4.711620000	-3.744754000	0.701070000
7	-2.646859000	-2.296931000	-0.357689000
1	-5.568572000	-0.967948000	-1.466206000
1	-3.343340000	-0.310156000	-0.684658000
1	-2.915278000	-1.408056000	1.563578000
1	-4.914649000	-2.707784000	2.141260000
6	-1.212219000	-2.057470000	-0.463825000
8	-0.787806000	-2.008148000	-1.788031000
1	-0.715547000	-2.863383000	0.093600000
1	1.802931000	1.415444000	0.213202000

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### 18-Fe-PNP

26	-0.009276000	0.102452000	-0.243162000
15	-2.239058000	-0.138191000	-0.227068000
15	2.229398000	-0.085965000	-0.202577000
8	-0.000074000	2.949813000	0.338647000
7	0.009747000	-1.602852000	-1.053329000

6	-1.159413000	-2.488087000	-1.141137000
1	-1.174142000	-3.175603000	-0.276766000
1	-1.082043000	-3.132443000	-2.033025000
6	1.213094000	-2.433788000	-1.185299000
1	1.142206000	-3.064312000	-2.087684000
1	1.284438000	-3.134563000	-0.334749000
6	-3.413628000	1.030472000	-1.124916000
1	-3.124148000	0.865644000	-2.171751000
6	2.996571000	-0.473424000	1.463463000
1	4.084577000	-0.482441000	1.321731000
6	2.478259000	-1.582032000	-1.267149000
1	2.600559000	-1.201914000	-2.287632000
1	3.378833000	-2.148267000	-1.009400000
6	3.376474000	1.157965000	-1.026036000
1	2.882888000	1.300617000	-1.997396000
6	-2.467776000	-1.699129000	-1.203415000
1	-3.323142000	-2.288154000	-0.856348000
1	-2.668984000	-1.392164000	-2.235235000
6	-2.915378000	0.731992000	2.366929000
1	-1.867689000	1.023243000	2.498002000
1	-3.329000000	0.488941000	3.352917000
1	-3.465248000	1.595445000	1.982869000
6	-2.380192000	-1.725039000	2.090003000
1	-2.522041000	-2.628361000	1.489766000
1	-2.837348000	-1.903375000	3.070608000
1	-1.305816000	-1.573181000	2.233308000
6	-3.022178000	-0.488397000	1.438752000
1	-4.079797000	-0.709593000	1.250268000
6	-0.010935000	1.808539000	0.059893000
6	-3.195661000	2.522028000	-0.826244000
1	-3.411600000	2.770569000	0.217086000
1	-3.870700000	3.118801000	-1.451531000
1	-2.173018000	2.835876000	-1.041288000
6	-4.894945000	0.645297000	-0.971122000
1	-5.075193000	-0.415806000	-1.171511000
1	-5.502995000	1.225954000	-1.674757000
1	-5.259138000	0.868882000	0.037451000
6	4.797930000	0.623779000	-1.278355000
1	5.329676000	0.445686000	-0.337187000
1	5.373622000	1.368093000	-1.841641000
1	4.806964000	-0.305000000	-1.855094000
6	2.553741000	-1.860550000	1.961160000
1	1.461572000	-1.917772000	2.022799000
1	2.959720000	-2.038686000	2.963947000
1	2.905745000	-2.668536000	1.313935000
6	2.629986000	0.598186000	2.506111000

1	2.943340000	1.602401000	2.212987000
1	3.112969000	0.362700000	3.462007000
1	1.546698000	0.617203000	2.660852000
6	3.442345000	2.524801000	-0.323650000
1	2.456540000	2.916201000	-0.066597000
1	3.932434000	3.249292000	-0.984782000
1	4.040312000	2.468420000	0.591660000
1	-0.022375000	0.020571000	1.229242000

-1605.938171

### TS9-Fe-PNP

26	0.000008000	0.099468000	-0.214731000
15	-2.227188000	-0.138300000	-0.199951000
15	2.227191000	-0.138293000	-0.199955000
8	-0.000037000	2.796995000	0.850155000
7	0.000003000	-1.835328000	-1.029377000
6	-1.198892000	-2.618879000	-0.780567000
1	-1.205125000	-2.996214000	0.259855000
1	-1.222248000	-3.511243000	-1.432548000
6	1.198945000	-2.618871000	-0.780736000
1	1.222298000	-3.511148000	-1.432836000
1	1.205251000	-2.996352000	0.259634000
6	-3.269718000	0.978287000	-1.294568000
1	-2.785414000	0.826151000	-2.269194000
6	3.107674000	-0.234332000	1.451511000
1	4.182792000	-0.218441000	1.234355000
6	2.460086000	-1.788560000	-1.024496000
1	2.571346000	-1.585327000	-2.095860000
1	3.363738000	-2.305192000	-0.687073000
6	3.269717000	0.978356000	-1.294512000
1	2.785448000	0.826226000	-2.269157000
6	-2.460058000	-1.788619000	-1.024389000
1	-3.363714000	-2.305231000	-0.686952000
1	-2.571287000	-1.585461000	-2.095771000
6	-2.748607000	0.974905000	2.332198000
1	-1.679587000	0.965056000	2.565896000
1	-3.307653000	0.925645000	3.274165000
1	-2.979828000	1.931412000	1.857213000
6	-2.781286000	-1.539710000	2.196562000
1	-3.113441000	-2.428693000	1.652483000
1	-3.285616000	-1.539491000	3.170144000
1	-1.703829000	-1.625380000	2.371286000
6	-3.107674000	-0.234237000	1.451529000
1	-4.182792000	-0.218294000	1.234374000
6	-0.000009000	1.723406000	0.385343000

6	-3.158024000	2.471815000	-0.950478000
1	-3.669952000	2.707219000	-0.011905000
1	-3.635990000	3.065902000	-1.738383000
1	-2.119255000	2.798954000	-0.864516000
6	-4.742325000	0.550317000	-1.410644000
1	-4.852359000	-0.503328000	-1.684866000
1	-5.241094000	1.148875000	-2.182305000
1	-5.281628000	0.715713000	-0.471504000
6	4.742343000	0.550438000	-1.410547000
1	5.281614000	0.715867000	-0.471394000
1	5.241114000	1.149001000	-2.182202000
1	4.852421000	-0.503207000	-1.684748000
6	2.781204000	-1.539828000	2.196467000
1	1.703736000	-1.625465000	2.371149000
1	3.285502000	-1.539687000	3.170065000
1	3.113339000	-2.428791000	1.652341000
6	2.748670000	0.974811000	2.332203000
1	2.980069000	1.931305000	1.857273000
1	3.307620000	0.925444000	3.274221000
1	1.679627000	0.965090000	2.565800000
6	3.157953000	2.471871000	-0.950394000
1	2.119164000	2.798990000	-0.864588000
1	3.636034000	3.065985000	-1.738210000
1	3.669724000	2.707260000	-0.011732000
1	0.000007000	-0.581370000	-1.781707000
1	0.000028000	0.365601000	-1.900441000
1	-0.000022000	-0.360359000	1.226722000

-1607.088122

### 19-Fe-PNP

26	1.109532000	0.368525000	-0.043543000
15	1.747587000	-1.749039000	-0.165328000
15	0.079270000	2.331161000	-0.091020000
8	3.303720000	1.235575000	1.625429000
7	-0.518587000	-0.261456000	-1.285017000
6	-0.176096000	-1.444233000	-2.106885000
1	0.552673000	-1.115908000	-2.852425000
1	-1.061903000	-1.818143000	-2.641349000
6	-1.034432000	0.846466000	-2.120389000
1	-1.915391000	0.522941000	-2.695588000
1	-0.245408000	1.110593000	-2.829313000
6	1.658417000	-2.802472000	1.391510000
1	0.582024000	-2.766796000	1.603255000
6	0.888380000	3.861332000	-0.825166000
1	0.147524000	4.667842000	-0.758714000

6	-1.372773000	2.039562000	-1.229606000
1	-2.241783000	1.809303000	-0.605490000
1	-1.624403000	2.922227000	-1.824786000
6	-0.792019000	2.913110000	1.469821000
1	-1.522371000	2.103796000	1.606167000
6	0.423237000	-2.535159000	-1.222137000
1	0.802311000	-3.367632000	-1.822897000
1	-0.341825000	-2.939839000	-0.550601000
6	4.566364000	-1.654072000	-0.305229000
1	4.525736000	-0.560225000	-0.321991000
1	5.486572000	-1.966486000	-0.813382000
1	4.641018000	-1.972173000	0.738017000
6	3.342546000	-1.860103000	-2.503479000
1	2.560565000	-2.375378000	-3.069979000
1	4.304659000	-2.127519000	-2.956902000
1	3.193168000	-0.781690000	-2.617409000
6	3.344522000	-2.256649000	-1.018053000
1	3.399045000	-3.350481000	-0.956796000
6	2.414308000	0.882583000	0.942546000
6	2.367125000	-2.166303000	2.597078000
1	3.455773000	-2.172771000	2.483661000
1	2.129909000	-2.733128000	3.505720000
1	2.042950000	-1.132969000	2.740127000
6	2.067623000	-4.271487000	1.205092000
1	1.575623000	-4.735500000	0.343363000
1	1.795465000	-4.849782000	2.096240000
1	3.150495000	-4.369535000	1.071605000
6	-1.555279000	4.239245000	1.331260000
1	-0.867277000	5.088024000	1.251960000
1	-2.178583000	4.405855000	2.218165000
1	-2.213096000	4.252553000	0.455211000
6	1.239134000	3.650322000	-2.307492000
1	1.907745000	2.792305000	-2.428040000
1	1.742899000	4.543155000	-2.697061000
1	0.352941000	3.478817000	-2.926409000
6	2.142437000	4.267061000	-0.034085000
1	1.923971000	4.488507000	1.013883000
1	2.587608000	5.166387000	-0.476509000
1	2.893137000	3.471067000	-0.061230000
6	0.115958000	2.905860000	2.708598000
1	0.639185000	1.951020000	2.801727000
1	-0.487977000	3.060903000	3.611045000
1	0.861184000	3.706820000	2.674089000
1	-1.273285000	-0.531440000	-0.640251000
1	0.254097000	-0.019501000	1.201390000
1	-3.719998000	-1.176947000	3.241257000

1	-1.973400000	-0.284410000	2.116412000
6	-3.485479000	-2.391804000	-0.034172000
6	-4.133871000	-0.145745000	0.567198000
6	-4.715511000	0.031761000	-0.833285000
8	-5.153649000	-1.218442000	-1.370313000
6	-4.074350000	-2.156055000	-1.421692000
1	-2.632859000	-3.075920000	-0.106354000
1	-3.759303000	0.814898000	0.938995000
1	-3.965566000	0.477668000	-1.503529000
1	-3.296814000	-1.782645000	-2.105839000
7	-3.026995000	-1.114257000	0.535658000
1	-5.591102000	0.685093000	-0.803941000
1	-4.942153000	-0.480188000	1.239363000
1	-4.245572000	-2.863786000	0.607581000
1	-4.484270000	-3.083701000	-1.828771000
6	-2.354344000	-1.263134000	1.809803000
8	-3.144827000	-1.852060000	2.857490000
1	-1.505559000	-1.935138000	1.673818000
1	1.852666000	0.705269000	-1.382882000

-2009.363739

### 20-Fe-PNP

26	0.105564000	-0.753353000	-0.149378000
15	-2.115439000	-1.017389000	-0.320578000
15	2.312248000	-0.428874000	-0.382794000
8	0.309507000	-1.969849000	2.473827000
7	-0.066424000	0.322397000	-1.711694000
6	-1.249190000	0.270435000	-2.582114000
1	-1.134866000	-0.536813000	-3.326746000
1	-1.337844000	1.206427000	-3.159905000
6	1.073422000	0.762440000	-2.523383000
1	0.851201000	1.739426000	-2.987279000
1	1.236444000	0.063835000	-3.362776000
6	-3.270633000	-0.319010000	0.987053000
1	-2.941702000	0.729113000	1.009809000
6	3.295788000	-1.881119000	-1.039159000
1	4.348492000	-1.572752000	-1.058818000
6	2.350046000	0.880329000	-1.692551000
1	2.358730000	1.833052000	-1.153412000
1	3.251756000	0.841476000	-2.311309000
6	3.361816000	0.360912000	0.963443000
1	2.753830000	1.238631000	1.221893000
6	-2.530042000	0.058045000	-1.776144000
1	-3.339894000	-0.355992000	-2.384218000
1	-2.881828000	1.010841000	-1.370738000

6	-2.282052000	-3.760600000	0.293654000
1	-1.189351000	-3.810836000	0.333326000
1	-2.662263000	-4.753231000	0.025101000
1	-2.645519000	-3.525508000	1.296929000
6	-2.231652000	-3.143636000	-2.153215000
1	-2.612939000	-2.491150000	-2.943900000
1	-2.566315000	-4.163674000	-2.375263000
1	-1.137316000	-3.127834000	-2.193181000
6	-2.729651000	-2.730032000	-0.756781000
1	-3.825382000	-2.682074000	-0.774077000
6	0.218398000	-1.437744000	1.424462000
6	-3.071269000	-0.893174000	2.397753000
1	-3.413198000	-1.930709000	2.466738000
1	-3.661397000	-0.308264000	3.113143000
1	-2.029643000	-0.853960000	2.718974000
6	-4.754381000	-0.364654000	0.583868000
1	-4.936237000	0.063856000	-0.406506000
1	-5.349509000	0.206472000	1.306385000
1	-5.136261000	-1.391571000	0.585371000
6	4.734842000	0.856285000	0.476181000
1	5.384625000	0.019280000	0.198675000
1	5.234388000	1.403223000	1.284685000
1	4.661827000	1.530132000	-0.381977000
6	2.859122000	-2.233109000	-2.472321000
1	1.789999000	-2.469469000	-2.503405000
1	3.412099000	-3.114416000	-2.817815000
1	3.054974000	-1.422698000	-3.179710000
6	3.141951000	-3.110138000	-0.125413000
1	3.482189000	-2.925638000	0.895860000
1	3.729426000	-3.944162000	-0.527045000
1	2.092549000	-3.417875000	-0.080468000
6	3.518102000	-0.487770000	2.235500000
1	2.571993000	-0.904492000	2.584168000
1	3.928782000	0.134487000	3.039192000
1	4.218054000	-1.314014000	2.076521000
1	-0.800768000	1.906915000	-0.377422000
1	-0.367035000	1.118118000	2.593241000
1	0.125661000	-0.635941000	4.033764000
1	1.297948000	1.276107000	3.211413000
6	-2.020084000	3.561415000	-0.158285000
6	0.220267000	3.293260000	0.700956000
6	0.727556000	4.219343000	-0.408779000
8	-0.288074000	5.148466000	-0.809484000
6	-1.467044000	4.467551000	-1.260471000
1	-2.897193000	3.017576000	-0.527064000
1	0.980713000	2.540322000	0.932766000

1	1.034543000	3.623451000	-1.283929000
1	-1.224932000	3.866572000	-2.153658000
7	-1.023832000	2.606053000	0.338927000
1	1.581223000	4.817703000	-0.075117000
1	0.047661000	3.883273000	1.610907000
1	-2.351172000	4.186835000	0.682002000
1	-2.183624000	5.245270000	-1.542734000
6	0.238448000	1.244492000	3.498699000
8	-0.012684000	0.220504000	4.466089000
1	-0.023581000	2.198715000	3.963007000
1	0.283098000	-2.140154000	-0.602817000

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### 21-Fe-PNP

26	-1.123383000	0.152913000	0.003593000
15	-1.219187000	-2.060002000	0.187692000
15	-0.661813000	2.319675000	0.028101000
8	-3.539722000	0.403118000	-1.561568000
7	0.655720000	-0.030457000	1.175295000
6	0.667664000	-1.245900000	2.023106000
1	-0.075864000	-1.087753000	2.808267000
1	1.649711000	-1.373613000	2.502271000
6	0.948618000	1.192526000	1.957197000
1	1.923162000	1.110011000	2.461577000
1	0.177999000	1.267045000	2.728645000
6	-0.981262000	-3.123555000	-1.340940000
1	0.038872000	-2.845480000	-1.628613000
6	-1.792626000	3.561522000	0.872844000
1	-1.326043000	4.546166000	0.743812000
6	0.906252000	2.412650000	1.039699000
1	1.748499000	2.391101000	0.339335000
1	0.987271000	3.341469000	1.612230000
6	-0.109954000	3.141052000	-1.570871000
1	0.777743000	2.539700000	-1.809353000
6	0.311827000	-2.467863000	1.178062000
1	0.182342000	-3.354300000	1.806623000
1	1.115074000	-2.680427000	0.464298000
6	-3.976283000	-2.553388000	0.531795000
1	-4.160751000	-1.474518000	0.546107000
1	-4.773990000	-3.042598000	1.103803000
1	-4.055911000	-2.894168000	-0.503889000
6	-2.594140000	-2.469477000	2.638886000
1	-1.683745000	-2.794254000	3.152405000
1	-3.443353000	-2.932379000	3.156113000
1	-2.677776000	-1.382810000	2.740883000

6	-2.608872000	-2.876606000	1.156643000
1	-2.435552000	-3.958097000	1.097656000
6	-2.557009000	0.299952000	-0.925514000
6	-1.905261000	-2.730189000	-2.503870000
1	-2.949328000	-2.996931000	-2.310599000
1	-1.596549000	-3.259741000	-3.413740000
1	-1.856903000	-1.656285000	-2.699666000
6	-1.013366000	-4.638472000	-1.084737000
1	-0.370001000	-4.932625000	-0.248370000
1	-0.662727000	-5.172173000	-1.976516000
1	-2.029076000	-4.990888000	-0.872247000
6	0.315630000	4.610788000	-1.430093000
1	-0.549361000	5.261860000	-1.262295000
1	0.803887000	4.948058000	-2.352375000
1	1.019513000	4.763831000	-0.605020000
6	-1.914081000	3.281243000	2.380112000
1	-2.287731000	2.267558000	2.556266000
1	-2.616834000	3.992425000	2.830608000
1	-0.959723000	3.390123000	2.904724000
6	-3.186748000	3.578421000	0.224042000
1	-3.154594000	3.834962000	-0.837960000
1	-3.820543000	4.320186000	0.724687000
1	-3.670591000	2.601268000	0.319751000
6	-1.103597000	2.949870000	-2.726847000
1	-1.397273000	1.902015000	-2.825964000
1	-0.640706000	3.269247000	-3.668494000
1	-2.008162000	3.550691000	-2.589830000
1	1.385331000	-0.137993000	0.470400000
1	-0.208193000	0.011116000	-1.270420000
6	4.456948000	-1.616552000	-0.056187000
6	4.144917000	0.623881000	-1.061003000
6	4.565730000	1.221337000	0.280468000
8	5.473750000	0.356285000	0.964078000
6	4.871462000	-0.913107000	1.233548000
1	3.897007000	-2.527570000	0.161803000
1	3.384219000	1.248588000	-1.538168000
1	3.683901000	1.402367000	0.911597000
1	3.998220000	-0.777380000	1.889741000
7	3.608306000	-0.726444000	-0.856000000
1	5.085806000	2.169338000	0.125180000
1	5.019079000	0.572906000	-1.724181000
1	5.348889000	-1.886398000	-0.638329000
1	5.618121000	-1.508370000	1.764012000
6	2.658683000	-1.241677000	-1.679773000
8	2.346447000	-2.434060000	-1.728329000
1	2.149192000	-0.478324000	-2.288680000

1 -1.878762000 0.289027000 1.363703000

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**TS10-Fe-PNP**

26	0.055562000	-0.849695000	0.025380000
15	-2.161481000	-0.876070000	-0.202303000
15	2.260007000	-0.669693000	-0.145690000
8	0.110462000	-2.824783000	2.136051000
7	0.010360000	0.608993000	-1.491635000
6	-1.197582000	0.555469000	-2.351268000
1	-1.096445000	-0.322428000	-2.993873000
1	-1.246333000	1.442517000	-3.000146000
6	1.235186000	0.662731000	-2.328821000
1	1.223927000	1.553188000	-2.974736000
1	1.209395000	-0.215453000	-2.979268000
6	-3.263029000	-0.282602000	1.191828000
1	-2.786567000	0.673544000	1.442817000
6	3.289877000	-2.102958000	-0.789456000
1	4.321039000	-1.732679000	-0.848930000
6	2.489637000	0.638972000	-1.457643000
1	2.622140000	1.605951000	-0.963519000
1	3.382669000	0.467071000	-2.066845000
6	3.249182000	0.047418000	1.283132000
1	2.845353000	1.066480000	1.332446000
6	-2.450405000	0.445992000	-1.488055000
1	-3.336503000	0.259457000	-2.102256000
1	-2.620285000	1.385312000	-0.952765000
6	-2.677841000	-3.643279000	-0.061037000
1	-1.601597000	-3.841931000	-0.077008000
1	-3.192826000	-4.519330000	-0.473340000
1	-2.985561000	-3.535765000	0.981969000
6	-2.603824000	-2.656035000	-2.374628000
1	-2.917028000	-1.846743000	-3.040991000
1	-3.084466000	-3.575250000	-2.730290000
1	-1.519646000	-2.778842000	-2.463563000
6	-2.998910000	-2.402420000	-0.910508000
1	-4.078172000	-2.206316000	-0.876875000
6	0.088206000	-2.019136000	1.282133000
6	-3.183030000	-1.153568000	2.455860000
1	-3.762924000	-2.076814000	2.349370000
1	-3.602814000	-0.600822000	3.304616000
1	-2.153072000	-1.418430000	2.706587000
6	-4.724602000	-0.021493000	0.793651000
1	-4.813927000	0.635737000	-0.077011000
1	-5.251174000	0.461358000	1.626117000

1	-5.255622000	-0.953884000	0.570659000
6	4.761463000	0.155042000	1.037611000
1	5.235967000	-0.832022000	1.031159000
1	5.228510000	0.737438000	1.840725000
1	4.992521000	0.649945000	0.088266000
6	2.859794000	-2.531750000	-2.201524000
1	1.805413000	-2.823709000	-2.214512000
1	3.463166000	-3.389438000	-2.521883000
1	3.005131000	-1.736739000	-2.939352000
6	3.239165000	-3.298539000	0.175321000
1	3.648207000	-3.057795000	1.160258000
1	3.825952000	-4.130639000	-0.231516000
1	2.209599000	-3.645659000	0.310296000
6	2.932378000	-0.611130000	2.634830000
1	1.854107000	-0.699067000	2.789762000
1	3.347251000	-0.002225000	3.446837000
1	3.370990000	-1.610370000	2.717334000
1	-0.051166000	1.467959000	-0.922725000
1	-0.022397000	0.355599000	1.020940000
6	-1.311148000	3.591517000	0.500199000
6	1.114615000	3.591836000	0.589078000
6	1.135929000	4.276518000	-0.773532000
8	-0.033852000	5.074583000	-0.964993000
6	-1.224093000	4.286210000	-0.854812000
1	-2.191702000	2.948596000	0.545270000
1	1.995639000	2.955178000	0.701445000
1	1.202428000	3.523952000	-1.574588000
1	-1.247639000	3.542509000	-1.667095000
7	-0.105992000	2.781406000	0.713126000
1	1.993289000	4.949094000	-0.852515000
1	1.150142000	4.358267000	1.379965000
1	-1.412496000	4.343795000	1.298181000
1	-2.064130000	4.972103000	-0.987200000
6	-0.143721000	1.905034000	1.824312000
8	-1.147750000	1.798779000	2.543246000
1	0.862412000	1.685000000	2.202495000
1	0.111813000	-1.933577000	-1.079600000

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### 22-Fe-PNP

26	0.248365000	-0.796951000	0.037321000
15	-1.920184000	-1.319823000	-0.192376000
15	2.380698000	-0.129962000	-0.176943000
8	0.801739000	-2.759519000	2.094569000
7	-0.124434000	0.604583000	-1.508132000

6	-1.306528000	0.289535000	-2.351262000
1	-1.025921000	-0.535790000	-3.010673000
1	-1.560967000	1.150213000	-2.986076000
6	1.052275000	0.912884000	-2.359953000
1	0.838251000	1.777428000	-3.004392000
1	1.216624000	0.048418000	-3.008422000
6	-3.068973000	-0.982671000	1.241606000
1	-2.743774000	0.018590000	1.559194000
6	3.646958000	-1.353254000	-0.815759000
1	4.591824000	-0.801138000	-0.884716000
6	2.290504000	1.177620000	-1.504016000
1	2.204790000	2.148383000	-1.006890000
1	3.194525000	1.206235000	-2.119880000
6	3.198251000	0.783348000	1.246008000
1	2.650543000	1.733508000	1.247245000
6	-2.496581000	-0.102820000	-1.478902000
1	-3.322222000	-0.487982000	-2.083463000
1	-2.871413000	0.772983000	-0.943599000
6	-1.622703000	-4.119901000	-0.075589000
1	-0.544286000	-4.045289000	-0.245031000
1	-1.957355000	-5.103671000	-0.424688000
1	-1.796279000	-4.069734000	1.001252000
6	-2.028989000	-3.149736000	-2.357516000
1	-2.606724000	-2.462017000	-2.981454000
1	-2.260246000	-4.167816000	-2.691357000
1	-0.963057000	-2.972367000	-2.537042000
6	-2.355707000	-3.017024000	-0.859882000
1	-3.438575000	-3.133645000	-0.725358000
6	0.571084000	-1.951497000	1.284149000
6	-2.833072000	-1.924332000	2.433952000
1	-3.206722000	-2.933964000	2.232525000
1	-3.375944000	-1.542772000	3.306211000
1	-1.776595000	-1.992452000	2.705040000
6	-4.558859000	-0.943781000	0.863686000
1	-4.773678000	-0.231472000	0.061553000
1	-5.148402000	-0.641738000	1.737511000
1	-4.921745000	-1.929082000	0.549539000
6	4.687617000	1.094308000	1.030900000
1	5.297651000	0.186815000	1.091865000
1	5.037277000	1.778133000	1.812864000
1	4.878085000	1.569904000	0.062866000
6	3.284177000	-1.862949000	-2.220090000
1	2.300974000	-2.343505000	-2.219170000
1	4.027780000	-2.601193000	-2.541898000
1	3.276215000	-1.062001000	-2.965248000
6	3.821274000	-2.528683000	0.158282000

1	4.127847000	-2.204308000	1.156157000
1	4.591935000	-3.210233000	-0.219766000
1	2.889208000	-3.093405000	0.256185000
6	2.942043000	0.118147000	2.608037000
1	1.873745000	-0.029421000	2.786227000
1	3.334818000	0.758072000	3.406538000
1	3.436902000	-0.854098000	2.690949000
1	-0.346640000	1.446063000	-0.929587000
1	-0.232878000	0.601233000	1.202759000
6	-2.072486000	3.070751000	0.489632000
6	0.212246000	3.770551000	0.561123000
6	-0.001572000	4.559574000	-0.728103000
8	-1.362861000	4.974397000	-0.865769000
6	-2.258096000	3.857512000	-0.803667000
1	-2.747129000	2.212828000	0.515832000
1	1.253836000	3.437185000	0.607040000
1	0.285155000	3.939785000	-1.593969000
1	-2.090490000	3.203830000	-1.675515000
7	-0.683416000	2.609404000	0.580141000
1	0.602728000	5.470760000	-0.734182000
1	0.035049000	4.429601000	1.429979000
1	-2.338775000	3.706762000	1.348156000
1	-3.268448000	4.270717000	-0.866801000
6	-0.436673000	1.674524000	1.740925000
8	-1.371219000	1.570307000	2.639192000
1	0.587200000	1.905826000	2.102748000
1	0.536632000	-1.868693000	-0.970979000

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### TS11-Fe-PNP

26	0.548447000	-0.654037000	-0.007521000
15	-1.255237000	-1.955717000	-0.239133000
15	2.289761000	0.738815000	-0.186141000
8	1.636224000	-2.127836000	2.246196000
7	-0.236978000	0.408726000	-1.441810000
6	-1.263831000	-0.173992000	-2.320133000
1	-0.781984000	-0.752016000	-3.128304000
1	-1.834417000	0.624606000	-2.826464000
6	0.608912000	1.273227000	-2.279820000
1	-0.004433000	2.046880000	-2.774855000
1	1.058213000	0.681129000	-3.096204000
6	-2.493605000	-2.098816000	1.168269000
1	-2.918543000	-1.087535000	1.198650000
6	3.884123000	0.027112000	-0.862654000
1	4.589071000	0.863121000	-0.944628000

6	1.718724000	1.948790000	-1.472534000
1	1.332120000	2.823463000	-0.941409000
1	2.536161000	2.294523000	-2.113116000
6	2.771524000	1.869942000	1.238528000
1	1.925834000	2.569656000	1.264245000
6	-2.231407000	-1.080329000	-1.556070000
1	-2.743582000	-1.781354000	-2.222628000
1	-3.003925000	-0.489262000	-1.056931000
6	-0.201046000	-4.552971000	0.073396000
1	0.787034000	-4.119168000	0.256957000
1	-0.059446000	-5.555083000	-0.347897000
1	-0.706909000	-4.668144000	1.035788000
6	-0.314727000	-3.645691000	-2.284589000
1	-0.905178000	-3.106206000	-3.030878000
1	-0.173610000	-4.669077000	-2.651608000
1	0.667174000	-3.167120000	-2.214809000
6	-1.002118000	-3.684567000	-0.909255000
1	-2.002890000	-4.115510000	-1.036557000
6	1.169138000	-1.498350000	1.375874000
6	-1.843093000	-2.342563000	2.539000000
1	-1.317364000	-3.300611000	2.584749000
1	-2.618998000	-2.351046000	3.313235000
1	-1.131284000	-1.552455000	2.787674000
6	-3.636786000	-3.088597000	0.893708000
1	-4.106409000	-2.921708000	-0.081619000
1	-4.411883000	-2.979563000	1.661016000
1	-3.282959000	-4.124615000	0.929281000
6	4.050925000	2.682045000	0.983165000
1	4.941058000	2.045230000	1.024187000
1	4.161772000	3.451329000	1.756188000
1	4.036005000	3.185212000	0.010698000
6	3.673215000	-0.562508000	-2.267685000
1	2.923202000	-1.359209000	-2.247393000
1	4.616450000	-0.987685000	-2.630218000
1	3.351717000	0.192010000	-2.991517000
6	4.462481000	-1.031367000	0.089274000
1	4.699482000	-0.621588000	1.074998000
1	5.388501000	-1.441964000	-0.329881000
1	3.754724000	-1.855308000	0.223903000
6	2.809331000	1.161071000	2.600831000
1	1.858797000	0.671417000	2.824690000
1	3.007193000	1.895424000	3.390386000
1	3.596816000	0.403334000	2.648577000
1	-1.171237000	1.617430000	-0.267584000
1	-0.650666000	0.576908000	1.623559000
6	-3.106369000	2.007803000	0.427717000

6	-1.320143000	3.638803000	0.276367000
6	-1.974815000	4.194405000	-0.987916000
8	-3.390022000	3.996804000	-0.957377000
6	-3.719425000	2.610208000	-0.834594000
1	-3.314508000	0.938091000	0.487799000
1	-0.234354000	3.752875000	0.227747000
1	-1.549192000	3.706540000	-1.879484000
1	-3.368930000	2.066505000	-1.726073000
7	-1.648013000	2.211343000	0.456199000
1	-1.808049000	5.271696000	-1.066156000
1	-1.683242000	4.179399000	1.157432000
1	-3.521609000	2.472671000	1.326533000
1	-4.809904000	2.549271000	-0.796198000
6	-0.997638000	1.549412000	2.059357000
8	-1.885981000	1.532176000	2.961863000
1	-0.155774000	2.265604000	2.130842000
1	1.315417000	-1.647636000	-0.769690000

-2008.159419

### 23-Fe-PNP

26	0.304016000	-0.822804000	-0.033618000
15	-1.841674000	-1.416522000	-0.301952000
15	2.421280000	-0.099257000	-0.128177000
8	0.627576000	-2.237978000	2.481472000
7	0.028039000	0.293159000	-1.560912000
6	-1.131310000	0.134874000	-2.448973000
1	-0.905575000	-0.605091000	-3.236920000
1	-1.339139000	1.081018000	-2.977952000
6	1.136680000	0.827846000	-2.363619000
1	0.817066000	1.741169000	-2.894718000
1	1.413284000	0.105952000	-3.152181000
6	-3.119042000	-1.032829000	1.020239000
1	-2.938592000	0.035158000	1.199111000
6	3.725603000	-1.334351000	-0.650330000
1	4.669651000	-0.782375000	-0.733011000
6	2.361023000	1.147465000	-1.504082000
1	2.250992000	2.133015000	-1.041833000
1	3.284386000	1.162847000	-2.091608000
6	3.170218000	0.903459000	1.278329000
1	2.594062000	1.835556000	1.219233000
6	-2.379269000	-0.294359000	-1.678216000
1	-3.129962000	-0.753698000	-2.328648000
1	-2.845278000	0.575387000	-1.206480000
6	-1.563680000	-4.193061000	0.076780000
1	-0.478524000	-4.065611000	0.140271000

1	-1.771026000	-5.207285000	-0.284285000
1	-1.971454000	-4.109115000	1.086612000
6	-1.586151000	-3.372475000	-2.307294000
1	-2.058085000	-2.727041000	-3.053351000
1	-1.747672000	-4.411015000	-2.619227000
1	-0.508085000	-3.179055000	-2.316142000
6	-2.163133000	-3.162795000	-0.895967000
1	-3.251675000	-3.292979000	-0.939013000
6	0.481200000	-1.619110000	1.495207000
6	-2.893605000	-1.750393000	2.359942000
1	-3.122106000	-2.818362000	2.289710000
1	-3.563756000	-1.321387000	3.113582000
1	-1.870356000	-1.640930000	2.723619000
6	-4.571625000	-1.211152000	0.546241000
1	-4.779444000	-0.683196000	-0.389279000
1	-5.256212000	-0.818274000	1.307364000
1	-4.816398000	-2.269132000	0.401555000
6	4.653864000	1.247614000	1.069302000
1	5.287816000	0.363624000	1.196808000
1	4.970571000	1.988551000	1.812519000
1	4.848782000	1.666438000	0.076374000
6	3.388379000	-1.925854000	-2.029816000
1	2.411413000	-2.418928000	-2.012155000
1	4.145587000	-2.669255000	-2.305403000
1	3.372804000	-1.163867000	-2.814647000
6	3.878364000	-2.447278000	0.398759000
1	4.215656000	-2.064238000	1.366040000
1	4.617515000	-3.181741000	0.058157000
1	2.925967000	-2.965880000	0.549971000
6	2.917663000	0.314450000	2.674450000
1	1.850529000	0.193689000	2.871379000
1	3.327992000	0.989774000	3.434509000
1	3.395089000	-0.660818000	2.806161000
1	-0.526980000	1.863588000	-0.189750000
1	-0.656141000	0.731621000	2.124157000
6	-2.163522000	3.081987000	0.159849000
6	0.147460000	3.728766000	0.398583000
6	0.052596000	4.486956000	-0.928175000
8	-1.286406000	4.940632000	-1.156694000
6	-2.222465000	3.854446000	-1.159118000
1	-2.843018000	2.225543000	0.136068000
1	1.161561000	3.346732000	0.548586000
1	0.366786000	3.832042000	-1.757385000
1	-1.999224000	3.179033000	-2.000978000
7	-0.806649000	2.617520000	0.454832000
1	0.686423000	5.378521000	-0.925257000

1	-0.073735000	4.415855000	1.225371000
1	-2.490060000	3.727225000	0.984362000
1	-3.209642000	4.298150000	-1.317163000
6	-1.014086000	1.670061000	2.580262000
8	-2.183952000	1.812121000	2.939161000
1	-0.225061000	2.382328000	2.878168000
1	0.726314000	-2.132507000	-0.559361000

-2008.167384

#### 24-Fe-PNP

8	-0.000789000	-3.257665000	-0.706595000
6	-0.000226000	-2.856977000	0.579266000
1	0.895459000	-3.137883000	1.170255000
1	-0.894679000	-3.139422000	1.171426000
26	0.000024000	0.100557000	0.044860000
15	2.243047000	0.016460000	-0.161977000
15	-2.243004000	0.016382000	-0.161635000
8	0.000303000	1.575910000	2.540065000
7	-0.000039000	-0.859539000	-1.800194000
6	1.214602000	-0.645069000	-2.624279000
1	1.183006000	0.377461000	-3.012874000
1	1.210989000	-1.328211000	-3.486141000
6	-1.215115000	-0.646122000	-2.623936000
1	-1.211499000	-1.329797000	-3.485378000
1	-1.184213000	0.376166000	-3.013209000
6	3.185384000	-1.074632000	1.040612000
1	2.866757000	-2.076210000	0.726538000
6	-3.224830000	1.597153000	-0.338608000
1	-4.260726000	1.286688000	-0.522827000
6	-2.471278000	-0.868487000	-1.783410000
1	-2.576776000	-1.934369000	-1.557609000
1	-3.371038000	-0.541914000	-2.313881000
6	-3.185360000	-1.073826000	1.041773000
1	-2.866814000	-2.075637000	0.728338000
6	2.471241000	-0.867226000	-1.784434000
1	3.370531000	-0.539581000	-2.315037000
1	2.577751000	-1.933201000	-1.559520000
6	3.176725000	2.439003000	0.947225000
1	2.151283000	2.741727000	1.179881000
1	3.774476000	3.348045000	0.814021000
1	3.577884000	1.905118000	1.812884000
6	2.745527000	2.420477000	-1.545112000
1	2.875783000	1.886211000	-2.490855000
1	3.327312000	3.347268000	-1.608436000
1	1.688114000	2.683698000	-1.442549000

6	3.225046000	1.597261000	-0.337875000
1	4.260790000	1.286769000	-0.522928000
6	0.000126000	0.943700000	1.557992000
6	2.723973000	-0.888713000	2.494523000
1	2.972557000	0.103479000	2.883007000
1	3.217013000	-1.629203000	3.134913000
1	1.643061000	-1.025453000	2.584070000
6	4.713754000	-0.993638000	0.903878000
1	5.045046000	-1.137501000	-0.130088000
1	5.180000000	-1.775036000	1.515035000
1	5.097902000	-0.029652000	1.254056000
6	-4.713725000	-0.992732000	0.904995000
1	-5.097686000	-0.028444400	1.254553000
1	-5.180081000	-1.773654000	1.516673000
1	-5.045052000	-1.137214000	-0.128871000
6	-2.745814000	2.419189000	-1.546846000
1	-1.688139000	2.681817000	-1.445416000
1	-3.327044000	3.346320000	-1.610320000
1	-2.877309000	1.884309000	-2.492068000
6	-3.175682000	2.440005000	0.945743000
1	-3.576195000	1.906822000	1.812143000
1	-3.773577000	3.348899000	0.812188000
1	-2.150080000	2.742945000	1.177400000
6	-2.724012000	-0.887043000	2.495574000
1	-1.643164000	-1.024100000	2.585317000
1	-3.217350000	-1.626939000	3.136424000
1	-2.972292000	0.105497000	2.883373000
1	0.000124000	-1.891581000	-1.476320000
1	-0.001257000	-1.691109000	0.726463000
1	0.000008000	1.436648000	-0.605684000

-1721.649093

### 25-Fe-PNP

8	0.002013000	-3.155454000	1.216105000
6	-0.000128000	-3.183083000	-0.196455000
1	-0.893278000	-3.691193000	-0.584321000
1	0.890868000	-3.693075000	-0.586720000
26	-0.000090000	0.113153000	-0.033021000
15	-2.234632000	0.064451000	0.159353000
15	2.234448000	0.064934000	0.159432000
8	0.000016000	0.883384000	-2.831881000
7	-0.000019000	-0.501798000	1.814109000
6	-1.192517000	-0.317561000	2.659447000
1	-1.215270000	0.708992000	3.061903000
1	-1.146316000	-0.988479000	3.533912000

6	1.192230000	-0.316483000	2.659571000
1	1.146291000	-0.987033000	3.534333000
1	1.214302000	0.710271000	3.061556000
6	-3.219348000	-1.149803000	-0.887526000
1	-2.924648000	-2.110533000	-0.445230000
6	3.157027000	1.690850000	0.123608000
1	4.211419000	1.456229000	0.312671000
6	2.473871000	-0.601861000	1.874714000
1	2.616610000	-1.683105000	1.779469000
1	3.359718000	-0.187133000	2.366176000
6	3.219035000	-1.149974000	-0.886787000
1	2.924017000	-2.110424000	-0.444083000
6	-2.473880000	-0.603321000	1.874274000
1	-3.360046000	-0.189407000	2.365847000
1	-2.615961000	-1.684607000	1.778466000
6	-3.028781000	2.369410000	-1.248563000
1	-1.980340000	2.584978000	-1.478542000
1	-3.578301000	3.317970000	-1.245978000
1	-3.434736000	1.754744000	-2.057064000
6	-2.660409000	2.620800000	1.243742000
1	-2.833747000	2.199946000	2.238389000
1	-3.194939000	3.576530000	1.190602000
1	-1.589135000	2.819242000	1.137921000
6	-3.157128000	1.690446000	0.124392000
1	-4.211622000	1.455807000	0.312827000
6	-0.000061000	0.512727000	-1.720185000
6	-2.789371000	-1.181892000	-2.362298000
1	-2.988768000	-0.234830000	-2.872448000
1	-3.346175000	-1.966130000	-2.888555000
1	-1.722840000	-1.397991000	-2.462650000
6	-4.742533000	-1.002707000	-0.742255000
1	-5.060534000	-0.982340000	0.305569000
1	-5.244351000	-1.848425000	-1.226663000
1	-5.101106000	-0.087614000	-1.225635000
6	4.742225000	-1.003151000	-0.741343000
1	5.101088000	-0.088384000	-1.225126000
1	5.243937000	-1.849227000	-1.225237000
1	5.060058000	-0.982321000	0.306523000
6	2.659890000	2.622046000	1.242067000
1	1.588801000	2.820974000	1.135263000
1	3.194947000	3.577474000	1.188841000
1	2.832182000	2.201641000	2.237088000
6	3.029341000	2.368884000	-1.249867000
1	3.435744000	1.753709000	-2.057750000
1	3.578790000	3.317486000	-1.247637000
1	1.981009000	2.584237000	-1.480539000

6	2.789268000	-1.182672000	-2.361614000
1	1.722675000	-1.398443000	-2.462019000
1	3.345870000	-1.967391000	-2.887366000
1	2.989104000	-0.235960000	-2.872240000
1	0.001052000	-2.178396000	1.486046000
1	0.000402000	-2.159222000	-0.624961000
1	-0.000161000	1.571891000	0.142031000

-1721.656336

### 1-Ru-PNP

44	-0.000014000	-0.181327000	-0.145744000
15	2.324125000	0.143959000	-0.193732000
15	-2.324085000	0.144081000	-0.193794000
8	-0.000028000	-3.015596000	0.893898000
7	0.000105000	1.949814000	-0.922832000
6	1.233097000	2.691227000	-0.558860000
1	1.184213000	2.881702000	0.516037000
1	1.261414000	3.661302000	-1.075697000
6	-1.232860000	2.691289000	-0.558873000
1	-1.261093000	3.661387000	-1.075670000
1	-1.183972000	2.881718000	0.516026000
6	3.391708000	-0.844005000	-1.382568000
1	2.865655000	-0.668092000	-2.330312000
6	-3.282564000	0.191335000	1.423482000
1	-4.346693000	0.209309000	1.158753000
6	-2.474231000	1.868067000	-0.904684000
1	-2.557013000	1.760007000	-1.992879000
1	-3.380254000	2.376832000	-0.561982000
6	-3.391519000	-0.843890000	-1.382764000
1	-2.865581000	-0.667645000	-2.330510000
6	2.474408000	1.867911000	-0.904625000
1	3.380465000	2.376616000	-0.561921000
1	2.557199000	1.759784000	-1.992813000
6	2.985356000	-1.068097000	2.256050000
1	1.926053000	-1.093724000	2.530013000
1	3.581071000	-1.054577000	3.176674000
1	3.215872000	-1.993655000	1.722911000
6	2.964730000	1.448574000	2.249319000
1	3.269023000	2.371528000	1.746368000
1	3.502064000	1.404245000	3.204115000
1	1.892471000	1.505236000	2.465251000
6	3.282285000	0.191161000	1.423713000
1	4.346480000	0.208757000	1.159228000
6	-0.000102000	-1.912137000	0.484742000
6	3.348833000	-2.354460000	-1.101891000

1	3.927985000	-2.611712000	-0.209029000
1	3.790654000	-2.899969000	-1.944075000
1	2.325079000	-2.713072000	-0.963015000
6	4.839112000	-0.345958000	-1.523689000
1	4.894245000	0.724839000	-1.743422000
1	5.334067000	-0.879216000	-2.344284000
1	5.420130000	-0.537550000	-0.615101000
6	-4.839063000	-0.346185000	-1.523648000
1	-5.419948000	-0.538189000	-0.615060000
1	-5.333942000	-0.879351000	-2.344348000
1	-4.894508000	0.724657000	-1.743078000
6	-2.964827000	1.448515000	2.249404000
1	-1.892615000	1.504835000	2.465655000
1	-3.502436000	1.404171000	3.204041000
1	-3.268722000	2.371661000	1.746568000
6	-2.986229000	-1.068145000	2.255685000
1	-3.217021000	-1.993542000	1.722376000
1	-3.582059000	-1.054544000	3.176230000
1	-1.926977000	-1.094203000	2.529802000
6	-3.348215000	-2.354394000	-1.102423000
1	-2.324351000	-2.712754000	-0.963744000
1	-3.789994000	-2.899830000	-1.944676000
1	-3.927177000	-2.612016000	-0.209551000
1	0.000104000	1.814418000	-1.933563000
1	-0.000054000	-0.632637000	-1.804009000
1	0.000158000	0.502304000	1.402771000

-1577.635325

## 2-Ru-PNP

44	-0.063823000	-0.242829000	-0.178190000
15	2.258333000	-0.307940000	0.146013000
15	-2.381970000	-0.050683000	0.137922000
8	-0.097324000	-1.137725000	-3.062243000
7	-0.033307000	0.424769000	1.985353000
6	1.178982000	-0.030553000	2.709733000
1	1.084280000	-1.110210000	2.849501000
1	1.226876000	0.438158000	3.703338000
6	-1.285423000	0.088862000	2.706289000
1	-1.286207000	0.550401000	3.704406000
1	-1.302395000	-0.996331000	2.834289000
6	3.360948000	0.896626000	-0.782969000
1	2.873852000	1.851462000	-0.546433000
6	-3.470575000	-1.580724000	0.081303000
1	-4.508505000	-1.233191000	0.151376000
6	-2.499282000	0.558609000	1.903219000

1	-2.513629000	1.654252000	1.863549000
1	-3.427780000	0.241234000	2.387393000
6	-3.336093000	1.290803000	-0.769869000
1	-2.750985000	2.178958000	-0.495198000
6	2.436549000	0.303237000	1.905367000
1	3.325895000	-0.106082000	2.393970000
1	2.566957000	1.390475000	1.857835000
6	2.872476000	-2.701498000	-1.201704000
1	1.806829000	-2.941728000	-1.270811000
1	3.439642000	-3.639543000	-1.228790000
1	3.143707000	-2.122167000	-2.087488000
6	2.786836000	-2.841629000	1.310332000
1	3.091404000	-2.407578000	2.267340000
1	3.287298000	-3.812873000	1.218217000
1	1.705865000	-3.015922000	1.334293000
6	3.162869000	-1.955168000	0.111999000
1	4.234249000	-1.727578000	0.169833000
6	-0.085166000	-0.786602000	-1.939217000
6	3.293960000	0.716125000	-2.307776000
1	3.846188000	-0.172527000	-2.630179000
1	3.752827000	1.580641000	-2.801739000
1	2.263398000	0.628776000	-2.662965000
6	4.816448000	0.956262000	-0.292237000
1	4.887259000	1.105561000	0.789811000
1	5.335539000	1.791436000	-0.777656000
1	5.363382000	0.041869000	-0.546348000
6	-4.784013000	1.488336000	-0.293054000
1	-5.422348000	0.650850000	-0.594421000
1	-5.201928000	2.395019000	-0.746883000
1	-4.856692000	1.597689000	0.793592000
6	-3.192349000	-2.525843000	1.261726000
1	-2.138712000	-2.823925000	1.275802000
1	-3.802270000	-3.430974000	1.157203000
1	-3.438984000	-2.075540000	2.228025000
6	-3.274513000	-2.328458000	-1.248483000
1	-3.495439000	-1.707662000	-2.120216000
1	-3.935518000	-3.202612000	-1.285082000
1	-2.240328000	-2.675342000	-1.336589000
6	-3.270167000	1.149376000	-2.298685000
1	-2.248515000	0.977337000	-2.647785000
1	-3.641491000	2.067125000	-2.770081000
1	-3.898677000	0.326168000	-2.653400000
1	0.017591000	1.439698000	1.902379000
1	0.014057000	1.423701000	-0.552816000
1	-0.150337000	-1.819690000	0.433008000
6	0.736033000	3.732345000	0.148747000

8	0.983259000	4.031531000	-0.953639000
8	0.514619000	3.506253000	1.277778000

-1766.231092

**TS1-Ru-PNP**

44	0.005109000	-0.269849000	-0.161216000
15	2.328568000	-0.189123000	0.152804000
15	-2.319630000	-0.215043000	0.163751000
8	0.004757000	-0.519976000	-3.171808000
7	0.005718000	-0.101924000	2.083788000
6	1.250884000	-0.633979000	2.693665000
1	1.234727000	-1.718900000	2.563596000
1	1.268159000	-0.419638000	3.771884000
6	-1.220125000	-0.675153000	2.695682000
1	-1.237152000	-0.471500000	3.776022000
1	-1.173479000	-1.757919000	2.555212000
6	3.242120000	1.338980000	-0.443536000
1	2.759106000	2.119253000	0.159638000
6	-3.408894000	-1.675847000	-0.279952000
1	-4.422994000	-1.418320000	0.050143000
6	-2.469000000	-0.094784000	2.026975000
1	-2.564015000	0.967166000	2.280844000
1	-3.369803000	-0.597413000	2.393277000
6	-3.250265000	1.318374000	-0.393652000
1	-2.798216000	2.084688000	0.250133000
6	2.478310000	-0.023921000	2.011567000
1	3.397181000	-0.484192000	2.388226000
1	2.533445000	1.046625000	2.240307000
6	3.369217000	-1.963867000	-1.770698000
1	2.345934000	-2.201365000	-2.080694000
1	4.001372000	-2.831075000	-1.995104000
1	3.723394000	-1.130353000	-2.382950000
6	3.038847000	-2.894326000	0.555513000
1	3.188118000	-2.745976000	1.629520000
1	3.663506000	-3.742726000	0.252177000
1	1.989935000	-3.159518000	0.387960000
6	3.424611000	-1.653306000	-0.265828000
1	4.447472000	-1.363682000	0.004609000
6	0.004759000	-0.422348000	-2.000480000
6	2.961880000	1.672220000	-1.917748000
1	3.434249000	0.954241000	-2.595260000
1	3.371075000	2.661989000	-2.152848000
1	1.888717000	1.686529000	-2.124598000
6	4.748105000	1.345221000	-0.136533000
1	4.961025000	1.114937000	0.912936000

1	5.165848000	2.335689000	-0.352109000
1	5.285011000	0.621595000	-0.759616000
6	-4.761846000	1.283122000	-0.119686000
1	-5.270153000	0.571099000	-0.779006000
1	-5.195992000	2.271850000	-0.309153000
1	-4.991045000	1.011625000	0.916465000
6	-2.968177000	-2.947852000	0.461956000
1	-1.929398000	-3.196990000	0.223296000
1	-3.606263000	-3.786874000	0.160279000
1	-3.052902000	-2.846375000	1.548582000
6	-3.418078000	-1.908078000	-1.799381000
1	-3.839655000	-1.060761000	-2.346675000
1	-4.023578000	-2.790216000	-2.038443000
1	-2.403420000	-2.082620000	-2.173042000
6	-2.942053000	1.713546000	-1.846751000
1	-1.864256000	1.768694000	-2.018819000
1	-3.375977000	2.698276000	-2.057850000
1	-3.370699000	1.006202000	-2.563368000
1	-0.010632000	0.907692000	2.237586000
1	-0.001707000	1.447235000	-0.170279000
1	0.015109000	-1.932590000	0.082056000
6	-0.047003000	3.279046000	0.607964000
8	-0.047359000	3.872759000	-0.409112000
8	-0.053737000	2.993548000	1.755829000

-1766.230496

### 3-Ru-PNP

44	0.003801000	-0.199730000	0.157731000
15	-2.341687000	-0.194529000	-0.175224000
15	2.348979000	-0.182226000	-0.176958000
8	0.005673000	-0.477891000	3.172712000
7	0.003110000	-0.106038000	-2.078259000
6	-1.227576000	-0.667567000	-2.696804000
1	-1.190496000	-1.753507000	-2.574675000
1	-1.237410000	-0.451961000	-3.773962000
6	1.235606000	-0.662323000	-2.697666000
1	1.243759000	-0.447069000	-3.774905000
1	1.203147000	-1.748379000	-2.575067000
6	-3.274742000	1.329556000	0.393206000
1	-2.876322000	2.098830000	-0.281572000
6	3.373830000	-1.669741000	0.300525000
1	4.397319000	-1.456367000	-0.031594000
6	2.486642000	-0.076940000	-2.037562000
1	2.575441000	0.984122000	-2.293915000
1	3.387283000	-0.580094000	-2.403047000

6	3.272350000	1.349129000	0.387695000
1	2.867922000	2.113782000	-0.288812000
6	-2.480169000	-0.086815000	-2.035549000
1	-3.379586000	-0.591537000	-2.401898000
1	-2.570774000	0.974593000	-2.289699000
6	-3.349018000	-1.898770000	1.821964000
1	-2.328529000	-2.050177000	2.188400000
1	-3.934923000	-2.789589000	2.075163000
1	-3.783753000	-1.053426000	2.361518000
6	-2.859326000	-2.949568000	-0.427306000
1	-2.943132000	-2.864667000	-1.514771000
1	-3.463835000	-3.809727000	-0.118101000
1	-1.814480000	-3.161038000	-0.177593000
6	-3.357052000	-1.689510000	0.299871000
1	-4.382108000	-1.481643000	-0.030842000
6	0.004755000	-0.346433000	2.012680000
6	-2.912485000	1.754039000	1.826232000
1	-3.240694000	1.021488000	2.569481000
1	-3.405551000	2.705026000	2.057544000
1	-1.834882000	1.898304000	1.940509000
6	-4.794590000	1.240397000	0.184590000
1	-5.057103000	0.946185000	-0.837050000
1	-5.249499000	2.218487000	0.377469000
1	-5.251034000	0.523353000	0.875314000
6	4.792601000	1.270351000	0.177571000
1	5.254686000	0.556722000	0.868079000
1	5.240913000	2.251637000	0.369707000
1	5.056099000	0.977715000	-0.844263000
6	2.882789000	-2.934264000	-0.423494000
1	1.839517000	-3.151455000	-0.172065000
1	3.492842000	-3.790153000	-0.113342000
1	2.964618000	-2.851133000	-1.511275000
6	3.368422000	-1.875646000	1.823107000
1	3.798265000	-1.026368000	2.360424000
1	3.960243000	-2.762129000	2.077729000
1	2.349278000	-2.032755000	2.190907000
6	2.909113000	1.774758000	1.820151000
1	1.830140000	1.906045000	1.937786000
1	3.391643000	2.732271000	2.046654000
1	3.248256000	1.048929000	2.565093000
1	-0.000778000	0.922238000	-2.216894000
1	0.022141000	1.851294000	0.071295000
1	0.007856000	-1.775536000	0.100444000
6	-0.028508000	2.850854000	-0.525636000
8	-0.062813000	3.849576000	0.209533000
8	-0.035452000	2.729610000	-1.774655000

-1766.252425

**TS2-Ru-PNP**

44	0.056606000	-0.230332000	-0.148287000
15	2.395063000	-0.080461000	0.201494000
15	-2.290069000	-0.327222000	0.168097000
8	0.117370000	-0.671305000	-3.142927000
7	0.026425000	-0.025799000	2.065264000
6	1.284104000	-0.423970000	2.745702000
1	1.332141000	-1.516422000	2.729892000
1	1.258868000	-0.108499000	3.797883000
6	-1.167502000	-0.635845000	2.708923000
1	-1.195088000	-0.369730000	3.774745000
1	-1.057222000	-1.722061000	2.640155000
6	3.283153000	1.423155000	-0.488881000
1	2.889099000	2.230872000	0.141529000
6	-3.231129000	-1.881346000	-0.268015000
1	-4.261268000	-1.720299000	0.073761000
6	-2.453891000	-0.170368000	2.021129000
1	-2.616501000	0.890899000	2.230497000
1	-3.315803000	-0.729226000	2.398787000
6	-3.273838000	1.135716000	-0.462601000
1	-2.905651000	1.934922000	0.191787000
6	2.504097000	0.183931000	2.047445000
1	3.430463000	-0.225996000	2.462337000
1	2.521098000	1.266753000	2.212716000
6	3.466598000	-1.899994000	-1.651228000
1	2.453208000	-2.128734000	-1.997231000
1	4.094294000	-2.779110000	-1.836066000
1	3.857610000	-1.081726000	-2.261855000
6	3.029828000	-2.782922000	0.680918000
1	3.121106000	-2.606209000	1.756526000
1	3.664670000	-3.641547000	0.434606000
1	1.991905000	-3.054555000	0.462215000
6	3.471528000	-1.567343000	-0.150411000
1	4.488172000	-1.290818000	0.154363000
6	0.089424000	-0.469428000	-1.992204000
6	2.871807000	1.736190000	-1.937078000
1	3.189434000	0.955270000	-2.634247000
1	3.339955000	2.674886000	-2.254383000
1	1.787921000	1.849695000	-2.028843000
6	4.809835000	1.383177000	-0.317755000
1	5.105729000	1.172672000	0.715385000
1	5.235463000	2.354189000	-0.595291000
1	5.265771000	0.626887000	-0.965482000

6	-4.791451000	0.988760000	-0.274861000
1	-5.209841000	0.232149000	-0.947625000
1	-5.283217000	1.941043000	-0.504435000
1	-5.057292000	0.716550000	0.752243000
6	-2.657405000	-3.098753000	0.475369000
1	-1.612190000	-3.270959000	0.198215000
1	-3.231678000	-3.993345000	0.208808000
1	-2.710210000	-2.986527000	1.562335000
6	-3.235781000	-2.120945000	-1.785623000
1	-3.728454000	-1.313301000	-2.332981000
1	-3.772006000	-3.049649000	-2.011983000
1	-2.214720000	-2.219517000	-2.168342000
6	-2.903091000	1.525258000	-1.903269000
1	-1.829862000	1.711362000	-2.001973000
1	-3.430271000	2.446473000	-2.176617000
1	-3.181839000	0.755157000	-2.629018000
1	-0.085201000	1.003312000	2.086666000
1	0.693921000	3.078120000	0.050690000
1	0.149277000	-1.782258000	-0.032104000
6	-0.313503000	3.349505000	0.455691000
8	-0.851359000	4.379450000	-0.010371000
8	-0.780891000	2.558237000	1.334141000

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### 3'-Ru-PNP

44	-0.000067000	-0.133187000	0.146598000
15	-2.339608000	-0.242709000	-0.159842000
15	2.339487000	-0.242938000	-0.159813000
8	-0.000064000	0.563726000	3.084787000
7	-0.000110000	-0.747142000	-2.006940000
6	-1.236234000	-1.454014000	-2.429810000
1	-1.210146000	-2.449021000	-1.978457000
1	-1.247763000	-1.578792000	-3.521409000
6	1.235988000	-1.454048000	-2.429833000
1	1.247520000	-1.578779000	-3.521438000
1	1.209846000	-2.449077000	-1.978530000
6	-3.282619000	1.373131000	-0.083033000
1	-2.722279000	1.972748000	-0.812204000
6	3.345907000	-1.537109000	0.740935000
1	4.396247000	-1.355481000	0.481349000
6	2.472923000	-0.677709000	-1.973360000
1	2.533659000	0.270179000	-2.520298000
1	3.385199000	-1.239853000	-2.194825000
6	3.282765000	1.372744000	-0.082902000
1	2.722624000	1.972462000	-0.812142000

6	-2.473123000	-0.677584000	-1.973368000
1	-3.385440000	-1.239701000	-2.194732000
1	-2.533841000	0.270256000	-2.520388000
6	-3.166622000	-1.404028000	2.262901000
1	-2.119768000	-1.565159000	2.539531000
1	-3.774697000	-2.160074000	2.772947000
1	-3.468388000	-0.424674000	2.641541000
6	-2.967045000	-2.956281000	0.284905000
1	-3.185008000	-3.130469000	-0.772833000
1	-3.541132000	-3.689859000	0.862407000
1	-1.902618000	-3.148648000	0.457268000
6	-3.346219000	-1.536709000	0.740952000
1	-4.396526000	-1.354954000	0.481319000
6	-0.000073000	0.315909000	1.939633000
6	-3.171481000	2.081934000	1.276752000
1	-3.774263000	1.584386000	2.042663000
1	-3.545496000	3.107875000	1.182947000
1	-2.139196000	2.131972000	1.632968000
6	-4.746198000	1.274188000	-0.543544000
1	-4.845816000	0.795391000	-1.522800000
1	-5.176147000	2.279738000	-0.620239000
1	-5.353836000	0.712578000	0.174258000
6	4.746371000	1.273551000	-0.543256000
1	5.353840000	0.711827000	0.174602000
1	5.176497000	2.279032000	-0.619885000
1	4.846014000	0.794761000	-1.522513000
6	2.966576000	-2.956619000	0.284817000
1	1.902115000	-3.148865000	0.457111000
1	3.540540000	-3.690293000	0.862319000
1	3.184576000	-3.130791000	-0.772917000
6	3.166278000	-1.404472000	2.262886000
1	3.468128000	-0.425159000	2.641567000
1	3.774265000	-2.160594000	2.772920000
1	2.119397000	-1.565506000	2.539471000
6	3.171590000	2.081552000	1.276877000
1	2.139271000	2.131793000	1.632969000
1	3.545818000	3.107422000	1.183139000
1	3.774177000	1.583877000	2.042859000
1	-0.000098000	0.184484000	-2.432478000
1	0.000268000	3.053892000	0.667998000
1	-0.000166000	-1.668071000	0.614790000
6	0.000595000	3.023728000	-0.443431000
8	0.001306000	4.102331000	-1.065665000
8	0.000248000	1.853325000	-0.963681000

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**4-Ru-PNP**

15	2.272237000	-0.464424000	-0.274064000
7	0.072793000	1.308624000	-1.387044000
6	-1.007467000	1.114504000	-2.386480000
6	1.425241000	1.520660000	-1.980198000
6	2.253468000	0.235935000	-1.995066000
1	3.260017000	0.421239000	-2.383422000
1	1.776938000	-0.508437000	-2.638389000
6	-2.362097000	1.142520000	-1.671868000
1	-3.174437000	0.918299000	-2.369351000
15	-2.355322000	-0.061206000	-0.248548000
6	-0.175233000	-1.508716000	1.593009000
8	-0.282689000	-2.295470000	2.446228000
44	-0.034860000	-0.236534000	0.233917000
6	3.058170000	-2.157646000	-0.412789000
1	4.134349000	-1.974358000	-0.516259000
6	2.812826000	-2.992849000	0.856135000
1	3.413329000	-3.908600000	0.812335000
1	3.075589000	-2.463957000	1.775174000
1	1.761161000	-3.284481000	0.925284000
6	2.574775000	-2.928271000	-1.653030000
1	2.899075000	-2.462761000	-2.587675000
1	2.985654000	-3.944017000	-1.629740000
1	1.482026000	-3.009089000	-1.665767000
6	-3.138161000	-1.583038000	-1.017096000
1	-2.601388000	-1.638804000	-1.974287000
6	-2.846431000	-2.884053000	-0.252619000
1	-3.253013000	-3.733657000	-0.813396000
1	-1.772544000	-3.040240000	-0.130132000
1	-3.308287000	-2.892225000	0.738849000
6	-4.639366000	-1.422769000	-1.312256000
1	-4.983724000	-2.266558000	-1.920728000
1	-5.232875000	-1.418011000	-0.392898000
1	-4.865039000	-0.505165000	-1.864158000
1	-0.972912000	1.918623000	-3.134541000
1	-0.848059000	0.164184000	-2.905662000
1	-2.534872000	2.143246000	-1.265601000
1	1.910359000	2.285548000	-1.367242000
1	1.329022000	1.919669000	-2.997653000
6	-3.583119000	0.643059000	0.974371000
1	-4.490091000	0.864119000	0.396740000
6	-3.055645000	1.948331000	1.594257000
1	-3.863218000	2.434157000	2.153619000
1	-2.246497000	1.736231000	2.301367000
1	-2.669349000	2.660533000	0.860499000

6	-3.921298000	-0.368620000	2.082891000
1	-4.582638000	0.103310000	2.818429000
1	-4.430640000	-1.257938000	1.705049000
1	-3.015491000	-0.690553000	2.609259000
6	3.469485000	0.633291000	0.657267000
1	3.010300000	1.620517000	0.523154000
6	4.898441000	0.662943000	0.092055000
1	5.479035000	1.431094000	0.616194000
1	5.413892000	-0.292310000	0.240477000
1	4.925829000	0.904248000	-0.974689000
6	3.479654000	0.337989000	2.167258000
1	4.001597000	1.146052000	2.691952000
1	2.468917000	0.268349000	2.580532000
1	4.008400000	-0.593752000	2.393507000
1	-0.151916000	2.196548000	-0.886042000
1	0.269963000	4.978693000	1.243055000
6	0.424108000	4.059728000	0.628072000
8	-0.545645000	3.730331000	-0.121874000
8	1.523146000	3.462791000	0.754762000
1	-0.279785000	1.201653000	1.410467000
1	0.517063000	1.197851000	1.326370000
1	-0.137753000	-1.396884000	-0.864961000

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### TS3-Ru-PNP

15	-2.264157000	-0.395721000	0.329740000
7	0.015517000	1.229746000	1.517651000
6	1.076470000	0.901768000	2.503798000
6	-1.325692000	1.503716000	2.113108000
6	-2.255078000	0.290488000	2.061605000
1	-3.259160000	0.565279000	2.402677000
1	-1.881483000	-0.497641000	2.720474000
6	2.434068000	0.897457000	1.793250000
1	3.215835000	0.530117000	2.464316000
15	2.355718000	-0.139842000	0.235074000
6	0.056106000	-1.510543000	-1.543629000
8	0.062419000	-2.285589000	-2.422249000
44	0.032277000	-0.278922000	-0.161897000
6	-3.148173000	-2.038596000	0.494202000
1	-4.114687000	-1.810662000	0.962306000
6	-3.399409000	-2.678525000	-0.882229000
1	-3.877892000	-3.655925000	-0.750853000
1	-4.056235000	-2.074328000	-1.511866000
1	-2.458971000	-2.835348000	-1.420412000
6	-2.387847000	-3.018530000	1.402467000

1	-2.224334000	-2.623875000	2.409331000
1	-2.968956000	-3.943066000	1.500558000
1	-1.411700000	-3.267024000	0.976600000
6	3.218498000	-1.713619000	0.792466000
1	2.744529000	-1.880272000	1.769495000
6	2.894686000	-2.934394000	-0.082560000
1	3.344188000	-3.831404000	0.359830000
1	1.816528000	-3.091865000	-0.153884000
1	3.292268000	-2.832867000	-1.096856000
6	4.732936000	-1.556597000	1.008462000
1	5.128765000	-2.452872000	1.499863000
1	5.264544000	-1.442342000	0.058556000
1	4.982546000	-0.697359000	1.639490000
1	1.085917000	1.647041000	3.312065000
1	0.854995000	-0.075223000	2.941238000
1	2.700422000	1.921026000	1.512476000
1	-1.760605000	2.330766000	1.543873000
1	-1.212719000	1.853812000	3.146893000
6	3.528692000	0.725155000	-0.942987000
1	4.479264000	0.846405000	-0.407485000
6	2.997102000	2.114401000	-1.332952000
1	3.739393000	2.623789000	-1.958615000
1	2.068435000	2.024531000	-1.904012000
1	2.787694000	2.754277000	-0.471804000
6	3.762765000	-0.122600000	-2.205540000
1	4.397078000	0.429444000	-2.908681000
1	4.258200000	-1.072683000	-1.991577000
1	2.814084000	-0.338703000	-2.710230000
6	-3.443801000	0.752179000	-0.575291000
1	-3.072743000	1.738587000	-0.268409000
6	-4.916479000	0.627281000	-0.152895000
1	-5.501078000	1.434917000	-0.608933000
1	-5.350283000	-0.320697000	-0.488435000
1	-5.049894000	0.695475000	0.931584000
6	-3.282639000	0.678484000	-2.103422000
1	-3.823721000	1.510692000	-2.568481000
1	-2.232195000	0.749317000	-2.395233000
1	-3.690602000	-0.250130000	-2.513567000
1	0.297762000	2.110818000	1.066524000
1	-0.722658000	5.016649000	-0.861575000
6	-0.405611000	3.993607000	-0.589850000
8	0.406774000	3.822021000	0.330492000
8	-0.967345000	3.073418000	-1.307306000
1	-0.004603000	1.064219000	-1.323236000
1	-0.470803000	1.962234000	-1.197165000
1	0.136299000	-1.462919000	0.965359000

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**5-Ru-PNP**

15	-2.265197000	-0.414146000	0.322834000
7	0.010039000	1.158530000	1.579928000
6	1.080960000	0.812924000	2.548442000
6	-1.328410000	1.404314000	2.194913000
6	-2.263606000	0.199251000	2.083010000
1	-3.267831000	0.465213000	2.430957000
1	-1.897121000	-0.618817000	2.708022000
6	2.433626000	0.830563000	1.829758000
1	3.219045000	0.444724000	2.486239000
15	2.349431000	-0.163053000	0.241781000
6	0.059374000	-1.486652000	-1.570052000
8	0.069257000	-2.227012000	-2.481622000
44	0.031512000	-0.312439000	-0.146894000
6	-3.184304000	-2.045004000	0.412954000
1	-4.152454000	-1.818119000	0.877809000
6	-3.428210000	-2.623277000	-0.991971000
1	-3.928958000	-3.594913000	-0.908358000
1	-4.062402000	-1.979836000	-1.605939000
1	-2.483121000	-2.777822000	-1.522813000
6	-2.455117000	-3.075622000	1.289675000
1	-2.302998000	-2.726448000	2.314980000
1	-3.051665000	-3.994457000	1.337923000
1	-1.475026000	-3.318245000	0.870014000
6	3.240640000	-1.740237000	0.746994000
1	2.774775000	-1.940771000	1.721555000
6	2.923635000	-2.938453000	-0.160963000
1	3.380150000	-3.844869000	0.254610000
1	1.846010000	-3.099265000	-0.234400000
1	3.318437000	-2.805416000	-1.172810000
6	4.754626000	-1.572770000	0.956768000
1	5.164201000	-2.477296000	1.421335000
1	5.278486000	-1.427499000	0.006630000
1	4.999187000	-0.727748000	1.608837000
1	1.093488000	1.536796000	3.376311000
1	0.865505000	-0.176647000	2.959502000
1	2.699328000	1.862442000	1.579493000
1	-1.763532000	2.264161000	1.676626000
1	-1.209150000	1.696476000	3.245928000
6	3.514299000	0.748199000	-0.911936000
1	4.469886000	0.849552000	-0.381354000
6	2.983589000	2.151775000	-1.247439000
1	3.714257000	2.676803000	-1.874008000

1	2.041060000	2.084395000	-1.798484000
1	2.803088000	2.766312000	-0.361054000
6	3.736071000	-0.052740000	-2.206671000
1	4.369552000	0.520290000	-2.893737000
1	4.226486000	-1.013104000	-2.029933000
1	2.782495000	-0.244892000	-2.711928000
6	-3.436512000	0.787540000	-0.529220000
1	-3.061660000	1.755114000	-0.169167000
6	-4.911857000	0.657486000	-0.116684000
1	-5.487243000	1.493144000	-0.532402000
1	-5.354785000	-0.267495000	-0.500987000
1	-5.047765000	0.671607000	0.969585000
6	-3.275420000	0.789995000	-2.058697000
1	-3.808780000	1.648561000	-2.483453000
1	-2.223312000	0.861898000	-2.344439000
1	-3.691841000	-0.113634000	-2.513835000
1	0.277906000	2.046225000	1.144719000
1	-0.613103000	5.140874000	-0.848598000
6	-0.343182000	4.110673000	-0.571519000
8	0.282478000	3.855730000	0.452456000
8	-0.774846000	3.239895000	-1.456787000
1	-0.046020000	1.050560000	-1.204276000
1	-0.465532000	2.261318000	-1.248107000
1	0.134325000	-1.530300000	0.987047000

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### 15-Ru-PNP

44	-1.050924000	0.496689000	-0.184671000
15	-2.607972000	-1.229922000	0.132294000
15	0.702504000	2.024480000	0.112686000
8	-1.684653000	1.126945000	-3.070283000
7	-0.555255000	0.002915000	1.966814000
6	-1.707311000	-0.578637000	2.694222000
1	-2.451711000	0.212455000	2.817134000
1	-1.395772000	-0.913845000	3.694740000
6	0.048679000	1.150719000	2.683201000
1	0.384612000	0.840380000	3.683754000
1	-0.729183000	1.909280000	2.804594000
6	-2.342006000	-2.847031000	-0.787722000
1	-1.334921000	-3.112544000	-0.438678000
6	0.426523000	3.880860000	0.048002000
1	1.407681000	4.347699000	0.201357000
6	1.228018000	1.701810000	1.879683000
1	2.025680000	0.951418000	1.850592000
1	1.638711000	2.598347000	2.354093000

6	2.304369000	1.701778000	-0.810113000
1	2.499733000	0.674190000	-0.482705000
6	-2.285797000	-1.751993000	1.901022000
1	-3.189106000	-2.139021000	2.382751000
1	-1.556163000	-2.569651000	1.871347000
6	-4.892594000	-0.383371000	-1.289327000
1	-4.383586000	0.558088000	-1.521553000
1	-5.972681000	-0.194354000	-1.292262000
1	-4.678643000	-1.089560000	-2.095473000
6	-4.890179000	0.067126000	1.194403000
1	-4.717746000	-0.334572000	2.197702000
1	-5.963694000	0.271488000	1.103768000
1	-4.349147000	1.014906000	1.106501000
6	-4.458663000	-0.910380000	0.088666000
1	-4.945164000	-1.876136000	0.273732000
6	-1.442195000	0.885801000	-1.943125000
6	-2.260526000	-2.672029000	-2.311960000
1	-3.242423000	-2.469981000	-2.751327000
1	-1.884463000	-3.595485000	-2.768673000
1	-1.587204000	-1.855252000	-2.583479000
6	-3.309605000	-3.977203000	-0.402725000
1	-3.374054000	-4.121520000	0.680911000
1	-2.971475000	-4.922218000	-0.844721000
1	-4.319357000	-3.783892000	-0.780799000
6	3.487925000	2.589696000	-0.396662000
1	3.353560000	3.620704000	-0.740904000
1	4.411777000	2.212212000	-0.851973000
1	3.636630000	2.610630000	0.687948000
6	-0.514391000	4.349988000	1.170271000
1	-1.476123000	3.829580000	1.111875000
1	-0.697565000	5.426316000	1.068779000
1	-0.093398000	4.182418000	2.166421000
6	-0.125548000	4.306892000	-1.322771000
1	0.548585000	4.053934000	-2.144699000
1	-0.278270000	5.392580000	-1.340711000
1	-1.089775000	3.825962000	-1.517960000
6	2.136941000	1.663877000	-2.336303000
1	1.283688000	1.047296000	-2.630061000
1	3.039543000	1.242283000	-2.795484000
1	2.000880000	2.665872000	-2.754915000
1	0.165452000	-0.723490000	1.902808000
1	0.106428000	-0.674069000	-0.607073000
6	3.594362000	-1.961719000	-1.193633000
6	4.312940000	-1.069714000	0.991668000
6	5.625099000	-1.834094000	0.810595000
8	5.951492000	-1.972727000	-0.575801000

6	4.936484000	-2.688859000	-1.284889000
1	2.801827000	-2.550614000	-1.662836000
1	4.010154000	-1.047356000	2.039769000
1	5.547390000	-2.828673000	1.276145000
1	4.840488000	-3.705844000	-0.874043000
7	3.262054000	-1.726560000	0.211984000
1	6.450858000	-1.288303000	1.273217000
1	4.435493000	-0.039676000	0.634343000
1	3.661554000	-0.997021000	-1.712039000
1	5.266326000	-2.753755000	-2.324510000
6	2.078495000	-2.086709000	0.747406000
8	1.741588000	-1.886567000	1.925460000
1	1.410327000	-2.583479000	0.031290000
1	-2.144215000	1.613057000	0.486099000

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### TS7-Ru-PNP

44	-0.531031000	0.430644000	-0.173946000
15	-2.639879000	-0.570931000	0.147085000
15	1.412729000	1.725536000	0.122549000
8	-0.500170000	0.389275000	-3.196921000
7	-0.530962000	0.416951000	2.059523000
6	-1.893595000	0.394183000	2.654850000
1	-2.335173000	1.382889000	2.502419000
1	-1.825908000	0.219966000	3.738530000
6	0.306774000	1.472586000	2.685405000
1	0.471328000	1.239731000	3.747136000
1	-0.258563000	2.406724000	2.638245000
6	-2.922886000	-2.348486000	-0.393227000
1	-2.300736000	-2.899804000	0.322040000
6	1.293657000	3.555168000	-0.300803000
1	2.318164000	3.945220000	-0.268343000
6	1.652490000	1.632116000	1.973368000
1	2.279730000	0.755440000	2.164200000
1	2.188010000	2.502823000	2.364985000
6	3.091466000	1.202795000	-0.535045000
1	3.153054000	0.160702000	-0.210199000
6	-2.752311000	-0.693401000	2.005511000
1	-3.786586000	-0.630347000	2.359066000
1	-2.353483000	-1.675358000	2.278028000
6	-4.193732000	0.596774000	-1.884894000
1	-3.323889000	1.184978000	-2.195099000
1	-5.097704000	1.146997000	-2.171125000
1	-4.187191000	-0.341919000	-2.446066000
6	-4.312555000	1.705471000	0.384984000

1	-4.417494000	1.566244000	1.465268000
1	-5.208058000	2.231266000	0.033388000
1	-3.444117000	2.346043000	0.201975000
6	-4.178156000	0.370608000	-0.364805000
1	-5.029373000	-0.262097000	-0.087058000
6	-0.512678000	0.399972000	-2.022879000
6	-2.371374000	-2.632153000	-1.799845000
1	-2.942260000	-2.111465000	-2.574918000
1	-2.432455000	-3.706499000	-2.010141000
1	-1.326259000	-2.323696000	-1.889133000
6	-4.369429000	-2.844169000	-0.238297000
1	-4.771349000	-2.645608000	0.760916000
1	-4.407505000	-3.927291000	-0.403708000
1	-5.033964000	-2.376961000	-0.973038000
6	4.287170000	1.956726000	0.068952000
1	4.301481000	3.008513000	-0.235773000
1	5.219621000	1.501415000	-0.285545000
1	4.296549000	1.917898000	1.162436000
6	0.445192000	4.341475000	0.711374000
1	-0.572288000	3.938849000	0.757327000
1	0.377802000	5.388876000	0.394522000
1	0.872275000	4.331181000	1.718329000
6	0.725305000	3.751877000	-1.717782000
1	1.286066000	3.210075000	-2.482754000
1	0.746658000	4.817088000	-1.977246000
1	-0.312130000	3.406514000	-1.756992000
6	3.155778000	1.198267000	-2.070737000
1	2.286921000	0.708220000	-2.519769000
1	4.052679000	0.657545000	-2.394343000
1	3.224102000	2.214333000	-2.471846000
1	-0.111103000	-0.515500000	2.238585000
1	0.272801000	-1.162084000	0.099836000
6	2.096668000	-2.592602000	-1.006168000
6	2.854816000	-2.198411000	1.283401000
6	4.225834000	-2.714413000	0.863363000
8	4.480243000	-2.454240000	-0.521514000
6	3.496542000	-3.093727000	-1.341176000
1	1.355044000	-3.156608000	-1.583215000
1	2.640989000	-2.483677000	2.315959000
1	4.295896000	-3.797262000	1.052798000
1	3.555840000	-4.185026000	-1.203770000
7	1.818893000	-2.757588000	0.419281000
1	5.013271000	-2.206315000	1.426116000
1	2.846382000	-1.099284000	1.237934000
1	1.995909000	-1.531350000	-1.290591000
1	3.748513000	-2.853894000	-2.377432000

6	0.480412000	-2.459069000	0.800763000
8	0.185895000	-2.317589000	2.038861000
1	-0.212927000	-2.996966000	0.134267000
1	-1.311551000	1.867419000	-0.150002000

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### 16-Ru-PNP

44	-0.513366000	0.400376000	-0.170790000
15	-2.641076000	-0.579118000	0.151919000
15	1.414935000	1.731877000	0.116651000
8	-0.467771000	0.307415000	-3.196096000
7	-0.529093000	0.421689000	2.049046000
6	-1.892558000	0.421749000	2.643849000
1	-2.326611000	1.412877000	2.484375000
1	-1.825456000	0.257247000	3.729023000
6	0.322429000	1.460052000	2.685738000
1	0.500137000	1.199350000	3.738722000
1	-0.237316000	2.398845000	2.673819000
6	-2.939112000	-2.357576000	-0.372328000
1	-2.336342000	-2.911535000	0.357429000
6	1.232364000	3.555793000	-0.298771000
1	2.241936000	3.981154000	-0.250643000
6	1.662458000	1.633749000	1.964751000
1	2.297063000	0.760181000	2.144571000
1	2.193537000	2.507131000	2.356815000
6	3.098443000	1.249913000	-0.559573000
1	3.199882000	0.216502000	-0.215643000
6	-2.762916000	-0.666369000	2.010093000
1	-3.798147000	-0.585327000	2.356975000
1	-2.374750000	-1.647242000	2.301012000
6	-4.157140000	0.581693000	-1.914648000
1	-3.275525000	1.145754000	-2.235874000
1	-5.048957000	1.144379000	-2.213957000
1	-4.169418000	-0.368153000	-2.456356000
6	-4.256152000	1.740017000	0.332374000
1	-4.370372000	1.625595000	1.414373000
1	-5.136321000	2.280242000	-0.035127000
1	-3.372977000	2.357879000	0.141361000
6	-4.151290000	0.387192000	-0.390100000
1	-5.018326000	-0.219389000	-0.102711000
6	-0.482615000	0.332683000	-2.025174000
6	-2.368386000	-2.662963000	-1.766885000
1	-2.909233000	-2.132149000	-2.556370000
1	-2.453597000	-3.736588000	-1.971542000
1	-1.313227000	-2.385382000	-1.837310000

6	-4.396643000	-2.825817000	-0.236502000
1	-4.810637000	-2.612076000	0.754546000
1	-4.450577000	-3.909335000	-0.393633000
1	-5.040873000	-2.353325000	-0.985697000
6	4.273721000	2.057634000	0.014421000
1	4.253423000	3.099582000	-0.322262000
1	5.217461000	1.620558000	-0.332591000
1	4.289842000	2.051563000	1.108442000
6	0.345869000	4.303706000	0.710315000
1	-0.655953000	3.862506000	0.750605000
1	0.238732000	5.348161000	0.395209000
1	0.767943000	4.308014000	1.719218000
6	0.674988000	3.744575000	-1.721270000
1	1.255831000	3.218936000	-2.482221000
1	0.675856000	4.811007000	-1.975681000
1	-0.354830000	3.378985000	-1.775825000
6	3.142993000	1.216225000	-2.095639000
1	2.291951000	0.678311000	-2.522908000
1	4.058512000	0.707719000	-2.418793000
1	3.162032000	2.224697000	-2.520003000
1	-0.125979000	-0.535780000	2.235486000
1	0.329026000	-1.279363000	0.231707000
6	2.072161000	-2.625518000	-0.965411000
6	2.870268000	-2.165472000	1.273558000
6	4.235672000	-2.694407000	0.852678000
8	4.468462000	-2.485458000	-0.545840000
6	3.461850000	-3.138189000	-1.326465000
1	1.316027000	-3.188928000	-1.525523000
1	2.680851000	-2.392650000	2.325190000
1	4.309972000	-3.769667000	1.080573000
1	3.519273000	-4.226542000	-1.166033000
7	1.820070000	-2.777673000	0.465516000
1	5.033227000	-2.165652000	1.381708000
1	2.861765000	-1.068258000	1.171288000
1	1.981482000	-1.565320000	-1.269382000
1	3.690788000	-2.922839000	-2.373688000
6	0.469069000	-2.349304000	0.838127000
8	0.217972000	-2.202269000	2.120882000
1	-0.224675000	-2.994634000	0.264934000
1	-1.275244000	1.803223000	-0.243718000

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#### TS8-Ru-PNP

44	0.449655000	-0.572607000	-0.194931000
15	2.493452000	0.583293000	0.066349000

15	-1.391900000	-2.000016000	0.188137000
8	0.257624000	-0.449348000	-3.230155000
7	0.497634000	-0.535949000	1.934881000
6	1.791482000	-0.311032000	2.601463000
1	2.376745000	-1.245650000	2.631398000
1	1.627231000	-0.021194000	3.653928000
6	-0.231746000	-1.576315000	2.677815000
1	-0.403590000	-1.246104000	3.717501000
1	0.375749000	-2.494051000	2.749751000
6	2.704370000	2.340410000	-0.568447000
1	1.991674000	2.889618000	0.056426000
6	-1.144567000	-3.816832000	-0.195153000
1	-2.067549000	-4.324077000	0.109672000
6	-1.584961000	-1.899601000	2.036630000
1	-2.290234000	-1.083914000	2.231369000
1	-2.016060000	-2.816852000	2.452536000
6	-3.118081000	-1.577272000	-0.432070000
1	-3.382825000	-0.725799000	0.204951000
6	2.603681000	0.790046000	1.912163000
1	3.643045000	0.796849000	2.257861000
1	2.171156000	1.768534000	2.146088000
6	4.137282000	-0.492317000	-1.948284000
1	3.287191000	-1.083063000	-2.306895000
1	5.057194000	-1.025934000	-2.214269000
1	4.141204000	0.460792000	-2.484947000
6	4.216850000	-1.648760000	0.304748000
1	4.259444000	-1.528059000	1.390966000
1	5.148289000	-2.132686000	-0.011731000
1	3.386796000	-2.321480000	0.067125000
6	4.066834000	-0.304109000	-0.424246000
1	4.889554000	0.347484000	-0.105872000
6	0.315939000	-0.470830000	-2.057864000
6	2.271355000	2.506462000	-2.049778000
1	2.021706000	1.560286000	-2.533439000
1	3.070532000	2.972097000	-2.636030000
1	1.386318000	3.145771000	-2.127974000
6	4.099096000	2.932608000	-0.299584000
1	4.402496000	2.817310000	0.746391000
1	4.093657000	4.004328000	-0.530224000
1	4.861734000	2.465755000	-0.931764000
6	-4.163427000	-2.679823000	-0.197785000
1	-3.996217000	-3.536283000	-0.859594000
1	-5.164265000	-2.288466000	-0.414567000
1	-4.163382000	-3.040536000	0.836168000
6	0.017207000	-4.420843000	0.610788000
1	0.956462000	-3.896442000	0.406826000

1	0.147551000	-5.471950000	0.327646000
1	-0.166664000	-4.390267000	1.688087000
6	-0.928356000	-4.028877000	-1.702312000
1	-1.778978000	-3.687237000	-2.298115000
1	-0.785608000	-5.095734000	-1.910134000
1	-0.036750000	-3.492599000	-2.043601000
6	-3.134070000	-1.082852000	-1.886718000
1	-2.427914000	-0.263685000	-2.040683000
1	-4.137431000	-0.721272000	-2.140834000
1	-2.883331000	-1.879473000	-2.593397000
1	-0.156229000	0.757770000	2.383131000
1	0.069251000	2.245572000	0.787389000
6	-1.689208000	4.066772000	-0.055455000
6	-2.574317000	1.895075000	0.436402000
6	-3.910835000	2.322967000	-0.156971000
8	-3.731416000	3.323517000	-1.164792000
6	-3.042456000	4.462566000	-0.638994000
1	-1.204389000	4.950207000	0.376238000
1	-2.733930000	1.172185000	1.239967000
1	-4.567305000	2.710345000	0.637858000
1	-3.658334000	4.941403000	0.138445000
7	-1.871649000	3.053797000	0.987954000
1	-4.405545000	1.478818000	-0.644612000
1	-1.970047000	1.404004000	-0.352081000
1	-1.042766000	3.689789000	-0.872707000
1	-2.915768000	5.159972000	-1.471229000
6	-0.584293000	2.674864000	1.576958000
8	-0.725104000	1.758819000	2.622328000
1	-0.110081000	3.599188000	1.937198000
1	1.294724000	-1.862398000	-0.429239000

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### 17-Ru-PNP

44	0.957466000	0.453406000	0.177326000
15	2.420263000	-1.359118000	-0.209114000
15	-0.589120000	2.213009000	-0.094246000
8	1.595821000	0.882477000	3.123436000
7	0.455977000	0.070127000	-1.857649000
6	1.488962000	-0.555203000	-2.700118000
1	2.268682000	0.180197000	-2.963894000
1	1.046848000	-0.889654000	-3.654890000
6	-0.206681000	1.133910000	-2.625020000
1	-0.690521000	0.707643000	-3.521433000
1	0.533958000	1.863154000	-2.994476000
6	1.998408000	-2.983410000	0.637417000

1	1.060805000	-3.253709000	0.133840000
6	0.067656000	3.967117000	-0.133514000
1	-0.805729000	4.630919000	-0.152893000
6	-1.268163000	1.853261000	-1.789032000
1	-2.125351000	1.188632000	-1.637119000
1	-1.635691000	2.754382000	-2.290509000
6	-2.141793000	2.238027000	0.958783000
1	-2.506578000	1.211669000	0.821722000
6	2.124098000	-1.763663000	-2.004361000
1	3.047573000	-2.075140000	-2.503502000
1	1.427810000	-2.607537000	-2.027655000
6	4.693743000	-0.868974000	1.388471000
1	4.190732000	0.014536000	1.795946000
1	5.774904000	-0.693094000	1.433186000
1	4.470681000	-1.718297000	2.039828000
6	4.734019000	0.025919000	-0.978691000
1	4.475024000	-0.144919000	-2.027950000
1	5.823998000	0.124161000	-0.916753000
1	4.287498000	0.976440000	-0.669190000
6	4.267969000	-1.121034000	-0.066136000
1	4.725656000	-2.053337000	-0.420085000
6	1.324876000	0.697021000	1.996103000
6	1.680477000	-2.823154000	2.132437000
1	2.555519000	-2.509739000	2.709638000
1	1.341022000	-3.782679000	2.540250000
1	0.890124000	-2.084936000	2.293781000
6	3.022120000	-4.100814000	0.382783000
1	3.241023000	-4.226012000	-0.682973000
1	2.632170000	-5.054385000	0.757631000
1	3.965130000	-3.903793000	0.903952000
6	-3.227894000	3.206123000	0.462978000
1	-2.921429000	4.249840000	0.591450000
1	-4.144420000	3.059694000	1.046854000
1	-3.478316000	3.050478000	-0.590591000
6	0.906734000	4.223616000	-1.397085000
1	1.745129000	3.520662000	-1.459267000
1	1.321089000	5.237850000	-1.360191000
1	0.318731000	4.140359000	-2.315132000
6	0.903733000	4.265872000	1.123567000
1	0.346214000	4.114639000	2.050582000
1	1.240638000	5.308962000	1.102175000
1	1.787350000	3.620345000	1.155953000
6	-1.866038000	2.429783000	2.457976000
1	-1.058706000	1.783730000	2.812530000
1	-2.770240000	2.189906000	3.029399000
1	-1.603323000	3.467396000	2.687688000

1	-0.638461000	-1.190641000	-1.670303000
1	-1.465341000	-1.137664000	0.283638000
6	-3.715240000	-2.448425000	1.077105000
6	-3.898935000	-1.104939000	-0.902250000
6	-5.398024000	-1.379691000	-0.927488000
8	-5.903032000	-1.606383000	0.393564000
6	-5.220606000	-2.695311000	1.022849000
1	-3.219318000	-3.320834000	1.518355000
1	-3.522424000	-0.975213000	-1.920415000
1	-5.607162000	-2.257247000	-1.559171000
1	-5.424463000	-3.627430000	0.472666000
7	-3.198477000	-2.228357000	-0.275615000
1	-5.942981000	-0.518818000	-1.323837000
1	-3.720762000	-0.164185000	-0.346749000
1	-3.516485000	-1.577897000	1.732943000
1	-5.634848000	-2.780539000	2.030995000
6	-1.746920000	-2.061175000	-0.275119000
8	-1.242628000	-2.009170000	-1.577837000
1	-1.329835000	-2.914862000	0.279750000
1	2.109622000	1.471835000	-0.098080000

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### 18-Ru-PNP

44	-0.002518000	0.184385000	-0.182022000
15	-2.333717000	-0.172927000	-0.221633000
15	2.333686000	-0.138475000	-0.194583000
8	-0.018115000	3.111784000	0.671985000
7	0.012037000	-1.704126000	-1.046735000
6	-1.172133000	-2.565303000	-1.038123000
1	-1.206400000	-3.169448000	-0.112249000
1	-1.116302000	-3.294716000	-1.865534000
6	1.212447000	-2.542235000	-1.035152000
1	1.173819000	-3.271709000	-1.863508000
1	1.257506000	-3.145511000	-0.109202000
6	-3.483084000	0.962904000	-1.186184000
1	-3.162369000	0.772757000	-2.219378000
6	3.162054000	-0.475907000	1.452694000
1	4.232669000	-0.602089000	1.249522000
6	2.492518000	-1.713998000	-1.173765000
1	2.617815000	-1.404805000	-2.217761000
1	3.380076000	-2.288778000	-0.887914000
6	3.473341000	1.012991000	-1.148259000
1	3.038581000	0.952152000	-2.155724000
6	-2.469797000	-1.763835000	-1.180198000
1	-3.343322000	-2.349899000	-0.873583000

1	-2.611719000	-1.477548000	-2.228253000
6	-3.143207000	0.720799000	2.322910000
1	-2.108247000	1.028098000	2.508216000
1	-3.609548000	0.489301000	3.287785000
1	-3.679045000	1.571364000	1.892899000
6	-2.556972000	-1.731731000	2.115750000
1	-2.665667000	-2.649261000	1.530829000
1	-3.053421000	-1.893192000	3.079984000
1	-1.490825000	-1.569402000	2.304755000
6	-3.183887000	-0.516566000	1.412152000
1	-4.227622000	-0.758672000	1.177437000
6	-0.013564000	1.990122000	0.316670000
6	-3.251705000	2.456479000	-0.909111000
1	-3.532348000	2.734940000	0.111123000
1	-3.865296000	3.054760000	-1.593288000
1	-2.206073000	2.734900000	-1.058016000
6	-4.970273000	0.590914000	-1.068726000
1	-5.149998000	-0.472544000	-1.257799000
1	-5.554081000	1.163669000	-1.798871000
1	-5.361708000	0.832450000	-0.074633000
6	4.931880000	0.530755000	-1.220763000
1	5.427451000	0.617403000	-0.247676000
1	5.491849000	1.153352000	-1.928730000
1	5.014267000	-0.508347000	-1.554286000
6	2.628506000	-1.775276000	2.079943000
1	1.542783000	-1.724187000	2.216695000
1	3.086944000	-1.922118000	3.065047000
1	2.858662000	-2.655705000	1.474105000
6	2.963176000	0.701110000	2.422810000
1	3.376126000	1.637597000	2.040621000
1	3.459170000	0.483034000	3.376043000
1	1.897140000	0.857103000	2.618787000
6	3.396900000	2.481916000	-0.703992000
1	2.365817000	2.833697000	-0.625799000
1	3.917164000	3.111956000	-1.435167000
1	3.885174000	2.637965000	0.262834000
1	-0.004330000	-0.094715000	1.362216000

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#### TS9-Ru-PNP

44	-0.000968000	-0.177388000	-0.141838000
15	2.337660000	0.147657000	-0.170352000
15	-2.334087000	0.194951000	-0.196478000
8	-0.030158000	-3.016873000	0.926582000
7	0.021485000	1.859829000	-1.052410000

6	1.235798000	2.629868000	-0.822372000
1	1.244907000	3.033806000	0.207121000
1	1.272057000	3.504637000	-1.496949000
6	-1.173223000	2.659860000	-0.822850000
1	-1.186078000	3.536339000	-1.496107000
1	-1.172075000	3.064114000	0.206825000
6	3.394029000	-0.962880000	-1.255984000
1	2.909174000	-0.822031000	-2.231901000
6	-3.275338000	0.402302000	1.407037000
1	-4.305193000	0.654165000	1.125727000
6	-2.456131000	1.851271000	-1.050765000
1	-2.575317000	1.641432000	-2.119681000
1	-3.339438000	2.409297000	-0.722471000
6	-3.399961000	-0.892473000	-1.300440000
1	-3.034445000	-0.614965000	-2.298092000
6	2.495562000	1.786893000	-1.048394000
1	3.396744000	2.328188000	-0.742720000
1	2.596712000	1.551916000	-2.114204000
6	3.000389000	-0.886841000	2.361176000
1	1.935371000	-0.979268000	2.597152000
1	3.551616000	-0.766546000	3.301243000
1	3.326675000	-1.823430000	1.902558000
6	2.828888000	1.623713000	2.188286000
1	3.081704000	2.525415000	1.623004000
1	3.349242000	1.679395000	3.151588000
1	1.751357000	1.630457000	2.383561000
6	3.242579000	0.334809000	1.458112000
1	4.310094000	0.399950000	1.215131000
6	-0.019417000	-1.928675000	0.490392000
6	3.289938000	-2.454267000	-0.900880000
1	3.812741000	-2.684401000	0.032724000
1	3.758201000	-3.052330000	-1.691472000
1	2.251397000	-2.778977000	-0.799976000
6	4.862111000	-0.520177000	-1.371084000
1	4.960976000	0.533938000	-1.648408000
1	5.367488000	-1.115807000	-2.140576000
1	5.401334000	-0.677784000	-0.430618000
6	-4.902339000	-0.574818000	-1.229025000
1	-5.330988000	-0.891031000	-0.271733000
1	-5.433294000	-1.116269000	-2.020727000
1	-5.108250000	0.492800000	-1.359230000
6	-2.710234000	1.560463000	2.245272000
1	-1.657651000	1.387186000	2.490497000
1	-3.273692000	1.640039000	3.182396000
1	-2.787512000	2.522611000	1.730514000
6	-3.278060000	-0.903686000	2.217639000

1	-3.785215000	-1.717893000	1.693554000
1	-3.798890000	-0.748679000	3.169728000
1	-2.254529000	-1.224908000	2.438605000
6	-3.129862000	-2.395339000	-1.122603000
1	-2.069911000	-2.629052000	-1.248613000
1	-3.695477000	-2.959802000	-1.873493000
1	-3.440447000	-2.757085000	-0.137863000
1	0.011560000	0.643816000	-1.894410000
1	0.006245000	-0.295097000	-2.078918000
1	0.004309000	0.277866000	1.402696000

-1577.594134

### 19-Ru-PNP

44	1.102243000	0.349931000	0.077723000
15	1.647656000	-1.916399000	-0.171754000
15	0.077109000	2.450758000	-0.060237000
8	3.442656000	1.156464000	1.806793000
7	-0.658574000	-0.242034000	-1.222935000
6	-0.355335000	-1.430948000	-2.057070000
1	0.367166000	-1.119626000	-2.815352000
1	-1.261728000	-1.775167000	-2.576525000
6	-1.136980000	0.898677000	-2.041460000
1	-2.048283000	0.619014000	-2.591428000
1	-0.359029000	1.122012000	-2.776062000
6	1.578378000	-3.062768000	1.315827000
1	0.569751000	-2.850542000	1.693497000
6	0.930317000	3.906696000	-0.883910000
1	0.235969000	4.753625000	-0.818006000
6	-1.403212000	2.116298000	-1.154685000
1	-2.251035000	1.917271000	-0.490933000
1	-1.667288000	2.987265000	-1.762217000
6	-0.755828000	3.137506000	1.478421000
1	-1.479895000	2.338767000	1.689264000
6	0.222270000	-2.557944000	-1.199668000
1	0.515502000	-3.407162000	-1.824522000
1	-0.539370000	-2.922429000	-0.501648000
6	4.437576000	-1.758087000	-0.526543000
1	4.365847000	-0.669123000	-0.607937000
1	5.329515000	-2.085212000	-1.074242000
1	4.584955000	-2.006621000	0.527264000
6	3.073309000	-2.073763000	-2.620312000
1	2.272307000	-2.625949000	-3.121279000
1	4.012101000	-2.327289000	-3.126864000
1	2.891202000	-1.002010000	-2.751714000
6	3.185904000	-2.420927000	-1.126903000

1	3.272777000	-3.509867000	-1.029190000
6	2.531762000	0.841021000	1.130486000
6	2.571004000	-2.675120000	2.423835000
1	3.596484000	-2.951190000	2.157924000
1	2.319985000	-3.211019000	3.346876000
1	2.547580000	-1.602522000	2.635813000
6	1.672089000	-4.561267000	0.986041000
1	0.957958000	-4.866328000	0.214598000
1	1.460202000	-5.151447000	1.885757000
1	2.677043000	-4.834845000	0.647015000
6	-1.521976000	4.452421000	1.265691000
1	-0.836503000	5.293300000	1.114190000
1	-2.124587000	4.679149000	2.153448000
1	-2.199843000	4.407163000	0.406643000
6	1.213357000	3.626877000	-2.368911000
1	1.834789000	2.732808000	-2.481891000
1	1.747502000	4.478682000	-2.806380000
1	0.296945000	3.482258000	-2.949602000
6	2.233016000	4.263134000	-0.149175000
1	2.062514000	4.547365000	0.892238000
1	2.722919000	5.108101000	-0.647498000
1	2.926318000	3.415543000	-0.158511000
6	0.186146000	3.221356000	2.689179000
1	0.729062000	2.283477000	2.832887000
1	-0.396387000	3.425863000	3.595605000
1	0.915698000	4.030215000	2.582308000
1	-1.418649000	-0.500285000	-0.578167000
1	0.110482000	-0.008294000	1.410090000
1	-3.760592000	-1.538486000	3.243357000
1	-1.970469000	-0.701232000	2.158952000
6	-3.748571000	-2.335318000	-0.188646000
6	-4.148404000	-0.136606000	0.735113000
6	-4.774741000	0.275247000	-0.595024000
8	-5.352586000	-0.848378000	-1.263266000
6	-4.368710000	-1.859590000	-1.498326000
1	-2.968049000	-3.075351000	-0.397762000
1	-3.659095000	0.727707000	1.199054000
1	-4.021213000	0.740678000	-1.246994000
1	-3.587978000	-1.464855000	-2.167289000
7	-3.147584000	-1.195195000	0.524418000
1	-5.582503000	0.992485000	-0.429349000
1	-4.954414000	-0.475828000	1.406910000
1	-4.523196000	-2.822303000	0.423498000
1	-4.879823000	-2.682940000	-2.003261000
6	-2.467392000	-1.583525000	1.745188000
8	-3.297190000	-2.216569000	2.734332000

1	-1.706705000	-2.324982000	1.492524000
1	1.880072000	0.646069000	-1.403197000

-1979.871780

### **20-Ru-PNP**

44	0.070973000	-0.797478000	-0.065372000
15	-2.267213000	-0.871882000	-0.359700000
15	2.383801000	-0.477378000	-0.389664000
8	0.230425000	-2.184820000	2.635225000
7	-0.060809000	0.459067000	-1.727667000
6	-1.234887000	0.418411000	-2.604674000
1	-1.147968000	-0.405745000	-3.336840000
1	-1.293562000	1.346267000	-3.201360000
6	1.121742000	0.795041000	-2.522811000
1	0.975290000	1.769929000	-3.022631000
1	1.267904000	0.061455000	-3.336813000
6	-3.369551000	-0.088376000	0.941359000
1	-2.977688000	0.938078000	0.945065000
6	3.364453000	-1.903464000	-1.106471000
1	4.418331000	-1.598638000	-1.101770000
6	2.390709000	0.871518000	-1.668935000
1	2.400398000	1.809192000	-1.103126000
1	3.294253000	0.852686000	-2.286765000
6	3.446225000	0.271485000	0.967342000
1	2.848913000	1.148751000	1.250973000
6	-2.535935000	0.268491000	-1.808940000
1	-3.360376000	-0.074524000	-2.442190000
1	-2.829940000	1.235908000	-1.391801000
6	-2.807296000	-3.576702000	0.207698000
1	-1.734407000	-3.733671000	0.362084000
1	-3.248769000	-4.525902000	-0.118020000
1	-3.253723000	-3.317448000	1.170875000
6	-2.486346000	-2.963893000	-2.220501000
1	-2.711147000	-2.261842000	-3.028572000
1	-2.931640000	-3.929449000	-2.486982000
1	-1.399762000	-3.092860000	-2.171853000
6	-3.041740000	-2.498303000	-0.862815000
1	-4.118705000	-2.317218000	-0.969465000
6	0.162707000	-1.651807000	1.582591000
6	-3.173620000	-0.654512000	2.355864000
1	-3.576251000	-1.667550000	2.450978000
1	-3.705944000	-0.023087000	3.077019000
1	-2.121292000	-0.677527000	2.646369000
6	-4.856484000	-0.051548000	0.553662000
1	-5.017933000	0.363758000	-0.446320000

1	-5.408912000	0.572517000	1.266163000
1	-5.300665000	-1.052579000	0.582735000
6	4.824370000	0.763300000	0.493325000
1	5.468492000	-0.073609000	0.203095000
1	5.326075000	1.292694000	1.312128000
1	4.757207000	1.452126000	-0.353530000
6	2.943838000	-2.188810000	-2.558890000
1	1.870857000	-2.401779000	-2.620953000
1	3.483404000	-3.067827000	-2.930276000
1	3.168365000	-1.355681000	-3.230432000
6	3.199203000	-3.171315000	-0.250101000
1	3.501904000	-3.024979000	0.789144000
1	3.811876000	-3.979589000	-0.666414000
1	2.153990000	-3.496362000	-0.251220000
6	3.582784000	-0.620519000	2.211523000
1	2.625896000	-1.033642000	2.538149000
1	3.996756000	-0.032413000	3.038830000
1	4.270417000	-1.452495000	2.029471000
1	-0.687855000	2.042195000	-0.431353000
1	-0.340698000	1.104418000	2.635780000
1	0.042660000	-0.698127000	4.090437000
1	1.340402000	1.090421000	3.227783000
6	-1.849530000	3.729595000	-0.162002000
6	0.343598000	3.331020000	0.760754000
6	0.928820000	4.286505000	-0.283823000
8	-0.033733000	5.274560000	-0.674299000
6	-1.222314000	4.666041000	-1.197498000
1	-2.733042000	3.241187000	-0.588680000
1	1.067213000	2.541312000	0.989392000
1	1.244812000	3.719667000	-1.175332000
1	-0.973189000	4.099996000	-2.111288000
7	-0.909231000	2.710544000	0.317241000
1	1.792266000	4.832970000	0.108609000
1	0.155124000	3.885717000	1.689707000
1	-2.186622000	4.325693000	0.697143000
1	-1.896841000	5.485966000	-1.463709000
6	0.288247000	1.167074000	3.532031000
8	-0.053621000	0.173541000	4.503134000
1	0.131884000	2.142083000	4.000716000
1	0.202366000	-2.221450000	-0.709738000

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### 21-Ru-PNP

44	-1.134311000	-0.140275000	0.071494000
15	-1.128452000	2.194612000	-0.183965000

15	-0.619663000	-2.426711000	-0.039147000
8	-3.664618000	-0.354931000	1.704051000
7	0.756382000	0.029396000	-1.163637000
6	0.776339000	1.253225000	-2.004168000
1	0.036117000	1.106974000	-2.794779000
1	1.761665000	1.372718000	-2.478068000
6	1.018815000	-1.203224000	-1.945593000
1	1.994014000	-1.138672000	-2.450737000
1	0.246271000	-1.261641000	-2.715899000
6	-0.846556000	3.291500000	1.311555000
1	0.092755000	2.876199000	1.694791000
6	-1.726633000	-3.640118000	-0.950685000
1	-1.251506000	-4.624795000	-0.859351000
6	0.964530000	-2.433205000	-1.038047000
1	1.793347000	-2.410055000	-0.321773000
1	1.075955000	-3.349730000	-1.625615000
6	-0.069222000	-3.306970000	1.527240000
1	0.804956000	-2.703217000	1.805608000
6	0.439957000	2.485135000	-1.161466000
1	0.363246000	3.373044000	-1.796715000
1	1.236746000	2.669760000	-0.432817000
6	-3.864049000	2.717668000	-0.614974000
1	-4.058592000	1.641800000	-0.666671000
1	-4.635734000	3.233168000	-1.199217000
1	-3.973711000	3.028928000	0.426649000
6	-2.415948000	2.642221000	-2.674706000
1	-1.486651000	2.959517000	-3.157882000
1	-3.243838000	3.119207000	-3.212797000
1	-2.512560000	1.557310000	-2.787627000
6	-2.473483000	3.036633000	-1.190031000
1	-2.289410000	4.115208000	-1.111303000
6	-2.677029000	-0.271305000	1.068725000
6	-1.916791000	3.120517000	2.401651000
1	-2.857067000	3.609761000	2.127623000
1	-1.569178000	3.585803000	3.331919000
1	-2.126288000	2.067296000	2.607735000
6	-0.617436000	4.777118000	0.988971000
1	0.157966000	4.926108000	0.230498000
1	-0.296599000	5.303978000	1.895931000
1	-1.535524000	5.261994000	0.638980000
6	0.382224000	-4.761916000	1.324387000
1	-0.470302000	-5.418527000	1.119687000
1	0.866632000	-5.131087000	2.236276000
1	1.097106000	-4.867003000	0.501530000
6	-1.834242000	-3.293072000	-2.444786000
1	-2.205180000	-2.271799000	-2.579757000

1	-2.534035000	-3.982738000	-2.931424000
1	-0.874998000	-3.381823000	-2.964397000
6	-3.125304000	-3.695367000	-0.313595000
1	-3.099166000	-4.010303000	0.732658000
1	-3.752888000	-4.410216000	-0.858883000
1	-3.611563000	-2.715304000	-0.359569000
6	-1.083085000	-3.187133000	2.675589000
1	-1.412898000	-2.153632000	2.808748000
1	-0.620917000	-3.524486000	3.611081000
1	-1.964939000	-3.812451000	2.505559000
1	1.490784000	0.123147000	-0.461910000
1	-0.100359000	-0.026242000	1.428827000
6	4.561362000	1.571942000	0.075453000
6	4.222585000	-0.660999000	1.087449000
6	4.645660000	-1.267866000	-0.249061000
8	5.566242000	-0.414695000	-0.930489000
6	4.979135000	0.859899000	-1.208554000
1	4.012143000	2.487655000	-0.150032000
1	3.453870000	-1.276936000	1.563111000
1	3.765821000	-1.442938000	-0.885095000
1	4.110290000	0.730971000	-1.871940000
7	3.698546000	0.693002000	0.872770000
1	5.155223000	-2.220422000	-0.087020000
1	5.093640000	-0.614523000	1.754999000
1	5.451466000	1.835208000	0.663390000
1	5.736169000	1.445759000	-1.734747000
6	2.750659000	1.220601000	1.691785000
8	2.444904000	2.414996000	1.729744000
1	2.234457000	0.465253000	2.304552000
1	-1.920959000	-0.246105000	-1.426390000

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#### TS10-Ru-PNP

44	0.145543000	-0.868749000	0.061317000
15	-2.186525000	-1.013470000	-0.213510000
15	2.428730000	-0.384068000	-0.190016000
8	0.428283000	-2.964487000	2.222250000
7	-0.053166000	0.685363000	-1.525826000
6	-1.273688000	0.533869000	-2.358735000
1	-1.115103000	-0.325003000	-3.015734000
1	-1.409486000	1.420206000	-2.995539000
6	1.161888000	0.841975000	-2.367535000
1	1.067201000	1.732363000	-3.006078000
1	1.212979000	-0.031260000	-3.023485000
6	-3.285419000	-0.484256000	1.203735000

1	-2.817215000	0.464196000	1.498633000
6	3.607662000	-1.681906000	-0.851893000
1	4.580780000	-1.185847000	-0.951958000
6	2.426172000	0.942868000	-1.509539000
1	2.456165000	1.911448000	-1.001334000
1	3.318445000	0.886476000	-2.140799000
6	3.329652000	0.459473000	1.227181000
1	2.848688000	1.445323000	1.242628000
6	-2.509379000	0.318483000	-1.485173000
1	-3.382970000	0.095626000	-2.104941000
1	-2.736868000	1.234040000	-0.932293000
6	-2.463619000	-3.812207000	-0.129958000
1	-1.380306000	-3.935507000	-0.225966000
1	-2.948712000	-4.712729000	-0.524753000
1	-2.700460000	-3.744811000	0.934333000
6	-2.571050000	-2.757678000	-2.412847000
1	-2.980242000	-1.963470000	-3.044224000
1	-2.978122000	-3.708295000	-2.776551000
1	-1.484021000	-2.783682000	-2.545746000
6	-2.928586000	-2.581186000	-0.927791000
1	-4.017245000	-2.478991000	-0.836782000
6	0.315783000	-2.146139000	1.389065000
6	-3.187638000	-1.421989000	2.418213000
1	-3.724805000	-2.361028000	2.248406000
1	-3.645010000	-0.936516000	3.288016000
1	-2.150398000	-1.656857000	2.672828000
6	-4.752111000	-0.231690000	0.818380000
1	-4.855549000	0.475253000	-0.010832000
1	-5.288599000	0.188368000	1.677700000
1	-5.261797000	-1.160540000	0.538441000
6	4.834312000	0.669800000	0.997616000
1	5.380089000	-0.278889000	1.038241000
1	5.241171000	1.316655000	1.783557000
1	5.045540000	1.143985000	0.033091000
6	3.174973000	-2.181416000	-2.239023000
1	2.167984000	-2.608431000	-2.202546000
1	3.869041000	-2.958571000	-2.579738000
1	3.182804000	-1.384635000	-2.989202000
6	3.740538000	-2.853905000	0.133701000
1	4.133204000	-2.539362000	1.104323000
1	4.427773000	-3.604711000	-0.273327000
1	2.771847000	-3.337014000	0.299861000
6	3.041202000	-0.195492000	2.587912000
1	1.965975000	-0.288275000	2.763394000
1	3.469132000	0.419906000	3.387982000
1	3.484489000	-1.192851000	2.667306000

1	-0.161309000	1.528250000	-0.933323000
1	-0.076802000	0.540669000	1.152807000
6	-1.669561000	3.424064000	0.538202000
6	0.720222000	3.740774000	0.577497000
6	0.621613000	4.487079000	-0.750024000
8	-0.651186000	5.120027000	-0.895320000
6	-1.718836000	4.171378000	-0.789847000
1	-2.466346000	2.679943000	0.588908000
1	1.685807000	3.230283000	0.637947000
1	0.785694000	3.789712000	-1.587638000
1	-1.662401000	3.461267000	-1.630652000
7	-0.368830000	2.758937000	0.673657000
1	1.372605000	5.279366000	-0.803955000
1	0.672696000	4.465778000	1.407958000
1	-1.836945000	4.131165000	1.365940000
1	-2.647446000	4.741066000	-0.877345000
6	-0.266362000	1.854402000	1.815839000
8	-1.232601000	1.751536000	2.625157000
1	0.772323000	1.847149000	2.189364000
1	0.290152000	-2.007731000	-1.113358000

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### 22-Ru-PNP

44	0.165620000	-0.838814000	0.076098000
15	-2.163140000	-1.067504000	-0.216613000
15	2.445361000	-0.309860000	-0.194326000
8	0.508507000	-2.917457000	2.248748000
7	-0.071058000	0.679529000	-1.531329000
6	-1.279984000	0.481753000	-2.373517000
1	-1.088488000	-0.373621000	-3.026730000
1	-1.439227000	1.360335000	-3.015159000
6	1.141548000	0.874892000	-2.370004000
1	1.018991000	1.763441000	-3.005764000
1	1.223734000	0.007042000	-3.029832000
6	-3.269072000	-0.552571000	1.198361000
1	-2.812135000	0.400711000	1.500680000
6	3.612330000	-1.606743000	-0.874355000
1	4.589197000	-1.117160000	-0.967253000
6	2.400049000	1.018067000	-1.509392000
1	2.390390000	1.984244000	-0.995721000
1	3.296304000	0.996760000	-2.137322000
6	3.354351000	0.534611000	1.216092000
1	2.870789000	1.518929000	1.241985000
6	-2.517808000	0.231456000	-1.511569000
1	-3.374701000	-0.034339000	-2.137425000

1	-2.786983000	1.145532000	-0.976229000
6	-2.325824000	-3.875850000	-0.095191000
1	-1.238976000	-3.963081000	-0.190183000
1	-2.778286000	-4.797662000	-0.478965000
1	-2.565348000	-3.803868000	0.967959000
6	-2.456259000	-2.853322000	-2.390771000
1	-2.890537000	-2.084470000	-3.036131000
1	-2.821731000	-3.823908000	-2.745197000
1	-1.367879000	-2.839219000	-2.515838000
6	-2.833933000	-2.673571000	-0.910516000
1	-3.926572000	-2.613908000	-0.828595000
6	0.372118000	-2.104887000	1.417840000
6	-3.163122000	-1.493091000	2.410005000
1	-3.683793000	-2.440326000	2.234784000
1	-3.633445000	-1.016416000	3.277496000
1	-2.123806000	-1.710040000	2.671748000
6	-4.737427000	-0.321136000	0.806169000
1	-4.848917000	0.393832000	-0.014865000
1	-5.285685000	0.079278000	1.667232000
1	-5.228416000	-1.255773000	0.512078000
6	4.855818000	0.748571000	0.968245000
1	5.404499000	-0.198659000	1.003320000
1	5.268790000	1.396684000	1.749763000
1	5.054846000	1.223528000	0.001619000
6	3.178263000	-2.085155000	-2.268853000
1	2.168442000	-2.506726000	-2.242509000
1	3.866007000	-2.865135000	-2.615330000
1	3.197567000	-1.280528000	-3.009960000
6	3.733290000	-2.792768000	0.095585000
1	4.114377000	-2.493567000	1.075543000
1	4.424616000	-3.537634000	-0.315013000
1	2.761670000	-3.276076000	0.241525000
6	3.086033000	-0.129093000	2.576981000
1	2.014497000	-0.218229000	2.774363000
1	3.529705000	0.480039000	3.373007000
1	3.526873000	-1.128392000	2.642462000
1	-0.208848000	1.531310000	-0.943705000
1	-0.146958000	0.650523000	1.207197000
6	-1.751639000	3.301365000	0.517125000
6	0.592652000	3.767516000	0.581082000
6	0.453831000	4.575345000	-0.706864000
8	-0.858792000	5.126263000	-0.838355000
6	-1.860935000	4.104526000	-0.774407000
1	-2.509140000	2.515720000	0.543070000
1	1.595774000	3.331565000	0.623514000
1	0.671621000	3.930731000	-1.574646000

1	-1.761813000	3.438859000	-1.647817000
7	-0.415781000	2.702567000	0.604104000
1	1.147873000	5.420111000	-0.715124000
1	0.486391000	4.441178000	1.450366000
1	-1.950787000	3.959421000	1.377148000
1	-2.825305000	4.616248000	-0.834307000
6	-0.263703000	1.746986000	1.763471000
8	-1.211232000	1.719397000	2.647644000
1	0.775663000	1.875040000	2.133237000
1	0.355103000	-1.995755000	-1.021527000

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44	-0.127936000	-0.865857000	0.104879000
15	-2.407197000	-0.404137000	-0.278920000
15	2.200730000	-1.082700000	-0.149979000
8	-0.478895000	-2.808716000	2.423490000
7	0.143525000	0.605948000	-1.399348000
6	-0.994541000	0.961795000	-2.255173000
1	-1.093810000	0.244739000	-3.090386000
1	-0.821688000	1.946082000	-2.727972000
6	1.352875000	0.559776000	-2.229032000
1	1.507190000	1.532049000	-2.732068000
1	1.237315000	-0.178417000	-3.043660000
6	-3.462844000	0.309114000	1.094241000
1	-2.870258000	1.184533000	1.393766000
6	2.855311000	-2.673156000	-0.889270000
1	3.937255000	-2.536039000	-1.005402000
6	2.607004000	0.225067000	-1.412063000
1	2.942697000	1.105863000	-0.857250000
1	3.435580000	-0.081345000	-2.059436000
6	3.350719000	-0.649645000	1.274220000
1	3.218467000	0.437577000	1.347159000
6	-2.311869000	1.018370000	-1.475083000
1	-3.173840000	1.047395000	-2.149397000
1	-2.349541000	1.924624000	-0.863076000
6	-3.374328000	-3.047369000	-0.336037000
1	-2.347664000	-3.422305000	-0.273154000
1	-3.986493000	-3.804380000	-0.840303000
1	-3.753940000	-2.937156000	0.682509000
6	-2.919828000	-1.964028000	-2.569598000
1	-3.056334000	-1.084987000	-3.205441000
1	-3.479497000	-2.790876000	-3.022258000
1	-1.857542000	-2.231330000	-2.576332000
6	-3.415785000	-1.731624000	-1.132077000

1	-4.449455000	-1.366524000	-1.173797000
6	-0.342311000	-2.038593000	1.547993000
6	-3.569658000	-0.600058000	2.328377000
1	-4.214376000	-1.465510000	2.143796000
1	-4.012433000	-0.034203000	3.156482000
1	-2.592574000	-0.963726000	2.655989000
6	-4.850731000	0.784411000	0.633259000
1	-4.798735000	1.457991000	-0.227899000
1	-5.341894000	1.328239000	1.449134000
1	-5.497217000	-0.059436000	0.367756000
6	4.835322000	-0.930530000	0.992548000
1	5.040836000	-2.006305000	0.978192000
1	5.452839000	-0.488582000	1.783168000
1	5.163560000	-0.507801000	0.037011000
6	2.252534000	-2.931515000	-2.280404000
1	1.163238000	-3.025059000	-2.225127000
1	2.654433000	-3.868704000	-2.683002000
1	2.491402000	-2.137072000	-2.993287000
6	2.593783000	-3.864715000	0.045320000
1	3.100175000	-3.758101000	1.008413000
1	2.957410000	-4.788645000	-0.419323000
1	1.521289000	-3.978332000	0.235231000
6	2.899568000	-1.243376000	2.618046000
1	1.866547000	-0.969576000	2.846947000
1	3.540974000	-0.861214000	3.420928000
1	2.969640000	-2.335105000	2.631785000
1	0.365999000	2.104514000	-0.207772000
1	-0.279204000	0.937105000	1.647694000
6	-0.465684000	3.969577000	0.223006000
6	1.820903000	3.319011000	0.665800000
6	2.261832000	4.106463000	-0.569591000
8	1.368771000	5.195053000	-0.821340000
6	0.021501000	4.742558000	-1.002238000
1	-1.475298000	3.583394000	0.066807000
1	2.476402000	2.459782000	0.830825000
1	2.295450000	3.443264000	-1.448616000
1	-0.037643000	4.105872000	-1.899405000
7	0.435727000	2.850303000	0.524115000
1	3.253560000	4.542251000	-0.421821000
1	1.879078000	3.961362000	1.552366000
1	-0.498911000	4.626365000	1.098649000
1	-0.586290000	5.636238000	-1.166703000
6	-0.230603000	1.929364000	2.167553000
8	-1.284764000	2.465372000	2.574005000
1	0.728029000	2.079113000	2.696822000
1	-0.273223000	-2.120161000	-0.821116000

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44	0.162751000	-0.868209000	0.077605000
15	-2.157952000	-1.070892000	-0.290817000
15	2.459160000	-0.403568000	-0.172306000
8	0.323916000	-2.485685000	2.653465000
7	0.015746000	0.478848000	-1.522529000
6	-1.171018000	0.479204000	-2.381884000
1	-1.077621000	-0.281406000	-3.178531000
1	-1.259720000	1.448015000	-2.906446000
6	1.189882000	0.797033000	-2.339382000
1	1.035301000	1.754651000	-2.869005000
1	1.329788000	0.039399000	-3.132188000
6	-3.362283000	-0.570570000	1.055215000
1	-2.962261000	0.407287000	1.354488000
6	3.558971000	-1.772800000	-0.819581000
1	4.576520000	-1.365884000	-0.869043000
6	2.465663000	0.902943000	-1.498948000
1	2.491750000	1.866738000	-0.982051000
1	3.364711000	0.845728000	-2.120930000
6	3.398229000	0.458952000	1.209573000
1	2.804270000	1.375870000	1.329875000
6	-2.453695000	0.235484000	-1.584277000
1	-3.295617000	-0.013184000	-2.238474000
1	-2.726087000	1.143079000	-1.037142000
6	-2.367788000	-3.878759000	-0.154448000
1	-1.276742000	-3.961223000	-0.121451000
1	-2.769416000	-4.802803000	-0.586957000
1	-2.729218000	-3.807614000	0.873742000
6	-2.272163000	-2.866402000	-2.460107000
1	-2.646650000	-2.099043000	-3.143111000
1	-2.601789000	-3.839566000	-2.842338000
1	-1.176903000	-2.847339000	-2.487917000
6	-2.784778000	-2.677608000	-1.021412000
1	-3.879738000	-2.609628000	-1.044642000
6	0.258726000	-1.847694000	1.668523000
6	-3.305894000	-1.473574000	2.297175000
1	-3.789311000	-2.438704000	2.114942000
1	-3.842479000	-0.989974000	3.121554000
1	-2.280371000	-1.656762000	2.626503000
6	-4.809940000	-0.394302000	0.567500000
1	-4.887155000	0.290301000	-0.282556000
1	-5.423115000	0.015291000	1.379200000
1	-5.253329000	-1.352514000	0.274253000

6	4.834546000	0.858733000	0.834105000
1	5.481051000	-0.021056000	0.745227000
1	5.257671000	1.498162000	1.617853000
1	4.881726000	1.413044000	-0.108656000
6	3.128481000	-2.190455000	-2.236580000
1	2.084172000	-2.520697000	-2.242841000
1	3.750984000	-3.026044000	-2.577100000
1	3.236886000	-1.380642000	-2.963177000
6	3.539486000	-2.989283000	0.121063000
1	3.888213000	-2.749089000	1.128336000
1	4.190577000	-3.776086000	-0.277670000
1	2.524632000	-3.392952000	0.201435000
6	3.356451000	-0.284909000	2.552854000
1	2.339078000	-0.571977000	2.828603000
1	3.752116000	0.365109000	3.342074000
1	3.973322000	-1.188447000	2.536196000
1	-0.225830000	2.053875000	-0.164826000
1	0.143071000	0.982935000	2.210564000
6	-1.661262000	3.428054000	0.408107000
6	0.716719000	3.819142000	0.355020000
6	0.540222000	4.597133000	-0.952744000
8	-0.763230000	5.187149000	-1.020478000
6	-1.801627000	4.204840000	-0.901369000
1	-2.426467000	2.650868000	0.490347000
1	1.695744000	3.330363000	0.379030000
1	0.685505000	3.921551000	-1.811624000
1	-1.753374000	3.512339000	-1.757403000
7	-0.336682000	2.814581000	0.526623000
1	1.256919000	5.420167000	-1.027999000
1	0.672993000	4.516928000	1.201231000
1	-1.802888000	4.109618000	1.255822000
1	-2.748604000	4.750617000	-0.943579000
6	-0.402574000	1.846355000	2.631082000
8	-1.584402000	1.760987000	2.969522000
1	0.227065000	2.701572000	2.932855000
1	0.381615000	-2.245514000	-0.639864000

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8	-0.001567000	3.356533000	-0.097118000
6	0.000205000	2.716990000	-1.286954000
1	0.897269000	2.886738000	-1.918058000
1	-0.893404000	2.889554000	-1.922213000
44	0.000061000	-0.181703000	-0.100242000
15	2.341077000	0.026350000	0.171285000

15	-2.341006000	0.025683000	0.171493000
8	0.000272000	-2.230065000	-2.334192000
7	-0.000177000	1.313388000	1.545538000
6	1.222302000	1.316212000	2.385950000
1	1.195781000	0.435722000	3.036035000
1	1.225733000	2.204202000	3.035135000
6	-1.222203000	1.314814000	2.386602000
1	-1.225969000	2.202410000	3.036326000
1	-1.194665000	0.433936000	3.036135000
6	3.312419000	0.806224000	-1.232636000
1	2.925994000	1.833534000	-1.223533000
6	-3.347524000	-1.422255000	0.791759000
1	-4.366762000	-1.043632000	0.938990000
6	-2.480530000	1.313364000	1.515388000
1	-2.572414000	2.282424000	1.014636000
1	-3.377185000	1.163481000	2.125335000
6	-3.311685000	0.806985000	-1.232029000
1	-2.924229000	1.833902000	-1.222342000
6	2.480184000	1.315183000	1.514096000
1	3.377300000	1.166649000	2.123693000
1	2.570903000	2.283907000	1.012471000
6	3.377372000	-2.560284000	-0.238410000
1	2.365481000	-2.915512000	-0.459744000
1	3.952177000	-3.404390000	0.159549000
1	3.844806000	-2.257740000	-1.179074000
6	2.820520000	-1.922983000	2.147571000
1	2.881476000	-1.156924000	2.926317000
1	3.422507000	-2.777110000	2.478398000
1	1.778749000	-2.250089000	2.067770000
6	3.347292000	-1.421253000	0.792967000
1	4.366600000	-1.042765000	0.939998000
6	0.000227000	-1.423967000	-1.485714000
6	2.968745000	0.209125000	-2.606593000
1	3.289349000	-0.832977000	-2.697855000
1	3.477884000	0.781566000	-3.390690000
1	1.893466000	0.250370000	-2.799658000
6	4.828662000	0.859079000	-0.988292000
1	5.075314000	1.291258000	-0.012755000
1	5.305099000	1.478043000	-1.757203000
1	5.278339000	-0.138067000	-1.043543000
6	-4.827856000	0.861106000	-0.987551000
1	-5.278384000	-0.135654000	-1.042897000
1	-5.303853000	1.480597000	-1.756311000
1	-5.074039000	1.293334000	-0.011918000
6	-2.820882000	-1.925110000	2.146001000
1	-1.779343000	-2.252852000	2.065822000

1	-3.423375000	-2.779027000	2.476448000
1	-2.881159000	-1.159458000	2.925208000
6	-3.377730000	-2.560451000	-0.240529000
1	-3.845200000	-2.257106000	-1.180917000
1	-3.952550000	-3.404849000	0.156783000
1	-2.365877000	-2.915567000	-0.462222000
6	-2.968623000	0.210307000	-2.606311000
1	-1.893233000	0.250042000	-2.799076000
1	-3.476700000	0.784092000	-3.390115000
1	-3.290850000	-0.831227000	-2.698397000
1	-0.000779000	2.225348000	0.953413000
1	-0.002142000	1.547822000	-1.209064000
1	0.000344000	-1.393560000	0.917920000

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8	-0.001729000	3.533246000	0.372254000
6	0.000045000	3.089354000	-0.903548000
1	0.897111000	3.356522000	-1.499991000
1	-0.893559000	3.359937000	-1.503639000
44	0.000069000	-0.180869000	-0.122015000
15	2.341088000	-0.018219000	0.178920000
15	-2.340992000	-0.018963000	0.179023000
8	0.000297000	-1.851292000	-2.651047000
7	-0.000174000	1.035962000	1.738954000
6	1.222309000	0.906223000	2.569285000
1	1.195793000	-0.065768000	3.072382000
1	1.225731000	1.680718000	3.350388000
6	-1.222200000	0.904707000	2.569714000
1	-1.225969000	1.678733000	3.351290000
1	-1.194647000	-0.067572000	3.072198000
6	3.312422000	0.973308000	-1.084442000
1	2.925980000	1.986318000	-0.913441000
6	-3.347492000	-1.546609000	0.563183000
1	-4.366736000	-1.195947000	0.768282000
6	-2.480524000	1.040659000	1.709181000
1	-2.572418000	2.076565000	1.367522000
1	-3.377180000	0.796457000	2.287853000
6	-3.311688000	0.973897000	-1.083708000
1	-2.924240000	1.986432000	-0.912196000
6	2.480186000	1.042712000	1.708180000
1	3.377310000	0.799911000	2.286721000
1	2.570892000	2.078429000	1.365610000
6	3.377409000	-2.507855000	-0.633579000
1	2.365522000	-2.823745000	-0.908165000
1	3.952221000	-3.404155000	-0.373724000
1	3.844841000	-2.060746000	-1.514751000

6	2.820560000	-2.254819000	1.823053000
1	2.881513000	-1.621164000	2.712862000
1	3.422552000	-3.150425000	2.015033000
1	1.778793000	-2.565256000	1.692661000
6	3.347318000	-1.545731000	0.564521000
1	4.366624000	-1.195162000	0.769406000
6	0.000250000	-1.189090000	-1.686056000
6	2.968745000	0.600363000	-2.535364000
1	3.289358000	-0.414302000	-2.789834000
1	3.477875000	1.289302000	-3.219380000
1	1.893464000	0.671526000	-2.719516000
6	4.828663000	0.986987000	-0.834819000
1	5.075311000	1.259913000	0.196664000
1	5.305092000	1.719465000	-1.496496000
1	5.278345000	0.011042000	-1.046633000
6	-4.827857000	0.988771000	-0.833754000
1	-5.278375000	0.013205000	-1.045606000
1	-5.303858000	1.721737000	-1.495199000
1	-5.074039000	1.261726000	0.197827000
6	-2.820840000	-2.256732000	1.821174000
1	-1.779297000	-2.567715000	1.690304000
1	-3.423328000	-3.152088000	2.012813000
1	-2.881127000	-1.623555000	2.711374000
6	-3.377691000	-2.507762000	-0.635685000
1	-3.845169000	-2.059917000	-1.516465000
1	-3.952499000	-3.404253000	-0.376514000
1	-2.365838000	-2.823461000	-0.910613000
6	-2.968625000	0.601428000	-2.534891000
1	-1.893236000	0.671070000	-2.718986000
1	-3.476705000	1.291630000	-3.218401000
1	-3.290842000	-0.412555000	-2.790082000
1	-0.001094000	2.522461000	1.049713000
1	-0.002280000	1.922534000	-1.011023000
1	0.000368000	-1.538132000	0.692282000

-1692.149083

### 25-Ru-PNP

8	-0.005094000	3.344788000	0.263726000
6	-0.001311000	2.909870000	-1.069568000
1	0.900855000	3.234722000	-1.606267000
1	-0.885233000	3.263584000	-1.618002000
44	0.000018000	-0.133190000	-0.135213000
15	2.334808000	-0.001989000	0.172760000
15	-2.334634000	-0.003365000	0.172659000
8	0.002147000	-1.781193000	-2.695164000

7	-0.000230000	1.086636000	1.623460000
6	1.198425000	1.056278000	2.475310000
1	1.209104000	0.144412000	3.095862000
1	1.182490000	1.906581000	3.179149000
6	-1.198765000	1.054831000	2.475475000
1	-1.183463000	1.904766000	3.179765000
1	-1.208601000	0.142584000	3.095490000
6	3.364325000	0.892011000	-1.119757000
1	2.948639000	1.906773000	-1.057296000
6	-3.263454000	-1.559577000	0.637945000
1	-4.318925000	-1.278907000	0.738988000
6	-2.479355000	1.133973000	1.638651000
1	-2.587463000	2.146494000	1.234831000
1	-3.368887000	0.917118000	2.239132000
6	-3.363116000	0.891461000	-1.119985000
1	-2.946043000	1.905667000	-1.057702000
6	2.478871000	1.136001000	1.638324000
1	3.368584000	0.919934000	2.238835000
1	2.586431000	2.148480000	1.234186000
6	3.125405000	-2.625092000	-0.458522000
1	2.073984000	-2.896723000	-0.598467000
1	3.676355000	-3.527880000	-0.170091000
1	3.518936000	-2.289656000	-1.421362000
6	2.776216000	-2.110242000	1.989583000
1	2.953860000	-1.414145000	2.814163000
1	3.312999000	-3.038212000	2.218944000
1	1.705528000	-2.338485000	1.956242000
6	3.263585000	-1.557913000	0.639328000
1	4.318913000	-1.277014000	0.741119000
6	0.001116000	-1.118617000	-1.727146000
6	3.127044000	0.393829000	-2.553699000
1	3.530724000	-0.611086000	-2.710733000
1	3.631548000	1.063081000	-3.260548000
1	2.063098000	0.375432000	-2.803395000
6	4.862480000	0.964710000	-0.784373000
1	5.043567000	1.330052000	0.231838000
1	5.364551000	1.648393000	-1.478932000
1	5.341334000	-0.015267000	-0.885701000
6	-4.861186000	0.966042000	-0.784732000
1	-5.341106000	-0.013479000	-0.885453000
1	-5.362474000	1.649832000	-1.479754000
1	-5.041913000	1.332225000	0.231233000
6	-2.776856000	-2.112104000	1.988394000
1	-1.706072000	-2.340000000	1.955678000
1	-3.313490000	-3.040303000	2.217174000
1	-2.955220000	-1.416273000	2.813044000

6	-3.124101000	-2.626422000	-0.460083000
1	-3.516787000	-2.290792000	-1.423192000
1	-3.675138000	-3.529398000	-0.172408000
1	-2.072495000	-2.897797000	-0.599142000
6	-3.126267000	0.392459000	-2.553685000
1	-2.062155000	0.370882000	-2.802359000
1	-3.628246000	1.063044000	-3.261056000
1	-3.532740000	-0.611316000	-2.710830000
1	-0.001492000	2.498482000	0.863993000
1	-0.020334000	1.792263000	-1.159926000
1	0.000224000	-1.501606000	0.629545000

-1692.162239

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