

Supporting Information

Aliphatic Mn-PNP Complexes for CO₂ Hydrogenation Reaction: A Base Free Mechanism

Kuber Singh Rawat, Biswarup Pathak ^{†, #, *}

[†]Discipline of Chemistry and [#]Discipline of Metallurgy Engineering and Materials Science, Indian Institute of Technology (IIT) Indore, Indore. M.P. 453552, India

Email: biswarup@iiti.ac.in

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S1. Gaussian full reference (reference number 62 in the manuscript)

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

Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

S2. Reaction free energies (ΔG) and activation barriers (ΔG^\ddagger) are calculated by using B3LYP and M06 functional

Table S1: Reaction free energies (ΔG) and activation barriers (ΔG^\ddagger) are calculated by using B3LYP and M06 functional for heterolytic H₂ cleavage.

Complexes	B3LYP		M06	
	ΔG	ΔG^\ddagger	ΔG	ΔG^\ddagger
Mn1	-16.8	5.1	-18.1	4.4
Mn1-PF₃	-20.5	2.9	-23.1	1.9
Mn1-2PF₃	-26.5	1.9	-26.3	0.3
Mn1-PH₃	-19.0	3.6	-17.3	5.3
Mn1-2PH₃	-13.7	4.5	-14.5	4.2
Mn1-PMe₃	-17.3	6.5	-14.6	6.7
Mn1-2PMe₃	-11.7	5.6	-10.4	-

S3. Table S2. Calculated bond distance (Å) between Mn-N bonds in Mn complexes.

Intermediate	Mn1	Mn1-PF ₃	Mn1-2PF ₃	Mn1-PH ₃	Mn1-2PH ₃	Mn1-PMe ₃	Mn1-2PMe ₃
1	1.91	1.90	1.89	1.92	1.93	1.94	1.97
2	2.11	2.09	2.09	2.10	2.14	2.13	2.15
3	2.29	2.26	2.28	2.23	2.25	2.24	2.25
4	2.15	2.13	2.14	2.14	2.16	2.17	2.20

S4. Cartesian coordinates and energies (in Hartree) in solvent phase for all the species.

H₂

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

-1.178427

CO₂

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

-188.657811

HCOOH

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

-189.823583

1-Mn1

25 -0.000016000 -0.014833000 -0.013168000
 15 2.296304000 -0.189513000 0.238459000
 15 -2.296326000 -0.189655000 0.238228000
 7 0.000003000 -1.822172000 0.615551000

6	2.414557000	-1.852225000	1.043384000
1	3.358743000	-2.363513000	0.844701000
1	2.338800000	-1.679332000	2.120051000
6	1.201497000	-2.659851000	0.590404000
1	1.374482000	-3.071981000	-0.418740000
1	1.079621000	-3.527941000	1.255081000
6	-1.201350000	-2.660044000	0.589631000
1	-1.079642000	-3.528313000	1.254103000
1	-1.373802000	-3.071886000	-0.419715000
6	-2.414745000	-1.852756000	1.042330000
1	-2.339593000	-1.680358000	2.119114000
1	-3.358773000	-2.364039000	0.842884000
6	-3.310964000	-0.340002000	-1.330061000
6	-3.177938000	0.896870000	-2.235484000
1	-3.508771000	0.647991000	-3.248330000
1	-2.151170000	1.256125000	-2.296881000
1	-3.802981000	1.717208000	-1.878115000
6	-3.148651000	0.958243000	1.456026000
6	-3.411984000	2.355851000	0.875028000
1	-3.659912000	3.048685000	1.685142000
1	-4.262896000	2.340450000	0.189899000
1	-2.549662000	2.759312000	0.343983000
6	3.148804000	0.958956000	1.455583000
6	3.412180000	2.356239000	0.873828000
1	3.660089000	3.049527000	1.683560000
1	2.549886000	2.759427000	0.342533000
1	4.263108000	2.340461000	0.188726000
6	3.310845000	-0.340755000	-1.329802000
6	3.178031000	0.895775000	-2.235733000
1	3.508774000	0.646405000	-3.248487000
1	3.803265000	1.716121000	-1.878710000
1	2.151336000	1.255223000	-2.297240000
6	-0.000016000	-0.079657000	-1.759874000
8	-0.000048000	-0.249860000	-2.912655000
6	-0.000060000	1.770657000	0.057877000
6	-4.411910000	0.405833000	2.135515000
1	-5.241378000	0.312329000	1.432688000
1	-4.250909000	-0.569210000	2.598525000
1	-4.727779000	1.095645000	2.925263000
6	4.412081000	0.406825000	2.135253000
1	4.728011000	1.096993000	2.924665000
1	4.251071000	-0.568003000	2.598703000
1	5.241501000	0.312974000	1.432415000
6	4.785812000	-0.729516000	-1.158816000
1	5.212965000	-0.983050000	-2.134537000
1	5.367743000	0.102757000	-0.756067000

1	4.925742000	-1.591811000	-0.503737000
6	-4.785989000	-0.728570000	-1.159137000
1	-5.367740000	0.103688000	-0.756093000
1	-5.213238000	-0.981716000	-2.134917000
1	-4.926040000	-1.591047000	-0.504318000
1	-2.788924000	-1.169148000	-1.824507000
1	2.788619000	-1.170005000	-1.823877000
1	-2.367090000	1.054610000	2.219911000
1	2.367326000	1.055792000	2.219497000
8	-0.000111000	2.935099000	0.099800000

-1699.439906

2-Mn1

25	-0.000023000	0.073973000	0.094398000
15	2.294818000	-0.197710000	0.254479000
15	-2.294863000	-0.197941000	0.254270000
7	-0.000024000	-1.964631000	0.622628000
6	2.433283000	-1.970061000	0.773049000
1	3.366538000	-2.432181000	0.442956000
1	2.409575000	-1.985971000	1.866347000
6	1.194313000	-2.690865000	0.236572000
1	1.291951000	-2.812879000	-0.864109000
1	1.176302000	-3.715987000	0.645631000
6	-1.194066000	-2.691004000	0.235877000
1	-1.176038000	-3.716200000	0.644742000
1	-1.291193000	-2.812807000	-0.864863000
6	-2.433396000	-1.970554000	0.771990000
1	-2.410249000	-1.986959000	1.865290000
1	-3.366439000	-2.432633000	0.441240000
6	-3.257991000	-0.107564000	-1.349522000
6	-2.992239000	1.191885000	-2.126038000
1	-3.409767000	1.108953000	-3.134150000
1	-1.927304000	1.402505000	-2.218333000
1	-3.463804000	2.050819000	-1.643991000
6	-3.178697000	0.761693000	1.603508000
6	-3.326728000	2.249203000	1.250861000
1	-3.627785000	2.813235000	2.139073000
1	-4.100025000	2.398516000	0.493246000
1	-2.396504000	2.679959000	0.876229000
6	3.178776000	0.762429000	1.603247000
6	3.326757000	2.249828000	1.250156000
1	3.628031000	2.814114000	2.138131000
1	2.396458000	2.680492000	0.875591000
1	4.099871000	2.398930000	0.492320000
6	3.257922000	-0.108229000	-1.349405000

6	2.992516000	1.191039000	-2.126359000
1	3.409682000	1.107549000	-3.134575000
1	3.464645000	2.049929000	-1.644792000
1	1.927651000	1.402137000	-2.218404000
6	0.000004000	-0.368994000	-1.617643000
8	0.000043000	-0.710857000	-2.724760000
6	-0.000173000	1.821202000	-0.251211000
6	-4.505326000	0.175550000	2.111955000
1	-5.304836000	0.281924000	1.378191000
1	-4.423080000	-0.881523000	2.372463000
1	-4.814263000	0.713899000	3.014155000
6	4.505482000	0.176464000	2.111749000
1	4.814351000	0.714916000	3.013906000
1	4.423402000	-0.880607000	2.372310000
1	5.304930000	0.282919000	1.377931000
6	4.764265000	-0.389135000	-1.255946000
1	5.171558000	-0.535201000	-2.261560000
1	5.295096000	0.455152000	-0.810416000
1	4.995005000	-1.282986000	-0.672770000
6	-4.764411000	-0.388021000	-1.256084000
1	-5.294950000	0.456192000	-0.810083000
1	-5.171823000	-0.533440000	-2.261745000
1	-4.995363000	-1.282110000	-0.673357000
1	-2.793455000	-0.928763000	-1.910041000
1	2.793130000	-0.929468000	-1.909628000
1	-2.449340000	0.682530000	2.418795000
1	2.449474000	0.683527000	2.418615000
8	-0.000217000	2.952294000	-0.524802000
1	0.000406000	0.645051000	1.823582000
1	-0.000779000	-0.136371000	1.868448000

-1700.601556

TS1-Mn1

15	-2.274927000	-0.151812000	-0.136764000
7	-0.020529000	-1.504551000	-1.382041000
6	1.178848000	-2.271014000	-1.673694000
6	-1.270791000	-2.149009000	-1.741077000
6	-2.404674000	-1.115552000	-1.719546000
1	-3.386335000	-1.573924000	-1.860655000
1	-2.238087000	-0.402089000	-2.528766000
6	2.412188000	-1.358827000	-1.606695000
1	2.425298000	-0.712441000	-2.488914000
15	2.275695000	-0.202065000	-0.151088000
6	0.022938000	1.110210000	1.510921000

8	0.033947000	1.755182000	2.477075000
25	0.005868000	0.092239000	0.061005000
6	0.036671000	1.470702000	-1.064284000
8	0.071461000	2.355346000	-1.814216000
6	-3.428247000	1.322278000	-0.286724000
1	-4.419895000	0.968383000	0.010422000
6	-2.995122000	2.436837000	0.680101000
1	-3.732615000	3.245414000	0.665367000
1	-2.898106000	2.088641000	1.709541000
1	-2.030332000	2.852873000	0.382278000
6	-3.524617000	1.862214000	-1.721787000
1	-3.968813000	1.137759000	-2.407178000
1	-4.156108000	2.756218000	-1.730436000
1	-2.544184000	2.148470000	-2.109575000
6	3.297667000	1.264229000	-0.717653000
1	2.793719000	1.523571000	-1.655517000
6	3.180510000	2.476557000	0.216808000
1	3.594295000	3.362022000	-0.275419000
1	2.142752000	2.689015000	0.478214000
1	3.742641000	2.325791000	1.141368000
6	4.763913000	0.940892000	-1.034773000
1	5.236187000	1.803389000	-1.515732000
1	5.332448000	0.725989000	-0.125861000
1	4.865747000	0.088215000	-1.710356000
1	1.316454000	-3.129858000	-0.987190000
1	1.113896000	-2.702980000	-2.683287000
1	3.345530000	-1.928031000	-1.591184000
1	-1.531007000	-2.998606000	-1.073880000
1	-1.200973000	-2.576991000	-2.751994000
6	3.259317000	-1.012147000	1.227460000
1	4.312329000	-0.932151000	0.939047000
6	2.919570000	-2.501631000	1.383462000
1	3.509965000	-2.925129000	2.202198000
1	1.863628000	-2.642583000	1.627376000
1	3.141376000	-3.077700000	0.483436000
6	3.043947000	-0.280659000	2.560789000
1	3.675436000	-0.727810000	3.335035000
1	3.286167000	0.781016000	2.506297000
1	2.003337000	-0.367807000	2.881139000
6	-3.082063000	-1.280296000	1.128153000
1	-2.452933000	-2.175135000	1.063625000
6	-4.531127000	-1.682886000	0.823710000
1	-4.864183000	-2.431030000	1.550287000
1	-5.212368000	-0.831319000	0.903487000
1	-4.646451000	-2.118114000	-0.170920000
6	-2.951354000	-0.717563000	2.550580000

1	-3.275348000	-1.467097000	3.279262000
1	-1.921655000	-0.440996000	2.782312000
1	-3.583302000	0.164156000	2.688370000
1	-0.036020000	-1.587460000	0.093858000
1	-0.025717000	-1.347861000	1.013515000

-1700.593505

3-Mn1

15	-2.225810000	-0.136450000	-0.045393000
7	-0.010789000	-1.839735000	-1.076093000
6	0.980582000	-1.728054000	-2.170389000
6	-1.360922000	-2.320005000	-1.483949000
6	-2.360316000	-1.168526000	-1.592863000
1	-3.367898000	-1.544275000	-1.787301000
1	-2.080609000	-0.513902000	-2.420307000
6	2.370841000	-1.451861000	-1.582452000
1	3.025634000	-1.037875000	-2.351326000
15	2.250186000	-0.259961000	-0.128593000
6	0.094558000	1.310040000	1.398048000
8	0.145075000	2.043201000	2.302568000
25	0.021964000	0.111388000	0.112613000
6	0.039304000	1.270265000	-1.235020000
8	0.055627000	2.088623000	-2.071319000
6	-3.389326000	1.319854000	-0.308959000
1	-4.372671000	0.999667000	0.049567000
6	-2.928663000	2.521413000	0.532330000
1	-3.672570000	3.322493000	0.472944000
1	-2.786308000	2.268894000	1.584012000
1	-1.978699000	2.909486000	0.158919000
6	-3.528381000	1.724778000	-1.784713000
1	-3.978865000	0.935967000	-2.391192000
1	-4.171487000	2.607522000	-1.860018000
1	-2.560249000	1.985214000	-2.218959000
6	3.340880000	1.154499000	-0.715849000
1	2.954367000	1.313091000	-1.729737000
6	3.099606000	2.453970000	0.064936000
1	3.634744000	3.278304000	-0.417179000
1	2.039499000	2.704976000	0.094872000
1	3.457033000	2.385963000	1.094565000
6	4.834891000	0.818472000	-0.813372000
1	5.365712000	1.628302000	-1.323974000
1	5.284655000	0.708524000	0.177077000
1	5.021797000	-0.102645000	-1.372368000
1	1.003829000	-2.644231000	-2.776196000
1	0.665214000	-0.905280000	-2.813682000

1	2.828315000	-2.383639000	-1.243310000
1	-1.699622000	-3.031566000	-0.727261000
1	-1.298286000	-2.867369000	-2.431091000
6	3.238035000	-1.145593000	1.202328000
1	4.227978000	-1.355941000	0.783274000
6	2.570190000	-2.473864000	1.585012000
1	3.142020000	-2.961283000	2.380907000
1	1.554633000	-2.294132000	1.946454000
1	2.519254000	-3.176959000	0.748736000
6	3.389168000	-0.250719000	2.440769000
1	3.899527000	-0.798492000	3.239256000
1	3.971885000	0.648124000	2.233925000
1	2.409741000	0.058366000	2.815500000
6	-3.083701000	-1.172447000	1.263174000
1	-2.404557000	-2.025751000	1.362675000
6	-4.482287000	-1.688971000	0.903621000
1	-4.865326000	-2.315980000	1.715632000
1	-5.195110000	-0.871065000	0.765033000
1	-4.483169000	-2.294977000	-0.005328000
6	-3.086055000	-0.428416000	2.606440000
1	-3.410604000	-1.100255000	3.407163000
1	-2.089351000	-0.057444000	2.853849000
1	-3.778683000	0.417951000	2.589985000
1	0.349924000	-2.496236000	-0.391550000
1	-0.036945000	-0.877522000	1.409017000

-1700.625748

TS2-Mn1

15	-2.228917000	-0.274327000	0.184298000
7	-0.004068000	0.486887000	1.996081000
6	1.072063000	-0.179248000	2.763315000
6	-1.337911000	0.515670000	2.663522000
6	-2.311933000	-0.478699000	2.032803000
1	-3.316236000	-0.356089000	2.445134000
1	-1.986162000	-1.499145000	2.242633000
6	2.421341000	0.121511000	2.101911000
1	3.204904000	-0.499362000	2.538656000
15	2.300112000	-0.135261000	0.245992000
6	0.074405000	-0.471306000	-1.879164000
8	0.098301000	-0.536682000	-3.039139000
25	0.034683000	-0.277300000	-0.123873000
6	0.074774000	-2.015413000	0.215912000
8	0.111041000	-3.169532000	0.389922000
6	-3.341632000	-1.615186000	-0.530356000

1	-4.336146000	-1.166467000	-0.612828000
6	-2.870820000	-2.009379000	-1.939368000
1	-3.604551000	-2.678649000	-2.399876000
1	-2.742472000	-1.146253000	-2.594027000
1	-1.913893000	-2.534141000	-1.896483000
6	-3.457047000	-2.857636000	0.366021000
1	-3.913035000	-2.631001000	1.332083000
1	-4.087012000	-3.603192000	-0.129641000
1	-2.481618000	-3.316646000	0.542478000
6	3.294826000	-1.711336000	-0.001299000
1	2.778176000	-2.408965000	0.667148000
6	3.159991000	-2.247609000	-1.433332000
1	3.598972000	-3.247791000	-1.499340000
1	2.116713000	-2.313282000	-1.742803000
1	3.689200000	-1.610244000	-2.146907000
6	4.769041000	-1.640786000	0.420509000
1	5.200777000	-2.646760000	0.413483000
1	5.356377000	-1.034095000	-0.273723000
1	4.907039000	-1.232559000	1.424715000
1	1.086164000	0.170877000	3.804190000
1	0.866966000	-1.251381000	2.771873000
1	2.686995000	1.161337000	2.297644000
1	-1.728244000	1.531103000	2.564893000
1	-1.227606000	0.317526000	3.734826000
6	3.353405000	1.205654000	-0.559018000
1	4.383040000	0.838480000	-0.563915000
6	3.331915000	2.542768000	0.194934000
1	3.808368000	3.315041000	-0.416470000
1	2.313420000	2.875757000	0.406800000
1	3.875804000	2.494250000	1.140697000
6	2.890594000	1.396745000	-2.012842000
1	3.553180000	2.103379000	-2.522460000
1	2.895545000	0.463562000	-2.578200000
1	1.873283000	1.790555000	-2.040971000
6	-3.168238000	1.314321000	-0.148007000
1	-2.545113000	2.065804000	0.344992000
6	-4.580528000	1.400141000	0.443539000
1	-5.006914000	2.386311000	0.232929000
1	-5.253025000	0.657958000	0.004700000
1	-4.588126000	1.265706000	1.527534000
6	-3.166293000	1.609284000	-1.655374000
1	-3.532655000	2.623290000	-1.841215000
1	-2.161196000	1.529518000	-2.072558000
1	-3.823043000	0.919135000	-2.192896000
1	0.265019000	1.456752000	1.854363000
1	-0.001282000	1.358240000	-0.511795000

6	-0.214280000	3.217013000	-0.318197000
8	-0.214932000	3.515844000	-1.450406000
8	-0.254432000	3.307935000	0.857273000

-1889.271547

4-Mn1

15	-2.268000000	-0.278199000	0.144490000
7	-0.075620000	0.546430000	1.929200000
6	1.066950000	0.070800000	2.748450000
6	-1.398780000	0.468780000	2.629640000
6	-2.343610000	-0.540449000	1.979090000
1	-3.351040000	-0.457169000	2.392220000
1	-1.990090000	-1.556870000	2.162050000
6	2.379680000	0.472860000	2.075000000
1	3.231350000	0.020839000	2.586080000
15	2.326810000	-0.005050000	0.273810000
6	0.148220000	-0.427570000	-1.859230000
8	0.243820000	-0.561280000	-3.002880000
25	0.030550000	-0.174030000	-0.093540000
6	0.077380000	-1.897960000	0.257340000
8	0.093530000	-3.032810000	0.503220000
6	-3.300080000	-1.638689000	-0.641270000
1	-4.297920000	-1.206369000	-0.762110000
6	-2.761690000	-1.998119000	-2.034810000
1	-3.461580000	-2.674389000	-2.535110000
1	-2.629350000	-1.120579000	-2.668950000
1	-1.797190000	-2.506110000	-1.964400000
6	-3.434220000	-2.895259000	0.232290000
1	-3.922260000	-2.686479000	1.186450000
1	-4.043721000	-3.634899000	-0.295890000
1	-2.462991000	-3.352619000	0.432900000
6	3.259990000	-1.636311000	0.266820000
1	2.747850000	-2.180030000	1.069190000
6	3.074760000	-2.443311000	-1.028560000
1	3.414829000	-3.470731000	-0.869070000
1	2.034100000	-2.481430000	-1.347720000
1	3.659940000	-2.027571000	-1.849890000
6	4.745690000	-1.522631000	0.637860000
1	5.166880000	-2.524171000	0.767990000
1	5.318690000	-1.028281000	-0.150200000
1	4.909880000	-0.974891000	1.568710000
1	1.021660000	0.501820000	3.755660000
1	0.991650000	-1.015010000	2.846410000
1	2.501100000	1.556960000	2.130580000
1	-1.838780000	1.467990000	2.593060000

1	-1.247300000	0.221140000	3.683520000
6	3.472790000	1.230919000	-0.547610000
1	4.398130000	1.188849000	0.037480000
6	2.927731000	2.664939000	-0.499680000
1	3.723151000	3.358559000	-0.788030000
1	2.108051000	2.794920000	-1.207390000
1	2.568871000	2.965950000	0.485710000
6	3.780980000	0.840619000	-2.001540000
1	4.376230000	1.629559000	-2.470590000
1	4.348400000	-0.086531000	-2.077950000
1	2.862680000	0.729469000	-2.584320000
6	-3.248130000	1.285351000	-0.173660000
1	-2.644219000	2.065891000	0.296980000
6	-4.644570000	1.311891000	0.459920000
1	-5.123959000	2.270311000	0.238070000
1	-5.292670000	0.525661000	0.062900000
1	-4.609540000	1.208391000	1.546440000
6	-3.299650000	1.566661000	-1.683450000
1	-3.724849000	2.558581000	-1.857700000
1	-2.304150000	1.556121000	-2.130360000
1	-3.931260000	0.839261000	-2.201780000
1	0.059440000	1.555890000	1.747320000
1	-0.029510000	1.617060000	-0.492180000
6	-0.277689000	2.775310000	-0.309640000
8	-0.479839000	3.359900000	-1.363800000
8	-0.258959000	3.108990000	0.886190000

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TS3-Mn1

15	-2.245456000	-0.419776000	0.163959000
7	-0.095788000	0.663172000	1.679201000
6	1.105029000	0.772813000	2.543341000
6	-1.317744000	0.566360000	2.530194000
6	-2.312643000	-0.474616000	2.005744000
1	-3.313182000	-0.331259000	2.419919000
1	-1.968218000	-1.473054000	2.283563000
6	2.335265000	1.119626000	1.710027000
1	3.253239000	1.021088000	2.291402000
15	2.337378000	0.039182000	0.201680000
6	0.136322000	-0.613045000	-1.821773000
8	0.203065000	-0.767696000	-2.968278000
25	0.049685000	-0.338403000	-0.056174000
6	0.131663000	-2.050814000	0.296468000
8	0.158650000	-3.170695000	0.605601000
6	-3.280931000	-1.838948000	-0.496235000

1	-4.281166000	-1.423772000	-0.649512000
6	-2.746199000	-2.321099000	-1.854013000
1	-3.441754000	-3.047599000	-2.284845000
1	-2.625150000	-1.506208000	-2.569446000
1	-1.776687000	-2.810699000	-1.740320000
6	-3.400193000	-3.009438000	0.491504000
1	-3.882647000	-2.714476000	1.425491000
1	-4.007210000	-3.800334000	0.040439000
1	-2.423471000	-3.437510000	0.727605000
6	3.391317000	-1.423431000	0.715009000
1	2.867616000	-1.751140000	1.621173000
6	3.363301000	-2.589312000	-0.289096000
1	2.376088000	-2.749974000	-0.719484000
1	4.063286000	-2.424444000	-1.109154000
1	3.662686000	-3.512243000	0.215565000
6	4.836148000	-1.062156000	1.090348000
1	5.346698000	-1.950546000	1.474823000
1	5.397928000	-0.714226000	0.219480000
1	4.895218000	-0.291740000	1.861784000
1	0.955524000	1.552284000	3.302783000
1	1.257847000	-0.172137000	3.081324000
1	2.264823000	2.154464000	1.370884000
1	-1.799398000	1.551617000	2.587086000
1	-1.039055000	0.300954000	3.554671000
6	3.319804000	1.027613000	-1.049039000
1	4.225609000	1.356186000	-0.527240000
6	2.525889000	2.267757000	-1.485325000
1	3.129739000	2.868071000	-2.171749000
1	1.612689000	1.981364000	-2.012947000
1	2.246514000	2.911823000	-0.650314000
6	3.722725000	0.195696000	-2.275676000
1	4.202234000	0.845731000	-3.013660000
1	4.431760000	-0.594138000	-2.028516000
1	2.852480000	-0.260576000	-2.753744000
6	-3.198003000	1.122739000	-0.303504000
1	-2.623400000	1.921461000	0.172913000
6	-4.630548000	1.194397000	0.242668000
1	-5.070828000	2.159062000	-0.027483000
1	-5.270276000	0.416026000	-0.181367000
1	-4.666416000	1.111401000	1.330759000
6	-3.163644000	1.335102000	-1.824097000
1	-3.552873000	2.326028000	-2.072265000
1	-2.150657000	1.261001000	-2.225243000
1	-3.784349000	0.596343000	-2.338948000
1	-0.196461000	1.989426000	1.229456000
1	-0.524367000	2.389677000	-0.860847000

6	-0.491120000	3.317457000	-0.248685000
8	-0.636238000	4.401701000	-0.780459000
8	-0.294661000	3.106521000	1.021157000

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5-Mn1

15	-2.240907000	-0.460220000	0.222423000
7	-0.048097000	0.434305000	1.721853000
6	1.140476000	0.753914000	2.540565000
6	-1.235135000	0.362272000	2.606880000
6	-2.289290000	-0.603695000	2.058925000
1	-3.274585000	-0.436631000	2.499060000
1	-1.982651000	-1.627707000	2.281809000
6	2.316474000	1.151499000	1.655235000
1	3.257610000	1.146514000	2.207105000
15	2.335953000	0.005359000	0.196656000
6	0.043694000	-0.304281000	-1.813166000
8	0.044134000	-0.225397000	-2.972140000
25	0.045923000	-0.395099000	-0.031879000
6	0.107203000	-2.146430000	-0.087549000
8	0.096159000	-3.309595000	-0.050629000
6	-3.321233000	-1.811572000	-0.499670000
1	-4.327269000	-1.385779000	-0.560169000
6	-2.858671000	-2.166035000	-1.922885000
1	-3.579724000	-2.847464000	-2.384491000
1	-2.767200000	-1.288089000	-2.564073000
1	-1.887938000	-2.664693000	-1.904998000
6	-3.389464000	-3.065073000	0.385818000
1	-3.832050000	-2.855411000	1.361869000
1	-4.011868000	-3.819523000	-0.105178000
1	-2.401201000	-3.503326000	0.540332000
6	3.431287000	-1.395014000	0.809655000
1	2.908511000	-1.679008000	1.731516000
6	3.465390000	-2.629724000	-0.106139000
1	3.869850000	-3.480379000	0.450996000
1	2.482833000	-2.912561000	-0.474994000
1	4.116190000	-2.469822000	-0.966955000
6	4.862065000	-0.964473000	1.167433000
1	5.388912000	-1.801895000	1.635463000
1	5.425167000	-0.685610000	0.272551000
1	4.897032000	-0.126175000	1.865377000
1	0.915829000	1.576872000	3.234078000
1	1.404087000	-0.113703000	3.163893000
1	2.160116000	2.162323000	1.275623000
1	-1.670660000	1.364025000	2.742826000

1	-0.933817000	0.026267000	3.606659000
6	3.325733000	0.940894000	-1.090109000
1	4.254304000	1.246311000	-0.595570000
6	2.576872000	2.203134000	-1.542450000
1	3.193025000	2.758114000	-2.255825000
1	1.643425000	1.943825000	-2.045539000
1	2.346493000	2.881012000	-0.718985000
6	3.670070000	0.064500000	-2.304323000
1	4.156437000	0.675579000	-3.070633000
1	4.353741000	-0.745287000	-2.050498000
1	2.771573000	-0.370356000	-2.749246000
6	-3.163272000	1.130640000	-0.147527000
1	-2.550626000	1.884586000	0.353316000
6	-4.577165000	1.213714000	0.444386000
1	-4.999994000	2.200730000	0.233061000
1	-5.248175000	0.472328000	0.002347000
1	-4.585402000	1.079721000	1.527639000
6	-3.176600000	1.434328000	-1.653140000
1	-3.540262000	2.451401000	-1.824019000
1	-2.186067000	1.352298000	-2.103683000
1	-3.845131000	0.752371000	-2.185774000
1	-0.252036000	2.084761000	1.133001000
1	-0.394296000	2.514753000	-0.941390000
6	-0.448838000	3.390745000	-0.272858000
8	-0.579795000	4.516729000	-0.685411000
8	-0.359104000	3.086243000	1.016537000

-1889.270285

1-Mn1-PF₃

25	0.019525000	-0.240338000	-0.066187000
15	-2.301882000	-0.369716000	-0.386247000
15	2.335787000	-0.390237000	-0.373459000
7	0.025449000	-1.931797000	-0.930960000
6	2.457063000	-2.007659000	-1.271248000
6	1.204763000	-2.806937000	-0.942629000
6	-1.175017000	-2.755206000	-1.103148000
6	-2.370541000	-1.882804000	-1.448962000
6	3.489694000	-0.584494000	1.093210000
6	3.239315000	0.725559000	-1.600713000
6	-3.455088000	-0.710970000	1.055235000
6	-3.237630000	0.874021000	-1.458379000
1	2.466009000	-1.775937000	-2.339084000
1	3.375495000	-2.547393000	-1.033220000
1	1.078304000	-3.602214000	-1.690291000
1	1.313670000	-3.312640000	0.028556000

1	-1.016233000	-3.481713000	-1.913002000
1	-1.373309000	-3.348106000	-0.197372000
1	-2.262469000	-1.532388000	-2.478690000
1	-3.322142000	-2.411622000	-1.366403000
15	-0.005982000	1.824231000	0.310958000
9	1.232211000	2.590934000	1.034712000
9	-0.226006000	2.980033000	-0.829111000
9	-1.109972000	2.459573000	1.327553000
6	0.013525000	-0.539237000	1.655490000
1	2.652832000	0.546313000	-2.509842000
6	4.685852000	0.274687000	-1.864520000
1	5.079282000	0.805602000	-2.736767000
1	5.335130000	0.516645000	-1.018920000
1	4.771478000	-0.795450000	-2.064223000
6	3.195713000	2.231704000	-1.317405000
1	2.181602000	2.625001000	-1.304541000
1	3.672616000	2.487516000	-0.369807000
1	3.737723000	2.757604000	-2.109943000
6	3.396157000	0.607199000	2.056471000
1	3.598002000	1.560306000	1.568018000
1	2.402219000	0.671456000	2.502127000
1	4.121786000	0.480647000	2.865958000
6	3.237013000	-1.904152000	1.841848000
1	3.918638000	-1.967832000	2.695889000
1	2.219360000	-1.961192000	2.229771000
1	3.415948000	-2.780342000	1.216505000
1	4.500361000	-0.624548000	0.675600000
6	-4.490786000	0.279757000	-2.125088000
1	-5.239331000	-0.009549000	-1.381753000
1	-4.950362000	1.037496000	-2.767441000
1	-4.277005000	-0.589139000	-2.747778000
6	-3.616475000	2.182890000	-0.749741000
1	-2.781419000	2.661712000	-0.245337000
1	-4.005282000	2.889707000	-1.488931000
1	-4.407841000	2.013751000	-0.014920000
1	-2.502785000	1.104704000	-2.238558000
1	-4.467452000	-0.633407000	0.643475000
6	-3.268464000	-2.131705000	1.612354000
1	-3.934316000	-2.274099000	2.469155000
1	-3.505336000	-2.904926000	0.879489000
1	-2.245412000	-2.289504000	1.962076000
6	-3.298940000	0.321427000	2.184124000
1	-4.103268000	0.181632000	2.913381000
1	-2.350960000	0.186251000	2.705706000
1	-3.335296000	1.350687000	1.832890000
8	0.006455000	-0.848439000	2.778883000

-2227.175111

2-Mn1-PF₃

25	0.003815000	-0.130356000	-0.165758000
15	-2.323170000	-0.394989000	-0.379831000
15	2.328649000	-0.404539000	-0.377091000
7	0.004662000	-2.054761000	-0.986758000
6	2.427217000	-2.075287000	-1.173881000
6	1.188106000	-2.858102000	-0.749705000
6	-1.189368000	-2.849633000	-0.776459000
6	-2.414409000	-2.049839000	-1.208552000
6	3.488256000	-0.539155000	1.100853000
6	3.246022000	0.654388000	-1.637238000
6	-3.479582000	-0.548246000	1.098786000
6	-3.247956000	0.691094000	-1.610219000
1	2.395957000	-1.913615000	-2.255047000
1	3.360674000	-2.587849000	-0.933981000
1	1.139150000	-3.789671000	-1.338936000
1	1.288979000	-3.176664000	0.306727000
1	-1.141015000	-3.773960000	-1.377236000
1	-1.308269000	-3.181354000	0.273939000
1	-2.356418000	-1.864015000	-2.284900000
1	-3.356277000	-2.561715000	-1.001955000
1	0.000940000	0.573111000	-1.876826000
1	0.007013000	-0.205266000	-1.961423000
15	0.006092000	1.890072000	0.411528000
9	1.210389000	2.566974000	1.261993000
9	-0.052251000	3.090085000	-0.699112000
9	-1.146997000	2.533451000	1.353642000
6	-0.005238000	-0.697339000	1.509154000
1	2.618884000	0.511096000	-2.525706000
6	4.659614000	0.145745000	-1.962984000
1	5.049278000	0.685055000	-2.831997000
1	5.349469000	0.328948000	-1.134925000
1	4.683917000	-0.920073000	-2.198276000
6	3.276359000	2.155158000	-1.322543000
1	2.281307000	2.577857000	-1.195748000
1	3.857019000	2.367152000	-0.422194000
1	3.754148000	2.688339000	-2.150571000
6	3.381415000	0.653504000	2.061145000
1	3.493333000	1.614472000	1.561681000
1	2.417072000	0.660164000	2.572313000
1	4.162822000	0.573827000	2.823507000
6	3.317831000	-1.854734000	1.879466000

1	4.045650000	-1.876831000	2.696950000
1	2.325318000	-1.937736000	2.323066000
1	3.492845000	-2.737629000	1.263942000
1	4.490963000	-0.543308000	0.661729000
6	-4.617963000	0.132486000	-2.029176000
1	-5.337993000	0.179072000	-1.207743000
1	-5.022006000	0.738922000	-2.845890000
1	-4.567560000	-0.899736000	-2.379852000
6	-3.381059000	2.160245000	-1.189755000
1	-2.425345000	2.617160000	-0.940880000
1	-3.814141000	2.735276000	-2.014162000
1	-4.048872000	2.270507000	-0.332193000
1	-2.580970000	0.646098000	-2.479919000
1	-4.483967000	-0.512303000	0.664168000
6	-3.339405000	-1.889780000	1.837813000
1	-4.064607000	-1.918196000	2.657404000
1	-3.537336000	-2.749725000	1.197353000
1	-2.347223000	-2.008104000	2.274935000
6	-3.338821000	0.611496000	2.095591000
1	-4.124097000	0.531010000	2.853929000
1	-2.376359000	0.573326000	2.608563000
1	-3.420705000	1.590474000	1.627094000
8	-0.016193000	-1.098327000	2.596594000

-2228.330497

TS1-Mn1-PF₃

25	0.014175000	-0.146937000	-0.125423000
15	-2.305772000	-0.379409000	-0.370925000
15	2.332128000	-0.392585000	-0.358006000
7	0.021910000	-2.076407000	-1.025479000
6	2.449727000	-2.060688000	-1.172254000
6	1.213061000	-2.865460000	-0.786367000
6	-1.193492000	-2.846928000	-0.861693000
6	-2.393757000	-2.001399000	-1.273246000
6	3.490528000	-0.524036000	1.117810000
6	3.242352000	0.663344000	-1.626845000
6	-3.466983000	-0.581553000	1.095874000
6	-3.232558000	0.757441000	-1.553811000
1	2.445865000	-1.889145000	-2.252328000
1	3.377849000	-2.574513000	-0.917171000
1	1.184490000	-3.790645000	-1.385068000
1	1.284440000	-3.180175000	0.270621000
1	-1.160022000	-3.751459000	-1.491380000
1	-1.315258000	-3.197960000	0.178652000
1	-2.312373000	-1.768071000	-2.338787000

1	-3.344265000	-2.512806000	-1.111707000
1	0.029085000	0.158685000	-1.827905000
1	0.031795000	-0.761854000	-1.744818000
15	-0.000313000	1.884746000	0.368714000
9	1.230467000	2.629672000	1.123487000
9	-0.160801000	3.030272000	-0.780148000
9	-1.117847000	2.532138000	1.354114000
6	-0.007496000	-0.682213000	1.571105000
1	2.634797000	0.476806000	-2.520543000
6	4.676318000	0.186254000	-1.908695000
1	5.064147000	0.700896000	-2.793266000
1	5.345530000	0.425330000	-1.077869000
1	4.738873000	-0.887202000	-2.098457000
6	3.223969000	2.173874000	-1.362321000
1	2.214525000	2.576879000	-1.307349000
1	3.747519000	2.433624000	-0.440051000
1	3.734939000	2.687513000	-2.182969000
6	3.370173000	0.680121000	2.061981000
1	3.514518000	1.632572000	1.553514000
1	2.387309000	0.707911000	2.535978000
1	4.122651000	0.599212000	2.852649000
6	3.305384000	-1.833702000	1.902144000
1	4.022734000	-1.855907000	2.728730000
1	2.307153000	-1.910739000	2.333725000
1	3.484574000	-2.720579000	1.292652000
1	4.497327000	-0.533851000	0.688831000
6	-4.533382000	0.153450000	-2.109949000
1	-5.280766000	0.015228000	-1.323502000
1	-4.964042000	0.839283000	-2.846351000
1	-4.381436000	-0.805772000	-2.606026000
6	-3.513051000	2.159789000	-0.995333000
1	-2.629396000	2.647321000	-0.589974000
1	-3.900168000	2.795698000	-1.797295000
1	-4.274952000	2.125844000	-0.212467000
1	-2.513355000	0.853609000	-2.375326000
1	-4.472304000	-0.508080000	0.666808000
6	-3.343773000	-1.954785000	1.776380000
1	-4.061135000	-2.007620000	2.601518000
1	-3.561371000	-2.783464000	1.101263000
1	-2.348848000	-2.105991000	2.198600000
6	-3.299284000	0.533963000	2.140051000
1	-4.085848000	0.440024000	2.895567000
1	-2.337952000	0.452842000	2.649830000
1	-3.358944000	1.532769000	1.712597000
8	-0.032354000	-1.064098000	2.666271000

-2228.325848

3-Mn1-PF₃

25	0.007747000	-0.120606000	-0.069154000
15	-2.275464000	-0.380878000	-0.372758000
15	2.288210000	-0.390697000	-0.370231000
7	0.010709000	-2.192010000	-0.976593000
6	2.432093000	-2.101965000	-1.118505000
6	1.241325000	-2.946975000	-0.683125000
6	-1.233477000	-2.936373000	-0.717556000
6	-2.405038000	-2.071616000	-1.165296000
6	3.493643000	-0.496458000	1.077506000
6	3.194638000	0.601083000	-1.692012000
6	-3.474933000	-0.517218000	1.077804000
6	-3.198815000	0.651914000	-1.649936000
1	2.414947000	-1.983298000	-2.206429000
1	3.377967000	-2.579242000	-0.860126000
1	1.240634000	-3.915316000	-1.201848000
1	1.262693000	-3.140153000	0.391212000
1	-1.233867000	-3.897028000	-1.250457000
1	-1.277803000	-3.145860000	0.352804000
1	-2.349216000	-1.921887000	-2.248069000
1	-3.362425000	-2.548704000	-0.952850000
1	0.021248000	0.349306000	-1.637659000
1	0.024857000	-1.943897000	-1.963557000
15	0.004665000	1.906818000	0.380238000
9	1.235218000	2.658357000	1.141774000
9	-0.105715000	3.045708000	-0.782046000
9	-1.128100000	2.609462000	1.319399000
6	-0.004047000	-0.651045000	1.632975000
1	2.577492000	0.373857000	-2.569149000
6	4.631578000	0.130892000	-1.965292000
1	5.006902000	0.613393000	-2.873296000
1	5.304661000	0.411144000	-1.150547000
1	4.708008000	-0.948851000	-2.111918000
6	3.155198000	2.119680000	-1.486100000
1	2.137083000	2.498805000	-1.429122000
1	3.689743000	2.423914000	-0.583639000
1	3.641848000	2.611702000	-2.334539000
6	3.405992000	0.735455000	1.988368000
1	3.537057000	1.672028000	1.447781000
1	2.435961000	0.780618000	2.486907000
1	4.180715000	0.676166000	2.759577000
6	3.303034000	-1.775407000	1.909514000
1	4.019799000	-1.773764000	2.736958000
1	2.304288000	-1.827373000	2.344286000

1	3.479180000	-2.686438000	1.334605000
1	4.491702000	-0.535018000	0.630266000
6	-4.555001000	0.073639000	-2.086323000
1	-5.289021000	0.116730000	-1.276950000
1	-4.953377000	0.670553000	-2.912923000
1	-4.492102000	-0.959798000	-2.431888000
6	-3.362213000	2.126759000	-1.260103000
1	-2.419974000	2.599209000	-0.992505000
1	-3.776829000	2.680936000	-2.108169000
1	-4.058226000	2.243724000	-0.425917000
1	-2.503537000	0.601532000	-2.495673000
1	-4.475952000	-0.506054000	0.634013000
6	-3.317697000	-1.833717000	1.856289000
1	-4.031592000	-1.846688000	2.686079000
1	-3.518402000	-2.716087000	1.246164000
1	-2.318966000	-1.926518000	2.285910000
6	-3.348717000	0.670075000	2.043992000
1	-4.136417000	0.607411000	2.801788000
1	-2.386135000	0.651604000	2.557501000
1	-3.432031000	1.635462000	1.547777000
8	-0.016091000	-0.947453000	2.761816000

-2228.363099

TS2-Mn1-PF₃

25	0.013086000	-0.289004000	-0.057050000
15	-2.275788000	-0.064841000	-0.369533000
15	2.308379000	-0.167257000	-0.444897000
7	0.008485000	-0.367749000	-2.280546000
6	2.446183000	-0.437259000	-2.297269000
6	1.173527000	-1.096249000	-2.821095000
6	-1.282132000	-0.804817000	-2.849754000
6	-2.391101000	0.038730000	-2.228603000
6	3.594509000	-1.393304000	0.175798000
6	3.130096000	1.520784000	-0.282009000
6	-3.501281000	-1.423472000	0.085002000
6	-3.150369000	1.511946000	0.173809000
1	2.568920000	0.542729000	-2.766808000
1	3.327998000	-1.029610000	-2.547339000
1	1.161222000	-1.089605000	-3.919055000
1	1.097553000	-2.134406000	-2.490685000
1	-1.279663000	-0.692631000	-3.941888000
1	-1.407523000	-1.865193000	-2.624431000
1	-2.229534000	1.086279000	-2.496086000
1	-3.376505000	-0.247477000	-2.598558000
1	0.026924000	1.389241000	-0.292484000

1	0.120644000	0.618113000	-2.518218000
15	0.030749000	0.143924000	1.983849000
9	1.347152000	0.010966000	2.929818000
9	-0.338448000	1.632525000	2.515593000
9	-0.935379000	-0.618336000	3.047856000
6	-0.067657000	-2.052374000	0.154319000
1	2.594410000	2.090644000	-1.049319000
6	4.622631000	1.531665000	-0.641084000
1	4.975051000	2.565360000	-0.710786000
1	5.223552000	1.033993000	0.123996000
1	4.825555000	1.049076000	-1.600798000
6	2.866035000	2.210045000	1.063095000
1	1.800003000	2.349989000	1.236562000
1	3.279850000	1.650952000	1.903526000
1	3.331543000	3.200559000	1.059707000
6	3.906163000	-1.272990000	1.672166000
1	4.245402000	-0.274700000	1.951736000
1	3.034380000	-1.512617000	2.281418000
1	4.703173000	-1.977232000	1.931787000
6	3.211661000	-2.838219000	-0.174756000
1	4.047282000	-3.501889000	0.068740000
1	2.345578000	-3.169998000	0.397376000
1	2.987883000	-2.974071000	-1.235439000
1	4.498613000	-1.138226000	-0.387028000
6	-4.381436000	1.875900000	-0.672376000
1	-5.158952000	1.109271000	-0.604881000
1	-4.813609000	2.808947000	-0.297622000
1	-4.144506000	2.027463000	-1.726476000
6	-3.527094000	1.511963000	1.663564000
1	-2.699779000	1.237071000	2.315176000
1	-3.848602000	2.517195000	1.951514000
1	-4.362151000	0.834142000	1.858564000
1	-2.379319000	2.272132000	0.023446000
1	-4.489105000	-0.955371000	0.009893000
6	-3.466952000	-2.619471000	-0.880899000
1	-4.206628000	-3.359400000	-0.559809000
1	-3.708986000	-2.345593000	-1.909264000
1	-2.491817000	-3.110081000	-0.868886000
6	-3.300630000	-1.924298000	1.524624000
1	-4.108154000	-2.617887000	1.780424000
1	-2.356227000	-2.461456000	1.619600000
1	-3.297534000	-1.125204000	2.262880000
8	-0.159517000	-3.203480000	0.303464000
6	0.008970000	2.978642000	-1.133514000
8	-0.090416000	3.697897000	-0.211168000
8	0.102404000	2.654547000	-2.268201000

-2417.011237

4-Mn1-PF₃

25	0.012552000	-0.245214000	-0.049710000
15	-2.319675000	-0.117733000	-0.353752000
15	2.336230000	-0.209724000	-0.431816000
7	-0.007130000	-0.753793000	-2.114977000
6	2.438406000	-0.783981000	-2.205469000
6	1.164694000	-1.543983000	-2.557347000
6	-1.282250000	-1.323984000	-2.607573000
6	-2.423585000	-0.406489000	-2.187765000
6	3.604188000	-1.326993000	0.388203000
6	3.145641000	1.484621000	-0.540509000
6	-3.498258000	-1.380389000	0.394222000
6	-3.206806000	1.529805000	-0.152988000
1	2.521257000	0.105125000	-2.835156000
1	3.324718000	-1.397150000	-2.376729000
1	1.113931000	-1.724128000	-3.638051000
1	1.128332000	-2.513280000	-2.055765000
1	-1.253683000	-1.421695000	-3.699538000
1	-1.394424000	-2.324648000	-2.186555000
1	-2.293168000	0.566886000	-2.667454000
1	-3.394414000	-0.801568000	-2.488601000
1	0.049332000	1.464189000	-0.689048000
1	0.080255000	0.188349000	-2.539019000
15	0.054060000	0.521566000	1.920814000
9	1.378715000	0.480253000	2.847326000
9	-0.279104000	2.071888000	2.216410000
9	-0.909488000	-0.074004000	3.071935000
6	-0.056939000	-1.913752000	0.526421000
1	2.623695000	1.918785000	-1.399642000
6	4.643540000	1.431636000	-0.875194000
1	4.996999000	2.439802000	-1.110232000
1	5.233383000	1.067660000	-0.030424000
1	4.857227000	0.798058000	-1.740176000
6	2.861613000	2.385464000	0.669265000
1	1.796893000	2.593058000	0.775095000
1	3.227395000	1.958480000	1.604236000
1	3.360852000	3.348038000	0.523801000
6	3.925355000	-0.962192000	1.842024000
1	4.259874000	0.069896000	1.952382000
1	3.060516000	-1.106013000	2.489450000
1	4.729427000	-1.610648000	2.203806000
6	3.220703000	-2.810179000	0.279177000
1	4.063429000	-3.422299000	0.614579000

1	2.366903000	-3.049580000	0.912717000
1	2.984466000	-3.116211000	-0.742254000
1	4.504883000	-1.167809000	-0.214006000
6	-4.479844000	1.649979000	-1.005736000
1	-5.243035000	0.927722000	-0.701197000
1	-4.906759000	2.648378000	-0.870505000
1	-4.291230000	1.519849000	-2.072068000
6	-3.517627000	1.879191000	1.309694000
1	-2.649056000	1.802367000	1.961318000
1	-3.869883000	2.913306000	1.360759000
1	-4.311842000	1.243807000	1.709381000
1	-2.470052000	2.249949000	-0.520228000
1	-4.494370000	-0.958094000	0.223644000
6	-3.440120000	-2.751441000	-0.298620000
1	-4.169034000	-3.417480000	0.172888000
1	-3.686841000	-2.702563000	-1.360299000
1	-2.458533000	-3.215907000	-0.188470000
6	-3.289882000	-1.549763000	1.906803000
1	-4.079293000	-2.192845000	2.307939000
1	-2.331655000	-2.024069000	2.119771000
1	-3.316332000	-0.607910000	2.451204000
8	-0.134472000	-3.015682000	0.879989000
6	-0.007765000	2.367989000	-1.494361000
8	-0.176017000	3.440437000	-0.939148000
8	0.121643000	1.986371000	-2.665987000

-2417.024436

1-Mn1-2PF₃

25	-0.010385000	-0.087032000	0.240281000
15	2.325129000	0.142447000	0.649768000
15	-2.302439000	0.174430000	0.685097000
7	-0.024325000	-0.872743000	1.959246000
6	-2.438191000	-0.692850000	2.322757000
6	-1.207498000	-1.574080000	2.479994000
6	1.184132000	-1.377345000	2.619043000
6	2.320667000	-0.387635000	2.424278000
6	-3.768031000	-0.512429000	-0.271799000
6	-2.841975000	1.912394000	1.206780000
6	3.697404000	-0.868691000	-0.140771000
6	3.042660000	1.889160000	0.775095000
1	-2.434701000	0.074045000	3.100240000
1	-3.371205000	-1.252140000	2.407999000
1	-1.067277000	-1.816344000	3.541011000
1	-1.342674000	-2.529338000	1.954940000
1	0.997064000	-1.500917000	3.694344000

1	1.454020000	-2.373447000	2.237616000
1	2.097144000	0.506024000	3.010779000
1	3.289664000	-0.775442000	2.745023000
15	0.073477000	1.308318000	-1.334372000
9	-1.178766000	1.610707000	-2.320442000
9	0.458100000	2.885748000	-1.124894000
9	1.141811000	1.110761000	-2.549804000
15	-0.153421000	-1.710069000	-1.026560000
9	1.079065000	-2.419828000	-1.810116000
9	-0.674147000	-3.099938000	-0.367712000
9	-1.140979000	-1.774962000	-2.314155000
1	-2.167253000	2.086455000	2.053034000
6	-4.288318000	1.958978000	1.726094000
1	-4.459444000	2.911225000	2.237211000
1	-5.005426000	1.898743000	0.903249000
1	-4.515373000	1.159632000	2.435506000
6	-2.597527000	3.032335000	0.189706000
1	-1.538904000	3.175306000	-0.013098000
1	-3.105699000	2.854404000	-0.758716000
1	-2.978883000	3.974311000	0.596543000
6	-3.930337000	0.109064000	-1.665743000
1	-4.079930000	1.188894000	-1.625811000
1	-3.061083000	-0.089687000	-2.293309000
1	-4.807116000	-0.326679000	-2.155278000
6	-3.763771000	-2.047472000	-0.357989000
1	-4.739359000	-2.380111000	-0.726005000
1	-3.013365000	-2.412903000	-1.055219000
1	-3.595886000	-2.530207000	0.606550000
1	-4.628541000	-0.226288000	0.340399000
6	4.159700000	2.019382000	1.825742000
1	5.020046000	1.392228000	1.574699000
1	4.510882000	3.055676000	1.847549000
1	3.836033000	1.764066000	2.834835000
6	3.539016000	2.482166000	-0.553398000
1	2.847889000	2.345952000	-1.381078000
1	3.693233000	3.557768000	-0.427135000
1	4.501084000	2.045654000	-0.832144000
1	2.176508000	2.470055000	1.109981000
1	4.619308000	-0.459941000	0.288776000
6	3.606848000	-2.352431000	0.251320000
1	4.415976000	-2.903956000	-0.236954000
1	3.706711000	-2.507926000	1.326533000
1	2.666341000	-2.795014000	-0.078439000
6	3.759566000	-0.716512000	-1.669458000
1	4.602327000	-1.301757000	-2.051107000
1	2.853147000	-1.090340000	-2.140380000

1 3.901590000 0.313490000 -1.988696000

-2754.901923

2-Mn1-2PF₃

25	0.002762000	0.050015000	0.251507000
15	2.355895000	0.039575000	0.669968000
15	-2.319346000	0.056743000	0.729974000
7	0.012820000	-1.200641000	1.921651000
6	-2.381236000	-1.008478000	2.252250000
6	-1.188765000	-1.959527000	2.211439000
6	1.215089000	-1.981144000	2.129933000
6	2.403178000	-1.026909000	2.188589000
6	-3.745380000	-0.613414000	-0.299184000
6	-2.965806000	1.692394000	1.423873000
6	3.741472000	-0.613377000	-0.429314000
6	3.066062000	1.665548000	1.322778000
1	-2.281258000	-0.342376000	3.113298000
1	-3.338250000	-1.528153000	2.335194000
1	-1.093489000	-2.447594000	3.195574000
1	-1.384222000	-2.773298000	1.490349000
1	1.152610000	-2.526021000	3.086219000
1	1.387142000	-2.755072000	1.355064000
1	2.260184000	-0.360052000	3.042421000
1	3.364765000	-1.529101000	2.304666000
1	0.015780000	1.497078000	1.308551000
1	0.031544000	0.875453000	1.796885000
15	-0.004054000	1.482032000	-1.291176000
9	-1.299824000	1.716114000	-2.234814000
9	0.241939000	3.070170000	-1.013830000
9	1.034124000	1.406342000	-2.531938000
15	-0.080847000	-1.531700000	-1.135138000
9	1.151411000	-1.968633000	-2.086748000
9	-0.431062000	-3.038211000	-0.676520000
9	-1.139021000	-1.481342000	-2.360802000
1	-2.305809000	1.823865000	2.289222000
6	-4.409917000	1.609527000	1.941315000
1	-4.632952000	2.497711000	2.540293000
1	-5.127571000	1.586266000	1.117153000
1	-4.582277000	0.733963000	2.571271000
6	-2.783723000	2.915230000	0.516625000
1	-1.737597000	3.111162000	0.289141000
1	-3.322193000	2.816064000	-0.427004000
1	-3.175002000	3.801860000	1.025557000
6	-3.942913000	0.122074000	-1.631119000
1	-4.123446000	1.188942000	-1.493781000

1	-3.076568000	0.007193000	-2.281231000
1	-4.813123000	-0.295819000	-2.147062000
6	-3.688264000	-2.135044000	-0.513529000
1	-4.642274000	-2.461627000	-0.939213000
1	-2.908174000	-2.424341000	-1.214003000
1	-3.537104000	-2.688762000	0.414071000
1	-4.614524000	-0.418151000	0.336076000
6	4.315574000	1.493006000	2.203176000
1	5.168377000	1.124911000	1.626544000
1	4.602541000	2.466433000	2.613403000
1	4.157501000	0.817420000	3.044362000
6	3.344591000	2.714152000	0.236687000
1	2.499082000	2.883210000	-0.427310000
1	3.581904000	3.671029000	0.711681000
1	4.209040000	2.432072000	-0.368929000
1	2.253122000	2.035999000	1.956750000
1	4.645282000	-0.221913000	0.048924000
6	3.853170000	-2.146661000	-0.430999000
1	4.672985000	-2.441210000	-1.093698000
1	4.071328000	-2.551998000	0.557914000
1	2.947013000	-2.621734000	-0.804292000
6	3.691714000	-0.068626000	-1.866156000
1	4.635860000	-0.304206000	-2.367754000
1	2.887205000	-0.527626000	-2.437362000
1	3.551862000	1.010334000	-1.908888000

-2756.055601

TS1-Mn1-2PF₃

25	-0.004753000	0.025227000	0.241752000
15	2.336394000	0.052390000	0.657640000
15	-2.325333000	0.073966000	0.698908000
7	-0.010668000	-1.156157000	1.993033000
6	-2.417627000	-0.967407000	2.242304000
6	-1.218052000	-1.910595000	2.267621000
6	1.213353000	-1.882171000	2.260882000
6	2.374900000	-0.893179000	2.257691000
6	-3.748038000	-0.592950000	-0.335740000
6	-2.965449000	1.718923000	1.376425000
6	3.723317000	-0.707940000	-0.366820000
6	3.055346000	1.721492000	1.181332000
1	-2.358233000	-0.284817000	3.093999000
1	-3.368292000	-1.500136000	2.305083000
1	-1.151188000	-2.376181000	3.263882000
1	-1.371084000	-2.732158000	1.548899000
1	1.158887000	-2.366767000	3.248839000

1	1.396920000	-2.689606000	1.528252000
1	2.206511000	-0.167563000	3.057231000
1	3.343408000	-1.364933000	2.428492000
1	0.007734000	1.197116000	1.479831000
1	-0.002234000	0.403298000	1.902972000
15	0.033863000	1.488173000	-1.258619000
9	-1.225966000	1.765919000	-2.239001000
9	0.296989000	3.059651000	-0.929228000
9	1.119167000	1.429350000	-2.463454000
15	-0.095528000	-1.558004000	-1.142799000
9	1.134906000	-2.051400000	-2.075331000
9	-0.485713000	-3.052070000	-0.655190000
9	-1.137350000	-1.513951000	-2.385811000
1	-2.310823000	1.848248000	2.245986000
6	-4.416391000	1.650833000	1.877333000
1	-4.637641000	2.543290000	2.470580000
1	-5.124626000	1.632165000	1.044864000
1	-4.606461000	0.779592000	2.508318000
6	-2.762114000	2.937366000	0.468150000
1	-1.709802000	3.134149000	0.275337000
1	-3.271944000	2.833398000	-0.490811000
1	-3.171630000	3.824417000	0.961968000
6	-3.919326000	0.138588000	-1.673903000
1	-4.106578000	1.205099000	-1.541985000
1	-3.038549000	0.024950000	-2.305097000
1	-4.776470000	-0.282935000	-2.208404000
6	-3.701373000	-2.116101000	-0.540654000
1	-4.661610000	-2.440822000	-0.953494000
1	-2.930378000	-2.413416000	-1.247572000
1	-3.542637000	-2.665214000	0.388852000
1	-4.623147000	-0.385325000	0.287117000
6	4.245641000	1.610995000	2.149902000
1	5.103531000	1.121963000	1.679646000
1	4.567793000	2.616336000	2.439164000
1	4.006157000	1.068816000	3.064877000
6	3.440160000	2.640455000	0.011477000
1	2.667116000	2.727356000	-0.749076000
1	3.635307000	3.646258000	0.395337000
1	4.357788000	2.293169000	-0.469150000
1	2.214101000	2.176724000	1.714470000
1	4.628971000	-0.319950000	0.112659000
6	3.775364000	-2.241839000	-0.277190000
1	4.619351000	-2.603195000	-0.872991000
1	3.919696000	-2.598954000	0.743374000
1	2.873770000	-2.703149000	-0.678699000
6	3.729864000	-0.250539000	-1.835377000

1	4.662890000	-0.580321000	-2.303646000
1	2.904716000	-0.689261000	-2.392388000
1	3.665480000	0.829837000	-1.947162000

-2756.052544

3-Mn1-2PF₃

25	0.014067000	0.026024000	0.166743000
15	2.305923000	0.089984000	0.660475000
15	-2.253924000	0.117180000	0.728471000
7	0.024502000	-1.179487000	2.098465000
6	-2.373091000	-0.931634000	2.282367000
6	-1.224023000	-1.931160000	2.325118000
6	1.271152000	-1.947204000	2.271490000
6	2.418448000	-0.947604000	2.219723000
6	-3.726325000	-0.551323000	-0.244422000
6	-2.872875000	1.761576000	1.425476000
6	3.702873000	-0.595399000	-0.407772000
6	3.030248000	1.716059000	1.299465000
1	-2.300318000	-0.257721000	3.141487000
1	-3.340481000	-1.430231000	2.348623000
1	-1.195458000	-2.449489000	3.292751000
1	-1.313149000	-2.682836000	1.540603000
1	1.269374000	-2.485286000	3.228825000
1	1.335152000	-2.685762000	1.470196000
1	2.319193000	-0.262828000	3.067051000
1	3.390272000	-1.431410000	2.313662000
1	0.028989000	1.270959000	1.150746000
1	0.044398000	-0.421060000	2.777817000
15	-0.013272000	1.426566000	-1.371030000
9	-1.351957000	1.722773000	-2.244493000
9	0.297066000	3.003331000	-1.112576000
9	0.953614000	1.336078000	-2.675382000
15	-0.085855000	-1.601484000	-1.139932000
9	1.106009000	-2.086077000	-2.147303000
9	-0.412415000	-3.135066000	-0.638265000
9	-1.187978000	-1.623512000	-2.345869000
1	-2.192972000	1.880375000	2.276920000
6	-4.314834000	1.724184000	1.953015000
1	-4.508200000	2.623212000	2.546422000
1	-5.038793000	1.716360000	1.133978000
1	-4.513822000	0.859709000	2.591152000
6	-2.660083000	2.972086000	0.509877000
1	-1.607748000	3.121763000	0.279498000
1	-3.210514000	2.886349000	-0.428618000
1	-3.017212000	3.873995000	1.017710000

6	-3.915349000	0.141964000	-1.599907000
1	-4.015558000	1.223748000	-1.503946000
1	-3.075757000	-0.059188000	-2.264364000
1	-4.825735000	-0.236024000	-2.076185000
6	-3.708906000	-2.079282000	-0.414565000
1	-4.660675000	-2.392908000	-0.855247000
1	-2.919423000	-2.409628000	-1.085465000
1	-3.601277000	-2.613546000	0.531368000
1	-4.584354000	-0.311427000	0.390795000
6	4.285921000	1.562820000	2.174738000
1	5.134232000	1.179513000	1.601126000
1	4.577419000	2.545904000	2.558051000
1	4.138969000	0.910762000	3.036423000
6	3.305788000	2.751016000	0.200031000
1	2.459197000	2.906161000	-0.464170000
1	3.538282000	3.714924000	0.663525000
1	4.173156000	2.465245000	-0.400125000
1	2.207371000	2.085696000	1.920365000
1	4.616633000	-0.211411000	0.057663000
6	3.783956000	-2.130139000	-0.394266000
1	4.592531000	-2.451751000	-1.058156000
1	4.001471000	-2.532899000	0.596730000
1	2.865987000	-2.587735000	-0.761597000
6	3.641294000	-0.072497000	-1.852080000
1	4.554557000	-0.366643000	-2.379623000
1	2.793525000	-0.493550000	-2.389262000
1	3.560270000	1.012269000	-1.909068000

-2756.097803

TS2-Mn1-2PF₃

25	0.000050000	-0.074962000	-0.077208000
15	-2.326378000	0.208648000	-0.472446000
15	2.326240000	0.209314000	-0.472445000
7	-0.000023000	0.021877000	-2.308156000
6	2.411840000	0.283672000	-2.339350000
6	1.238528000	-0.481056000	-2.939185000
6	-1.238604000	-0.480889000	-2.939265000
6	-2.411850000	0.283854000	-2.339306000
6	3.714252000	-1.010604000	-0.097500000
6	3.084202000	1.886403000	-0.049334000
6	-3.714226000	-1.011658000	-0.097955000
6	-3.084524000	1.885451000	-0.048556000
1	2.341988000	1.335841000	-2.628823000
1	3.366785000	-0.091537000	-2.708707000
1	1.200627000	-0.333486000	-4.026098000

1	1.309971000	-1.553609000	-2.750554000
1	-1.200670000	-0.333175000	-4.026157000
1	-1.310202000	-1.553482000	-2.750855000
1	-2.341673000	1.336132000	-2.628299000
1	-3.366827000	-0.090920000	-2.708992000
1	0.000551000	1.586247000	-0.198959000
1	0.000008000	1.035336000	-2.435172000
15	-0.000446000	0.176660000	2.007175000
9	1.189674000	-0.419642000	2.931603000
9	0.001293000	1.625709000	2.724710000
9	-1.193623000	-0.415923000	2.930103000
15	0.001012000	-2.155338000	0.141243000
9	-1.169525000	-2.934973000	0.955724000
9	0.005352000	-3.192887000	-1.121001000
9	1.169115000	-2.932354000	0.961635000
1	2.485736000	2.554959000	-0.675503000
6	4.550985000	2.044659000	-0.478584000
1	4.829725000	3.100880000	-0.417089000
1	5.223646000	1.493977000	0.183722000
1	4.734176000	1.716051000	-1.504777000
6	2.886800000	2.322623000	1.406480000
1	1.834979000	2.439746000	1.651235000
1	3.335925000	1.623158000	2.114338000
1	3.365438000	3.294987000	1.559087000
6	3.888088000	-1.270585000	1.404700000
1	4.097562000	-0.353413000	1.957155000
1	3.001344000	-1.730079000	1.837889000
1	4.733629000	-1.948189000	1.560142000
6	3.623650000	-2.324020000	-0.891927000
1	4.523010000	-2.914491000	-0.690660000
1	2.770964000	-2.933034000	-0.602451000
1	3.583315000	-2.162060000	-1.970915000
1	4.606807000	-0.492915000	-0.459617000
6	-4.551279000	2.043924000	-0.477809000
1	-5.223977000	1.492620000	0.183939000
1	-4.830140000	3.100063000	-0.415437000
1	-4.734297000	1.716166000	-1.504307000
6	-2.887226000	2.320898000	1.407512000
1	-1.835403000	2.437665000	1.652501000
1	-3.365610000	3.293321000	1.560526000
1	-3.336640000	1.621191000	2.114936000
1	-2.486061000	2.554332000	-0.674364000
1	-4.606982000	-0.493404000	-0.458757000
6	-3.624427000	-2.324094000	-0.894116000
1	-4.523157000	-2.915222000	-0.691958000
1	-3.586134000	-2.160766000	-1.972968000

1	-2.770941000	-2.933059000	-0.606870000
6	-3.887028000	-1.273483000	1.404045000
1	-4.733305000	-1.950215000	1.559280000
1	-3.000491000	-1.734714000	1.835804000
1	-4.094746000	-0.356825000	1.957990000
6	-0.000891000	3.166302000	-0.787884000
8	-0.000740000	3.015934000	-1.967928000
8	-0.001355000	3.796043000	0.207598000

-2944.740780

4-Mn1-2PF₃

25	0.000077000	-0.042600000	-0.105786000
15	-2.355312000	0.209673000	-0.480958000
15	2.355297000	0.209662000	-0.481088000
7	-0.000012000	-0.023160000	-2.248087000
6	2.418269000	0.245512000	-2.343407000
6	1.232098000	-0.532615000	-2.896995000
6	-1.232172000	-0.532592000	-2.896910000
6	-2.418268000	0.245610000	-2.343277000
6	3.724853000	-1.017067000	-0.076489000
6	3.106159000	1.891748000	-0.073609000
6	-3.724806000	-1.017188000	-0.076550000
6	-3.106218000	1.891726000	-0.073426000
1	2.341040000	1.290407000	-2.653824000
1	3.365519000	-0.142555000	-2.719019000
1	1.164443000	-0.400477000	-3.983397000
1	1.313601000	-1.602470000	-2.696994000
1	-1.164581000	-0.400483000	-3.983322000
1	-1.313708000	-1.602442000	-2.696887000
1	-2.340941000	1.290506000	-2.653660000
1	-3.365547000	-0.142370000	-2.718905000
1	0.000183000	1.732233000	-0.287501000
1	-0.000037000	1.001103000	-2.397537000
15	0.000061000	0.241896000	2.000207000
9	1.190478000	-0.360851000	2.908838000
9	0.000070000	1.689254000	2.700295000
9	-1.190547000	-0.360748000	2.908698000
15	0.000021000	-2.115684000	0.187818000
9	-1.170511000	-2.861362000	1.014201000
9	0.000210000	-3.152806000	-1.059167000
9	1.170425000	-2.861345000	1.014470000
1	2.524461000	2.554231000	-0.720941000
6	4.581577000	2.027142000	-0.480231000
1	4.866698000	3.082041000	-0.432417000
1	5.239109000	1.482369000	0.201908000

1	4.776882000	1.680899000	-1.498474000
6	2.880559000	2.351969000	1.371394000
1	1.827431000	2.529333000	1.573236000
1	3.269963000	1.642564000	2.104333000
1	3.398759000	3.302656000	1.528475000
6	3.902079000	-1.242048000	1.430740000
1	4.119982000	-0.312923000	1.959353000
1	3.015241000	-1.686230000	1.879069000
1	4.744359000	-1.920563000	1.597706000
6	3.627604000	-2.345096000	-0.845411000
1	4.530667000	-2.928765000	-0.642014000
1	2.780219000	-2.951735000	-0.536184000
1	3.576518000	-2.203022000	-1.926533000
1	4.618141000	-0.510398000	-0.451884000
6	-4.581639000	2.027046000	-0.480072000
1	-5.239121000	1.482244000	0.202096000
1	-4.866836000	3.081925000	-0.432280000
1	-4.776943000	1.680775000	-1.498306000
6	-2.880719000	2.352007000	1.371552000
1	-1.827599000	2.529181000	1.573570000
1	-3.398744000	3.302821000	1.528445000
1	-3.270409000	1.642734000	2.104474000
1	-2.524518000	2.554213000	-0.720754000
1	-4.618111000	-0.510486000	-0.451867000
6	-3.627521000	-2.345110000	-0.845660000
1	-4.530622000	-2.928768000	-0.642396000
1	-3.576356000	-2.202909000	-1.926759000
1	-2.780185000	-2.951821000	-0.536432000
6	-3.902033000	-1.242407000	1.430643000
1	-4.744288000	-1.920979000	1.597511000
1	-3.015184000	-1.686618000	1.878928000
1	-4.119998000	-0.313356000	1.959368000
6	-0.000058000	2.846530000	-0.810745000
8	-0.000345000	2.789669000	-2.044614000
8	0.000091000	3.715428000	0.039127000

-2944.748755

1-Mn1-PH₃

25	0.007234000	0.036727000	-0.022385000
15	-2.302023000	0.001033000	-0.349832000
15	2.312563000	-0.007482000	-0.350846000
7	0.010122000	-1.278638000	-1.423633000
6	2.447726000	-1.220585000	-1.750771000
6	1.193932000	-2.086456000	-1.729443000
6	-1.183166000	-2.054175000	-1.768779000

6	-2.415777000	-1.159712000	-1.793961000
6	3.451921000	-0.683266000	0.981815000
6	3.259099000	1.448019000	-1.105083000
6	-3.442241000	-0.722073000	0.957045000
6	-3.256441000	1.483483000	-1.036040000
1	2.461466000	-0.631707000	-2.672007000
1	3.366713000	-1.809541000	-1.712547000
1	1.081054000	-2.575278000	-2.709678000
1	1.308139000	-2.901310000	-0.994863000
1	-1.061978000	-2.521220000	-2.758812000
1	-1.328411000	-2.884652000	-1.057702000
1	-2.379582000	-0.534392000	-2.690518000
1	-3.349990000	-1.725835000	-1.811643000
15	-0.001213000	1.996090000	1.098480000
1	1.081657000	2.310268000	1.960237000
1	-0.091564000	3.301401000	0.524030000
1	-1.016196000	2.212228000	2.066606000
6	0.004148000	-0.792996000	1.498591000
1	2.663425000	1.638330000	-2.006243000
6	4.690489000	1.097055000	-1.541705000
1	5.104833000	1.913972000	-2.141513000
1	5.347429000	0.965193000	-0.677445000
1	4.737351000	0.187954000	-2.144349000
6	3.260193000	2.737412000	-0.275094000
1	2.253496000	3.074009000	-0.031217000
1	3.820192000	2.622960000	0.655711000
1	3.741767000	3.538622000	-0.845235000
6	3.301675000	0.107297000	2.290755000
1	3.488094000	1.174333000	2.159910000
1	2.297581000	-0.011787000	2.702365000
1	4.014700000	-0.264941000	3.033504000
6	3.204270000	-2.180302000	1.227932000
1	3.864037000	-2.531595000	2.028140000
1	2.176122000	-2.367213000	1.540258000
1	3.410559000	-2.785510000	0.343307000
1	4.474646000	-0.564455000	0.610898000
6	-4.607062000	1.119325000	-1.674886000
1	-5.321823000	0.772566000	-0.922991000
1	-5.040811000	2.006575000	-2.147934000
1	-4.521710000	0.347847000	-2.441199000
6	-3.453616000	2.643522000	-0.050289000
1	-2.530701000	2.950180000	0.439754000
1	-3.845538000	3.514907000	-0.584536000
1	-4.180730000	2.386632000	0.723645000
1	-2.579906000	1.826380000	-1.828519000
1	-4.465236000	-0.572877000	0.595742000

6	-3.208744000	-2.230847000	1.135693000
1	-3.867905000	-2.611755000	1.922654000
1	-3.422014000	-2.794508000	0.225952000
1	-2.180078000	-2.437562000	1.436516000
6	-3.276405000	0.002214000	2.303039000
1	-4.003840000	-0.386242000	3.023302000
1	-2.279201000	-0.167082000	2.711636000
1	-3.430194000	1.078833000	2.225922000
8	-0.000932000	-1.450443000	2.474247000

-1929.211361

2-Mn1-PH₃

25	0.004834000	0.143060000	-0.049583000
15	-2.300707000	-0.001682000	-0.347924000
15	2.307385000	-0.012210000	-0.347350000
7	0.005382000	-1.318249000	-1.564265000
6	2.437568000	-1.287796000	-1.690312000
6	1.184469000	-2.158600000	-1.615645000
6	-1.183188000	-2.143813000	-1.630045000
6	-2.424107000	-1.256799000	-1.709717000
6	3.462402000	-0.619815000	1.010046000
6	3.232027000	1.429486000	-1.142849000
6	-3.452044000	-0.628056000	1.005576000
6	-3.238531000	1.449240000	-1.109222000
1	2.435236000	-0.743406000	-2.639353000
1	3.362840000	-1.865132000	-1.633351000
1	1.157448000	-2.814820000	-2.504653000
1	1.262290000	-2.842617000	-0.743827000
1	-1.157377000	-2.794949000	-2.522886000
1	-1.276199000	-2.831898000	-0.763134000
1	-2.397651000	-0.697735000	-2.650001000
1	-3.358008000	-1.822009000	-1.677299000
1	0.015041000	1.497360000	-1.298606000
1	0.004853000	0.834565000	-1.713675000
15	0.006793000	1.906441000	1.369023000
1	1.086039000	2.116705000	2.265020000
1	-0.052672000	3.256133000	0.916477000
1	-1.017242000	2.045660000	2.340435000
6	-0.002024000	-0.977967000	1.298745000
1	2.613286000	1.609607000	-2.030526000
6	4.655085000	1.091749000	-1.613312000
1	5.050827000	1.914238000	-2.218244000
1	5.334049000	0.958977000	-0.766353000
1	4.691476000	0.186018000	-2.221894000
6	3.234996000	2.716353000	-0.307757000

1	2.231473000	3.015790000	-0.002445000
1	3.849891000	2.612213000	0.589648000
1	3.658212000	3.537832000	-0.894963000
6	3.252738000	0.157659000	2.318499000
1	3.356082000	1.236379000	2.191287000
1	2.260966000	-0.041102000	2.730073000
1	3.992030000	-0.159894000	3.060953000
6	3.329258000	-2.129170000	1.271153000
1	4.030146000	-2.420132000	2.060757000
1	2.325202000	-2.389519000	1.607395000
1	3.560533000	-2.729458000	0.390018000
1	4.477697000	-0.429753000	0.648331000
6	-4.623938000	1.092599000	-1.670362000
1	-5.328962000	0.846134000	-0.871460000
1	-5.036050000	1.951404000	-2.210595000
1	-4.591776000	0.251056000	-2.364362000
6	-3.337148000	2.675281000	-0.192367000
1	-2.369065000	2.976288000	0.209619000
1	-3.740292000	3.525868000	-0.751307000
1	-4.012941000	2.491406000	0.646866000
1	-2.585635000	1.709174000	-1.951536000
1	-4.467487000	-0.406639000	0.661794000
6	-3.346487000	-2.146493000	1.222918000
1	-4.040064000	-2.445139000	2.016067000
1	-3.603936000	-2.717105000	0.329506000
1	-2.342357000	-2.435727000	1.535330000
6	-3.212472000	0.106718000	2.333951000
1	-3.955296000	-0.212527000	3.072248000
1	-2.224152000	-0.130824000	2.731888000
1	-3.287723000	1.190803000	2.238656000
8	-0.010367000	-1.724207000	2.199437000

-1930.371047

TS1-Mn1-PH₃

25	-0.000034000	0.120367000	-0.033629000
15	-2.301032000	-0.004669000	-0.333067000
15	2.300989000	-0.004633000	-0.333040000
7	-0.000035000	-1.360834000	-1.571219000
6	2.436346000	-1.270080000	-1.692991000
6	1.201713000	-2.167514000	-1.638519000
6	-1.201782000	-2.167511000	-1.638629000
6	-2.436436000	-1.270101000	-1.693038000
6	3.452528000	-0.622226000	1.021767000
6	3.238908000	1.429574000	-1.126155000
6	-3.452583000	-0.622276000	1.021720000

6	-3.238870000	1.429556000	-1.126247000
1	2.434395000	-0.714986000	-2.635917000
1	3.365425000	-1.840933000	-1.643565000
1	1.187723000	-2.812289000	-2.534307000
1	1.275657000	-2.847676000	-0.768786000
1	-1.187762000	-2.812196000	-2.534481000
1	-1.275744000	-2.847767000	-0.768968000
1	-2.434562000	-0.714990000	-2.635954000
1	-3.365491000	-1.840991000	-1.643579000
1	-0.000071000	1.004478000	-1.549289000
1	-0.000043000	0.088092000	-1.782904000
15	-0.000070000	1.973295000	1.252392000
1	1.050836000	2.214454000	2.174650000
1	0.000701000	3.284491000	0.698864000
1	-1.051759000	2.215266000	2.173541000
6	-0.000001000	-0.934830000	1.375054000
1	2.603687000	1.637576000	-1.995459000
6	4.647116000	1.072847000	-1.627625000
1	5.051381000	1.904391000	-2.214290000
1	5.335713000	0.901604000	-0.795444000
1	4.657335000	0.185578000	-2.263128000
6	3.289790000	2.700763000	-0.269443000
1	2.301830000	3.015588000	0.065633000
1	3.925390000	2.567197000	0.609552000
1	3.715461000	3.523098000	-0.853549000
6	3.230792000	0.152236000	2.330747000
1	3.342307000	1.230596000	2.207637000
1	2.232309000	-0.040496000	2.727834000
1	3.958593000	-0.172157000	3.081585000
6	3.313119000	-2.132250000	1.273076000
1	4.003721000	-2.430785000	2.068777000
1	2.304441000	-2.391406000	1.596821000
1	3.553681000	-2.727868000	0.390739000
1	4.470740000	-0.431356000	0.668508000
6	-4.647421000	1.073053000	-1.626913000
1	-5.335792000	0.902912000	-0.794319000
1	-5.051500000	1.904248000	-2.214198000
1	-4.658292000	0.185193000	-2.261586000
6	-3.288925000	2.701146000	-0.270083000
1	-2.300656000	3.015968000	0.064083000
1	-3.714905000	3.523270000	-0.854262000
1	-3.923882000	2.568119000	0.609456000
1	-2.603985000	1.637004000	-1.995928000
1	-4.470793000	-0.431513000	0.668405000
6	-3.313044000	-2.132282000	1.273054000
1	-4.003457000	-2.430826000	2.068916000

1	-3.553779000	-2.727923000	0.390777000
1	-2.304291000	-2.391400000	1.596585000
6	-3.230967000	0.152277000	2.330667000
1	-3.958668000	-0.172244000	3.081545000
1	-2.232426000	-0.040198000	2.727737000
1	-3.342738000	1.230606000	2.207505000
8	0.000045000	-1.652156000	2.300888000

-1930.365392

3-Mn1-PH₃

25	0.004935000	0.108622000	0.039089000
15	-2.255407000	0.033820000	-0.337615000
15	2.261624000	0.014720000	-0.341810000
7	0.002977000	-1.394986000	-1.611343000
6	2.431958000	-1.269557000	-1.698760000
6	1.231272000	-2.209044000	-1.643356000
6	-1.240411000	-2.184082000	-1.661138000
6	-2.421288000	-1.220651000	-1.721229000
6	3.494519000	-0.609463000	0.944279000
6	3.151235000	1.455686000	-1.176703000
6	-3.472595000	-0.611198000	0.955521000
6	-3.163775000	1.487221000	-1.128393000
1	2.431846000	-0.736187000	-2.654802000
1	3.372322000	-1.819423000	-1.635788000
1	1.230320000	-2.892286000	-2.504551000
1	1.246800000	-2.812456000	-0.733123000
1	-1.244814000	-2.860794000	-2.527503000
1	-1.276841000	-2.793902000	-0.755934000
1	-2.387264000	-0.664580000	-2.663848000
1	-3.373330000	-1.752777000	-1.693555000
1	0.012052000	1.219916000	-1.211914000
1	0.014468000	-0.775504000	-2.419120000
15	0.018119000	1.838884000	1.460384000
1	1.102534000	2.053475000	2.353693000
1	-0.045159000	3.184380000	1.008232000
1	-0.990602000	1.983342000	2.451509000
6	-0.010127000	-1.047452000	1.368951000
1	2.556600000	1.547325000	-2.092803000
6	4.612765000	1.188748000	-1.562889000
1	4.976988000	1.990045000	-2.214496000
1	5.262175000	1.168755000	-0.683141000
1	4.741029000	0.244636000	-2.098455000
6	3.016511000	2.783064000	-0.422273000
1	1.970847000	3.026082000	-0.234978000
1	3.549746000	2.770329000	0.531884000

1	3.444793000	3.594528000	-1.020269000
6	3.390690000	0.205603000	2.241145000
1	3.537206000	1.274974000	2.079099000
1	2.410219000	0.065624000	2.701953000
1	4.149363000	-0.128257000	2.956672000
6	3.314406000	-2.104566000	1.252806000
1	4.043157000	-2.408101000	2.012007000
1	2.319817000	-2.313424000	1.648246000
1	3.478512000	-2.737721000	0.378250000
1	4.492524000	-0.471931000	0.516921000
6	-4.585018000	1.183363000	-1.625414000
1	-5.279964000	1.045997000	-0.792136000
1	-4.957094000	2.025113000	-2.219084000
1	-4.632413000	0.291559000	-2.254223000
6	-3.159138000	2.754356000	-0.264653000
1	-2.153432000	3.025714000	0.055696000
1	-3.561746000	3.595801000	-0.838251000
1	-3.787454000	2.639568000	0.622483000
1	-2.519245000	1.676112000	-1.994316000
1	-4.478087000	-0.403214000	0.576820000
6	-3.352941000	-2.127543000	1.178742000
1	-4.063108000	-2.437288000	1.952790000
1	-3.582101000	-2.705046000	0.280928000
1	-2.353995000	-2.401229000	1.521522000
6	-3.279622000	0.124406000	2.290046000
1	-4.029017000	-0.210196000	3.015049000
1	-2.291826000	-0.092290000	2.701322000
1	-3.373900000	1.207041000	2.192323000
8	-0.027732000	-1.783632000	2.289076000

-1930.401285

TS2-Mn1-PH₃

25	-0.012485000	-0.299675000	-0.122252000
15	2.262568000	-0.048530000	0.168737000
15	-2.281651000	-0.043934000	0.186662000
7	-0.007108000	-0.181770000	2.059851000
6	-2.457539000	-0.071429000	2.049979000
6	-1.233437000	-0.756792000	2.648404000
6	1.226178000	-0.746357000	2.642070000
6	2.442739000	-0.056001000	2.031736000
6	-3.559930000	-1.307617000	-0.381308000
6	-3.083443000	1.630381000	-0.175663000
6	3.489887000	-1.369879000	-0.393809000
6	3.117632000	1.591670000	-0.246606000
1	-2.502720000	0.966450000	2.392921000

1	-3.379367000	-0.557861000	2.373859000
1	-1.230052000	-0.647834000	3.741929000
1	-1.238565000	-1.824961000	2.419701000
1	1.230262000	-0.627078000	3.734488000
1	1.235752000	-1.816373000	2.422846000
1	2.482837000	0.984798000	2.365592000
1	3.367332000	-0.535376000	2.356835000
1	-0.123434000	1.427461000	-0.105873000
1	-0.012067000	0.822838000	2.231052000
15	-0.016826000	-0.300862000	-2.386128000
1	-0.020404000	-1.558874000	-3.053535000
1	-1.060894000	0.276995000	-3.161789000
1	1.042525000	0.255992000	-3.149913000
6	0.004685000	-2.054796000	-0.147365000
1	-2.551071000	2.271620000	0.535014000
6	-4.580897000	1.719557000	0.149442000
1	-4.908776000	2.761989000	0.084023000
1	-5.181905000	1.146963000	-0.561849000
1	-4.812650000	1.362272000	1.156982000
6	-2.785844000	2.173717000	-1.577048000
1	-1.718013000	2.155287000	-1.783820000
1	-3.310041000	1.607112000	-2.350896000
1	-3.122519000	3.212902000	-1.648235000
6	-3.454468000	-1.555520000	-1.892929000
1	-3.634101000	-0.651847000	-2.478679000
1	-2.467073000	-1.941984000	-2.155423000
1	-4.191508000	-2.302783000	-2.203766000
6	-3.456663000	-2.636800000	0.382273000
1	-4.272176000	-3.297549000	0.070451000
1	-2.516500000	-3.146484000	0.171559000
1	-3.539045000	-2.509601000	1.463528000
1	-4.540359000	-0.872975000	-0.169166000
6	4.606378000	1.676925000	0.120461000
1	5.221527000	1.056000000	-0.535756000
1	4.951581000	2.709078000	0.002954000
1	4.801425000	1.379562000	1.154909000
6	2.886764000	2.049533000	-1.691864000
1	1.829479000	2.049639000	-1.945060000
1	3.261700000	3.069567000	-1.821211000
1	3.421508000	1.413639000	-2.401657000
1	2.584182000	2.284915000	0.411597000
1	4.484566000	-0.931108000	-0.294899000
6	3.443949000	-2.639722000	0.469957000
1	4.248643000	-3.315444000	0.161865000
1	3.583798000	-2.436348000	1.532856000
1	2.498866000	-3.170127000	0.346671000

6	3.263087000	-1.738217000	-1.867121000
1	3.990662000	-2.492456000	-2.183495000
1	2.267439000	-2.164330000	-2.010689000
1	3.366272000	-0.880517000	-2.534689000
8	0.010374000	-3.225151000	-0.242158000
6	0.075385000	2.966079000	0.543489000
8	0.116617000	2.799900000	1.721759000
8	0.085089000	3.660574000	-0.413045000

-2119.053010

4-Mn1-PH₃

25	0.017803000	-0.186694000	-0.127042000
15	2.325516000	-0.038873000	0.186942000
15	-2.295920000	-0.085163000	0.190065000
7	0.016487000	-0.278271000	2.011511000
6	-2.436695000	-0.182014000	2.046903000
6	-1.201494000	-0.890964000	2.592488000
6	1.247858000	-0.859436000	2.594367000
6	2.465675000	-0.124110000	2.045455000
6	-3.421381000	-1.459764000	-0.429248000
6	-3.242465000	1.512747000	-0.138307000
6	3.496220000	-1.369159000	-0.438202000
6	3.210929000	1.594383000	-0.136088000
1	-2.456856000	0.846668000	2.415714000
1	-3.354781000	-0.672778000	2.373303000
1	-1.176442000	-0.824437000	3.687833000
1	-1.203616000	-1.949491000	2.322608000
1	1.222355000	-0.790183000	3.689532000
1	1.276243000	-1.918624000	2.327958000
1	2.462681000	0.906327000	2.411649000
1	3.395412000	-0.589825000	2.375594000
1	0.203247000	1.626476000	0.104433000
1	-0.002553000	0.729057000	2.244759000
15	-0.009431000	0.294680000	-2.346987000
1	-1.071596000	-0.141608000	-3.174126000
1	-0.023775000	1.652191000	-2.749559000
1	1.041020000	-0.125765000	-3.198156000
6	0.038609000	-1.905629000	-0.448442000
1	-2.734114000	2.207494000	0.537591000
6	-4.723706000	1.456763000	0.261298000
1	-5.140252000	2.468700000	0.258557000
1	-5.308806000	0.863700000	-0.446923000
1	-4.873938000	1.040835000	1.260684000
6	-3.066744000	2.055858000	-1.560912000
1	-2.020290000	2.268642000	-1.775619000

1	-3.462256000	1.372908000	-2.316968000
1	-3.611023000	3.000183000	-1.658180000
6	-3.234398000	-1.688434000	-1.935467000
1	-3.396781000	-0.781372000	-2.520132000
1	-2.227609000	-2.054285000	-2.146243000
1	-3.945733000	-2.441592000	-2.288267000
6	-3.233218000	-2.778086000	0.338427000
1	-3.933800000	-3.522483000	-0.053384000
1	-2.227115000	-3.179272000	0.215605000
1	-3.436758000	-2.673427000	1.405540000
1	-4.443258000	-1.114669000	-0.249855000
6	4.670782000	1.623830000	0.338376000
1	5.316025000	1.026628000	-0.311668000
1	5.043654000	2.652288000	0.308793000
1	4.788245000	1.260502000	1.361961000
6	3.089013000	2.090246000	-1.580635000
1	2.048221000	2.168687000	-1.892329000
1	3.527231000	3.089367000	-1.662922000
1	3.620527000	1.442258000	-2.281927000
1	2.633698000	2.279143000	0.494638000
1	4.506692000	-0.985272000	-0.270942000
6	3.359484000	-2.691042000	0.334069000
1	4.081573000	-3.412933000	-0.060536000
1	3.565636000	-2.576543000	1.399723000
1	2.365678000	-3.124807000	0.218607000
6	3.297211000	-1.606229000	-1.942171000
1	4.034136000	-2.329274000	-2.305085000
1	2.303317000	-2.013021000	-2.138726000
1	3.412203000	-0.693743000	-2.529336000
8	0.065714000	-3.049248000	-0.695336000
6	-0.105675000	2.641282000	0.627177000
8	-0.167703000	2.574714000	1.867177000
8	-0.262940000	3.542970000	-0.191034000

-2119.071404

1-Mn1-2PH₃

25	0.000025000	-0.065854000	-0.091419000
15	2.289030000	0.088959000	0.334199000
15	-2.289052000	0.088986000	0.334066000
7	-0.000040000	-1.058986000	1.566589000
6	-2.394127000	-0.808382000	1.961877000

6	-1.197333000	-1.749324000	2.040895000
6	1.197216000	-1.749328000	2.040982000
6	2.394018000	-0.808394000	1.962018000
6	-3.656185000	-0.667205000	-0.720539000
6	-3.018831000	1.764317000	0.845170000
6	3.656114000	-0.667306000	-0.720389000
6	3.018876000	1.764312000	0.845163000
1	-2.285907000	-0.049990000	2.741594000
1	-3.350463000	-1.314323000	2.111751000
1	-1.069926000	-2.079930000	3.084091000
1	-1.393144000	-2.666254000	1.455560000
1	1.069743000	-2.079946000	3.084164000
1	1.393050000	-2.666248000	1.455640000
1	2.285763000	-0.049996000	2.741728000
1	3.350338000	-1.314344000	2.111933000
15	0.000063000	1.527541000	-1.660764000
1	-1.048687000	1.601575000	-2.625681000
1	0.000222000	2.939577000	-1.412310000
1	1.048667000	1.601394000	-2.625871000
15	0.000105000	-1.736280000	-1.520035000
1	1.035351000	-2.056521000	-2.449228000
1	-0.000063000	-3.009674000	-0.877672000
1	-1.034982000	-2.056380000	-2.449464000
1	-2.229526000	2.141155000	1.507084000
6	-4.325705000	1.673225000	1.650386000
1	-4.604929000	2.668135000	2.013551000
1	-5.151681000	1.313962000	1.029597000
1	-4.246149000	1.017056000	2.518187000
6	-3.192811000	2.768890000	-0.301824000
1	-2.302347000	2.865840000	-0.921105000
1	-4.029140000	2.490582000	-0.948157000
1	-3.418463000	3.759395000	0.106870000
6	-3.542417000	-0.200056000	-2.180900000
1	-3.599235000	0.884199000	-2.280553000
1	-2.596771000	-0.518819000	-2.620869000
1	-4.354095000	-0.631267000	-2.776496000
6	-3.660442000	-2.201955000	-0.642964000
1	-4.435097000	-2.603377000	-1.304783000
1	-2.706498000	-2.626522000	-0.960166000
1	-3.867496000	-2.565637000	0.364932000
1	-4.607231000	-0.308982000	-0.312728000
6	4.325648000	1.673343000	1.650567000
1	5.151675000	1.313793000	1.030016000
1	4.604932000	2.668351000	2.013420000
1	4.245913000	1.017479000	2.518592000
6	3.193020000	2.768673000	-0.301999000

1	2.302643000	2.865557000	-0.921400000
1	3.418700000	3.759242000	0.106527000
1	4.029389000	2.490162000	-0.948183000
1	2.229507000	2.141315000	1.506916000
1	4.607185000	-0.309180000	-0.312556000
6	3.660220000	-2.202045000	-0.642758000
1	4.434827000	-2.603574000	-1.304558000
1	3.867208000	-2.565746000	0.365156000
1	2.706226000	-2.626476000	-0.959980000
6	3.542393000	-0.200146000	-2.180780000
1	4.354049000	-0.631394000	-2.776376000
1	2.596734000	-0.518859000	-2.620772000
1	3.599260000	0.884112000	-2.280462000

-2158.968528

2-Mn1-2PH₃

25	0.003248000	0.095243000	0.074719000
15	-2.291756000	0.054775000	-0.340893000
15	2.293937000	0.049980000	-0.351333000
7	0.000943000	-1.151302000	-1.670705000
6	2.408689000	-1.003485000	-1.885982000
6	1.194119000	-1.932649000	-1.892128000
6	-1.194965000	-1.930475000	-1.883525000
6	-2.405180000	-0.996294000	-1.876380000
6	3.668390000	-0.637213000	0.749389000
6	3.033095000	1.667036000	-1.007097000
6	-3.656573000	-0.623387000	0.779645000
6	-3.043167000	1.667925000	-0.989155000
1	2.337491000	-0.325481000	-2.741359000
1	3.359343000	-1.537242000	-1.958064000
1	1.149940000	-2.454865000	-2.866342000
1	1.352764000	-2.738578000	-1.139826000
1	-1.157393000	-2.456481000	-2.856027000
1	-1.352533000	-2.733028000	-1.126883000
1	-2.322762000	-0.314010000	-2.727433000
1	-3.358693000	-1.522876000	-1.958039000
1	0.003063000	1.592393000	-0.776476000
1	0.004999000	1.024861000	-1.346575000
15	0.009642000	1.476627000	1.846195000
1	1.073813000	1.475905000	2.795193000
1	-0.022163000	2.898242000	1.729790000
1	-1.016626000	1.431797000	2.834917000
15	0.007232000	-1.685637000	1.448232000
1	-1.053758000	-1.953128000	2.353654000
1	0.071722000	-2.998096000	0.908573000

1	1.018802000	-1.877339000	2.427444000
1	2.364157000	1.863259000	-1.853409000
6	4.464370000	1.555173000	-1.551023000
1	4.723303000	2.461227000	-2.109126000
1	5.192686000	1.457855000	-0.740892000
1	4.589486000	0.703610000	-2.223665000
6	2.910518000	2.852870000	-0.042301000
1	1.884572000	2.993608000	0.299656000
1	3.549928000	2.730272000	0.835572000
1	3.223847000	3.775219000	-0.542987000
6	3.634309000	-0.020574000	2.155509000
1	3.663157000	1.069851000	2.136156000
1	2.732410000	-0.317355000	2.694030000
1	4.496471000	-0.364771000	2.736739000
6	3.668264000	-2.172300000	0.836830000
1	4.515647000	-2.500333000	1.448599000
1	2.762863000	-2.559505000	1.305482000
1	3.765443000	-2.647808000	-0.140144000
1	4.605919000	-0.344723000	0.267468000
6	-4.430662000	1.530902000	-1.632910000
1	-5.204858000	1.346580000	-0.882769000
1	-4.695956000	2.462018000	-2.145134000
1	-4.472913000	0.724743000	-2.368397000
6	-3.033853000	2.813311000	0.030401000
1	-2.051632000	2.949539000	0.484170000
1	-3.307740000	3.753440000	-0.460030000
1	-3.759556000	2.645322000	0.830542000
1	-2.327692000	1.922372000	-1.780127000
1	-4.597995000	-0.277796000	0.341842000
6	-3.712743000	-2.159547000	0.815207000
1	-4.524865000	-2.478195000	1.477633000
1	-3.902277000	-2.592809000	-0.167779000
1	-2.790527000	-2.598650000	1.198262000
6	-3.553862000	-0.058162000	2.204999000
1	-4.425176000	-0.367065000	2.792457000
1	-2.663388000	-0.430515000	2.714444000
1	-3.511458000	1.031620000	2.223912000

-2160.134396

TS1-Mn1-2PH₃

25	-0.000083000	0.061076000	0.082739000
15	-2.296997000	0.058141000	-0.324078000
15	2.296744000	0.058192000	-0.324154000
7	-0.000206000	-1.183931000	-1.677138000
6	2.409674000	-0.987179000	-1.871289000

6	1.213463000	-1.937533000	-1.897490000
6	-1.213803000	-1.937719000	-1.897244000
6	-2.410088000	-0.987448000	-1.871054000
6	3.652529000	-0.636074000	0.793115000
6	3.067637000	1.658861000	-0.983017000
6	-3.652569000	-0.635684000	0.793714000
6	-3.067674000	1.658815000	-0.983123000
1	2.330784000	-0.300044000	-2.718964000
1	3.363527000	-1.511535000	-1.955500000
1	1.183316000	-2.453925000	-2.873162000
1	1.355710000	-2.729981000	-1.136751000
1	-1.183704000	-2.454233000	-2.872851000
1	-1.355886000	-2.730086000	-1.136383000
1	-2.331234000	-0.300408000	-2.718809000
1	-3.363937000	-1.511814000	-1.955173000
1	-0.000146000	1.152528000	-1.227482000
1	-0.000253000	0.268872000	-1.611215000
15	0.000007000	1.617895000	1.681683000
1	1.046749000	1.694963000	2.648654000
1	0.001379000	3.020501000	1.413679000
1	-1.047913000	1.696778000	2.647219000
15	0.000251000	-1.633780000	1.547477000
1	-1.035269000	-1.862743000	2.497751000
1	0.001892000	-2.963034000	1.035132000
1	1.034860000	-1.860659000	2.499226000
1	2.339246000	1.926668000	-1.757045000
6	4.442712000	1.493398000	-1.647982000
1	4.722300000	2.423287000	-2.154833000
1	5.222593000	1.284537000	-0.910119000
1	4.459331000	0.694929000	-2.392348000
6	3.107207000	2.808833000	0.030670000
1	2.139635000	2.978526000	0.501663000
1	3.844953000	2.628414000	0.816763000
1	3.396299000	3.737069000	-0.473572000
6	3.556115000	-0.044041000	2.208145000
1	3.608132000	1.045452000	2.210286000
1	2.618980000	-0.327366000	2.689250000
1	4.378467000	-0.416869000	2.828029000
6	3.659742000	-2.172292000	0.847445000
1	4.462370000	-2.510528000	1.511530000
1	2.724432000	-2.576319000	1.237254000
1	3.833276000	-2.622513000	-0.131390000
1	4.603629000	-0.322860000	0.351566000
6	-4.442856000	1.493470000	-1.647875000
1	-5.222596000	1.284223000	-0.909973000
1	-4.722649000	2.423518000	-2.154322000

1	-4.459479000	0.695276000	-2.392541000
6	-3.106796000	2.808901000	0.030445000
1	-2.139055000	2.978489000	0.501149000
1	-3.395897000	3.737131000	-0.473801000
1	-3.844337000	2.628659000	0.816777000
1	-2.339346000	1.926349000	-1.757304000
1	-4.603800000	-0.321917000	0.352844000
6	-3.660423000	-2.171914000	0.847693000
1	-4.462244000	-2.509954000	1.512848000
1	-3.835613000	-2.621745000	-0.131025000
1	-2.724727000	-2.576512000	1.235993000
6	-3.554827000	-0.043872000	2.208732000
1	-4.375956000	-0.417614000	2.829683000
1	-2.616716000	-0.326316000	2.688434000
1	-3.607934000	1.045575000	2.211073000

-2160.127286

3-Mn1-2PH₃

25	0.005988000	-0.025751000	0.151703000
15	-2.218719000	0.057022000	-0.338104000
15	2.229760000	0.109126000	-0.331534000
7	0.013424000	-1.140640000	-1.805729000
6	2.413263000	-0.817734000	-1.958408000
6	1.282583000	-1.838446000	-2.071979000
6	-1.203102000	-1.947215000	-2.000937000
6	-2.411471000	-1.021888000	-1.877990000
6	3.650868000	-0.627838000	0.682720000
6	2.918505000	1.789212000	-0.869434000
6	-3.672112000	-0.572975000	0.701520000
6	-2.899927000	1.679887000	-1.050591000
1	2.320468000	-0.084897000	-2.766643000
1	3.390552000	-1.290488000	-2.067268000
1	1.277632000	-2.309787000	-3.065905000
1	1.393233000	-2.628968000	-1.325845000
1	-1.194978000	-2.450996000	-2.978844000
1	-1.220279000	-2.718672000	-1.227948000
1	-2.449011000	-0.359378000	-2.748631000
1	-3.344707000	-1.587834000	-1.868897000
1	0.005209000	1.299794000	-0.790434000
1	-0.035886000	-0.347960000	-2.442653000
15	-0.010631000	1.272065000	1.960879000
1	1.186835000	1.675083000	2.622355000
1	-0.586543000	2.576133000	1.980989000
1	-0.652476000	0.853923000	3.171418000
15	-0.027269000	-1.816388000	1.466277000

1	-0.914943000	-1.828987000	2.584994000
1	-0.365430000	-3.147059000	1.047742000
1	1.083763000	-2.260717000	2.247314000
1	2.257530000	2.005433000	-1.715886000
6	4.370309000	1.791273000	-1.366901000
1	4.597278000	2.748637000	-1.848576000
1	5.077602000	1.672294000	-0.541017000
1	4.567450000	1.000767000	-2.096109000
6	2.689657000	2.896681000	0.164580000
1	1.637622000	2.951482000	0.444422000
1	3.284314000	2.744394000	1.069156000
1	2.979905000	3.866118000	-0.255057000
6	3.569747000	-0.145607000	2.138645000
1	3.622322000	0.941754000	2.219758000
1	2.633648000	-0.465006000	2.601075000
1	4.396187000	-0.562035000	2.724848000
6	3.684838000	-2.163287000	0.624710000
1	4.480779000	-2.540069000	1.276221000
1	2.748045000	-2.605753000	0.964942000
1	3.885992000	-2.537794000	-0.381018000
1	4.585637000	-0.263586000	0.246499000
6	-4.374710000	1.655932000	-1.472417000
1	-5.039871000	1.657821000	-0.604140000
1	-4.609111000	2.550324000	-2.059912000
1	-4.622282000	0.784594000	-2.085120000
6	-2.585239000	2.905290000	-0.187650000
1	-1.514476000	2.965057000	0.002079000
1	-2.896492000	3.818097000	-0.707839000
1	-3.108428000	2.884157000	0.771863000
1	-2.281752000	1.767559000	-1.951134000
1	-4.577711000	-0.385037000	0.116909000
6	-3.604019000	-2.084380000	0.966013000
1	-4.528146000	-2.413213000	1.453817000
1	-3.492882000	-2.670764000	0.051123000
1	-2.779498000	-2.341086000	1.630724000
6	-3.770169000	0.196982000	2.024561000
1	-4.599999000	-0.185192000	2.629047000
1	-2.852942000	0.083168000	2.607619000
1	-3.939066000	1.264238000	1.870066000

-2160.156238

TS2-Mn1-2PH₃

25	-0.000344000	-0.346335000	-0.185892000
15	2.249888000	-0.060586000	0.167337000
15	-2.250331000	-0.059959000	0.167884000

7	-0.000049000	-0.249271000	2.055962000
6	-2.418954000	-0.016363000	2.041951000
6	-1.240802000	-0.760383000	2.666367000
6	1.240150000	-0.762686000	2.665532000
6	2.419049000	-0.019552000	2.041530000
6	-3.639453000	-1.263646000	-0.291787000
6	-3.023827000	1.625001000	-0.227124000
6	3.638598000	-1.264195000	-0.294058000
6	3.024430000	1.624612000	-0.224988000
1	-2.384047000	1.032918000	2.350489000
1	-3.373424000	-0.419487000	2.384738000
1	-1.229836000	-0.622896000	3.757547000
1	-1.300701000	-1.833482000	2.468534000
1	1.229695000	-0.626323000	3.756858000
1	1.298529000	-1.835643000	2.466484000
1	2.385673000	1.029404000	2.351361000
1	3.373100000	-0.424370000	2.383483000
1	-0.001233000	1.289139000	-0.091862000
1	0.000876000	0.761813000	2.178837000
15	-0.001369000	-0.159700000	-2.407413000
1	-1.050970000	-0.691957000	-3.215577000
1	0.008786000	1.106664000	-3.059851000
1	1.036583000	-0.710263000	-3.218494000
15	0.000597000	-2.558316000	-0.352221000
1	1.032899000	-3.262019000	-1.042144000
1	0.007455000	-3.452577000	0.770603000
1	-1.036163000	-3.265496000	-1.031759000
1	-2.442113000	2.272059000	0.436636000
6	-4.503986000	1.786750000	0.145496000
1	-4.782621000	2.845035000	0.103679000
1	-5.154180000	1.255209000	-0.554927000
1	-4.725692000	1.426321000	1.153722000
6	-2.758081000	2.097819000	-1.659737000
1	-1.690550000	2.107469000	-1.872372000
1	-3.259025000	1.467796000	-2.399451000
1	-3.135215000	3.117765000	-1.791688000
6	-3.636231000	-1.548472000	-1.800422000
1	-3.729149000	-0.636959000	-2.393877000
1	-2.712993000	-2.046581000	-2.102595000
1	-4.473517000	-2.203330000	-2.064986000
6	-3.593404000	-2.575170000	0.507506000
1	-4.433887000	-3.212577000	0.211819000
1	-2.679853000	-3.140053000	0.322506000
1	-3.674628000	-2.411873000	1.583922000
1	-4.579504000	-0.767253000	-0.034895000
6	4.504207000	1.785521000	0.149501000

1	5.155016000	1.254516000	-0.550750000
1	4.783202000	2.843765000	0.109051000
1	4.724710000	1.424040000	1.157606000
6	2.760596000	2.099030000	-1.657375000
1	1.693408000	2.108837000	-1.871441000
1	3.137929000	3.119113000	-1.787719000
1	3.262548000	1.469835000	-2.397120000
1	2.442155000	2.271087000	0.438834000
1	4.578740000	-0.768371000	-0.036414000
6	3.592172000	-2.576733000	0.503526000
1	4.432830000	-3.213750000	0.207500000
1	3.672753000	-2.414809000	1.580193000
1	2.678750000	-3.141444000	0.317362000
6	3.635605000	-1.547259000	-1.803030000
1	4.473879000	-2.200529000	-2.068395000
1	2.713206000	-2.046600000	-2.105676000
1	3.727011000	-0.634989000	-2.395544000
6	0.001048000	3.204920000	0.670564000
8	0.001533000	2.921046000	1.808663000
8	0.000970000	3.757376000	-0.356561000

-2348.809424

4-Mn1-2PH₃

25	-0.005009000	-0.243581000	-0.164689000
15	2.309406000	-0.056311000	0.186807000
15	-2.319394000	-0.044526000	0.189313000
7	-0.003569000	-0.343124000	1.992666000
6	-2.439988000	-0.136526000	2.055111000
6	-1.235094000	-0.908712000	2.584831000
6	1.223484000	-0.924070000	2.579699000
6	2.433764000	-0.159389000	2.051619000
6	-3.663754000	-1.253635000	-0.354371000
6	-3.108292000	1.650856000	-0.100980000
6	3.636311000	-1.281953000	-0.365559000
6	3.121968000	1.629501000	-0.096596000
1	-2.403752000	0.888495000	2.433060000
1	-3.378859000	-0.579417000	2.391900000
1	-1.197290000	-0.852803000	3.681178000
1	-1.292469000	-1.965884000	2.310771000
1	1.188124000	-0.873460000	3.676398000
1	1.270229000	-1.980207000	2.299757000
1	2.405561000	0.864301000	2.433418000
1	3.369617000	-0.611601000	2.384165000
1	-0.091751000	1.582490000	0.076393000
1	0.005287000	0.668603000	2.208271000

15	0.005972000	0.165840000	-2.379643000
1	-1.049203000	-0.283085000	-3.220995000
1	0.026997000	1.495014000	-2.878023000
1	1.054444000	-0.313603000	-3.211621000
15	-0.014823000	-2.422867000	-0.580280000
1	1.019493000	-3.029907000	-1.341929000
1	-0.021015000	-3.408797000	0.452474000
1	-1.062585000	-3.011698000	-1.337373000
1	-2.545902000	2.269756000	0.604619000
6	-4.592638000	1.747473000	0.276400000
1	-4.894678000	2.799113000	0.300959000
1	-5.228663000	1.245344000	-0.457924000
1	-4.804041000	1.321341000	1.260825000
6	-2.848118000	2.218911000	-1.500588000
1	-1.781167000	2.313670000	-1.694654000
1	-3.302549000	1.611408000	-2.287196000
1	-3.277893000	3.222951000	-1.572661000
6	-3.706304000	-1.406782000	-1.881915000
1	-3.835393000	-0.449579000	-2.389738000
1	-2.793063000	-1.866513000	-2.265536000
1	-4.545768000	-2.048299000	-2.169182000
6	-3.576627000	-2.622960000	0.338048000
1	-4.432825000	-3.234315000	0.034404000
1	-2.676987000	-3.175479000	0.067469000
1	-3.606661000	-2.542094000	1.425971000
1	-4.603670000	-0.798379000	-0.030825000
6	4.605302000	1.701687000	0.291296000
1	5.238719000	1.194299000	-0.441802000
1	4.922911000	2.748486000	0.323909000
1	4.804125000	1.266827000	1.274465000
6	2.881833000	2.205298000	-1.497212000
1	1.819090000	2.342708000	-1.689548000
1	3.349293000	3.192429000	-1.568942000
1	3.313755000	1.581859000	-2.284110000
1	2.562345000	2.254820000	0.605637000
1	4.582958000	-0.836444000	-0.048541000
6	3.540074000	-2.650077000	0.328328000
1	4.387664000	-3.270258000	0.018396000
1	3.578990000	-2.569717000	1.415931000
1	2.633142000	-3.193786000	0.064361000
6	3.669515000	-1.438964000	-1.892990000
1	4.505476000	-2.083878000	-2.183007000
1	2.753245000	-1.897663000	-2.270248000
1	3.798508000	-0.483759000	-2.404431000
6	0.018527000	2.604687000	0.649833000
8	0.051296000	2.504159000	1.890803000

8 0.062357000 3.558841000 -0.123375000

-2348.833489

1-Mn1-PMe₃

25	0.034454000	-0.186061000	-0.052138000
15	-2.342574000	-0.410355000	-0.361350000
15	2.389127000	-0.430052000	-0.326368000
7	0.047708000	-1.936017000	-0.901523000
6	2.486462000	-2.120130000	-1.093538000
6	1.189616000	-2.847469000	-0.792110000
6	-1.131467000	-2.763955000	-1.134077000
6	-2.351801000	-1.918520000	-1.442201000
6	3.537267000	-0.614651000	1.156641000
6	3.431524000	0.467591000	-1.646301000
6	-3.435994000	-0.934080000	1.086698000
6	-3.482646000	0.676330000	-1.442714000
1	2.568133000	-1.976171000	-2.173581000
1	3.367830000	-2.672128000	-0.760146000
1	1.083167000	-3.684610000	-1.499605000
1	1.224788000	-3.304922000	0.210628000
1	-0.952820000	-3.445209000	-1.982526000
1	-1.327870000	-3.419720000	-0.269718000
1	-2.281037000	-1.550036000	-2.469876000
1	-3.280186000	-2.486662000	-1.347982000
15	-0.037303000	2.109563000	0.192800000
1	2.857304000	0.215043000	-2.545855000
6	4.849599000	-0.105934000	-1.807753000
1	5.302233000	0.287936000	-2.723730000
1	5.492850000	0.193527000	-0.975663000
1	4.867805000	-1.194912000	-1.874837000
6	3.503520000	1.994260000	-1.576702000
1	2.516821000	2.452491000	-1.578571000
1	4.047836000	2.337677000	-0.693180000
1	4.041899000	2.373361000	-2.451806000
6	3.596353000	0.654698000	2.013576000
1	3.926713000	1.527482000	1.447857000
1	2.616185000	0.874193000	2.441424000
1	4.298430000	0.511946000	2.841594000
6	3.140002000	-1.820150000	2.025528000
1	3.831326000	-1.898071000	2.871425000
1	2.133638000	-1.707258000	2.429491000
1	3.186450000	-2.763179000	1.478593000
1	4.532497000	-0.809900000	0.746145000
6	-4.750326000	-0.050398000	-1.930424000
1	-5.425035000	-0.276682000	-1.099932000

1	-5.297188000	0.600700000	-2.620343000
1	-4.540551000	-0.979342000	-2.459310000
6	-3.896302000	2.042275000	-0.878451000
1	-3.053871000	2.666612000	-0.596758000
1	-4.462180000	2.588920000	-1.639868000
1	-4.551073000	1.935166000	-0.010282000
1	-2.838310000	0.854035000	-2.312927000
1	-4.437044000	-1.085109000	0.668991000
6	-2.962984000	-2.271207000	1.681642000
1	-3.565324000	-2.509586000	2.564396000
1	-3.071873000	-3.097736000	0.978642000
1	-1.918364000	-2.220297000	1.995491000
6	-3.519708000	0.125808000	2.194061000
1	-4.172373000	-0.235985000	2.995283000
1	-2.536715000	0.317643000	2.626547000
1	-3.932347000	1.072191000	1.843347000
6	1.358640000	3.076319000	0.949446000
1	1.129688000	4.145176000	0.918995000
1	1.458278000	2.770366000	1.991326000
1	2.304574000	2.901478000	0.452182000
6	-0.376623000	3.151844000	-1.311668000
1	0.481532000	3.092345000	-1.984093000
1	-1.240766000	2.756103000	-1.846153000
1	-0.555847000	4.199930000	-1.055211000
6	-1.295059000	2.747101000	1.400831000
1	-2.284830000	2.356365000	1.205058000
1	-0.994701000	2.405747000	2.393298000
1	-1.326642000	3.840102000	1.393640000
6	0.018473000	-0.315668000	1.676342000
8	-0.001044000	-0.479638000	2.842815000

-2047.121934

2-Mn1-PMe₃

25	0.008276000	-0.129071000	-0.059424000
15	-2.329736000	-0.411231000	-0.361594000
15	2.369947000	-0.546540000	-0.230376000
7	0.036101000	-2.148797000	-0.728762000
6	2.431974000	-2.400961000	-0.453479000
6	1.060258000	-2.968830000	-0.121633000
6	-1.206304000	-2.892373000	-0.734394000
6	-2.339312000	-2.028736000	-1.271303000
6	3.707978000	-0.377196000	1.095371000
6	3.215480000	-0.019000000	-1.837772000
6	-3.549661000	-0.702307000	1.056023000
6	-3.338765000	0.662030000	-1.562253000

1	2.654738000	-2.601942000	-1.504048000
1	3.228726000	-2.842368000	0.150496000
1	1.011030000	-4.005751000	-0.501075000
1	0.943032000	-3.049425000	0.980469000
1	-1.119984000	-3.793324000	-1.371551000
1	-1.473345000	-3.274347000	0.269734000
1	-2.132837000	-1.786988000	-2.318393000
1	-3.312423000	-2.523958000	-1.223591000
15	0.023191000	2.167373000	0.263767000
1	2.591751000	-0.547653000	-2.568665000
6	4.660484000	-0.515296000	-1.998551000
1	5.006466000	-0.325486000	-3.020104000
1	5.341411000	0.008207000	-1.322740000
1	4.758990000	-1.586914000	-1.811325000
6	3.113589000	1.476505000	-2.158328000
1	2.087221000	1.834728000	-2.079569000
1	3.738537000	2.082210000	-1.497960000
1	3.454319000	1.660839000	-3.182459000
6	4.333820000	1.007166000	1.293709000
1	4.678093000	1.457357000	0.361500000
1	3.639199000	1.697841000	1.768319000
1	5.202539000	0.916052000	1.954394000
6	3.186259000	-0.922975000	2.432685000
1	4.006604000	-0.979483000	3.155925000
1	2.414564000	-0.271494000	2.846275000
1	2.754120000	-1.921974000	2.338086000
1	4.498639000	-1.045366000	0.738096000
6	-4.483060000	-0.076740000	-2.278072000
1	-5.227996000	-0.447921000	-1.567790000
1	-4.997233000	0.615008000	-2.953827000
1	-4.135696000	-0.920003000	-2.874723000
6	-3.892827000	1.951725000	-0.940278000
1	-3.141844000	2.521165000	-0.396471000
1	-4.291157000	2.600486000	-1.726855000
1	-4.714611000	1.731187000	-0.254479000
1	-2.588655000	0.935715000	-2.313368000
1	-4.538099000	-0.707043000	0.582387000
6	-3.353793000	-2.060054000	1.750226000
1	-4.085434000	-2.155915000	2.559410000
1	-3.499702000	-2.902787000	1.074491000
1	-2.358643000	-2.141029000	2.192689000
6	-3.518848000	0.409799000	2.114040000
1	-4.263073000	0.195210000	2.888228000
1	-2.542292000	0.459700000	2.596500000
1	-3.751522000	1.391939000	1.706679000
6	1.558067000	3.063474000	0.785463000

1	1.377522000	4.141616000	0.812717000
1	1.833337000	2.730308000	1.786567000
1	2.380248000	2.856351000	0.105413000
6	-0.437601000	3.239401000	-1.185988000
1	0.352132000	3.181441000	-1.938176000
1	-1.362819000	2.891267000	-1.642804000
1	-0.555577000	4.283759000	-0.884407000
6	-1.075316000	2.859745000	1.584500000
1	-2.121157000	2.669316000	1.365712000
1	-0.833434000	2.367134000	2.528175000
1	-0.921502000	3.936938000	1.688688000
6	-0.082897000	-0.428608000	1.660104000
8	-0.180109000	-0.627220000	2.810814000
1	0.015705000	0.458341000	-1.909896000
1	0.093197000	-0.311483000	-1.943635000

-2048.284263

TS1-Mn1-PMe₃

25	0.006302000	-0.119100000	-0.048494000
15	-2.343431000	-0.417074000	-0.344932000
15	2.379086000	-0.493991000	-0.271784000
7	0.018118000	-2.165770000	-0.849997000
6	2.445555000	-2.293912000	-0.780411000
6	1.135186000	-2.972949000	-0.415519000
6	-1.217032000	-2.913427000	-0.776375000
6	-2.380863000	-2.049306000	-1.239960000
6	3.661519000	-0.527279000	1.113320000
6	3.309988000	0.218056000	-1.764213000
6	-3.541146000	-0.713687000	1.088557000
6	-3.367122000	0.617182000	-1.566217000
1	2.568842000	-2.322215000	-1.865978000
1	3.306878000	-2.796238000	-0.333839000
1	1.108062000	-3.969417000	-0.891219000
1	1.092096000	-3.152134000	0.676127000
1	-1.168829000	-3.815273000	-1.413766000
1	-1.398709000	-3.279118000	0.249304000
1	-2.246788000	-1.817600000	-2.300456000
1	-3.343682000	-2.552117000	-1.125163000
15	0.000434000	2.170856000	0.251235000
1	2.706312000	-0.195475000	-2.580557000
6	4.749331000	-0.298220000	-1.915544000
1	5.147543000	-0.001751000	-2.891589000
1	5.406298000	0.130084000	-1.153385000
1	4.818250000	-1.386081000	-1.848392000
6	3.272585000	1.740783000	-1.916449000

1	2.255157000	2.123453000	-1.868583000
1	3.870818000	2.245985000	-1.154731000
1	3.688275000	2.022422000	-2.889588000
6	4.130751000	0.844997000	1.605040000
1	4.505875000	1.478177000	0.798891000
1	3.327422000	1.378176000	2.113814000
1	4.945284000	0.715312000	2.325510000
6	3.172741000	-1.375821000	2.296278000
1	3.988782000	-1.502459000	3.015638000
1	2.340933000	-0.895948000	2.812710000
1	2.844859000	-2.371481000	1.990989000
1	4.520092000	-1.037490000	0.664652000
6	-4.572170000	-0.115732000	-2.181964000
1	-5.306265000	-0.391288000	-1.419099000
1	-5.077815000	0.549455000	-2.889912000
1	-4.293229000	-1.018268000	-2.725315000
6	-3.840521000	1.971991000	-1.022716000
1	-3.044944000	2.544966000	-0.553576000
1	-4.241364000	2.577558000	-1.841851000
1	-4.644242000	1.843343000	-0.293507000
1	-2.634111000	0.801258000	-2.360655000
1	-4.533279000	-0.780857000	0.628211000
6	-3.268362000	-2.038346000	1.820703000
1	-3.981949000	-2.145699000	2.644283000
1	-3.383317000	-2.908583000	1.174028000
1	-2.264111000	-2.055483000	2.249373000
6	-3.551140000	0.431244000	2.110369000
1	-4.280128000	0.211356000	2.897399000
1	-2.573965000	0.537845000	2.583113000
1	-3.827591000	1.388947000	1.672177000
6	1.489712000	3.056131000	0.912007000
1	1.320671000	4.136496000	0.913537000
1	1.650990000	2.725910000	1.939265000
1	2.380637000	2.836091000	0.333362000
6	-0.361342000	3.216888000	-1.240833000
1	-0.498145000	4.267094000	-0.968830000
1	0.467269000	3.138683000	-1.945643000
1	-1.256310000	2.851629000	-1.742973000
6	-1.180810000	2.887766000	1.487618000
1	-2.211361000	2.661828000	1.236986000
1	-0.965504000	2.445541000	2.462129000
1	-1.057870000	3.972180000	1.550483000
6	-0.063740000	-0.400118000	1.678841000
8	-0.142359000	-0.581611000	2.835470000
1	0.062682000	-0.045179000	-1.949089000
1	0.083926000	-0.967163000	-1.718691000

-2048.273906

3-Mn1-PMe₃

25	0.015053000	-0.117118000	-0.026732000
15	-2.278971000	-0.390280000	-0.364869000
15	2.332708000	-0.489256000	-0.266773000
7	0.029282000	-2.239650000	-0.745956000
6	2.444682000	-2.340694000	-0.611030000
6	1.150126000	-3.017506000	-0.196210000
6	-1.253492000	-2.949672000	-0.641609000
6	-2.347921000	-2.058823000	-1.206599000
6	3.682326000	-0.420912000	1.064385000
6	3.218091000	0.108643000	-1.832348000
6	-3.541778000	-0.659576000	1.035004000
6	-3.289468000	0.633619000	-1.607359000
1	2.592278000	-2.478104000	-1.686600000
1	3.303908000	-2.788481000	-0.109184000
1	1.124922000	-4.057784000	-0.552558000
1	1.035800000	-3.028392000	0.890173000
1	-1.215461000	-3.908545000	-1.178799000
1	-1.417575000	-3.169651000	0.413136000
1	-2.150881000	-1.886326000	-2.268682000
1	-3.331990000	-2.524088000	-1.124417000
15	0.000185000	2.152875000	0.274836000
1	2.608439000	-0.388152000	-2.596015000
6	4.672336000	-0.359347000	-1.987212000
1	5.033250000	-0.122591000	-2.993851000
1	5.332702000	0.148369000	-1.278981000
1	4.787931000	-1.436304000	-1.841160000
6	3.094397000	1.611935000	-2.091569000
1	2.057895000	1.931487000	-1.997635000
1	3.710315000	2.200947000	-1.407412000
1	3.431788000	1.843125000	-3.107509000
6	4.197333000	0.977494000	1.418165000
1	4.501374000	1.551579000	0.541413000
1	3.443868000	1.551593000	1.956138000
1	5.070474000	0.888688000	2.073469000
6	3.231454000	-1.152392000	2.337118000
1	4.060375000	-1.190843000	3.052161000
1	2.395912000	-0.639212000	2.814742000
1	2.919377000	-2.181403000	2.143879000
1	4.516280000	-0.980740000	0.627992000
6	-4.420679000	-0.126002000	-2.321756000
1	-5.167852000	-0.499039000	-1.614450000
1	-4.937796000	0.552890000	-3.008350000

1	-4.061951000	-0.970368000	-2.910742000
6	-3.864802000	1.930180000	-1.017811000
1	-3.129269000	2.514287000	-0.468627000
1	-4.249522000	2.562808000	-1.824169000
1	-4.700151000	1.716568000	-0.345831000
1	-2.526141000	0.894896000	-2.347375000
1	-4.523342000	-0.675731000	0.547056000
6	-3.357352000	-1.999026000	1.767914000
1	-4.096026000	-2.073405000	2.572905000
1	-3.503764000	-2.863743000	1.119156000
1	-2.367939000	-2.065802000	2.226797000
6	-3.527847000	0.469306000	2.074426000
1	-4.278316000	0.266640000	2.846256000
1	-2.554463000	0.531070000	2.562920000
1	-3.759892000	1.442764000	1.647160000
6	1.515209000	3.080638000	0.817629000
1	1.329838000	4.157997000	0.784190000
1	1.747811000	2.800119000	1.845778000
1	2.368875000	2.848175000	0.188259000
6	-0.445569000	3.204974000	-1.190604000
1	0.377028000	3.179462000	-1.906470000
1	-1.325867000	2.804517000	-1.688584000
1	-0.627878000	4.242352000	-0.895226000
6	-1.115740000	2.886292000	1.566341000
1	-2.159571000	2.711910000	1.325282000
1	-0.904691000	2.403540000	2.522494000
1	-0.948440000	3.962881000	1.659025000
6	-0.067479000	-0.435389000	1.702553000
8	-0.162439000	-0.592297000	2.867879000
1	0.046664000	0.237250000	-1.650436000
1	0.208105000	-2.075859000	-1.734838000

-2048.311789

TS-2Mn1-PMe₃

15	-2.210154000	-0.327895000	0.158878000
7	-0.029616000	0.592171000	1.967742000
6	1.033853000	-0.037291000	2.780391000
6	-1.378835000	0.613888000	2.600426000
6	-2.302061000	-0.452787000	2.013112000
1	-3.314742000	-0.354674000	2.411229000
1	-1.935500000	-1.447241000	2.275517000
6	2.394605000	0.238235000	2.134559000
1	3.164919000	-0.386605000	2.589786000
15	2.310418000	-0.049722000	0.281133000
6	0.144982000	-0.456037000	-1.876057000

8	0.205974000	-0.534225000	-3.033909000
25	0.056317000	-0.230270000	-0.125832000
6	0.140127000	-1.952989000	0.275848000
8	0.152981000	-3.099114000	0.497896000
6	-3.232266000	-1.758708000	-0.512247000
1	-4.251844000	-1.375346000	-0.612310000
6	-2.734115000	-2.162279000	-1.909034000
1	-3.397763000	-2.923685000	-2.331065000
1	-2.705242000	-1.318382000	-2.600271000
1	-1.726889000	-2.581424000	-1.857281000
6	-3.272691000	-2.977176000	0.421364000
1	-3.716545000	-2.741577000	1.390770000
1	-3.879204000	-3.764575000	-0.037473000
1	-2.273397000	-3.385672000	0.587976000
6	3.326954000	-1.623126000	0.101312000
1	2.870710000	-2.257340000	0.870253000
6	3.118872000	-2.332942000	-1.245253000
1	3.562869000	-3.332348000	-1.203572000
1	2.061350000	-2.443509000	-1.484256000
1	3.595351000	-1.796306000	-2.067688000
6	4.819648000	-1.469151000	0.424942000
1	5.287062000	-2.456923000	0.488292000
1	5.342595000	-0.911124000	-0.356077000
1	4.996422000	-0.960502000	1.376115000
1	1.024708000	0.351543000	3.807515000
1	0.832479000	-1.109236000	2.825525000
1	2.681020000	1.278129000	2.309748000
1	-1.800037000	1.605851000	2.426208000
1	-1.289879000	0.488411000	3.685028000
6	3.406675000	1.312334000	-0.400511000
1	4.348920000	1.253038000	0.155146000
6	2.792928000	2.701931000	-0.186687000
1	3.535829000	3.470534000	-0.420894000
1	1.944623000	2.842453000	-0.856838000
1	2.451161000	2.875056000	0.836066000
6	3.684922000	1.096234000	-1.895763000
1	4.216041000	1.961957000	-2.303417000
1	4.299451000	0.215941000	-2.084742000
1	2.749499000	0.985663000	-2.451765000
6	-3.245138000	1.178163000	-0.259587000
1	-2.675154000	1.995904000	0.189357000
6	-4.661462000	1.206004000	0.328978000
1	-5.148152000	2.151079000	0.066909000
1	-5.285491000	0.401183000	-0.068997000
1	-4.663049000	1.128763000	1.418519000
6	-3.260437000	1.379433000	-1.781979000

1	-3.695002000	2.352367000	-2.029308000
1	-2.251856000	1.343253000	-2.197023000
1	-3.866896000	0.612652000	-2.273046000
1	0.228389000	1.561849000	1.805182000
1	-0.089971000	1.387946000	-0.557419000
6	-0.488714000	3.261114000	-0.323047000
8	-0.574863000	3.550146000	-1.454110000
8	-0.491394000	3.329395000	0.853266000

-2236.965647

4-Mn1-PMe₃

25	-0.021632000	-0.134264000	-0.215112000
15	2.336367000	-0.412431000	0.087830000
15	-2.396480000	-0.488553000	0.020385000
7	-0.049473000	-2.171884000	0.544336000
6	-2.474594000	-2.321850000	0.411036000
6	-1.164781000	-2.983335000	0.018667000
6	1.223517000	-2.916760000	0.477866000
6	2.345659000	-2.034008000	1.000685000
6	-3.719306000	-0.439020000	-1.325412000
6	-3.246989000	0.167470000	1.574889000
6	3.546230000	-0.743795000	-1.329685000
6	3.333799000	0.669142000	1.280401000
1	-2.619906000	-2.425793000	1.489027000
1	-3.322875000	-2.797859000	-0.083114000
1	-1.121011000	-4.005348000	0.418428000
1	-1.054557000	-3.044742000	-1.066661000
1	1.155872000	-3.836166000	1.074506000
1	1.386095000	-3.211101000	-0.559370000
1	2.146356000	-1.803703000	2.050174000
1	3.315170000	-2.532175000	0.944256000
15	0.002558000	2.163408000	-0.608892000
1	-2.647739000	-0.321729000	2.349852000
6	-4.705952000	-0.282285000	1.737712000
1	-5.059891000	-0.019705000	2.739628000
1	-5.363048000	0.214689000	1.019111000
1	-4.828673000	-1.361571000	1.618721000
6	-3.104655000	1.677219000	1.790466000
1	-2.067408000	1.996171000	1.698840000
1	-3.712849000	2.254749000	1.089969000
1	-3.439200000	1.935574000	2.799608000
6	-4.242878000	0.949933000	-1.702678000
1	-4.545046000	1.539696000	-0.836168000
1	-3.498130000	1.516598000	-2.259656000
1	-5.119845000	0.839695000	-2.348659000

6	-3.254539000	-1.191947000	-2.580559000
1	-4.084254000	-1.262765000	-3.291239000
1	-2.432803000	-0.671823000	-3.074392000
1	-2.922621000	-2.209821000	-2.364072000
1	-4.549513000	-0.997558000	-0.880883000
6	4.449522000	-0.075917000	2.032902000
1	5.197149000	-0.490475000	1.349331000
1	4.967762000	0.627599000	2.692190000
1	4.072138000	-0.884736000	2.658274000
6	3.924374000	1.927021000	0.627267000
1	3.191674000	2.500769000	0.063197000
1	4.323272000	2.585207000	1.404847000
1	4.750731000	1.674646000	-0.042242000
1	2.576934000	0.978233000	2.007898000
1	4.534291000	-0.751982000	-0.855722000
6	3.331410000	-2.111027000	-2.000646000
1	4.059710000	-2.229112000	-2.809011000
1	3.473154000	-2.947210000	-1.315033000
1	2.335921000	-2.184507000	-2.445249000
6	3.527373000	0.347537000	-2.408415000
1	4.268736000	0.108700000	-3.177754000
1	2.551264000	0.398499000	-2.892023000
1	3.772319000	1.334024000	-2.020189000
6	-1.517340000	3.038642000	-1.196248000
1	-1.336311000	4.116105000	-1.232120000
1	-1.752730000	2.690407000	-2.202603000
1	-2.365393000	2.843195000	-0.547011000
6	0.460386000	3.243655000	0.821622000
1	-0.304899000	3.174986000	1.594409000
1	1.389890000	2.907821000	1.275190000
1	0.559024000	4.282910000	0.497070000
6	1.127474000	2.800231000	-1.932089000
1	2.168774000	2.627379000	-1.681145000
1	0.909033000	2.275982000	-2.864067000
1	0.971470000	3.872155000	-2.076045000
6	0.046967000	-0.472354000	-1.925737000
8	0.128623000	-0.667930000	-3.077786000
1	-0.122513000	0.338703000	1.610610000
1	-0.232047000	-1.990527000	1.545511000
6	0.040143000	0.140331000	2.761389000
8	0.469742000	1.129966000	3.349729000
8	-0.270610000	-1.007532000	3.129403000

-2236.987923

1-Mn1-2PMe₃

25	-0.010073000	-0.116598000	-0.108761000
15	-2.410719000	-0.095127000	-0.656805000
15	2.323474000	0.117715000	-0.691266000
7	0.007074000	-1.251881000	-1.714297000
6	2.294545000	-0.737035000	-2.346421000
6	1.210530000	-1.798090000	-2.322068000
6	-1.149567000	-2.062270000	-2.067785000
6	-2.369725000	-1.160724000	-2.184353000
6	3.677728000	-0.818496000	0.279254000
6	3.126682000	1.737994000	-1.310828000
6	-3.878408000	-0.910443000	0.235250000
6	-3.048036000	1.576920000	-1.310015000
1	2.009890000	0.032913000	-3.069441000
1	3.264119000	-1.136507000	-2.642762000
1	1.011226000	-2.123071000	-3.357172000
1	1.581722000	-2.700227000	-1.800055000
1	-0.997298000	-2.573819000	-3.031708000
1	-1.344562000	-2.867663000	-1.334000000
1	-2.227959000	-0.517433000	-3.052582000
1	-3.296113000	-1.722805000	-2.322859000
15	-0.104147000	1.656672000	1.339745000
15	0.169377000	-1.691880000	1.486116000
1	2.369988000	2.043261000	-2.044514000
6	4.457962000	1.553686000	-2.060036000
1	4.739443000	2.495990000	-2.543205000
1	5.266335000	1.290710000	-1.374040000
1	4.410788000	0.790754000	-2.837495000
6	3.262002000	2.895525000	-0.314570000
1	2.320090000	3.136375000	0.168538000
1	4.002319000	2.693011000	0.461517000
1	3.592612000	3.793178000	-0.848542000
6	4.689175000	-1.636547000	-0.538412000
1	4.201579000	-2.399929000	-1.147487000
1	5.295107000	-1.012780000	-1.198267000
1	5.372217000	-2.153027000	0.145730000
6	4.406459000	0.060358000	1.306162000
1	5.008997000	-0.570051000	1.968757000
1	5.085483000	0.764949000	0.821895000
1	3.718634000	0.628800000	1.932400000
1	3.081995000	-1.535898000	0.844347000
6	-3.887470000	1.559405000	-2.599111000
1	-4.829566000	1.023572000	-2.469306000
1	-4.132127000	2.589453000	-2.881993000
1	-3.358476000	1.112139000	-3.441067000
6	-3.776190000	2.409248000	-0.242966000
1	-3.251267000	2.431868000	0.710086000

1	-3.879353000	3.444004000	-0.586076000
1	-4.782652000	2.027309000	-0.061395000
1	-2.102415000	2.080348000	-1.540141000
1	-3.520997000	-1.946587000	0.283865000
6	-4.101731000	-0.431928000	1.676057000
1	-4.764123000	-1.128954000	2.200471000
1	-3.174151000	-0.367671000	2.237310000
1	-4.579230000	0.549663000	1.701332000
6	-5.222252000	-0.921831000	-0.513021000
1	-5.919378000	-1.594657000	-0.000968000
1	-5.681175000	0.068830000	-0.522691000
1	-5.138256000	-1.263509000	-1.545516000
6	1.230257000	-1.531767000	3.015311000
1	0.742912000	-0.845064000	3.710988000
1	1.353464000	-2.498398000	3.512445000
1	2.211779000	-1.126868000	2.771427000
6	-1.310656000	-2.416468000	2.357405000
1	-2.056806000	-2.724772000	1.625263000
1	-1.018396000	-3.284600000	2.955331000
1	-1.758648000	-1.673440000	3.017721000
6	0.846323000	-3.293766000	0.819283000
1	1.841409000	-3.149099000	0.398976000
1	0.896700000	-4.057242000	1.600541000
1	0.193854000	-3.639416000	0.017049000
6	1.326194000	2.014786000	2.488511000
1	1.172287000	2.958075000	3.020755000
1	1.400427000	1.210541000	3.220055000
1	2.264128000	2.065261000	1.946524000
6	-0.376480000	3.385347000	0.671717000
1	0.357384000	3.599554000	-0.106046000
1	-1.363245000	3.445588000	0.214824000
1	-0.303430000	4.146251000	1.454834000
6	-1.381964000	1.692861000	2.698752000
1	-2.389848000	1.659495000	2.295282000
1	-1.241245000	0.810191000	3.326396000
1	-1.275919000	2.588220000	3.318256000

-2394.790437

2-Mn1-2PMe₃

25	0.013436000	0.012467000	-0.139595000
15	-2.381500000	-0.265552000	-0.635319000
15	2.345081000	-0.120150000	-0.707915000
7	0.055651000	-1.812752000	-1.275119000
6	2.327324000	-1.484726000	-1.983095000
6	1.265186000	-2.508829000	-1.604055000

6	-1.128534000	-2.610647000	-1.336692000
6	-2.286145000	-1.721077000	-1.795049000
6	3.693910000	-0.663983000	0.519251000
6	3.117995000	1.219819000	-1.814664000
6	-3.810869000	-0.883061000	0.462213000
6	-3.122083000	1.119468000	-1.708969000
1	2.024510000	-1.000664000	-2.916854000
1	3.310103000	-1.931651000	-2.139876000
1	1.111033000	-3.185995000	-2.467050000
1	1.679752000	-3.168345000	-0.807442000
1	-1.021279000	-3.438504000	-2.061742000
1	-1.419652000	-3.110196000	-0.377051000
1	-2.037093000	-1.344039000	-2.788660000
1	-3.236259000	-2.256151000	-1.858110000
15	-0.120568000	2.033643000	0.955130000
15	0.179167000	-1.228013000	1.839996000
1	2.388014000	1.220591000	-2.633891000
6	4.490418000	0.882737000	-2.418720000
1	4.743699000	1.618449000	-3.190238000
1	5.279913000	0.923205000	-1.664727000
1	4.515537000	-0.103621000	-2.884025000
6	3.127410000	2.638339000	-1.237608000
1	2.143481000	2.926196000	-0.875292000
1	3.840215000	2.747703000	-0.418026000
1	3.415968000	3.352690000	-2.016501000
6	4.769564000	-1.635086000	0.009767000
1	4.338137000	-2.569162000	-0.355356000
1	5.371759000	-1.204393000	-0.791583000
1	5.447372000	-1.888218000	0.833074000
6	4.339468000	0.525486000	1.245365000
1	4.927659000	0.168033000	2.097150000
1	5.017804000	1.073330000	0.587700000
1	3.598311000	1.228802000	1.625338000
1	3.110051000	-1.211174000	1.260968000
6	-3.969689000	0.693331000	-2.919517000
1	-4.896667000	0.201946000	-2.619708000
1	-4.242447000	1.581876000	-3.500370000
1	-3.433119000	0.019264000	-3.588243000
6	-3.882264000	2.173292000	-0.887282000
1	-3.344488000	2.483546000	0.009024000
1	-4.051865000	3.068313000	-1.495135000
1	-4.860884000	1.802826000	-0.576259000
1	-2.217512000	1.596037000	-2.099836000
1	-3.398305000	-1.847863000	0.778747000
6	-4.076897000	-0.052036000	1.723632000
1	-4.711417000	-0.617628000	2.414419000

1	-3.162627000	0.204274000	2.248285000
1	-4.601482000	0.876132000	1.488396000
6	-5.149818000	-1.169045000	-0.240139000
1	-5.808775000	-1.714626000	0.444640000
1	-5.663403000	-0.244312000	-0.510742000
1	-5.046302000	-1.773662000	-1.141740000
6	1.213993000	-0.575442000	3.250325000
1	0.707889000	0.282429000	3.696902000
1	1.339917000	-1.340134000	4.021793000
1	2.195328000	-0.251937000	2.907387000
6	-1.286975000	-1.692551000	2.892387000
1	-2.008757000	-2.264916000	2.310148000
1	-0.960719000	-2.300377000	3.740949000
1	-1.777348000	-0.799115000	3.275608000
6	0.888197000	-2.937052000	1.702708000
1	1.894071000	-2.912614000	1.286483000
1	0.918311000	-3.420402000	2.683189000
1	0.261085000	-3.518496000	1.027876000
6	1.304828000	2.772268000	1.907536000
1	1.023443000	3.743569000	2.324576000
1	1.584202000	2.108796000	2.725149000
1	2.170049000	2.907507000	1.263631000
6	-0.533295000	3.527308000	-0.084741000
1	0.262633000	3.703426000	-0.809824000
1	-1.451749000	3.343319000	-0.640158000
1	-0.657776000	4.424831000	0.527988000
6	-1.396281000	2.285397000	2.290217000
1	-2.394558000	2.126738000	1.889131000
1	-1.234948000	1.565596000	3.095012000
1	-1.336825000	3.295378000	2.705483000
1	0.056974000	1.099845000	-1.459518000
1	-0.131770000	0.378763000	-1.780959000

-2395.954583

TS1-Mn1-PMe₃

25	0.001731000	-0.028541000	-0.113006000
15	-2.401138000	-0.223389000	-0.616493000
15	2.343724000	-0.066027000	-0.677496000
7	0.032831000	-1.676721000	-1.527277000
6	2.359724000	-1.330936000	-2.062287000
6	1.259070000	-2.361619000	-1.852001000
6	-1.156349000	-2.479222000	-1.623591000
6	-2.337500000	-1.562389000	-1.922843000
6	3.706300000	-0.680948000	0.509336000
6	3.121781000	1.344029000	-1.699592000

6	-3.818197000	-0.931121000	0.439934000
6	-3.145682000	1.249953000	-1.566358000
1	2.135220000	-0.765554000	-2.971588000
1	3.335009000	-1.796627000	-2.199595000
1	1.145192000	-2.950410000	-2.780764000
1	1.575096000	-3.088815000	-1.082119000
1	-1.070350000	-3.221257000	-2.437102000
1	-1.361612000	-3.064538000	-0.701985000
1	-2.153621000	-1.086526000	-2.887267000
1	-3.279446000	-2.108138000	-1.990839000
15	-0.128794000	1.963477000	1.003470000
15	0.195441000	-1.339474000	1.776736000
1	2.381657000	1.408407000	-2.506223000
6	4.486477000	1.027377000	-2.334623000
1	4.744498000	1.809380000	-3.057411000
1	5.280360000	1.008714000	-1.584440000
1	4.499821000	0.074684000	-2.865336000
6	3.167647000	2.726810000	-1.041774000
1	2.191089000	3.034518000	-0.678306000
1	3.873755000	2.769164000	-0.210513000
1	3.491190000	3.469964000	-1.778998000
6	4.774010000	-1.628572000	-0.057486000
1	4.336747000	-2.542695000	-0.464654000
1	5.372919000	-1.161611000	-0.841062000
1	5.456529000	-1.926070000	0.746713000
6	4.363457000	0.463355000	1.294778000
1	4.954535000	0.055431000	2.121517000
1	5.040722000	1.043626000	0.664921000
1	3.629129000	1.147689000	1.719952000
1	3.128425000	-1.264866000	1.226586000
6	-4.005730000	0.933730000	-2.801399000
1	-4.322320000	1.873017000	-3.269038000
1	-3.462452000	0.366313000	-3.557534000
1	-4.907849000	0.375916000	-2.545017000
6	-3.899050000	2.234843000	-0.658277000
1	-3.359475000	2.465436000	0.259017000
1	-4.062231000	3.178316000	-1.189691000
1	-4.880696000	1.846693000	-0.379261000
1	-2.237002000	1.746925000	-1.919088000
1	-3.401726000	-1.917892000	0.674311000
6	-4.060974000	-0.200266000	1.768106000
1	-4.688092000	-0.815878000	2.421778000
1	-3.137721000	0.011294000	2.298636000
1	-4.584493000	0.745483000	1.613554000
6	-5.168220000	-1.157006000	-0.262088000
1	-5.821886000	-1.748741000	0.388477000

1	-5.678954000	-0.211649000	-0.455982000
1	-5.081417000	-1.692953000	-1.208086000
6	1.228209000	-0.765613000	3.223593000
1	0.698046000	0.040572000	3.734813000
1	1.389818000	-1.578782000	3.936965000
1	2.192157000	-0.382488000	2.893766000
6	-1.244287000	-1.918728000	2.809747000
1	-1.982851000	-2.423025000	2.186780000
1	-0.901465000	-2.613776000	3.581904000
1	-1.720451000	-1.069045000	3.298253000
6	0.947559000	-3.022193000	1.510560000
1	1.918239000	-2.936829000	1.025784000
1	1.063395000	-3.555105000	2.458370000
1	0.293772000	-3.596107000	0.852913000
6	1.286630000	2.645770000	2.013841000
1	1.027450000	3.624558000	2.428176000
1	1.502682000	1.965328000	2.836872000
1	2.184625000	2.748906000	1.412087000
6	-0.508978000	3.492041000	0.003387000
1	0.254150000	3.626681000	-0.763855000
1	-1.464286000	3.367220000	-0.503570000
1	-0.550873000	4.388049000	0.629761000
6	-1.404854000	2.189835000	2.346432000
1	-2.405752000	2.006739000	1.964261000
1	-1.213786000	1.471582000	3.146986000
1	-1.364132000	3.199767000	2.764886000
1	-0.071319000	0.711998000	-1.655913000
1	-0.047828000	-0.245986000	-1.804346000

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3-Mn1-PMe₃

25	-0.000723000	-0.027300000	-0.105377000
15	-2.337911000	-0.232619000	-0.613975000
15	2.292001000	-0.072830000	-0.685621000
7	0.034186000	-1.765509000	-1.533611000
6	2.376805000	-1.460997000	-1.960576000
6	1.299078000	-2.493259000	-1.681608000
6	-1.173926000	-2.594344000	-1.518226000
6	-2.342120000	-1.673481000	-1.832026000
6	3.682449000	-0.594868000	0.529100000
6	3.065929000	1.257802000	-1.808494000
6	-3.788224000	-0.879941000	0.464935000
6	-3.098317000	1.181987000	-1.639358000
1	2.175615000	-0.998472000	-2.932768000
1	3.359888000	-1.921923000	-2.028219000

1	1.241118000	-3.224389000	-2.502443000
1	1.501892000	-3.044073000	-0.764974000
1	-1.113791000	-3.405608000	-2.259991000
1	-1.278857000	-3.052673000	-0.530902000
1	-2.207596000	-1.282093000	-2.842798000
1	-3.285315000	-2.218096000	-1.823966000
15	-0.132429000	1.984203000	0.967143000
15	0.206212000	-1.282107000	1.805839000
1	2.324181000	1.252039000	-2.615435000
6	4.439755000	0.927942000	-2.414336000
1	4.685706000	1.666284000	-3.185968000
1	5.231064000	0.975173000	-1.662721000
1	4.477453000	-0.056879000	-2.882742000
6	3.077770000	2.679587000	-1.239858000
1	2.099699000	2.966963000	-0.865111000
1	3.804458000	2.797545000	-0.433681000
1	3.351468000	3.388963000	-2.028874000
6	4.775377000	-1.554174000	0.033069000
1	4.367768000	-2.513204000	-0.294370000
1	5.357388000	-1.135530000	-0.789465000
1	5.471125000	-1.765970000	0.853331000
6	4.317120000	0.606294000	1.244596000
1	4.910378000	0.262877000	2.099109000
1	4.988758000	1.156976000	0.582233000
1	3.568709000	1.302855000	1.619879000
1	3.110672000	-1.142270000	1.279039000
6	-3.931129000	0.803516000	-2.875021000
1	-4.818998000	0.222308000	-2.619385000
1	-4.271185000	1.718378000	-3.373771000
1	-3.356781000	0.236650000	-3.609429000
6	-3.879368000	2.191687000	-0.782788000
1	-3.358224000	2.463917000	0.134548000
1	-4.039892000	3.113093000	-1.352768000
1	-4.862744000	1.807296000	-0.505372000
1	-2.184965000	1.667761000	-1.990954000
1	-3.383816000	-1.858338000	0.750835000
6	-4.039914000	-0.093605000	1.758179000
1	-4.669734000	-0.681036000	2.435393000
1	-3.120332000	0.142178000	2.283112000
1	-4.564010000	0.843667000	1.560785000
6	-5.138727000	-1.126369000	-0.231188000
1	-5.801820000	-1.679205000	0.444232000
1	-5.639653000	-0.187076000	-0.473110000
1	-5.059433000	-1.707635000	-1.150896000
6	1.211555000	-0.609940000	3.237548000
1	0.676216000	0.236216000	3.671940000

1	1.348970000	-1.367362000	4.014939000
1	2.186950000	-0.258448000	2.905492000
6	-1.242905000	-1.805165000	2.866707000
1	-1.955454000	-2.386806000	2.280636000
1	-0.905810000	-2.410343000	3.713716000
1	-1.751983000	-0.923505000	3.252919000
6	0.980968000	-2.992189000	1.741788000
1	1.994145000	-2.952715000	1.340005000
1	1.020903000	-3.438854000	2.739544000
1	0.380921000	-3.637881000	1.097140000
6	1.287652000	2.747889000	1.917873000
1	0.998006000	3.720656000	2.326308000
1	1.572070000	2.094045000	2.741775000
1	2.152398000	2.887741000	1.274333000
6	-0.548743000	3.477028000	-0.072112000
1	0.233172000	3.633226000	-0.814907000
1	-1.476414000	3.300619000	-0.611368000
1	-0.650706000	4.378616000	0.539656000
6	-1.395458000	2.258492000	2.318105000
1	-2.399775000	2.098622000	1.933040000
1	-1.226504000	1.542164000	3.124889000
1	-1.330774000	3.271413000	2.726497000
1	-0.090014000	0.816869000	-1.509596000
1	-0.039597000	-1.146719000	-2.338282000

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4-Mn1-PMe₃

25	-0.013438000	0.155409000	-0.056556000
15	2.418747000	-0.142329000	-0.474580000
15	-2.385669000	-0.313964000	-0.396814000
7	-0.036456000	-0.280284000	-2.211368000
6	-2.422905000	-0.720108000	-2.227937000
6	-1.284276000	-0.023487000	-2.954269000
6	1.167720000	0.153654000	-2.938325000
6	2.363157000	-0.543491000	-2.305373000
6	-3.722612000	1.028931000	-0.203273000
6	-3.147550000	-1.941929000	0.211069000
6	3.827681000	1.135215000	-0.535150000
6	3.163300000	-1.703575000	0.317834000
1	-2.264889000	-1.799578000	-2.294648000
1	-3.383124000	-0.502954000	-2.691902000
1	-1.203918000	-0.411200000	-3.979948000
1	-1.449216000	1.049442000	-3.028076000
1	1.100904000	-0.117450000	-4.001892000
1	1.252361000	1.243219000	-2.883948000

1	2.226083000	-1.618960000	-2.417340000
1	3.288641000	-0.271351000	-2.811313000
15	0.119392000	0.124885000	2.269532000
15	-0.223075000	2.449489000	-0.200851000
1	-2.453560000	-2.659305000	-0.237181000
6	-4.549861000	-2.260754000	-0.329483000
1	-4.807656000	-3.295149000	-0.078531000
1	-5.313194000	-1.619943000	0.116952000
1	-4.615617000	-2.163050000	-1.414706000
6	-3.077444000	-2.165305000	1.723389000
1	-2.066129000	-2.017031000	2.094375000
1	-3.757092000	-1.510433000	2.272338000
1	-3.359173000	-3.197961000	1.951335000
6	-4.813174000	1.104375000	-1.282672000
1	-4.401055000	1.307355000	-2.273268000
1	-5.406357000	0.190841000	-1.343117000
1	-5.496633000	1.926497000	-1.044140000
6	-4.350839000	1.035731000	1.198618000
1	-4.927160000	1.956003000	1.338514000
1	-5.036722000	0.198128000	1.336698000
1	-3.603467000	0.991023000	1.989486000
1	-3.137994000	1.945250000	-0.289951000
6	3.929900000	-2.650355000	-0.619163000
1	4.781187000	-2.163405000	-1.099383000
1	4.315042000	-3.494367000	-0.037287000
1	3.286912000	-3.066755000	-1.395361000
6	3.999684000	-1.405650000	1.573213000
1	3.515357000	-0.700931000	2.249500000
1	4.157779000	-2.335022000	2.129053000
1	4.983454000	-1.005495000	1.322281000
1	2.271209000	-2.235835000	0.651106000
1	3.410258000	1.853200000	-1.250546000
6	4.087315000	1.887768000	0.777714000
1	4.672626000	2.790815000	0.576031000
1	3.168990000	2.191263000	1.270738000
1	4.660311000	1.280723000	1.479920000
6	5.168810000	0.643646000	-1.108372000
1	5.828652000	1.503138000	-1.268327000
1	5.676490000	-0.029301000	-0.415998000
1	5.071051000	0.127354000	-2.063675000
6	-1.209521000	3.345352000	1.102365000
1	-0.662546000	3.317045000	2.045589000
1	-1.359926000	4.391224000	0.821850000
1	-2.178719000	2.875929000	1.257432000
6	1.241896000	3.595836000	-0.158732000
1	1.936182000	3.356356000	-0.963531000

1	0.914821000	4.632775000	-0.273146000
1	1.764077000	3.500082000	0.791342000
6	-1.016057000	3.197483000	-1.716171000
1	-2.019007000	2.801421000	-1.871775000
1	-1.081589000	4.283910000	-1.615619000
1	-0.412112000	2.964637000	-2.594824000
6	-1.328501000	0.560376000	3.357711000
1	-1.033216000	0.525665000	4.409880000
1	-1.686305000	1.562186000	3.126261000
1	-2.141731000	-0.144227000	3.204472000
6	0.572271000	-1.506573000	3.032122000
1	0.015795000	-2.318565000	2.564537000
1	1.629282000	-1.703767000	2.859020000
1	0.391496000	-1.494065000	4.110236000
6	1.369056000	1.195099000	3.137145000
1	2.370002000	0.947229000	2.792985000
1	1.184147000	2.248515000	2.919201000
1	1.321970000	1.045819000	4.219274000
1	0.054611000	-1.800487000	0.058341000
1	0.032219000	-1.311898000	-2.146411000
6	0.076659000	-2.903327000	-0.316191000
8	0.124677000	-3.031539000	-1.557717000
8	0.045095000	-3.726770000	0.600821000

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