

Electronic Supplementary Information

Radical reactions of diamine bis(phenolate) vanadium(III) complexes. Activation of O₂ and TEMPO

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1. Sulfoxidation results:

Table S1. Sulfoxidation of Thioanisole using vanadium complexes **6** and **8** as catalyst precursors.

	Catalyst	Solvent	Oxidant ^{b,c}	<i>n</i> Ox./ <i>n</i> S	mol % cat. ^a	T/°C	<i>t</i> /h	conv. (%)	ee (%)	sulfone (%)
1	6	DCE	H ₂ O ₂	1.2	1	10	24	>99	0	21
2	8	DCE	TBHP	1.2	2	10	20	54	0	0
3	8	DCE	H ₂ O ₂	1.2	2	10	20	93	0	5

^a Thioanisole (1 mmol). ^b H₂O₂ 20% (w/v) aqueous solution. ^c TBHP 5.5 M in decane.

2. NMR data for TEMPO-CH₂Ph:

¹H NMR (300 MHz, C₆D₆, ppm): δ 7.35 (d, 2H, ⁴J_{HH} = 6.5 Hz, Ph), 7.16 (m, 3H, Ph), 4.90 (s, 2H, CH₂Ph), 1.49 (m, 3H, CH₂ TEMPO), 1.33 (m, 2H, CH₂ TEMPO), 1.16 (m, 1H, CH₂ TEMPO). ¹³C-¹H NMR (75 MHz, C₆D₆, ppm): δ 135.2 (C_{ipso}-Ph), 128.9, 128.7 and 127.9 (CH-Ph), 79.7 (CH₂Ph), 60.4 (C_{ipso}-TEMPO), 40.4 (CH₂ TEMPO), 33.7 (CH₃ TEMPO), 20.7 (CH₃ TEMPO), 17.8 (CH₂ TEMPO).

3. Atom coordinates for the optimized molecules:

2*

23	7.948246000	3.607444000	5.532697000	6	9.310065000	6.883526000	8.042896000
17	7.569617000	1.757075000	6.885758000	1	10.098899000	7.490155000	7.586922000
8	6.404303000	3.492374000	4.513127000	1	8.760158000	7.540286000	8.721512000
8	9.589975000	3.086097000	4.844450000	6	9.467042000	4.468372000	7.920631000
7	8.304721000	5.592098000	4.571339000	1	10.195766000	4.289185000	7.123695000
7	8.173400000	4.865514000	7.288238000	1	9.331013000	3.526223000	8.453642000
6	11.917681000	3.148442000	4.461769000	6	9.886261000	5.659386000	8.782414000
6	10.633673000	3.709626000	4.293937000	1	10.972267000	5.707112000	8.891866000
6	13.008083000	3.794278000	3.889727000	1	9.465841000	5.577270000	9.788700000
1	13.996334000	3.355698000	4.020025000	6	5.681331000	4.892398000	7.668106000
6	7.004835000	6.227210000	4.237580000	1	4.931022000	4.704638000	8.441517000
1	7.187237000	7.257203000	3.892438000	1	5.503378000	4.179607000	6.857016000
1	6.427185000	6.291143000	5.166702000	1	5.506388000	5.905412000	7.291137000
6	6.211324000	5.480476000	3.211063000	6	7.061386000	4.711281000	8.272595000
6	5.937102000	4.124389000	3.433785000	1	7.143184000	3.695115000	8.663432000
6	9.111212000	5.451348000	3.330509000	1	7.212466000	5.417976000	9.099881000
1	9.186306000	6.432584000	2.836487000	6	12.059814000	1.872076000	5.234775000
1	8.531946000	4.802424000	2.663915000	1	11.685613000	1.978979000	6.258527000
6	5.150494000	3.406866000	2.509685000	1	11.464426000	1.072967000	4.781492000
6	10.482815000	4.894423000	3.557002000	1	13.103907000	1.551328000	5.276849000
6	4.663503000	4.077282000	1.393346000	6	14.086324000	5.637343000	2.540174000
1	4.057601000	3.520714000	0.679943000	1	14.903572000	5.740131000	3.262141000
6	11.606921000	5.515884000	3.008968000	1	14.474527000	5.053287000	1.697374000
1	11.475019000	6.437937000	2.444452000	1	13.846117000	6.635628000	2.163609000
6	12.882767000	4.979923000	3.156572000	6	4.871523000	1.956326000	2.760503000
6	9.019331000	6.402262000	5.567948000	1	4.253498000	1.530467000	1.965963000
1	9.063408000	7.458714000	5.257243000	1	5.802050000	1.382919000	2.826684000
1	10.052484000	6.042080000	5.605424000	1	4.359820000	1.813845000	3.717869000
6	5.709508000	6.114986000	2.073709000	6	4.374706000	6.114420000	-0.071159000
1	5.935802000	7.167957000	1.911898000	1	4.669015000	5.595244000	-0.989969000
6	8.385428000	6.303463000	6.948319000	1	3.279031000	6.142645000	-0.055796000
1	7.411996000	6.798495000	6.947559000	1	4.730145000	7.146007000	-0.144476000
6	4.925717000	5.431124000	1.149526000				

7*

23	1.130991000	3.626328000	5.053846000	6	3.411726000	2.532340000	7.291235000
17	1.999812000	5.316205000	6.351733000	1	3.590835000	2.133672000	8.299541000
8	-0.481631000	3.510029000	5.886852000	1	3.550223000	3.614389000	7.338247000
8	2.660496000	3.214946000	4.148773000	6	1.185121000	2.737612000	8.163031000
8	0.279166000	3.842716000	3.474003000	1	0.160341000	2.939848000	7.851366000
8	0.697020000	5.041925000	4.019380000	1	1.591880000	3.666978000	8.562793000
6	2.705578000	2.764549000	2.885465000	6	-1.692389000	3.114520000	5.474084000
7	1.965560000	2.341042000	6.954512000	6	0.438163000	0.736925000	5.880114000
7	0.590932000	1.444694000	4.593301000	1	-0.459156000	1.121830000	6.369027000
6	2.142691000	1.038697000	1.299491000	1	0.267386000	-0.334901000	5.690976000
1	1.696933000	0.069254000	1.083321000	6	-3.145149000	1.694369000	4.182714000
6	-4.273317000	2.311254000	4.713753000	1	-3.269869000	0.887614000	3.461928000
6	1.355683000	0.323120000	8.199098000	6	2.720258000	1.780551000	0.268956000
1	2.153905000	-0.352040000	8.518131000	6	4.434384000	1.935559000	6.340978000
1	0.431480000	-0.264452000	8.190221000	1	5.424472000	2.275546000	6.660304000
6	-4.081118000	3.339117000	5.643681000	1	4.274964000	2.275752000	5.317931000
1	-4.948790000	3.834753000	6.075120000	1	4.461491000	0.840812000	6.360609000
6	3.284798000	3.545184000	1.874209000	6	-2.815846000	3.751930000	6.039343000
6	1.617824000	0.741558000	3.771262000	6	1.640047000	0.900494000	6.791499000
1	2.459977000	0.524844000	4.432114000	6	-1.851942000	2.083065000	4.537452000
1	1.201899000	-0.221745000	3.441323000	6	2.135337000	1.520616000	2.605008000
6	-0.692769000	1.402407000	3.860001000	6	1.242764000	1.548306000	9.123213000
1	-0.954511000	0.345647000	3.689685000	1	2.105407000	1.611823000	9.792949000
1	-0.512841000	1.850347000	2.877214000	1	0.353048000	1.513517000	9.757294000

6	3.280898000	3.024144000	0.582771000	1	-1.905489000	5.598063000	6.652535000
1	3.722363000	3.618743000	-0.215190000	6	3.854109000	4.889587000	2.209788000
1	2.501608000	0.404490000	6.345032000	1	3.113353000	5.492873000	2.744102000
6	-5.657302000	1.902586000	4.294295000	1	4.722550000	4.798887000	2.871300000
1	-5.646365000	0.956122000	3.746942000	1	4.163989000	5.421770000	1.307174000
1	-6.319738000	1.784594000	5.158000000	6	2.747138000	1.264136000	-1.142694000
1	-6.112136000	2.655812000	3.640219000	1	3.769227000	1.033740000	-1.465052000
6	-2.609031000	4.852800000	7.035668000	1	2.155009000	0.350706000	-1.244741000
1	-3.554461000	5.346276000	7.273749000	1	2.347050000	2.002290000	-1.845733000
1	-2.180096000	4.472059000	7.969714000				

6*

23	6.733005000	12.123755000	14.046060000	1	6.261257000	16.900374000	11.364380000
17	8.864532000	12.905099000	13.952080000	6	7.873837000	13.452656000	10.540880000
8	6.755858000	12.436889000	15.842567000	6	4.082656000	10.975108000	13.029047000
8	6.556571000	12.484780000	12.260060000	1	4.739905000	10.103851000	12.965450000
8	6.869606000	10.571599000	14.010476000	1	4.365628000	11.627784000	12.199433000
6	7.668516000	15.855523000	10.115136000	6	4.315694000	10.779441000	15.477780000
7	4.461632000	11.679839000	14.283674000	1	3.822418000	9.854546000	15.164081000
7	5.633938000	14.286808000	14.197457000	1	5.300555000	10.520344000	15.864531000
6	7.104135000	13.448657000	16.643755000	6	5.253225000	14.848599000	12.885737000
6	6.920922000	13.576059000	11.566463000	1	4.886678000	15.879811000	13.018983000
6	7.555232000	13.117265000	17.939047000	1	4.411125000	14.255660000	12.513997000
6	8.223297000	14.601852000	9.837475000	6	3.461614000	11.531225000	16.494206000
1	8.963482000	14.516701000	9.043695000	1	4.099765000	12.102650000	17.176291000
6	7.000015000	14.792747000	16.249618000	1	2.857117000	10.853082000	17.102398000
6	6.569223000	15.207954000	14.867230000	6	2.619980000	12.465360000	15.628321000
1	6.110425000	16.209692000	14.930234000	1	2.222361000	13.326400000	16.174968000
1	7.447309000	15.292852000	14.216585000	1	1.772877000	11.925522000	15.193878000
6	3.607617000	12.878612000	14.533951000	6	7.661395000	11.674047000	18.329520000
1	3.093232000	13.131370000	13.602124000	1	6.682879000	11.181024000	18.309754000
6	6.340773000	14.813990000	11.858570000	1	8.299159000	11.127532000	17.627648000
6	7.902311000	14.142796000	18.808470000	1	8.076582000	11.570381000	19.335031000
1	8.257134000	13.884806000	19.804596000	6	8.217502000	16.576069000	19.398058000
6	7.809894000	15.489778000	18.443196000	1	7.864253000	16.371002000	20.413669000
6	7.345834000	15.787670000	17.165115000	1	9.308949000	16.669064000	19.449001000
1	7.255382000	16.829614000	16.862343000	1	7.820289000	17.547907000	19.092334000
6	2.627238000	10.547893000	12.886023000	6	8.485439000	12.116686000	12.251720000
1	2.516070000	10.009776000	11.939780000	1	9.040147000	11.755325000	11.123590000
1	1.937896000	11.397524000	12.855843000	1	7.716259000	11.368566000	10.033725000
1	2.299691000	9.872693000	13.682377000	1	9.167900000	12.173531000	9.399977000
6	4.433091000	14.073092000	15.003734000	6	8.097158000	17.072312000	9.343424000
1	3.790656000	14.970230000	14.994840000	1	9.130136000	17.351529000	9.581529000
1	4.746916000	13.918403000	16.037350000	1	8.052157000	16.898572000	8.263064000
6	6.720045000	15.940450000	11.133216000	1	7.462417000	17.933264000	9.570445000

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17	1.772711000	5.485775000	6.019605000	6	-4.106082000	3.357455000	5.675643000
8	-0.498147000	3.405476000	5.965244000	1	-4.966983000	3.854765000	6.119151000
8	2.707635000	3.071131000	4.275732000	6	3.391983000	3.527818000	2.021445000
8	-0.182037000	4.472519000	2.641053000	6	1.547824000	0.718676000	3.721097000
8	0.423193000	4.134727000	3.688626000	1	2.372512000	0.422467000	4.374046000
6	2.743374000	2.728279000	2.972688000	1	1.085691000	-0.202524000	3.338650000
7	1.949315000	2.430869000	6.906378000	6	-0.738644000	1.439885000	3.847416000
7	0.552324000	1.430157000	4.576312000	1	-1.013261000	0.398751000	3.616496000
6	2.108243000	1.138851000	1.269940000	1	-0.546273000	1.939850000	2.889319000
1	1.611933000	0.211700000	0.988000000	6	3.413625000	2.713270000	7.134773000
6	-4.313557000	2.369419000	4.705389000	1	3.607643000	2.668251000	8.213326000
6	1.407450000	0.417714000	8.194463000	1	3.562120000	3.750975000	6.829509000
1	2.174206000	-0.308501000	8.477004000	6	1.228859000	2.819165000	8.152718000
1	0.445153000	-0.103867000	8.237944000	1	0.176813000	2.958075000	7.902920000

1	1.614557000	3.776478000	8.508580000	1	3.877516000	3.699433000	-0.051299000
6	-1.722948000	3.090993000	5.516428000	1	2.516821000	0.496612000	6.314044000
6	0.436580000	0.741964000	5.877111000	6	-5.703852000	2.004897000	4.265113000
1	-0.468227000	1.101759000	6.368991000	1	-5.701271000	1.112514000	3.633277000
1	0.314053000	-0.340817000	5.717014000	1	-6.357786000	1.807772000	5.121285000
6	-3.194854000	1.750400000	4.160474000	1	-6.164288000	2.815530000	3.688408000
1	-3.328386000	0.975920000	3.406586000	6	-2.615799000	4.782702000	7.141140000
6	2.742940000	1.908818000	0.296413000	1	-3.560621000	5.246697000	7.434841000
6	4.429494000	1.826621000	6.436512000	1	-2.148306000	4.363872000	8.039821000
1	5.417354000	2.271917000	6.591294000	1	-1.940207000	5.562451000	6.775499000
1	4.254616000	1.780551000	5.361195000	6	4.055083000	4.802642000	2.446055000
1	4.473565000	0.814020000	6.851249000	1	3.337115000	5.477036000	2.924728000
6	-2.836848000	3.728469000	6.098387000	1	4.842179000	4.613327000	3.183893000
6	1.650899000	0.973985000	6.770064000	1	4.499884000	5.318334000	1.591519000
6	-1.897386000	2.100505000	4.544040000	6	2.729892000	1.501720000	-1.151021000
6	2.108970000	1.539137000	2.603506000	1	3.727918000	1.569035000	-1.596383000
6	1.415200000	1.648833000	9.115026000	1	2.378522000	0.473381000	-1.273033000
1	2.364135000	1.721482000	9.655857000	1	2.069201000	2.147766000	-1.740859000
1	0.621538000	1.618951000	9.866084000	23	1.105720000	3.558902000	5.065927000
6	3.379169000	3.088513000	0.699540000				

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23	6.330519000	12.079846000	14.223753000	6	7.952784000	13.604681000	10.977953000
17	8.418856000	12.959687000	14.495601000	6	4.006549000	10.808617000	12.734424000
8	6.115617000	12.166134000	16.044619000	1	4.695652000	9.959035000	12.714457000
8	6.443534000	12.476129000	12.427611000	1	4.378226000	11.531965000	12.005378000
8	6.633105000	10.463781000	14.094265000	6	3.881642000	10.432127000	15.172834000
6	7.719488000	16.031114000	10.720866000	1	3.479348000	9.523774000	14.717777000
7	4.160656000	11.433701000	14.082400000	1	4.806628000	10.166341000	15.681245000
7	5.228035000	14.053768000	14.359950000	6	5.003098000	14.716189000	13.046067000
6	6.300119000	13.124223000	16.958888000	1	4.570795000	15.711810000	13.225268000
6	6.865578000	13.620119000	11.866705000	1	4.247763000	14.124438000	12.519579000
6	6.558188000	12.717901000	18.285246000	6	2.860297000	11.074581000	16.104502000
6	8.350060000	14.818127000	10.422580000	1	3.368000000	11.613501000	16.910676000
1	9.193388000	14.819112000	9.734113000	1	2.207591000	10.330386000	16.568307000
6	6.209230000	14.488786000	16.641285000	6	2.105487000	12.042265000	15.195619000
6	5.978120000	14.983023000	15.238287000	1	1.595595000	12.843480000	15.739780000
1	5.425567000	15.934989000	15.286835000	1	1.353716000	11.509789000	14.605119000
1	6.935013000	15.179247000	14.743140000	6	6.658582000	11.255229000	18.596595000
6	3.215902000	12.574534000	14.286872000	1	5.717496000	10.734847000	18.386348000
1	2.829646000	12.875674000	13.309064000	1	7.423146000	10.777012000	17.976276000
6	6.213783000	14.815738000	12.178035000	1	6.910344000	11.095420000	19.647885000
6	6.726031000	13.691905000	19.260636000	6	6.851825000	16.087038000	20.046764000
1	6.931439000	13.376613000	20.281946000	1	6.350276000	15.804162000	20.977725000
6	6.640199000	15.058136000	18.972241000	1	7.917281000	16.205122000	20.277449000
6	6.370356000	15.430323000	17.658709000	1	6.472262000	17.066671000	19.743415000
1	6.290003000	16.487766000	17.411660000	6	8.650720000	12.313632000	10.681869000
6	2.607137000	10.347494000	12.348160000	1	9.071682000	11.891884000	11.600395000
1	2.659976000	9.891880000	11.354827000	1	7.954901000	11.568682000	10.282177000
1	1.889191000	11.171602000	12.285964000	1	9.458269000	12.458974000	9.960068000
1	2.201940000	9.591316000	13.027071000	6	8.207959000	17.318653000	10.117865000
6	3.914656000	13.750896000	14.956142000	1	9.152371000	17.638520000	10.573735000
1	3.264974000	14.638366000	14.898190000	1	8.388320000	17.214963000	9.043005000
1	4.071047000	13.538167000	16.014424000	1	7.484494000	18.126323000	10.259838000
6	6.642918000	16.010183000	11.606729000	8	6.515277000	9.204795000	13.964281000
1	6.125257000	16.936481000	11.850511000				

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23	6.172348000	12.222467000	13.767252000	8	6.120370000	12.904712000	12.074336000
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8	6.290170000	12.139207000	15.582650000	6	7.931379000	16.325534000	10.581995000

7	3.931351000	12.062396000	13.974759000	8	6.851373000	8.152132000	10.901563000
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1	6.432795000	16.036177000	15.387270000	1	3.942815000	7.739788000	7.477709000
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6	6.401547000	15.249020000	12.123096000	1	5.457636000	5.110400000	12.001656000
6	7.718649000	12.988790000	18.792720000	6	9.721596000	6.594967000	12.656912000
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1	9.584274000	15.037297000	19.859989000	1	5.895534000	6.977498000	18.062925000
1	8.291800000	16.229774000	19.711272000	6	4.678869000	2.351199000	16.572742000
6	7.961631000	12.547806000	9.952939000	1	5.119173000	2.138915000	17.552330000
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23	6.875673000	7.900320000	12.710042000	1	3.236383000	4.885746000	7.192188000
17	4.552522000	7.725150000	12.661350000	1	4.229195000	5.639445000	5.945997000
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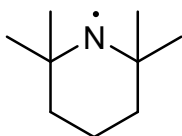
8	-4.142221000	-11.909433000	-10.400329000
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TEMPO

7	1.787881000	5.735048000	2.786953000	1	1.660817000	8.894420000	2.369257000
6	0.589927000	6.443963000	3.317912000	1	2.310115000	9.427819000	3.908825000
6	3.024271000	6.410078000	2.300419000	1	2.139490000	7.517414000	0.621440000
8	1.573965000	4.572097000	2.313021000	1	2.537028000	5.821331000	0.283573000
6	1.011517000	7.712459000	4.068673000	1	3.826936000	7.040426000	0.387049000
6	-0.106672000	5.483475000	4.281247000	1	0.048045000	7.530276000	1.487162000
6	-0.357092000	6.765095000	2.154584000	1	-1.315136000	7.127394000	2.540820000
6	3.294466000	7.679153000	3.116439000	1	-0.533955000	5.857171000	1.572456000
6	2.867111000	6.722474000	0.806589000	1	0.565726000	5.201616000	5.097092000
6	4.174635000	5.421748000	2.488816000	1	-0.413251000	4.575739000	3.759611000
6	2.054867000	8.534688000	3.327763000	1	-0.989308000	5.968146000	4.709936000
1	4.088202000	8.242718000	2.612540000	1	4.269671000	5.138915000	3.541425000
1	3.690067000	7.388777000	4.099063000	1	5.112762000	5.884177000	2.166832000
1	1.424850000	7.422578000	5.044033000	1	4.001091000	4.516813000	1.904856000
1	0.109463000	8.300873000	4.272186000				

TEMPO-CH₂Ph

7	1.332750000	6.057727000	1.769699000	1	-0.701103000	7.665901000	1.477584000
6	0.415623000	6.450078000	2.888891000	1	-0.177631000	4.393334000	3.326645000
6	2.581960000	6.875202000	1.618855000	1	-1.210327000	5.219056000	2.132637000
8	1.792036000	4.739652000	2.109476000	1	-1.328759000	5.631551000	3.849674000
6	1.181174000	6.623849000	4.211551000	1	3.789938000	5.169430000	0.972343000
6	-0.633158000	5.346535000	3.054228000	1	4.415347000	6.754485000	0.496517000
6	-0.357085000	7.721691000	2.514070000	1	3.022718000	6.073808000	-0.355931000
6	3.312416000	7.039063000	2.962196000	6	1.395093000	3.824793000	1.111121000
6	2.248510000	8.236258000	0.992041000	6	2.021153000	2.482257000	1.384709000
6	3.503393000	6.162815000	0.623876000	6	2.920902000	2.282585000	2.431430000
6	2.396736000	7.535504000	4.076120000	1	3.169253000	3.115057000	3.080606000
1	4.164031000	7.717089000	2.826509000	6	3.489244000	1.027553000	2.642171000
1	3.725440000	6.063347000	3.246844000	1	4.187983000	0.886428000	3.462223000
1	1.513849000	5.632682000	4.543971000	6	3.166891000	-0.039798000	1.811653000
1	0.493124000	7.002189000	4.977636000	1	3.611194000	-1.016995000	1.977286000
1	2.080867000	8.568436000	3.880337000	6	2.267054000	0.153035000	0.764926000
1	2.946419000	7.566089000	5.023907000	1	2.006572000	-0.674225000	0.110621000
1	1.861329000	8.968637000	1.700093000	6	1.698887000	1.403516000	0.555893000
1	1.522218000	8.115644000	0.183540000	1	0.995877000	1.546331000	-0.262366000
1	3.163066000	8.659875000	0.565943000	1	1.702577000	4.189918000	0.122206000
1	0.212788000	8.641622000	2.640553000	1	0.299937000	3.730674000	1.088887000
1	-1.236566000	7.800513000	3.160399000				



7	1.772079000	5.711174000	2.749141000	6	1.012216000	7.737193000	4.065784000
6	0.647658000	6.444200000	3.311667000	6	-0.052589000	5.472358000	4.268465000
6	2.980033000	6.411659000	2.336977000	6	-0.321213000	6.754289000	2.152272000

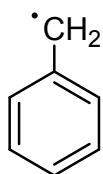
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6	2.840162000	6.714540000	0.830898000	1	3.811721000	7.019361000	0.427480000
6	4.127559000	5.411295000	2.517183000	1	0.064237000	7.531172000	1.487347000
6	2.058463000	8.564303000	3.334167000	1	-1.277934000	7.099057000	2.558836000
1	4.081333000	8.254549000	2.591095000	1	-0.498887000	5.853447000	1.558734000
1	3.704716000	7.428896000	4.097865000	1	0.623302000	5.176848000	5.076801000
1	1.411053000	7.466649000	5.053259000	1	-0.357858000	4.568000000	3.734982000
1	0.097541000	8.314540000	4.246668000	1	-0.939006000	5.938183000	4.713149000
1	1.665830000	8.928159000	2.375863000	1	4.217148000	5.117209000	3.567427000
1	2.314657000	9.456094000	3.917299000	1	5.079040000	5.852265000	2.200132000
1	2.125096000	7.517729000	0.635260000	1	3.941361000	4.509088000	1.928134000

2,2,6,6-tetramethylpiperidine

7	1.874387000	5.725187000	2.994980000	1	2.331750000	9.414762000	3.959327000
6	0.632826000	6.432640000	3.322354000	1	2.039936000	7.498851000	0.676421000
6	2.996865000	6.398075000	2.334250000	1	2.440561000	5.817782000	0.307602000
6	1.004481000	7.714814000	4.080838000	1	3.716864000	7.040444000	0.378365000
6	-0.148419000	5.504289000	4.256138000	1	0.150072000	7.524986000	1.464372000
6	-0.270458000	6.757149000	2.117142000	1	-1.248733000	7.115279000	2.457365000
6	3.307817000	7.681049000	3.117900000	1	-0.437970000	5.859262000	1.511541000
6	2.779495000	6.712634000	0.841889000	1	0.470686000	5.223583000	5.112437000
6	4.187311000	5.441632000	2.443426000	1	-0.444349000	4.585870000	3.734527000
6	2.068398000	8.535314000	3.360198000	1	-1.061720000	5.987877000	4.618442000
1	4.079967000	8.249691000	2.585970000	1	4.352971000	5.165247000	3.488157000
1	3.730473000	7.393380000	4.089546000	1	5.098540000	5.901541000	2.046652000
1	1.392693000	7.426663000	5.066526000	1	4.003811000	4.522977000	1.873004000
1	0.098092000	8.307977000	4.250973000	1	1.657906000	4.860813000	2.507222000
1	1.677148000	8.922752000	2.410665000				

Toluene

6	1.182249000	-0.188542000	0.073516000	1	1.808648000	-2.243962000	0.109773000
6	0.963782000	-1.562717000	0.061006000	1	-0.505660000	-3.136250000	-0.015117000
6	-0.332979000	-2.064088000	-0.008607000	1	-2.423213000	-1.560575000	-0.112032000
6	-1.406823000	-1.180017000	-0.063384000	1	-2.026887000	0.877750000	-0.090145000
6	-1.182741000	0.193288000	-0.050715000	1	0.470908000	2.562729000	-1.030784000
6	0.113889000	0.710483000	0.014643000	1	1.265317000	2.460134000	0.540235000
6	0.354674000	2.194248000	-0.004340000	1	-0.479165000	2.742013000	0.444168000
1	2.198003000	0.195486000	0.131761000				



6	1.136309000	-0.147615000	-0.069772000	1	2.137573000	0.273466000	-0.108158000
6	0.960623000	-1.518313000	-0.018335000	1	1.827750000	-2.172805000	-0.016657000
6	-0.324918000	-2.066570000	0.031398000	1	-0.458443000	-3.143250000	0.071754000
6	-1.437462000	-1.219281000	0.028599000	1	-2.438079000	-1.640654000	0.066840000
6	-1.273051000	0.152804000	-0.022519000	1	-2.140942000	0.807111000	-0.024578000
6	0.022534000	0.735433000	-0.073259000	1	1.186273000	2.569266000	-0.162694000
6	0.195681000	2.129414000	-0.124426000	1	-0.657027000	2.799585000	-0.127013000