

Supporting Information

Unravelling the catalytically preferential pathway between direct and indirect hydrogenation of CO₂ to CH₃OH using N-heterocyclic carbene-based Mn(I) catalysts: A theoretical approach

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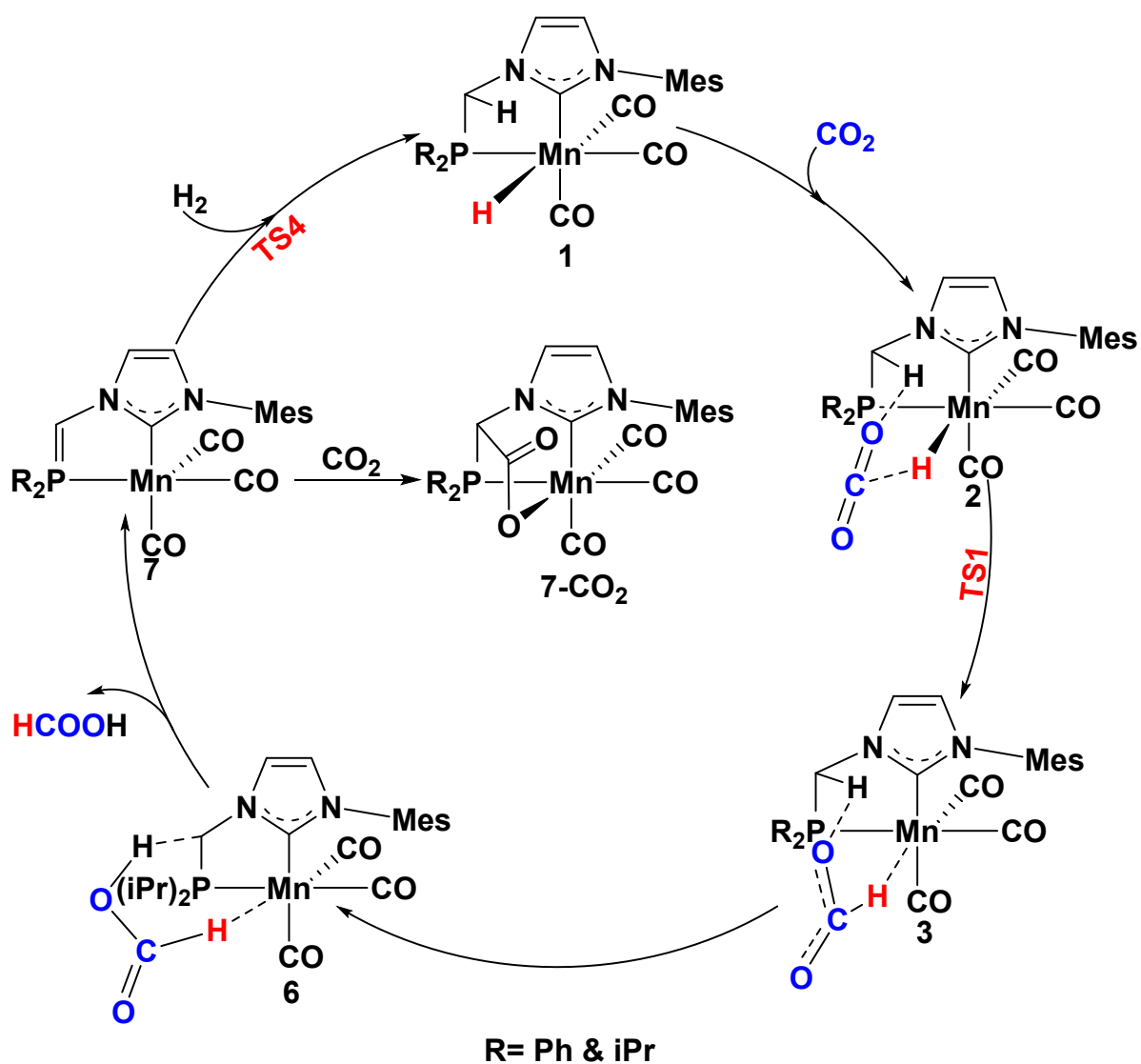
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1. Gaussian full references

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

2. Scheme of ligand participated CO₂ hydrogenation to HCOOH



Scheme S1: Mechanistic pathway for the ligand participated CO₂ hydrogenation to HCOOH.

3. Energy profile diagram for the ligand participated CO₂ hydrogenation to HCOOH

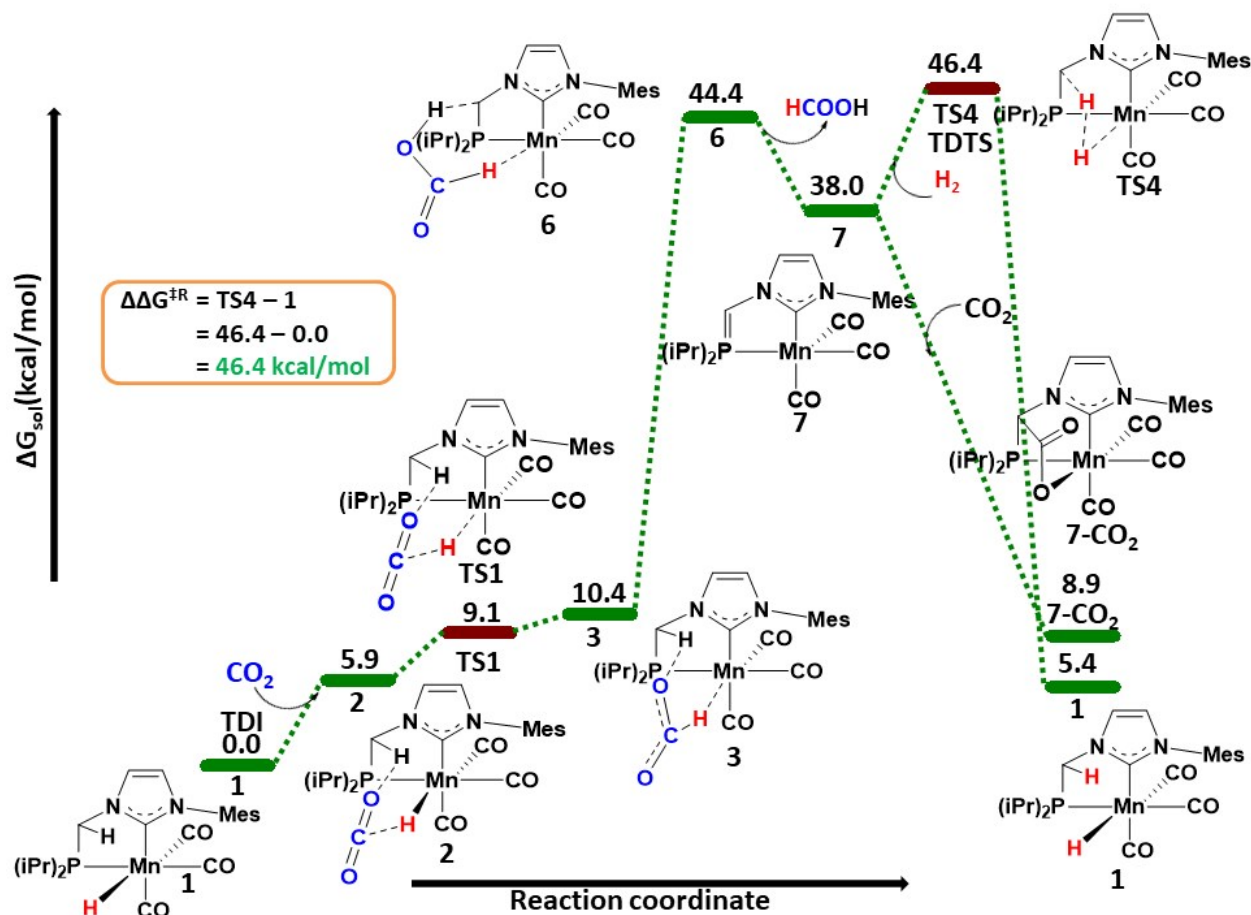


Figure S1: Energy profile diagram for ligand participated CO₂ hydrogenation to HCOOH.

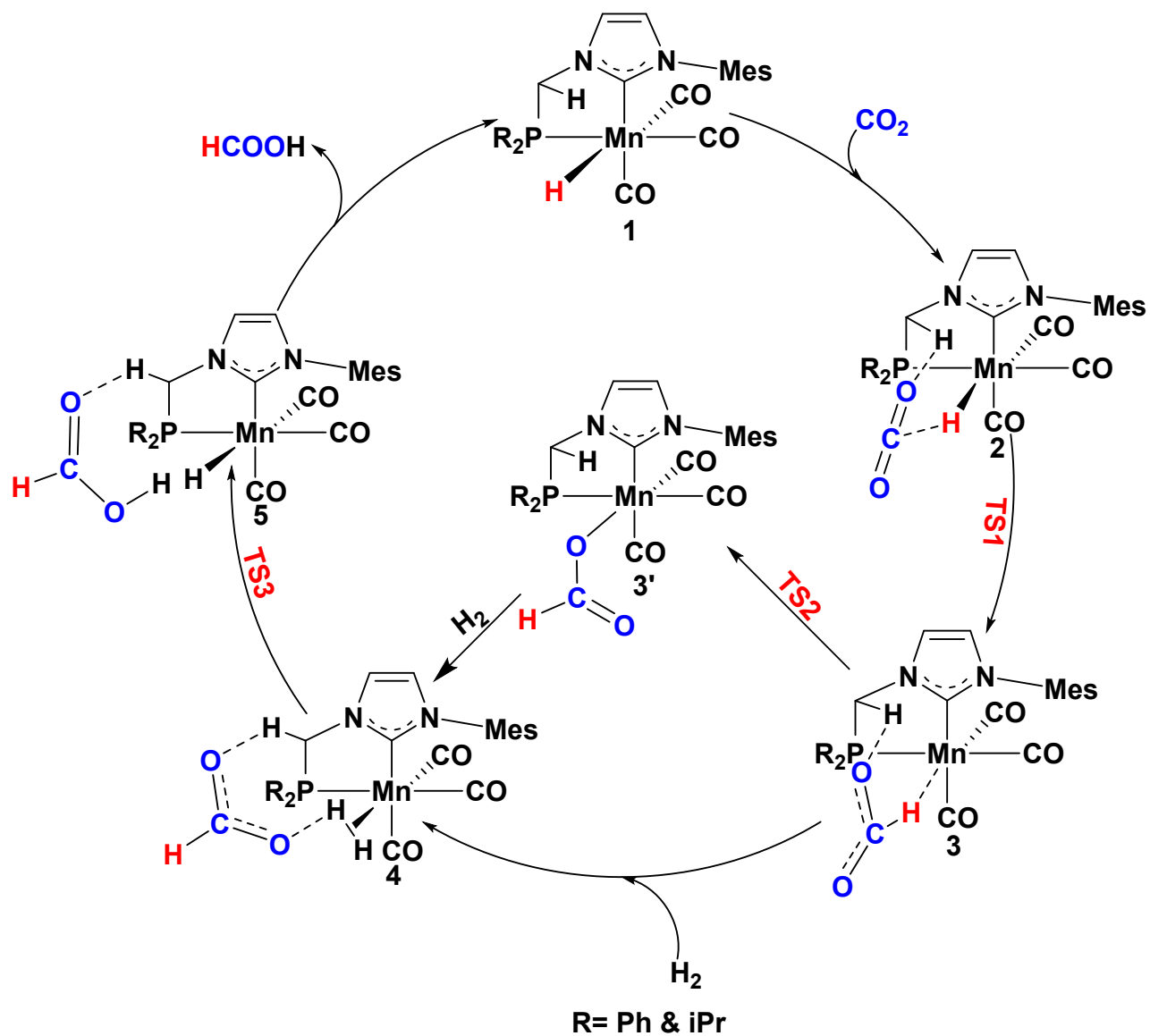
$\Delta\Delta G^{\ddagger R}$ denote the total reaction free energy barrier of the catalytic cycle.

4. Table of the ligand participated reaction free energy for CO₂ hydrogenation reaction to HCOOH by N-heterocyclic carbene-based Mn(I)-iPr and Mn(I)-Ph complexes

Table S1: Ligand participated reaction free energy for CO₂ hydrogenation reaction to HCOOH by N-heterocyclic carbene-based Mn(I)-iPr and Mn(I)-Ph complexes. $\Delta\Delta G^\ddagger$ is the total reaction free energy barriers for reaction. All free energies are calculated in kcal/mol.

Complexes	Relative Free Energies for intermediates and transition states (kcal/mol)								$\Delta\Delta G^\ddagger$
	1 + CO ₂	2	TS1	3	6	7 + HCOOH	TS4	1	
Mn(I)-iPr	0.0	5.9	9.1	10.4	44.4	38.0	46.4	5.4	46.4
Mn(I)-Ph	0.0	4.4	10.0	9.5	41.1	38.5	45.6	5.4	45.6

5. Scheme of ligand assisted CO₂ hydrogenation to HCOOH



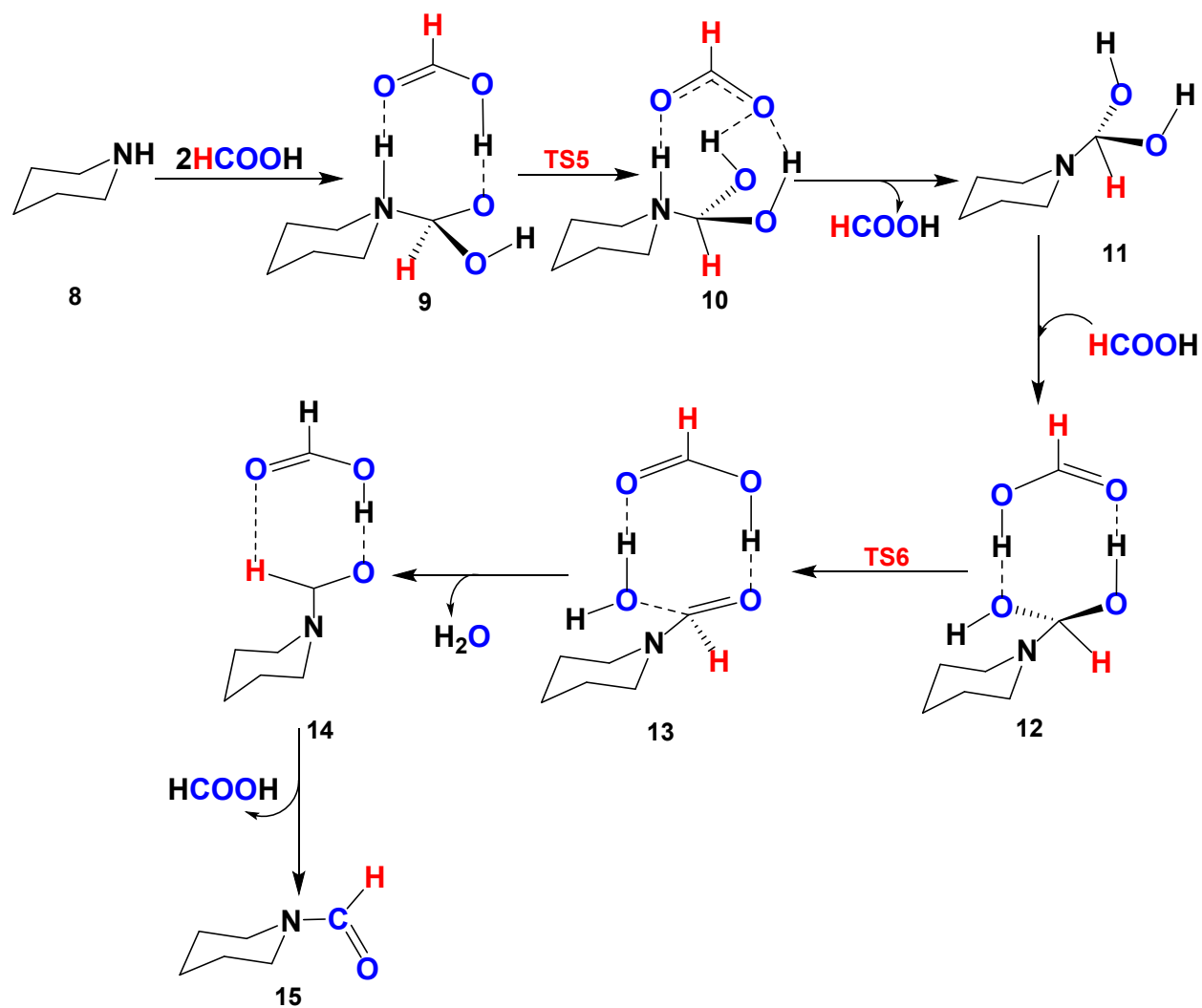
Scheme S2: Mechanistic pathway for the revised Noyori type hydrogenation of CO₂ to HCOOH.

6. Table of the ligand assisted reaction free energy for the hydrogenation of CO₂ to HCOOH by N-heterocyclic carbene-based Mn(I)-iPr and Mn(I)-Ph complexes

Table S2: Ligand assisted reaction free energy for CO₂ hydrogenation reaction to HCOOH by N-heterocyclic carbene-based Mn(I)-iPr and Mn(I)-Ph complexes. $\Delta\Delta G^\ddagger$ represents the total reaction free energy barriers for reaction. All free energies are calculated in kcal/mol.

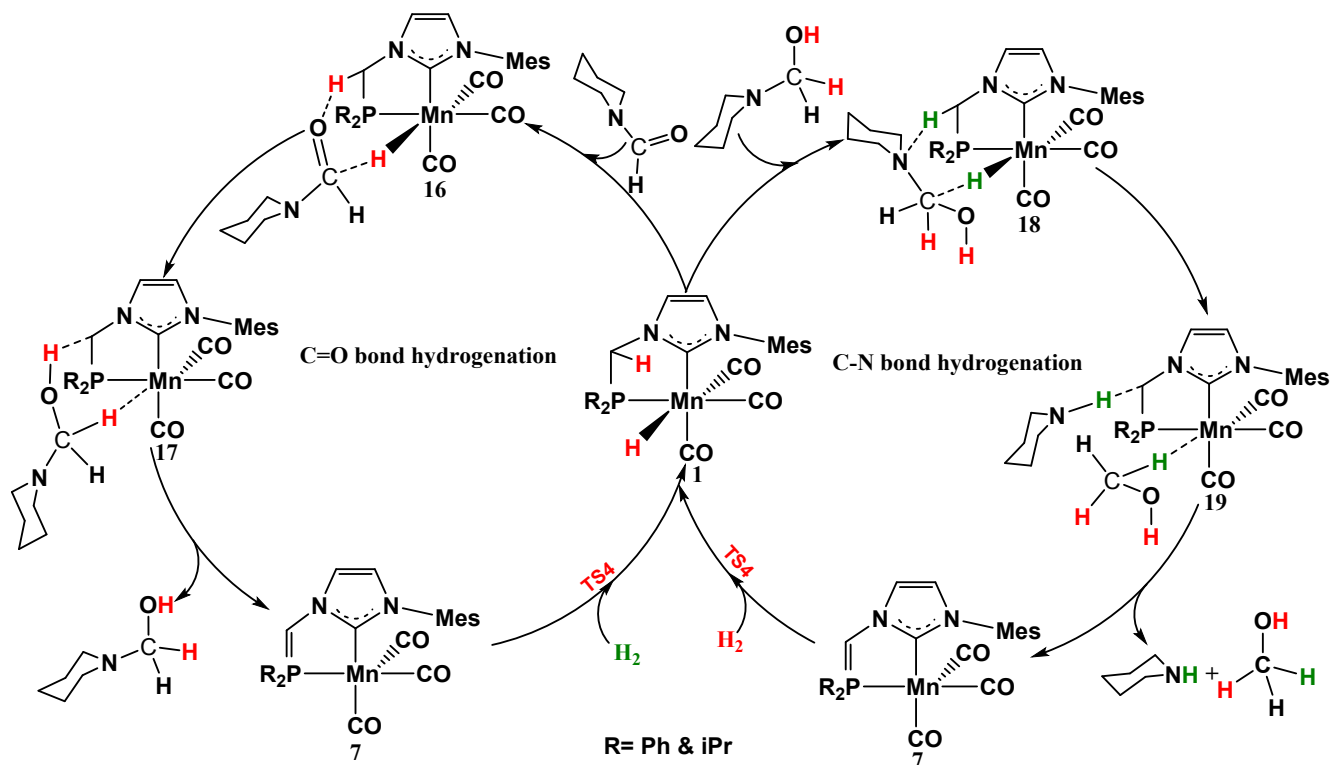
Complexes	Relative Free Energies for intermediates and transition states (kcal/mol)										$\Delta\Delta G^\ddagger$
	1 + CO ₂	2	TS1	3	TS2	3'	4	TS3	5	1 + HCOOH	
Mn(I)-iPr	0.0	5.9	9.1	10.4	17.1	-3.2	17.3	16.1	6.3	5.4	25.7
Mn(I)-Ph	0.0	4.4	10.0	9.5	16.6	-3.8	18.9	16.9	5.7	5.4	25.8

7. Scheme of HCOOH amidation to *N*-formylpiperidine



Scheme S3: Reaction mechanism for the conversion of HCOOH to *N*-formylpiperidine.

8. Scheme of *N*-formylpiperidine hydrogenation to CH₃OH going through C=O bond hydrogenation followed by C–N bond hydrogenation using N-heterocyclic carbene-based Mn(I) catalysts



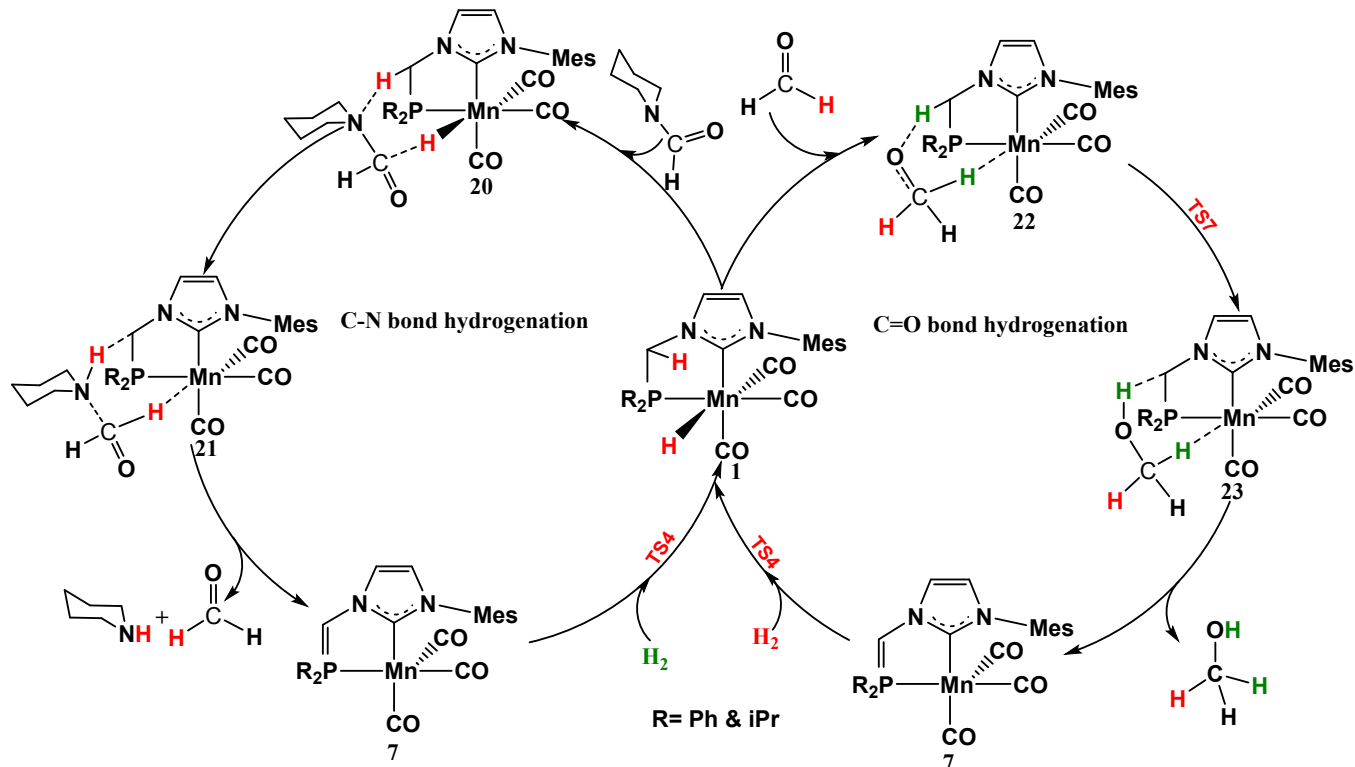
Scheme S4: Hydrogenation of *N*-formylpiperidine to the CH₃OH via C=O bond hydrogenation followed by C–N bond hydrogenation.

9. Table of *N*-formylpiperidine hydrogenation to methanol *via* C=O bond hydrogenation followed by C–N bond hydrogenation reaction by N-heterocyclic carbene-based Mn(I) catalysts

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

Complexes	Relative Free Energies for intermediates and transition states (kcal/mol)											$\Delta\Delta G^{\ddagger R}$
	1	16	17	7	TS4	1	18	19	7	TS4	1	
Mn(I)-iPr	0.0	5.3	48.5	46.4	54.8	13.8	21.2	51.0	33.6	42.0	1.0	54.8
Mn(I)-Ph	0.0	5.2	47.4	46.8	54.0	13.8	16.9	48.0	34.1	41.2	1.0	54.0

10. Scheme of *N*-formylpiperidine hydrogenation to CH₃OH going through C–N bond hydrogenation followed by C=O bond hydrogenation using NHC-based Mn(I) catalysts



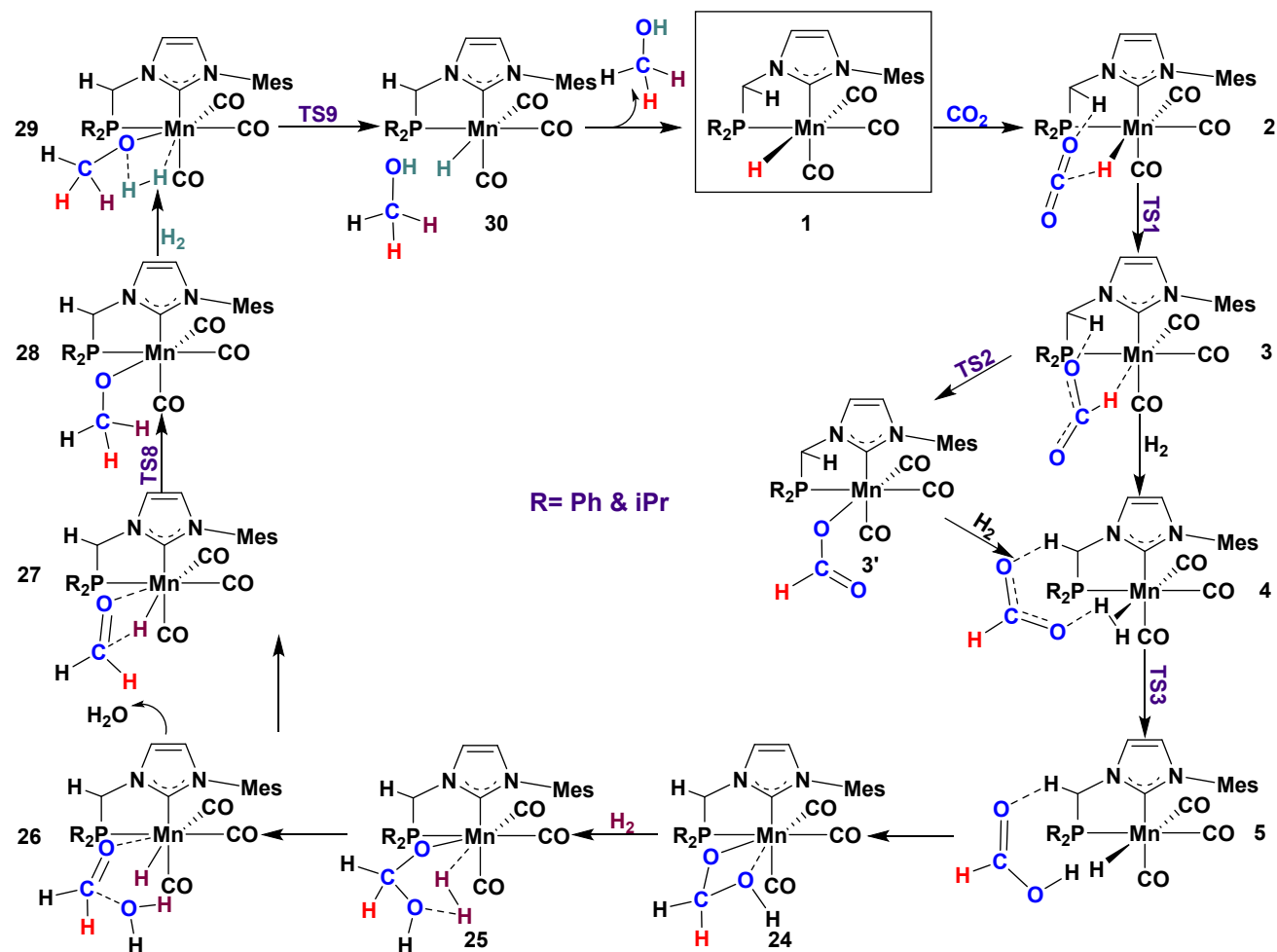
Scheme S5: Hydrogenation of *N*-formylpiperidine to the CH₃OH via C–N bond hydrogenation followed by C=O bond hydrogenation.

11. Table of *N*-formylpiperidine hydrogenation to methanol *via* C–N bond hydrogenation followed by C=O bond hydrogenation reaction N-heterocyclic carbene-based Mn(I) complexes

Table S4: *N*-formyl hydrogenation to methanol via C–N bond hydrogenation followed by C=O bond hydrogenation reaction by N-heterocyclic carbene-based Mn(I)-iPr and Mn(I)-Ph complexes. $\Delta\Delta G^{\ddagger R}$ represents the total reaction free energy barriers for reaction. All free energies are calculated in kcal/mol.

Complexes	Relative Free Energies for intermediates and transition states (kcal/mol)												$\Delta\Delta G^{\ddagger R}$
	1	20	21	7	TS4	1	22	TS7	23	7	TS4	1	
Mn(I)-iPr	0.0	11.0	58.6	47.3	55.7	14.7	27.0	35.4	38.1	33.6	42.0	1.0	55.7
Mn(I)-Ph	0.0	7.5	55.3	47.7	54.9	14.7	26.3	34.9	35.4	34.1	41.2	1.0	54.9

12. Scheme for direct CO₂ hydrogenation to CH₃OH using N-heterocyclic carbene-based Mn(I) catalysts



Scheme S6: Mechanistic pathway for the direct CO₂ hydrogenation to CH₃OH using NHC-based Mn(I) catalysts.

13. Figure of the intermediate having coordinated H_2 molecule (7-H_2)

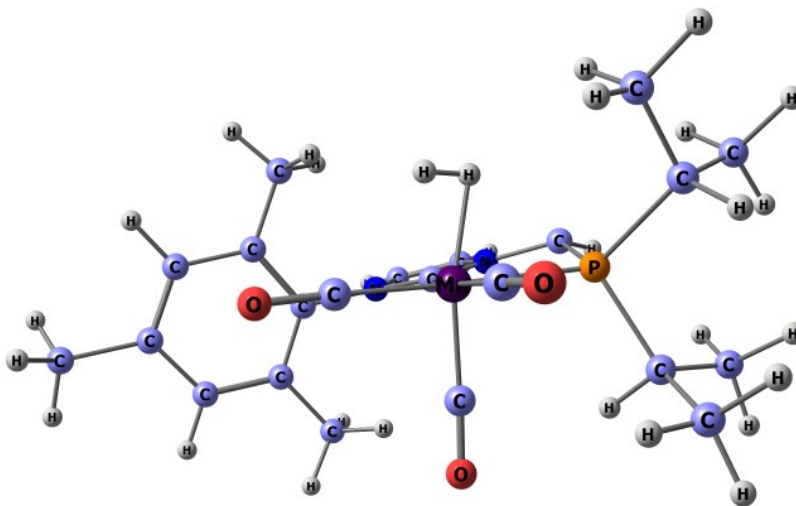


Figure S2: Intermediate (7-H_2) generated by the in-corporation of H_2 molecule with the intermediate **7** of catalyst **1**

14. Table of direct CO₂ hydrogenation to CH₃OH by N-heterocyclic carbene-based Mn(I) complexes

Table S5: Direct CO₂ hydrogenation to CH₃OH by N-heterocyclic carbene-based Mn(I)-iPr and Mn(I)-Ph complexes. $\Delta\Delta G^{\ddagger R}$ represents the total reaction free energy barriers for reaction. All free energies are calculated in kcal/mol.

Complexes	Relative Free Energies for intermediates and transition states (kcal/mol)											$\Delta\Delta G^{\ddagger R}$
	5	24	25	26	27	TS8	28	29	TS9	30	1	
Mn(I)-iPr	6.3	14.1	19.4	15.3	11.9	34.4	2.0	6.0	34.9	-5.5	-4.1	36.3
Mn(I)-Ph	5.7	17.4	20.0	22.2	13.6	35.4	1.8	6.5	35.6	-2.0	-4.1	35.6

15. Transition states of CO₂ hydrogenation reaction to methanol catalyzed by NHC-based Mn(I) catalyst I

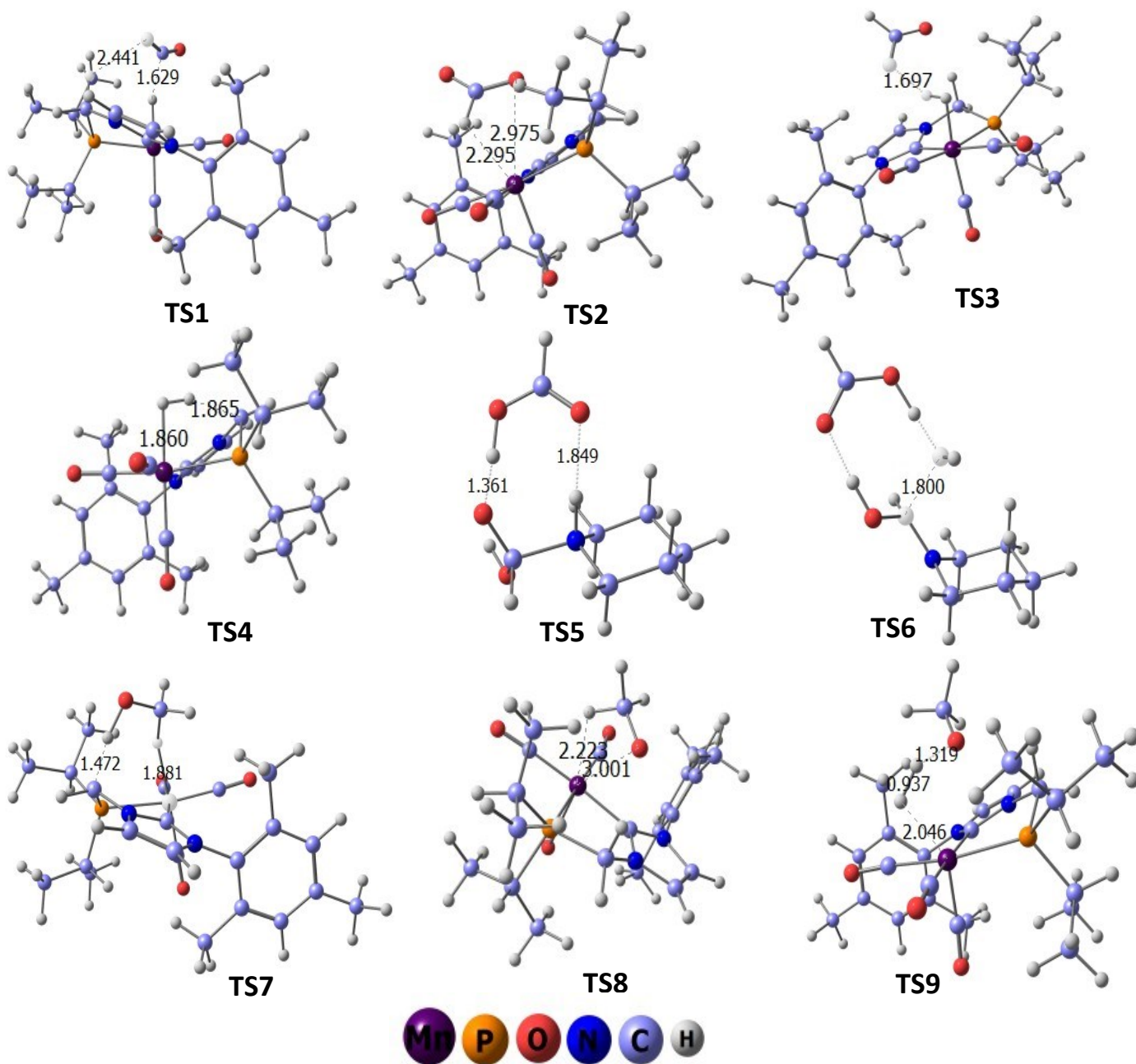


Figure S3: Optimized geometries of the transition states for the hydrogenation of CO₂ to methanol catalyzed by NHC-based Mn(I) catalyst I. Bond lengths and bond angles are in Å and °, respectively.

16. Microkinetic model

Text S1: The microkinetic modeling has been done using Livermore Solver for Ordinary Differential Equations (LSODA) algorithm as implemented in the Complex Pathway Simulator (COPASI) software (version 4.24).¹⁻² Here, we have only considered the most favorable CO₂ hydrogenation pathway for the microkinetic modelling. For the dimerization reactions, which are proceeding without barrier, the rate constants have been calculated by diffusion-controlled

method.³ In such cases, the rate constant is calculated using the following equation, $k = \frac{8k_B T}{3\eta}$,

where k_B is the Boltzmann constant, T is the temperature, and η is the solvent's viscosity.^{4,5} All the rate constants have been calculated at 383.15 K. Moreover, we have also considered an error range up to ± 1.5 kcal/mol (to account the DFT calculation errors) in the reaction free energy barrier and calculated the rate constant for each step. We have considered the 0.005 M concentration of N-heterocyclic carbene based Mn(I) catalysts and various concentration of CO₂ and H₂ to understand the effect of gaseous molecular concentrations on the product formation. The concentration of H₂ has been taken fixed to study the effect of the concentration of CO₂ and vice versa during the course of the reaction. Most of these conditions are closely related to experimental conditions.⁶

17. Table of the important steps in the direct pathway with free energy barriers and rate constants

Table S6: Gibbs free energy and rate constant of the important steps of direct mechanism.

All free energies are in kcal/mol and rate constants are in $\text{M}^{-1}\text{S}^{-1}$.

Steps	Reaction free energy barrier at 298.15 K in kcal/mol	Rate constant (at 383.15 K) (k) in $\text{M}^{-1}\text{S}^{-1}$	Rate constant value by considering ± 1.5 kcal/mol error bar with the reaction free energy barrier at 383.15 K in $\text{M}^{-1}\text{S}^{-1}$	
			$- 1.5$ kcal/mol	$+ 1.5$ kcal/mol
$1 + \text{CO}_2 \rightarrow 3$		$8.2147\text{E} + 06$	$8.2147\text{E} + 06$	$8.2147\text{E} + 06$
$3 + \text{H}_2\text{O} = 5$	5.7	$4.47\text{E} + 09$	$3.21\text{E} + 10$	$6.24\text{E} + 08$
$5 = 3 + \text{H}_2\text{O}$	9.8	$2.05\text{E} + 07$	$1.47\text{E} + 08$	$2.86\text{E} + 06$
$5 + \text{H}_2 \rightarrow 25$		$8.2147\text{E} + 06$	$8.2147\text{E} + 06$	$8.2147\text{E} + 06$
$25 = 28 + \text{H}_2\text{O}$	15	$2.22\text{E} + 04$	$1.59\text{E} + 05$	$3.09\text{E} + 03$
$28 + \text{H}_2\text{O} = 25$	32.4	$2.63\text{E} - 06$	$1.88\text{E} - 05$	$3.66\text{E} - 07$
$28 + \text{H}_2 \rightarrow 29$		$8.2147\text{E} + 06$	$8.2147\text{E} + 06$	$8.2147\text{E} + 06$
$29 = 1 + \text{CH}_3\text{OH}$	28.9	$2.61\text{E} - 04$	$1.87\text{E} - 03$	$3.64\text{E} - 05$
$1 + \text{CH}_3\text{OH} = 29$	39	$4.51\text{E} - 10$	$3.24\text{E} - 09$	$6.29\text{E} - 11$

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

H₂

1	0.000000000	0.000000000	0.371980000
1	0.000000000	0.000000000	-0.371980000

-1.179867

CO₂

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

-188.600082

H₂O

8	0.000000000	0.000000000	0.117230000
1	0.000000000	0.768920000	-0.468920000
1	0.000000000	-0.768920000	-0.468920000

-76.435231

HCOOH

1	-0.683780000	-1.344930000	0.000000000
8	-1.035140000	-0.434280000	0.000000000
8	1.166660000	0.102970000	0.000000000
6	0.000000000	0.422790000	0.000000000
1	-0.368420000	1.458620000	0.000000000

-189.771329

CH₃OH

8	0.752570000	-0.122940000	0.000010000
6	-0.670160000	0.020210000	0.000010000
1	-1.089250000	-0.989250000	0.000370000
1	-1.031140000	0.546760000	-0.894910000
1	-1.030860000	0.547500000	0.894580000
1	1.151660000	0.757250000	-0.000150000

-115.710945

1-Mn-iPr

25	-0.498040000	-0.961640000	-0.117390000
6	-1.333760000	-2.543470000	-0.121760000
6	1.019010000	-1.784410000	-0.598290000
1	-0.755200000	-0.884370000	-1.685320000
6	-0.150700000	-0.978540000	1.645950000
8	-1.881930000	-3.571320000	-0.141340000
8	1.928300000	-2.421580000	-0.941490000
8	0.098160000	-1.045670000	2.783630000
7	-0.688480000	1.990530000	-0.658320000
6	0.167700000	0.954880000	-0.392030000
6	-0.021620000	3.198430000	-0.814630000
6	1.295500000	2.929410000	-0.631480000
7	1.393890000	1.561960000	-0.375040000
1	2.164970000	3.567460000	-0.652680000
1	-0.536170000	4.120990000	-1.034420000
6	-2.115520000	1.780020000	-0.854260000
1	-2.674120000	2.621210000	-0.438360000
15	-2.517390000	0.139380000	-0.061360000
1	-2.333680000	1.708220000	-1.925450000
6	2.652810000	0.901770000	-0.155010000
6	3.339880000	0.390680000	-1.269300000
6	3.161690000	0.809640000	1.147590000
6	4.563930000	-0.243360000	-1.046140000
6	4.389270000	0.155210000	1.322510000
6	5.100000000	-0.379170000	0.242480000
1	5.101550000	-0.662000000	-1.893810000
1	4.792940000	0.059770000	2.327780000
6	2.439500000	1.424670000	2.321050000
1	2.749230000	0.955280000	3.258690000
1	2.661300000	2.497270000	2.395500000
1	1.356370000	1.321720000	2.234340000
6	2.747550000	0.493590000	-2.652440000
1	1.772530000	-0.003080000	-2.698470000
1	2.588090000	1.537670000	-2.946510000
1	3.403380000	0.027770000	-3.392760000
6	6.405090000	-1.110110000	0.448710000
1	7.173380000	-0.758210000	-0.249290000
1	6.785240000	-0.979980000	1.466560000
1	6.278940000	-2.186050000	0.274660000
6	-4.000000000	-0.471390000	-1.034660000
1	-4.397040000	-1.284610000	-0.412990000
6	-3.582250000	-1.067920000	-2.389290000
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1	-5.494800000	0.980350000	-0.304790000

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1	-2.856240000	-1.874980000	-2.284410000
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6	-3.552360000	-0.733410000	2.383600000
6	-4.137180000	1.679330000	1.888640000
1	-3.915510000	2.586460000	1.316760000
1	-5.151840000	1.357920000	1.636900000
1	-4.144190000	1.960330000	2.949140000
1	-4.519910000	-1.081580000	2.003190000
1	-3.668250000	-0.550750000	3.458110000
1	-2.827750000	-1.543520000	2.260220000

-1636.662704

2-Mn-iPr

25	-0.453360000	-0.301560000	-0.957190000
6	-1.293340000	-0.351550000	-2.536780000
6	1.064280000	0.121750000	-1.808010000
1	-0.708520000	1.264360000	-0.958300000
6	-0.101770000	-2.063450000	-0.888580000
8	-1.843100000	-0.355880000	-3.563450000
8	1.972820000	0.417520000	-2.469370000
8	0.150990000	-3.202130000	-0.896660000
7	-0.648130000	0.369510000	1.967550000
6	0.209190000	0.087570000	0.937290000
6	0.023100000	0.640080000	3.151990000
6	1.345050000	0.516510000	2.875350000
7	1.441950000	0.180520000	1.524570000
1	2.219810000	0.630280000	3.496070000
1	-0.492680000	0.894380000	4.064830000
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1	-2.601630000	0.006750000	2.627900000
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1	-2.378040000	1.521930000	1.728800000
6	2.707010000	-0.048260000	0.878980000
6	3.378130000	1.040820000	0.299670000
6	3.247230000	-1.342860000	0.886520000
6	4.619930000	0.801200000	-0.296130000
6	4.488390000	-1.536070000	0.266610000
6	5.186460000	-0.479750000	-0.330800000
1	5.146710000	1.630650000	-0.762470000
1	4.916280000	-2.535650000	0.251370000

6	2.535660000	-2.483060000	1.571880000
1	2.934260000	-3.446380000	1.242300000
1	2.659660000	-2.423690000	2.660830000
1	1.463180000	-2.473900000	1.367500000
6	2.752010000	2.412260000	0.265780000
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1	2.355620000	2.709050000	1.242210000
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1	6.973400000	-1.648440000	-0.701410000
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1	-5.496520000	-0.136490000	0.892030000
1	-4.760360000	1.393650000	1.391820000
1	-5.913950000	1.359380000	0.058360000
1	-3.170490000	2.649010000	-0.293390000
1	-4.415960000	2.459060000	-1.530920000
1	-2.764270000	1.889900000	-1.838510000
6	-3.068870000	-2.076940000	0.579660000
1	-2.126770000	-2.530190000	0.915280000
6	-3.505830000	-2.801270000	-0.705940000
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1	-3.629090000	-3.872180000	-0.507690000
1	-2.773880000	-2.694600000	-1.511710000
6	-0.531360000	3.706470000	-0.032050000
8	-0.783430000	3.382980000	1.064920000
8	-0.282600000	4.088050000	-1.107860000

-1825.253450

TS1-Mn-iPr

25	-0.446340000	0.342740000	-0.892460000
6	-1.299000000	1.032540000	-2.316360000
6	1.064800000	1.190670000	-1.388330000
1	-0.854960000	1.714900000	-0.091210000
6	0.003050000	-1.170400000	-1.743770000
8	-1.852630000	1.493470000	-3.226940000
8	1.972420000	1.786940000	-1.790440000

8	0.304440000	-2.120310000	-2.345030000
7	-0.656760000	-0.398510000	2.007090000
6	0.211330000	-0.227320000	0.964080000
6	-0.001590000	-0.719900000	3.185740000
6	1.320910000	-0.769050000	2.882290000
7	1.432900000	-0.469050000	1.525980000
1	2.185350000	-0.987740000	3.489230000
1	-0.524590000	-0.875140000	4.116400000
6	-2.090720000	-0.190800000	1.853730000
1	-2.637030000	-0.875720000	2.504450000
15	-2.427420000	-0.425670000	0.036980000
1	-2.340750000	0.838760000	2.121910000
6	2.692370000	-0.443400000	0.830240000
6	3.433380000	0.749820000	0.827700000
6	3.148300000	-1.613120000	0.205200000
6	4.656580000	0.755230000	0.151910000
6	4.375500000	-1.555240000	-0.468340000
6	5.138900000	-0.382550000	-0.509750000
1	5.236600000	1.674730000	0.123470000
1	4.739670000	-2.448200000	-0.970710000
6	2.369830000	-2.903020000	0.288850000
1	2.725280000	-3.622420000	-0.453640000
1	2.480130000	-3.361340000	1.280070000
1	1.301900000	-2.747630000	0.122400000
6	2.905200000	1.987360000	1.508700000
1	1.924010000	2.267780000	1.114580000
1	2.776140000	1.831750000	2.585920000
1	3.581970000	2.832970000	1.362820000
6	6.438850000	-0.325490000	-1.275710000
1	6.308600000	0.219920000	-2.218970000
1	7.216710000	0.194800000	-0.705810000
1	6.807480000	-1.326350000	-1.520500000
6	-4.047510000	0.463170000	-0.265730000
1	-4.263680000	0.243940000	-1.319420000
6	-3.886730000	1.988030000	-0.130900000
6	-5.222150000	-0.039570000	0.590130000
1	-5.470520000	-1.083940000	0.389140000
1	-5.017830000	0.066160000	1.662020000
1	-6.116130000	0.555960000	0.369720000
1	-3.653750000	2.285560000	0.897220000
1	-4.829510000	2.474010000	-0.407110000
1	-3.105750000	2.382900000	-0.781970000
6	-2.728600000	-2.267790000	-0.200490000
1	-1.705340000	-2.648930000	-0.294140000
6	-3.432230000	-2.498730000	-1.548480000
6	-3.395850000	-3.047100000	0.941930000

1	-2.821180000	-2.988570000	1.871800000
1	-4.415730000	-2.713530000	1.149650000
1	-3.447810000	-4.107740000	0.666750000
1	-4.487430000	-2.208130000	-1.506080000
1	-3.391420000	-3.561490000	-1.812070000
1	-2.955950000	-1.939700000	-2.361570000
6	-0.752830000	3.120670000	0.726260000
8	-0.880800000	2.777870000	1.865460000
8	-0.608200000	3.936760000	-0.129650000

-1825.248272

3-Mn-iPr

25	0.453260000	0.263170000	0.908990000
6	1.312160000	0.781090000	2.415280000
6	-1.103350000	0.967390000	1.531250000
1	0.814490000	1.878010000	0.160850000
6	0.044540000	-1.336690000	1.583220000
8	1.876300000	1.082010000	3.380770000
8	-2.032290000	1.438940000	2.027130000
8	-0.247240000	-2.365300000	2.036290000
7	0.662940000	-0.352590000	-2.029120000
6	-0.206820000	-0.207740000	-0.985980000
6	0.007150000	-0.630630000	-3.216220000
6	-1.316830000	-0.681160000	-2.915530000
7	-1.429160000	-0.421570000	-1.553290000
1	-2.182280000	-0.871070000	-3.530520000
1	0.529610000	-0.754260000	-4.151840000
6	2.095590000	-0.119390000	-1.889500000
1	2.646670000	-0.782910000	-2.558730000
15	2.487010000	-0.370880000	-0.088910000
1	2.307280000	0.924460000	-2.138360000
6	-2.693660000	-0.385470000	-0.864900000
6	-3.389040000	0.834580000	-0.798660000
6	-3.201470000	-1.573410000	-0.317860000
6	-4.620820000	0.841200000	-0.137750000
6	-4.433970000	-1.510570000	0.345390000
6	-5.154310000	-0.315140000	0.447800000
1	-5.169690000	1.777220000	-0.063830000
1	-4.838000000	-2.418560000	0.786630000
6	-2.481090000	-2.890070000	-0.478340000
1	-2.797450000	-3.603570000	0.287320000
1	-2.699980000	-3.334350000	-1.457780000
1	-1.397240000	-2.779410000	-0.408690000
6	-2.810830000	2.103320000	-1.373580000
1	-2.038080000	2.517900000	-0.717250000

1	-2.344570000	1.942350000	-2.349840000
1	-3.586090000	2.866100000	-1.484900000
6	-6.467650000	-0.255650000	1.190150000
1	-7.234310000	0.262080000	0.602670000
1	-6.841250000	-1.255530000	1.430990000
1	-6.355930000	0.294560000	2.132650000
6	4.066900000	0.588860000	0.196390000
1	4.437470000	0.197040000	1.152740000
6	3.794430000	2.093770000	0.367290000
6	5.137190000	0.364340000	-0.886950000
1	5.423520000	-0.682660000	-0.998920000
1	4.799980000	0.733880000	-1.861890000
1	6.040750000	0.926990000	-0.624630000
1	3.408140000	2.540970000	-0.553170000
1	4.733410000	2.600830000	0.617100000
1	3.081600000	2.305290000	1.166340000
6	2.847270000	-2.196940000	0.132500000
1	1.845730000	-2.624780000	-0.001220000
6	3.291570000	-2.454630000	1.583520000
6	3.787860000	-2.890490000	-0.862750000
1	3.536060000	-2.681780000	-1.907020000
1	4.833270000	-2.615420000	-0.699370000
1	3.714440000	-3.975660000	-0.722960000
1	4.322020000	-2.119050000	1.745780000
1	3.257290000	-3.528350000	1.798590000
1	2.653530000	-1.949830000	2.314910000
6	0.665090000	2.939130000	-0.483420000
8	0.991680000	2.785350000	-1.660460000
8	0.262410000	3.836300000	0.245260000

-1825.246239

TS2-Mn-iPr

25	-0.437830000	0.224210000	-0.845200000
6	-1.215900000	0.869570000	-2.351870000
6	1.112990000	0.948850000	-1.448360000
1	-0.727450000	1.797980000	0.000520000
6	-0.084590000	-1.346860000	-1.611020000
8	-1.640190000	1.267980000	-3.351390000
8	2.020640000	1.459070000	-1.947320000
8	0.168970000	-2.359840000	-2.119030000
7	-0.551150000	-0.688520000	2.028550000
6	0.278290000	-0.387190000	0.988720000
6	0.151540000	-1.039460000	3.169320000
6	1.467300000	-0.978530000	2.838280000
7	1.527280000	-0.580930000	1.506770000

1	2.359050000	-1.174890000	3.412480000
1	-0.339170000	-1.285130000	4.098100000
6	-1.995520000	-0.499610000	1.971540000
1	-2.493740000	-1.298550000	2.524830000
15	-2.475280000	-0.438200000	0.169370000
1	-2.227460000	0.465770000	2.421700000
6	2.772890000	-0.387440000	0.811900000
6	3.368750000	0.884030000	0.846850000
6	3.361270000	-1.479450000	0.156590000
6	4.586020000	1.047240000	0.178890000
6	4.576570000	-1.262590000	-0.505040000
6	5.202210000	-0.009850000	-0.504270000
1	5.053610000	2.028900000	0.175250000
1	5.042230000	-2.092220000	-1.031860000
6	2.730440000	-2.849630000	0.192860000
1	2.899950000	-3.332250000	1.163840000
1	1.650080000	-2.809040000	0.038870000
1	3.157070000	-3.495950000	-0.578830000
6	2.692000000	2.041000000	1.537100000
1	3.336780000	2.923400000	1.544090000
1	1.758940000	2.313170000	1.032320000
1	2.426370000	1.801010000	2.572210000
6	6.523630000	0.197470000	-1.205320000
1	6.576090000	1.187110000	-1.670940000
1	7.358410000	0.126510000	-0.496080000
1	6.687470000	-0.553850000	-1.984100000
6	-4.084100000	0.555160000	0.100760000
1	-4.861350000	-0.202210000	-0.052490000
6	-4.095130000	1.498670000	-1.110850000
6	-4.423490000	1.320260000	1.390200000
1	-4.539780000	0.656580000	2.253690000
1	-3.668340000	2.075360000	1.627910000
1	-5.379480000	1.838100000	1.249600000
1	-3.312010000	2.258900000	-1.034060000
1	-5.059820000	2.017070000	-1.159320000
1	-3.963530000	0.963280000	-2.054600000
6	-3.001500000	-2.183390000	-0.263710000
1	-2.071230000	-2.759530000	-0.182210000
6	-3.468230000	-2.218200000	-1.730120000
6	-4.047350000	-2.808580000	0.669610000
1	-3.698550000	-2.878790000	1.704510000
1	-4.990070000	-2.250340000	0.665080000
1	-4.272460000	-3.828160000	0.334910000
1	-4.415610000	-1.682610000	-1.859990000
1	-3.631450000	-3.255030000	-2.044300000
1	-2.734540000	-1.775620000	-2.410380000

6	-0.998480000	2.817250000	0.658590000
8	-1.211270000	2.537060000	1.839110000
8	-0.980100000	3.808570000	-0.059170000

-1825.235571

3'-Mn-iPr

25	-0.438220000	0.557200000	-0.750020000
6	-1.298910000	1.445530000	-2.073210000
6	1.112100000	1.410190000	-1.154490000
1	-0.553630000	3.610260000	-0.423290000
6	-0.021710000	-0.780370000	-1.856190000
8	-1.849250000	1.971150000	-2.947130000
8	2.036750000	2.011690000	-1.498280000
8	0.271440000	-1.634790000	-2.587810000
7	-0.638490000	-0.801560000	1.917120000
6	0.232390000	-0.448710000	0.927050000
6	0.012910000	-1.364150000	3.004140000
6	1.333520000	-1.383550000	2.686120000
7	1.446980000	-0.824530000	1.415090000
1	2.195980000	-1.732340000	3.231930000
1	-0.511160000	-1.689880000	3.889160000
6	-2.064770000	-0.503250000	1.833200000
1	-2.634790000	-1.259020000	2.376160000
15	-2.438220000	-0.432400000	0.013200000
1	-2.255920000	0.486180000	2.255670000
6	2.709090000	-0.606450000	0.758950000
6	3.380560000	0.602720000	1.004210000
6	3.229880000	-1.605060000	-0.076880000
6	4.613460000	0.798050000	0.374280000
6	4.463230000	-1.357360000	-0.693070000
6	5.166660000	-0.165350000	-0.480080000
1	5.143980000	1.732900000	0.538080000
1	4.881500000	-2.113770000	-1.353140000
6	2.510780000	-2.916350000	-0.280650000
1	2.862560000	-3.416580000	-1.186730000
1	2.685830000	-3.593970000	0.564760000
1	1.430630000	-2.781600000	-0.368530000
6	2.770650000	1.659620000	1.891320000
1	1.750930000	1.910500000	1.578780000
1	2.704110000	1.318900000	2.931500000
1	3.367140000	2.575330000	1.873720000
6	6.474040000	0.098190000	-1.188410000
1	7.147600000	0.704250000	-0.573620000
1	6.989590000	-0.833170000	-1.444040000
1	6.303520000	0.647550000	-2.123300000

6	-4.096670000	0.415930000	-0.123390000
1	-4.348380000	0.305000000	-1.186170000
6	-3.991290000	1.920080000	0.181210000
6	-5.207750000	-0.238810000	0.713780000
1	-5.394690000	-1.275900000	0.426280000
1	-4.975830000	-0.214570000	1.784860000
1	-6.144010000	0.314040000	0.571900000
1	-3.681050000	2.113440000	1.211820000
1	-4.974130000	2.382500000	0.032910000
1	-3.281140000	2.427710000	-0.472590000
6	-2.651100000	-2.219220000	-0.529610000
1	-1.615830000	-2.522140000	-0.720950000
6	-3.401050000	-2.267560000	-1.872110000
6	-3.223990000	-3.209420000	0.494730000
1	-2.593210000	-3.284390000	1.386350000
1	-4.237860000	-2.954730000	0.814060000
1	-3.262000000	-4.208870000	0.044650000
1	-4.468830000	-2.058340000	-1.746190000
1	-3.308410000	-3.266530000	-2.312780000
1	-2.996740000	-1.550870000	-2.596290000
6	-0.825090000	3.243440000	0.593150000
8	-0.875690000	1.960910000	0.724280000
8	-1.048020000	4.065800000	1.486170000

-1825.267955

4-Mn-iPr

25	-0.304060000	-1.007310000	-0.532160000
6	-1.028100000	-2.230960000	-1.661250000
6	1.362530000	-1.505270000	-1.084390000
1	-0.370820000	4.355750000	-1.267790000
6	-0.230890000	-2.155400000	0.844410000
8	-1.463450000	-3.029440000	-2.375150000
8	2.343650000	-1.940810000	-1.505720000
8	-0.161560000	-2.875420000	1.747390000
7	-0.606090000	1.259120000	1.426460000
6	0.285610000	0.493220000	0.744870000
6	0.024190000	2.255280000	2.152740000
6	1.355650000	2.100530000	1.940370000
7	1.499920000	1.014770000	1.079540000
1	2.207150000	2.654660000	2.301890000
1	-0.527320000	2.991750000	2.714360000
6	-2.056240000	1.157030000	1.292790000
1	-2.494100000	0.983220000	2.279900000
15	-2.444420000	-0.255870000	0.145150000
1	-2.411300000	2.107210000	0.881860000

6	2.776300000	0.586460000	0.572020000
6	3.265820000	1.191280000	-0.599810000
6	3.498170000	-0.388500000	1.275700000
6	4.508000000	0.762510000	-1.076970000
6	4.739020000	-0.780950000	0.757770000
6	5.254590000	-0.224440000	-0.418160000
1	4.902880000	1.208810000	-1.986930000
1	5.310240000	-1.541460000	1.284910000
6	2.950180000	-1.016020000	2.533570000
1	2.127920000	-1.702960000	2.307340000
1	3.724760000	-1.587190000	3.052440000
1	2.556780000	-0.265370000	3.226940000
6	2.484670000	2.272160000	-1.304650000
1	1.436670000	2.001650000	-1.465520000
1	2.471450000	3.195210000	-0.711850000
1	2.934650000	2.505920000	-2.273510000
6	6.576890000	-0.682290000	-0.985160000
1	7.217750000	0.169250000	-1.240870000
1	7.121090000	-1.317120000	-0.279440000
1	6.424700000	-1.260960000	-1.904900000
6	-3.726870000	0.310090000	-1.114540000
1	-4.464750000	-0.501940000	-1.081390000
6	-3.181310000	0.390810000	-2.548300000
6	-4.425020000	1.624620000	-0.726840000
1	-4.842730000	1.603650000	0.284640000
1	-3.733170000	2.469140000	-0.797240000
1	-5.254860000	1.802880000	-1.421290000
1	-2.434390000	1.183090000	-2.632640000
1	-4.009770000	0.622920000	-3.228700000
1	-2.742780000	-0.554290000	-2.880140000
6	-3.391040000	-1.435140000	1.254070000
1	-2.702840000	-1.598600000	2.093980000
6	-3.644290000	-2.784370000	0.562210000
6	-4.702870000	-0.855280000	1.809260000
1	-4.566610000	0.107290000	2.311630000
1	-5.451620000	-0.722890000	1.021530000
1	-5.123530000	-1.550690000	2.545150000
1	-4.271820000	-2.671690000	-0.329280000
1	-4.170860000	-3.456840000	1.248760000
1	-2.719700000	-3.282430000	0.260920000
6	-1.079640000	3.594000000	-0.853540000
8	-0.986830000	2.430570000	-1.345570000
8	-1.872230000	3.989730000	0.037380000
1	-0.246660000	-0.036700000	-1.963850000
1	-0.454130000	0.519210000	-1.429820000

-1826.415114

TS3-Mn-iPr

25	0.379300000	-0.496940000	0.976840000
6	1.148760000	-1.316260000	2.396460000
6	-1.172600000	-0.290080000	1.902290000
1	0.948600000	4.938750000	0.555860000
6	-0.173860000	-2.068470000	0.309670000
8	1.636030000	-1.859890000	3.294500000
8	-2.098170000	-0.208360000	2.585480000
8	-0.549610000	-3.088910000	-0.088280000
7	0.669350000	1.000940000	-1.611360000
6	-0.233370000	0.476130000	-0.738990000
6	0.051430000	1.674790000	-2.650990000
6	-1.285270000	1.543010000	-2.447630000
7	-1.443420000	0.802230000	-1.280350000
1	-2.131760000	1.896110000	-3.014830000
1	0.608670000	2.185430000	-3.420520000
6	2.109570000	0.945930000	-1.383760000
1	2.627990000	0.836310000	-2.338540000
15	2.425040000	-0.450190000	-0.206330000
1	2.422830000	1.878640000	-0.891480000
6	-2.730830000	0.378550000	-0.790870000
6	-3.437230000	1.215310000	0.088140000
6	-3.251580000	-0.843880000	-1.248340000
6	-4.680850000	0.767700000	0.548980000
6	-4.494730000	-1.250910000	-0.749560000
6	-5.217880000	-0.464370000	0.156100000
1	-5.234820000	1.392350000	1.245780000
1	-4.907470000	-2.201310000	-1.080350000
6	-2.539870000	-1.666140000	-2.295640000
1	-1.458020000	-1.680030000	-2.153280000
1	-2.894590000	-2.700160000	-2.288710000
1	-2.727370000	-1.256140000	-3.296360000
6	-2.881920000	2.549530000	0.514760000
1	-1.825550000	2.501170000	0.792370000
1	-2.946520000	3.278080000	-0.303950000
1	-3.446850000	2.951090000	1.360630000
6	-6.533550000	-0.945830000	0.719190000
1	-7.210600000	-0.111140000	0.928220000
1	-7.038510000	-1.632450000	0.032140000
1	-6.376100000	-1.482780000	1.663640000
6	4.035520000	0.013750000	0.628890000
1	4.433960000	-0.945500000	0.984440000
6	3.804400000	0.933660000	1.841400000
6	5.058310000	0.662630000	-0.324730000

1	5.233560000	0.085630000	-1.234290000
1	4.741070000	1.670830000	-0.609320000
1	6.018290000	0.761160000	0.195370000
1	3.334430000	1.875490000	1.538410000
1	4.773500000	1.174660000	2.294210000
1	3.190810000	0.462630000	2.612840000
6	2.727230000	-1.986460000	-1.236590000
1	1.748380000	-2.131300000	-1.712480000
6	3.003010000	-3.191230000	-0.318880000
6	3.783510000	-1.899950000	-2.347930000
1	3.650680000	-1.029210000	-2.997180000
1	4.799010000	-1.875440000	-1.941780000
1	3.709320000	-2.791960000	-2.981420000
1	3.987000000	-3.110430000	0.156560000
1	2.998800000	-4.114530000	-0.909130000
1	2.256170000	-3.303170000	0.471710000
6	1.266960000	3.869670000	0.494620000
8	0.395820000	3.028890000	0.877770000
8	2.422160000	3.644930000	0.060190000
1	0.999990000	0.858430000	1.782980000
1	0.694390000	1.397110000	1.237500000

-1826.417087

5-Mn-iPr

25	0.423920000	-0.318400000	0.984620000
6	1.247960000	-0.591360000	2.552470000
6	-1.058480000	0.215720000	1.845820000
1	0.611550000	5.235910000	0.105030000
6	-0.102120000	-2.031360000	0.839160000
8	1.791000000	-0.764460000	3.566350000
8	-1.948040000	0.572960000	2.499870000
8	-0.452750000	-3.141240000	0.804580000
7	0.658950000	0.500570000	-1.901210000
6	-0.221260000	0.183820000	-0.905320000
6	0.016380000	0.817510000	-3.088940000
6	-1.312560000	0.683710000	-2.847640000
7	-1.441140000	0.297460000	-1.514020000
1	-2.172530000	0.821990000	-3.483840000
1	0.553210000	1.108850000	-3.978150000
6	2.096360000	0.559770000	-1.671700000
1	2.626140000	0.213920000	-2.561900000
15	2.432780000	-0.461350000	-0.150860000
1	2.380810000	1.593490000	-1.457000000
6	-2.715380000	0.031250000	-0.900600000
6	-3.405100000	1.092620000	-0.292380000

6	-3.242970000	-1.267480000	-0.963490000
6	-4.641430000	0.814460000	0.298730000
6	-4.479980000	-1.499160000	-0.348390000
6	-5.187720000	-0.475880000	0.293500000
1	-5.180690000	1.620700000	0.790630000
1	-4.896990000	-2.503200000	-0.373290000
6	-2.534510000	-2.369230000	-1.712630000
1	-2.902820000	-3.351190000	-1.404000000
1	-2.704040000	-2.273380000	-2.792930000
1	-1.455680000	-2.348140000	-1.550610000
6	-2.816810000	2.480150000	-0.258600000
1	-1.887060000	2.503640000	0.316890000
1	-2.576350000	2.841680000	-1.264990000
1	-3.512470000	3.187230000	0.200960000
6	-6.495630000	-0.759350000	0.993230000
1	-7.196050000	0.076490000	0.891330000
1	-6.977900000	-1.658800000	0.597330000
1	-6.332630000	-0.918490000	2.066910000
6	4.008670000	0.288270000	0.537470000
1	4.392590000	-0.487150000	1.213310000
6	3.730290000	1.555190000	1.365720000
6	5.075570000	0.593390000	-0.530980000
1	5.331550000	-0.268930000	-1.147860000
1	4.750940000	1.402730000	-1.194910000
1	5.995570000	0.931570000	-0.039630000
1	3.282820000	2.343570000	0.751160000
1	4.678050000	1.938660000	1.762950000
1	3.062690000	1.366930000	2.207610000
6	2.842480000	-2.188610000	-0.768290000
1	1.866820000	-2.496930000	-1.167920000
6	3.174880000	-3.098060000	0.428270000
6	3.885380000	-2.362520000	-1.882560000
1	3.748360000	-1.665990000	-2.715750000
1	4.905710000	-2.249600000	-1.504500000
1	3.805490000	-3.377050000	-2.292150000
1	4.162900000	-2.862610000	0.840520000
1	3.195950000	-4.145370000	0.105510000
1	2.441540000	-3.015110000	1.235170000
6	0.878650000	4.167570000	0.062190000
8	0.325780000	3.505920000	1.068110000
8	1.590200000	3.698900000	-0.809280000
1	0.930820000	1.189400000	1.061800000
1	0.551810000	2.520060000	1.028910000

-1826.432629

6-Mn-iPr

25	1.530610000	0.928860000	-0.638980000
6	2.797990000	1.157040000	-1.894140000
6	1.411690000	2.717970000	-0.468350000
6	0.275670000	0.504320000	-1.817730000
8	3.565320000	1.342130000	-2.748360000
8	1.427770000	3.871610000	-0.341800000
8	-0.600210000	0.183820000	-2.529810000
7	1.215900000	0.730460000	1.934360000
6	0.253610000	0.742840000	0.992010000
6	0.697090000	0.756100000	3.219130000
6	-0.658240000	0.789010000	3.057750000
7	-0.919390000	0.758110000	1.679720000
1	-1.457950000	0.831080000	3.779960000
1	1.306510000	0.763600000	4.109400000
6	2.497130000	0.589150000	1.273320000
15	2.564180000	-0.875250000	0.234460000
1	3.349250000	1.055190000	1.753410000
6	-2.235830000	0.670020000	1.103050000
6	-3.004820000	-0.488360000	1.337370000
6	-2.720410000	1.732530000	0.320650000
6	-4.274970000	-0.560930000	0.756560000
6	-3.996230000	1.602840000	-0.246490000
6	-4.787940000	0.469080000	-0.041630000
1	-4.868590000	-1.458950000	0.909400000
1	-4.376640000	2.415200000	-0.861390000
6	-1.907860000	2.975320000	0.059990000
1	-2.561640000	3.823880000	-0.161280000
1	-1.275780000	3.241440000	0.910980000
1	-1.246590000	2.831070000	-0.800220000
6	-2.513680000	-1.642950000	2.179850000
1	-1.426060000	-1.722570000	2.189900000
1	-2.843210000	-1.541820000	3.221590000
1	-2.917350000	-2.585790000	1.799470000
6	-6.151100000	0.331410000	-0.675170000
1	-6.937800000	0.282730000	0.087590000
1	-6.377000000	1.175070000	-1.334390000
1	-6.214290000	-0.591790000	-1.263090000
1	-1.278145749	-1.333201674	-0.502696851
8	-1.721934112	-2.172146358	-0.738167420
8	-3.656562399	-2.815043927	-1.652050862
6	-2.924139558	-1.927961116	-1.276940057
1	-3.178134211	-0.857459922	-1.355102133
6	4.342000000	-1.352110000	-0.090690000
1	4.574590000	-2.085120000	0.693970000
6	5.337420000	-0.190220000	0.031340000

6	4.443390000	-2.050030000	-1.458330000
1	3.746300000	-2.890900000	-1.550000000
1	4.235070000	-1.350960000	-2.274420000
1	5.456200000	-2.444560000	-1.602050000
1	5.117390000	0.620750000	-0.667670000
1	6.346090000	-0.555900000	-0.195360000
1	5.358840000	0.226220000	1.042710000
6	1.770420000	-2.477740000	0.831480000
1	2.490950000	-3.244650000	0.517800000
6	0.452850000	-2.722390000	0.082310000
6	1.612690000	-2.564340000	2.355760000
1	2.554060000	-2.363980000	2.879390000
1	0.865790000	-1.857080000	2.725730000
1	1.281260000	-3.571580000	2.636260000
1	-0.268990000	-1.925470000	0.275210000
1	0.004610000	-3.671930000	0.397050000
1	0.608610000	-2.764160000	-1.000120000

-1825.191961

7-Mn-iPr

25	-0.480470000	-0.837290000	-0.212930000
6	-1.319600000	-2.266000000	-0.941110000
6	1.121620000	-1.592620000	-0.601170000
6	-0.526290000	-1.518560000	1.410600000
8	-1.846400000	-3.182130000	-1.424420000
8	2.066040000	-2.211850000	-0.858960000
8	-0.546020000	-1.929140000	2.499340000
7	-0.685460000	2.063850000	0.378310000
6	0.185060000	1.005950000	0.145720000
6	0.017700000	3.229570000	0.627820000
6	1.350000000	2.916750000	0.568640000
7	1.447120000	1.583080000	0.274850000
1	2.222480000	3.537970000	0.703660000
1	-0.478090000	4.169270000	0.813060000
6	-2.077080000	1.932990000	0.360230000
1	-2.645250000	2.722500000	0.830650000
15	-2.563680000	0.282530000	0.040890000
6	2.695660000	0.888090000	0.147800000
6	3.317400000	0.829540000	-1.110280000
6	3.257750000	0.293560000	1.288410000
6	4.539450000	0.156390000	-1.205630000
6	4.480030000	-0.373220000	1.143530000
6	5.134070000	-0.452270000	-0.091890000
1	5.032800000	0.093860000	-2.173060000
1	4.927670000	-0.844740000	2.015260000

6	2.557880000	0.368960000	2.621940000
1	3.087320000	-0.218780000	3.376670000
1	2.489980000	1.402210000	2.982080000
1	1.534250000	-0.010030000	2.549190000
6	2.659820000	1.441940000	-2.321400000
1	1.681970000	0.981580000	-2.505180000
1	2.483720000	2.515280000	-2.189200000
1	3.274830000	1.303790000	-3.214660000
6	6.430210000	-1.213500000	-0.234910000
1	7.113160000	-0.716410000	-0.932180000
1	6.943080000	-1.321210000	0.726100000
1	6.244740000	-2.222800000	-0.624440000
6	-3.493810000	0.193060000	-1.595460000
1	-3.779990000	-0.860150000	-1.705100000
6	-2.520640000	0.558500000	-2.730000000
6	-4.753360000	1.066220000	-1.655100000
1	-5.522960000	0.732920000	-0.954300000
1	-4.516090000	2.113780000	-1.435060000
1	-5.188300000	1.025010000	-2.661970000
1	-2.122010000	1.570110000	-2.590500000
1	-3.038100000	0.532170000	-3.696560000
1	-1.677910000	-0.140000000	-2.789370000
6	-3.714740000	-0.324210000	1.392500000
1	-3.012320000	-0.496640000	2.217470000
6	-4.364650000	-1.667830000	1.030020000
6	-4.749390000	0.702320000	1.878120000
1	-4.281410000	1.652610000	2.152370000
1	-5.520230000	0.903050000	1.128940000
1	-5.253380000	0.313790000	2.771860000
1	-5.089130000	-1.561440000	0.214740000
1	-4.903810000	-2.065260000	1.898300000
1	-3.623460000	-2.415490000	0.730990000

-1635.430899

TS4-Mn-iPr

25	-0.532850000	-1.106940000	-0.102570000
6	-1.452510000	-2.603780000	0.314610000
6	0.968190000	-2.044190000	-0.470740000
1	-1.031320000	-1.311950000	-1.882330000
6	-0.040770000	-0.854690000	1.587810000
8	-2.040710000	-3.557220000	0.618310000
8	1.885010000	-2.717150000	-0.687650000
8	0.282880000	-0.698760000	2.692110000
7	-0.713910000	1.499900000	-1.412380000
6	0.180190000	0.676990000	-0.790990000

6	-0.083750000	2.623720000	-1.922640000
6	1.238480000	2.514540000	-1.597850000
7	1.385320000	1.325250000	-0.903080000
1	2.074160000	3.168300000	-1.792570000
1	-0.620290000	3.394570000	-2.453310000
6	-2.093200000	1.105290000	-1.540620000
1	-2.714740000	1.931600000	-1.884720000
15	-2.511330000	0.207140000	-0.039690000
1	-1.515980000	-0.617870000	-1.959280000
6	2.628590000	0.832730000	-0.380010000
6	3.453160000	0.057150000	-1.209030000
6	2.979990000	1.146350000	0.943690000
6	4.652280000	-0.426370000	-0.671910000
6	4.184170000	0.634420000	1.439090000
6	5.029530000	-0.156700000	0.648890000
1	5.297060000	-1.040400000	-1.296220000
1	4.467260000	0.857490000	2.465390000
6	2.103830000	2.036410000	1.790270000
1	1.053610000	1.740040000	1.737640000
1	2.412370000	2.006130000	2.838580000
1	2.160750000	3.078220000	1.451250000
6	3.056760000	-0.247120000	-2.632550000
1	2.022400000	-0.597230000	-2.695090000
1	3.129570000	0.646270000	-3.264450000
1	3.703620000	-1.017290000	-3.061000000
6	6.302890000	-0.730430000	1.223900000
1	6.093310000	-1.639440000	1.802310000
1	7.013990000	-0.999170000	0.436440000
1	6.793240000	-0.021500000	1.899620000
6	-4.163810000	-0.615510000	-0.337280000
1	-4.320140000	-1.232050000	0.557290000
6	-4.132810000	-1.546520000	-1.562470000
6	-5.331000000	0.379250000	-0.460710000
1	-5.497450000	0.946400000	0.457630000
1	-5.166060000	1.088740000	-1.279530000
1	-6.256910000	-0.167010000	-0.679080000
1	-4.002310000	-0.974930000	-2.486300000
1	-5.084640000	-2.087230000	-1.627890000
1	-3.335730000	-2.291140000	-1.511730000
6	-2.674130000	1.311540000	1.481790000
1	-1.620560000	1.483270000	1.735280000
6	-3.317910000	0.553800000	2.652390000
6	-3.310340000	2.685810000	1.235560000
1	-2.831880000	3.204950000	0.398290000
1	-4.381190000	2.621230000	1.023810000
1	-3.187910000	3.313170000	2.127480000

1	-4.387460000	0.386240000	2.484240000
1	-3.215710000	1.130630000	3.579730000
1	-2.844380000	-0.421000000	2.816840000

-1636.597436

8

6	-0.832610000	-1.165640000	0.204460000
6	0.630830000	-1.310540000	-0.227880000
6	1.455510000	-0.098460000	0.234590000
6	0.801610000	1.214080000	-0.227000000
6	-0.668520000	1.267010000	0.203690000
1	-2.371050000	0.159700000	-0.089040000
1	-1.433250000	-1.994750000	-0.185590000
1	-0.882550000	-1.210560000	1.310990000
1	1.046720000	-2.239520000	0.181330000
1	0.668520000	-1.385900000	-1.322520000
1	2.484300000	-0.168060000	-0.139220000
1	1.516100000	-0.102770000	1.332890000
1	1.338500000	2.078280000	0.183340000
1	0.850630000	1.284460000	-1.321510000
1	-1.151370000	2.168820000	-0.188630000
1	-0.713440000	1.320330000	1.310100000
7	-1.382010000	0.093050000	-0.314200000

-251.818954

9

6	-1.365540000	1.975070000	-0.297320000
1	-0.704680000	2.531300000	-0.965130000
8	-2.268430000	1.238450000	-0.682850000
1	-2.686140000	-0.282870000	-0.097780000
8	-1.231750000	2.396660000	0.970030000
8	-2.990430000	-1.137100000	0.320340000
1	-1.881920000	1.930520000	1.525920000
6	-2.225420000	-2.163530000	-0.029880000
1	-2.591010000	-3.094840000	0.429170000
8	-1.247450000	-2.119300000	-0.753760000
6	1.671310000	0.835650000	-1.075570000
6	0.913780000	0.043170000	1.110780000
6	2.078710000	-0.957470000	1.196330000
6	2.858120000	-0.142280000	-1.065480000
1	1.315570000	1.005680000	-2.098450000
1	0.027060000	-0.350890000	1.621340000
1	1.744460000	-1.927490000	0.803020000
1	2.558290000	-1.069950000	-1.572780000

7	0.535700000	0.382700000	-0.264690000
1	2.359980000	-1.112390000	2.246090000
1	1.189130000	0.977610000	1.620100000
1	1.998500000	1.808350000	-0.678250000
1	3.696240000	0.281690000	-1.633410000
1	0.081230000	-0.418770000	-0.702130000
6	3.281420000	-0.461630000	0.377080000
1	4.084720000	-1.208090000	0.385600000
1	3.688810000	0.447710000	0.843840000

-631.347677

TS5

6	-0.852850000	1.689370000	-0.339710000
1	-0.390960000	2.346260000	-1.091900000
8	-1.974790000	1.131220000	-0.682750000
1	-2.464190000	-0.025650000	-0.159970000
8	-0.847220000	2.398410000	0.874180000
8	-2.918700000	-0.953730000	0.197030000
1	-1.657070000	2.139310000	1.341430000
6	-2.168650000	-1.995900000	-0.008470000
1	-2.657060000	-2.940710000	0.282150000
8	-1.022400000	-1.995820000	-0.468430000
6	1.460780000	0.757860000	-1.135090000
6	0.809290000	0.259090000	1.202300000
6	1.800610000	-0.906530000	1.246730000
6	2.471930000	-0.390650000	-1.124760000
1	1.027620000	0.898360000	-2.129400000
1	-0.070320000	0.057980000	1.817440000
1	1.279320000	-1.830840000	0.969670000
1	1.994870000	-1.291940000	-1.530820000
7	0.332470000	0.501990000	-0.192310000
1	2.146180000	-1.024490000	2.279980000
1	1.262530000	1.187650000	1.557470000
1	1.929840000	1.698920000	-0.826620000
1	3.297810000	-0.132860000	-1.797050000
1	-0.160760000	-0.360080000	-0.493660000
6	2.981930000	-0.668410000	0.296190000
1	3.650810000	-1.535850000	0.295710000
1	3.570710000	0.190360000	0.648290000

-631.341715

10

6	-0.855400000	-1.514030000	-0.004770000
1	-0.369700000	-2.494250000	-0.008530000

8	-1.582990000	-1.369580000	1.155260000
1	-2.177520000	-0.591800000	1.019840000
8	-1.583910000	-1.361340000	-1.163060000
8	-2.870750000	0.764380000	0.003000000
1	-2.178890000	-0.585020000	-1.021430000
6	-2.184620000	1.831650000	0.005670000
1	-2.746380000	2.787060000	0.004450000
8	-0.925110000	1.911550000	0.009670000
6	1.135950000	-0.576350000	1.239770000
6	1.130600000	-0.559730000	-1.246410000
6	2.218980000	0.513620000	-1.253360000
6	2.224280000	0.496870000	1.256530000
1	0.462660000	-0.482970000	2.091460000
1	0.453830000	-0.454850000	-2.093930000
1	1.745520000	1.501450000	-1.310990000
1	1.750990000	1.483750000	1.329320000
7	0.295450000	-0.468210000	-0.000920000
1	2.813330000	0.386720000	-2.164660000
1	1.565610000	-1.565950000	-1.270200000
1	1.571190000	-1.582720000	1.247990000
1	2.822380000	0.357960000	2.163600000
1	-0.189400000	0.494870000	0.005630000
6	3.099170000	0.430140000	-0.000750000
1	3.832880000	1.243170000	0.003100000
1	3.663600000	-0.512970000	-0.008210000

-631.354000

11

6	1.730520000	-0.000280000	0.308230000
1	1.863380000	-0.000990000	1.400370000
8	2.372000000	-1.165600000	-0.147300000
1	2.163880000	-1.266120000	-1.090660000
8	2.372190000	1.165570000	-0.145610000
1	2.165790000	1.266490000	-1.089290000
6	-0.393710000	-1.211960000	0.329120000
6	-0.393520000	1.212170000	0.328400000
6	-1.795920000	1.255590000	-0.284960000
6	-1.796120000	-1.255610000	-0.284170000
1	0.175600000	-2.093570000	0.032280000
1	0.175880000	2.093520000	0.030970000
1	-1.701130000	1.332160000	-1.376340000
1	-1.701400000	-1.332940000	-1.375510000
7	0.332290000	-0.000080000	-0.107190000
1	-2.308730000	2.160430000	0.062590000
1	-0.472670000	1.231370000	1.432890000

1	-0.472870000	-1.230420000	1.433630000
1	-2.309050000	-2.160150000	0.064010000
6	-2.598650000	0.000160000	0.077280000
1	-3.569520000	0.000090000	-0.432170000
1	-2.804240000	0.000520000	1.157470000

-441.567965

12

6	2.436740000	-1.412880000	0.424650000
6	1.804660000	-0.421250000	1.415960000
6	1.815950000	1.368460000	-0.263080000
6	2.470230000	0.438710000	-1.301370000
1	1.144980000	-0.938970000	2.120170000
1	1.640820000	-1.973180000	-0.080340000
1	3.050610000	-2.136030000	0.976280000
1	1.164680000	2.104660000	-0.737190000
1	2.607280000	1.924770000	0.258800000
1	1.698630000	-0.019540000	-1.935780000
1	3.107420000	1.034910000	-1.966650000
1	2.602380000	0.052120000	2.006600000
6	3.289200000	-0.663940000	-0.612150000
7	1.047240000	0.652580000	0.764610000
6	-0.328090000	0.418660000	0.562700000
1	-0.764570000	0.000980000	1.477990000
8	-0.642820000	-0.675210000	-0.421130000
1	-0.354570000	-0.368130000	-1.295880000
8	-0.954270000	1.574440000	0.134030000
1	-1.916510000	1.388510000	0.086130000
6	-3.966240000	-0.405810000	-0.133600000
1	-5.021820000	-0.712140000	-0.124550000
8	-3.165900000	-1.419670000	-0.395790000
1	-2.195370000	-1.128730000	-0.414610000
8	-3.621490000	0.749870000	0.080070000
1	4.150390000	-0.202830000	-0.105530000
1	3.695970000	-1.361520000	-1.353810000

-631.337536

TS6

6	2.444670000	-1.385730000	0.428590000
6	1.760860000	-0.431910000	1.418420000
6	1.779690000	1.395410000	-0.244820000
6	2.476990000	0.490140000	-1.272110000
1	1.086370000	-0.972820000	2.087990000
1	1.670440000	-1.950650000	-0.103050000

1	3.059320000	-2.102480000	0.986370000
1	1.121090000	2.120800000	-0.722930000
1	2.534680000	1.955000000	0.323090000
1	1.722410000	0.023170000	-1.918480000
1	3.113290000	1.107390000	-1.917650000
1	2.517480000	0.066680000	2.039470000
6	3.305100000	-0.599910000	-0.573350000
7	0.999010000	0.615360000	0.726820000
6	-0.343390000	0.472490000	0.605460000
1	-0.811730000	-0.035420000	1.449450000
8	-0.731400000	-0.887790000	-0.508330000
1	-0.503300000	-0.567910000	-1.395110000
8	-0.993490000	1.512540000	0.075220000
1	-1.976390000	1.299370000	0.075370000
6	-3.871480000	-0.365340000	-0.106800000
1	-4.944860000	-0.612200000	-0.071370000
8	-3.114720000	-1.370590000	-0.394530000
1	-1.993980000	-1.126130000	-0.462270000
8	-3.509110000	0.801090000	0.123020000
1	3.744130000	-1.278260000	-1.313850000
1	4.143040000	-0.126920000	-0.040210000

-631.336205

13

6	-2.572000000	1.232630000	0.447800000
6	-1.764100000	0.338230000	1.396410000
6	-1.778810000	-1.508540000	-0.271370000
6	-2.581610000	-0.640850000	-1.249500000
1	-1.068500000	0.928330000	1.997950000
1	-1.865680000	1.838740000	-0.130360000
1	-3.193460000	1.911760000	1.043580000
1	-1.088500000	-2.175060000	-0.788850000
1	-2.456760000	-2.117230000	0.342110000
1	-1.880290000	-0.122840000	-1.915160000
1	-3.207240000	-1.292420000	-1.870640000
1	-2.434410000	-0.201210000	2.079520000
6	-3.439810000	0.387210000	-0.496480000
7	-0.997470000	-0.655750000	0.634460000
6	0.335360000	-0.661760000	0.637240000
1	0.787210000	0.071520000	1.317900000
8	0.650750000	2.093560000	-0.540800000
1	0.795120000	3.000830000	-0.837730000
8	1.045970000	-1.426620000	-0.051930000
1	2.551230000	-1.196940000	-0.039990000
6	3.988330000	0.130140000	-0.105000000

1	5.086880000	0.197900000	-0.129450000
8	3.281870000	1.132160000	-0.122820000
1	1.545910000	1.715570000	-0.439140000
8	3.579300000	-1.114800000	-0.047540000
1	-3.966700000	1.034220000	-1.206940000
1	-4.209770000	-0.139690000	0.086030000

-631.376429

14

6	-2.577590000	1.412020000	-0.380070000
6	-1.498160000	1.223360000	0.692760000
6	-1.648240000	-1.249170000	0.470110000
6	-2.729310000	-1.103670000	-0.608400000
1	-0.763340000	2.032530000	0.668000000
1	-2.088680000	1.539380000	-1.354610000
1	-3.134270000	2.332630000	-0.169640000
1	-1.008870000	-2.114170000	0.292420000
1	-2.112310000	-1.358970000	1.459870000
1	-2.247340000	-1.111140000	-1.594560000
1	-3.395750000	-1.972660000	-0.564390000
1	-1.956250000	1.214520000	1.691520000
6	-3.522120000	0.200440000	-0.427090000
7	-0.798780000	-0.051810000	0.499040000
6	0.523600000	-0.109100000	0.309270000
1	1.037240000	0.862000000	0.324660000
8	1.168500000	-1.162680000	0.122100000
1	2.721160000	-0.976440000	-0.059420000
6	4.086540000	0.384910000	-0.250700000
1	5.175370000	0.488120000	-0.383960000
8	3.337680000	1.347880000	-0.188180000
8	3.731510000	-0.884500000	-0.172880000
1	-4.250670000	0.318440000	-1.237030000
1	-4.094780000	0.150050000	0.510340000

-554.946313

15

6	-1.572280000	1.078190000	-0.400660000
6	-0.310320000	1.342360000	0.431000000
6	0.170140000	-1.089380000	0.558800000
6	-1.081810000	-1.400090000	-0.271720000
1	0.163620000	2.286060000	0.144980000
1	-1.314080000	1.139540000	-1.466120000
1	-2.310620000	1.862430000	-0.195520000
1	0.979220000	-1.791590000	0.353500000

1	-0.067330000	-1.141960000	1.631540000
1	-0.796200000	-1.463900000	-1.329810000
1	-1.472510000	-2.381630000	0.020930000
1	-0.575860000	1.411680000	1.496360000
6	-2.150830000	-0.311310000	-0.088090000
7	0.658280000	0.259250000	0.259890000
6	1.924050000	0.479940000	-0.168230000
1	2.125130000	1.549790000	-0.361880000
8	2.789380000	-0.380120000	-0.338080000
1	-2.510050000	-0.327710000	0.951270000
1	-3.018140000	-0.514680000	-0.726480000

-365.171837

16-Mn-iPr

25	-0.021470000	0.461410000	-0.963980000
6	0.982940000	0.343890000	-2.436100000
6	-0.866980000	-1.052840000	-1.391420000
1	1.016560000	-0.515410000	-0.284220000
6	-1.210550000	1.580650000	-1.724720000
8	1.660020000	0.266690000	-3.381670000
8	-1.321410000	-2.071950000	-1.722240000
8	-1.965180000	2.265660000	-2.291650000
7	-0.027540000	1.064010000	1.984420000
6	-0.774690000	0.577300000	0.945640000
6	-0.705640000	1.006400000	3.192920000
6	-1.926840000	0.480690000	2.917600000
7	-1.954190000	0.227320000	1.545940000
1	-2.772180000	0.265250000	3.552010000
1	-0.263650000	1.333960000	4.120880000
6	1.327550000	1.565440000	1.779850000
1	1.510710000	2.408340000	2.448870000
15	1.414460000	1.995210000	-0.030620000
1	2.051250000	0.774970000	1.999910000
6	-3.107620000	-0.302450000	0.869270000
6	-3.268270000	-1.693140000	0.792690000
6	-4.050390000	0.591580000	0.334780000
6	-4.396590000	-2.187080000	0.127590000
6	-5.158780000	0.051750000	-0.325980000
6	-5.344790000	-1.332460000	-0.446080000
1	-4.526930000	-3.263420000	0.044020000
1	-5.892710000	0.728100000	-0.758150000
6	-3.894560000	2.082530000	0.504660000
1	-4.593290000	2.624160000	-0.138300000
1	-4.090340000	2.379630000	1.542790000
1	-2.884330000	2.415380000	0.258550000

6	-2.255530000	-2.624940000	1.408830000
1	-1.235500000	-2.298360000	1.192700000
1	-2.357070000	-2.658010000	2.500830000
1	-2.376350000	-3.642370000	1.027830000
6	-6.526780000	-1.883900000	-1.207020000
1	-6.748100000	-2.915550000	-0.915560000
1	-7.427020000	-1.282130000	-1.041930000
1	-6.327030000	-1.882170000	-2.286270000
6	3.242690000	1.972180000	-0.426710000
1	3.277100000	2.309860000	-1.470460000
6	3.812640000	0.544200000	-0.375270000
6	4.096490000	2.926420000	0.424300000
1	3.817350000	3.973360000	0.288000000
1	4.028740000	2.687100000	1.491960000
1	5.150570000	2.830130000	0.136580000
1	3.827170000	0.148270000	0.645270000
1	4.846110000	0.557780000	-0.741880000
1	3.240740000	-0.148340000	-0.993440000
6	0.835300000	3.784360000	-0.164390000
1	-0.250560000	3.650070000	-0.224890000
6	1.299390000	4.373310000	-1.507420000
6	1.110590000	4.733510000	1.010680000
1	0.658710000	4.374680000	1.941070000
1	2.176670000	4.894810000	1.191140000
1	0.662920000	5.711750000	0.794990000
1	2.370070000	4.604540000	-1.497870000
1	0.761940000	5.306410000	-1.712310000
1	1.104340000	3.691790000	-2.343100000
6	2.112070000	-3.422580000	-1.372970000
6	1.581220000	-3.590270000	0.056190000
6	3.882040000	-3.393330000	0.974040000
6	4.455950000	-3.231790000	-0.440130000
1	0.591900000	-3.139640000	0.154720000
1	2.053570000	-2.361560000	-1.641280000
1	1.458480000	-3.968760000	-2.062760000
1	4.440410000	-2.810310000	1.707940000
1	3.920130000	-4.451160000	1.273720000
1	4.534230000	-2.162850000	-0.670020000
1	5.470770000	-3.647170000	-0.462450000
1	1.496690000	-4.658710000	0.304470000
6	3.561220000	-3.920460000	-1.482740000
7	2.484490000	-2.957090000	1.021080000
6	2.069750000	-1.979380000	1.854140000
1	0.992340000	-1.771280000	1.765500000
8	2.784310000	-1.353270000	2.647940000
1	3.585540000	-5.008160000	-1.319560000

1	3.947630000	-3.742390000	-2.492800000
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-2001.826054

17-Mn-iPr

25	-0.318670000	-0.399950000	-0.848120000
6	-1.263390000	-0.026560000	-2.344770000
6	1.014120000	0.700500000	-1.405930000
1	-1.153870000	1.067260000	0.031990000
6	0.454840000	-1.783060000	-1.645800000
8	-1.815520000	0.167160000	-3.345220000
8	1.801660000	1.407450000	-1.869800000
8	0.986040000	-2.673320000	-2.165380000
7	-0.335910000	-1.223950000	2.005150000
6	0.491720000	-0.877060000	0.982610000
6	0.373780000	-1.418170000	3.173970000
6	1.691660000	-1.202440000	2.880620000
7	1.748730000	-0.868030000	1.539140000
1	2.577820000	-1.255880000	3.493310000
1	-0.109870000	-1.682980000	4.101280000
6	-1.786190000	-1.265510000	1.853450000
1	-2.227010000	-1.917000000	2.608350000
15	-2.129050000	-1.632280000	0.138500000
1	-2.196270000	0.537460000	1.932390000
6	2.970350000	-0.584360000	0.836820000
6	3.456160000	0.733060000	0.809200000
6	3.655880000	-1.645880000	0.220810000
6	4.650260000	0.974920000	0.119640000
6	4.836170000	-1.350590000	-0.470740000
6	5.346290000	-0.047350000	-0.535840000
1	5.035170000	1.991380000	0.082880000
1	5.372120000	-2.159280000	-0.962490000
6	3.170510000	-3.069620000	0.343070000
1	3.608080000	-3.699560000	-0.435940000
1	3.455140000	-3.492900000	1.314580000
1	2.084100000	-3.141650000	0.267510000
6	2.704190000	1.872450000	1.451410000
1	1.916370000	2.240380000	0.784240000
1	2.228400000	1.577540000	2.390710000
1	3.375290000	2.711830000	1.655610000
6	6.601850000	0.252760000	-1.319440000
1	7.125700000	1.126410000	-0.918300000
1	7.295180000	-0.594780000	-1.310740000
1	6.361270000	0.468280000	-2.368520000
6	-3.944040000	-1.224740000	-0.126020000
1	-4.270930000	-1.922100000	-0.906480000

6	-4.177770000	0.207440000	-0.631900000
6	-4.781270000	-1.477590000	1.141960000
1	-4.652760000	-2.483940000	1.548860000
1	-4.518950000	-0.760490000	1.925880000
1	-5.845280000	-1.346770000	0.909180000
1	-3.780950000	0.943580000	0.072050000
1	-5.255370000	0.387840000	-0.733590000
1	-3.727640000	0.378340000	-1.611360000
6	-1.998720000	-3.470490000	-0.285100000
1	-0.931650000	-3.665500000	-0.117480000
6	-2.315310000	-3.743610000	-1.764670000
6	-2.800590000	-4.399660000	0.634780000
1	-2.604560000	-4.198030000	1.693300000
1	-3.877990000	-4.307120000	0.460200000
1	-2.528610000	-5.444910000	0.439830000
1	-3.392870000	-3.689520000	-1.957650000
1	-1.986040000	-4.752190000	-2.043230000
1	-1.821080000	-3.038440000	-2.439660000
6	-1.082110000	1.774350000	0.921780000
8	-2.198270000	1.542520000	1.738870000
1	-0.152200000	1.563610000	1.455620000
6	-1.467330000	5.841600000	-0.402070000
6	-0.385190000	5.444130000	0.613310000
6	-0.761320000	4.141490000	1.326170000
7	-1.001410000	3.076140000	0.342710000
6	-2.082780000	3.399330000	-0.595390000
6	-1.748590000	4.679740000	-1.366060000
1	-1.164170000	6.737500000	-0.957220000
1	-2.391500000	6.097240000	0.136560000
1	-0.240680000	6.237280000	1.357190000
1	0.571150000	5.299400000	0.093310000
1	0.049770000	3.817750000	1.988830000
1	-1.653770000	4.305090000	1.955850000
1	-2.191290000	2.556840000	-1.286550000
1	-3.046250000	3.518550000	-0.069200000
1	-2.578860000	4.926440000	-2.039100000
1	-0.862950000	4.495830000	-1.988410000

-2001.757243

18-Mn-iPr

25	0.373370000	1.059080000	1.005840000
6	-0.079800000	1.930800000	2.501420000
6	1.272480000	-0.138110000	1.981450000
1	-0.820200000	0.034720000	1.242850000
6	1.757400000	2.160740000	0.680370000

8	-0.360660000	2.511430000	3.471340000
8	1.771260000	-0.896630000	2.707740000
8	2.671830000	2.868780000	0.533010000
7	-0.394480000	0.122800000	-1.743780000
6	0.583830000	0.086420000	-0.786610000
6	-0.047130000	-0.598270000	-2.879060000
6	1.191590000	-1.100020000	-2.643090000
7	1.562060000	-0.674490000	-1.367550000
1	1.843260000	-1.708320000	-3.250260000
1	-0.701250000	-0.690040000	-3.731780000
6	-1.642980000	0.836710000	-1.527740000
1	-1.987850000	1.273890000	-2.467560000
15	-1.308850000	2.083780000	-0.177330000
1	-2.406990000	0.144120000	-1.161500000
6	2.862100000	-0.929580000	-0.804380000
6	3.046900000	-2.063250000	0.001720000
6	3.911860000	-0.050360000	-1.113620000
6	4.318320000	-2.279670000	0.542220000
6	5.165860000	-0.305790000	-0.545270000
6	5.385070000	-1.406660000	0.291700000
1	4.473940000	-3.141770000	1.186620000
1	5.986340000	0.375140000	-0.759010000
6	3.712310000	1.106500000	-2.061240000
1	4.524280000	1.832480000	-1.968780000
1	3.692230000	0.756570000	-3.101380000
1	2.771440000	1.629190000	-1.877700000
6	1.909940000	-3.016520000	0.269620000
1	0.996570000	-2.481220000	0.534380000
1	1.687490000	-3.622610000	-0.617610000
1	2.156150000	-3.696180000	1.089550000
6	6.729020000	-1.633810000	0.942370000
1	6.979600000	-2.699400000	0.983450000
1	7.530170000	-1.115510000	0.406070000
1	6.726100000	-1.259530000	1.974200000
6	-3.015480000	2.427730000	0.528190000
1	-2.924110000	3.445040000	0.930090000
6	-3.377100000	1.485810000	1.688320000
6	-4.147060000	2.409950000	-0.519770000
1	-3.945350000	3.027920000	-1.396300000
1	-4.347730000	1.388980000	-0.863940000
1	-5.072350000	2.778620000	-0.061330000
1	-3.436350000	0.446460000	1.353310000
1	-4.360880000	1.763740000	2.085850000
1	-2.657370000	1.526690000	2.506010000
6	-0.787990000	3.655540000	-1.068420000
1	0.157010000	3.334480000	-1.527050000

6	-0.464900000	4.746810000	-0.031710000
6	-1.694140000	4.215890000	-2.173600000
1	-1.993460000	3.460470000	-2.907430000
1	-2.599060000	4.671660000	-1.759610000
1	-1.158060000	5.002590000	-2.718970000
1	-1.379570000	5.147030000	0.421640000
1	0.050900000	5.582810000	-0.518220000
1	0.179590000	4.380740000	0.772020000
6	-1.972440000	-3.622360000	-1.573320000
6	-1.762210000	-3.092870000	-0.151550000
6	-4.070000000	-2.337350000	-0.023490000
6	-4.363850000	-2.843010000	-1.438470000
1	-1.019810000	-3.704310000	0.371370000
1	-2.241070000	-4.685710000	-1.521480000
1	-1.029790000	-3.545170000	-2.127700000
1	-4.964880000	-2.389360000	0.602300000
1	-3.767750000	-1.272050000	-0.073350000
1	-4.768030000	-3.861700000	-1.375930000
1	-5.136260000	-2.212560000	-1.896310000
1	-1.360710000	-2.063710000	-0.196080000
6	-3.085980000	-2.846050000	-2.289290000
7	-3.014910000	-3.134770000	0.614910000
6	-2.823160000	-2.783070000	2.012560000
1	-1.892480000	-3.256400000	2.354780000
8	-3.930520000	-3.196840000	2.804170000
1	-2.754550000	-1.809590000	-2.446450000
1	-3.279990000	-3.272170000	-3.281110000
1	-2.737100000	-1.698210000	2.179160000
1	-4.072210000	-4.137170000	2.616230000

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19-Mn-iPr

25	0.369930000	1.178890000	0.803180000
6	-0.133130000	2.039120000	2.319290000
6	1.826580000	0.500910000	1.662100000
1	-0.907790000	-0.999700000	1.511050000
6	1.350620000	2.536240000	0.254550000
8	-0.433030000	2.610290000	3.281960000
8	2.750290000	0.203520000	2.287470000
8	2.021150000	3.403000000	-0.131710000
7	-0.531550000	0.013840000	-1.781030000
6	0.509830000	0.080970000	-0.890640000
6	-0.211990000	-0.801140000	-2.849430000
6	1.063710000	-1.253580000	-2.644650000
7	1.490860000	-0.720190000	-1.451390000

1	1.688930000	-1.903550000	-3.236940000
1	-0.912270000	-1.003640000	-3.644210000
6	-1.798710000	0.656410000	-1.579680000
1	-2.290390000	0.891030000	-2.520940000
15	-1.641370000	1.883590000	-0.317940000
1	-2.639480000	-1.220530000	-0.748230000
6	2.818560000	-0.902480000	-0.934560000
6	3.075750000	-1.957130000	-0.045280000
6	3.828420000	-0.020000000	-1.358820000
6	4.386720000	-2.114720000	0.420370000
6	5.119850000	-0.211200000	-0.856550000
6	5.417850000	-1.251560000	0.033860000
1	4.601370000	-2.923170000	1.115630000
1	5.910450000	0.467520000	-1.168430000
6	3.536430000	1.083300000	-2.346290000
1	4.345460000	1.818730000	-2.358120000
1	3.429460000	0.684670000	-3.362760000
1	2.607280000	1.606410000	-2.108180000
6	1.973560000	-2.852880000	0.460700000
1	1.486530000	-2.397360000	1.330810000
1	1.203770000	-3.028780000	-0.294980000
1	2.373540000	-3.821070000	0.777030000
6	6.810870000	-1.411380000	0.595230000
1	7.036710000	-2.459220000	0.818830000
1	7.570310000	-1.038900000	-0.099910000
1	6.917410000	-0.847040000	1.530720000
6	-3.250260000	1.953350000	0.644040000
1	-3.237650000	2.925640000	1.152220000
6	-3.308540000	0.847280000	1.709180000
6	-4.489040000	1.870740000	-0.264310000
1	-4.536130000	2.678090000	-0.998450000
1	-4.501480000	0.920040000	-0.807880000
1	-5.400090000	1.923660000	0.345200000
1	-3.247420000	-0.143360000	1.251400000
1	-4.258230000	0.907660000	2.255400000
1	-2.502860000	0.931630000	2.442680000
6	-1.406000000	3.617920000	-1.041570000
1	-0.424440000	3.512260000	-1.520450000
6	-1.301100000	4.700980000	0.043160000
6	-2.409030000	4.024510000	-2.130560000
1	-2.554490000	3.236220000	-2.876600000
1	-3.384490000	4.284760000	-1.707920000
1	-2.038220000	4.912950000	-2.657470000
1	-2.270890000	4.884270000	0.519870000
1	-0.972370000	5.648170000	-0.402130000
1	-0.586360000	4.439760000	0.828490000

6	-2.393230000	-4.544540000	-0.302360000
6	-2.108260000	-3.197480000	-0.978350000
6	-4.322720000	-2.363140000	-0.442770000
6	-4.697570000	-3.668900000	0.268810000
1	-1.045050000	-2.947180000	-0.908060000
1	-2.036730000	-4.504380000	0.735650000
1	-1.834750000	-5.341940000	-0.809250000
1	-4.846420000	-1.514430000	0.011530000
1	-4.656990000	-2.424130000	-1.499210000
1	-4.470330000	-3.562390000	1.338350000
1	-5.775870000	-3.851000000	0.177930000
1	-2.345850000	-3.287900000	-2.058630000
6	-3.900420000	-4.848470000	-0.312400000
7	-2.881010000	-2.131790000	-0.337810000
6	-1.013030000	-1.759200000	2.291350000
1	-0.916690000	-2.740020000	1.813830000
8	0.014480000	-1.525050000	3.259690000
1	-4.224550000	-5.022470000	-1.349310000
1	-4.111980000	-5.770170000	0.243910000
1	-2.016090000	-1.666140000	2.721480000
1	-0.078030000	-2.171890000	3.971280000

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20-Mn-iPr

25	0.596170000	1.102650000	1.087460000
6	0.274140000	2.208270000	2.456610000
6	1.551320000	0.009280000	2.135590000
1	-0.617700000	0.226890000	1.629930000
6	1.982400000	2.081660000	0.485720000
8	0.042170000	2.920890000	3.348860000
8	2.104040000	-0.679110000	2.890520000
8	2.893990000	2.740830000	0.178680000
7	-0.591330000	-0.366740000	-1.244790000
6	0.540240000	-0.215040000	-0.487860000
6	-0.434880000	-1.323310000	-2.237740000
6	0.835350000	-1.785070000	-2.118380000
7	1.416640000	-1.098700000	-1.053240000
1	1.376480000	-2.535530000	-2.672360000
1	-1.231000000	-1.597040000	-2.911920000
6	-1.768590000	0.451640000	-0.993550000
1	-2.314720000	0.615990000	-1.924610000
15	-1.089560000	1.991690000	-0.186020000
1	-2.424240000	-0.044960000	-0.273860000
6	2.811820000	-1.214290000	-0.715150000
6	3.226180000	-2.187420000	0.204990000

6	3.720860000	-0.357970000	-1.362930000
6	4.594800000	-2.261370000	0.499850000
6	5.074580000	-0.468580000	-1.032370000
6	5.529060000	-1.409060000	-0.096920000
1	4.931610000	-3.001360000	1.222500000
1	5.789310000	0.195610000	-1.513080000
6	3.255670000	0.623080000	-2.411390000
1	4.035550000	1.355750000	-2.634450000
1	3.000630000	0.106170000	-3.345250000
1	2.363410000	1.166430000	-2.091920000
6	2.253680000	-3.149970000	0.836720000
1	1.244740000	-2.744780000	0.915540000
1	2.172800000	-4.064580000	0.234750000
1	2.592340000	-3.441520000	1.834920000
6	6.990630000	-1.476060000	0.278670000
1	7.269320000	-2.473650000	0.633440000
1	7.635840000	-1.223280000	-0.569510000
1	7.217480000	-0.766200000	1.084620000
6	-2.576310000	2.839540000	0.570970000
1	-2.144020000	3.744640000	1.017250000
6	-3.184200000	1.998290000	1.706290000
6	-3.666210000	3.259130000	-0.428720000
1	-3.307890000	3.989760000	-1.156440000
1	-4.064120000	2.397670000	-0.977690000
1	-4.503730000	3.717190000	0.111570000
1	-3.730100000	1.137240000	1.306710000
1	-3.903570000	2.607300000	2.266180000
1	-2.431070000	1.629150000	2.404950000
6	-0.483460000	3.067240000	-1.609180000
1	0.509660000	2.637110000	-1.783450000
6	-0.276550000	4.507260000	-1.109800000
6	-1.241480000	3.012300000	-2.943000000
1	-1.267830000	1.998390000	-3.355380000
1	-2.269410000	3.376840000	-2.867250000
1	-0.724010000	3.642060000	-3.677530000
1	-1.228830000	5.030110000	-0.968800000
1	0.307720000	5.075810000	-1.842430000
1	0.270990000	4.534250000	-0.161180000
6	-5.133985545	-0.190567986	0.669900085
6	-4.621532362	-0.747190498	2.005214797
6	-3.663129137	-2.730623882	0.855677523
6	-4.144011143	-2.198261354	-0.498875952
1	-4.328017592	0.054493411	2.688671929
1	-4.386882977	0.496849645	0.253226242
1	-6.045604248	0.391026649	0.849943907
1	-2.716196290	-3.265561093	0.770017323

1	-4.408846013	-3.426005179	1.271144192
1	-3.337569056	-1.607600259	-0.954821758
1	-4.345851753	-3.043880823	-1.166788755
1	-5.426144967	-1.319047902	2.492813923
6	-5.395956592	-1.323554236	-0.334381104
7	-3.470230956	-1.626979378	1.798636791
6	-2.362049649	-1.560591121	2.583419009
1	-2.358286198	-0.686626086	3.257313305
8	-1.427403845	-2.361808012	2.554298449
1	-6.226356042	-1.945541158	0.029280835
1	-5.707848155	-0.911139907	-1.300945864

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21-Mn-iPr

25	-0.117055697	-0.904523451	1.021809328
6	0.575064303	-1.589233451	2.538599328
6	-1.517625697	-0.168983451	1.913779328
1	0.723315697	0.795303451	1.323080672
6	-1.080085697	-2.367593451	0.719299328
8	1.025974303	-2.042973451	3.507059328
8	-2.386185697	0.220466549	2.567649328
8	-1.734365697	-3.314633451	0.559539328
7	0.591194303	0.210816549	-1.646710672
6	-0.451955697	0.002786549	-0.792040672
6	0.171804303	0.859976549	-2.792340672
6	-1.172065697	1.074636549	-2.660010672
7	-1.536985697	0.548076549	-1.432290672
1	-1.888245697	1.539296549	-3.319320672
1	0.850164303	1.115756549	-3.590780672
6	1.965424303	-0.159973451	-1.284250672
1	2.556594303	-0.287483451	-2.194080672
15	1.758924303	-1.613033451	-0.253030672
1	2.283285697	1.372883451	-0.079769328
6	-2.882815697	0.526146549	-0.925530672
6	-3.341365697	1.610576549	-0.159920672
6	-3.691765697	-0.585033451	-1.213820672
6	-4.649955697	1.550786549	0.332139328
6	-4.989895697	-0.603113451	-0.689520672
6	-5.482935697	0.451536549	0.089179328
1	-5.018515697	2.374926549	0.938509328
1	-5.627065697	-1.460683451	-0.893250672
6	-3.191605697	-1.708483451	-2.088680672
1	-3.845335697	-2.581593451	-2.015300672
1	-3.156635697	-1.400083451	-3.141040672
1	-2.181635697	-2.020073451	-1.812400672

6	-2.445325697	2.780466549	0.156589328
1	-1.618595697	2.496566549	0.819249328
1	-2.004355697	3.204636549	-0.752190672
1	-3.008075697	3.571706549	0.659709328
6	-6.868895697	0.391996549	0.686009328
1	-7.331345697	1.383846549	0.727679328
1	-7.527305697	-0.267763451	0.111859328
1	-6.831195697	0.007236549	1.713309328
6	3.395784303	-1.991753451	0.564579328
1	3.183444303	-2.860913451	1.199919328
6	3.847254303	-0.837453451	1.468679328
6	4.518384303	-2.361813451	-0.419290672
1	4.306884303	-3.280333451	-0.970180672
1	4.692604303	-1.558943451	-1.145240672
1	5.455134303	-2.517953451	0.130439328
1	4.138514303	0.025306549	0.863929328
1	4.719034303	-1.143833451	2.059289328
1	3.069534303	-0.524393451	2.169089328
6	1.314134303	-3.150993451	-1.270410672
1	0.239804303	-3.002893451	-1.428190672
6	1.493654303	-4.442823451	-0.459200672
6	1.955974303	-3.235333451	-2.661580672
1	1.779954303	-2.322803451	-3.240370672
1	3.035624303	-3.404993451	-2.621800672
1	1.512924303	-4.070303451	-3.219580672
1	2.552084303	-4.700053451	-0.341480672
1	1.004934303	-5.282223451	-0.968760672
1	1.052734303	-4.366393451	0.540839328
6	4.215415697	3.332503451	-0.207559328
6	3.366265697	2.876203451	0.979760672
6	1.295755697	3.194593451	-0.308649328
6	2.099095697	3.662183451	-1.523819328
1	3.898485697	2.145793451	1.592400672
1	4.519805697	2.452493451	-0.789639328
1	5.129785697	3.801353451	0.174020672
1	0.382525697	2.680613451	-0.601849328
1	1.010015697	4.030403451	0.335140672
1	2.295995697	2.804533451	-2.178589328
1	1.485775697	4.369443451	-2.093849328
1	3.096845697	3.723913451	1.620160672
6	3.429545697	4.300503451	-1.102889328
7	2.091535697	2.248713451	0.526510672
6	1.217525697	1.771523451	1.822580672
1	1.990405697	1.353423451	2.494560672
8	0.402285697	2.632103451	2.255690672
1	3.232335697	5.229343451	-0.549479328

1 4.021115697 4.571313451 -1.984889328

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22-Mn-iPr

25	-0.420883651	-0.459651563	0.941470604
6	-1.262733651	-1.120541563	2.390130604
6	1.080726349	-1.367521563	1.370210604
1	-0.965256349	-2.030288437	-0.019340604
6	0.090356349	1.017198437	1.812220604
8	-1.798893651	-1.555861563	3.323250604
8	1.981556349	-2.012121563	1.707840604
8	0.425286349	1.944018437	2.429730604
7	-0.663243651	0.249208437	-1.976229396
6	0.221726349	0.109258437	-0.947119396
6	-0.030923651	0.563198437	-3.166889396
6	1.296216349	0.640438437	-2.883579396
7	1.432256349	0.362898437	-1.525629396
1	2.147606349	0.862148437	-3.507449396
1	-0.569143651	0.688948437	-4.093229396
6	-2.098023651	0.047728437	-1.780749396
1	-2.658733651	0.691588437	-2.460259396
15	-2.388723651	0.407848437	0.019060604
1	-2.333603651	-1.005681563	-1.970399396
6	2.692266349	0.383808437	-0.830829396
6	3.484106349	-0.776021563	-0.835879396
6	3.090506349	1.563978437	-0.185139396
6	4.700576349	-0.736131563	-0.147929396
6	4.311136349	1.550328437	0.501540604
6	5.124496349	0.411188437	0.536240604
1	5.320846349	-1.629231563	-0.127069396
1	4.630196349	2.450988437	1.020480604
6	2.259876349	2.821598437	-0.264039396
1	2.566886349	3.541438437	0.499030604
1	2.374826349	3.302118437	-1.244129396
1	1.195596349	2.618808437	-0.128319396
6	3.026886349	-2.022951563	-1.549659396
1	1.995496349	-2.278801563	-1.289719396
1	3.054946349	-1.893721563	-2.638239396
1	3.663646349	-2.873821563	-1.294179396
6	6.416906349	0.400488437	1.317070604
1	7.215676349	-0.103541563	0.761920604
1	6.753356349	1.414428437	1.554320604
1	6.291746349	-0.137441563	2.265380604
6	-4.067533651	-0.315881563	0.396730604
1	-4.263503651	0.014428437	1.424970604

6	-4.020223651	-1.854231563	0.390800604
6	-5.193283651	0.204078437	-0.511469396
1	-5.324963651	1.285898437	-0.438889396
1	-5.014223651	-0.052231563	-1.561869396
1	-6.141833651	-0.262261563	-0.219969396
1	-3.733813651	-2.256721563	-0.585979396
1	-5.013653651	-2.243521563	0.642680604
1	-3.316893651	-2.244941563	1.127990604
6	-2.514963651	2.279908437	0.167530604
1	-1.460663651	2.564948437	0.256030604
6	-3.211243651	2.650988437	1.487350604
6	-3.091513651	3.049228437	-1.029639396
1	-2.508293651	2.884868437	-1.941199396
1	-4.133403651	2.793538437	-1.240399396
1	-3.054653651	4.124368437	-0.815319396
1	-4.288923651	2.459458437	1.441640604
1	-3.072423651	3.718188437	1.693770604
1	-2.802653651	2.096078437	2.339290604
6	-1.040336349	-3.196768437	-0.691550604
1	-1.592436349	-3.720008437	0.117889396
8	-1.598846349	-3.052078437	-1.832900604
1	0.040843651	-3.440848437	-0.652300604

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TS7-Mn-iPr

25	0.465670000	0.546600000	0.887280000
6	1.320770000	0.964540000	2.425490000
6	-1.003310000	1.492210000	1.375380000
1	1.227110000	2.090040000	0.127660000
6	-0.158310000	-0.942820000	1.634340000
8	1.846480000	1.175000000	3.436310000
8	-1.882250000	2.138040000	1.758220000
8	-0.570620000	-1.902590000	2.137570000
7	0.661220000	-0.160870000	-1.993570000
6	-0.229990000	0.006360000	-0.983970000
6	0.032350000	-0.501930000	-3.173140000
6	-1.303380000	-0.570960000	-2.898090000
7	-1.447240000	-0.259360000	-1.554010000
1	-2.150160000	-0.808080000	-3.522580000
1	0.574990000	-0.653580000	-4.093110000
6	2.089400000	0.100230000	-1.785450000
1	2.677750000	-0.389650000	-2.563200000
15	2.434390000	-0.377180000	-0.078600000
1	2.108020000	1.571100000	-1.827490000
6	-2.707210000	-0.276200000	-0.860640000

6	-3.460740000	0.909200000	-0.798520000
6	-3.155690000	-1.478260000	-0.293590000
6	-4.679430000	0.873350000	-0.116470000
6	-4.383660000	-1.463050000	0.383090000
6	-5.155390000	-0.301040000	0.484690000
1	-5.266640000	1.785900000	-0.042090000
1	-4.739890000	-2.382680000	0.840970000
6	-2.378470000	-2.763880000	-0.440600000
1	-2.622400000	-3.461370000	0.365110000
1	-2.623640000	-3.255490000	-1.390750000
1	-1.299290000	-2.598920000	-0.431530000
6	-2.966380000	2.176300000	-1.449510000
1	-1.929590000	2.390570000	-1.177160000
1	-2.993760000	2.098350000	-2.543060000
1	-3.580070000	3.031740000	-1.155630000
6	-6.472550000	-0.297220000	1.223900000
1	-7.303930000	-0.060570000	0.548720000
1	-6.679500000	-1.268150000	1.683900000
1	-6.476260000	0.459530000	2.017050000
6	4.138190000	0.294470000	0.303800000
1	4.450780000	-0.250160000	1.203460000
6	4.124190000	1.798740000	0.627550000
6	5.147770000	0.021010000	-0.827370000
1	5.228600000	-1.036600000	-1.086660000
1	4.876140000	0.575840000	-1.731680000
1	6.143260000	0.363190000	-0.518840000
1	3.807300000	2.384640000	-0.239930000
1	5.137560000	2.116580000	0.901490000
1	3.469190000	2.043150000	1.466240000
6	2.508900000	-2.245410000	0.161150000
1	1.454460000	-2.517110000	0.022800000
6	2.904530000	-2.601930000	1.603210000
6	3.330850000	-3.034900000	-0.865710000
1	3.109320000	-2.730410000	-1.894380000
1	4.406640000	-2.922670000	-0.698780000
1	3.099640000	-4.104060000	-0.779910000
1	3.977730000	-2.453670000	1.768100000
1	2.683490000	-3.656370000	1.807270000
1	2.365500000	-2.001930000	2.344000000
6	1.151880000	2.954390000	-0.634420000
1	1.515790000	3.797630000	-0.024450000
8	1.912710000	2.714590000	-1.742180000
1	0.079870000	3.098240000	-0.835630000

-1751.138971

23-Mn-iPr

25	-0.416960000	-0.176850000	-0.989480000
6	-1.309570000	-0.500090000	-2.533890000
6	1.131540000	0.138580000	-1.888960000
1	-0.815670000	2.269180000	-1.066600000
6	0.014190000	-1.884330000	-0.825500000
8	-1.876120000	-0.744110000	-3.514290000
8	2.056140000	0.300180000	-2.563180000
8	0.313720000	-2.997800000	-0.699370000
7	-0.659070000	0.842390000	1.787080000
6	0.237120000	0.398820000	0.863150000
6	-0.023440000	1.237890000	2.943930000
6	1.316180000	1.029060000	2.754960000
7	1.460670000	0.519400000	1.480570000
1	2.162750000	1.202580000	3.400630000
1	-0.561900000	1.645750000	3.784950000
6	-2.082310000	0.971970000	1.493900000
1	-2.662010000	0.945030000	2.417070000
15	-2.463340000	-0.238320000	0.243210000
1	-1.911780000	2.659970000	0.785660000
6	2.726150000	0.192550000	0.884930000
6	3.420990000	1.200810000	0.195550000
6	3.231590000	-1.109810000	1.016860000
6	4.651710000	0.871180000	-0.379190000
6	4.463860000	-1.395240000	0.413500000
6	5.184920000	-0.421940000	-0.288410000
1	5.197170000	1.635910000	-0.927240000
1	4.866870000	-2.402020000	0.495950000
6	2.497630000	-2.160620000	1.813480000
1	2.825800000	-3.164710000	1.531330000
1	2.687180000	-2.037140000	2.887340000
1	1.416870000	-2.103080000	1.668530000
6	2.831920000	2.581380000	0.051800000
1	1.850220000	2.540450000	-0.431260000
1	2.679430000	3.062260000	1.024500000
1	3.480660000	3.223550000	-0.549670000
6	6.488980000	-0.762140000	-0.969850000
1	7.199420000	0.069710000	-0.915720000
1	6.961000000	-1.642770000	-0.522850000
1	6.324490000	-0.980430000	-2.032890000
6	-4.048270000	0.287490000	-0.594910000
1	-4.285740000	-0.533580000	-1.282720000
6	-3.852490000	1.568970000	-1.420340000
6	-5.216260000	0.469420000	0.389200000
1	-5.486050000	-0.457280000	0.899860000
1	-4.976040000	1.224090000	1.146660000

1	-6.105010000	0.817320000	-0.151810000
1	-3.664150000	2.426830000	-0.769550000
1	-4.761750000	1.774030000	-1.998120000
1	-3.024980000	1.491760000	-2.130790000
6	-2.761370000	-1.977270000	0.935660000
1	-1.737220000	-2.286500000	1.175800000
6	-3.307740000	-2.934800000	-0.133410000
6	-3.565140000	-2.049450000	2.241200000
1	-3.212560000	-1.320280000	2.978400000
1	-4.634100000	-1.881350000	2.082200000
1	-3.455330000	-3.047170000	2.685090000
1	-4.361120000	-2.727510000	-0.353020000
1	-3.243340000	-3.972090000	0.217420000
1	-2.748870000	-2.869430000	-1.073360000
6	-1.017670000	3.338670000	-0.853540000
1	-1.683330000	3.691360000	-1.656830000
8	-1.565200000	3.540660000	0.424390000
1	-0.061620000	3.871030000	-0.944950000

-1751.134796

24-Mn-iPr

25	-0.510130000	0.571810000	-0.610190000
6	-1.462200000	1.528180000	-1.815520000
6	-0.020620000	-0.570810000	-1.892960000
6	0.986120000	1.535180000	-0.929270000
8	-2.073410000	2.068250000	-2.641390000
8	0.344500000	-1.264020000	-2.754520000
8	1.885390000	2.198030000	-1.234260000
7	-0.606280000	-1.115290000	1.867910000
6	0.230970000	-0.602810000	0.920140000
6	0.086610000	-1.783050000	2.866920000
6	1.401570000	-1.703220000	2.536400000
7	1.469710000	-0.983930000	1.344640000
1	2.286120000	-2.079830000	3.025360000
1	-0.408870000	-2.246110000	3.706110000
6	-2.050390000	-0.906690000	1.835000000
15	-2.480330000	-0.546180000	0.060690000
1	-2.557500000	-1.793150000	2.225280000
6	2.711130000	-0.621840000	0.714550000
6	3.327430000	0.576560000	1.106870000
6	3.269420000	-1.477230000	-0.246780000
6	4.536870000	0.918210000	0.493030000
6	4.476800000	-1.088290000	-0.839160000
6	5.121740000	0.104420000	-0.485700000
1	5.020700000	1.851560000	0.770700000

1	4.920830000	-1.731300000	-1.595500000
6	2.607570000	-2.783990000	-0.606900000
1	3.040380000	-3.203360000	-1.519160000
1	2.731640000	-3.522600000	0.195060000
1	1.534190000	-2.663030000	-0.767560000
6	2.683050000	1.471000000	2.136470000
1	1.626170000	1.641370000	1.908230000
1	2.722810000	1.021700000	3.136490000
1	3.187890000	2.439410000	2.182400000
6	6.398510000	0.524630000	-1.174120000
1	7.030800000	1.128780000	-0.515140000
1	6.980250000	-0.341180000	-1.506780000
1	6.177590000	1.131980000	-2.061370000
1	-2.307720000	-0.030090000	2.433140000
1	0.324480000	3.281090000	1.042660000
6	-2.864810000	-2.236800000	-0.649390000
1	-3.727870000	-2.617960000	-0.091660000
6	-1.708550000	-3.230480000	-0.452590000
6	-3.253570000	-2.112350000	-2.132290000
1	-4.132660000	-1.476850000	-2.280930000
1	-2.433960000	-1.698210000	-2.728180000
1	-3.491990000	-3.101840000	-2.539770000
1	-0.799050000	-2.902880000	-0.960580000
1	-1.989970000	-4.203340000	-0.872890000
1	-1.466870000	-3.386400000	0.603300000
6	-4.149230000	0.302170000	0.123050000
1	-4.422180000	0.397580000	-0.936380000
6	-4.074230000	1.718080000	0.716640000
6	-5.233600000	-0.527800000	0.833710000
1	-5.423490000	-1.493140000	0.355900000
1	-4.976570000	-0.708890000	1.884400000
1	-6.177770000	0.029460000	0.824150000
1	-3.821210000	1.692900000	1.781650000
1	-5.057420000	2.194890000	0.615240000
1	-3.326940000	2.343010000	0.229270000
1	-0.874737541	3.530683564	-0.821339146
1	-1.103090000	3.412070000	2.116140000
6	-0.755530000	3.041970000	1.136100000
8	-1.421792004	3.609176272	-0.028413365
8	-1.021240000	1.716810000	1.021880000

-1826.420254

25-Mn-iPr

25	0.512780000	-0.593610000	-0.532880000
6	1.465820000	-1.672780000	-1.646320000

6	0.016590000	0.421840000	-1.909320000
6	-0.976860000	-1.589600000	-0.765420000
8	2.078930000	-2.264560000	-2.429930000
8	-0.353510000	1.034460000	-2.829450000
8	-1.886040000	-2.264460000	-1.007760000
7	0.599590000	1.292810000	1.792610000
6	-0.234280000	0.696970000	0.890930000
6	-0.096430000	2.037280000	2.733390000
6	-1.411030000	1.923860000	2.410910000
7	-1.474930000	1.107200000	1.283730000
1	-2.297630000	2.337520000	2.865050000
1	0.396810000	2.571240000	3.530800000
6	2.046270000	1.103180000	1.765720000
15	2.470570000	0.602680000	0.022810000
1	2.541650000	2.026030000	2.079800000
6	-2.714490000	0.702080000	0.677770000
6	-3.335380000	-0.462270000	1.156410000
6	-3.266330000	1.483780000	-0.347800000
6	-4.546690000	-0.842490000	0.570430000
6	-4.476210000	1.057430000	-0.909670000
6	-5.128190000	-0.100090000	-0.465850000
1	-5.034840000	-1.750920000	0.915370000
1	-4.915330000	1.641670000	-1.715280000
6	-2.601820000	2.757680000	-0.808690000
1	-2.926880000	3.024610000	-1.817890000
1	-2.855280000	3.593680000	-0.143890000
1	-1.513550000	2.670430000	-0.815600000
6	-2.693700000	-1.281790000	2.248360000
1	-1.630020000	-1.446220000	2.048630000
1	-2.759940000	-0.773760000	3.218600000
1	-3.183290000	-2.254560000	2.343820000
6	-6.407550000	-0.563150000	-1.121430000
1	-7.040100000	-1.119380000	-0.421870000
1	-6.987830000	0.279610000	-1.511070000
1	-6.189710000	-1.229190000	-1.966300000
1	2.321300000	0.282190000	2.431320000
1	-0.269820000	-3.197170000	1.274880000
6	2.833680000	2.237570000	-0.819190000
1	3.675620000	2.683280000	-0.276150000
6	1.652260000	3.217490000	-0.730760000
6	3.256430000	2.003220000	-2.279070000
1	4.170550000	1.405970000	-2.357880000
1	2.470960000	1.493550000	-2.846580000
1	3.449520000	2.963810000	-2.771220000
1	0.781220000	2.853310000	-1.279680000
1	1.943280000	4.176920000	-1.174910000

1	1.345090000	3.412740000	0.301140000
6	4.155170000	-0.206580000	0.153350000
1	4.446350000	-0.348710000	-0.895860000
6	4.099360000	-1.593250000	0.812930000
6	5.210590000	0.680130000	0.838220000
1	5.374390000	1.632940000	0.326510000
1	4.941420000	0.892080000	1.880020000
1	6.171080000	0.151610000	0.854500000
1	3.819660000	-1.526030000	1.869300000
1	5.095250000	-2.051040000	0.755500000
1	3.380210000	-2.257740000	0.336560000
1	1.136090000	-4.608130000	0.375620000
1	1.140990000	-3.216540000	2.386810000
6	0.801210000	-2.912600000	1.375140000
8	1.539910000	-3.729490000	0.407470000
8	1.039920000	-1.601440000	1.192230000
1	-0.194820000	-4.896320000	-2.191910000
1	0.202880000	-4.400770000	-1.803130000

-1827.591714

26-Mn-iPr

25	0.489940000	0.366560000	-0.965340000
6	1.354010000	0.569570000	-2.522520000
6	-0.101600000	2.068380000	-0.933130000
6	-0.942450000	-0.259470000	-1.832750000
8	1.925130000	0.689590000	-3.529110000
8	-0.517540000	3.154700000	-0.994270000
8	-1.793120000	-0.700960000	-2.492550000
7	0.707090000	-0.422390000	1.931250000
6	-0.163060000	-0.103630000	0.926120000
6	0.051940000	-0.745770000	3.109710000
6	-1.274350000	-0.614570000	2.855090000
7	-1.387970000	-0.222490000	1.521280000
1	-2.141270000	-0.762100000	3.479580000
1	0.579850000	-1.043990000	4.001780000
6	2.146370000	-0.479480000	1.716460000
15	2.477580000	0.521970000	0.179200000
1	2.667270000	-0.090510000	2.595810000
6	-2.653450000	-0.003300000	0.875910000
6	-3.291460000	-1.097370000	0.268810000
6	-3.218330000	1.280030000	0.895010000
6	-4.521670000	-0.871450000	-0.355360000
6	-4.448120000	1.459460000	0.248570000
6	-5.109930000	0.400490000	-0.384500000
1	-5.023250000	-1.702690000	-0.845910000

1	-4.895130000	2.450730000	0.239560000
6	-2.550250000	2.419910000	1.623590000
1	-2.937040000	3.383400000	1.280970000
1	-2.734540000	2.350850000	2.703480000
1	-1.468200000	2.418390000	1.480110000
6	-2.655900000	-2.465730000	0.285160000
1	-1.602830000	-2.421960000	-0.006190000
1	-2.687910000	-2.907300000	1.288980000
1	-3.173900000	-3.144290000	-0.398100000
6	-6.413820000	0.624390000	-1.113210000
1	-7.114450000	-0.200540000	-0.943730000
1	-6.898310000	1.553110000	-0.796130000
1	-6.246450000	0.690740000	-2.195810000
1	2.447560000	-1.517070000	1.548980000
1	-0.079910000	-4.757700000	0.603600000
6	3.052090000	2.169920000	0.862070000
1	3.933090000	1.967840000	1.483140000
6	1.975400000	2.805780000	1.755810000
6	3.450330000	3.112500000	-0.283990000
1	4.284220000	2.720930000	-0.875870000
1	2.607880000	3.288560000	-0.962180000
1	3.760620000	4.083590000	0.119690000
1	1.071260000	3.038770000	1.188410000
1	2.355140000	3.745080000	2.175270000
1	1.689530000	2.162590000	2.594770000
6	4.034480000	-0.246040000	-0.531700000
1	4.305230000	0.429910000	-1.352800000
6	3.772480000	-1.636060000	-1.135480000
6	5.206520000	-0.297770000	0.464030000
1	5.499480000	0.689790000	0.831580000
1	4.973230000	-0.930230000	1.328900000
1	6.084710000	-0.732910000	-0.027250000
1	3.425970000	-2.350630000	-0.380680000
1	4.706010000	-2.026410000	-1.558140000
1	3.027410000	-1.605960000	-1.931950000
1	-0.562370000	-3.283590000	-2.286780000
1	1.637120000	-4.875370000	-0.140460000
6	0.976700000	-4.435300000	0.626260000
8	0.279110000	-3.407490000	-1.828000000
8	1.390320000	-3.659840000	1.467490000
1	0.995620000	-1.134180000	-0.918230000
1	0.541190000	-2.501020000	-1.555000000

-1827.598214

27-Mn-iPr

25	0.522930000	0.194610000	-0.990360000
6	1.415500000	0.533160000	-2.503990000
6	-0.145290000	1.864060000	-0.891860000
6	-0.840500000	-0.486650000	-1.922860000
8	2.007920000	0.741070000	-3.484650000
8	-0.603270000	2.935190000	-0.925380000
8	-1.643930000	-0.968130000	-2.612390000
7	0.696390000	-0.802200000	1.841160000
6	-0.162090000	-0.418590000	0.846440000
6	0.025860000	-1.208920000	2.985240000
6	-1.297520000	-1.066220000	2.720890000
7	-1.396210000	-0.586660000	1.414270000
1	-2.172200000	-1.258600000	3.322100000
1	0.541490000	-1.563410000	3.864030000
6	2.144060000	-0.771280000	1.668880000
15	2.466630000	0.358300000	0.218410000
1	2.617110000	-0.421250000	2.590740000
6	-2.653440000	-0.240730000	0.804740000
6	-3.391330000	-1.231110000	0.137400000
6	-3.123650000	1.077620000	0.937250000
6	-4.607010000	-0.857600000	-0.448390000
6	-4.337920000	1.404840000	0.323750000
6	-5.087410000	0.455050000	-0.382430000
1	-5.183750000	-1.611270000	-0.979940000
1	-4.707070000	2.424820000	0.402390000
6	-2.377920000	2.099110000	1.760490000
1	-2.671000000	3.114660000	1.482160000
1	-2.598070000	1.967850000	2.827980000
1	-1.296940000	2.014150000	1.641760000
6	-2.895800000	-2.650500000	0.009260000
1	-2.268830000	-2.754600000	-0.882700000
1	-2.304790000	-2.966830000	0.872590000
1	-3.736020000	-3.342910000	-0.100310000
6	-6.369630000	0.842640000	-1.079680000
1	-7.088010000	0.016090000	-1.089410000
1	-6.846570000	1.703170000	-0.599450000
1	-6.173000000	1.116910000	-2.124110000
1	2.509440000	-1.775560000	1.437980000
1	-0.093260000	-3.389070000	-0.553510000
6	2.933800000	1.984330000	1.027190000
1	3.804460000	1.789520000	1.665010000
6	1.797600000	2.507780000	1.918160000
6	3.315590000	3.017510000	-0.044890000
1	4.200970000	2.721260000	-0.617180000
1	2.493870000	3.175980000	-0.752630000
1	3.538030000	3.982100000	0.426730000

1	0.907850000	2.737020000	1.328230000
1	2.115630000	3.433080000	2.413300000
1	1.513800000	1.797100000	2.701240000
6	4.090040000	-0.261670000	-0.488860000
1	4.334770000	0.483940000	-1.255970000
6	3.943420000	-1.620810000	-1.191530000
6	5.236500000	-0.301120000	0.536450000
1	5.455200000	0.679000000	0.969830000
1	5.021220000	-0.997180000	1.356050000
1	6.153490000	-0.650940000	0.047880000
1	3.681590000	-2.417130000	-0.486780000
1	4.899110000	-1.890680000	-1.656490000
1	3.180570000	-1.595610000	-1.971470000
1	1.507230000	-3.568250000	-1.511460000
6	0.994650000	-3.568370000	-0.532810000
8	1.586800000	-3.806840000	0.505490000
1	1.064670000	-1.296510000	-1.071340000

-1751.168443

TS8-Mn-iPr

25	0.505240000	0.185250000	-0.907310000
6	1.366570000	0.445460000	-2.489800000
6	0.242960000	1.922990000	-0.730330000
6	-1.107670000	0.058070000	-1.758420000
8	1.927700000	0.661400000	-3.478170000
8	0.020300000	3.060310000	-0.652110000
8	-2.056670000	0.023190000	-2.411490000
7	0.697850000	-0.497460000	2.030940000
6	-0.157430000	-0.209050000	1.006440000
6	0.022020000	-0.742240000	3.213330000
6	-1.297520000	-0.567830000	2.944120000
7	-1.387810000	-0.230900000	1.596850000
1	-2.172880000	-0.652000000	3.568330000
1	0.531100000	-1.019740000	4.123100000
6	2.102940000	-0.802280000	1.804940000
15	2.578990000	0.046450000	0.226310000
1	2.701160000	-0.485810000	2.663550000
6	-2.642780000	-0.104000000	0.907330000
6	-3.240310000	-1.281150000	0.420530000
6	-3.229940000	1.160450000	0.758710000
6	-4.452480000	-1.152380000	-0.263860000
6	-4.443270000	1.234980000	0.062060000
6	-5.062130000	0.094360000	-0.462260000
1	-4.926150000	-2.046290000	-0.663320000
1	-4.910520000	2.207710000	-0.075080000

6	-2.613720000	2.400440000	1.360400000
1	-2.854900000	3.285740000	0.765250000
1	-3.000950000	2.569160000	2.373660000
1	-1.527940000	2.328870000	1.437640000
6	-2.604040000	-2.630180000	0.653320000
1	-1.511460000	-2.611190000	0.551020000
1	-2.819450000	-2.981830000	1.671220000
1	-3.009520000	-3.371560000	-0.040870000
6	-6.344650000	0.201220000	-1.252380000
1	-6.136710000	0.204880000	-2.330040000
1	-7.009060000	-0.646430000	-1.053260000
1	-6.887810000	1.122570000	-1.019080000
1	2.192590000	-1.876080000	1.626330000
1	-0.708440000	-2.685290000	-1.478530000
6	3.375840000	1.659420000	0.753060000
1	4.326230000	1.376230000	1.222550000
6	2.545870000	2.430710000	1.791630000
6	3.683040000	2.532840000	-0.475130000
1	4.301590000	2.015990000	-1.215980000
1	2.767070000	2.860980000	-0.975220000
1	4.228410000	3.430970000	-0.162890000
1	1.590730000	2.769600000	1.383840000
1	3.100070000	3.322670000	2.107010000
1	2.338880000	1.839870000	2.689130000
6	4.043750000	-0.920870000	-0.429950000
1	4.570780000	-0.185920000	-1.051830000
6	3.631050000	-2.106680000	-1.312280000
6	4.994150000	-1.379960000	0.691460000
1	5.293830000	-0.572600000	1.367560000
1	4.542530000	-2.180040000	1.287040000
1	5.909660000	-1.785400000	0.245250000
1	2.980330000	-2.792970000	-0.761920000
1	4.529460000	-2.639270000	-1.646900000
1	3.088680000	-1.779770000	-2.202890000
1	0.787810000	-3.540950000	-1.886500000
6	0.391210000	-2.681460000	-1.284820000
8	0.761560000	-2.657330000	0.019500000
1	0.764920000	-1.789370000	-1.895100000

-1751.132535

28-Mn-iPr

25	0.525480000	-0.688620000	-0.577790000
6	1.409990000	-1.854580000	-1.636890000
6	0.150290000	0.371540000	-1.964630000
6	-1.019680000	-1.585740000	-0.870600000

8	1.983220000	-2.558310000	-2.360710000
8	-0.151890000	1.026310000	-2.880700000
8	-1.940410000	-2.222000000	-1.166540000
7	0.670600000	1.233850000	1.719540000
6	-0.176410000	0.659670000	0.817040000
6	-0.008910000	1.990820000	2.662960000
6	-1.325090000	1.906270000	2.340830000
7	-1.407420000	1.094830000	1.210060000
1	-2.202870000	2.336150000	2.797080000
1	0.496360000	2.511090000	3.461840000
6	2.098370000	0.942230000	1.747750000
15	2.552270000	0.336360000	0.048210000
1	2.653900000	1.833990000	2.050200000
6	-2.660090000	0.657470000	0.655670000
6	-3.231990000	-0.516080000	1.170080000
6	-3.272040000	1.421060000	-0.349170000
6	-4.460930000	-0.924480000	0.639670000
6	-4.497650000	0.968960000	-0.851530000
6	-5.104290000	-0.200090000	-0.371220000
1	-4.914430000	-1.840500000	1.010880000
1	-4.987130000	1.539930000	-1.637280000
6	-2.629360000	2.687020000	-0.859880000
1	-3.237070000	3.143580000	-1.645800000
1	-2.502670000	3.423450000	-0.057460000
1	-1.636090000	2.489770000	-1.273680000
6	-2.520460000	-1.317730000	2.232070000
1	-1.465800000	-1.474790000	1.975950000
1	-2.538300000	-0.797550000	3.198200000
1	-2.997460000	-2.292180000	2.367070000
6	-6.402970000	-0.690110000	-0.966380000
1	-6.958830000	-1.315780000	-0.260760000
1	-7.048070000	0.142740000	-1.265680000
1	-6.213190000	-1.295010000	-1.862460000
1	2.285360000	0.128410000	2.452720000
1	-0.334530000	-3.403330000	1.059190000
6	3.135630000	1.876540000	-0.847040000
1	4.040250000	2.215860000	-0.328370000
6	2.101470000	3.012620000	-0.788270000
6	3.504670000	1.537090000	-2.301690000
1	4.299850000	0.787310000	-2.367780000
1	2.640110000	1.160290000	-2.857040000
1	3.860900000	2.438230000	-2.814740000
1	1.173890000	2.745350000	-1.300600000
1	2.508150000	3.900460000	-1.287280000
1	1.849140000	3.298500000	0.237700000
6	4.146380000	-0.611470000	0.319810000

1	4.580830000	-0.668050000	-0.686600000
6	3.911730000	-2.045020000	0.815560000
6	5.140460000	0.123030000	1.238250000
1	5.370190000	1.140160000	0.906050000
1	4.767920000	0.175060000	2.267680000
1	6.086660000	-0.430370000	1.265990000
1	3.400550000	-2.060130000	1.781090000
1	4.879640000	-2.551020000	0.920370000
1	3.300950000	-2.621970000	0.121260000
1	1.022350000	-3.473670000	2.198690000
6	0.716320000	-3.080440000	1.210410000
8	0.885720000	-1.702790000	1.167630000
1	1.310240000	-3.633860000	0.453840000

-1751.184119

29-Mn-iPr

25	0.529600000	0.706970000	0.544460000
6	1.441660000	1.932220000	1.509740000
6	0.128790000	-0.240450000	1.999960000
6	-1.006060000	1.653630000	0.734620000
8	2.044040000	2.674720000	2.167770000
8	-0.183180000	-0.828080000	2.957030000
8	-1.930360000	2.316890000	0.945400000
7	0.665780000	-1.364020000	-1.666660000
6	-0.184910000	-0.739530000	-0.801660000
6	-0.011340000	-2.167890000	-2.571090000
6	-1.329280000	-2.063380000	-2.260140000
7	-1.414360000	-1.192490000	-1.175370000
1	-2.206260000	-2.514030000	-2.697520000
1	0.495730000	-2.729800000	-3.340090000
6	2.096210000	-1.081830000	-1.696370000
15	2.539340000	-0.399620000	-0.022240000
1	2.650130000	-1.989720000	-1.949850000
6	-2.664730000	-0.734780000	-0.632810000
6	-3.243570000	0.413910000	-1.192160000
6	-3.260970000	-1.451880000	0.415170000
6	-4.470000000	0.840360000	-0.669400000
6	-4.482930000	-0.982000000	0.908740000
6	-5.100380000	0.160380000	0.379530000
1	-4.930070000	1.737620000	-1.076470000
1	-4.961000000	-1.516520000	1.726600000
6	-2.599870000	-2.683700000	0.982700000
1	-3.199390000	-3.111890000	1.790510000
1	-2.462330000	-3.454650000	0.215500000
1	-1.608600000	-2.451810000	1.384330000

6	-2.539570000	1.174970000	-2.288510000
1	-1.484990000	1.350230000	-2.041970000
1	-2.554660000	0.615500000	-3.232450000
1	-3.023090000	2.139990000	-2.462380000
6	-6.397000000	0.668680000	0.963610000
1	-6.941470000	1.296290000	0.251050000
1	-7.053150000	-0.155570000	1.263140000
1	-6.206620000	1.275690000	1.858090000
1	2.290950000	-0.299730000	-2.434090000
1	-0.239870000	3.373730000	-1.346100000
6	3.065150000	-1.910810000	0.955070000
1	3.952270000	-2.312990000	0.451440000
6	1.986040000	-3.006090000	0.957310000
6	3.454460000	-1.509390000	2.388100000
1	4.290030000	-0.802350000	2.412080000
1	2.612860000	-1.053140000	2.918950000
1	3.760390000	-2.397940000	2.952930000
1	1.071290000	-2.674680000	1.455000000
1	2.358660000	-3.881960000	1.501870000
1	1.718430000	-3.334330000	-0.051800000
6	4.156950000	0.500440000	-0.308790000
1	4.550980000	0.637120000	0.706600000
6	3.960740000	1.890220000	-0.930190000
6	5.173610000	-0.320240000	-1.122670000
1	5.385590000	-1.302010000	-0.688660000
1	4.832410000	-0.467570000	-2.153720000
1	6.123820000	0.224570000	-1.172420000
1	3.503580000	1.830240000	-1.920670000
1	4.936920000	2.382630000	-1.021270000
1	3.316230000	2.522060000	-0.319670000
1	1.073210000	3.332300000	-2.536950000
6	0.794700000	3.008970000	-1.514600000
8	0.927170000	1.631630000	-1.393960000
1	1.437510000	3.589270000	-0.820510000
1	0.434775055	3.287168796	-0.061445663
1	0.303113796	3.672892706	0.561049346

-1752.357689

TS9-Mn-iPr

25	0.511830000	-0.118930000	0.989200000
6	1.355080000	-0.547600000	2.545090000
6	-0.028420000	-1.785950000	0.798390000
6	-1.013590000	0.249470000	1.915930000
8	1.875170000	-0.884000000	3.521970000
8	-0.430660000	-2.876250000	0.737540000

8	-1.938770000	0.403720000	2.589350000
7	0.698400000	0.767560000	-1.892580000
6	-0.155970000	0.446320000	-0.875430000
6	0.022120000	1.093190000	-3.057190000
6	-1.300740000	0.959670000	-2.780350000
7	-1.392550000	0.564090000	-1.449020000
1	-2.177850000	1.109080000	-3.390060000
1	0.533900000	1.391750000	-3.958750000
6	2.146020000	0.801270000	-1.726540000
15	2.522570000	-0.260650000	-0.243530000
1	2.628120000	0.450620000	-2.642820000
6	-2.650130000	0.255680000	-0.818500000
6	-3.326920000	1.269600000	-0.121640000
6	-3.176230000	-1.038010000	-0.959420000
6	-4.554050000	0.948680000	0.466690000
6	-4.402570000	-1.313990000	-0.341650000
6	-5.101980000	-0.337840000	0.377760000
1	-5.084360000	1.717180000	1.024120000
1	-4.818680000	-2.314980000	-0.427940000
6	-2.475430000	-2.088860000	-1.785080000
6	-2.475430000	-2.088860000	-1.785080000
1	-2.820190000	-3.090590000	-1.515600000
1	-2.676870000	-1.941840000	-2.853900000
1	-1.392510000	-2.058640000	-1.654170000
6	-2.723640000	2.641620000	0.028320000
1	-1.824560000	2.604030000	0.650630000
1	-2.422300000	3.063340000	-0.936180000
1	-3.430390000	3.330020000	0.498970000
6	-6.400220000	-0.668790000	1.074160000
1	-6.885830000	-1.543160000	0.629330000
1	-6.223130000	-0.893320000	2.133770000
1	-7.103470000	0.169880000	1.033350000
1	2.460340000	1.818070000	-1.487360000
1	0.405460000	3.256910000	-1.040200000
6	2.947200000	-1.922560000	-1.006450000
1	3.895410000	-1.766570000	-1.539020000
6	1.896190000	-2.393960000	-2.023750000
6	3.171250000	-2.984750000	0.084000000
1	3.912520000	-2.678250000	0.829080000
1	2.243250000	-3.218750000	0.613130000
1	3.532590000	-3.913360000	-0.373420000
1	0.918330000	-2.536580000	-1.557520000
1	2.202010000	-3.358550000	-2.445760000
1	1.771710000	-1.696740000	-2.857700000
6	4.212530000	0.289730000	0.367820000
1	4.650740000	-0.649050000	0.729710000

6	4.169440000	1.279180000	1.539810000
6	5.098960000	0.820210000	-0.773430000
1	5.129740000	0.150550000	-1.639990000
1	4.762650000	1.806210000	-1.110600000
1	6.127950000	0.933930000	-0.412850000
1	3.671070000	2.207560000	1.253930000
1	5.195220000	1.497100000	1.862920000
1	3.630910000	0.872380000	2.398910000
1	1.480320000	4.441040000	-0.269240000
6	0.855690000	3.548970000	-0.072550000
8	1.587320000	2.513120000	0.510820000
1	0.022550000	3.886890000	0.573670000
1	1.093550000	2.222260000	1.698930000
1	0.684660000	1.912660000	2.483610000

-1752.312066

30-Mn-iPr

25	-0.519340000	-0.181270000	-0.978680000
6	-1.400510000	-0.295950000	-2.534260000
6	0.043250000	-1.890820000	-1.041140000
6	0.915100000	0.470990000	-1.832080000
8	-1.982750000	-0.348950000	-3.540430000
8	0.444820000	-2.976220000	-1.177160000
8	1.762890000	0.931090000	-2.478300000
7	-0.693270000	0.455270000	1.963150000
6	0.159960000	0.179890000	0.928860000
6	-0.016910000	0.720240000	3.144670000
6	1.304140000	0.593880000	2.861840000
7	1.394450000	0.263610000	1.510590000
1	2.181650000	0.704760000	3.479100000
1	-0.528440000	0.972420000	4.060340000
6	-2.136520000	0.533110000	1.777610000
15	-2.496180000	-0.374720000	0.185410000
1	-2.644880000	0.090760000	2.638870000
6	2.649950000	0.050320000	0.842010000
6	3.304390000	1.157590000	0.277590000
6	3.188990000	-1.243530000	0.800520000
6	4.525340000	0.934260000	-0.365130000
6	4.411860000	-1.418440000	0.139480000
6	5.089770000	-0.345810000	-0.451810000
1	5.038890000	1.776020000	-0.824180000
1	4.839260000	-2.416830000	0.084250000
6	2.501420000	-2.403040000	1.478770000
1	2.860550000	-3.356390000	1.081880000
1	2.698990000	-2.394680000	2.558470000

1	1.418000000	-2.369100000	1.349230000
6	2.697850000	2.536120000	0.356480000
1	1.646000000	2.530990000	0.058670000
1	2.726950000	2.926760000	1.380990000
1	3.236460000	3.235380000	-0.288420000
6	6.387150000	-0.559850000	-1.194940000
1	7.114730000	0.226160000	-0.964230000
1	6.838980000	-1.525390000	-0.947470000
1	6.221180000	-0.539550000	-2.279510000
1	-2.435040000	1.581440000	1.682970000
1	0.043350000	4.522660000	-0.797310000
6	-3.073910000	-2.053440000	0.789550000
1	-3.949370000	-1.875690000	1.425730000
6	-1.997790000	-2.741100000	1.644260000
6	-3.488000000	-2.933420000	-0.400010000
1	-4.316510000	-2.500850000	-0.970590000
1	-2.649430000	-3.089240000	-1.087430000
1	-3.812890000	-3.918060000	-0.043390000
1	-1.095870000	-2.947350000	1.063610000
1	-2.380780000	-3.699730000	2.014100000
1	-1.707130000	-2.145180000	2.515660000
6	-4.059910000	0.435700000	-0.458980000
1	-4.332830000	-0.184320000	-1.322700000
6	-3.802750000	1.862810000	-0.971900000
6	-5.228130000	0.420290000	0.542130000
1	-5.527520000	-0.589820000	0.835830000
1	-4.986730000	0.984100000	1.451290000
1	-6.104650000	0.898210000	0.088840000
1	-3.484980000	2.534460000	-0.167250000
1	-4.730040000	2.265210000	-1.396720000
1	-3.033800000	1.886430000	-1.745790000
1	-1.041450000	5.328500000	0.359440000
6	-0.907150000	4.430000000	-0.250940000
8	-0.911440000	3.310600000	0.627420000
1	-1.724640000	4.385260000	-0.986000000
1	-0.823830000	2.502040000	0.078250000
1	-0.949860000	1.350010000	-0.964670000

-1752.375936

1-Mn-Ph

25	-0.050230000	-0.560020000	-0.777550000
6	0.824650000	-1.240170000	-2.186610000
6	-1.569820000	-1.254260000	-1.436030000
1	0.128000000	-1.970550000	-0.051780000
6	-0.250950000	1.073060000	-1.507740000

8	1.386520000	-1.696810000	-3.097280000
8	-2.474920000	-1.769780000	-1.949150000
8	-0.375340000	2.113450000	-2.015020000
7	-0.007740000	0.185110000	2.141200000
6	-0.812570000	-0.015540000	1.049330000
6	-0.734200000	0.510060000	3.278980000
6	-2.036540000	0.532540000	2.900730000
7	-2.067070000	0.213470000	1.542350000
1	-2.938460000	0.745150000	3.453060000
1	-0.265490000	0.692400000	4.233570000
6	1.421100000	-0.083060000	2.099530000
1	1.971260000	0.650710000	2.694180000
15	1.905420000	-0.095180000	0.296050000
1	1.623950000	-1.084220000	2.494030000
6	-3.302310000	0.092300000	0.814180000
6	-3.941940000	-1.157470000	0.790610000
6	-3.847870000	1.227990000	0.198640000
6	-5.159390000	-1.254070000	0.110650000
6	-5.067330000	1.080740000	-0.474600000
6	-5.734300000	-0.149050000	-0.531510000
1	-5.663080000	-2.217040000	0.068060000
1	-5.504180000	1.947920000	-0.964080000
6	-3.146100000	2.561470000	0.264050000
1	-3.746970000	3.342610000	-0.209610000
1	-2.950360000	2.863080000	1.299480000
1	-2.180200000	2.525150000	-0.247460000
6	-3.307700000	-2.358170000	1.446790000
1	-2.319360000	-2.558970000	1.018690000
1	-3.163280000	-2.200850000	2.522190000
1	-3.926240000	-3.249460000	1.312520000
6	-7.028410000	-0.295820000	-1.295730000
1	-7.730020000	-0.954520000	-0.772430000
1	-7.518580000	0.670800000	-1.449160000
1	-6.846430000	-0.735160000	-2.284900000
6	2.646600000	1.559180000	-0.013730000
6	2.247200000	2.690830000	0.713340000
6	3.511860000	1.723260000	-1.108730000
6	2.726130000	3.958770000	0.369850000
6	3.989470000	2.989790000	-1.449680000
6	3.601900000	4.111040000	-0.708150000
1	1.548020000	2.599660000	1.539640000
1	3.816800000	0.860910000	-1.695830000
1	2.409000000	4.825870000	0.942640000
1	4.661160000	3.100270000	-2.296370000
1	3.971690000	5.096760000	-0.975830000
6	3.350000000	-1.233750000	0.310150000

6	4.604780000	-0.819570000	0.790510000
6	3.180800000	-2.561190000	-0.111200000
6	5.670830000	-1.719770000	0.845780000
6	4.250190000	-3.459900000	-0.055110000
6	5.495580000	-3.041530000	0.421160000
1	4.755380000	0.206990000	1.111490000
1	2.212650000	-2.888040000	-0.475600000
1	6.637080000	-1.388390000	1.215960000
1	4.108750000	-4.483770000	-0.389520000
1	6.326870000	-3.740150000	0.459180000

-1862.903307

2-Mn-Ph

25	0.103160000	-0.232040000	-0.921830000
6	-0.768960000	-0.115290000	-2.483870000
6	1.624440000	0.167520000	-1.786760000
1	0.000910000	1.346410000	-0.771050000
6	0.279850000	-2.022040000	-1.001470000
8	-1.332420000	-0.036430000	-3.498610000
8	2.523710000	0.472420000	-2.454670000
8	0.410470000	-3.175980000	-1.087990000
7	0.056380000	-0.061240000	2.087930000
6	0.860420000	-0.135330000	0.981030000
6	0.787920000	0.020630000	3.265120000
6	2.093660000	-0.008830000	2.901890000
7	2.121690000	-0.106730000	1.509810000
1	2.999810000	0.029970000	3.485550000
1	0.319250000	0.096550000	4.233840000
6	-1.394770000	0.015290000	2.014300000
1	-1.849290000	-0.752350000	2.646150000
15	-1.869050000	-0.195040000	0.211110000
1	-1.728770000	0.998160000	2.354710000
6	3.359560000	-0.116570000	0.775210000
6	3.898960000	1.109300000	0.354590000
6	4.008780000	-1.339820000	0.549530000
6	5.127790000	1.087260000	-0.312580000
6	5.235650000	-1.311310000	-0.124590000
6	5.807680000	-0.111130000	-0.564880000
1	5.555250000	2.025820000	-0.657870000
1	5.752650000	-2.249560000	-0.311990000
6	3.401140000	-2.640810000	1.010730000
1	4.080810000	-3.476660000	0.823920000
1	3.168780000	-2.623040000	2.081520000
1	2.464660000	-2.845910000	0.482860000
6	3.145060000	2.398040000	0.565880000

1	2.223600000	2.392860000	-0.027010000
1	2.857360000	2.537410000	1.613840000
1	3.744300000	3.258430000	0.256670000
6	7.113490000	-0.108630000	-1.323470000
1	7.700810000	0.790190000	-1.108190000
1	7.724800000	-0.982910000	-1.077450000
1	6.932980000	-0.128180000	-2.405920000
6	-2.896650000	-1.723770000	0.198820000
6	-2.470210000	-2.851210000	0.920400000
6	-4.019820000	-1.834470000	-0.635610000
6	-3.171450000	-4.055600000	0.834450000
6	-4.715990000	-3.043080000	-0.726190000
6	-4.298700000	-4.153950000	0.012230000
1	-1.576740000	-2.802760000	1.538000000
1	-4.356040000	-0.980260000	-1.215450000
1	-2.830370000	-4.918030000	1.400240000
1	-5.584150000	-3.113800000	-1.375550000
1	-4.841360000	-5.092260000	-0.059570000
6	-3.103560000	1.151750000	-0.016040000
6	-4.262320000	1.198180000	0.779790000
6	-2.874880000	2.169310000	-0.951580000
6	-5.168680000	2.250840000	0.647070000
6	-3.786900000	3.221840000	-1.087070000
6	-4.931860000	3.265680000	-0.288140000
1	-4.462660000	0.407190000	1.497820000
1	-1.978270000	2.146280000	-1.561220000
1	-6.058990000	2.278180000	1.269140000
1	-3.597210000	4.004700000	-1.815850000
1	-5.638950000	4.083930000	-0.392440000
6	-0.314450000	3.642300000	0.583780000
8	-0.088880000	4.234030000	-0.398390000
8	-0.538410000	3.095400000	1.594010000

-2051.496397

TS1-Mn-Ph

25	-0.045710000	-0.349640000	-0.851020000
6	0.847520000	-0.828680000	-2.339140000
6	-1.555680000	-1.043410000	-1.553070000
1	0.247740000	-1.840430000	-0.213020000
6	-0.373290000	1.309220000	-1.460590000
8	1.426810000	-1.123300000	-3.300290000
8	-2.454650000	-1.534960000	-2.091840000
8	-0.590700000	2.366280000	-1.888450000
7	0.013590000	0.134240000	2.118370000
6	-0.798710000	0.033240000	1.022030000

6	-0.705290000	0.348830000	3.284320000
6	-2.010960000	0.405580000	2.917920000
7	-2.050060000	0.212850000	1.538330000
1	-2.909190000	0.563400000	3.493720000
1	-0.231590000	0.434040000	4.249780000
6	1.453410000	-0.059310000	2.036190000
1	1.973010000	0.632380000	2.704100000
15	1.910580000	0.169420000	0.242740000
1	1.704110000	-1.087570000	2.309220000
6	-3.277950000	0.229940000	0.787490000
6	-3.987410000	-0.972890000	0.630840000
6	-3.742320000	1.449920000	0.274460000
6	-5.186980000	-0.930780000	-0.083970000
6	-4.945550000	1.437980000	-0.444440000
6	-5.676880000	0.260770000	-0.636870000
1	-5.743960000	-1.853540000	-0.229070000
1	-5.315700000	2.371480000	-0.861510000
6	-3.006010000	2.743550000	0.525410000
1	-1.923010000	2.622510000	0.459870000
1	-3.303240000	3.507570000	-0.197890000
1	-3.229820000	3.128460000	1.528650000
6	-3.450670000	-2.272300000	1.176190000
1	-2.579710000	-2.604300000	0.601890000
1	-3.126150000	-2.180590000	2.217530000
1	-4.206430000	-3.060120000	1.118580000
6	-6.958910000	0.256600000	-1.435130000
1	-7.767640000	-0.239600000	-0.886260000
1	-7.286230000	1.271980000	-1.678520000
1	-6.827630000	-0.287140000	-2.378790000
6	2.487920000	1.906300000	0.096670000
6	2.028650000	2.911950000	0.960760000
6	3.288210000	2.261180000	-1.002500000
6	2.382920000	4.246670000	0.741480000
6	3.641020000	3.594150000	-1.218140000
6	3.190270000	4.590770000	-0.345800000
1	1.384900000	2.669700000	1.801270000
1	3.640470000	1.496460000	-1.689550000
1	2.022070000	5.015810000	1.418610000
1	4.263370000	3.853790000	-2.069800000
1	3.462270000	5.628470000	-0.516380000
6	3.437280000	-0.840050000	0.103780000
6	4.658000000	-0.385300000	0.632650000
6	3.373740000	-2.113310000	-0.481510000
6	5.792730000	-1.196950000	0.580530000
6	4.511270000	-2.923980000	-0.530820000
6	5.721190000	-2.467520000	-0.001840000

1	4.726970000	0.603890000	1.076050000
1	2.440230000	-2.474770000	-0.896580000
1	6.731940000	-0.836260000	0.990490000
1	4.448400000	-3.907230000	-0.987780000
1	6.605980000	-3.096460000	-0.044370000
6	0.170420000	-3.268930000	0.521200000
8	0.050890000	-4.041800000	-0.380360000
8	0.278970000	-2.998840000	1.682020000

-2051.487525

3-Mn-Ph

25	-0.067030555	-0.338044460	-0.860764256
6	0.828039445	-0.877984460	-2.340844256
6	-1.610200555	-0.961544460	-1.592704256
1	0.143620555	-2.061205540	-0.040555744
6	-0.329280555	1.302615540	-1.523864256
8	1.400909445	-1.192254460	-3.295474256
8	-2.516590555	-1.390274460	-2.164544256
8	-0.517250555	2.355385540	-1.970244256
7	0.003509445	0.244405540	2.099335744
6	-0.813270555	0.118935540	1.010445744
6	-0.712400555	0.491665540	3.258705744
6	-2.019670555	0.543125540	2.893135744
7	-2.062470555	0.314625540	1.520895744
1	-2.916540555	0.713155540	3.467655744
1	-0.237250555	0.594305540	4.221715744
6	1.442689445	0.025205540	2.027535744
1	1.968929445	0.721015540	2.685395744
15	1.914679445	0.218965540	0.237405744
1	1.666059445	-1.006734460	2.310505744
6	-3.294090555	0.274055540	0.776045744
6	-3.959790555	-0.954924460	0.645075744
6	-3.801130555	1.469955540	0.243455744
6	-5.167370555	-0.963994460	-0.061464256
6	-5.008250555	1.406375540	-0.461974256
6	-5.701600555	0.200055540	-0.628134256
1	-5.694370555	-1.907214460	-0.183914256
1	-5.416280555	2.319845540	-0.888204256
6	-3.084400555	2.781285540	0.452755744
1	-3.568440555	3.585085540	-0.108014256
1	-3.079090555	3.064385540	1.512335744
1	-2.041330555	2.728655540	0.130415744
6	-3.372300555	-2.227844460	1.200785744
1	-2.513600555	-2.555594460	0.604715744
1	-3.012090555	-2.105814460	2.226905744

1	-4.109750555	-3.034364460	1.188145744
6	-6.981150555	0.147215540	-1.428074256
1	-7.673240555	-0.601774460	-1.029254256
1	-7.492220555	1.115145540	-1.435074256
1	-6.773280555	-0.123164460	-2.471274256
6	2.433729445	1.966955540	0.046205744
6	1.932399445	2.974455540	0.884465744
6	3.235359445	2.321375540	-1.051704256
6	2.247749445	4.314255540	0.640355744
6	3.547989445	3.660195540	-1.292024256
6	3.056489445	4.659775540	-0.445584256
1	1.285229445	2.728245540	1.721125744
1	3.620979445	1.553045540	-1.716224256
1	1.856159445	5.085995540	1.296975744
1	4.171829445	3.921645540	-2.141944256
1	3.298129445	5.701555540	-0.635464256
6	3.454839445	-0.761484460	0.104155744
6	4.668029445	-0.272404460	0.620645744
6	3.412759445	-2.043584460	-0.463044256
6	5.818879445	-1.060354460	0.571395744
6	4.567169445	-2.829724460	-0.508664256
6	5.769769445	-2.340074460	0.006325744
1	4.717959445	0.723715540	1.050735744
1	2.486229445	-2.439764460	-0.862364256
1	6.752519445	-0.675474460	0.971785744
1	4.520259445	-3.821794460	-0.947544256
1	6.666969445	-2.951344460	-0.032104256
6	0.281210555	-3.186335540	0.495024256
8	0.161690555	-4.076025540	-0.336315744
8	0.496190555	-3.060415540	1.698444256

-2051.488318

TS2-Mn-Ph

25	-0.096830000	-0.481370000	-0.747550000
6	0.829860000	-1.069060000	-2.209570000
6	-1.676450000	-0.973930000	-1.520210000
1	-0.649020000	-2.653070000	-0.315310000
6	-0.296680000	1.129670000	-1.466270000
8	1.426960000	-1.381530000	-3.145070000
8	-2.603070000	-1.275930000	-2.136940000
8	-0.475630000	2.164210000	-1.954800000
7	-0.014090000	0.260930000	2.177970000
6	-0.826450000	0.060170000	1.097500000
6	-0.737420000	0.562180000	3.318820000
6	-2.045320000	0.573130000	2.949440000

7	-2.080250000	0.269220000	1.593510000
1	-2.945640000	0.763070000	3.512340000
1	-0.265640000	0.727860000	4.274810000
6	1.429710000	0.064340000	2.132300000
1	1.935010000	0.823700000	2.733920000
15	1.909440000	0.127010000	0.339410000
1	1.677650000	-0.936440000	2.490180000
6	-3.304650000	0.181680000	0.841980000
6	-3.968040000	-1.054700000	0.788390000
6	-3.801670000	1.335850000	0.217760000
6	-5.160340000	-1.118670000	0.060770000
6	-4.994720000	1.218060000	-0.505060000
6	-5.683730000	0.002060000	-0.597650000
1	-5.684330000	-2.069100000	-0.006060000
1	-5.393990000	2.096990000	-1.005600000
6	-3.095880000	2.663070000	0.349270000
1	-3.500860000	3.392370000	-0.357240000
1	-3.215580000	3.072360000	1.360240000
1	-2.022700000	2.576740000	0.164040000
6	-3.395360000	-2.270320000	1.473240000
1	-2.378670000	-2.483320000	1.127650000
1	-3.332750000	-2.128220000	2.558370000
1	-4.010670000	-3.152840000	1.281250000
6	-6.942850000	-0.111180000	-1.422800000
1	-7.456120000	0.851710000	-1.510000000
1	-6.706920000	-0.451680000	-2.439220000
1	-7.642500000	-0.834490000	-0.991270000
6	2.319460000	1.887320000	0.011390000
6	1.781630000	2.928310000	0.783460000
6	3.067720000	2.202020000	-1.135780000
6	2.009810000	4.261050000	0.427580000
6	3.293540000	3.533280000	-1.488270000
6	2.766920000	4.566680000	-0.706120000
1	1.171970000	2.715490000	1.656300000
1	3.479190000	1.407810000	-1.753170000
1	1.590360000	5.057970000	1.035210000
1	3.877410000	3.762110000	-2.375210000
1	2.940480000	5.602560000	-0.982870000
6	3.517330000	-0.742710000	0.257440000
6	4.690830000	-0.103650000	0.697850000
6	3.582800000	-2.060340000	-0.219930000
6	5.912320000	-0.777650000	0.662860000
6	4.810630000	-2.727370000	-0.256290000
6	5.973880000	-2.091000000	0.183080000
1	4.656450000	0.920440000	1.057840000
1	2.690350000	-2.585620000	-0.537910000

1	6.813210000	-0.277130000	1.006690000
1	4.847620000	-3.748210000	-0.624820000
1	6.925810000	-2.613940000	0.152550000
6	0.312850000	-3.123140000	0.097590000
8	0.762030000	-4.068830000	-0.569420000
8	0.742350000	-2.574190000	1.149730000

-2051.476926

3'-Mn-Ph

25	-0.038000000	-0.604250000	-0.757980000
6	0.859640000	-1.303360000	-2.172410000
6	-1.588600000	-1.319810000	-1.379160000
1	-0.341060000	-3.697460000	-0.823280000
6	-0.380030000	0.924030000	-1.625170000
8	1.425040000	-1.743010000	-3.080930000
8	-2.519360000	-1.790780000	-1.876040000
8	-0.622220000	1.899570000	-2.204200000
7	0.041410000	0.254710000	2.146650000
6	-0.786310000	0.081810000	1.075570000
6	-0.656700000	0.615510000	3.288860000
6	-1.964040000	0.689380000	2.925290000
7	-2.021730000	0.364270000	1.572660000
1	-2.850030000	0.935410000	3.489250000
1	-0.170670000	0.775290000	4.238720000
6	1.474980000	0.006090000	2.060360000
1	2.022260000	0.682430000	2.721350000
15	1.928170000	0.203330000	0.265410000
1	1.690190000	-1.032820000	2.322160000
6	-3.246140000	0.312240000	0.819070000
6	-3.956700000	-0.897310000	0.786760000
6	-3.682480000	1.467150000	0.152670000
6	-5.144870000	-0.930670000	0.049590000
6	-4.871630000	1.380060000	-0.580650000
6	-5.612510000	0.192380000	-0.645090000
1	-5.704470000	-1.861470000	-0.002290000
1	-5.225080000	2.259340000	-1.114110000
6	-2.912020000	2.761120000	0.247610000
1	-3.281290000	3.489600000	-0.479040000
1	-3.009170000	3.204150000	1.246770000
1	-1.844830000	2.614630000	0.063380000
6	-3.424720000	-2.122780000	1.487280000
1	-2.410300000	-2.364930000	1.151380000
1	-3.367510000	-1.974290000	2.571920000
1	-4.061820000	-2.989810000	1.295830000
6	-6.865280000	0.111580000	-1.484230000

1	-7.579900000	-0.608630000	-1.072780000
1	-7.363480000	1.083520000	-1.559310000
1	-6.624530000	-0.213220000	-2.504740000
6	2.256590000	1.988810000	0.023810000
6	1.768050000	2.964880000	0.905410000
6	2.907500000	2.393830000	-1.154380000
6	1.946570000	4.322820000	0.623040000
6	3.089250000	3.749360000	-1.430380000
6	2.610020000	4.717700000	-0.541330000
1	1.235060000	2.680900000	1.807280000
1	3.278210000	1.649820000	-1.854760000
1	1.563670000	5.069040000	1.313520000
1	3.599870000	4.048430000	-2.341210000
1	2.747320000	5.772900000	-0.759430000
6	3.558650000	-0.623690000	0.159170000
6	4.757980000	0.058690000	0.424170000
6	3.594300000	-1.992660000	-0.152710000
6	5.976600000	-0.621900000	0.372430000
6	4.815740000	-2.668240000	-0.200000000
6	6.007500000	-1.984810000	0.058790000
1	4.746680000	1.117750000	0.662670000
1	2.669250000	-2.528340000	-0.331760000
1	6.899920000	-0.086560000	0.575700000
1	4.831330000	-3.727490000	-0.439250000
1	6.956890000	-2.511410000	0.017130000
6	0.170210000	-3.564260000	0.157410000
8	0.450340000	-4.562760000	0.826610000
8	0.425410000	-2.341910000	0.488000000

-2051.509460

4-Mn-Ph

25	0.115410000	0.174260000	1.005860000
6	-0.805330000	0.381390000	2.555720000
6	1.711340000	0.185860000	1.891480000
1	-0.122950000	-5.037230000	-1.118070000
6	0.240300000	1.956700000	0.761820000
8	-1.402420000	0.523310000	3.534530000
8	2.642960000	0.227200000	2.568970000
8	0.353060000	3.098730000	0.634300000
7	0.031440000	-0.458040000	-1.948550000
6	0.849510000	-0.183180000	-0.894500000
6	0.751570000	-0.743300000	-3.096370000
6	2.062660000	-0.619820000	-2.765430000
7	2.105080000	-0.273750000	-1.417580000
1	2.962770000	-0.751970000	-3.344560000

1	0.271900000	-1.028710000	-4.019080000
6	-1.412000000	-0.631980000	-1.819730000
1	-1.929960000	-0.169380000	-2.663390000
15	-1.907740000	0.091100000	-0.191500000
1	-1.620730000	-1.714340000	-1.808410000
6	3.337070000	-0.108280000	-0.692200000
6	3.919640000	-1.241160000	-0.098630000
6	3.928300000	1.163010000	-0.637750000
6	5.120740000	-1.059650000	0.594880000
6	5.128250000	1.292410000	0.071940000
6	5.734250000	0.195840000	0.698070000
1	5.585020000	-1.919780000	1.071760000
1	5.599960000	2.270270000	0.133410000
6	3.301910000	2.344130000	-1.337200000
1	3.881470000	3.254380000	-1.162320000
1	3.246430000	2.180660000	-2.419910000
1	2.281200000	2.525180000	-0.990750000
6	3.273160000	-2.598660000	-0.209890000
1	2.209260000	-2.583990000	0.045980000
1	3.330740000	-2.979480000	-1.237200000
1	3.773570000	-3.320670000	0.441140000
6	7.007770000	0.360860000	1.492390000
1	7.693870000	-0.476610000	1.325900000
1	7.529870000	1.286460000	1.230900000
1	6.791980000	0.394740000	2.567860000
6	-2.588310000	1.760790000	-0.522610000
6	-2.280540000	2.460420000	-1.698640000
6	-3.309190000	2.412070000	0.493770000
6	-2.707200000	3.781650000	-1.865010000
6	-3.735370000	3.729490000	0.323360000
6	-3.436550000	4.417650000	-0.857750000
1	-1.696790000	1.993550000	-2.485750000
1	-3.545530000	1.889510000	1.416620000
1	-2.463360000	4.312550000	-2.780800000
1	-4.296470000	4.218560000	1.114440000
1	-3.764630000	5.444910000	-0.987590000
6	-3.318670000	-0.940180000	0.353500000
6	-4.648800000	-0.592630000	0.066320000
6	-3.045890000	-2.138780000	1.032740000
6	-5.693300000	-1.428670000	0.468080000
6	-4.094600000	-2.972110000	1.426570000
6	-5.418470000	-2.616340000	1.152660000
1	-4.874900000	0.324640000	-0.467530000
1	-2.022140000	-2.445720000	1.216140000
1	-6.719330000	-1.151590000	0.242960000
1	-3.872970000	-3.901200000	1.943490000

1	-6.232220000	-3.264980000	1.464770000
6	-0.481490000	-3.976530000	-1.134600000
8	-1.197950000	-3.643110000	-2.110050000
8	-0.108400000	-3.262070000	-0.156530000
1	0.033480000	-1.599860000	0.741860000
1	0.103110000	-1.448850000	1.529610000

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TS3-Mn-Ph

25	0.101760000	0.098130000	0.998570000
6	-0.790410000	0.261380000	2.566700000
6	1.693390000	-0.021220000	1.873120000
1	-0.061530000	-5.033570000	-1.046810000
6	0.282260000	1.883260000	0.851630000
8	-1.367870000	0.381760000	3.561400000
8	2.629470000	-0.077160000	2.544580000
8	0.420290000	3.029890000	0.793500000
7	0.013750000	-0.295490000	-1.993990000
6	0.837350000	-0.144420000	-0.917800000
6	0.724190000	-0.407010000	-3.177250000
6	2.036170000	-0.301270000	-2.844750000
7	2.088070000	-0.140760000	-1.462850000
1	2.931200000	-0.332490000	-3.445360000
1	0.239690000	-0.575380000	-4.125940000
6	-1.426900000	-0.485120000	-1.871580000
1	-1.952270000	0.040930000	-2.672220000
15	-1.916980000	0.101460000	-0.182350000
1	-1.623080000	-1.563980000	-1.924960000
6	3.325290000	-0.013920000	-0.738230000
6	3.937530000	-1.184590000	-0.256550000
6	3.889040000	1.258950000	-0.565670000
6	5.140980000	-1.044430000	0.440380000
6	5.093630000	1.345740000	0.144630000
6	5.728150000	0.209590000	0.659390000
1	5.626450000	-1.935280000	0.831910000
1	5.542350000	2.324600000	0.298110000
6	3.255480000	2.496320000	-1.154460000
1	3.521750000	3.384180000	-0.573870000
1	3.603530000	2.658400000	-2.182740000
1	2.166640000	2.429570000	-1.189460000
6	3.300790000	-2.534260000	-0.465810000
1	2.340960000	-2.617910000	0.053770000
1	3.088750000	-2.721700000	-1.524570000
1	3.954040000	-3.332370000	-0.102720000
6	7.003970000	0.327740000	1.458480000

1	7.680240000	-0.510110000	1.258060000
1	7.536600000	1.257510000	1.234730000
1	6.789200000	0.321850000	2.534780000
6	-2.656030000	1.764180000	-0.402900000
6	-2.256840000	2.601260000	-1.455890000
6	-3.528510000	2.262770000	0.578910000
6	-2.741150000	3.909800000	-1.537660000
6	-4.010920000	3.569940000	0.493240000
6	-3.619690000	4.396050000	-0.565830000
1	-1.557780000	2.248800000	-2.208960000
1	-3.838110000	1.629750000	1.405850000
1	-2.426140000	4.548330000	-2.358100000
1	-4.689500000	3.942730000	1.255140000
1	-3.993430000	5.413910000	-0.629630000
6	-3.318010000	-0.992900000	0.254910000
6	-4.577450000	-0.819620000	-0.345670000
6	-3.116130000	-2.059640000	1.141990000
6	-5.618560000	-1.703120000	-0.058250000
6	-4.161970000	-2.941740000	1.427090000
6	-5.412270000	-2.764860000	0.829800000
1	-4.748620000	0.005770000	-1.030540000
1	-2.146710000	-2.214970000	1.600170000
1	-6.588420000	-1.563480000	-0.527330000
1	-3.994040000	-3.767290000	2.112370000
1	-6.223580000	-3.452140000	1.052570000
6	-0.263750000	-3.935830000	-1.011140000
8	-0.798160000	-3.418680000	-2.013140000
8	0.096980000	-3.377430000	0.077500000
1	0.013320000	-1.894700000	0.650870000
1	-0.037230000	-1.517590000	1.408160000

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5-Mn-Ph

25	-0.016190000	-0.280050000	1.008750000
6	-0.906210000	-0.557170000	2.542720000
6	1.478280000	-0.940880000	1.756850000
1	0.896850000	-5.080830000	-1.620720000
6	0.352410000	1.436270000	1.423350000
8	-1.478040000	-0.749020000	3.535550000
8	2.382190000	-1.402670000	2.318220000
8	0.569800000	2.529740000	1.749450000
7	-0.056850000	-0.246150000	-2.004290000
6	0.752970000	-0.159470000	-0.905960000
6	0.652050000	-0.145250000	-3.190740000
6	1.951580000	0.027630000	-2.839620000

7	1.996650000	0.014530000	-1.445580000
1	2.842140000	0.155290000	-3.434350000
1	0.178440000	-0.219430000	-4.156990000
6	-1.486820000	-0.473730000	-1.873410000
1	-2.033070000	0.029410000	-2.675130000
15	-1.939010000	0.125700000	-0.169470000
1	-1.692710000	-1.547440000	-1.908450000
6	3.213000000	0.225390000	-0.705850000
6	4.016750000	-0.882100000	-0.389320000
6	3.573560000	1.537880000	-0.361810000
6	5.195260000	-0.647570000	0.326680000
6	4.757350000	1.719960000	0.363660000
6	5.574150000	0.641300000	0.724180000
1	5.824280000	-1.494130000	0.592470000
1	5.046400000	2.728440000	0.650300000
6	2.749440000	2.723930000	-0.801560000
1	2.949500000	3.593200000	-0.169660000
1	2.992140000	3.000310000	-1.835820000
1	1.677710000	2.521160000	-0.764800000
6	3.608110000	-2.282580000	-0.771780000
1	2.823750000	-2.655670000	-0.106570000
1	3.214370000	-2.332340000	-1.791960000
1	4.457320000	-2.967800000	-0.697980000
6	6.824970000	0.856040000	1.542850000
1	7.629450000	0.181380000	1.230760000
1	7.190440000	1.884470000	1.459260000
1	6.631640000	0.660800000	2.605400000
6	-2.423410000	1.885880000	-0.367230000
6	-2.029910000	2.656050000	-1.471460000
6	-3.087150000	2.513140000	0.701440000
6	-2.315950000	4.024680000	-1.516540000
6	-3.375690000	3.877140000	0.652360000
6	-2.991640000	4.637160000	-0.458460000
1	-1.488890000	2.205220000	-2.297600000
1	-3.378980000	1.933310000	1.573710000
1	-2.006160000	4.609540000	-2.378270000
1	-3.893250000	4.347640000	1.483530000
1	-3.212530000	5.700140000	-0.494430000
6	-3.519080000	-0.758050000	0.143780000
6	-4.744000000	-0.267900000	-0.340420000
6	-3.493360000	-1.981400000	0.831780000
6	-5.922100000	-0.989560000	-0.135420000
6	-4.673450000	-2.702380000	1.031910000
6	-5.889080000	-2.208020000	0.550810000
1	-4.783920000	0.679610000	-0.869260000
1	-2.552350000	-2.368600000	1.207380000

1	-6.863840000	-0.599750000	-0.511700000
1	-4.640780000	-3.645910000	1.569190000
1	-6.806920000	-2.766420000	0.712760000
6	0.436030000	-4.112940000	-1.365460000
8	-0.142950000	-3.417270000	-2.179800000
8	0.603310000	-3.839650000	-0.078020000
1	0.216270000	-2.937460000	0.155380000
1	-0.449070000	-1.766560000	0.598600000

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6-Mn-Ph

25	0.707850000	-1.702860000	0.113380000
6	2.026380000	-2.644370000	0.904280000
6	0.281180000	-3.123850000	-0.883940000
6	-0.374860000	-2.058320000	1.508920000
8	2.825180000	-3.297550000	1.433730000
8	0.073010000	-4.036310000	-1.569310000
8	-1.072350000	-2.366620000	2.387330000
7	0.397620000	-0.279840000	-2.033610000
6	-0.556510000	-0.555280000	-1.121060000
6	-0.098910000	0.411400000	-3.125920000
6	-1.434640000	0.554080000	-2.883680000
7	-1.698220000	-0.030940000	-1.638700000
1	-2.217620000	1.010270000	-3.467920000
1	0.506590000	0.711140000	-3.966920000
6	1.678260000	-0.698650000	-1.505530000
15	2.037070000	0.196730000	0.018080000
1	2.432510000	-1.000740000	-2.224090000
6	-2.970520000	0.018530000	-0.970900000
6	-3.438200000	1.267620000	-0.516430000
6	-3.693350000	-1.168280000	-0.773140000
6	-4.674170000	1.301680000	0.136140000
6	-4.921600000	-1.079030000	-0.101720000
6	-5.429050000	0.141160000	0.356110000
1	-5.041320000	2.253200000	0.512950000
1	-5.491350000	-1.990080000	0.064120000
6	-3.171790000	-2.505910000	-1.234560000
1	-3.986770000	-3.229840000	-1.321010000
1	-2.666460000	-2.437570000	-2.202110000
1	-2.445210000	-2.906620000	-0.520240000
6	-2.622830000	2.527570000	-0.683570000
1	-1.560950000	2.351470000	-0.492660000
1	-2.706340000	2.933810000	-1.698630000
1	-2.963970000	3.298150000	0.012610000
6	-6.735950000	0.215040000	1.107250000

1	-7.375820000	1.013630000	0.715310000
1	-7.290050000	-0.726420000	1.046060000
1	-6.558240000	0.431790000	2.167870000
6	3.847830000	0.170200000	0.287820000
6	4.473920000	1.218870000	0.981270000
6	4.623340000	-0.909300000	-0.168640000
6	5.852190000	1.189380000	1.208870000
6	6.001030000	-0.931170000	0.056780000
6	6.619450000	0.116260000	0.747120000
1	3.892210000	2.063910000	1.337040000
1	4.159890000	-1.735500000	-0.697780000
1	6.323930000	2.007670000	1.745710000
1	6.589040000	-1.770310000	-0.304150000
1	7.690750000	0.094340000	0.925630000
6	1.582430000	1.968490000	-0.108350000
6	0.986450000	2.613850000	0.984650000
6	1.810050000	2.682960000	-1.296340000
6	0.622500000	3.960670000	0.892040000
6	1.437440000	4.024860000	-1.389230000
6	0.843030000	4.664690000	-0.294720000
1	0.788240000	2.067250000	1.900770000
1	2.275700000	2.187530000	-2.143740000
1	0.154630000	4.449650000	1.741570000
1	1.609930000	4.571130000	-2.312570000
1	0.550240000	5.708320000	-0.369920000
1	-0.188376072	0.851288602	0.963530759
8	-0.649387975	1.396110090	1.630742086
8	-2.073909656	1.125317787	3.324852644
6	-1.446810938	0.643265324	2.410647293
1	-1.472349838	-0.424191820	2.146078522

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7-Mn-Ph

25	-0.084550000	0.216330000	-0.758300000
6	0.874350000	0.143100000	-2.297200000
6	-1.643690000	0.305710000	-1.689200000
6	0.030440000	1.980330000	-0.668360000
8	1.495980000	0.094400000	-3.274420000
8	-2.551620000	0.403310000	-2.399570000
8	0.086430000	3.133870000	-0.564500000
7	-0.038210000	-0.250290000	2.169510000
6	-0.850530000	-0.134020000	1.058150000
6	-0.791810000	-0.485210000	3.302330000
6	-2.107170000	-0.495610000	2.917450000
7	-2.135710000	-0.270440000	1.565110000

1	-3.007980000	-0.649890000	3.491510000
1	-0.341840000	-0.605300000	4.275110000
6	1.364210000	-0.069520000	2.132560000
1	1.907940000	-0.547720000	2.940180000
15	1.919650000	-0.078720000	0.470630000
6	-3.345580000	-0.183670000	0.798480000
6	-3.876560000	-1.348010000	0.222720000
6	-3.961550000	1.071270000	0.655320000
6	-5.067630000	-1.233050000	-0.504280000
6	-5.147150000	1.137110000	-0.083020000
6	-5.714870000	-0.002700000	-0.668890000
1	-5.493130000	-2.124560000	-0.959310000
1	-5.636060000	2.100480000	-0.209270000
6	-3.341370000	2.304790000	1.262080000
1	-3.922590000	3.197370000	1.016080000
1	-3.277330000	2.229360000	2.353530000
1	-2.319930000	2.449310000	0.895240000
6	-3.163620000	-2.671770000	0.345890000
1	-2.237910000	-2.668970000	-0.242330000
1	-2.880170000	-2.891070000	1.380400000
1	-3.790260000	-3.490060000	-0.019270000
6	-6.975130000	0.106830000	-1.493460000
1	-7.487520000	-0.856770000	-1.577060000
1	-7.675930000	0.829590000	-1.062020000
1	-6.742470000	0.446010000	-2.511090000
6	3.224290000	1.193370000	0.244760000
6	3.308370000	2.276290000	1.131000000
6	4.082520000	1.144210000	-0.866470000
6	4.247680000	3.289620000	0.917650000
6	5.019050000	2.158190000	-1.077390000
6	5.104530000	3.233460000	-0.185310000
1	2.635560000	2.312400000	1.983180000
1	4.027630000	0.312160000	-1.562760000
1	4.306680000	4.122680000	1.612970000
1	5.680270000	2.109070000	-1.938190000
1	5.833750000	4.021790000	-0.350900000
6	2.772670000	-1.665650000	0.068540000
6	4.051150000	-1.952190000	0.579280000
6	2.099340000	-2.656190000	-0.667210000
6	4.637810000	-3.199970000	0.361100000
6	2.683110000	-3.908750000	-0.876950000
6	3.954460000	-4.183060000	-0.364930000
1	4.592250000	-1.195820000	1.141530000
1	1.119630000	-2.445320000	-1.088750000
1	5.629670000	-3.404920000	0.755000000
1	2.151300000	-4.662380000	-1.451340000

1	4.414780000	-5.151990000	-0.536720000
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TS4-Mn-Ph

25	0.044090000	-1.205250000	-0.431870000
6	1.023730000	-2.131920000	-1.640610000
6	-1.416410000	-2.234560000	-0.708740000
1	0.553470000	-2.438740000	0.863560000
6	-0.480040000	-0.030810000	-1.669630000
8	1.636850000	-2.702260000	-2.441790000
8	-2.308270000	-2.938110000	-0.928960000
8	-0.827210000	0.707060000	-2.493160000
7	0.092580000	0.097480000	2.188380000
6	-0.752570000	-0.198710000	1.159290000
6	-0.588370000	0.699300000	3.234130000
6	-1.893230000	0.803310000	2.843890000
7	-1.977650000	0.257600000	1.573320000
1	-2.754790000	1.215980000	3.345030000
1	-0.094590000	1.005810000	4.142900000
6	1.486080000	-0.256520000	2.095410000
1	2.082370000	0.183840000	2.893750000
15	1.948640000	-0.018440000	0.376400000
1	0.992130000	-1.904850000	1.353960000
6	-3.169630000	0.225660000	0.773000000
6	-4.053190000	-0.854890000	0.911210000
6	-3.408510000	1.281400000	-0.124050000
6	-5.193980000	-0.874930000	0.098760000
6	-4.556610000	1.212200000	-0.920270000
6	-5.455680000	0.140510000	-0.828290000
1	-5.882810000	-1.712070000	0.183210000
1	-4.752180000	2.013080000	-1.629840000
6	-2.482610000	2.471270000	-0.194300000
1	-2.675580000	3.064450000	-1.091990000
1	-2.624070000	3.122950000	0.677020000
1	-1.431120000	2.176280000	-0.203080000
6	-3.782960000	-1.957950000	1.904370000
1	-2.751810000	-2.316300000	1.838100000
1	-3.934800000	-1.610890000	2.933710000
1	-4.449500000	-2.807590000	1.733970000
6	-6.665510000	0.078810000	-1.730620000
1	-7.409810000	-0.632430000	-1.359180000
1	-7.146770000	1.058710000	-1.822510000
1	-6.380570000	-0.238500000	-2.741920000
6	2.091810000	1.751870000	-0.119040000
6	1.991280000	2.776640000	0.831610000

6	2.220580000	2.084440000	-1.477990000
6	2.026320000	4.116680000	0.431630000
6	2.265040000	3.421610000	-1.875780000
6	2.164430000	4.440820000	-0.920990000
1	1.880360000	2.527810000	1.883510000
1	2.281760000	1.297770000	-2.226140000
1	1.944560000	4.904320000	1.175900000
1	2.365760000	3.668520000	-2.929100000
1	2.189210000	5.481610000	-1.231940000
6	3.642700000	-0.700700000	0.220590000
6	4.766530000	0.131460000	0.101720000
6	3.824450000	-2.094000000	0.252730000
6	6.049150000	-0.420610000	0.020130000
6	5.105400000	-2.641980000	0.176280000
6	6.221710000	-1.806380000	0.057670000
1	4.646300000	1.209760000	0.072190000
1	2.966590000	-2.752670000	0.336220000
1	6.910470000	0.235150000	-0.072910000
1	5.230590000	-3.720780000	0.201470000
1	7.218010000	-2.234550000	-0.008220000

-1862.839284

16-Mn-Ph

6	1.054040000	-4.132720000	-1.365940000
6	0.534390000	-4.242230000	0.072400000
6	2.862840000	-4.318550000	0.944920000
6	3.416210000	-4.225000000	-0.483640000
1	-0.391090000	-3.675800000	0.193560000
1	1.129670000	-3.071930000	-1.629740000
1	0.323580000	-4.586620000	-2.045140000
1	3.499760000	-3.797270000	1.661310000
1	2.795600000	-5.374030000	1.248790000
1	3.607330000	-3.172540000	-0.723640000
1	4.378310000	-4.749610000	-0.526970000
1	0.323520000	-5.294760000	0.315420000
6	2.426750000	-4.807450000	-1.504120000
7	1.523580000	-3.731290000	1.024770000
6	1.219950000	-2.763050000	1.916660000
1	0.172460000	-2.431070000	1.843400000
8	1.996920000	-2.268830000	2.741990000
1	2.322770000	-5.889310000	-1.334100000
1	2.811510000	-4.680480000	-2.522450000
25	-0.186630000	0.082510000	-0.856050000
6	0.844290000	-0.213630000	-2.290530000
6	-1.258250000	-1.267850000	-1.322620000

1	0.659060000	-1.046070000	-0.138450000
6	-1.138640000	1.387550000	-1.661690000
8	1.522800000	-0.427350000	-3.211440000
8	-1.876130000	-2.192200000	-1.664670000
8	-1.735190000	2.192610000	-2.253620000
7	-0.255410000	0.631450000	2.101180000
6	-1.019540000	0.307890000	1.013250000
6	-0.996580000	0.669450000	3.272700000
6	-2.275210000	0.377840000	2.920370000
7	-2.272870000	0.163470000	1.541890000
1	-3.178820000	0.306270000	3.504770000
1	-0.553510000	0.890190000	4.231260000
6	1.170680000	0.893790000	1.963670000
1	1.489680000	1.662530000	2.671230000
15	1.410270000	1.351250000	0.174180000
1	1.743920000	-0.019450000	2.152280000
6	-3.467470000	-0.098010000	0.784380000
6	-3.914080000	-1.420480000	0.650450000
6	-4.159200000	0.988600000	0.223820000
6	-5.073790000	-1.646300000	-0.099910000
6	-5.309670000	0.712500000	-0.523230000
6	-5.775590000	-0.596560000	-0.704290000
1	-5.423710000	-2.667900000	-0.229460000
1	-5.850680000	1.539510000	-0.976990000
6	-3.704800000	2.408270000	0.458260000
1	-4.224150000	3.099380000	-0.210640000
1	-3.913210000	2.717210000	1.490530000
1	-2.631500000	2.527430000	0.297800000
6	-3.171630000	-2.562580000	1.297960000
1	-2.090160000	-2.431250000	1.217100000
1	-3.407750000	-2.634240000	2.367220000
1	-3.436430000	-3.515190000	0.831840000
6	-6.988930000	-0.871500000	-1.560620000
1	-7.509190000	-1.780310000	-1.241070000
1	-7.701660000	-0.040770000	-1.528590000
1	-6.698190000	-1.012220000	-2.609750000
6	1.215900000	3.178800000	0.083410000
6	0.848400000	3.984000000	1.170680000
6	1.358800000	3.771130000	-1.184030000
6	0.643810000	5.357710000	0.997770000
6	1.168590000	5.142380000	-1.352990000
6	0.809300000	5.940630000	-0.260470000
1	0.709300000	3.556280000	2.158100000
1	1.612330000	3.154050000	-2.042640000
1	0.355310000	5.968420000	1.849040000
1	1.287280000	5.585360000	-2.337760000

1	0.651370000	7.007250000	-0.392890000
6	3.213430000	1.068780000	-0.044450000
6	4.160620000	2.094490000	0.103330000
6	3.651940000	-0.236380000	-0.319120000
6	5.524630000	1.815760000	-0.020690000
6	5.015210000	-0.513100000	-0.433300000
6	5.954830000	0.512340000	-0.287250000
1	3.839350000	3.110370000	0.311570000
1	2.921620000	-1.029920000	-0.437490000
1	6.249380000	2.617300000	0.092530000
1	5.341540000	-1.527890000	-0.642420000
1	7.015610000	0.297310000	-0.382560000

-2228.066875

17-Mn-Ph

25	-0.045295901	-0.096169492	-0.752276550
6	-0.921175901	0.656640508	-2.147376550
6	1.562944099	0.357890508	-1.462866550
1	-0.102664099	1.652899492	0.107936550
6	0.022794099	-1.673159492	-1.576046550
8	-1.484295901	1.100500508	-3.056146550
8	2.524194099	0.665540508	-2.025236550
8	0.093964099	-2.690789492	-2.123046550
7	-0.185305901	-0.756199492	2.138713450
6	0.633044099	-0.814019492	1.051793450
6	0.477104099	-1.161449492	3.280313450
6	1.748114099	-1.498509492	2.904143450
7	1.828984099	-1.276169492	1.540643450
1	2.585054099	-1.871099492	3.473503450
1	0.000274099	-1.172229492	4.247953450
6	-1.547505901	-0.233039492	2.052733450
1	-2.168845901	-0.613799492	2.864303450
15	-2.088675901	-0.534569492	0.384463450
1	-1.249794099	1.671849492	2.040536550
6	2.998574099	-1.531949492	0.745073450
6	3.965814099	-0.523769492	0.605753450
6	3.133154099	-2.790129492	0.132463450
6	5.086954099	-0.800569492	-0.185616550
6	4.265494099	-3.013679492	-0.658536550
6	5.248034099	-2.029989492	-0.834836550
1	5.840994099	-0.027239492	-0.312876550
1	4.381654099	-3.977339492	-1.149296550
6	2.112114099	-3.880609492	0.348713450
1	2.202614099	-4.656489492	-0.416126550
1	2.251664099	-4.357139492	1.327393450

1	1.089294099	-3.499069492	0.322263450
6	3.787204099	0.838530508	1.230313450
1	3.128944099	1.464320508	0.616293450
1	3.345694099	0.780660508	2.229263450
1	4.747034099	1.356710508	1.310613450
6	6.431274099	-2.278019492	-1.739446550
1	7.297224099	-1.676279492	-1.445276550
1	6.728684099	-3.331829492	-1.733436550
1	6.184784099	-2.013899492	-2.776026550
6	0.248785901	2.301369492	0.979056550
8	-0.861504099	2.578369492	1.784096550
1	1.012565901	1.742949492	1.525686550
6	1.579545901	6.120259492	-0.460713450
6	2.432885901	5.314679492	0.529286550
6	1.570555901	4.308779492	1.297746550
7	0.854395901	3.433129492	0.357886550
6	-0.024794099	4.173469492	-0.555513450
6	0.790075901	5.175129492	-1.378493450
1	2.210535901	6.793659492	-1.053153450
1	0.875365901	6.752689492	0.099566550
1	2.934445901	5.981389492	1.241526550
1	3.212515901	4.767819492	-0.017573450
1	2.196745901	3.679749492	1.940926550
1	0.863505901	4.847939492	1.953116550
1	-0.511964099	3.448019492	-1.217303450
1	-0.820714099	4.701379492	-0.001793450
1	0.116255901	5.741839492	-2.032543450
1	1.485165901	4.619979492	-2.022173450
6	-2.684405901	-2.260569492	0.086343450
6	-3.192335901	-2.628839492	-1.170836550
6	-2.544265901	-3.237709492	1.080093450
6	-3.572235901	-3.948089492	-1.420566550
6	-2.916545901	-4.562799492	0.827153450
6	-3.432765901	-4.919449492	-0.421386550
1	-3.289295901	-1.882699492	-1.956106550
1	-2.142795901	-2.963499492	2.051923450
1	-3.967625901	-4.221129492	-2.395196550
1	-2.802745901	-5.313349492	1.604873450
1	-3.722105901	-5.948019492	-0.618376550
6	-3.574995901	0.505310508	0.112983450
6	-4.874615901	-0.011879492	0.232993450
6	-3.408005901	1.865250508	-0.193516550
6	-5.984935901	0.817550508	0.047523450
6	-4.516795901	2.691790508	-0.378626550
6	-5.809185901	2.169270508	-0.261536550
1	-5.025675901	-1.060839492	0.467463450

1	-2.412195901	2.285620508	-0.268266550
1	-6.985375901	0.404700508	0.143943450
1	-4.370135901	3.741750508	-0.615926550
1	-6.672965901	2.811260508	-0.410706550

-2227.999693

18-Mn-Ph

6	-4.910513836	-2.467858542	0.049972305
6	-3.850353260	-2.760356171	1.115907466
6	-2.392221487	-3.819356709	-0.529279190
6	-3.396685684	-3.546957129	-1.654145463
1	-3.859593035	-1.976574717	1.881700914
1	-4.756532967	-1.452616159	-0.334784768
1	-5.904155500	-2.485765404	0.512016972
1	-1.366009007	-3.797549140	-0.914501753
1	-2.562669838	-4.831228159	-0.119883088
1	-3.145082329	-2.591552486	-2.135208098
1	-3.311632326	-4.329664761	-2.417902668
1	-4.093629414	-3.719664880	1.612065410
6	-4.827307451	-3.481273341	-1.100273224
7	-2.508831511	-2.798745107	0.519781948
6	-1.437066389	-2.806971412	1.481075255
1	-1.545615275	-1.927481613	2.125315362
8	-1.324696716	-4.003429032	2.283135793
1	-5.114684543	-4.476395378	-0.730150450
1	-5.537572674	-3.219935160	-1.894177095
25	0.664860000	0.782480000	1.132840000
6	0.041290000	1.474810000	2.663030000
6	2.031100000	0.061880000	2.042740000
1	-0.104510000	-0.566660000	1.498290000
6	1.522830000	2.296510000	0.667370000
8	-0.363350000	1.913380000	3.662140000
8	2.848580000	-0.382440000	2.737850000
8	2.079310000	3.289160000	0.424720000
7	0.086910000	-0.395700000	-1.582920000
6	1.061840000	-0.174320000	-0.647000000
6	0.568450000	-1.064360000	-2.698830000
6	1.893160000	-1.261940000	-2.478100000
7	2.177810000	-0.715060000	-1.227100000
1	2.656040000	-1.729960000	-3.080100000
1	-0.064620000	-1.334920000	-3.529360000
6	-1.303740000	-0.038170000	-1.344270000
1	-1.764420000	0.338570000	-2.261260000
15	-1.292660000	1.213080000	0.035530000
1	-1.843840000	-0.927170000	-0.997700000

6	3.507850000	-0.695280000	-0.676580000
6	3.929680000	-1.780490000	0.107620000
6	4.347950000	0.388620000	-0.973950000
6	5.230600000	-1.748710000	0.618590000
6	5.638710000	0.380710000	-0.429990000
6	6.094770000	-0.674170000	0.369960000
1	5.569380000	-2.572800000	1.242060000
1	6.300360000	1.218480000	-0.637750000
6	3.897020000	1.504680000	-1.884230000
1	4.546350000	2.378150000	-1.781590000
1	3.925100000	1.186800000	-2.934490000
1	2.874820000	1.821020000	-1.669010000
6	2.994240000	-2.922680000	0.410930000
1	2.094030000	-2.565560000	0.918730000
1	2.664630000	-3.430450000	-0.501920000
1	3.475220000	-3.663850000	1.054190000
6	7.474500000	-0.641430000	0.983150000
1	7.918540000	-1.641660000	1.026390000
1	8.151280000	0.008270000	0.419100000
1	7.431810000	-0.259620000	2.011300000
6	-1.439940000	2.840510000	-0.812570000
6	-0.849400000	3.047560000	-2.069750000
6	-2.009810000	3.934410000	-0.140590000
6	-0.850480000	4.317650000	-2.652950000
6	-2.011010000	5.202560000	-0.725610000
6	-1.433630000	5.397870000	-1.984410000
1	-0.371570000	2.227160000	-2.597840000
1	-2.459710000	3.797810000	0.839010000
1	-0.389890000	4.461920000	-3.626450000
1	-2.460070000	6.037880000	-0.195470000
1	-1.432300000	6.385300000	-2.437190000
6	-2.953330000	0.949150000	0.780780000
6	-4.122900000	1.344780000	0.107880000
6	-3.063190000	0.290760000	2.013810000
6	-5.378100000	1.086040000	0.662140000
6	-4.320790000	0.037360000	2.569140000
6	-5.478740000	0.434050000	1.896150000
1	-4.055450000	1.863880000	-0.843900000
1	-2.166450000	-0.030440000	2.531560000
1	-6.275080000	1.394670000	0.132450000
1	-4.391860000	-0.470530000	3.526830000
1	-6.455500000	0.236240000	2.328960000
1	-0.486240784	-2.740347374	0.947134325
1	-1.986631746	-3.968874017	2.986513995

-2229.228096

19-Mn-Ph

6	2.907910000	4.432220000	-0.465610000
6	1.980910000	3.624200000	0.460110000
6	0.153310000	3.747240000	-1.145930000
6	1.016370000	4.549450000	-2.135430000
1	2.560020000	2.915950000	1.059300000
1	3.491620000	3.729510000	-1.075540000
1	3.624560000	5.011920000	0.131790000
1	-0.568590000	3.124360000	-1.681820000
1	-0.425330000	4.446860000	-0.523040000
1	1.502470000	3.847290000	-2.828220000
1	0.382610000	5.214330000	-2.738140000
1	1.486830000	4.312470000	1.163280000
6	2.090170000	5.353280000	-1.384820000
7	0.932270000	2.883250000	-0.250780000
6	-0.222180000	1.803820000	2.566760000
1	0.827670000	1.676860000	2.856270000
8	-1.121850000	1.440070000	3.611420000
1	1.598610000	6.126710000	-0.775710000
1	2.746260000	5.878190000	-2.090560000
25	-0.407490000	-1.042000000	0.705170000
6	0.353070000	-1.692800000	2.214000000
6	-2.040480000	-1.090730000	1.511440000
1	-0.401270000	1.244930000	1.634800000
6	-0.649850000	-2.674530000	0.071110000
8	0.808950000	-2.161980000	3.172650000
8	-3.010380000	-1.244700000	2.119390000
8	-0.835530000	-3.729100000	-0.371890000
7	-0.087180000	0.161400000	-2.002760000
6	-0.988150000	-0.146430000	-1.015800000
6	-0.723000000	0.742480000	-3.083390000
6	-2.055180000	0.812380000	-2.776960000
7	-2.205880000	0.277440000	-1.518960000
1	-2.890660000	1.206350000	-3.334510000
1	-0.179530000	1.082220000	-3.950710000
6	1.322010000	-0.023580000	-1.880840000
1	1.826100000	-0.244080000	-2.814960000
15	1.719010000	-0.825220000	-0.378020000
1	1.350810000	2.127400000	-0.799680000
6	-3.463320000	0.202050000	-0.829490000
6	-3.841130000	1.255200000	0.018720000
6	-4.278660000	-0.924760000	-1.033930000
6	-5.069820000	1.148780000	0.682430000
6	-5.499880000	-0.980670000	-0.355800000
6	-5.909310000	0.043020000	0.510240000

1	-5.370590000	1.947280000	1.356660000
1	-6.141380000	-1.847680000	-0.497100000
6	-3.836700000	-2.045210000	-1.942330000
1	-4.602890000	-2.822380000	-2.005660000
1	-3.628860000	-1.686900000	-2.956650000
1	-2.915860000	-2.509750000	-1.576260000
6	-2.967100000	2.470370000	0.204800000
1	-1.905580000	2.218620000	0.199630000
1	-3.131210000	3.194320000	-0.603180000
1	-3.195840000	2.970780000	1.149890000
6	-7.207730000	-0.070790000	1.272700000
1	-7.578090000	0.910440000	1.585740000
1	-7.985760000	-0.554310000	0.672240000
1	-7.071260000	-0.675200000	2.178730000
6	2.551130000	-2.448190000	-0.685180000
6	2.213970000	-3.179580000	-1.833770000
6	3.448560000	-3.004960000	0.240050000
6	2.770410000	-4.441450000	-2.059470000
6	4.003580000	-4.266890000	0.013650000
6	3.667590000	-4.988260000	-1.136920000
1	1.512580000	-2.759150000	-2.549440000
1	3.723000000	-2.454500000	1.134910000
1	2.501520000	-4.996480000	-2.954230000
1	4.699280000	-4.685080000	0.736150000
1	4.101560000	-5.968820000	-1.312020000
6	3.056330000	0.131960000	0.470910000
6	4.014360000	0.796010000	-0.312950000
6	3.162310000	0.197780000	1.867030000
6	5.060060000	1.498780000	0.286790000
6	4.203170000	0.913290000	2.470020000
6	5.155740000	1.562630000	1.681710000
1	3.927770000	0.776990000	-1.395420000
1	2.439400000	-0.303720000	2.497800000
1	5.793160000	2.006920000	-0.333590000
1	4.263600000	0.962470000	3.553770000
1	5.962940000	2.119980000	2.148700000
1	-0.399810000	2.854210000	2.333470000
1	-1.002220000	0.503360000	3.816390000

-2229.178556

20-Mn-Ph

6	-1.061545369	-4.454225573	-2.426977591
6	-1.014145369	-3.270365573	-1.454407591
6	-3.471505369	-2.961665573	-1.641917591
6	-3.559225369	-4.135175573	-2.625257591

1	-0.239425369	-3.403305573	-0.695547591
1	-1.167315369	-5.385645573	-1.855217591
1	-0.111665369	-4.508865573	-2.972477591
1	-4.352995369	-2.896095573	-1.003007591
1	-3.390405369	-2.014125573	-2.196077591
1	-3.778005369	-5.052685573	-2.063467591
1	-4.396195369	-3.965365573	-3.312857591
1	-0.774995369	-2.345635573	-1.998487591
6	-2.242655369	-4.307555573	-3.398697591
7	-2.299305369	-3.100385573	-0.778357591
6	-2.387175369	-2.950135573	0.566542409
1	-1.410655369	-3.045875573	1.071252409
8	-3.425655369	-2.735795573	1.195852409
1	-2.077335369	-3.425915573	-4.036127591
1	-2.300575369	-5.175065573	-4.066377591
25	0.303600000	0.303740000	1.049980000
6	-0.580510000	0.510770000	2.597340000
6	1.336540000	-0.951620000	1.794660000
1	-0.651970000	-0.922290000	0.751550000
6	1.368450000	1.722410000	1.382200000
8	-1.149410000	0.642950000	3.601910000
8	1.921050000	-1.801250000	2.331730000
8	2.030660000	2.631450000	1.680760000
7	0.152200000	0.023390000	-1.940390000
6	0.989510000	-0.038860000	-0.857870000
6	0.804260000	-0.271530000	-3.129570000
6	2.098260000	-0.515680000	-2.798140000
7	2.194710000	-0.368480000	-1.414530000
1	2.953830000	-0.770430000	-3.403580000
1	0.299900000	-0.276300000	-4.083360000
6	-1.245650000	0.387530000	-1.777440000
1	-1.603030000	0.950030000	-2.643110000
15	-1.335400000	1.316860000	-0.159820000
1	-1.864700000	-0.506420000	-1.654140000
6	3.441460000	-0.443460000	-0.699020000
6	3.891750000	-1.688770000	-0.238720000
6	4.177420000	0.738910000	-0.513010000
6	5.103100000	-1.726780000	0.462600000
6	5.376760000	0.651730000	0.201360000
6	5.849100000	-0.567610000	0.706090000
1	5.458940000	-2.681460000	0.842700000
1	5.952300000	1.558510000	0.372450000
6	3.717240000	2.049740000	-1.103700000
1	4.283730000	2.885310000	-0.684900000
1	3.860980000	2.057030000	-2.191720000
1	2.657880000	2.237450000	-0.917880000

6	3.103530000	-2.947660000	-0.501330000
1	2.037530000	-2.796790000	-0.318460000
1	3.211540000	-3.272290000	-1.544100000
1	3.446050000	-3.763300000	0.140780000
6	7.118670000	-0.618750000	1.522610000
1	7.569430000	-1.616080000	1.504990000
1	7.861230000	0.098620000	1.157280000
1	6.913260000	-0.369300000	2.571480000
6	-1.098280000	3.087670000	-0.595910000
6	-0.617780000	3.524020000	-1.839010000
6	-1.298210000	4.031710000	0.426790000
6	-0.361610000	4.881680000	-2.061880000
6	-1.050830000	5.385580000	0.200570000
6	-0.581240000	5.815110000	-1.046450000
1	-0.426130000	2.818310000	-2.641340000
1	-1.645690000	3.704530000	1.403990000
1	0.011690000	5.205580000	-3.029630000
1	-1.214600000	6.103220000	0.999430000
1	-0.381320000	6.868520000	-1.220870000
6	-3.125160000	1.180080000	0.231030000
6	-4.073610000	2.055440000	-0.326430000
6	-3.559380000	0.126290000	1.048960000
6	-5.434300000	1.871960000	-0.069600000
6	-4.921310000	-0.058250000	1.299570000
6	-5.860360000	0.814270000	0.742590000
1	-3.753120000	2.883170000	-0.952410000
1	-2.843180000	-0.557070000	1.487400000
1	-6.160160000	2.555410000	-0.501850000
1	-5.231950000	-0.885220000	1.930750000
1	-6.919360000	0.675480000	0.942830000

-2228.063215

21-Mn-Ph

6	0.356616034	4.869749881	-1.201344206
6	0.433116034	3.360779881	-1.434814206
6	2.785576034	3.328719881	-0.643364206
6	2.744086034	4.839839881	-0.419794206
1	-0.527373966	2.872279881	-1.257554206
1	-0.028063966	5.067379881	-0.192954206
1	-0.365433966	5.294959881	-1.908204206
1	3.412986034	2.837609881	0.100075794
1	3.173106034	3.087439881	-1.641154206
1	2.469256034	5.027359881	0.623965794
1	3.752856034	5.241419881	-0.571004206
1	0.722006034	3.147639881	-2.471004206

6	1.738066034	5.519289881	-1.358774206
7	1.438266034	2.694899881	-0.557814206
6	0.918086034	2.543799881	0.971465794
1	-0.077273966	3.026019881	0.970645794
8	1.760096034	2.830009881	1.866055794
1	2.073576034	5.415859881	-2.401144206
1	1.680436034	6.592839881	-1.145994206
25	-0.226746034	-0.330709881	1.082184206
6	0.694583966	-0.595719881	2.618814206
6	-1.577616034	0.459310119	1.985264206
1	0.627026034	1.358899881	0.920035794
6	-0.998326034	-1.936469881	1.204894206
8	1.264473966	-0.798989881	3.605154206
8	-2.386496034	0.955000119	2.648674206
8	-1.508096034	-2.971889881	1.314474206
7	-0.092066034	0.119680119	-1.864415794
6	-0.956146034	0.039850119	-0.814835794
6	-0.757106034	0.376010119	-3.047905794
6	-2.086756034	0.450640119	-2.744135794
7	-2.192456034	0.244660119	-1.377675794
1	-2.952866034	0.617970119	-3.364965794
1	-0.238956034	0.488130119	-3.987575794
6	1.353023966	0.032030119	-1.659995794
1	1.865633966	-0.232679881	-2.586425794
15	1.594123966	-1.038239881	-0.247345794
1	1.562996034	1.668149881	-0.969384206
6	-3.443816034	0.132490119	-0.679295794
6	-4.011626034	1.280120119	-0.105945794
6	-4.061986034	-1.127139881	-0.606715794
6	-5.224636034	1.138710119	0.576644206
6	-5.269686034	-1.220669881	0.094594206
6	-5.862136034	-0.102479881	0.696234206
1	-5.672736034	2.015030119	1.038574206
1	-5.757576034	-2.189699881	0.172444206
6	-3.471146034	-2.331859881	-1.298115794
1	-3.881116034	-3.257679881	-0.886485794
1	-3.699816034	-2.313049881	-2.371365794
1	-2.384126034	-2.371739881	-1.202975794
6	-3.319806034	2.616720119	-0.200655794
1	-2.340476034	2.585320119	0.287604206
1	-3.151286034	2.911680119	-1.242355794
1	-3.909936034	3.398700119	0.284314206
6	-7.141516034	-0.242199881	1.485984206
1	-7.686566034	0.705510119	1.541084206
1	-7.805796034	-0.993379881	1.045714206
1	-6.927426034	-0.558239881	2.515054206

6	1.521283966	-2.834049881	-0.677175794
6	1.093393966	-3.253179881	-1.943475794
6	1.794973966	-3.797679881	0.307834206
6	0.952293966	-4.616359881	-2.227565794
6	1.662173966	-5.157149881	0.022484206
6	1.238603966	-5.569869881	-1.247095794
1	0.865963966	-2.515749881	-2.708455794
1	2.109603966	-3.483099881	1.300404206
1	0.618623966	-4.930529881	-3.213085794
1	1.880343966	-5.893799881	0.790914206
1	1.129593966	-6.628249881	-1.467245794
6	3.336783966	-0.783649881	0.266274206
6	4.378433966	-1.527319881	-0.313805794
6	3.644033966	0.202970119	1.216374206
6	5.706073966	-1.283139881	0.046774206
6	4.973493966	0.443500119	1.574974206
6	6.006273966	-0.297569881	0.993224206
1	4.156533966	-2.302179881	-1.041665794
1	2.865033966	0.806990119	1.672144206
1	6.503213966	-1.864659881	-0.408525794
1	5.194413966	1.210210119	2.312434206
1	7.038493966	-0.112159881	1.278034206

-2227.987038

22-Mn-Ph

6	0.501200000	-3.422450000	0.718640000
8	1.283600000	-3.406010000	1.736790000
25	-0.017210000	-0.763350000	-0.788030000
6	0.952510000	-1.418430000	-2.165630000
6	-1.473840000	-1.705450000	-1.289970000
1	0.478550000	-2.243840000	0.116940000
6	-0.534290000	0.692370000	-1.695720000
8	1.590530000	-1.851400000	-3.030130000
8	-2.348110000	-2.370450000	-1.654920000
8	-0.883240000	1.592460000	-2.340750000
7	0.047140000	-0.086960000	2.140720000
6	-0.776390000	-0.199840000	1.057790000
6	-0.647460000	0.259860000	3.286960000
6	-1.950970000	0.381010000	2.918480000
7	-2.009760000	0.099370000	1.556050000
1	-2.832220000	0.636950000	3.485140000
1	-0.164630000	0.375280000	4.244720000
6	1.487040000	-0.304850000	2.014840000
1	2.030300000	0.282070000	2.757680000
15	1.877610000	0.134210000	0.250620000

1	1.708540000	-1.371190000	2.149750000
6	-3.212450000	0.166520000	0.768650000
6	-4.036170000	-0.966280000	0.697910000
6	-3.514610000	1.363710000	0.099320000
6	-5.183570000	-0.887300000	-0.099590000
6	-4.665480000	1.388630000	-0.696520000
6	-5.506820000	0.273810000	-0.812590000
1	-5.826240000	-1.760610000	-0.181170000
1	-4.908920000	2.299960000	-1.237790000
6	-2.655900000	2.593600000	0.266360000
1	-2.886830000	3.337530000	-0.500090000
1	-2.829670000	3.056480000	1.246170000
1	-1.589660000	2.366140000	0.205370000
6	-3.692070000	-2.227810000	1.449250000
1	-2.634470000	-2.486220000	1.342060000
1	-3.885130000	-2.116070000	2.523430000
1	-4.286150000	-3.070990000	1.087450000
6	-6.712630000	0.310860000	-1.720690000
1	-7.490130000	-0.383040000	-1.385600000
1	-7.148240000	1.314130000	-1.771590000
1	-6.433980000	0.022920000	-2.742670000
6	2.033960000	1.962300000	0.182110000
6	2.023860000	2.783580000	1.318660000
6	2.112620000	2.556970000	-1.089440000
6	2.096940000	4.173880000	1.186060000
6	2.200170000	3.943360000	-1.219720000
6	2.188880000	4.755960000	-0.080770000
1	1.953830000	2.355690000	2.312790000
1	2.100970000	1.934130000	-1.979840000
1	2.081390000	4.798970000	2.074530000
1	2.263600000	4.387730000	-2.208720000
1	2.245260000	5.836070000	-0.181500000
6	3.568810000	-0.525460000	-0.008060000
6	4.649470000	0.291850000	-0.375050000
6	3.762220000	-1.912590000	0.125690000
6	5.907470000	-0.271490000	-0.609350000
6	5.023700000	-2.465100000	-0.101990000
6	6.096920000	-1.649520000	-0.476220000
1	4.519770000	1.363990000	-0.478900000
1	2.946770000	-2.559770000	0.439120000
1	6.736750000	0.369770000	-0.894980000
1	5.163710000	-3.536250000	0.012200000
1	7.074790000	-2.085800000	-0.660110000
1	0.806290000	-3.992880000	-0.185060000
1	-0.590770000	-3.514240000	0.890060000

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TS7-Mn-Ph

6	0.573050000	-3.270690000	0.834690000
8	1.327840000	-3.047270000	1.949830000
25	0.014930000	-0.877450000	-0.746350000
6	1.021390000	-1.422150000	-2.155840000
6	-1.430140000	-1.838220000	-1.273750000
1	0.703670000	-2.415750000	0.070010000
6	-0.557680000	0.546210000	-1.654170000
8	1.672780000	-1.747350000	-3.054290000
8	-2.302760000	-2.486520000	-1.665650000
8	-0.943050000	1.436960000	-2.286530000
7	0.050340000	-0.147830000	2.129400000
6	-0.781100000	-0.280270000	1.063910000
6	-0.636300000	0.241650000	3.260860000
6	-1.945920000	0.375890000	2.895740000
7	-2.014600000	0.055880000	1.547430000
1	-2.819410000	0.662680000	3.459640000
1	-0.148530000	0.378300000	4.213320000
6	1.484710000	-0.433390000	1.988790000
1	2.052650000	0.021810000	2.802720000
15	1.887760000	0.117310000	0.315810000
1	1.502890000	-1.903400000	2.036220000
6	-3.205100000	0.141710000	0.746190000
6	-4.040090000	-0.980000000	0.647570000
6	-3.484020000	1.350010000	0.083890000
6	-5.171740000	-0.880990000	-0.171800000
6	-4.620030000	1.396340000	-0.730780000
6	-5.470850000	0.291350000	-0.875540000
1	-5.821930000	-1.746500000	-0.273960000
1	-4.844730000	2.316060000	-1.266240000
6	-2.612920000	2.567470000	0.276310000
1	-2.815060000	3.316990000	-0.492870000
1	-2.804320000	3.028950000	1.253250000
1	-1.548360000	2.326400000	0.242190000
6	-3.730440000	-2.251180000	1.398440000
1	-2.667290000	-2.503170000	1.348470000
1	-3.982970000	-2.153390000	2.461580000
1	-4.300610000	-3.091900000	0.994550000
6	-6.662130000	0.360730000	-1.801090000
1	-7.376710000	-0.442940000	-1.598930000
1	-7.188430000	1.316900000	-1.706710000
1	-6.344440000	0.266590000	-2.847450000
6	1.958850000	1.955720000	0.190420000

6	1.954340000	2.756730000	1.340690000
6	1.952040000	2.571160000	-1.072300000
6	1.950570000	4.150760000	1.231840000
6	1.958750000	3.962980000	-1.181440000
6	1.955140000	4.755990000	-0.028190000
1	1.949690000	2.295080000	2.323520000
1	1.940830000	1.961820000	-1.972270000
1	1.942920000	4.761390000	2.130660000
1	1.956810000	4.426830000	-2.163850000
1	1.950600000	5.839130000	-0.112490000
6	3.595200000	-0.462970000	-0.024590000
6	4.590150000	0.397300000	-0.516540000
6	3.901650000	-1.822980000	0.168700000
6	5.866710000	-0.091630000	-0.810010000
6	5.179750000	-2.303670000	-0.121670000
6	6.165020000	-1.442470000	-0.616160000
1	4.381390000	1.450990000	-0.666690000
1	3.158440000	-2.502640000	0.573350000
1	6.625820000	0.587760000	-1.187960000
1	5.404140000	-3.354220000	0.040940000
1	7.157320000	-1.821120000	-0.845350000
1	0.912890000	-4.134440000	0.240600000
1	-0.508640000	-3.362910000	1.015660000

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23-Mn-Ph

6	-0.411743522	3.276128083	0.744539079
8	-1.384213522	3.223478083	1.732139079
25	0.000783522	0.789271917	-0.777819079
6	-1.005616478	1.283401917	-2.205819079
6	1.477543522	1.629281917	-1.414879079
1	-0.629113522	2.535598083	-0.089360921
6	0.478343522	-0.717268083	-1.598759079
8	-1.645886478	1.568921917	-3.125739079
8	2.369203522	2.184341917	-1.897249079
8	0.801633522	-1.673428083	-2.165079079
7	-0.025876478	0.202981917	2.127960921
6	0.801873522	0.279271917	1.052850921
6	0.679533522	-0.071648083	3.281770921
6	1.993463522	-0.193338083	2.922640921
7	2.051183522	0.022661917	1.556170921
1	2.874883522	-0.413358083	3.504030921
1	0.199193522	-0.151398083	4.244440921
6	-1.466796478	0.427351917	1.996570921
1	-2.012316478	-0.016478083	2.830530921

15	-1.889826478	-0.114418083	0.350810921
1	-1.534113522	2.228038083	1.957999079
6	3.241653522	-0.112068083	0.761310921
6	4.083973522	0.998761917	0.599850921
6	3.522443522	-1.358148083	0.176640921
6	5.220123522	0.846761917	-0.202429079
6	4.662223522	-1.456498083	-0.630609079
6	5.516183522	-0.365978083	-0.838299079
1	5.876663522	1.700831917	-0.350239079
1	4.886903522	-2.408248083	-1.106259079
6	2.654363522	-2.563168083	0.443700921
1	2.863393522	-3.361878083	-0.272589079
1	2.841973522	-2.957268083	1.450410921
1	1.589473522	-2.328908083	0.387480921
6	3.759293522	2.318711917	1.252320921
1	2.772993522	2.679841917	0.944610921
1	3.737653522	2.236211917	2.344910921
1	4.495633522	3.080001917	0.982340921
6	6.708003522	-0.481728083	-1.758159079
1	7.527633522	0.170391917	-1.439049079
1	7.085513522	-1.508388083	-1.802339079
1	6.435273522	-0.188258083	-2.780209079
6	-2.018376478	-1.951738083	0.177460921
6	-1.804066478	-2.783498083	1.284460921
6	-2.249126478	-2.531948083	-1.081069079
6	-1.829946478	-4.175058083	1.140290921
6	-2.285916478	-3.919728083	-1.223569079
6	-2.073676478	-4.744848083	-0.112169079
1	-1.614836478	-2.343618083	2.259840921
1	-2.401126478	-1.898348083	-1.951759079
1	-1.659156478	-4.810228083	2.005360921
1	-2.469966478	-4.357858083	-2.200689079
1	-2.093856478	-5.825218083	-0.225159079
6	-3.586046478	0.497861917	0.010560921
6	-4.695816478	-0.360958083	-0.029809079
6	-3.780396478	1.873101917	-0.204239079
6	-5.974346478	0.146191917	-0.282749079
6	-5.057456478	2.376721917	-0.454079079
6	-6.158346478	1.514351917	-0.497459079
1	-4.569946478	-1.426038083	0.134500921
1	-2.941306478	2.557951917	-0.152699079
1	-6.823556478	-0.531098083	-0.309979079
1	-5.191026478	3.442781917	-0.614719079
1	-7.151586478	1.907021917	-0.696959079
1	-0.443583522	4.239318083	0.220919079
1	0.606536478	3.094808083	1.107199079

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24-Mn-Ph

25	-0.051240000	-0.484240000	-0.870980000
6	0.835440000	-0.931660000	-2.386740000
6	-0.338820000	1.180530000	-1.452230000
6	-1.594030000	-1.061790000	-1.646100000
8	1.392900000	-1.190250000	-3.368270000
8	-0.553080000	2.247750000	-1.859320000
8	-2.493960000	-1.465610000	-2.245860000
7	0.007650000	0.096300000	2.114000000
6	-0.803670000	-0.051870000	1.024990000
6	-0.714750000	0.314050000	3.275530000
6	-2.022490000	0.340440000	2.910070000
7	-2.056930000	0.122780000	1.533920000
1	-2.922770000	0.495620000	3.483480000
1	-0.242600000	0.417880000	4.239920000
6	1.448810000	-0.104460000	2.045210000
15	1.912860000	0.119510000	0.252090000
1	1.961230000	0.600720000	2.704420000
6	-3.274060000	0.154440000	0.766560000
6	-3.957930000	-1.047390000	0.528660000
6	-3.743550000	1.393390000	0.303320000
6	-5.150070000	-0.983960000	-0.199360000
6	-4.935860000	1.404310000	-0.431020000
6	-5.649470000	0.228130000	-0.693820000
1	-5.688190000	-1.906150000	-0.405460000
1	-5.311350000	2.352980000	-0.807530000
6	-3.002720000	2.672020000	0.609280000
1	-3.400600000	3.503200000	0.021400000
1	-3.092670000	2.936190000	1.670240000
1	-1.935470000	2.585460000	0.389770000
6	-3.388950000	-2.363990000	0.992470000
1	-2.427630000	-2.558170000	0.499890000
1	-3.215830000	-2.367170000	2.075300000
1	-4.065650000	-3.188750000	0.754310000
6	-6.908580000	0.254360000	-1.527430000
1	-7.642570000	-0.475200000	-1.169020000
1	-7.377630000	1.243300000	-1.518600000
1	-6.684960000	0.004430000	-2.572460000
1	1.687330000	-1.127840000	2.343440000
1	1.724550000	-2.915440000	0.971440000
1	-0.534285933	-2.432505496	2.116552131
1	0.631300000	-4.287730000	0.648150000
6	0.668820000	-3.187060000	0.783470000

8	0.091560000	-2.586960000	-0.278780000
8	0.368203107	-2.220533165	1.843123729
6	2.365620000	1.894660000	0.121100000
6	3.204320000	2.315910000	-0.923830000
6	1.778670000	2.857720000	0.956920000
6	3.467330000	3.673800000	-1.114120000
6	2.043830000	4.216320000	0.763680000
6	2.889300000	4.627700000	-0.270040000
1	3.657870000	1.584160000	-1.586540000
1	1.102180000	2.562540000	1.753170000
1	4.120960000	3.985580000	-1.923830000
1	1.583790000	4.951130000	1.418490000
1	3.092430000	5.684040000	-0.420970000
6	3.502040000	-0.773050000	0.072880000
6	3.529460000	-1.974040000	-0.652180000
6	4.686510000	-0.284460000	0.651200000
6	4.728990000	-2.676650000	-0.798050000
6	5.881740000	-0.990230000	0.504510000
6	5.904190000	-2.186090000	-0.222920000
1	2.614070000	-2.362920000	-1.087070000
1	4.679560000	0.652010000	1.201820000
1	4.741150000	-3.605010000	-1.361610000
1	6.793850000	-0.605760000	0.952310000
1	6.836250000	-2.731700000	-0.341390000

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25-Mn-Ph

25	-0.045740000	-0.662640000	-0.585370000
6	0.872230000	-1.454190000	-1.946350000
6	-0.398970000	0.755240000	-1.616520000
6	-1.579240000	-1.448400000	-1.134760000
8	1.453630000	-1.846750000	-2.866210000
8	-0.647620000	1.660590000	-2.302050000
8	-2.512830000	-1.955860000	-1.594520000
7	0.006620000	0.586400000	2.148370000
6	-0.809830000	0.251990000	1.105880000
6	-0.701390000	1.112150000	3.219050000
6	-2.005270000	1.127590000	2.838870000
7	-2.050630000	0.604080000	1.548050000
1	-2.895860000	1.453930000	3.352500000
1	-0.223090000	1.419570000	4.136030000
6	1.442670000	0.341600000	2.112750000
15	1.910410000	0.269190000	0.312680000
1	1.975930000	1.118390000	2.666620000
6	-3.274890000	0.434930000	0.812690000

6	-3.973360000	-0.775350000	0.953620000
6	-3.734380000	1.482090000	0.001710000
6	-5.170580000	-0.920610000	0.247710000
6	-4.932930000	1.283440000	-0.696710000
6	-5.662240000	0.093760000	-0.585890000
1	-5.720730000	-1.854960000	0.332000000
1	-5.301620000	2.077810000	-1.341580000
6	-2.990440000	2.792320000	-0.088980000
1	-3.285090000	3.345280000	-0.984930000
1	-3.207330000	3.425370000	0.781100000
1	-1.908410000	2.649290000	-0.123710000
6	-3.423140000	-1.885740000	1.814140000
1	-2.387980000	-2.121790000	1.543990000
1	-3.415710000	-1.605590000	2.874540000
1	-4.022460000	-2.793850000	1.708530000
6	-6.933440000	-0.114930000	-1.374180000
1	-7.699800000	-0.615350000	-0.772090000
1	-7.346360000	0.833570000	-1.731500000
1	-6.746300000	-0.746670000	-2.251840000
1	1.665360000	-0.642620000	2.530480000
1	-0.889670000	-3.624120000	0.271620000
1	0.746840000	-4.861600000	-0.638460000
1	0.326540000	-3.988450000	1.544800000
6	0.148120000	-3.416480000	0.611280000
8	1.043560000	-3.967960000	-0.413490000
8	0.407710000	-2.112460000	0.812600000
1	-0.815292198	-3.263420749	-1.818166342
1	-0.340640708	-3.257103264	-1.243979323
6	2.267880000	2.004760000	-0.166530000
6	1.711290000	3.096500000	0.518050000
6	3.006910000	2.241210000	-1.338650000
6	1.907430000	4.399600000	0.050320000
6	3.203770000	3.542980000	-1.801750000
6	2.654250000	4.626740000	-1.108450000
1	1.110640000	2.944780000	1.409610000
1	3.435590000	1.407850000	-1.889010000
1	1.470470000	5.234840000	0.590720000
1	3.780890000	3.709440000	-2.706960000
1	2.803190000	5.639600000	-1.471700000
6	3.545170000	-0.557970000	0.345690000
6	3.612310000	-1.932260000	0.069020000
6	4.717450000	0.144810000	0.675300000
6	4.844610000	-2.590800000	0.116250000
6	5.944460000	-0.520470000	0.720780000
6	6.010040000	-1.889560000	0.438170000
1	2.710010000	-2.487860000	-0.161020000

1	4.678990000	1.210120000	0.884560000
1	4.887510000	-3.654030000	-0.103050000
1	6.846780000	0.030440000	0.971860000
1	6.966240000	-2.405030000	0.468670000

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26-Mn-Ph

25	-0.060930000	-0.246690000	-0.905460000
6	0.847330000	-0.650310000	-2.404150000
6	-0.392150000	1.433820000	-1.451660000
6	-1.567380000	-0.930460000	-1.623320000
8	1.434420000	-0.889460000	-3.378520000
8	-0.612150000	2.508250000	-1.835050000
8	-2.465990000	-1.416380000	-2.172590000
7	-0.013960000	0.214040000	2.117550000
6	-0.829500000	0.112750000	1.024580000
6	-0.731190000	0.424820000	3.285880000
6	-2.037850000	0.474580000	2.923930000
7	-2.078870000	0.284540000	1.542920000
1	-2.935670000	0.621570000	3.503090000
1	-0.255210000	0.502120000	4.250730000
6	1.425420000	0.014280000	2.030720000
15	1.888480000	0.225970000	0.235240000
1	1.949480000	0.711710000	2.689030000
6	-3.306490000	0.264310000	0.793450000
6	-3.955330000	-0.967360000	0.611590000
6	-3.823890000	1.470140000	0.297890000
6	-5.162720000	-0.968840000	-0.092930000
6	-5.029540000	1.415440000	-0.413100000
6	-5.710380000	0.209150000	-0.618980000
1	-5.675910000	-1.914070000	-0.253340000
1	-5.443060000	2.337290000	-0.815660000
6	-3.130100000	2.786200000	0.552160000
1	-3.481630000	3.552790000	-0.143700000
1	-3.328360000	3.142830000	1.570970000
1	-2.046410000	2.704830000	0.443830000
6	-3.336540000	-2.244050000	1.121870000
1	-2.368570000	-2.418620000	0.640250000
1	-3.148580000	-2.205930000	2.200460000
1	-3.981300000	-3.101870000	0.913920000
6	-6.987900000	0.168790000	-1.423570000
1	-7.675770000	-0.595540000	-1.046780000
1	-7.506160000	1.132800000	-1.404930000
1	-6.776450000	-0.071550000	-2.473430000
1	1.671700000	-1.008980000	2.326090000

1	-0.519480000	-3.909760000	1.100520000
1	-0.035130000	-3.889550000	-2.566290000
1	1.328020000	-3.591750000	1.108850000
6	0.355070000	-3.481030000	1.620830000
8	0.282010000	-4.000440000	-1.660350000
8	0.262060000	-2.957800000	2.716900000
1	0.174950000	-3.116610000	-1.248500000
1	0.238330000	-1.854320000	-0.218320000
6	2.502260000	1.953050000	0.097120000
6	2.050800000	2.966630000	0.956090000
6	3.319260000	2.295150000	-0.993630000
6	2.431100000	4.295080000	0.742470000
6	3.697880000	3.621900000	-1.204340000
6	3.256320000	4.625780000	-0.335480000
1	1.392210000	2.735740000	1.788310000
1	3.663900000	1.524810000	-1.678390000
1	2.076190000	5.069870000	1.416360000
1	4.333240000	3.871390000	-2.049450000
1	3.548740000	5.658610000	-0.501880000
6	3.401940000	-0.805490000	0.101910000
6	3.335290000	-2.057510000	-0.527130000
6	4.617750000	-0.381830000	0.666800000
6	4.465740000	-2.878220000	-0.583390000
6	5.744520000	-1.204180000	0.609170000
6	5.670450000	-2.453730000	-0.017140000
1	2.404200000	-2.395970000	-0.966240000
1	4.689540000	0.592080000	1.142610000
1	4.400210000	-3.844200000	-1.075750000
1	6.679610000	-0.867840000	1.048250000
1	6.549360000	-3.090620000	-0.064900000

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27-Mn-Ph

25	-0.024780000	-0.429530000	-0.950220000
6	0.850110000	-0.787440000	-2.472360000
6	-0.432110000	1.246450000	-1.475260000
6	-1.485970000	-1.218510000	-1.624520000
8	1.411460000	-1.023280000	-3.463820000
8	-0.675680000	2.311370000	-1.873170000
8	-2.357460000	-1.791540000	-2.135480000
7	0.031910000	-0.196800000	2.053430000
6	-0.780720000	-0.201200000	0.952330000
6	-0.681050000	-0.047510000	3.233650000
6	-1.984800000	0.061850000	2.874880000
7	-2.028790000	-0.032360000	1.483570000

1	-2.878880000	0.195060000	3.463110000
1	-0.205730000	-0.046750000	4.201910000
6	1.469950000	-0.377280000	1.936920000
15	1.896960000	0.068660000	0.176460000
1	1.994900000	0.231880000	2.677260000
6	-3.249940000	0.094260000	0.732870000
6	-4.006280000	-1.060290000	0.475710000
6	-3.660310000	1.369460000	0.315340000
6	-5.191220000	-0.914920000	-0.251560000
6	-4.852050000	1.463900000	-0.414920000
6	-5.623280000	0.334830000	-0.715760000
1	-5.781450000	-1.800370000	-0.475990000
1	-5.180120000	2.442260000	-0.758480000
6	-2.876200000	2.606980000	0.679060000
1	-3.128280000	3.437940000	0.014910000
1	-3.101180000	2.920390000	1.706680000
1	-1.798450000	2.444640000	0.619610000
6	-3.543230000	-2.410600000	0.961070000
1	-2.533360000	-2.632170000	0.605040000
1	-3.507280000	-2.453770000	2.055760000
1	-4.210950000	-3.201560000	0.609660000
6	-6.876650000	0.450360000	-1.550560000
1	-7.653480000	-0.241140000	-1.206880000
1	-7.286960000	1.464820000	-1.524230000
1	-6.666080000	0.207280000	-2.599910000
1	1.728820000	-1.429100000	2.089780000
1	-0.607060000	-3.949180000	0.400430000
1	1.251960000	-3.827160000	0.597410000
6	0.251070000	-3.697790000	1.049400000
8	0.109700000	-3.356650000	2.209660000
1	0.365660000	-1.889700000	-0.433360000
6	2.389940000	1.839170000	0.240510000
6	1.860630000	2.712480000	1.203430000
6	3.187400000	2.364490000	-0.790200000
6	2.144690000	4.080540000	1.150900000
6	3.471660000	3.730270000	-0.839550000
6	2.953120000	4.592430000	0.132630000
1	1.213450000	2.340930000	1.992560000
1	3.591630000	1.705580000	-1.554100000
1	1.729330000	4.744220000	1.904260000
1	4.094200000	4.120700000	-1.639710000
1	3.172560000	5.655530000	0.092160000
6	3.480430000	-0.833750000	-0.066590000
6	3.478080000	-2.051640000	-0.763330000
6	4.685350000	-0.358610000	0.479780000
6	4.660550000	-2.781960000	-0.912990000

6	5.865640000	-1.089140000	0.327390000
6	5.855510000	-2.301950000	-0.370230000
1	2.552110000	-2.425310000	-1.186180000
1	4.707730000	0.586260000	1.014700000
1	4.646780000	-3.720270000	-1.460290000
1	6.791680000	-0.710270000	0.750800000
1	6.775510000	-2.866670000	-0.493040000

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TS8-Mn-Ph

25	-0.118760000	-0.096880000	-0.861510000
6	0.760170000	-0.372000000	-2.436230000
6	-0.202700000	1.658050000	-1.089750000
6	-1.721890000	-0.294340000	-1.714830000
8	1.321850000	-0.527960000	-3.434390000
8	-0.288350000	2.806200000	-1.225860000
8	-2.655890000	-0.406100000	-2.381270000
7	-0.031170000	0.112500000	2.146560000
6	-0.847860000	0.091810000	1.052550000
6	-0.749920000	0.247520000	3.322360000
6	-2.055190000	0.348320000	2.964230000
7	-2.096050000	0.266080000	1.574660000
1	-2.951080000	0.470300000	3.551850000
1	-0.276770000	0.250860000	4.291850000
6	1.368430000	-0.279600000	2.089420000
15	1.927530000	-0.050760000	0.332140000
1	1.945630000	0.299960000	2.811860000
6	-3.329420000	0.203700000	0.836580000
6	-3.957490000	-1.053310000	0.725090000
6	-3.873190000	1.369170000	0.280570000
6	-5.148890000	-1.117500000	-0.001500000
6	-5.074860000	1.250300000	-0.432400000
6	-5.719450000	0.020530000	-0.591850000
1	-5.643820000	-2.079720000	-0.113500000
1	-5.507060000	2.143860000	-0.878020000
6	-3.208750000	2.718880000	0.406060000
1	-2.364950000	2.706540000	1.098140000
1	-2.834600000	3.059490000	-0.565140000
1	-3.926340000	3.468220000	0.758030000
6	-3.374980000	-2.278290000	1.387780000
1	-2.280480000	-2.321260000	1.320770000
1	-3.627630000	-2.291240000	2.456490000
1	-3.789430000	-3.188070000	0.944060000
6	-6.986180000	-0.095950000	-1.405370000
1	-7.701710000	-0.780390000	-0.936720000

1	-7.475710000	0.874750000	-1.532240000
1	-6.767570000	-0.490090000	-2.406110000
1	1.442430000	-1.346490000	2.306560000
1	-1.461330000	-2.826920000	-0.670030000
1	-0.081460000	-3.931090000	-0.723540000
6	-0.377010000	-2.893960000	-0.420820000
8	-0.045210000	-2.535910000	0.850580000
1	0.137680000	-2.273090000	-1.227720000
6	2.855840000	1.537260000	0.270320000
6	3.528160000	2.073620000	1.380470000
6	2.950580000	2.202800000	-0.963280000
6	4.255920000	3.260560000	1.263470000
6	3.688360000	3.382110000	-1.083260000
6	4.336860000	3.918280000	0.032450000
1	3.504660000	1.569930000	2.341200000
1	2.449970000	1.801780000	-1.838570000
1	4.763970000	3.666590000	2.133660000
1	3.748010000	3.882760000	-2.045230000
1	4.903340000	4.840840000	-0.056620000
6	3.228800000	-1.325390000	0.081390000
6	2.903320000	-2.675380000	0.307310000
6	4.512210000	-0.982150000	-0.375120000
6	3.868030000	-3.662280000	0.091570000
6	5.465880000	-1.980440000	-0.594590000
6	5.147470000	-3.321110000	-0.360210000
1	1.888300000	-2.921200000	0.640590000
1	4.779070000	0.053870000	-0.556090000
1	3.612650000	-4.703190000	0.271400000
1	6.456720000	-1.705930000	-0.946090000
1	5.891360000	-4.094860000	-0.530450000

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28-Mn-Ph

25	-0.027240000	-0.762350000	-0.660700000
6	0.861960000	-1.530420000	-2.037890000
6	-0.377270000	0.704050000	-1.630080000
6	-1.559630000	-1.534080000	-1.232050000
8	1.417720000	-1.989360000	-2.946110000
8	-0.618620000	1.639000000	-2.277580000
8	-2.481640000	-2.045030000	-1.711310000
7	0.038260000	0.296600000	2.150440000
6	-0.780480000	0.056090000	1.085350000
6	-0.664580000	0.744350000	3.258890000
6	-1.967790000	0.807550000	2.880030000
7	-2.017390000	0.389460000	1.551460000

1	-2.855310000	1.103730000	3.416860000
1	-0.183770000	0.969340000	4.198260000
6	1.470600000	0.036620000	2.092260000
15	1.928240000	0.101690000	0.289800000
1	2.016640000	0.758670000	2.704710000
6	-3.239970000	0.297520000	0.799870000
6	-3.967030000	-0.902810000	0.856470000
6	-3.665890000	1.404320000	0.051910000
6	-5.158420000	-0.975830000	0.129610000
6	-4.859610000	1.277720000	-0.670610000
6	-5.615620000	0.099570000	-0.644800000
1	-5.730340000	-1.900700000	0.148290000
1	-5.202330000	2.119590000	-1.267630000
6	-2.886780000	2.696860000	0.048400000
1	-3.188940000	3.331370000	-0.789100000
1	-3.057340000	3.260310000	0.974820000
1	-1.811220000	2.525920000	-0.032260000
6	-3.449590000	-2.077110000	1.649490000
1	-2.422030000	-2.326310000	1.362960000
1	-3.433090000	-1.860030000	2.724310000
1	-4.074070000	-2.960180000	1.491280000
6	-6.880740000	-0.031070000	-1.459290000
1	-7.669120000	-0.540650000	-0.894350000
1	-7.262390000	0.945980000	-1.771380000
1	-6.698900000	-0.621170000	-2.366580000
1	1.677860000	-0.982310000	2.425760000
1	-0.894670000	-3.809960000	0.127780000
1	0.525360000	-4.280520000	1.084040000
6	0.181800000	-3.594960000	0.286460000
8	0.439170000	-2.276930000	0.643270000
1	0.690220000	-3.917910000	-0.647780000
6	2.297740000	1.865090000	-0.058730000
6	1.807450000	2.906660000	0.744040000
6	2.977520000	2.184040000	-1.247240000
6	2.013560000	4.240320000	0.376510000
6	3.186190000	3.515230000	-1.609770000
6	2.706170000	4.548070000	-0.797110000
1	1.250390000	2.693250000	1.651120000
1	3.350700000	1.390250000	-1.889240000
1	1.628570000	5.036310000	1.007970000
1	3.718740000	3.744690000	-2.528400000
1	2.864410000	5.584450000	-1.081540000
6	3.552100000	-0.748810000	0.244950000
6	3.571290000	-2.129260000	-0.012250000
6	4.759150000	-0.072940000	0.488040000
6	4.784470000	-2.821110000	-0.031130000

6	5.969950000	-0.770210000	0.468490000
6	5.984870000	-2.144050000	0.206770000
1	2.632150000	-2.647850000	-0.168080000
1	4.761110000	0.995180000	0.682700000
1	4.789870000	-3.888270000	-0.234500000
1	6.899310000	-0.238810000	0.654390000
1	6.927980000	-2.683320000	0.187140000

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29-Mn-Ph

25	-0.010280000	-0.769830000	-0.609340000
6	0.930720000	-1.559200000	-1.941600000
6	-0.362310000	0.660920000	-1.628580000
6	-1.545930000	-1.543390000	-1.173090000
8	1.555460000	-2.005690000	-2.809980000
8	-0.611110000	1.570260000	-2.309150000
8	-2.482860000	-2.037360000	-1.640740000
7	0.044970000	0.386130000	2.164400000
6	-0.771490000	0.106230000	1.106430000
6	-0.659680000	0.878520000	3.252430000
6	-1.961620000	0.928680000	2.867970000
7	-2.008610000	0.458410000	1.556780000
1	-2.850010000	1.247420000	3.390180000
1	-0.181230000	1.138810000	4.183810000
6	1.475520000	0.115230000	2.119760000
15	1.935930000	0.140550000	0.319520000
1	2.025770000	0.838720000	2.726320000
6	-3.230340000	0.345700000	0.806850000
6	-3.959210000	-0.851420000	0.896690000
6	-3.656710000	1.433950000	0.032320000
6	-5.154540000	-0.939390000	0.177880000
6	-4.854560000	1.292520000	-0.680510000
6	-5.614120000	0.117980000	-0.619730000
1	-5.728750000	-1.861950000	0.222920000
1	-5.198110000	2.119730000	-1.297310000
6	-2.873900000	2.723850000	-0.008040000
1	-3.166720000	3.329680000	-0.869810000
1	-3.052520000	3.319120000	0.896680000
1	-1.797810000	2.548280000	-0.071660000
6	-3.441720000	-2.007360000	1.716490000
1	-2.416560000	-2.268660000	1.431700000
1	-3.418760000	-1.763620000	2.785510000
1	-4.070850000	-2.891370000	1.583870000
6	-6.884950000	-0.028670000	-1.422480000
1	-7.667460000	-0.531890000	-0.843910000

1	-7.271730000	0.942620000	-1.746100000
1	-6.708200000	-0.631630000	-2.322270000
1	1.673070000	-0.900550000	2.469140000
1	-0.872280000	-3.794320000	0.193360000
1	0.481380000	-4.237230000	1.250270000
6	0.192560000	-3.575250000	0.411700000
8	0.431350000	-2.247410000	0.745320000
1	0.761480000	-3.925050000	-0.476180000
6	2.271520000	1.894100000	-0.096570000
6	1.916640000	2.961720000	0.740940000
6	2.787060000	2.172560000	-1.375010000
6	2.094500000	4.282750000	0.316320000
6	2.972350000	3.490260000	-1.793180000
6	2.625470000	4.550220000	-0.947610000
1	1.487810000	2.780580000	1.721150000
1	3.040770000	1.355980000	-2.046680000
1	1.812760000	5.100290000	0.974160000
1	3.375280000	3.689290000	-2.782120000
1	2.761340000	5.576740000	-1.276020000
6	3.568950000	-0.694390000	0.293810000
6	3.582620000	-2.099050000	0.251310000
6	4.783230000	0.009680000	0.330570000
6	4.797790000	-2.786540000	0.243810000
6	5.996370000	-0.684840000	0.319580000
6	6.006130000	-2.082250000	0.273930000
1	2.636650000	-2.630850000	0.244940000
1	4.789500000	1.094770000	0.360580000
1	4.799040000	-3.872450000	0.209160000
1	6.931750000	-0.132500000	0.344310000
1	6.950630000	-2.619260000	0.261080000
1	-0.182500779	-3.125313016	-0.956190192
1	-0.421142898	-3.087243780	-1.659760975

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TS9-Mn-Ph

25	-0.043650000	-0.579180000	-0.840050000
6	0.851330000	-1.019140000	-2.369340000
6	-0.381430000	1.043030000	-1.447820000
6	-1.574920000	-1.220340000	-1.604410000
8	1.416990000	-1.216910000	-3.358930000
8	-0.622830000	2.091640000	-1.887710000
8	-2.503540000	-1.555410000	-2.204740000
7	0.017520000	-0.027060000	2.129930000
6	-0.795240000	-0.168970000	1.035330000
6	-0.701820000	0.259990000	3.280500000

6	-2.006350000	0.316770000	2.907490000
7	-2.044800000	0.056430000	1.540160000
1	-2.903220000	0.516720000	3.472370000
1	-0.229060000	0.389610000	4.241660000
6	1.464960000	-0.183690000	2.057470000
15	1.916740000	0.044320000	0.264420000
1	1.952300000	0.536440000	2.719080000
6	-3.265730000	0.099160000	0.776850000
6	-3.982560000	-1.092100000	0.579160000
6	-3.711900000	1.336570000	0.289880000
6	-5.175610000	-1.019570000	-0.143870000
6	-4.910470000	1.356130000	-0.436410000
6	-5.651550000	0.191570000	-0.665370000
1	-5.737420000	-1.933450000	-0.322340000
1	-5.267340000	2.303600000	-0.832950000
6	-2.953010000	2.611390000	0.566930000
1	-3.282160000	3.412480000	-0.100060000
1	-3.114110000	2.947260000	1.599130000
1	-1.876770000	2.485190000	0.431870000
6	-3.452390000	-2.407320000	1.088310000
1	-2.524890000	-2.674040000	0.572360000
1	-3.224800000	-2.368630000	2.159170000
1	-4.173730000	-3.211100000	0.919380000
6	-6.928800000	0.221020000	-1.470300000
1	-7.237240000	1.245260000	-1.700650000
1	-6.801790000	-0.311720000	-2.420720000
1	-7.748850000	-0.268890000	-0.932540000
1	1.755850000	-1.199040000	2.335920000
1	-0.276080000	-2.632830000	2.339430000
1	0.823770000	-4.016370000	2.135760000
6	0.137140000	-3.339080000	1.606160000
8	0.807340000	-2.656040000	0.562150000
1	-0.694270000	-3.942920000	1.214610000
6	2.319430000	1.831740000	0.115480000
6	1.737800000	2.789170000	0.961000000
6	3.108410000	2.264270000	-0.963450000
6	1.957720000	4.152510000	0.743420000
6	3.327340000	3.626050000	-1.178370000
6	2.753850000	4.574230000	-0.324600000
1	1.098750000	2.485970000	1.784810000
1	3.557760000	1.536870000	-1.633960000
1	1.501620000	4.882540000	1.406350000
1	3.942640000	3.945360000	-2.014760000
1	2.921770000	5.633800000	-0.495030000
6	3.539250000	-0.792780000	0.101460000
6	3.622230000	-2.014810000	-0.581370000

6	4.700340000	-0.233100000	0.663140000
6	4.852610000	-2.666250000	-0.704080000
6	5.926210000	-0.890860000	0.544530000
6	6.003910000	-2.107830000	-0.142120000
1	2.728890000	-2.466490000	-0.994960000
1	4.652900000	0.721180000	1.180130000
1	4.906300000	-3.610420000	-1.238290000
1	6.818450000	-0.451410000	0.981860000
1	6.959020000	-2.616540000	-0.240070000
1	0.425790000	-2.996670000	-0.388380000
1	-0.071160000	-3.145370000	-1.434720000

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30-Mn-Ph

25	-0.058680000	-0.305170000	-0.946410000
6	0.826300000	-0.620330000	-2.473690000
6	-0.436130000	1.397980000	-1.402370000
6	-1.539030000	-1.012550000	-1.674590000
8	1.397030000	-0.833580000	-3.463830000
8	-0.672680000	2.478620000	-1.759290000
8	-2.420830000	-1.522490000	-2.230090000
7	0.002680000	-0.098490000	2.065410000
6	-0.812440000	-0.115040000	0.964880000
6	-0.712610000	0.026280000	3.247260000
6	-2.018990000	0.109570000	2.890250000
7	-2.062450000	0.023370000	1.499000000
1	-2.915250000	0.220250000	3.479880000
1	-0.236210000	0.036370000	4.215020000
6	1.442530000	-0.280250000	1.955080000
15	1.877940000	0.145090000	0.191720000
1	1.965790000	0.336250000	2.690370000
6	-3.293560000	0.084890000	0.756470000
6	-3.987450000	-1.111180000	0.510350000
6	-3.775430000	1.334420000	0.339360000
6	-5.194920000	-1.030500000	-0.189360000
6	-4.982520000	1.361930000	-0.371410000
6	-5.701340000	0.193110000	-0.648570000
1	-5.741610000	-1.946630000	-0.400480000
1	-5.366090000	2.319830000	-0.715180000
6	-3.051980000	2.613610000	0.683640000
1	-3.351450000	3.423700000	0.013290000
1	-3.284480000	2.927020000	1.709640000
1	-1.968010000	2.505500000	0.616250000
6	-3.427030000	-2.436280000	0.960910000
1	-2.456620000	-2.633600000	0.494060000

1	-3.260000000	-2.461480000	2.043480000
1	-4.102700000	-3.254910000	0.699330000
6	-6.979350000	0.239470000	-1.452230000
1	-7.708030000	-0.493390000	-1.089430000
1	-7.443970000	1.229870000	-1.414230000
1	-6.782420000	0.007770000	-2.506780000
1	1.695150000	-1.332860000	2.116630000
1	0.891450000	-5.235290000	1.707520000
1	1.943370000	-4.256750000	0.658660000
6	0.898920000	-4.448110000	0.946890000
8	0.283920000	-3.296300000	1.515660000
1	0.353280000	-4.813920000	0.065130000
6	2.406890000	1.904710000	0.242940000
6	1.902410000	2.794890000	1.203790000
6	3.209790000	2.405780000	-0.795600000
6	2.217520000	4.155720000	1.142130000
6	3.524910000	3.764420000	-0.853840000
6	3.032010000	4.643200000	0.116780000
1	1.250960000	2.442900000	1.998400000
1	3.593250000	1.733510000	-1.558600000
1	1.821440000	4.832940000	1.893800000
1	4.151430000	4.136480000	-1.659600000
1	3.275540000	5.700750000	0.069410000
6	3.437030000	-0.796360000	-0.052120000
6	3.396780000	-2.023600000	-0.731080000
6	4.658530000	-0.342960000	0.475470000
6	4.559200000	-2.785350000	-0.880450000
6	5.818580000	-1.104950000	0.322540000
6	5.771130000	-2.327260000	-0.356910000
1	2.457020000	-2.382800000	-1.135930000
1	4.709790000	0.608660000	0.996170000
1	4.515930000	-3.731740000	-1.412060000
1	6.758020000	-0.743240000	0.731140000
1	6.675610000	-2.916470000	-0.480030000
1	0.155640000	-2.645740000	0.793150000
1	0.281330000	-1.815720000	-0.544130000

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7-CO₂-Mn-iPr

25	-0.421376000	1.054001000	-0.503477000
6	-1.207214000	2.323192000	-1.548941000
6	0.932658000	2.203632000	-0.152171000
6	0.434161000	0.367292000	-1.911427000
8	-1.628066000	3.158459000	-2.228041000
8	1.763114000	2.982306000	0.041345000

8	0.986222000	-0.055214000	-2.841735000
7	-0.681263000	-0.886635000	1.673471000
6	0.258390000	-0.345564000	0.851835000
6	-0.126785000	-1.753901000	2.600896000
6	1.209293000	-1.771529000	2.341193000
7	1.425852000	-0.906782000	1.269108000
1	2.019031000	-2.304900000	2.813513000
1	-0.716189000	-2.259783000	3.349443000
6	-2.074803000	-0.485214000	1.502889000
1	-2.727709000	-1.156124000	2.058365000
15	-2.285914000	-0.452274000	-0.367287000
6	2.709899000	-0.657715000	0.667992000
6	3.525288000	0.351527000	1.205550000
6	3.097350000	-1.434605000	-0.434013000
6	4.754677000	0.590636000	0.582510000
6	4.336033000	-1.155395000	-1.024032000
6	5.172801000	-0.144990000	-0.535046000
1	5.396295000	1.376993000	0.973388000
1	4.648447000	-1.737433000	-1.887380000
6	2.217942000	-2.545678000	-0.952442000
1	2.612266000	-2.952458000	-1.887150000
1	2.150577000	-3.366058000	-0.227576000
1	1.198626000	-2.199561000	-1.141281000
6	3.098413000	1.139509000	2.419733000
1	2.054274000	1.456839000	2.357378000
1	3.196559000	0.538775000	3.332608000
1	3.716765000	2.032737000	2.539214000
6	6.490417000	0.167442000	-1.203509000
1	7.299708000	0.251125000	-0.469515000
1	6.767839000	-0.603892000	-1.928201000
1	6.438268000	1.123637000	-1.738895000
6	-4.098179000	-0.054739000	-0.670235000
1	-4.359419000	-0.678855000	-1.534534000
6	-4.301636000	1.417111000	-1.060211000
6	-5.013089000	-0.441095000	0.507844000
1	-4.895469000	-1.483153000	0.816522000
1	-4.831211000	0.196373000	1.378620000
1	-6.058421000	-0.302137000	0.208100000
1	-3.929392000	2.095689000	-0.286218000
1	-5.371722000	1.614896000	-1.193404000
1	-3.800977000	1.661464000	-1.999762000
6	-2.040851000	-2.216164000	-0.929171000
1	-1.032812000	-2.449775000	-0.566472000
6	-2.022713000	-2.279187000	-2.466106000
6	-3.022907000	-3.236247000	-0.337483000
1	-3.036552000	-3.216376000	0.756886000

1	-4.043908000	-3.070366000	-0.696951000
1	-2.729465000	-4.247254000	-0.644906000
1	-3.012734000	-2.073947000	-2.889523000
1	-1.732132000	-3.284659000	-2.792065000
1	-1.313816000	-1.569771000	-2.902105000
6	-2.223113000	1.000514000	1.962799000
8	-1.538711000	1.821668000	1.249965000
8	-2.949051000	1.263153000	2.927133000

-1824.077403

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