Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Adsorption and Decomposition of Dimethyl Methylphosphonate on Size-Selected $(MoO_3)_3$ Clusters

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Supporting Information

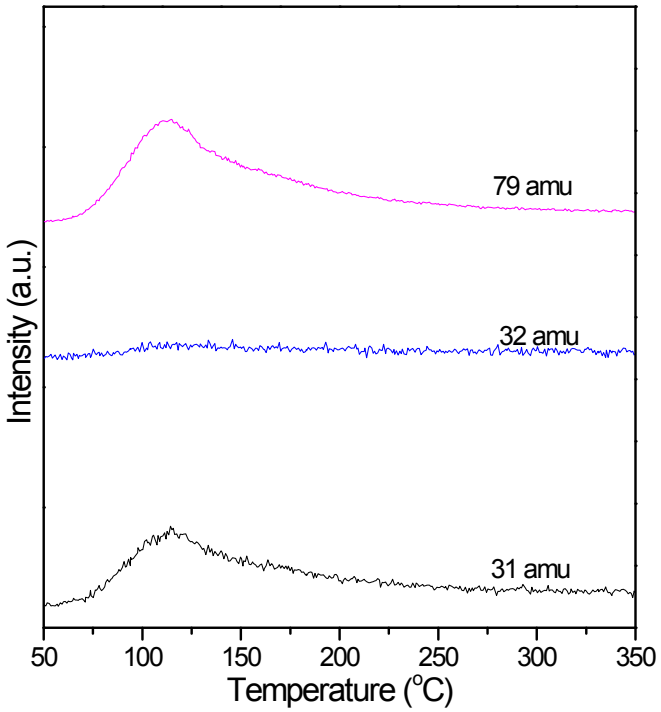

Figure S1. TPD Profiles of DMMP on HOPG**.** 79 amu is the major fragment of DMMP, 32 amu is methanol, 31 amu is methoxy which is a fragment of both methanol and DMMP.

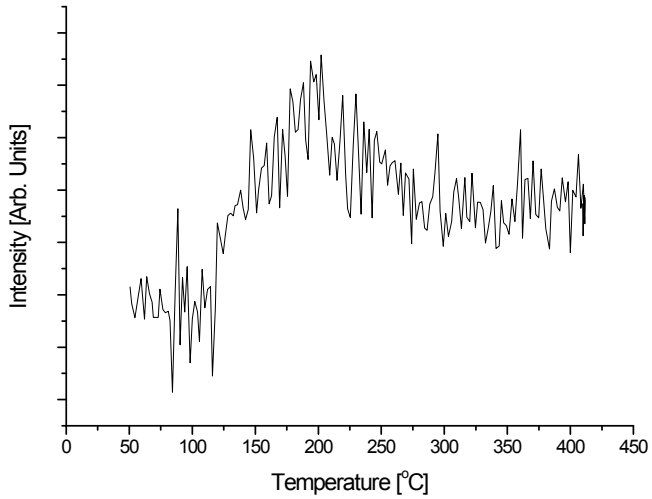

Figure S2 Subtraction of DMMP Contribution from 15 amu.

Table S1 Calculated decomposition energies (in kcal/mol) of DMMP in gas phase

Reaction		DFT functional[a]		
		B3LYP	CAM-B3LYP	B3LYP+D3
1	P=O	127	130.7	128.5
2	P-CH_3	79.3	84.0	82.0
3	PO-CH_3 (1)	76.8	83.3	78.7
4	P-OCH_3 (1)	86.6	93.1	89.5
5	CH_3OH loss (intramolecular)	64.8	67.5	64.1

[a] All calculations were carried out using 6-31+G(d,p) basis set

Atomic coordinates (B3LYP+D3)

DMMP molecule

15	0.088663000	-0.019321000	-0.046044000
8	0.090948000	-0.101696000	1.441772000
6	1.701715000	0.103974000	-0.850768000
1	1.577748000	0.156737000	-1.934450000
1	2.214168000	0.999035000	-0.490714000
1	2.292054000	-0.777337000	-0.587391000
8	-0.673052000	-1.272400000	-0.760118000
8	-0.676993000	1.242246000	-0.704968000
6	-0.784244000	-2.535371000	-0.073219000
1	-0.977868000	-2.381499000	0.991336000
1	-1.616543000	-3.066694000	-0.538289000
1	0.135120000	-3.118220000	-0.199955000
6	-2.021071000	1.543550000	-0.274014000
1	-2.708691000	0.758893000	-0.605697000
1	-2.061461000	1.643251000	0.814631000
1	-2.286558000	2.490248000	-0.746028000

DMMP on Mo_3O_9

42	1.217994000	-0.592783000	-0.100912000
8	1.805172000	0.212826000	-1.728211000
8	1.826194000	-2.403893000	-0.051643000
8	-0.477293000	-0.668296000	-0.192328000
8	1.569599000	0.320006000	1.308903000
42	3.380694000	-3.119082000	-0.913199000
42	3.367598000	-0.236494000	-2.740997000
8	3.828486000	-2.073997000	-2.452551000
8	4.689628000	-3.430399000	0.146528000
8	2.910189000	-4.637454000	-1.515323000
8	2.914408000	-0.122819000	-4.375446000
8	4.661897000	0.863726000	-2.540724000
15	4.903300000	0.093011000	0.650790000
8	3.862310000	-0.659755000	-0.182138000
6	4.536168000	1.840338000	0.786169000
1	4.531219000	2.263156000	-0.221642000
1	3.548592000	1.944519000	1.242642000
1	5.294442000	2.332695000	1.398303000

8	5.064158000	-0.529757000	2.113792000
8	6.369710000	0.059806000	0.040161000
6	4.062238000	-1.349446000	2.774888000
1	3.972735000	-2.304980000	2.256361000
1	4.441973000	-1.505596000	3.784395000
1	3.101620000	-0.831996000	2.807389000
6	6.959315000	-1.172815000	-0.453662000
1	8.008483000	-0.942966000	-0.635285000
1	6.862022000	-1.971462000	0.284660000
1	6.469667000	-1.460855000	-1.386659000

DMMP on Mo_3O_8

42	1.039118000	-0.242622000	-0.120169000
8	1.581301000	0.043342000	-2.003872000
8	1.422986000	-2.161880000	0.218434000
8	-0.057511000	0.724505000	0.729163000
42	3.013615000	-3.031731000	-0.268459000
42	3.221656000	-0.483394000	-2.741527000
8	3.523870000	-2.173339000	-1.886632000
8	4.219977000	-2.780248000	0.939347000
8	2.736048000	-4.709180000	-0.441989000
8	3.092494000	-0.596893000	-4.442083000
8	4.488186000	0.611390000	-2.346430000
15	3.556502000	0.844398000	1.823092000
8	2.931718000	0.349938000	0.510733000
6	3.250818000	2.589798000	2.090313000
1	3.653530000	3.143784000	1.238910000
1	2.172308000	2.752318000	2.160128000
1	3.738023000	2.914259000	3.012176000
8	2.964818000	0.177023000	3.136286000

8	5.121127000	0.603193000	1.798201000
6	2.972945000	-1.261449000	3.380322000
1	3.955303000	-1.681931000	3.161983000
1	2.725616000	-1.375472000	4.434799000
1	2.214562000	-1.737365000	2.755750000
6	5.870522000	0.040500000	0.669004000
1	6.906163000	0.323269000	0.853546000
1	5.751870000	-1.043027000	0.677087000
1	5.513228000	0.460768000	-0.272174000

DMMP on Mo_3O_9H

42	1.164004000	-0.564688000	-0.120694000
8	1.778615000	0.146605000	-1.752693000
8	1.761002000	-2.376663000	0.019143000
8	-0.537367000	-0.580270000	-0.173256000
8	1.609405000	0.382457000	1.249583000
42	3.143426000	-3.199349000	-1.007583000
42	3.340780000	-0.208663000	-2.864755000
8	3.411051000	-2.112287000	-2.522017000
8	4.586559000	-3.446763000	-0.101906000
8	2.608238000	-4.730053000	-1.527128000
8	2.757257000	-0.100295000	-4.445999000
15	4.889943000	0.160614000	0.624812000
8	3.914042000	-0.564468000	-0.278542000
6	4.505233000	1.894924000	0.871370000
1	4.511628000	2.404657000	-0.095613000
1	3.502601000	1.948178000	1.303710000
1	5.238790000	2.350517000	1.539519000
8	5.102531000	-0.525428000	2.046668000

8	6.360435000	0.200961000	-0.041227000
6	4.154970000	-1.470127000	2.630953000
1	4.173759000	-2.398639000	2.059744000
1	4.512646000	-1.637431000	3.646376000
1	3.152678000	-1.037793000	2.646236000
6	7.101356000	-1.051709000	-0.181782000
1	7.904189000	-0.843003000	-0.888262000
1	7.511558000	-1.332072000	0.790301000
1	6.449582000	-1.845319000	-0.556459000
8	4.974896000	0.722144000	-2.685574000
1	5.587753000	0.654029000	-1.930743000

DMMP on $Mo_3O_9H_2$ (A1)

42	1.012009000	-0.459897000	-0.083220000
8	1.596856000	0.400354000	-1.702048000
8	1.597601000	-2.228559000	-0.166568000
8	-0.686824000	-0.384334000	0.071507000
42	2.744774000	-3.425699000	-1.189555000
42	2.655586000	-0.393729000	-3.080431000
8	2.594435000	-2.185928000	-2.628831000
8	2.023352000	-4.886280000	-1.657263000
8	1.983706000	-0.195842000	-4.623638000
15	5.357917000	0.149295000	0.740334000
8	4.835491000	-0.745885000	-0.375759000
6	4.613511000	1.780065000	0.781755000
1	4.735434000	2.248418000	-0.198425000
1	3.550838000	1.670286000	1.010720000
1	5.106927000	2.383189000	1.546825000
8	5.250315000	-0.548206000	2.177862000
8	6.921920000	0.472819000	0.621445000

6	4.167746000	-1.440038000	2.567907000
1	4.127495000	-2.298367000	1.893822000
1	4.418442000	-1.769029000	3.576174000
1	3.216641000	-0.905282000	2.562345000
6	7.884320000	-0.607937000	0.550915000
1	8.857723000	-0.132933000	0.431116000
1	7.861927000	-1.190989000	1.475691000
1	7.674310000	-1.249539000	-0.309911000
8	4.423806000	0.190797000	-2.871043000
1	4.827202000	-0.136670000	-2.024950000
8	1.764691000	0.333444000	1.257414000
8	4.470378000	-3.409693000	-0.439422000
1	4.844414000	-2.494982000	-0.358689000

DMMP on $Mo_3O_9H_2$ (A2)

42	2.017925000	0.429483000	-0.508173000
8	2.784669000	0.172332000	-2.192346000
8	1.870781000	-1.330940000	0.288158000
8	0.480085000	1.161855000	-0.631529000
42	2.379080000	-2.997637000	-0.481711000
42	3.739370000	-1.112183000	-3.296807000
8	3.084149000	-2.438316000	-2.089659000
8	1.049801000	-4.002489000	-0.784310000
8	3.011582000	-1.362352000	-4.804595000
15	6.275429000	-0.861937000	0.691073000
8	7.679968000	-0.560968000	1.065267000
6	5.029662000	-0.749746000	1.986965000
1	5.377689000	-1.315688000	2.854123000
1	4.909133000	0.301637000	2.258628000
1	4.063798000	-1.130247000	1.651748000
8	5.723715000	0.030807000	-0.570836000
8	6.016714000	-2.356245000	0.073795000
6	5.987356000	1.468021000	-0.575768000

1	7.047685000	1.647542000	-0.386587000
1	5.707983000	1.815904000	-1.570557000
1	5.354020000	1.954123000	0.168007000
6	7.034384000	-2.962811000	-0.776849000
1	6.863125000	-4.038645000	-0.733552000
1	6.913054000	-2.605559000	-1.802634000
1	8.028011000	-2.719147000	-0.395537000
8	5.586970000	-0.751007000	-3.190970000
1	5.915886000	-0.535994000	-2.289661000
8	3.048474000	1.385770000	0.486172000
8	3.730313000	-3.767241000	0.570077000
1	4.639519000	-3.393494000	0.498174000

DMMP on $Mo_3O_9H_2$ (A3)

42	2.156300000	-0.258632000	0.064850000
8	2.823278000	-0.224013000	-1.675522000
8	2.486288000	-2.033860000	0.773927000
8	0.479047000	0.067233000	0.071545000
8	2.991515000	0.913599000	1.018296000
42	3.428562000	-3.385700000	-0.162322000
42	3.954165000	-1.138356000	-2.964528000
8	3.699263000	-2.683210000	-1.833187000
8	2.460855000	-4.764058000	-0.337495000
8	3.114607000	-1.463792000	-4.395232000
15	6.406654000	-0.031686000	0.371079000
8	5.460772000	-1.157137000	0.039078000
6	8.145648000	-0.491866000	0.274374000
1	8.330820000	-1.320411000	0.963014000
1	8.380336000	-0.809923000	-0.744609000
1	8.770899000	0.360429000	0.548405000
8	6.350216000	1.198241000	-0.672731000
8	6.178963000	0.625513000	1.808935000

6	5.286412000	2.200664000	-0.664196000
1	5.024126000	2.459391000	0.361624000
1	5.694712000	3.060689000	-1.194052000
1	4.411895000	1.806588000	-1.183397000
6	5.262827000	0.093353000	2.807096000
1	5.854552000	-0.135887000	3.695342000
1	4.520718000	0.863308000	3.012870000
1	4.760111000	-0.799964000	2.432814000
8	5.575701000	-0.179923000	-3.118152000
1	6.061292000	0.246912000	-2.388414000
8	5.074371000	-3.757678000	0.673753000
1	5.666687000	-2.982796000	0.558675000

DMMP on $Mo_3O_9H_2$ (A4)

42	-1.928652000	0.601169000	0.782171000
8	-1.213278000	1.662354000	-0.689512000
8	-1.425054000	-1.149255000	0.401788000
8	-3.631764000	0.715168000	0.785705000
42	0.115886000	-2.134363000	-0.233248000
42	0.088083000	0.974822000	-1.869209000
8	0.179596000	-0.850156000	-1.689526000
8	-0.438415000	-3.532811000	-0.998145000
8	-0.447621000	1.213796000	-3.455806000
15	1.896957000	0.997799000	1.498093000
8	0.951300000	0.296012000	0.551445000
6	1.478332000	2.704594000	1.850569000
1	1.465498000	3.250089000	0.901296000
1	0.477976000	2.721297000	2.293350000
1	2.219193000	3.140309000	2.526449000
8	2.114452000	0.151019000	2.849273000

8	3.392839000	1.077332000	0.910495000
6	0.985150000	-0.265070000	3.678546000
1	0.289670000	-0.863520000	3.086228000
1	1.425123000	-0.855402000	4.483026000
1	0.464182000	0.610474000	4.069490000
6	4.138679000	-0.150451000	0.680338000
1	5.022044000	0.139875000	0.110290000
1	4.431893000	-0.581326000	1.641356000
1	3.535546000	-0.865330000	0.110099000
8	1.783668000	1.840094000	-1.737525000
1	2.527171000	1.480833000	-1.226840000
8	-1.295624000	1.166751000	2.296286000
8	1.485939000	-2.478749000	1.051130000
1	1.905090000	-1.839345000	1.645832000

DMMP on $Mo_3O_9H_3$ (B1)

42	0.779159000	-0.451158000	-0.115689000
8	1.053016000	-0.247843000	-1.974281000
8	1.445676000	-2.226080000	0.155696000
8	-0.871086000	-0.336884000	0.273965000
42	2.642708000	-3.315715000	-0.869135000
42	2.322835000	-0.746637000	-3.308970000
8	2.508618000	-2.494925000	-2.565728000
8	2.116175000	-4.930769000	-0.926181000
8	1.612450000	-0.801710000	-4.850128000
15	5.671382000	0.466758000	0.625495000
8	4.584358000	-0.073691000	-0.298683000
6	5.613586000	2.248908000	0.830064000
1	5.762177000	2.728563000	-0.140446000
1	4.629707000	2.519568000	1.223662000
1	6.392214000	2.566603000	1.526705000
8	5.605355000	-0.211655000	2.073946000
8	7.157165000	0.193699000	0.116161000

6	4.428397000	-0.906325000	2.587316000
1	4.282983000	-1.838196000	2.037893000
1	4.653685000	-1.111636000	3.633259000
1	3.539033000	-0.277105000	2.505410000
6	7.598208000	-1.164704000	-0.162582000
1	8.642997000	-1.079054000	-0.458239000
1	7.507847000	-1.779971000	0.736179000
1	7.010006000	-1.593660000	-0.977762000
8	3.930968000	0.207889000	-3.008895000
1	4.314100000	0.215610000	-2.104130000
8	4.381849000	-2.858392000	-0.227607000
1	4.569401000	-1.895801000	-0.311835000
8	2.078304000	0.691518000	0.695237000
1	2.969015000	0.562849000	0.299361000

DMMP on $Mo_3O_9H_3$ (B2)

42	1.745496000	0.245774000	-0.685261000
8	2.345498000	-0.198859000	-2.421481000
8	1.887984000	-1.492311000	0.113279000
8	0.128794000	0.760192000	-0.740373000
42	2.417527000	-3.258339000	-0.441791000
42	3.584751000	-1.345387000	-3.294531000
8	3.202485000	-2.793388000	-2.109818000
8	1.054544000	-4.232298000	-0.706683000
8	3.045433000	-1.673779000	-4.869695000
15	6.212758000	-0.749212000	0.771821000
8	7.628141000	-0.608551000	1.194334000
6	4.922084000	-0.689352000	2.026359000
1	5.149800000	-1.434677000	2.792544000
1	4.915956000	0.304370000	2.480733000
1	3.941474000	-0.896271000	1.591401000
8	5.774677000	0.402790000	-0.348758000
8	5.828540000	-2.110703000	-0.024491000

6	6.591612000	1.612791000	-0.466953000
1	7.649361000	1.350433000	-0.436069000
1	6.325935000	2.057237000	-1.426537000
1	6.347016000	2.299640000	0.347286000
6	6.803169000	-2.746088000	-0.909152000
1	6.427772000	-3.754787000	-1.080806000
1	6.847135000	-2.201224000	-1.853900000
1	7.779812000	-2.773800000	-0.422365000
8	5.322004000	-0.632075000	-2.982513000
1	5.528280000	-0.267109000	-2.098225000
8	3.785720000	-3.887676000	0.718773000
1	4.634021000	-3.405066000	0.692728000
8	3.092759000	1.351361000	0.080918000
1	4.028180000	1.116949000	-0.076844000

DMMP on $Mo_3O_9H_3$ (B3)

42	2.827881000	-0.063146000	-0.409182000
8	3.004398000	-0.587021000	-2.196046000
8	3.218850000	-1.794984000	0.299118000
8	1.215868000	0.366600000	-0.091152000
42	3.773991000	-3.503143000	-0.390376000
42	4.118135000	-1.527639000	-3.383535000
8	4.386288000	-2.959084000	-2.127805000
8	2.403857000	-4.493130000	-0.534520000
8	3.209824000	-2.021160000	-4.729964000
15	7.343783000	-0.970263000	-0.402062000
8	6.476182000	0.068448000	-1.075357000
6	7.782060000	-2.391812000	-1.402891000
1	6.867133000	-2.910223000	-1.702092000
1	8.304838000	-2.038615000	-2.294697000
1	8.428270000	-3.063186000	-0.833371000
8	8.732885000	-0.358225000	0.123628000
8	6.636416000	-1.660346000	0.877589000
6	8.933820000	1.068691000	0.294025000

1	8.426977000	1.624782000	-0.497710000
1	8.555574000	1.380932000	1.271479000
1	10.011113000	1.227155000	0.244830000
6	6.186643000	-0.882559000	2.022923000
1	5.581697000	-1.562039000	2.622365000
1	7.056090000	-0.547510000	2.594790000
1	5.575581000	-0.038185000	1.698036000
8	5.742473000	-0.593469000	-3.645022000
1	6.130156000	-0.156452000	-2.853649000
8	5.265156000	-4.115100000	0.637631000
1	5.957440000	-3.468003000	0.861901000
8	4.221935000	1.140111000	0.039284000
1	5.100474000	0.956241000	-0.369402000

Atomic coordinates (CAM-B3LYP)

DMMP molecule ($PC_3O_3H_9$)

15	0.084064000	-0.024749000	-0.053434000
8	0.079829000	-0.104799000	1.427236000
6	1.691212000	0.107269000	-0.843224000
1	1.577913000	0.157454000	-1.927093000
1	2.195114000	1.005751000	-0.482871000
1	2.289314000	-0.766178000	-0.575496000
8	-0.660984000	-1.277366000	-0.757334000
8	-0.682559000	1.224271000	-0.707034000
6	-0.781349000	-2.531503000	-0.075066000
1	-0.943396000	-2.373839000	0.992713000
1	-1.634391000	-3.047013000	-0.516578000
1	0.121595000	-3.130348000	-0.226882000
6	-2.013137000	1.538865000	-0.276709000
1	-2.708174000	0.761146000	-0.604023000
1	-2.048069000	1.640737000	0.810346000

1	-2.273047000	2.485698000	-0.748467000

$PC_2O_3H_6^{\bullet}$ (product of P-CH_3 bond cleavage reaction)

15	-0.665841000	-0.262543000	0.234939000
8	-1.236953000	-0.397853000	1.618119000
8	-0.751074000	-1.580867000	-0.724175000
8	-1.434478000	0.762133000	-0.777138000
6	-0.444666000	-2.875258000	-0.163222000
1	-1.040592000	-3.057641000	0.734440000
1	-0.698407000	-3.598781000	-0.938479000
1	0.621199000	-2.951750000	0.073526000
6	-1.879325000	2.040078000	-0.274153000
1	-2.492797000	1.910157000	0.620834000
1	-1.024870000	2.686751000	-0.051198000
1	-2.470787000	2.481745000	-1.076666000

$PC_2O_3H_6^{\bullet}$ (product of PO-CH_3 bond cleavage reaction)

15	0.068656000	-0.052149000	-0.140642000
8	0.070766000	-0.183811000	1.396639000
6	1.705906000	0.119560000	-0.867991000
1	1.626525000	0.175454000	-1.956627000

1	2.187627000	1.026041000	-0.492768000
1	2.299066000	-0.753766000	-0.587887000
8	-0.683585000	-1.328468000	-0.571462000
8	-0.652010000	1.294309000	-0.647506000
6	-2.026588000	1.570092000	-0.280826000
1	-2.682191000	0.786035000	-0.666588000
1	-2.118705000	1.637615000	0.805601000
1	-2.271892000	2.527063000	-0.740509000

$PC_2O_2H_6^{\bullet}$ (product of P-OCH_3 bond cleavage reaction)

15	0.045528000	-0.141238000	-0.114822000
8	0.013838000	-0.183235000	1.393366000
6	1.721467000	0.127511000	-0.834951000
1	1.653997000	0.171740000	-1.923908000
1	2.119821000	1.069403000	-0.445458000
1	2.364149000	-0.701039000	-0.530547000
8	-0.739423000	1.135349000	-0.802936000
6	-2.005818000	1.566864000	-0.269021000
1	-2.780228000	0.817126000	-0.463159000
1	-1.929353000	1.748224000	0.806186000
1	-2.255657000	2.491739000	-0.790602000

TS for CH_3OH elimination reaction

15	0.398656000	-0.364716000	0.181139000
8	-0.080574000	-0.113789000	1.566062000
6	1.591001000	0.474933000	-0.722224000
1	0.099590000	0.951051000	-1.268469000
1	2.182018000	1.172902000	-0.133236000
1	2.164843000	-0.135962000	-1.415526000
8	0.190352000	-1.837226000	-0.427430000
8	-0.893101000	0.546964000	-0.949105000
6	-0.991935000	-2.602610000	-0.107087000
1	-1.160898000	-2.615071000	0.972114000
1	-1.857010000	-2.174506000	-0.622475000
1	-0.803891000	-3.612316000	-0.472183000
6	-1.832557000	1.480090000	-0.370179000
1	-2.326660000	0.989468000	0.469540000
1	-1.310970000	2.371229000	-0.008387000
1	-2.557273000	1.751190000	-1.140518000

$PC_2O_2H_5$ (product of CH_3OH elimination reaction)

15	0.577909000	-0.430400000	0.163868000
8	-0.258689000	0.017449000	1.311013000
6	1.771954000	0.303738000	-0.675683000
1	2.085227000	1.294111000	-0.376543000
1	2.243292000	-0.208254000	-1.503027000
8	0.303815000	-1.915960000	-0.392674000
6	-0.855244000	-2.674243000	0.031173000
1	-1.165577000	-2.381196000	1.035685000
1	-1.669881000	-2.505270000	-0.678024000
1	-0.553873000	-3.722025000	0.012894000

DMMP on Mo_3O_9

42	1.203503000	-0.592091000	-0.086827000
8	1.749425000	0.222574000	-1.710002000
8	1.809204000	-2.391944000	-0.067582000
8	-0.477974000	-0.664389000	-0.136252000
8	1.579696000	0.298593000	1.313511000
42	3.339570000	-3.091849000	-0.961369000
42	3.284385000	-0.209550000	-2.752504000
8	3.737924000	-2.042527000	-2.495908000
8	4.663295000	-3.408638000	0.054390000
8	2.866344000	-4.595700000	-1.553782000
8	2.802748000	-0.078271000	-4.361001000
8	4.566425000	0.885912000	-2.576406000
15	4.883637000	0.077802000	0.587317000
8	3.827998000	-0.657736000	-0.233568000
6	4.543660000	1.820505000	0.738267000
1	4.554324000	2.263868000	-0.259613000
1	3.557961000	1.944464000	1.191761000
1	5.307189000	2.288526000	1.361312000

8	5.059299000	-0.549978000	2.035354000
8	6.338887000	0.041198000	-0.025097000
6	4.092923000	-1.366940000	2.729069000
1	4.012179000	-2.334224000	2.232905000
1	4.490888000	-1.496026000	3.734258000
1	3.125241000	-0.865734000	2.768885000
6	7.051818000	-1.180794000	-0.301233000
1	8.073908000	-0.882113000	-0.526275000
1	7.029801000	-1.839541000	0.568044000
1	6.608260000	-1.680160000	-1.163392000

Mo_3O_9-$PC_2O_3H_6$• (product of P-CH_3 bond cleavage reaction)

42	1.187464000	-1.152281000	-0.152467000
8	1.837851000	0.016463000	-1.500739000
8	1.910082000	-2.880484000	-0.445806000
8	-0.474775000	-1.278525000	-0.382869000
8	1.382397000	-0.566008000	1.428076000
42	3.467291000	-3.377794000	-1.416859000
42	3.399883000	-0.153569000	-2.564279000
8	3.867536000	-1.990572000	-2.656898000
8	4.800845000	-3.834972000	-0.479053000
8	3.063182000	-4.739191000	-2.321263000
8	2.982502000	0.321136000	-4.124089000
8	4.689967000	0.853324000	-2.108471000
15	4.941314000	-0.481914000	0.852519000
8	3.903724000	-1.082543000	-0.086835000
8	4.875240000	-0.951016000	2.373466000
8	6.443993000	-0.879968000	0.530476000
6	3.952158000	-0.418825000	3.352614000
1	2.924726000	-0.501075000	3.000052000

1	4.102370000	-1.028213000	4.241816000
1	4.207524000	0.620154000	3.569311000
6	6.956436000	-1.183043000	-0.786072000
1	8.036629000	-1.239454000	-0.665712000
1	6.561946000	-2.146925000	-1.107885000
1	6.694548000	-0.392599000	-1.490012000

Mo_3O_9-$PC_2O_3H_6$• (product of PO-CH_3 bond cleavage reaction)

42	1.218340000	-0.617866000	-0.041150000
8	1.705573000	0.172094000	-1.701476000
8	1.883198000	-2.394970000	-0.021681000
8	-0.461654000	-0.716711000	-0.013240000
8	1.646303000	0.329442000	1.299617000
42	3.349230000	-3.120277000	-0.993436000
42	3.181073000	-0.231566000	-2.824488000
8	3.654503000	-2.046258000	-2.538083000
8	4.745560000	-3.429650000	-0.085085000
8	2.843948000	-4.622953000	-1.559014000
8	2.655650000	-0.094976000	-4.418130000
8	4.469960000	0.861898000	-2.665456000
15	4.907325000	0.133012000	0.567371000
8	3.899307000	-0.632302000	-0.265670000
6	4.592301000	1.878037000	0.704848000
1	4.661490000	2.321741000	-0.291039000
1	3.586376000	2.008462000	1.109204000
1	5.327184000	2.338998000	1.367402000

8	4.842955000	-0.589938000	2.002095000
8	6.415379000	0.051715000	0.113838000
6	7.082221000	-1.189605000	-0.225974000
1	8.146652000	-0.992426000	-0.117362000
1	6.763892000	-1.992450000	0.439072000
1	6.844986000	-1.439954000	-1.260271000

Mo_3O_9-$PC_2O_2H_6$• (product of P-OCH_3 bond cleavage reaction)

42	1.224808000	-0.544101000	-0.147791000
8	1.826209000	0.174242000	-1.803427000
8	1.807631000	-2.347107000	-0.017254000
8	-0.455722000	-0.590049000	-0.230913000
8	1.588590000	0.422319000	1.200980000
42	3.334874000	-3.128853000	-0.838072000
42	3.359390000	-0.343265000	-2.802311000
8	3.740823000	-2.168421000	-2.431946000
8	4.663715000	-3.371978000	0.189657000
8	2.864438000	-4.668201000	-1.330855000
8	2.924803000	-0.264183000	-4.427339000
8	4.695329000	0.691628000	-2.635486000
15	4.827835000	0.041355000	0.723798000
8	3.857712000	-0.632035000	-0.251177000
6	4.532442000	1.823486000	0.889483000
1	4.617695000	2.259684000	-0.110376000
1	3.528644000	1.969292000	1.290350000

1	5.282223000	2.254196000	1.554268000
8	6.361084000	-0.014083000	0.275868000
6	6.953824000	-1.075261000	-0.504383000
1	8.029098000	-0.917401000	-0.446757000
1	6.685883000	-2.049792000	-0.094405000
1	6.612893000	-0.984906000	-1.536831000

TS for CH_3OH elimination reaction

42	1.034983000	-0.793296000	-0.043874000
8	1.440789000	0.176997000	-1.624886000
8	1.806012000	-2.531369000	-0.176554000
8	-0.633363000	-1.020420000	-0.042537000
8	1.385186000	-0.000192000	1.415262000
42	3.342035000	-3.038737000	-1.168468000
42	2.937179000	-0.059658000	-2.775567000
8	3.545660000	-1.862925000	-2.637688000
8	4.741724000	-3.263293000	-0.223120000
8	2.996351000	-4.551007000	-1.822998000
8	2.358484000	0.120473000	-4.346528000
8	4.148350000	1.111806000	-2.604735000
15	4.627445000	0.201845000	0.563806000
8	3.641532000	-0.587262000	-0.277327000
6	4.997585000	1.849080000	0.477095000
1	4.556652000	2.381940000	-0.359601000
1	4.997876000	2.367312000	1.431041000
1	6.354769000	0.924311000	-0.017739000

8	4.868903000	-0.383898000	2.013316000
8	6.236937000	-0.157433000	-0.180456000
6	4.141541000	-1.484564000	2.607848000
1	4.292795000	-2.391466000	2.022058000
1	4.565723000	-1.601333000	3.603466000
1	3.083929000	-1.229911000	2.676140000
6	7.197030000	-1.169877000	0.214818000
1	8.050427000	-1.072872000	-0.454541000
1	7.490434000	-1.011585000	1.253455000
1	6.715592000	-2.138039000	0.085581000

Mo_3O_9-$PC_2O_2H_5$ (product of CH_3OH elimination reaction)

42	0.933332000	-0.916862000	-0.159252000
8	1.423581000	0.029627000	-1.727806000
8	1.835716000	-2.588155000	-0.181756000
8	-0.715247000	-1.239719000	-0.260621000
8	1.149450000	-0.058040000	1.290763000
42	3.485444000	-3.035829000	-1.016889000
42	3.012727000	-0.122556000	-2.763288000
8	3.732613000	-1.860396000	-2.485737000
8	4.786323000	-3.116420000	0.069098000
8	3.317717000	-4.588780000	-1.643508000
8	2.557838000	-0.030633000	-4.380592000
8	4.116516000	1.141209000	-2.527120000
15	4.389031000	0.338096000	0.795952000
8	3.569204000	-0.502764000	-0.150867000
6	5.178997000	1.711131000	0.484695000
1	5.145239000	2.097024000	-0.525409000
1	5.722894000	2.208406000	1.275259000

8	4.512994000	-0.188944000	2.270898000
6	3.833888000	-1.350112000	2.813720000
1	4.126706000	-2.239073000	2.255319000
1	4.177621000	-1.416362000	3.843765000
1	2.756421000	-1.190008000	2.778800000

DMMP on Mo_3O_8

42	0.951133000	-0.189253000	-0.190217000
8	1.631530000	0.187217000	-2.021123000
8	1.248970000	-2.162799000	-0.054521000
8	-0.045378000	0.781106000	0.748673000
42	2.830012000	-3.028820000	-0.451262000
42	3.261341000	-0.357961000	-2.708170000
8	3.545548000	-2.068364000	-1.922952000
8	3.908651000	-2.962502000	0.875512000
8	2.533345000	-4.654903000	-0.817893000
8	3.196952000	-0.422508000	-4.398903000
8	4.516089000	0.706323000	-2.261183000
15	3.500904000	0.795241000	1.801502000
8	2.870280000	0.126673000	0.585094000
6	3.104934000	2.527841000	1.929791000
1	3.424658000	3.028662000	1.013818000
1	2.025222000	2.639144000	2.051156000
1	3.619612000	2.961027000	2.788721000
8	3.010118000	0.206795000	3.184100000

8	5.068656000	0.641527000	1.743863000
6	3.340273000	-1.132719000	3.624982000
1	4.364723000	-1.138609000	4.000857000
1	2.642622000	-1.360404000	4.428400000
1	3.235191000	-1.850023000	2.809472000
6	5.807667000	-0.114565000	0.744543000
1	6.855112000	0.028287000	1.002664000
1	5.535177000	-1.168517000	0.807996000
1	5.597452000	0.282058000	-0.248979000

Mo_3O_8-$PC_2O_3H_6$• (product of P-CH_3 bond cleavage reaction)

42	1.592759000	-0.604548000	-0.213537000
8	2.110101000	0.045514000	-1.942141000
8	2.479257000	-2.298072000	-0.436610000
8	-0.067226000	-0.834653000	-0.156615000
42	3.556402000	-3.270174000	-1.627991000
42	2.881707000	-0.482524000	-3.573940000
8	3.618274000	-2.185633000	-3.175690000
8	5.096829000	-3.497219000	-0.962306000
8	2.900337000	-4.792160000	-1.952951000
8	1.719490000	-0.593401000	-4.794449000
8	4.060649000	0.615218000	-4.080401000
15	3.885329000	1.220422000	1.384265000
8	2.393478000	0.416106000	1.129893000
8	3.873465000	1.232361000	3.004991000
8	4.899619000	0.022298000	0.950113000
6	3.203374000	0.361434000	3.922234000
1	3.795389000	-0.539797000	4.097657000

1	3.101097000	0.915274000	4.855358000
1	2.215528000	0.092439000	3.543842000
6	5.144597000	-1.196078000	1.665424000
1	5.769253000	-1.816575000	1.024156000
1	5.670745000	-0.978929000	2.597945000
1	4.210701000	-1.726123000	1.873749000

Mo_3O_8-$PC_2O_3H_6$• (product of PO-CH_3 bond cleavage reaction)

42	0.864715000	0.072152000	-0.346043000
8	2.162573000	0.464619000	-1.687860000
8	0.983314000	-1.781390000	-0.027562000
8	-0.639405000	0.737700000	-0.666444000
42	2.628483000	-2.792161000	0.058572000
42	3.936751000	-0.237530000	-1.767232000
8	3.879742000	-2.037919000	-1.145453000
8	3.173419000	-3.105792000	1.631652000
8	2.234590000	-4.300355000	-0.578244000
8	4.319234000	-0.317486000	-3.405705000
8	5.113585000	0.772956000	-1.081301000
15	2.822492000	0.815736000	1.683428000
8	1.363541000	1.230521000	1.237155000
6	3.938680000	2.202549000	1.617620000
1	4.017741000	2.550224000	0.586839000
1	3.564154000	3.000692000	2.260799000
1	4.924872000	1.880946000	1.957241000

8	2.825567000	0.429235000	3.216832000
8	3.167385000	-0.338192000	0.736552000
6	2.049046000	-0.664605000	3.751898000
1	2.383162000	-1.606461000	3.314180000
1	2.234688000	-0.661433000	4.824229000
1	0.987279000	-0.493805000	3.560746000

Mo_3O_8-$PC_2O_2H_6$• (product of P-OCH_3 bond cleavage reaction)

42	1.727853000	-0.771994000	0.117974000
8	2.532959000	-0.021939000	-1.460497000
8	2.606899000	-2.464170000	-0.130069000
8	0.081161000	-0.965250000	-0.127271000
42	3.552754000	-3.505059000	-1.373006000
42	3.498135000	-0.450299000	-3.012310000
8	3.950725000	-2.271914000	-2.756244000
8	4.955228000	-4.149791000	-0.683503000
8	2.614152000	-4.789309000	-1.944116000
8	2.561709000	-0.234594000	-4.402568000
8	4.873829000	0.523052000	-3.152666000
15	2.954833000	0.654854000	3.118426000
8	2.297896000	0.065879000	1.677032000
6	3.887715000	2.050894000	2.401929000
1	4.694221000	1.668829000	1.771265000
1	3.225087000	2.690622000	1.813919000
1	4.325814000	2.635681000	3.214967000
8	1.714576000	1.554537000	3.702341000

6	0.731718000	0.927980000	4.530760000
1	1.191713000	0.211235000	5.219075000
1	0.246425000	1.719900000	5.101507000
1	-0.014623000	0.418413000	3.914634000

DMMP on Mo_3O_8: TS for CH_3OH elimination reaction

42	1.185451000	0.037819000	-0.574469000
8	2.221641000	0.113159000	-2.221539000
8	1.303636000	-1.941884000	-0.209201000
8	-0.298167000	0.709486000	-0.188519000
42	2.700946000	-3.093697000	-0.377445000
42	3.514897000	-0.990469000	-3.020524000
8	3.355974000	-2.635327000	-2.120778000
8	3.928529000	-2.727986000	0.770201000
8	2.205137000	-4.703624000	-0.188708000
8	3.271421000	-1.148265000	-4.687189000
8	5.056909000	-0.324711000	-2.757109000
15	3.442280000	1.132029000	1.728834000
8	2.468435000	0.158500000	1.079921000
6	2.986217000	2.459938000	2.669972000
1	3.643553000	3.323296000	2.633051000
1	1.923017000	2.684602000	2.662361000
1	3.471584000	1.161397000	3.662762000
8	3.882701000	0.230132000	3.214084000

8	4.823516000	1.282591000	1.004260000
6	3.409698000	-1.103569000	3.573610000
1	3.646549000	-1.770813000	2.745823000
1	3.947612000	-1.386641000	4.476548000
1	2.333565000	-1.070644000	3.745447000
6	5.664950000	0.174940000	0.571454000
1	6.566852000	0.204276000	1.182358000
1	5.150776000	-0.780987000	0.687365000
1	5.897441000	0.347828000	-0.478078000

Mo_3O_8-$PC_2O_2H_5$ (product of CH_3OH elimination reaction)

42	3.652969000	0.132935000	-0.942963000
8	3.179688000	-0.753856000	-2.568985000
8	2.860821000	-1.351588000	0.095404000
8	2.908658000	1.652195000	-1.060410000
42	2.012659000	-3.011628000	-0.042209000
42	2.268176000	-2.177284000	-3.393000000
8	1.772600000	-3.238809000	-1.908843000
8	2.974555000	-4.234357000	0.620780000
8	0.542863000	-3.005933000	0.794283000
8	0.916425000	-1.640764000	-4.251450000
8	3.258381000	-3.018101000	-4.471695000
15	3.996962000	0.779440000	1.653102000
8	5.327888000	0.367828000	-1.065024000
6	3.551729000	-0.007966000	3.011340000
1	3.750775000	0.375405000	4.005778000
1	3.035718000	-0.953841000	2.903323000
8	4.742256000	2.153490000	2.046333000
6	5.233488000	3.053904000	1.032420000

1	5.683815000	3.884643000	1.572923000
1	5.983931000	2.558926000	0.412631000
1	4.411373000	3.413393000	0.410063000

DMMP on Mo_3O_9H

42	1.175635000	-0.554836000	-0.121469000
8	1.757963000	0.156233000	-1.745125000
8	1.755563000	-2.362675000	0.001793000
8	-0.510983000	-0.564079000	-0.146331000
8	1.630003000	0.376645000	1.239069000
42	3.130548000	-3.179921000	-1.016502000
42	3.335752000	-0.206910000	-2.835226000
8	3.400881000	-2.116731000	-2.527759000
8	4.558075000	-3.432427000	-0.114872000
8	2.599736000	-4.700498000	-1.519582000
8	2.747687000	-0.092588000	-4.398040000
15	4.862523000	0.139717000	0.583007000
8	3.875960000	-0.566972000	-0.319416000
6	4.496774000	1.864979000	0.854984000
1	4.507197000	2.397108000	-0.098729000
1	3.499005000	1.930418000	1.294805000
1	5.239860000	2.297445000	1.526673000

8	5.087559000	-0.560033000	1.983139000
8	6.320754000	0.175797000	-0.084234000
6	4.158661000	-1.475296000	2.615801000
1	4.143681000	-2.411610000	2.058897000
1	4.551144000	-1.634605000	3.618408000
1	3.164984000	-1.028458000	2.664038000
6	7.123733000	-1.032086000	-0.145901000
1	7.922036000	-0.824688000	-0.856210000
1	7.538511000	-1.231543000	0.842462000
1	6.520677000	-1.879675000	-0.478525000
8	4.967837000	0.709259000	-2.674594000
1	5.609804000	0.648093000	-1.946382000

Mo_3O_9H -$PC_2O_3H_6$• (product of P-CH_3 bond cleavage reaction)

42	1.300010000	-0.574982000	-0.208200000
8	1.866205000	0.280239000	-1.905799000
8	1.694175000	-2.437113000	-0.093700000
8	-0.371401000	-0.552335000	-0.430762000
8	1.562470000	0.274171000	1.228808000
42	3.225594000	-3.093104000	-1.016850000
42	3.415060000	-0.249892000	-2.752334000
8	3.602942000	-2.074354000	-2.676738000
8	4.539476000	-3.560910000	-0.067158000
8	2.662596000	-4.528106000	-1.699016000
8	3.106814000	0.080141000	-4.364566000
15	4.599630000	0.041253000	0.650905000
8	3.661709000	-0.790694000	-0.431641000
8	5.063135000	-1.113803000	1.704726000
8	6.027978000	0.082935000	-0.226427000
6	4.248335000	-1.403262000	2.846238000
1	3.457427000	-2.107164000	2.574067000

1	4.899846000	-1.861465000	3.589951000
1	3.802968000	-0.492358000	3.257556000
6	6.973559000	-1.008981000	-0.282076000
1	7.726134000	-0.721877000	-1.016360000
1	7.431840000	-1.137229000	0.697941000
1	6.482167000	-1.938094000	-0.575258000
8	4.961907000	0.690155000	-2.492147000
1	5.488150000	0.546941000	-1.634713000

Mo_3O_9H -$PC_2O_3H_6$• (product of PO-CH_3 bond cleavage reaction)

42	1.144935000	-0.495204000	-0.172279000
8	1.771781000	0.320673000	-1.787064000
8	1.630581000	-2.331213000	-0.149223000
8	-0.533292000	-0.479768000	-0.298536000
8	1.489964000	0.350259000	1.260651000
42	3.138213000	-3.108110000	-1.012499000
42	3.283581000	-0.212904000	-2.793800000
8	3.571798000	-2.059283000	-2.556933000
8	4.426033000	-3.482922000	0.020199000
8	2.608026000	-4.589104000	-1.610207000
8	2.869603000	0.004088000	-4.409218000
15	4.805336000	0.082078000	0.479338000
8	3.697136000	-0.673088000	-0.253191000
6	4.362723000	1.791732000	0.764813000
1	4.219059000	2.292875000	-0.195303000
1	3.436068000	1.835193000	1.340378000
1	5.170959000	2.279401000	1.313053000
8	5.209697000	-0.552353000	1.863788000

8	6.180209000	0.049649000	-0.310502000
6	4.354333000	-1.416884000	2.644195000
1	4.299757000	-2.394799000	2.166435000
1	4.834401000	-1.497461000	3.617581000
1	3.359956000	-0.978682000	2.752021000
8	4.685874000	0.743010000	-2.542024000
1	6.049871000	0.330873000	-1.239319000

Mo_3O_9H -$PC_2O_2H_6$• (product of P-OCH_3 bond cleavage reaction)

42	1.285323000	-0.476634000	-0.100141000
8	1.828810000	0.320388000	-1.825928000
8	1.705254000	-2.329791000	0.071105000
8	-0.387114000	-0.491069000	-0.308970000
8	1.539250000	0.446212000	1.292682000
42	3.245655000	-3.011147000	-0.808728000
42	3.366476000	-0.259229000	-2.674086000
8	3.545642000	-2.084411000	-2.529917000
8	4.615985000	-3.320071000	0.131448000
8	2.749539000	-4.527089000	-1.352936000
8	3.014213000	0.008538000	-4.290056000
15	4.763241000	-0.115915000	0.735242000
8	3.653663000	-0.673989000	-0.365870000
6	4.396469000	1.679620000	0.757859000
1	4.305638000	2.103639000	-0.246078000
1	3.474847000	1.855821000	1.314813000
1	5.219997000	2.177926000	1.277097000
8	6.095885000	0.060919000	-0.320464000

6	7.109795000	-0.959480000	-0.322620000
1	7.921883000	-0.596428000	-0.952860000
1	7.475872000	-1.117314000	0.693912000
1	6.718657000	-1.900928000	-0.715920000
8	4.928543000	0.666895000	-2.493639000
1	5.492007000	0.493601000	-1.652048000

DMMP on Mo_3O_9H: TS for intramolecular CH_3OH elimination reaction

42	1.179304000	-0.589663000	-0.142754000
8	1.752712000	0.080755000	-1.787876000
8	1.786675000	-2.388906000	0.019087000
8	-0.507228000	-0.612449000	-0.149844000
8	1.642656000	0.359696000	1.196765000
42	3.135424000	-3.243480000	-0.994050000
42	3.293037000	-0.307098000	-2.914004000
8	3.399330000	-2.199491000	-2.515150000
8	4.569582000	-3.466350000	-0.091834000
8	2.601195000	-4.775185000	-1.458714000
8	2.655774000	-0.280446000	-4.459983000
15	4.876248000	0.348035000	0.393207000
8	3.919654000	-0.544536000	-0.356318000
6	4.607295000	1.878972000	1.047548000
1	5.402264000	2.606157000	0.917629000
1	3.588946000	2.245877000	0.960799000
1	4.755336000	0.707287000	2.293479000
8	4.993708000	-0.346279000	2.053293000

8	6.376184000	0.183239000	-0.122503000
6	4.219163000	-1.465384000	2.579508000
1	4.406380000	-2.320234000	1.931882000
1	4.589724000	-1.649993000	3.586424000
1	3.163097000	-1.196265000	2.585483000
6	7.051396000	-1.099468000	-0.093546000
1	7.907731000	-1.002969000	-0.758282000
1	7.388026000	-1.293648000	0.926320000
1	6.386192000	-1.896709000	-0.430881000
8	4.919964000	0.626095000	-2.858180000
1	5.605273000	0.658506000	-2.172737000

Mo_3O_9H-$PC_2O_2H_5$ (product of intramolecular CH_3OH elimination reaction)

42	1.269158000	-0.445278000	-0.177506000
8	1.818278000	0.295329000	-1.921665000
8	1.665000000	-2.299260000	0.033044000
8	-0.405868000	-0.433247000	-0.361405000
8	1.564001000	0.510798000	1.185230000
42	3.198280000	-3.022147000	-0.828337000
42	3.351227000	-0.316514000	-2.758571000
8	3.510050000	-2.139757000	-2.572605000
8	4.560872000	-3.332405000	0.123035000
8	2.678493000	-4.541193000	-1.341045000
8	2.995812000	-0.086166000	-4.379431000
15	4.745639000	-0.071366000	0.618024000
8	3.640258000	-0.694800000	-0.447691000
6	4.398769000	1.672718000	0.605214000
1	5.229143000	2.372371000	0.573994000
1	3.436910000	2.034809000	0.951509000
8	6.099230000	0.041489000	-0.405019000

6	7.097753000	-0.992704000	-0.334612000
1	7.915878000	-0.682518000	-0.984626000
1	7.459088000	-1.087604000	0.691512000
1	6.693811000	-1.951721000	-0.667430000
8	4.928274000	0.592265000	-2.615708000
1	5.489763000	0.458333000	-1.774755000

DMMP on Mo_3O_9H: TS for intermolecular CH_3OH elimination reaction

42	1.495359000	-0.869305000	0.024682000
8	1.529266000	-0.088729000	-1.584826000
8	1.802213000	-2.682645000	-0.200095000
8	-0.058723000	-0.694731000	0.646058000
8	2.601036000	-0.027752000	1.279015000
42	3.141170000	-3.369798000	-1.447137000
42	3.271126000	-0.174756000	-2.809633000
8	3.214036000	-2.149623000	-2.829491000
8	4.645655000	-3.659127000	-0.708699000
8	2.592980000	-4.848846000	-2.046391000
8	2.544837000	0.383815000	-4.223033000
15	4.220391000	0.132018000	0.561376000
8	3.742992000	-0.828471000	-0.582942000
6	4.033570000	1.935706000	0.519163000
1	3.243307000	2.198212000	-0.187747000
1	3.711486000	2.253112000	1.511860000
1	4.961524000	2.427683000	0.237886000
8	5.019485000	-0.442196000	1.811698000

8	5.822436000	0.320567000	-0.333766000
6	4.452738000	-1.181557000	2.908876000
1	4.053931000	-2.133665000	2.554842000
1	5.283257000	-1.361096000	3.590019000
1	3.670846000	-0.603799000	3.400097000
6	6.765724000	-0.774015000	-0.342012000
1	7.497875000	-0.555029000	-1.120125000
1	7.252436000	-0.811816000	0.630740000
1	6.257337000	-1.718251000	-0.551828000
8	4.850952000	0.615649000	-2.526705000
1	5.456171000	0.489833000	-1.422675000

Mo_3O_9H-$PC_2O_2H_5$ (product of intermolecular CH_3OH elimination reaction)

42	1.157874000	-0.834933000	-0.034641000
8	1.447311000	-0.032934000	-1.741033000
8	1.772315000	-2.610691000	-0.178843000
8	-0.380954000	-0.564476000	0.571056000
8	2.190418000	0.307650000	1.279209000
42	3.368860000	-3.162972000	-1.117327000
42	3.005305000	-0.243564000	-2.825352000
8	3.625993000	-2.032848000	-2.614162000
8	4.710958000	-3.424573000	-0.117192000
8	2.989549000	-4.677431000	-1.748086000
8	2.469280000	-0.116366000	-4.417134000
15	3.711327000	0.260710000	0.849927000
8	3.712344000	-0.700296000	-0.343184000
6	4.336575000	1.892287000	0.502670000
1	3.787539000	2.314548000	-0.339881000
1	4.219625000	2.521490000	1.386639000
1	5.391812000	1.818395000	0.233688000
8	4.600317000	-0.208290000	2.070699000

6	4.450875000	-1.499417000	2.700372000
1	4.670388000	-2.290815000	1.982164000
1	5.175080000	-1.517143000	3.512519000
1	3.441017000	-1.600165000	3.104199000
8	4.152095000	0.991933000	-2.638830000

DMMP on $Mo_3O_9H_2$ (A1)

42	0.821684000	-0.488083000	-0.195752000
8	1.413933000	0.317532000	-1.867083000
8	1.266304000	-2.238828000	-0.411429000
8	-0.836991000	-0.275571000	0.077505000
42	2.564783000	-3.501928000	-1.227231000
42	2.565566000	-0.481575000	-3.096842000
8	2.499326000	-2.237860000	-2.742919000
8	1.914518000	-4.970792000	-1.717440000
8	2.100535000	-0.193330000	-4.685506000
15	5.501172000	0.143275000	0.773258000
8	5.011615000	-0.726979000	-0.367786000
6	4.687347000	1.728257000	0.874735000
1	4.825294000	2.265188000	-0.066244000
1	3.620577000	1.561427000	1.046291000
1	5.114798000	2.308026000	1.694313000
8	5.403946000	-0.600259000	2.177234000
8	7.041246000	0.520724000	0.680897000

6	4.270531000	-1.403288000	2.579713000
1	4.251713000	-2.329853000	2.003505000
1	4.427706000	-1.622273000	3.634490000
1	3.338176000	-0.852562000	2.440535000
6	8.053526000	-0.497686000	0.577859000
1	8.998370000	0.028994000	0.456606000
1	8.072962000	-1.096759000	1.490458000
1	7.865771000	-1.131669000	-0.291351000
8	4.276462000	0.114809000	-2.744757000
1	4.698649000	-0.194459000	-1.887488000
8	1.742429000	0.214750000	1.072009000
8	4.240686000	-3.350019000	-0.394602000
1	4.680309000	-2.470360000	-0.326897000

DMMP on $Mo_3O_9H_2$ (A2)

42	1.725393000	0.349744000	-0.700009000
8	2.255233000	-0.058339000	-2.398275000
8	1.555782000	-1.419349000	0.119523000
8	0.282764000	1.237571000	-0.656278000
42	2.252884000	-3.004287000	-0.554451000
42	3.512218000	-1.196521000	-3.409110000
8	2.842525000	-2.597979000	-2.198477000
8	1.095980000	-4.217078000	-0.648706000
8	2.996383000	-1.528975000	-4.970560000
15	6.453867000	-0.859277000	0.736287000
8	7.861371000	-0.687441000	1.149723000
6	5.210758000	-0.690905000	2.016147000
1	5.384486000	-1.448541000	2.782673000
1	5.317993000	0.297251000	2.468801000
1	4.201511000	-0.780672000	1.613434000
8	6.000647000	0.103905000	-0.492680000
8	6.098975000	-2.303073000	0.072662000

6	6.232941000	1.530252000	-0.406322000
1	7.215561000	1.719896000	0.029300000
1	6.199348000	1.909443000	-1.426936000
1	5.432580000	1.985241000	0.179934000
6	7.092402000	-2.960750000	-0.755200000
1	6.818455000	-4.014435000	-0.783410000
1	7.065853000	-2.537031000	-1.760873000
1	8.079566000	-2.836302000	-0.309006000
8	5.271081000	-0.670076000	-3.029697000
1	5.610736000	-0.435149000	-2.138540000
8	2.974176000	1.167087000	0.136215000
8	3.700451000	-3.522943000	0.487096000
1	4.608409000	-3.156438000	0.356843000

DMMP on $Mo_3O_9H_2$ (A3)

42	1.855348000	-0.405819000	-0.131175000
8	2.451009000	-0.441110000	-1.847122000
8	2.234162000	-2.210877000	0.498229000
8	0.198081000	-0.060955000	-0.044815000
8	2.755337000	0.723980000	0.797461000
42	3.313236000	-3.460730000	-0.358358000
42	3.801977000	-1.138618000	-3.118891000
8	3.661939000	-2.751839000	-1.959773000
8	2.502373000	-4.917852000	-0.556264000
8	3.108618000	-1.517901000	-4.597323000
15	6.580666000	-0.109274000	0.463743000
8	5.637631000	-1.253578000	0.246267000
6	8.310705000	-0.509864000	0.250597000
1	8.570948000	-1.338615000	0.911821000
1	8.484319000	-0.807056000	-0.785712000
1	8.926713000	0.358540000	0.489049000
8	6.358206000	1.077329000	-0.601821000
8	6.473747000	0.565761000	1.900563000

6	5.500975000	2.218948000	-0.343188000
1	5.916555000	2.799045000	0.481903000
1	5.511872000	2.808129000	-1.258554000
1	4.486868000	1.890871000	-0.109094000
6	5.371912000	0.319159000	2.808315000
1	5.599226000	0.897764000	3.701898000
1	4.430155000	0.644153000	2.364681000
1	5.323603000	-0.743498000	3.051079000
8	5.352167000	-0.078015000	-3.037480000
1	5.793053000	0.304030000	-2.257133000
8	4.873463000	-3.706718000	0.604005000
1	5.426730000	-2.878365000	0.578931000

DMMP on $Mo_3O_9H_2$ (A4)

42	-1.999723000	0.534427000	0.664536000
8	-1.239617000	1.581874000	-0.797848000
8	-1.484723000	-1.162722000	0.266381000
8	-3.687876000	0.657875000	0.635454000
42	0.109123000	-2.193171000	-0.298159000
42	0.087108000	0.939024000	-1.930444000
8	0.181884000	-0.834654000	-1.785835000
8	-0.426236000	-3.551041000	-1.113509000
8	-0.421737000	1.237594000	-3.499470000
15	1.860552000	0.928771000	1.457103000
8	0.904327000	0.305011000	0.474561000
6	1.446418000	2.592680000	1.944172000
1	1.463113000	3.226210000	1.054095000
1	0.434558000	2.587076000	2.356908000
1	2.167695000	2.966489000	2.672838000
8	2.084051000	-0.001290000	2.739774000
8	3.334946000	1.047312000	0.850906000
6	1.123716000	-0.090974000	3.827053000

1	0.102182000	-0.076725000	3.444376000
1	1.337562000	-1.028412000	4.337474000
1	1.283924000	0.746447000	4.508575000
6	4.183631000	-0.110252000	0.675696000
1	5.050986000	0.236698000	0.117080000
1	4.490904000	-0.487031000	1.652071000
1	3.661645000	-0.890436000	0.116670000
8	1.749575000	1.827924000	-1.805949000
1	2.464842000	1.515301000	-1.231776000
8	-1.401838000	1.077835000	2.187662000
8	1.395779000	-2.511509000	1.061543000
1	1.737086000	-1.892319000	1.721507000

$Mo_3O_9H_2$ (A4) -$PC_2O_3H_6$• (product of P-CH_3 bond cleavage reaction)

42	-1.368981000	0.934725000	0.737667000
8	-0.952251000	1.544163000	-0.925054000
8	-1.755496000	-0.838574000	0.583874000
8	-2.737633000	1.749918000	1.273141000
42	-0.627391000	-2.139301000	-0.424899000
42	0.360852000	0.661756000	-2.157736000
8	-0.283024000	-1.137771000	-2.006379000
8	-1.800394000	-3.285824000	-0.769835000
8	-0.219566000	1.278755000	-3.604617000
15	1.558493000	0.572562000	1.318133000
8	0.805012000	-0.125805000	0.132611000
8	1.853829000	-0.488221000	2.502632000
8	3.086657000	0.495849000	0.609571000
6	0.994753000	-0.733064000	3.628107000
1	0.066926000	-1.210298000	3.305468000
1	1.548010000	-1.409570000	4.278444000
1	0.769770000	0.196577000	4.151340000
6	4.234599000	0.970963000	1.321543000

1	5.082634000	0.875080000	0.643645000
1	4.113786000	2.021107000	1.602915000
1	4.403330000	0.361367000	2.212460000
8	2.212062000	0.879124000	-2.053007000
1	2.702252000	0.681010000	-1.226789000
8	0.001732000	1.260014000	1.952581000
8	0.864108000	-2.930185000	0.406596000
1	1.568006000	-2.378800000	0.783021000

$Mo_3O_9H_2$ (A4) -$PC_2O_3H_6$• (product of PO-CH_3 bond cleavage reaction)

42	-2.029925000	0.781978000	0.500565000
8	-1.164878000	1.524867000	-1.076573000
8	-1.693486000	-1.042508000	0.492928000
8	-3.688845000	1.016183000	0.321721000
42	-0.113751000	-2.073072000	0.008016000
42	0.226455000	0.725416000	-1.996746000
8	0.120089000	-1.050166000	-1.752813000
8	-0.683942000	-3.502221000	-0.653416000
8	-0.127747000	0.967742000	-3.614685000
15	1.849505000	0.647619000	1.406176000
8	0.721798000	0.250550000	0.405868000
6	1.459161000	2.180989000	2.240482000
1	1.288586000	2.976798000	1.512565000
1	0.556636000	2.045285000	2.837490000
1	2.299668000	2.448203000	2.884004000
8	2.268732000	-0.467469000	2.328687000
8	3.108159000	1.084343000	0.435181000
6	4.344687000	0.338869000	0.431071000

1	5.100975000	1.001858000	0.012682000
1	4.606792000	0.047963000	1.448071000
1	4.242035000	-0.553361000	-0.190635000
8	1.896811000	1.497658000	-1.876505000
1	2.440756000	1.395661000	-1.046800000
8	-1.591125000	1.546998000	1.949989000
8	1.091087000	-2.440340000	1.325415000
1	1.618240000	-1.722168000	1.853228000

$Mo_3O_9H_2$ (A4) -$PC_2O_2H_6$• (product of P-OCH_3 bond cleavage reaction)

42	-2.004879000	0.607794000	0.602857000
8	-1.186823000	1.565640000	-0.864540000
8	-1.608650000	-1.209499000	0.412244000
8	-3.672727000	0.790132000	0.452420000
42	0.105018000	-1.971970000	-0.052831000
42	0.268756000	0.924460000	-1.833344000
8	0.224490000	-0.868118000	-1.807853000
8	-0.206397000	-3.380305000	-0.909968000
8	-0.078210000	1.341547000	-3.419266000
15	1.841656000	0.607942000	1.551319000
8	0.736095000	0.167339000	0.435281000
6	1.402402000	2.339291000	1.913901000
1	1.309389000	2.928436000	0.997201000
1	0.456916000	2.360739000	2.458843000
1	2.188690000	2.772659000	2.537306000
8	3.164912000	0.992171000	0.558845000
6	4.186912000	0.005128000	0.368159000

1	5.031051000	0.506935000	-0.105436000
1	4.500268000	-0.406521000	1.330846000
1	3.835963000	-0.804706000	-0.279501000
8	1.905682000	1.741051000	-1.608122000
1	2.476123000	1.518392000	-0.812551000
8	-1.595611000	1.215466000	2.132986000
8	1.219563000	-2.394383000	1.382549000
1	1.561835000	-1.720654000	2.004847000

DMMP on $Mo_3O_9H_2$ (A4) : TS for intramolecular CH_3OH elimination reaction

42	-1.975973000	0.408821000	0.603684000
8	-1.458364000	1.451455000	-0.960120000
8	-1.503090000	-1.280954000	0.131699000
8	-3.642698000	0.523487000	0.879312000
42	-0.014818000	-2.343140000	-0.613193000
42	-0.276663000	0.838982000	-2.256613000
8	-0.036460000	-0.910856000	-2.013474000
8	-0.617653000	-3.724960000	-1.341983000
8	-1.020409000	1.014074000	-3.747265000
15	1.670200000	1.012844000	1.353714000
8	1.109610000	0.551520000	0.045787000
6	1.844801000	2.597299000	1.939477000
1	1.317203000	3.355389000	1.367257000
1	1.724677000	2.704225000	3.014954000
1	3.390142000	2.013683000	1.496445000
8	1.708668000	-0.171801000	2.433443000
8	3.485812000	1.036527000	1.015363000

6	1.212236000	-0.035173000	3.789190000
1	0.216457000	0.406865000	3.770568000
1	1.174739000	-1.047006000	4.189274000
1	1.907658000	0.569986000	4.374180000
6	4.468682000	0.019337000	1.302550000
1	5.429145000	0.379173000	0.935642000
1	4.508262000	-0.177175000	2.374918000
1	4.174125000	-0.880866000	0.762880000
8	1.335003000	1.792206000	-2.403327000
1	1.985436000	1.565599000	-1.718801000
8	-1.097386000	0.932352000	1.991072000
8	1.317598000	-2.512985000	0.717791000
1	1.530674000	-1.836088000	1.381398000

$Mo_3O_9H_2$ (A4)-$PC_2O_2H_5$ (product of intramolecular CH_3OH elimination reaction)

42	-2.073508000	0.435394000	0.495615000
8	-1.408550000	0.966727000	-1.288205000
8	-1.399097000	-1.390902000	0.017873000
8	-3.731051000	0.287167000	0.639238000
42	0.039985000	-2.120788000	-0.762602000
42	0.089547000	0.856899000	-2.333616000
8	0.613963000	-1.009925000	-2.125870000
8	-0.529606000	-3.507297000	-1.505542000
8	-0.261482000	1.208319000	-3.950604000
15	0.824918000	0.713339000	1.679840000
8	1.085848000	-0.227868000	0.532086000
6	1.758549000	2.235669000	1.560343000
1	1.465520000	2.937760000	2.343301000
1	2.823140000	2.006548000	1.642583000
8	1.221894000	-0.029266000	3.040958000
6	0.895053000	0.506440000	4.331791000

1	-0.170046000	0.740985000	4.389037000
1	1.144607000	-0.267931000	5.055505000
1	1.490128000	1.400770000	4.536907000
8	1.288981000	1.934890000	-1.778562000
1	1.571206000	2.671228000	0.575685000
8	-0.706774000	1.099040000	1.800496000
8	1.340536000	-2.853691000	0.369533000
1	1.730286000	-2.178274000	0.952394000

DMMP on $Mo_3O_9H_2$ (A4) : TS for intermolecular CH_3OH elimination reaction

42	1.576488000	-0.628753000	-0.185726000
8	1.999888000	0.415262000	-1.676624000
8	1.602929000	-2.366366000	-0.627563000
8	0.002495000	-0.300918000	0.308061000
42	3.133865000	-3.429400000	-1.419092000
42	3.442169000	-0.229826000	-2.842550000
8	3.203681000	-2.017032000	-2.826505000
8	2.387926000	-4.735617000	-2.146439000
8	3.046206000	0.282691000	-4.395435000
15	4.348074000	-0.092078000	0.613586000
8	3.882218000	-1.029216000	-0.551925000
6	4.325971000	1.726450000	0.609333000
1	3.630969000	2.066990000	-0.161750000
1	3.935719000	2.050568000	1.574978000
1	5.314561000	2.139267000	0.426676000
8	5.074290000	-0.774732000	1.864785000
8	5.998184000	0.033521000	-0.250119000

6	4.402667000	-1.185280000	3.071756000
1	3.732580000	-2.021635000	2.869426000
1	5.196461000	-1.494204000	3.750631000
1	3.835083000	-0.358659000	3.498350000
6	6.936549000	-1.047330000	-0.268919000
1	7.799302000	-0.721408000	-0.852325000
1	7.245427000	-1.266673000	0.752871000
1	6.502695000	-1.937140000	-0.736134000
8	5.060793000	0.441975000	-2.441238000
1	5.620081000	0.236152000	-1.382017000
8	2.710849000	-0.110719000	1.241014000
8	4.571277000	-3.817903000	-0.246816000
1	5.037236000	-3.171676000	0.299376000

$Mo_3O_9H_2$ (A4) -$PC_2O_2H_5$ (product of intermolecular CH_3OH elimination reaction)

42	-1.999940000	0.527392000	0.903211000
8	-1.505941000	1.115794000	-0.919785000
8	-1.267237000	-1.252478000	0.333908000
8	-3.633412000	0.290601000	1.161890000
42	0.140471000	-1.889397000	-0.573132000
42	-0.071958000	1.141544000	-2.051441000
8	0.572430000	-0.697677000	-1.915017000
8	-0.412175000	-3.280941000	-1.318471000
8	-0.525464000	1.529854000	-3.634510000
15	0.948771000	0.967009000	1.978812000
8	1.194114000	-0.017419000	0.854940000
6	1.798397000	2.522057000	1.782572000
1	1.573037000	2.911329000	0.786853000
1	1.481375000	3.224109000	2.555048000
1	2.873344000	2.347489000	1.860019000
8	1.461548000	0.446572000	3.399692000
6	0.899728000	-0.721886000	4.016678000
1	0.999880000	-1.592875000	3.363568000

1	1.466190000	-0.885059000	4.931981000
1	-0.151966000	-0.551336000	4.257529000
8	1.099126000	2.255061000	-1.506249000
8	-0.608918000	1.240833000	2.131887000
8	1.576799000	-2.559583000	0.427187000
1	1.977116000	-1.829462000	0.936648000

DMMP on $Mo_3O_9H_3$ (B1)

42	0.657980000	-0.409360000	-0.303080000
8	1.097210000	-0.181077000	-2.127882000
8	1.144055000	-2.237970000	-0.060164000
8	-0.992249000	-0.148654000	-0.076912000
42	2.424446000	-3.349574000	-0.932925000
42	2.420507000	-0.764106000	-3.359746000
8	2.508148000	-2.513801000	-2.627144000
8	1.886977000	-4.937304000	-1.114245000
8	1.828362000	-0.786859000	-4.936758000
15	5.696990000	0.430151000	0.674174000
8	4.587121000	-0.161881000	-0.173121000
6	5.552978000	2.196114000	0.900903000
1	5.597550000	2.690262000	-0.071691000
1	4.591534000	2.418534000	1.370309000
1	6.364814000	2.555957000	1.534795000
8	5.778731000	-0.268991000	2.103659000
8	7.152357000	0.252978000	0.076305000

6	4.632456000	-0.855511000	2.761101000
1	4.281858000	-1.722198000	2.199057000
1	4.984339000	-1.162204000	3.744335000
1	3.828217000	-0.123521000	2.864873000
6	7.686635000	-1.049877000	-0.239955000
1	8.680950000	-0.873305000	-0.645097000
1	7.751152000	-1.655204000	0.666064000
1	7.062183000	-1.543385000	-0.987277000
8	4.032805000	0.113253000	-2.938362000
1	4.364713000	0.109901000	-2.016165000
8	4.079940000	-2.944298000	-0.105194000
1	4.378937000	-2.011469000	-0.162212000
8	1.972611000	0.573879000	0.644204000
1	2.897979000	0.419573000	0.358208000

DMMP on $Mo_3O_9H_3$ (B2)

42	1.623362000	0.205473000	-0.749993000
8	2.301687000	-0.113304000	-2.485335000
8	1.605821000	-1.581239000	-0.089198000
8	0.083003000	0.869725000	-0.889859000
42	2.261845000	-3.295733000	-0.628930000
42	3.496280000	-1.288725000	-3.363624000
8	3.040822000	-2.781425000	-2.281117000
8	0.999615000	-4.369992000	-0.920011000
8	3.013952000	-1.493342000	-4.962865000
15	6.353091000	-0.721563000	0.821294000
8	7.791664000	-0.537400000	1.099639000
6	5.207477000	-0.608500000	2.193072000
1	5.482439000	-1.354651000	2.941249000
1	5.288575000	0.385788000	2.637646000
1	4.178048000	-0.771890000	1.868665000
8	5.793874000	0.351757000	-0.301364000
8	5.938687000	-2.124539000	0.139478000

6	6.518277000	1.598626000	-0.493308000
1	7.590661000	1.407715000	-0.477509000
1	6.207046000	1.985391000	-1.462929000
1	6.247218000	2.304117000	0.294801000
6	6.865361000	-2.794578000	-0.757335000
1	6.541265000	-3.833088000	-0.802369000
1	6.804646000	-2.340765000	-1.747754000
1	7.877039000	-2.726164000	-0.356501000
8	5.243783000	-0.693938000	-2.944341000
1	5.474242000	-0.365184000	-2.054779000
8	3.669232000	-3.790334000	0.523936000
1	4.492699000	-3.267314000	0.559156000
8	3.009179000	1.147210000	0.136884000
1	3.947828000	0.948452000	-0.032770000

DMMP on $Mo_3O_9H_3$ (B3)

42	2.661535000	-0.342559000	-0.478957000
8	2.788344000	-0.397819000	-2.274345000
8	2.861811000	-2.093262000	0.053029000
8	1.174770000	0.287454000	-0.002885000
42	3.518022000	-3.613593000	-1.037998000
42	3.914357000	-1.175945000	-3.683346000
8	3.674512000	-2.868103000	-2.713431000
8	2.517955000	-4.952807000	-0.806953000
8	3.097428000	-1.142073000	-5.152752000
15	7.418949000	-1.009726000	0.005114000
8	6.412992000	-0.254753000	-0.828690000
6	8.136911000	-2.423185000	-0.813166000
1	7.344415000	-3.157077000	-0.983875000
1	8.561675000	-2.106397000	-1.768474000
1	8.917312000	-2.856526000	-0.185505000
8	8.588022000	-0.049190000	0.527228000
8	6.837708000	-1.620403000	1.359290000

6	9.033831000	1.090246000	-0.230508000
1	8.180122000	1.648057000	-0.618270000
1	9.607921000	1.707166000	0.459076000
1	9.675684000	0.765638000	-1.053368000
6	6.350380000	-0.774738000	2.426262000
1	6.076462000	-1.447742000	3.236857000
1	7.143665000	-0.100619000	2.753371000
1	5.476168000	-0.212389000	2.091697000
8	5.670048000	-0.536431000	-3.472728000
1	6.077251000	-0.398796000	-2.589520000
8	5.242008000	-3.705922000	-0.178310000
1	5.406882000	-3.229789000	0.649156000
8	4.106499000	0.640057000	0.176164000
1	5.002149000	0.458889000	-0.215399000