

## Supporting Information

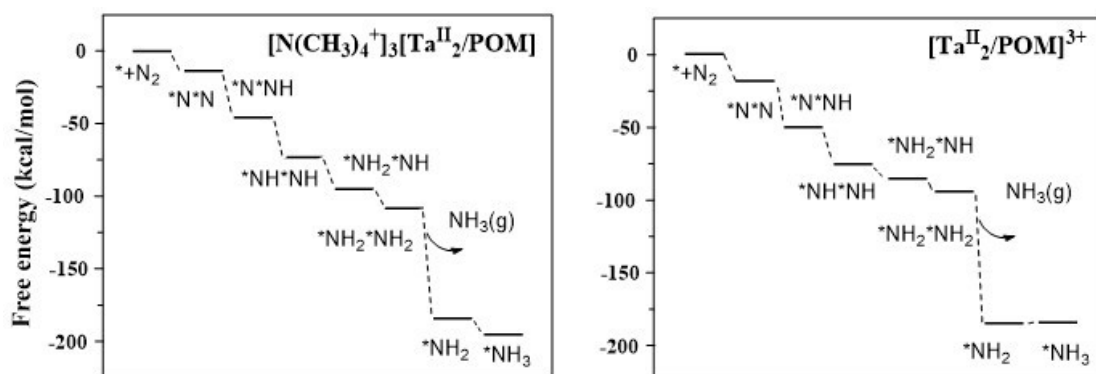
# Reduction of N<sub>2</sub> to NH<sub>3</sub> Catalyzed by A Keggin-Type Polyoxometalate-Supported Dual-Atom Catalyst

Yu Wang<sup>‡, §</sup>, Rui-Cheng Qin<sup>†</sup>, Dan Wang<sup>†</sup>, and Chun-Guang Liu<sup>†\*</sup>

*†Department of Chemistry, Faculty of Science, Beihua University, Jilin City,  
132013, P. R. China.*

*‡ State Key Lab of Urban Water Resource and Environment, School of Science,  
Harbin Institute of Technology Shenzhen, Shenzhen 518055, PR China.*

*§ College of Chemical Engineering, Northeast Electric Power University, Jilin  
City, 132012, P. R. China*



**Figure S1.** Free energy diagram for enzymatic pathway on  $[\text{N}(\text{CH}_3)_4^+]_3[\text{Ta}^{\text{II}}_2/\text{POM}]$  and  $[\text{Ta}^{\text{II}}_2/\text{POM}]^{3+}$ .

## XYZ coordinates

$[\text{N}(\text{CH}_3)_4^+]_3[\text{Ta}^{\text{II}}_2/\text{POM}]$  (POM =  $[\text{PW}_{11}\text{O}_{39}]^{7-}$ )

Atomic	Coordinates (Angstroms)		
	X	Y	Z
O	-1.06143900	-0.75513700	0.96631700
O	-0.90869100	0.62166900	-1.13942900
O	0.61103100	-1.42328300	-0.77722000
O	2.89093100	-2.63287700	-1.29540400
W	2.19394500	-1.32124500	-2.64748900
O	3.02599500	0.00149100	-1.56344700
W	2.88341900	1.75686400	-0.66095400
O	1.56189200	2.14221600	-2.00240200
W	0.12437400	1.71468900	-3.17917300
O	1.04612900	-0.02778100	-3.35151500
O	0.99882600	0.72326500	0.49075500
O	-1.48624800	0.69343600	-3.68347100
W	-2.71568900	-0.13888400	-2.52169300
O	-3.21888500	1.51966000	-1.76984100
W	-2.06819400	2.75351500	-0.70352900
O	-1.01922900	2.95383000	-2.31895600
O	-1.64467100	-1.77226100	-2.61340600
W	-0.62143000	-3.21646000	-1.93510200
O	0.68096300	-4.01969900	-0.71944700
O	-1.20185100	-4.56300400	-2.79235300
O	-1.89835300	-3.15127900	-0.42910000

W	-3.13715800	-2.19095700	0.60861300
O	-2.27991200	-2.78417500	2.22255100
O	2.00734700	-0.89340200	3.81699200
W	3.10728100	-0.25090700	2.36049300
O	3.63488500	0.82906100	0.90231900
O	0.88161900	-2.69898900	-2.99932900
O	-4.05404500	-0.47004800	-3.53606400
O	-3.36046200	-1.00125600	-0.84770800
O	-4.60333500	-3.07563500	0.56156900
O	-3.66169700	-0.62827000	1.77562700
W	-2.62430200	0.78159400	2.42999500
O	-1.61187000	-0.47528100	3.63786900
O	-3.63966800	1.58665300	3.53682500
O	-2.76560900	1.79963000	0.89632200
O	-0.70826800	1.53151400	2.72359500
W	0.69405200	2.67776700	1.76369500
O	1.74604600	1.28222500	2.87110600
O	0.80048400	-3.07835000	1.75525600
O	-2.94033800	4.22266800	-0.68311100
O	-0.59312800	3.13356400	0.43938800
O	0.54390300	2.53914200	-4.60762000
O	3.36184100	-1.55755800	-3.87408000
O	2.99247100	-1.79673000	1.31686000
O	0.76651200	4.11202300	2.69491200
O	2.17021000	3.01093700	0.56924800
O	4.27908700	2.56224800	-1.24875000
O	4.60781300	-0.30948100	3.17411000
O	3.04670700	-4.58798900	0.70846900
W	2.09757000	-3.24428500	0.27819300
N	-7.02478600	-0.11864300	-0.43813000
N	0.92372600	6.52462400	-0.62148100
N	6.75074100	-0.69924300	-1.09344800
C	-6.60256700	-1.14500900	-1.46578100
H	-7.41347600	-1.86702600	-1.57967300
H	-6.39548300	-0.63818600	-2.40870600
H	-5.69905300	-1.64112200	-1.11672600
C	-7.19463100	-0.78761100	0.90160600
H	-7.51595900	-0.03713300	1.62617500
H	-7.94790500	-1.57188800	0.80738800
H	-6.24097700	-1.21915900	1.20408300
C	-5.96968000	0.95873200	-0.32674600
H	-5.84318800	1.43082900	-1.30056900
H	-6.30076800	1.68634400	0.41664500
H	-5.02886700	0.50456700	-0.02402400

C	-8.32254600	0.50123000	-0.86232100
H	-9.08653300	-0.27608600	-0.92312400
H	-8.61297400	1.25497300	-0.12819000
H	-8.18507400	0.96688400	-1.83953200
C	-0.30145800	6.42173200	0.25728700
H	-0.23862400	5.50934200	0.84740800
H	-0.32621200	7.29474300	0.91220000
H	-1.18814900	6.38680300	-0.37683200
C	0.90461200	7.83733000	-1.34648700
H	0.92882000	8.64859600	-0.61645100
H	1.77718000	7.89458600	-1.99952100
H	-0.00848100	7.89670100	-1.94115800
C	2.16463400	6.42943400	0.23041400
H	2.19632200	5.44534000	0.69907000
H	3.03603700	6.56254100	-0.41337100
H	2.12832500	7.21442900	0.98789600
C	0.92611700	5.39732000	-1.62882400
H	1.81762100	5.49173500	-2.25121500
H	0.94125200	4.44855700	-1.09831800
H	0.02408000	5.46443600	-2.23693800
C	6.21716600	-0.17167100	-2.40497700
H	6.95251100	0.51841600	-2.82279200
H	6.04782000	-1.01273000	-3.07843600
H	5.27329800	0.33883000	-2.22129500
C	8.08158500	-1.35050600	-1.32216100
H	8.44617900	-1.75323500	-0.37556400
H	7.95855000	-2.15729500	-2.04656200
H	8.78154700	-0.60627900	-1.70671800
C	5.78247700	-1.71328300	-0.53083100
H	6.16840500	-2.06818600	0.42623000
H	4.81482800	-1.23559500	-0.39723800
H	5.68643500	-2.53696700	-1.23854500
C	6.90237600	0.43486300	-0.11069300
H	7.56186400	1.18723600	-0.54697800
H	5.91982300	0.85969500	0.09495400
H	7.33188400	0.03817600	0.81091700
P	-0.05867500	-0.19017300	-0.14077500
Ta	-0.51259800	-2.02066900	2.52375900
Ta	0.32027800	0.09327100	3.82624700

Four possible adsorption configurations of N<sub>2</sub> on [N(CH<sub>3</sub>)<sub>4</sub><sup>+</sup>]<sub>3</sub>[Ta<sup>II</sup><sub>2</sub>/POM]

Bridge-on configuration

Atomic

Coordinates (Angstroms)

	X	Y	Z
O	-0.83703400	-0.93349900	0.96753300
O	-0.96786700	0.59519000	-1.06766400
O	0.75657100	-1.28516800	-0.96112400
O	3.10343900	-2.16378400	-1.67346200
W	2.24125300	-0.85617000	-2.88490800
O	2.92106900	0.52537100	-1.80001200
W	2.65344700	2.23607100	-0.82302600
O	1.20225800	2.47527500	-2.06635000
W	-0.21022500	1.89118300	-3.17640100
O	0.86636000	0.28901700	-3.48013900
O	1.01399000	0.76403900	0.50713900
O	-1.74282000	0.73230500	-3.61011600
W	-2.78886400	-0.31583000	-2.45014000
O	-3.43313800	1.25186400	-1.58637200
W	-2.38714100	2.56155900	-0.55288700
O	-1.45372000	2.94789500	-2.18254900
O	-1.55631700	-1.79351500	-2.75049500
W	-0.31587000	-3.12916200	-2.25401400
O	1.11337700	-3.87200100	-1.13545700
O	-0.79113900	-4.47723600	-3.17201400
O	-1.47302900	-3.31072300	-0.64163700
W	-2.69039600	-2.56331600	0.55514000
O	-1.70842700	-3.07198700	2.09504700
O	1.89035700	-0.97107600	3.10705300
W	3.07580700	0.12999900	1.96875200
O	3.59840300	1.35541700	0.67611700
O	1.05059500	-2.36535000	-3.30517900
O	-4.14969600	-0.74053100	-3.39694600
O	-3.17454300	-1.31164400	-0.80395800
O	-4.03962200	-3.62029800	0.55278100
O	-3.45862500	-1.10973400	1.79376800
W	-2.65598700	0.40176900	2.48853600
O	-1.51762500	-0.71533100	3.61797600
O	-3.78338800	1.02348100	3.60847100
O	-2.93051400	1.47354700	1.00857300
O	-0.81952900	1.44906300	2.79373200
W	0.47102600	2.74013400	1.81254000
O	1.70485200	1.44075800	2.88290900
O	1.17583400	-2.93826500	1.40044600
O	-3.40669900	3.92959700	-0.43169700
O	-0.92488700	3.05493200	0.55062600

O	0.00154100	2.81758300	-4.58752900
O	3.35120600	-0.88819800	-4.17966300
O	3.21497000	-1.36177500	0.86435400
O	0.42211400	4.16200500	2.76044900
O	1.80932100	3.24988300	0.54752200
O	3.84814900	3.29750400	-1.41909000
O	4.50699300	0.09287000	2.90892900
O	3.53022000	-4.13078500	0.28989500
W	2.37836000	-2.93391200	-0.10502100
N	-6.92538000	-1.08033400	-0.22626700
N	0.01394100	6.68828600	-0.37471200
N	6.88840300	-1.08988700	-0.40684100
C	-6.39785300	-1.99660100	-1.30740700
H	-7.09385400	-2.83056300	-1.41608800
H	-6.31054200	-1.43457400	-2.23761600
H	-5.41630300	-2.36044700	-1.01018000
C	-6.91805600	-1.80559400	1.09552500
H	-7.31841500	-1.13759600	1.86032700
H	-7.54005700	-2.69817000	1.00655300
H	-5.89357300	-2.08625900	1.33843700
C	-6.05069900	0.14915300	-0.12551400
H	-6.05431200	0.66355800	-1.08623900
H	-6.45270500	0.79250000	0.65938500
H	-5.03514700	-0.15682300	0.11521400
C	-8.32515300	-0.66595300	-0.56793200
H	-8.95661500	-1.55457500	-0.62485300
H	-8.69568100	0.00738600	0.20709500
H	-8.31443900	-0.15452600	-1.53185700
C	-1.17066200	6.37237200	0.50936000
H	-0.94565800	5.48305200	1.09549500
H	-1.34256200	7.22576300	1.16829100
H	-2.04242700	6.18356600	-0.11833900
C	-0.23047200	7.98476800	-1.08852100
H	-0.34291800	8.78260100	-0.35207500
H	0.61777500	8.19470800	-1.74231400
H	-1.14195000	7.89174100	-1.68123800
C	1.25644100	6.79726300	0.47234100
H	1.43314600	5.84006800	0.96322300
H	2.09805600	7.04661100	-0.17623600
H	1.10414700	7.58132700	1.21654600
C	0.20246100	5.58722900	-1.39376000
H	1.06495500	5.83537900	-2.01443800
H	0.37530200	4.64987200	-0.87187400
H	-0.69871700	5.50809000	-2.00141200

C	5.89137300	-0.41850900	-1.32418400
H	6.33143200	0.50985000	-1.69242400
H	5.66647000	-1.09142600	-2.15149000
H	4.97822000	-0.21107400	-0.77187100
C	8.13547100	-1.40733900	-1.17742800
H	8.85279900	-1.89237900	-0.51282600
H	7.87849200	-2.07519900	-2.00115600
H	8.55549000	-0.47958600	-1.56989700
C	6.29136900	-2.36586900	0.13701400
H	7.03292200	-2.85187600	0.77396000
H	5.39620300	-2.11800800	0.70571400
H	6.01956600	-3.01223900	-0.69759500
C	7.21873100	-0.16717400	0.73763700
H	7.62138700	0.76191700	0.33059900
H	6.31284300	0.03420600	1.31133600
H	7.96070300	-0.65358300	1.37402500
P	0.00242200	-0.19612600	-0.16521100
Ta	-0.06310800	-2.11558400	2.59020900
N	0.44406200	-1.26286500	5.62348300
N	0.29252300	-2.00142300	4.70905900
Ta	0.35706500	0.09700900	3.78333700

#### Side-on configuration

Atomic	Coordinates (Angstroms)		
	X	Y	Z
O	-0.91312000	-1.04178800	0.77418200
O	-1.10195300	0.85529200	-0.91540300
O	0.62606100	-1.00797100	-1.23560200
O	2.95997800	-1.68762000	-2.22727000
W	1.98344700	-0.16382700	-3.12913100
O	2.76825700	0.93987600	-1.81951600
W	2.55895000	2.37687100	-0.48428700
O	1.04414000	2.88987100	-1.54729200
W	-0.46149400	2.56992400	-2.65770400
O	0.61549500	1.07598300	-3.38521700
O	0.94040300	0.74610900	0.54742500
O	-2.00317100	1.51240600	-3.29063600
W	-2.99028500	0.25939500	-2.29682800
O	-3.58224600	1.57323200	-1.08540700
W	-2.43700800	2.60618300	0.17958100
O	-1.62201300	3.37730100	-1.39858900
O	-1.77106600	-1.14297800	-2.96189500

W	-0.52882000	-2.53722800	-2.79030400
O	0.98360500	-3.48995300	-1.90025200
O	-1.03573200	-3.68362900	-3.93739800
O	-1.59239900	-3.07103500	-1.22273700
W	-2.75633100	-2.57218500	0.15759100
O	-1.67603100	-3.49245800	1.45429600
O	2.56569200	-1.43630800	3.15410000
W	3.36652600	-0.26558400	1.83932500
O	3.60029900	1.20240600	0.70580200
O	0.81236700	-1.59543900	-3.74582300
O	-4.39784300	0.02319300	-3.24222500
O	-3.30066300	-1.09346000	-0.88984500
O	-4.12257600	-3.59772200	0.00012200
O	-3.33888800	-1.50481100	1.76048100
W	-2.35714600	-0.18921100	2.64986800
O	-1.11523500	-1.57459300	3.40755400
O	-3.30374000	0.15958000	4.02446300
O	-2.81187100	1.17924000	1.49648700
O	-0.51365100	0.71637200	3.04275800
W	0.58904400	2.28356500	2.29157500
O	1.93336300	0.83557300	2.91243300
O	1.24862600	-3.12500300	0.77001700
O	-3.45043900	3.88377700	0.69028300
O	-0.88833500	2.87149900	1.25864500
O	-0.31801700	3.78510700	-3.83995800
O	3.01986600	0.06121600	-4.46545600
O	3.24948200	-1.49450600	0.46525300
O	0.59896800	3.42200900	3.56927500
O	1.84546800	3.12232600	1.11045100
O	3.73026100	3.53564800	-0.93153500
O	4.97498000	-0.35002100	2.43223200
O	3.50053200	-4.01712900	-0.80746200
W	2.33849400	-2.76791300	-0.84940500
N	-6.99697000	-0.98576700	-0.02009400
N	0.08936700	6.62357200	1.00537800
N	6.87376000	-0.92998300	-1.10847400
C	-6.54360300	-1.58139900	-1.33447600
H	-7.27853100	-2.32879500	-1.63994900
H	-6.46131100	-0.78753700	-2.07724000
H	-5.56982200	-2.04563300	-1.19031600
C	-6.99618100	-2.05839000	1.03887800
H	-7.30502800	-1.61341000	1.98646300
H	-7.69633400	-2.84140600	0.74131600
H	-5.99042600	-2.47127200	1.12087800



C	-6.05997200	0.12688900	0.39374400
H	-6.04519100	0.88671700	-0.38718800
H	-6.42247600	0.54580600	1.33435500
H	-5.05876900	-0.27886300	0.51905900
C	-8.38040100	-0.42967800	-0.17955000
H	-9.05782200	-1.23471500	-0.47017900
H	-8.70038600	0.00463500	0.76931400
H	-8.36107000	0.33905200	-0.95380700
C	-1.03960300	6.12920400	1.87917700
H	-0.83575700	5.10140300	2.17378400
H	-1.09815300	6.77209200	2.75944100
H	-1.96891900	6.16646300	1.30958400
C	-0.14360100	8.06519200	0.66295300
H	-0.16724400	8.65131800	1.58352100
H	0.66596300	8.41193000	0.01849800
H	-1.09740900	8.15158500	0.13982700
C	1.39808500	6.47841700	1.74108200
H	1.57769000	5.42096400	1.93635100
H	2.19453400	6.87998500	1.11198100
H	1.33563800	7.03516200	2.67789400
C	0.14323600	5.80941100	-0.26704100
H	0.95820500	6.18780400	-0.88636400
H	0.32285500	4.76821400	-0.01213400
H	-0.81035800	5.90126000	-0.78657900
C	5.79857300	-0.08674400	-1.75632300
H	6.23856100	0.86897900	-2.04637600
H	5.41680000	-0.61508400	-2.62937400
H	4.98861200	0.07157400	-1.04784200
C	7.98842400	-1.14781100	-2.08852700
H	8.76025800	-1.76210300	-1.62106300
H	7.58821400	-1.65529400	-2.96764100
H	8.40204600	-0.17947600	-2.37551100
C	6.29425500	-2.26385800	-0.70226200
H	7.08713800	-2.86202900	-0.24907900
H	5.48671400	-2.09514200	0.00852900
H	5.89663000	-2.76129800	-1.58683400
C	7.40008400	-0.22180500	0.11330000
H	7.78079000	0.75553700	-0.18878800
H	6.59171500	-0.10822100	0.83848600
H	8.20377500	-0.82274000	0.54368500
P	-0.10693900	-0.10880400	-0.20015000
Ta	0.01430400	-2.86601900	2.12221700
N	0.82072700	-2.87047500	4.16483700
N	0.67431600	-4.01469700	3.83922800

Ta	0.79090100	-0.77497500	3.62023500
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End-on configuration

Atomic	Coordinates (Angstroms)		
	X	Y	Z
O	-0.87147100	-1.04146100	0.80883300
O	-1.11019400	0.80414000	-0.92085600
O	0.64633500	-1.04806300	-1.20362800
O	2.98939000	-1.76241700	-2.18714900
W	1.99035300	-0.28528100	-3.13052600
O	2.77237600	0.86008900	-1.84488600
W	2.56582100	2.33780700	-0.55992400
O	1.05075100	2.82066600	-1.64412900
W	-0.45661100	2.46473700	-2.74649300
O	0.62133900	0.95084000	-3.41374600
O	0.94839600	0.77044300	0.51795500
O	-1.99145600	1.37375700	-3.32281600
W	-2.97732000	0.14555800	-2.28583900
O	-3.57772900	1.51655500	-1.13266800
W	-2.45053000	2.61655800	0.08244400
O	-1.62392800	3.31508600	-1.52111400
O	-1.75145200	-1.26558700	-2.89675500
W	-0.50561200	-2.65817400	-2.66909200
O	1.02430700	-3.55447700	-1.78255100
O	-1.01738100	-3.84613400	-3.77081100
O	-1.57323500	-3.12489700	-1.08331000
W	-2.75496100	-2.59601400	0.28149900
O	-1.69319400	-3.39695000	1.61841600
O	2.47106400	-1.34741800	3.22277100
W	3.33633600	-0.23222400	1.87261200
O	3.59141200	1.20115700	0.69399700
O	0.81744300	-1.73158500	-3.68294500
O	-4.38178000	-0.12658300	-3.22796400
O	-3.28784700	-1.13938300	-0.82675800
O	-4.11769300	-3.63283100	0.14953300
O	-3.34079400	-1.41858100	1.83587600
W	-2.39812400	-0.06511800	2.68840800
O	-1.09728800	-1.39850700	3.52924300
O	-3.35857900	0.32815800	4.03967700
O	-2.83628500	1.24491000	1.47049700
O	-0.56085200	0.87004500	2.99777000
W	0.57430300	2.39021700	2.19995700

O	1.90180000	0.94133100	2.87451900
O	1.30994100	-3.08216300	0.83844300
O	-3.46957600	3.91319200	0.52860200
O	-0.90242400	2.93645900	1.14128800
O	-0.31468300	3.63401000	-3.97442800
O	3.01717800	-0.09151000	-4.47902100
O	3.29696700	-1.49857300	0.51946200
O	0.59111000	3.57803400	3.43157100
O	1.84729300	3.16423300	0.99050800
O	3.75209100	3.46583300	-1.04577800
O	4.92473200	-0.30432300	2.51658700
O	3.56578300	-4.05802700	-0.69770200
W	2.40615500	-2.80724400	-0.76311300
N	-7.01470600	-1.06978300	-0.12010500
N	0.08400500	6.66068500	0.74722100
N	6.89145400	-0.90369300	-0.98515100
C	-6.51264700	-1.75063800	-1.37442100
H	-7.24115800	-2.51148900	-1.66174700
H	-6.39078000	-1.00601400	-2.16138500
H	-5.55052700	-2.21200000	-1.15918000
C	-7.03969100	-2.06662100	1.00967300
H	-7.38789600	-1.56238000	1.91299200
H	-7.71938100	-2.87835200	0.74307100
H	-6.03269500	-2.45916400	1.15390000
C	-6.10270200	0.07990200	0.24586500
H	-6.07867800	0.78855100	-0.58142700
H	-6.49565800	0.55235200	1.14808800
H	-5.09877400	-0.30124400	0.41938700
C	-8.39657300	-0.54106600	-0.36314500
H	-9.05804600	-1.37197700	-0.61503100
H	-8.75021600	-0.04151000	0.54069400
H	-8.35808800	0.16938800	-1.19056700
C	-1.05324200	6.20943500	1.63351900
H	-0.85404400	5.19604000	1.97707500
H	-1.11737100	6.89253900	2.48260400
H	-1.97799900	6.22221200	1.05545800
C	-0.14018800	8.08677600	0.34056700
H	-0.16518500	8.71334100	1.23414500
H	0.67384500	8.40076700	-0.31497000
H	-1.09123400	8.15481100	-0.19025000
C	1.38655300	6.54265700	1.49861200
H	1.56052700	5.49411500	1.74104700
H	2.18924700	6.91380600	0.85887800
H	1.31903200	7.13944100	2.41010300

C	0.14391100	5.79161100	-0.48830400
H	0.96817900	6.13672100	-1.11468000
H	0.31252700	4.76099500	-0.18722800
H	-0.80372800	5.86873500	-1.02106600
C	5.78810500	-0.13871500	-1.68167800
H	6.19047600	0.81952600	-2.01451600
H	5.43676500	-0.72506000	-2.53005800
H	4.96624800	0.01925300	-0.98717500
C	8.02721000	-1.11544300	-1.94175000
H	8.81855400	-1.67491300	-1.43920100
H	7.66040100	-1.67678300	-2.80252700
H	8.40271700	-0.14333600	-2.26604500
C	6.36493000	-2.24171200	-0.52482000
H	7.17605000	-2.78275700	-0.03365800
H	5.53895400	-2.07515800	0.16534900
H	6.00332200	-2.79661000	-1.39062000
C	7.36995400	-0.11857300	0.20885800
H	7.70781700	0.86145000	-0.13270400
H	6.54803000	-0.01125900	0.91926900
H	8.19552200	-0.66120700	0.67411600
P	-0.08241500	-0.11180000	-0.20934500
Ta	0.03752600	-2.56137400	2.08759800
N	0.84783200	-4.52465000	4.54817900
N	0.55639600	-3.86147100	3.68508900
Ta	0.73877500	-0.57048400	3.67522600

### End-on configuration

Atomic	Coordinates (Angstroms)		
	X	Y	Z
O	-0.84634500	-0.95232900	0.89529700
O	-1.08300200	0.68107700	-1.01899400
O	0.66490100	-1.19896300	-1.09365800
O	2.98318300	-2.05560400	-1.98013700
W	2.01780200	-0.66252300	-3.07589200
O	2.80225600	0.60466500	-1.92080100
W	2.61001700	2.22752800	-0.79649000
O	1.10845700	2.59815600	-1.94227400
W	-0.39062700	2.14742800	-3.01316200
O	0.65768400	0.54317000	-3.50092500
O	0.98210000	0.78854900	0.42603100
O	-1.94328100	1.00892800	-3.48253300
W	-2.95066100	-0.08267000	-2.33785900

O	-3.53717500	1.39514700	-1.32273600
W	-2.40384100	2.61812100	-0.22072500
O	-1.55821700	3.12017900	-1.88461200
O	-1.74133900	-1.57470000	-2.75385700
W	-0.50693200	-2.94757400	-2.37169200
O	0.99628800	-3.75287800	-1.37603700
O	-1.03529400	-4.24688200	-3.33045300
O	-1.59736400	-3.21316200	-0.73502000
W	-2.82576000	-2.53818600	0.51552300
O	-1.77311400	-3.21665800	1.97505000
O	2.44844200	-1.06315400	3.28075000
W	3.32963300	-0.07530400	1.89330200
O	3.61653500	1.21735400	0.55979300
O	0.82043900	-2.15365000	-3.47519100
O	-4.35012400	-0.43337400	-3.26067800
O	-3.31443400	-1.22215400	-0.75128400
O	-4.19082100	-3.57389700	0.47243400
O	-3.39091300	-1.18395000	1.89903100
W	-2.44339600	0.23670700	2.66166800
O	-1.23323100	-1.04182100	3.56740600
O	-3.42391300	0.78697000	3.94322500
O	-2.83087500	1.41681100	1.29402300
O	-0.57842200	1.16199500	2.89405100
W	0.60327200	2.56101100	1.95108800
O	1.91031400	1.20242900	2.77112100
O	1.26748700	-3.05342200	1.18164700
O	-3.39776000	3.97809800	0.06819500
O	-0.85861400	3.00858100	0.82125600
O	-0.22988300	3.17944200	-4.35575900
O	3.05158800	-0.62933600	-4.43270000
O	3.27344200	-1.48632000	0.66735600
O	0.62316800	3.88412900	3.03735400
O	1.88442200	3.19679000	0.66816800
O	3.80335800	3.29433400	-1.39103100
O	4.91316500	-0.08779800	2.55437800
O	3.54290000	-4.16742300	-0.24045600
W	2.39789600	-2.91862800	-0.43860100
N	-7.03482400	-0.93538500	-0.07607900
N	0.13548800	6.67259900	0.13027400
N	6.88602900	-1.02754000	-0.88738800
C	-6.53536400	-1.75543700	-1.24510600
H	-7.27754500	-2.52719900	-1.45839700
H	-6.39033100	-1.10132300	-2.10511300
H	-5.58481400	-2.21011900	-0.97289000

C	-7.09394000	-1.80585700	1.15205500
H	-7.45635100	-1.20609800	1.98887000
H	-7.77479700	-2.63687700	0.95803600
H	-6.09382000	-2.18597500	1.36075200
C	-6.10109000	0.22704600	0.17950000
H	-6.04397000	0.83968100	-0.71974200
H	-6.49743100	0.80484700	1.01672200
H	-5.10998000	-0.15486000	0.41486200
C	-8.40237000	-0.40736900	-0.39214100
H	-9.07836900	-1.24722300	-0.56299000
H	-8.75541400	0.19268900	0.44855900
H	-8.33943300	0.20974100	-1.28987700
C	-1.00075800	6.32570300	1.06475100
H	-0.78774900	5.37038800	1.54108100
H	-1.07808100	7.11372200	1.81644100
H	-1.92301500	6.24760600	0.48768300
C	-0.08567000	8.04533100	-0.43156500
H	-0.09668600	8.76833500	0.38619200
H	0.72270400	8.27824100	-1.12682600
H	-1.04227400	8.05986700	-0.95650900
C	1.43907100	6.63516500	0.88808300
H	1.60521100	5.62193500	1.25404700
H	2.24271800	6.92230100	0.20771900
H	1.37734000	7.33681300	1.72198700
C	0.19078400	5.67297000	-1.00265200
H	1.02382300	5.93749800	-1.65592100
H	0.34239800	4.67941400	-0.58921500
H	-0.75187800	5.70466700	-1.54886500
C	5.78351500	-0.38066800	-1.69548500
H	6.16766600	0.54733600	-2.12222800
H	5.47519800	-1.06751500	-2.48345800
H	4.93604700	-0.17272400	-1.04640200
C	8.05205200	-1.32173800	-1.78355800
H	8.84222700	-1.79477500	-1.19729600
H	7.72342800	-1.99234900	-2.57902700
H	8.41298100	-0.38563400	-2.21318800
C	6.37770600	-2.31434100	-0.28342200
H	7.18517900	-2.76891500	0.29382300
H	5.52574900	-2.08945300	0.35699100
H	6.05958700	-2.97951300	-1.08664500
C	7.31498600	-0.09265600	0.21434400
H	7.63931400	0.84746300	-0.23525400
H	6.47375500	0.07878700	0.88821100
H	8.14007400	-0.55522100	0.75979600

P	-0.04602600	-0.13982300	-0.22785700
Ta	-0.06767000	-2.31459600	2.24098800
N	0.73654500	-2.18599700	6.40246600
N	0.69918800	-1.61497200	5.43758500
Ta	0.69000700	-0.28362300	3.70202300