

DFT Study on Reduction of Carbon Dioxide by $(\text{tBuArN})_3\text{M}\equiv\text{N}$ (M=Nb, V, Ta): the Electronic Structure and Catalyzing Activity

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NbN1

N	0.42075700	-0.68346300	-3.12910800
C	-1.89519100	-1.55378900	0.32328000
C	-1.66559500	-2.85799200	0.82240600
C	-2.33144700	-0.58047700	1.23787200
C	-1.88263500	-3.18562600	2.16094800
H	-1.29122300	-3.61407400	0.13883400
C	-2.55666900	-0.88322200	2.58881800
H	-2.50501800	0.42633300	0.86965400
C	-2.33410800	-2.18733700	3.03866200
H	-2.50900800	-2.43150300	4.08565200
C	-0.46890600	2.37665500	-0.32677700
C	0.14628900	2.48996600	0.93351200
C	-1.79248700	2.86066000	-0.44740200
C	-0.50508200	3.08276000	2.02377100
H	1.16134100	2.12050500	1.04376100
C	-2.46379400	3.45442000	0.62286400
H	-2.30047000	2.74935500	-1.40048100
C	-1.80733000	3.56603300	1.85742800
H	-2.31775700	4.03624900	2.69725500
C	2.28157100	-0.68731900	0.68480300
C	1.51922600	-0.92515200	1.84603900
C	3.41365300	0.15112000	0.81684400
C	1.87226000	-0.38270900	3.08726900
H	0.64962700	-1.57037800	1.76366100
C	3.79051800	0.69836100	2.04492100
H	3.99542600	0.38382300	-0.07010300
C	3.01455700	0.42139100	3.17912600
H	3.30463800	0.83592700	4.14328600
C	-2.66462100	-1.79790200	-2.02803100
C	-2.92574500	-0.73426200	-3.11410200
C	-2.10342500	-3.06632300	-2.70796800
C	-4.02222700	-2.13238600	-1.37069800
H	-3.35484400	0.16807900	-2.66475000
H	-1.98940400	-0.46680900	-3.60757900
H	-3.62837000	-1.11427900	-3.86767300
H	-1.94237400	-3.86808200	-1.97927000
H	-2.79630800	-3.44486400	-3.47178400
H	-1.14951400	-2.82828300	-3.18508100

H	-4.73049600	-2.45640300	-2.14200200
H	-3.94132200	-2.93362500	-0.63101600
H	-4.44238900	-1.25397100	-0.86962200
C	0.61261500	2.71912400	-2.53853500
C	-0.40809700	2.66941800	-3.69747100
C	0.76468300	4.17877700	-2.05428500
C	1.98524600	2.26764400	-3.07759200
H	-0.51666800	1.63693300	-4.03866500
H	-1.38868700	3.04112900	-3.38188800
H	-0.07540000	3.28709900	-4.54276500
H	1.47833500	4.24324200	-1.22612100
H	1.13957300	4.79931100	-2.87647600
H	-0.18234700	4.60739800	-1.71511800
H	2.30928300	2.91810900	-3.90078400
H	2.73720100	2.31490200	-2.28237800
H	1.92577700	1.24015900	-3.44162600
C	2.86513500	-2.19875400	-1.21005500
C	3.68816500	-1.49689300	-2.31339300
C	3.82552300	-2.85652100	-0.19348100
C	2.04698300	-3.33344000	-1.86193200
H	3.00813800	-1.04376500	-3.03868400
H	4.32892600	-0.71282500	-1.89661300
H	4.33611600	-2.21332800	-2.83635100
H	3.26617400	-3.33700700	0.61628200
H	4.42081400	-3.62512200	-0.70000800
H	4.51754000	-2.14057800	0.25740200
H	2.71052600	-4.04903100	-2.36535600
H	1.47276300	-3.87031600	-1.09911500
H	1.35244700	-2.92044200	-2.59583100
N	1.89575300	-1.26435300	-0.54779200
N	0.22726400	1.79683300	-1.41862200
N	-1.69015600	-1.22334700	-1.04136900
C	5.01601500	1.58165800	2.14319600
H	5.14590100	1.97358900	3.15710200
H	5.92988100	1.03467200	1.87894000
H	4.94870900	2.43714400	1.46094400
C	1.04292800	-0.68795800	4.31479400
H	1.45771600	-0.20692900	5.20685500
H	0.00989200	-0.34749900	4.18983500
H	0.99556700	-1.76671100	4.50614100
C	-3.07732400	0.18286400	3.52778900
H	-2.53508400	1.12425000	3.39589300
H	-4.13784700	0.39589600	3.33764600
H	-2.98966100	-0.12639900	4.57474900

C	-1.61466300	-4.58527300	2.67026700
H	-0.80128900	-4.59629900	3.40679800
H	-2.49752000	-5.01083500	3.16343100
H	-1.32990000	-5.25703600	1.85521700
C	-3.88766000	3.94344100	0.46809400
H	-4.59296200	3.30644800	1.01718400
H	-4.00837100	4.96210100	0.85616400
H	-4.19614900	3.94477000	-0.58157700
C	0.21518600	3.25421400	3.34346500
H	0.69021300	4.24265400	3.41047600
H	-0.47374500	3.17158300	4.19150200
H	1.00246600	2.50536700	3.46375800
Nb	0.19981800	-0.33344700	-1.46556400

NbN2

C	-0.42271400	2.41382800	-0.27562200
C	-0.37000800	3.01025500	-1.55627100
C	-1.68494400	2.23590000	0.31122000
C	-1.52352100	3.43238400	-2.21637500
H	0.59651000	3.12177300	-2.03612400
C	-2.86157500	2.64600200	-0.33429700
H	-1.73517000	1.77518900	1.29293800
C	-2.76838500	3.24563900	-1.59175000
H	-3.67585900	3.57300000	-2.09736400
C	-0.77288000	-0.95088300	2.14077600
C	-1.92139100	-1.47684400	1.52683600
C	-0.95194000	-0.09957900	3.25219100
C	-3.20750200	-1.19287700	2.00698600
H	-1.79328000	-2.12916600	0.66844000
C	-2.22192300	0.20286700	3.74788600
H	-0.07398200	0.33768800	3.71706600
C	-3.34463200	-0.35432500	3.11725500
H	-4.33954600	-0.12898500	3.49908200
C	-0.40669400	-1.40218300	-1.96308900
C	-1.57685700	-0.65720900	-2.20819600
C	-0.52403300	-2.80267100	-1.87767900
C	-2.81897800	-1.27645400	-2.37865500
H	-1.49152600	0.42255200	-2.27771400
C	-1.75302800	-3.44786200	-2.05620700
H	0.36444400	-3.38648900	-1.65796700
C	-2.89223000	-2.67463800	-2.30899800

H	-3.85162500	-3.16938000	-2.45409100
C	1.63472200	3.07346200	0.98083000
C	0.79692200	4.31026500	1.37189500
C	2.29450500	2.53053600	2.26289000
C	2.74625000	3.49036900	-0.00553100
H	0.34493200	4.79534000	0.50199700
H	-0.00709200	4.04127600	2.06544000
H	1.44297300	5.04375200	1.86652800
H	2.93540300	1.67720800	2.03602000
H	2.91504100	3.30747500	2.72517100
H	1.53031100	2.22457600	2.98585000
H	3.35491900	4.29338600	0.43092900
H	3.40956400	2.64603000	-0.21837800
H	2.32360500	3.87339100	-0.94025000
C	1.32083300	-2.27825700	2.44496300
C	2.25656100	-1.56532200	3.44330900
C	0.38978400	-3.23824100	3.21748200
C	2.17141200	-3.12333900	1.47750000
H	2.92158000	-0.88547300	2.90653700
H	1.68805300	-0.99583400	4.18626500
H	2.87503100	-2.29395700	3.98210900
H	-0.29180600	-3.75993900	2.53756400
H	0.99669000	-3.99061700	3.73270100
H	-0.21335700	-2.72074000	3.96911500
H	2.68974100	-3.91398200	2.03442600
H	1.52637400	-3.60145500	0.73197100
H	2.93385100	-2.52397100	0.97223600
C	1.84228700	-0.87233800	-2.92861600
C	2.82970400	-2.03181300	-2.67195100
C	1.12835900	-1.10233100	-4.27855700
C	2.63126100	0.44768300	-3.04219800
H	3.36537100	-1.89481600	-1.72905600
H	2.30830100	-2.99451800	-2.64270400
H	3.57076000	-2.08470300	-3.47976100
H	0.40986100	-0.30273800	-4.48725100
H	1.87148000	-1.11137700	-5.08341900
H	0.59186900	-2.05478800	-4.30749100
H	3.34628700	0.38677000	-3.87145900
H	1.94759100	1.28034200	-3.23991500
H	3.19408300	0.66455800	-2.13216000
N	0.84233200	-0.73457100	-1.80955700
N	0.52259700	-1.28045200	1.64499000
N	0.75464400	1.99266100	0.40877800
C	-1.83987900	-4.95648700	-1.97716500

H	-2.87743000	-5.30085400	-2.03012200
H	-1.28874200	-5.43327100	-2.79719700
H	-1.40817000	-5.33224600	-1.04269100
C	-4.06366400	-0.45694700	-2.63854800
H	-4.63324600	-0.85149900	-3.48859200
H	-4.73513900	-0.46440000	-1.77056500
H	-3.81324300	0.58632500	-2.84636900
C	-4.20066200	2.46645700	0.34505300
H	-4.31089000	1.45026000	0.73669900
H	-4.30841800	3.14940700	1.19750300
H	-5.02913800	2.66427000	-0.34264800
C	-1.44534700	4.07239300	-3.58504500
H	-2.03675400	3.51688700	-4.32287100
H	-1.83391600	5.09852800	-3.57081400
H	-0.41409100	4.11181600	-3.94676300
C	-2.39115300	1.14057500	4.92306900
H	-2.75391000	2.12487300	4.60054200
H	-3.11756500	0.75202400	5.64633100
H	-1.44378200	1.29698700	5.44697700
C	-4.41968200	-1.82877200	1.36251200
H	-4.66146300	-2.79009300	1.83551000
H	-5.30663500	-1.19260000	1.45558000
H	-4.24334900	-2.02544000	0.30130100
Nb	1.19905900	-0.02738000	0.11953200
C	4.44493900	-0.18270700	0.20639500
N	2.95090700	-0.09214300	0.25099700
O	4.87100900	-1.33661500	0.38499500
O	4.99852000	0.90693200	-0.02026600

NbNO

C	-1.08366200	2.06011700	1.02077700
C	-1.37344200	3.22281100	0.28046500
C	-2.13978900	1.36599600	1.62369700
C	-2.68078500	3.69427300	0.15428300
H	-0.56080400	3.75467500	-0.20123000
C	-3.46328500	1.82089000	1.51463600
H	-1.91862400	0.47110200	2.19565900
C	-3.71681500	2.98138200	0.78006500
H	-4.73898900	3.34538200	0.69512300
C	-0.39816000	-1.90063600	1.37742400
C	-1.63546000	-2.31175800	0.86002400

C	-0.26722100	-1.75043500	2.76890100
C	-2.71900400	-2.58875200	1.70371000
H	-1.73777000	-2.43541300	-0.21241800
C	-1.33625400	-2.00885800	3.63233400
H	0.68116600	-1.41703100	3.17439000
C	-2.55519400	-2.43038700	3.08414300
H	-3.39113000	-2.64341000	3.74798900
C	-1.20382600	-0.37315700	-2.22582400
C	-2.48605900	0.08705000	-1.88430000
C	-1.07426100	-1.63418900	-2.82561500
C	-3.62391100	-0.67903800	-2.15474000
H	-2.58272500	1.06159700	-1.41698500
C	-2.19757800	-2.42446900	-3.10244800
H	-0.08245000	-2.00018800	-3.07053300
C	-3.46297800	-1.93201000	-2.76379200
H	-4.34252000	-2.53500700	-2.98152700
C	1.09732900	2.30876100	2.23452100
C	0.21713200	2.69955500	3.43870900
C	2.19959700	1.36406400	2.74342600
C	1.74698600	3.57307600	1.63644400
H	-0.56041100	3.41765300	3.16784700
H	-0.26454600	1.82118100	3.87948500
H	0.84837400	3.16089900	4.20480600
H	2.90718600	1.07721900	1.96478500
H	2.77369600	1.86465900	3.52976700
H	1.76328600	0.45862200	3.17398500
H	2.38631700	4.05495300	2.38476200
H	2.36679800	3.32120300	0.77209100
H	0.99141800	4.30313300	1.33229400
C	1.70459600	-2.81149000	0.38133500
C	2.74712400	-2.73061800	1.51423500
C	0.97703400	-4.17042000	0.45299400
C	2.41826500	-2.73759100	-0.98024600
H	3.26173700	-1.76642000	1.50472600
H	2.27991800	-2.86611300	2.49360900
H	3.49689500	-3.52204200	1.39823900
H	0.22067500	-4.25703800	-0.33292000
H	1.70751900	-4.97355200	0.31231500
H	0.48759700	-4.32746300	1.41681100
H	3.09867300	-3.58963500	-1.08500700
H	1.69236400	-2.78441900	-1.79780900
H	3.00156300	-1.82205500	-1.08609600
C	0.44015100	1.26221800	-3.17853400
C	1.51236100	0.45476100	-3.93747700

C	-0.71567300	1.59591700	-4.14284800
C	1.03454800	2.59416000	-2.68799400
H	2.35380100	0.21532900	-3.28261500
H	1.09819400	-0.47982500	-4.32706400
H	1.89237500	1.03105000	-4.78832200
H	-1.50952200	2.15258300	-3.63688500
H	-0.32602500	2.22142000	-4.95224500
H	-1.15595600	0.70231300	-4.59138900
H	1.42335000	3.16027700	-3.54098300
H	0.26119000	3.19930900	-2.20730500
H	1.85960600	2.45627200	-1.98667300
N	-0.06229900	0.46511700	-1.98585200
N	0.71221000	-1.67340100	0.49035300
N	0.26768900	1.59568900	1.18500900
C	-2.03646700	-3.77772200	-3.75745400
H	-3.00199000	-4.27189300	-3.89587500
H	-1.56266200	-3.68954600	-4.74193400
H	-1.40393700	-4.44088200	-3.15628500
C	-5.00409900	-0.15450700	-1.82949800
H	-5.53277100	0.15424200	-2.73988300
H	-5.62130700	-0.91877600	-1.34499600
H	-4.95129400	0.71213300	-1.16594500
C	-4.58420700	1.06618000	2.19201900
H	-4.69161700	0.05785300	1.77759600
H	-4.39183800	0.94993600	3.26440800
H	-5.54108200	1.58314400	2.07648300
C	-2.98089500	4.95736600	-0.62030300
H	-3.81772600	4.81337600	-1.31226800
H	-3.25847400	5.77809500	0.05237700
H	-2.11506300	5.28593300	-1.20157700
C	-1.18997600	-1.81162700	5.12433900
H	-1.59807300	-0.84298300	5.43881000
H	-1.72655700	-2.58444700	5.68408100
H	-0.14054200	-1.83850900	5.43094900
C	-4.02599200	-3.09447600	1.13603800
H	-4.10507800	-4.18389800	1.24232800
H	-4.88614300	-2.65981300	1.65625700
H	-4.11211700	-2.86077800	0.07186000
Nb	0.89436500	0.24268900	-0.20115900
C	3.88089800	1.10234700	-0.76078500
N	2.67279900	0.56860300	-0.52335000
O	4.18229500	2.26560500	-0.90242300
C	5.55328700	-0.31889500	0.16181500
O	4.90306000	0.10896300	-0.95366100

C	6.65863400	-1.27980600	-0.20029300
H	7.36864600	-0.79240500	-0.87456600
H	7.16698500	-1.60597900	0.70650700
H	6.24451300	-2.14307200	-0.72954700
O	5.26420500	0.03596400	1.28231700
NbN3			
C	-0.72675700	-1.28916000	1.85704800
C	-1.45907800	-0.54596200	2.80042200
C	-1.35954300	-2.36615500	1.22286300
C	-2.77697500	-0.86943700	3.12316500
H	-0.97939900	0.28438100	3.30044500
C	-2.67890000	-2.72657800	1.54211300
H	-0.81004100	-2.93989700	0.48587200
C	-3.37300900	-1.96897800	2.48724900
H	-4.39313800	-2.24573400	2.74672200
C	-0.37177100	-1.15048300	-1.87622100
C	-1.75379800	-1.05139300	-2.07114100
C	0.25147100	-2.40678600	-1.98530800
C	-2.51127700	-2.18130000	-2.41054600
H	-2.23353900	-0.08554400	-1.96632700
C	-0.48560700	-3.54672200	-2.31316200
H	1.31994700	-2.47205100	-1.81842100
C	-1.86481300	-3.41440600	-2.53227800
H	-2.44592500	-4.29324500	-2.80468800
C	-1.10603300	2.32664600	0.00014400
C	-2.32219300	1.63573600	0.13339400
C	-1.06714400	3.43739400	-0.85762500
C	-3.47432300	2.04432000	-0.54539000
H	-2.36546400	0.78543400	0.80334000
C	-2.20553900	3.86300300	-1.55633400
H	-0.13692500	3.97567500	-0.99610000
C	-3.40232100	3.16037900	-1.38936300
H	-4.29302400	3.48914800	-1.92103500
C	1.60504500	-1.86927400	2.50866500
C	1.84777500	-3.23523900	1.83701200
C	2.94732800	-1.14921800	2.73192400
C	0.98889200	-2.10237500	3.90524800
H	0.91839400	-3.80657200	1.76338600
H	2.26291800	-3.09653600	0.83858300
H	2.55247600	-3.82528500	2.43428200
H	2.80126100	-0.19208100	3.23861000
H	3.58078700	-1.77177600	3.37181400
H	3.47907900	-0.97712900	1.79890900
H	1.70550400	-2.67251700	4.50494500

H	0.79505000	-1.15938700	4.42451500
H	0.05838000	-2.67179200	3.86600800
C	0.87843600	0.74500800	-2.90704500
C	1.64921800	-0.21177800	-3.84025200
C	-0.34645800	1.29733200	-3.66353200
C	1.81950400	1.89599500	-2.52007900
H	2.55569400	-0.58468000	-3.36120700
H	1.03327600	-1.05296800	-4.16639900
H	1.95083200	0.34613900	-4.73307000
H	-0.94641900	1.95310900	-3.03106900
H	0.00623600	1.87417400	-4.52514500
H	-0.98318300	0.49438500	-4.04230400
H	2.06312800	2.47397100	-3.41692900
H	1.35381700	2.57886200	-1.80647600
H	2.75753500	1.51039000	-2.11405000
C	0.28783100	2.88745700	1.94922500
C	1.04815200	4.14728800	1.47309900
C	-1.04576400	3.33475400	2.59285900
C	1.12725500	2.22010500	3.05643200
H	1.93904400	3.87251900	0.90572600
H	0.41947400	4.79528800	0.85942200
H	1.36496300	4.73373100	2.34290100
H	-1.63234500	2.47896200	2.93784100
H	-0.82705600	3.96856100	3.45832600
H	-1.66539400	3.91261300	1.90469600
H	1.18867300	2.90164100	3.91084000
H	0.67957600	1.28827400	3.40402700
H	2.14187400	2.00909600	2.72481500
N	0.02845900	1.92303100	0.79181400
N	0.42921000	0.02471200	-1.64365500
N	0.67476800	-1.02659200	1.63281300
C	-2.12237800	5.04385900	-2.49699200
H	-3.11585700	5.43022100	-2.74172300
H	-1.53815000	5.86194200	-2.06334600
H	-1.63578600	4.76580700	-3.44017500
C	-4.78578500	1.32016000	-0.33731800
H	-5.46053700	1.90219800	0.30286200
H	-5.30980100	1.15506100	-1.28503900
H	-4.63261200	0.35023500	0.14416000
C	-3.33412200	-3.91642600	0.87898900
H	-3.70930400	-3.66111900	-0.11793400
H	-2.62555700	-4.74067700	0.75115000
H	-4.17844900	-4.28362100	1.46982200
C	-3.54272600	-0.07751400	4.15877800

H	-4.48665300	0.30378700	3.75323000
H	-3.79451500	-0.69826100	5.02678200
H	-2.96407900	0.77744200	4.51860500
C	0.18368600	-4.89756300	-2.42747100
H	-0.07298800	-5.54345700	-1.57880800
H	-0.12992000	-5.42230900	-3.33619800
H	1.27255800	-4.80274900	-2.45120500
C	-3.99773100	-2.05255700	-2.65647700
H	-4.20401400	-1.38842300	-3.50380900
H	-4.45209600	-3.02266100	-2.87677300
H	-4.51121000	-1.62882900	-1.78630400
Nb	1.21890200	0.29992100	0.18407600
C	3.97641300	1.87738200	0.52089200
N	2.84403200	1.46082500	0.58101000
O	5.06539300	2.33778200	0.52071900
C	3.90739900	-1.06356000	-0.99559200
O	4.33859700	-0.11265000	-1.63995000
C	4.70236500	-2.35539800	-0.86170100
H	4.93506800	-2.54412500	0.19126500
H	4.11181200	-3.20587100	-1.21771200
H	5.62812700	-2.28392400	-1.43332800
O	2.74692200	-1.08785000	-0.37370400

TS_NbN12

C	-0.54935900	2.42716200	-0.28828500
C	-0.56749300	3.01825900	-1.56888400
C	-1.78861100	2.19931300	0.34037200
C	-1.76215100	3.39742900	-2.18949400
H	0.37530700	3.16091100	-2.08799500
C	-2.99861600	2.56018200	-0.26203500
H	-1.78559000	1.73295500	1.32074600
C	-2.97319700	3.16331200	-1.52617300
H	-3.90967100	3.44934500	-2.00317700
C	-0.75481500	-0.99069100	2.16095700
C	-1.87693200	-1.56175700	1.53157700
C	-0.98446400	-0.16632200	3.28240700
C	-3.17583700	-1.34737400	2.00718700
H	-1.71234500	-2.19542200	0.66531900
C	-2.27151900	0.06617200	3.77644000
H	-0.13113200	0.30724300	3.75869300
C	-3.36114600	-0.53486700	3.13295300

H	-4.36755000	-0.36785000	3.51457800
C	-0.38693900	-1.42370500	-1.98699400
C	-1.56946600	-0.68682500	-2.19095300
C	-0.49839500	-2.83050000	-1.93258200
C	-2.81170500	-1.31281900	-2.34852000
H	-1.49732800	0.39522500	-2.23475600
C	-1.72340200	-3.48045900	-2.10425800
H	0.39482800	-3.41555000	-1.73770000
C	-2.87605600	-2.71099400	-2.31415200
H	-3.83520500	-3.20875600	-2.45223200
C	1.52551700	3.17759000	0.86226300
C	0.68722600	4.43228300	1.19416700
C	2.19720100	2.71130900	2.16880200
C	2.62616800	3.55355100	-0.15334000
H	0.22601700	4.87125200	0.30518300
H	-0.11136600	4.19505600	1.90508300
H	1.33315800	5.19227000	1.64825900
H	2.80582300	1.82422300	1.98595600
H	2.84260800	3.50185600	2.57213500
H	1.43789900	2.46727400	2.92002400
H	3.27475200	4.34343700	0.24813500
H	3.24544200	2.68133700	-0.37356900
H	2.19120900	3.92608700	-1.08670100
C	1.40974400	-2.17267100	2.49769600
C	2.36375000	-1.38454500	3.42148700
C	0.55148900	-3.12867000	3.35548200
C	2.25045100	-3.03791600	1.53834300
H	2.99090700	-0.72074600	2.82197700
H	1.80543100	-0.78262800	4.14656500
H	3.01576000	-2.06547100	3.98397100
H	-0.14911600	-3.69491000	2.73292200
H	1.20653000	-3.84297000	3.86691500
H	-0.02809200	-2.59951300	4.11713700
H	2.88498700	-3.73100000	2.10521000
H	1.59403000	-3.62493800	0.88666800
H	2.89720200	-2.41307200	0.92057700
C	1.87082500	-0.93657400	-2.92769700
C	2.88011600	-2.05723100	-2.59310600
C	1.19678100	-1.24577700	-4.28277300
C	2.64068900	0.39000000	-3.08971600
H	3.36129400	-1.85242800	-1.63418000
H	2.38626400	-3.03268100	-2.53375000
H	3.65745100	-2.12762700	-3.36545200
H	0.45910500	-0.47731600	-4.53675400

H	1.95652500	-1.26386900	-5.07247800
H	0.68807600	-2.21362100	-4.28453200
H	3.39696800	0.30136200	-3.87990300
H	1.95078600	1.19621100	-3.36153500
H	3.14274600	0.66170000	-2.15944800
N	0.85536100	-0.75193600	-1.83712300
N	0.55593100	-1.24845600	1.67394700
N	0.66301600	2.05712000	0.35641300
C	-1.80157100	-4.99164900	-2.08738100
H	-2.74993500	-5.34006700	-1.66421600
H	-1.72683500	-5.40894300	-3.10064400
H	-0.98871100	-5.42583400	-1.49723700
C	-4.06743500	-0.49316800	-2.54821200
H	-4.70711700	-0.92180400	-3.32894300
H	-4.66431900	-0.45108400	-1.62794600
H	-3.82721700	0.53696700	-2.82278000
C	-4.31063600	2.34219500	0.45875800
H	-4.23737700	1.51459500	1.16967100
H	-4.60767100	3.23585000	1.02457500
H	-5.12181000	2.12261100	-0.24420400
C	-1.73979100	4.06067100	-3.54943100
H	-2.71536500	3.99850900	-4.04255200
H	-1.47961400	5.12473000	-3.47207100
H	-0.99790300	3.59686500	-4.20788100
C	-2.48405700	0.98511200	4.95976300
H	-2.46393600	2.03949800	4.65540200
H	-3.45085300	0.80278000	5.44069600
H	-1.70070400	0.85506800	5.71408300
C	-4.35429400	-2.03001000	1.34834400
H	-4.58500900	-2.98575400	1.83853000
H	-5.25921000	-1.41472000	1.40365900
H	-4.14543500	-2.24562900	0.29702300
Nb	1.18814500	0.02235700	0.10836800
C	5.02811400	-0.05776400	0.21895700
N	2.90925200	0.02392000	0.25865700
O	5.24768400	-1.19469400	0.49140600
O	5.32673300	1.05648000	-0.07081200
TS_NbN03			
C	-0.63827017	-1.48534794	1.79873735
C	-1.33793283	-0.92878082	2.88740029
C	-1.28978485	-2.43721779	1.00564604

C	-2.63954527	-1.32119862	3.19711257
H	-0.84114157	-0.18771293	3.50277227
C	-2.59530832	-2.86339832	1.30392968
H	-0.76495673	-2.85912745	0.15566849
C	-3.25440658	-2.29727244	2.39657790
H	-4.26320104	-2.62605256	2.63885689
C	-0.19233674	-0.84599009	-2.06981373
C	-1.57464671	-0.71167372	-2.28053848
C	0.40407514	-2.10303097	-2.26621546
C	-2.34588881	-1.79215899	-2.72018433
H	-2.04090331	0.25143601	-2.11087674
C	-0.34976341	-3.20236277	-2.69517403
H	1.46796215	-2.20759651	-2.08520157
C	-1.71852006	-3.02802438	-2.92924341
H	-2.30859480	-3.87121936	-3.28459387
C	-1.45035236	2.08903867	0.19555989
C	-2.58477268	1.31781398	0.48094176
C	-1.56291924	3.10300431	-0.77337721
C	-3.80828190	1.54862462	-0.16319931
H	-2.51043088	0.54024324	1.23067745
C	-2.77062287	3.35460932	-1.43187140
H	-0.69183752	3.70162311	-1.01527644
C	-3.88715622	2.56768683	-1.11691564
H	-4.83360204	2.75999337	-1.61860158
C	1.71603585	-2.05167825	2.31330475
C	2.01715653	-3.29870024	1.45539469
C	3.01940894	-1.30327490	2.63517350
C	1.14106342	-2.52597463	3.66769102
H	1.10551486	-3.87790502	1.28203364
H	2.43806740	-3.01301153	0.49030894
H	2.73193436	-3.95108835	1.97097895
H	2.82185485	-0.40746003	3.23027126
H	3.67856266	-1.95698894	3.21533025
H	3.55907970	-1.00846213	1.73926720
H	1.89546551	-3.14499265	4.16371693
H	0.91232687	-1.68517919	4.32825734
H	0.23853945	-3.12923738	3.55316568
C	1.12781966	1.09222567	-2.88146035
C	2.04664021	0.22741705	-3.77066030
C	-0.04042255	1.60982142	-3.74852194
C	1.93134103	2.30139293	-2.37759747
H	2.88727010	-0.17014405	-3.19815676
H	1.50504408	-0.61293045	-4.21153843
H	2.44529223	0.83720438	-4.58853646

H	-0.72998364	2.21370072	-3.15571192
H	0.35877661	2.23023522	-4.55820646
H	-0.60131480	0.79032795	-4.20323539
H	2.21729902	2.92632117	-3.22945092
H	1.34664876	2.91705669	-1.68972363
H	2.84482147	1.99651495	-1.86527963
C	0.06257805	2.90920364	1.99674014
C	0.80688677	4.12594430	1.40941552
C	-1.25558226	3.38007765	2.64907759
C	0.93172401	2.30037527	3.11527776
H	1.72084033	3.80375111	0.90474081
H	0.18125220	4.67870049	0.70366859
H	1.08763022	4.81869600	2.21096136
H	-1.81069729	2.53826067	3.07433236
H	-1.02089944	4.07691196	3.46007312
H	-1.90868009	3.89638394	1.94259534
H	1.02107360	3.02376807	3.93248620
H	0.47891402	1.39138669	3.51900963
H	1.93677009	2.06640827	2.76632548
N	-0.22191978	1.87549721	0.91136974
N	0.60824790	0.29373025	-1.70594084
N	0.74321712	-1.14710670	1.56722811
C	-2.86229560	4.43457666	-2.48626947
H	-3.87258186	4.85096077	-2.54414037
H	-2.16851369	5.25536563	-2.28063831
H	-2.61506673	4.04267297	-3.48126247
C	-5.02845648	0.73525969	0.20655044
H	-5.53225995	1.15849978	1.08514161
H	-5.76053013	0.71574154	-0.60673859
H	-4.75864491	-0.29555501	0.45380318
C	-3.25073098	-3.94737345	0.47954818
H	-3.16381933	-3.73802271	-0.59043084
H	-2.77188408	-4.91870071	0.65514132
H	-4.31056215	-4.05389099	0.72825104
C	-3.38310533	-0.70176783	4.35825202
H	-4.11473496	0.03908199	4.01221616
H	-3.93532217	-1.45654141	4.92801681
H	-2.70087339	-0.19226741	5.04451263
C	0.29937093	-4.55473738	-2.88698786
H	0.16783812	-5.18889140	-2.00131311
H	-0.13708770	-5.09121718	-3.73553641
H	1.37494717	-4.46092561	-3.06220585
C	-3.82446959	-1.62627062	-2.99040637
H	-4.05421858	-1.79241159	-4.04972623

H	-4.42187317	-2.34447231	-2.41734956
H	-4.16467803	-0.62142569	-2.72796599
Nb	1.10213679	0.43020060	0.28141936
C	4.01568261	1.39096789	0.67750527
N	2.70030197	1.31002304	0.62425371
O	4.77025248	2.09469597	1.29864031
C	4.19400919	-0.65154634	-0.76985511
O	4.73574686	0.43890569	-0.23456397
C	5.21404266	-1.44392134	-1.55126450
H	5.95856874	-1.85061321	-0.85942820
H	4.72543735	-2.25884988	-2.08480794
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C	-2.23550569	0.45118532	0.94411872
C	-2.81998737	-0.38407588	1.92526355
C	-1.66171073	1.65650552	1.37963037
C	-2.85319652	-0.02728620	3.27308359
H	-3.23666560	-1.33630093	1.61184512
C	-1.67414350	2.03551701	2.73012833
H	-1.20715815	2.30542096	0.63696569
C	-2.27576758	1.19114045	3.66633275
H	-2.29536933	1.48082803	4.71621287
C	1.13841591	1.81299003	-1.18491902
C	2.02121529	1.87924127	-0.09365362
C	0.43821323	2.99122777	-1.52889592
C	2.22309789	3.06768280	0.62199675
H	2.56417500	0.97991727	0.18089917
C	0.62161485	4.18850146	-0.83444773
H	-0.27225238	2.94974195	-2.34889625
C	1.52237567	4.21638218	0.24074891
H	1.67822912	5.14612412	0.78678544
C	1.40097523	-1.67327552	1.10704193
C	1.00249059	-0.95657352	2.25355916
C	2.78682884	-1.85227952	0.90497389
C	1.93244984	-0.45076009	3.16827960
H	-0.05982452	-0.81616096	2.42817459
C	3.73529983	-1.37361255	1.81348729
H	3.11831787	-2.37238071	0.01144726

C	3.29745325	-0.67587741	2.94589112
H	4.02789743	-0.30607922	3.66408038
C	-3.53211103	0.09216533	-1.15157877
C	-3.29607648	0.63082709	-2.57718159
C	-4.12483465	-1.32932677	-1.25595083
C	-4.55582921	1.02502357	-0.46858950
H	-2.90261921	1.65263712	-2.53419156
H	-2.57547900	-0.00329164	-3.09751216
H	-4.23593283	0.64478450	-3.14478597
H	-4.36461135	-1.73396080	-0.26638063
H	-5.05076304	-1.32590958	-1.84685422
H	-3.39737024	-1.98529347	-1.74067328
H	-5.46264800	1.07929148	-1.08184059
H	-4.84447792	0.67429016	0.52605032
H	-4.15462280	2.03872954	-0.36391310
C	1.58060068	0.55506710	-3.28342073
C	0.53461451	0.86375381	-4.37614473
C	2.76172390	1.54156731	-3.41589874
C	2.13415154	-0.86413871	-3.51920583
H	-0.29753670	0.16153794	-4.28329600
H	0.15099674	1.88548762	-4.28069284
H	0.97242460	0.76510002	-5.37871509
H	3.51801448	1.35657842	-2.64570793
H	3.23540693	1.41068164	-4.39565670
H	2.44693974	2.58560768	-3.33285517
H	2.59414143	-0.93675228	-4.51370088
H	2.89477148	-1.10190705	-2.76702061
H	1.32562924	-1.59432670	-3.44589135
C	0.34022650	-3.67784006	0.07057630
C	1.10631233	-4.19444720	-1.16663566
C	0.85799301	-4.39810860	1.33500940
C	-1.14817870	-4.04922949	-0.08996073
H	0.73275430	-3.68280003	-2.05721233
H	2.18239433	-4.01069784	-1.07628078
H	0.96362651	-5.27634573	-1.29159153
H	0.34637046	-4.03163884	2.23154665
H	0.66151294	-5.47278080	1.24601613
H	1.93268739	-4.26628504	1.48567439
H	-1.26402469	-5.13606168	-0.19525879
H	-1.71574059	-3.72486032	0.78947359
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N	0.43017885	-2.18020003	0.20186904
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C	5.21034884	-1.61366660	1.57351643
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H	5.50953200	-1.29357423	0.56887190
C	1.47417373	0.33345111	4.37752462
H	2.14863535	0.18814239	5.22922344
H	1.44484251	1.40925740	4.16324354
H	0.46433915	0.04424585	4.68099408
C	-1.07800457	3.36063724	3.15046171
H	-0.11272986	3.53141032	2.66363899
H	-1.72915822	4.19786740	2.86577311
H	-0.93508800	3.41017674	4.23495095
C	-3.48169494	-0.94094898	4.30283094
H	-2.74867596	-1.27080437	5.04944914
H	-4.28884489	-0.43674714	4.84926765
H	-3.90319236	-1.83560936	3.83546086
C	-0.15665265	5.43038650	-1.21114634
H	-0.91748794	5.67125534	-0.45770254
H	0.49822481	6.30610092	-1.29554464
H	-0.67151121	5.30224094	-2.16783023
C	3.22962576	3.11800472	1.75081953
H	4.23180501	3.37059449	1.37826166
H	2.96244621	3.87715092	2.49423435
H	3.30596278	2.15058640	2.25484028
N	-0.89528966	-1.69235761	-2.45563586
Ta	-0.40802618	-0.75225110	-1.09118768

TaN2

C	-0.50750616	2.39370170	0.23523722
C	-0.45279696	3.23996059	-0.89428393
C	-1.76765846	2.11497857	0.78483805
C	-1.60439820	3.80239685	-1.44498977
H	0.51265399	3.43788483	-1.34742851
C	-2.94238353	2.66244060	0.24651931
H	-1.81909312	1.46477113	1.65253303
C	-2.84785014	3.50455984	-0.86340451
H	-3.75374051	3.93715357	-1.28614700
C	-0.84416786	-1.36545429	1.88266276
C	-2.00782705	-1.75329235	1.19945709
C	-0.99114393	-0.76798495	3.15135127
C	-3.28081271	-1.57530419	1.75858089

H	-1.90205695	-2.21505265	0.22270398
C	-2.24776029	-0.57586123	3.73033890
H	-0.09980242	-0.43961151	3.67622986
C	-3.38713332	-0.98775415	3.02331099
H	-4.37163531	-0.84829515	3.46792223
C	-0.55278185	-0.93035110	-2.19051226
C	-1.71850182	-0.14744091	-2.28102869
C	-0.67317926	-2.31909160	-2.38571821
C	-2.96350067	-0.71709905	-2.56826824
H	-1.63213766	0.92450986	-2.13306219
C	-1.90401277	-2.91252968	-2.68764289
H	0.21387512	-2.93712791	-2.28804742
C	-3.04118599	-2.10052985	-2.77803547
H	-4.00262333	-2.55338715	-3.01620728
C	1.55714218	2.75983047	1.59524678
C	0.71314598	3.86841180	2.25935267
C	2.24147971	1.95522428	2.71654861
C	2.65293141	3.39275021	0.71213679
H	0.24080497	4.52718259	1.52510505
H	-0.07654520	3.44262941	2.88795190
H	1.36028384	4.48370528	2.89377051
H	2.90614162	1.19908213	2.29705897
H	2.84188908	2.62513925	3.34359771
H	1.49419196	1.46701338	3.35171993
H	3.25969365	4.08770428	1.30800240
H	3.32023594	2.62071584	0.31400701
H	2.21652763	3.96851360	-0.11113490
C	1.23547467	-2.75035087	1.83866189
C	2.16826585	-2.30472796	2.98329433
C	0.29020236	-3.85808683	2.35069017
C	2.09171462	-3.35005495	0.70578887
H	2.85169939	-1.53193936	2.62475207
H	1.59946976	-1.91555896	3.83486650
H	2.76835754	-3.15017321	3.34190653
H	-0.38138104	-4.20057734	1.55639087
H	0.88775464	-4.71377964	2.68263324
H	-0.32392188	-3.53062784	3.19454964
H	2.57964635	-4.26570167	1.06350876
H	1.45433198	-3.61962617	-0.14381138
H	2.88000875	-2.66783381	0.37164828
C	1.67611034	-0.18211591	-3.05503313
C	2.64881392	-1.37910542	-3.10426860
C	0.92220829	-0.07929186	-4.39762188
C	2.48067531	1.12074595	-2.87460598

H	3.20600490	-1.47192334	-2.16842179
H	2.11001651	-2.31511128	-3.28760786
H	3.37094589	-1.25075798	-3.92074201
H	0.20868623	0.75137111	-4.38886539
H	1.64305040	0.09937792	-5.20273315
H	0.37243421	-0.99390953	-4.63702350
H	3.16900504	1.25215059	-3.71824702
H	1.80414026	1.98208244	-2.85039331
H	3.07579459	1.11438492	-1.95934334
N	0.70563270	-0.31590913	-1.90262750
N	0.44470976	-1.57764118	1.29946070
N	0.67508219	1.82259397	0.80227775
C	-1.99463869	-4.40525626	-2.91749229
H	-3.03523259	-4.73769581	-2.98532622
H	-1.49153323	-4.69818969	-3.84749782
H	-1.51488929	-4.96388623	-2.10623836
C	-4.20701662	0.14096678	-2.64045928
H	-4.85347776	-0.15770232	-3.47378313
H	-4.80236369	0.05637298	-1.72241696
H	-3.95288017	1.19714896	-2.76169571
C	-4.27992884	2.36836788	0.88785301
H	-4.35426816	1.31627612	1.17941592
H	-4.42273575	2.96375384	1.79925606
H	-5.10913219	2.60088913	0.21187729
C	-1.52459385	4.70613877	-2.65566691
H	-2.10638935	4.30604424	-3.49497160
H	-1.92312890	5.70488953	-2.43775777
H	-0.49182284	4.82597105	-2.99443405
C	-2.38268681	0.09803594	5.07810312
H	-2.64601182	1.15812034	4.97039697
H	-3.16718102	-0.36890221	5.68416340
H	-1.44651450	0.05171063	5.64218906
C	-4.51149227	-2.06145301	1.02525425
H	-4.73462226	-3.10719234	1.27601972
H	-5.39635596	-1.47140612	1.28725650
H	-4.37009865	-2.01245434	-0.05813264
C	4.33490218	-0.22767863	0.06789930
N	2.86215628	-0.15979061	0.19056748
O	4.77912839	-1.38877798	-0.03831074
O	4.89412647	0.88729733	0.06516525
Ta	1.11460511	-0.05571538	0.09277927

TaNO

C	1.03080200	1.17588200	1.96583300
C	1.38587400	0.49272700	3.14194500
C	2.01149000	1.91675100	1.29383000
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C	3.32357500	1.99117700	1.78157600
H	1.73698900	2.45094600	0.39059800
C	3.64353700	1.30770400	2.95947200
H	4.65709300	1.36813300	3.35198400
C	0.38514700	1.32277700	-1.97002400
C	1.72908200	1.00150600	-2.21708700
C	0.00084800	2.67219700	-1.97762000
C	2.67330600	1.99849800	-2.48709800
H	2.03005700	-0.04031700	-2.20778700
C	0.92850500	3.69009500	-2.22880000
H	-1.03673500	2.92106100	-1.78222300
C	2.25898100	3.33637100	-2.48563300
H	2.98592100	4.11923300	-2.69366400
C	1.41649600	-2.15907700	-0.19451800
C	2.62912700	-1.65155100	0.29674300
C	1.42303100	-2.86419600	-1.40893500
C	3.83058100	-1.84851700	-0.39485300
H	2.62593500	-1.11327800	1.23817400
C	2.60888800	-3.06783000	-2.12436100
H	0.48891600	-3.25342000	-1.79968600
C	3.80325300	-2.55411400	-1.60415600
H	4.73154300	-2.71469400	-2.14903500
C	-1.27450800	2.12775900	2.17807200
C	-0.51323500	3.34152900	2.74676900
C	-2.29392500	2.65770600	1.15421900
C	-2.01476100	1.41287400	3.32506900
H	0.19655700	3.06039600	3.52803000
H	0.03439700	3.87426600	1.96418900
H	-1.23773400	4.03460000	3.18612800
H	-2.87878400	1.84605500	0.71919100
H	-2.98873500	3.34807200	1.64494200
H	-1.78326500	3.20003900	0.35399900
H	-2.71246200	2.10088000	3.81576600
H	-2.58542400	0.56353400	2.94296700
H	-1.31418600	1.05346500	4.08446500
C	-1.30874200	-0.21417500	-2.97205500
C	-2.24260200	0.88077000	-3.52268400
C	-0.28946700	-0.61304800	-4.05867200

C	-2.15851400	-1.44792600	-2.62420700
H	-2.99124000	1.16168000	-2.77728300
H	-1.68623800	1.76964700	-3.83173300
H	-2.77500100	0.50098000	-4.40150000
H	0.38540600	-1.39344100	-3.69592800
H	-0.82637600	-1.00147700	-4.93019400
H	0.31388300	0.23529900	-4.39015300
H	-2.53354600	-1.89565900	-3.54992000
H	-1.57056900	-2.21206200	-2.10552500
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C	-0.21917200	-3.17236600	1.41293800
C	-1.13942600	-4.10601400	0.60354700
C	1.01465800	-3.95656100	1.90129200
C	-0.97442500	-2.66816000	2.65465700
H	-2.05120600	-3.58540700	0.30089100
H	-0.62975800	-4.49085400	-0.28459700
H	-1.43197100	-4.96792400	1.21422000
H	1.70364000	-3.31322700	2.45679300
H	0.68217400	-4.75601600	2.57081400
H	1.56653700	-4.41773000	1.07883200
H	-1.27720700	-3.51972000	3.27244200
H	-0.33438600	-2.02003000	3.25952700
H	-1.87751200	-2.12127400	2.38218400
N	0.20138200	-1.98122600	0.56377100
N	-0.57961600	0.27619100	-1.73262500
N	-0.32603500	1.16215300	1.47886300
C	2.59147600	-3.80816200	-3.44256900
H	3.59010000	-4.16133500	-3.71528000
H	1.92383500	-4.67482800	-3.40536300
H	2.23758600	-3.16349300	-4.25677200
C	5.13826400	-1.34956700	0.17692200
H	5.66197800	-2.14981700	0.71519100
H	5.81375200	-0.99760500	-0.60970100
H	4.97544500	-0.53193400	0.88387400
C	4.37602800	2.78735500	1.04401600
H	4.97710600	2.14133000	0.39229600
H	3.92277300	3.55501600	0.41139000
H	5.06548800	3.27740500	1.73903600
C	3.04867500	-0.15552500	4.93757100
H	4.00670000	-0.67863200	4.85026500
H	3.14482300	0.55523200	5.76762400
H	2.28793400	-0.88869000	5.21958600
C	0.50322400	5.14083000	-2.20020100
H	0.49133800	5.53238500	-1.17524400

H	1.18536300	5.76855200	-2.78103000
H	-0.50482500	5.27033200	-2.60634700
C	4.10420700	1.63273800	-2.80983100
H	4.26855500	1.60399800	-3.89448500
H	4.80897200	2.36174800	-2.39719400
H	4.35802200	0.64553900	-2.41453200
C	-3.84297900	-1.12293100	0.60937300
N	-2.58915800	-0.66886800	0.49732400
O	-4.25097000	-2.26101600	0.61036800
C	-5.41733400	0.45476700	-0.23893200
O	-4.79511700	-0.06323000	0.85038400
C	-6.47702500	1.44859800	0.17130700
H	-6.03367500	2.24221700	0.77974000
H	-6.94035100	1.87302200	-0.71890000
H	-7.23323500	0.95027600	0.78499000
O	-5.14213200	0.15228900	-1.37907900
Ta	-0.83483200	-0.29716000	0.17883800

TaN3

C	-0.88404800	-1.23489400	1.84943400
C	-1.57337200	-0.44318000	2.78060200
C	-1.57223400	-2.29238300	1.23623900
C	-2.91132600	-0.68702400	3.10380600
H	-1.05163600	0.36976700	3.26692900
C	-2.90511200	-2.57928500	1.56329300
H	-1.05642200	-2.90270800	0.50445600
C	-3.56284900	-1.76347600	2.48957200
H	-4.59826400	-1.97757100	2.74737300
C	-0.50454100	-1.19149700	-1.85678800
C	-1.88372000	-1.04432900	-2.04463400
C	0.07009900	-2.46912500	-1.96575000
C	-2.68444400	-2.14599700	-2.37331600
H	-2.32633200	-0.06089200	-1.94128600
C	-0.70889900	-3.58369800	-2.28863800
H	1.13626500	-2.57394400	-1.80510100
C	-2.08245200	-3.40209500	-2.50265000
H	-2.69518300	-4.25831100	-2.77839000
C	-1.08406200	2.34051400	-0.05613500
C	-2.33343100	1.71471800	0.08854000

C	-0.99707400	3.44695000	-0.91410300
C	-3.46810000	2.17754900	-0.58454900
H	-2.41652400	0.86950100	0.76081000
C	-2.11904500	3.93311200	-1.60120700
H	-0.04261900	3.93868500	-1.06027800
C	-3.34789000	3.29189400	-1.42586500
H	-4.22551900	3.66672200	-1.94891000
C	1.41319300	-1.93959800	2.48940400
C	1.59117300	-3.31680100	1.82165300
C	2.78802300	-1.28772200	2.72929000
C	0.77772500	-2.14396900	3.88157400
H	0.63523900	-3.84213700	1.74620000
H	2.01484000	-3.20444300	0.82366100
H	2.26349900	-3.93989900	2.42277300
H	2.68276500	-0.32020800	3.22656900
H	3.37840900	-1.93637600	3.38433900
H	3.34624300	-1.14962200	1.80611700
H	1.46146800	-2.75057600	4.48383300
H	0.62755900	-1.19400500	4.40254400
H	-0.17957900	-2.66624900	3.83672300
C	0.80050100	0.64684800	-2.91775700
C	1.52479600	-0.34886300	-3.84650100
C	-0.40862100	1.23589100	-3.66927500
C	1.79106000	1.76691200	-2.56097600
H	2.41786700	-0.75630100	-3.36990000
H	0.87318600	-1.16711300	-4.16123100
H	1.84415000	0.18657000	-4.74698800
H	-0.97257600	1.92743800	-3.04212100
H	-0.04568500	1.78133700	-4.54708500
H	-1.08318500	0.45337100	-4.02436300
H	2.03374400	2.33012500	-3.46741500
H	1.36694100	2.47209300	-1.84322300
H	2.72513800	1.35280700	-2.17397300
C	0.33503300	2.84976500	1.88738600
C	1.14189700	4.07802100	1.40701100
C	-0.98000700	3.35443900	2.52647500
C	1.14514900	2.16239100	3.00558500
H	2.02237300	3.77015700	0.84035000
H	0.53776100	4.74590200	0.79017000
H	1.47962000	4.65684700	2.27411200
H	-1.60094000	2.52748200	2.88059500
H	-0.73601600	3.98779400	3.38549800
H	-1.57610200	3.95051500	1.83328900
H	1.21594100	2.84538300	3.85810100

H	0.66900900	1.24467800	3.35198300
H	2.15843400	1.92270700	2.68978100
N	0.04077300	1.88641200	0.72969500
N	0.34138200	-0.04093000	-1.63376600
N	0.53171200	-1.04174400	1.60903400
C	-1.98349400	5.11126800	-2.53903900
H	-2.95666200	5.55720800	-2.76336200
H	-1.34325300	5.89109900	-2.11399300
H	-1.53255700	4.80903800	-3.49251400
C	-4.80854800	1.50521600	-0.38628100
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H	-5.24668200	1.19291900	-1.34133400
H	-4.71836900	0.61993800	0.24910200
C	-3.60448700	-3.78066200	0.96908800
H	-3.19538400	-4.03447200	-0.01150000
H	-3.48681900	-4.66037600	1.61474900
H	-4.67929200	-3.60497900	0.85885600
C	-3.64036800	0.20345200	4.08411500
H	-4.07554800	1.07519300	3.57946200
H	-4.45872300	-0.32986500	4.57698500
H	-2.96754000	0.58191800	4.85974000
C	-0.08646500	-4.95745100	-2.39413100
H	-0.19837800	-5.51796200	-1.45749800
H	-0.55852300	-5.55060600	-3.18367500
H	0.98378600	-4.89581800	-2.61076900
C	-4.17267600	-1.97355000	-2.57312600
H	-4.39416100	-1.10043500	-3.19572500
H	-4.61633400	-2.85114500	-3.05189900
H	-4.68385600	-1.82443700	-1.61447800
C	3.93403200	1.71340700	0.47633300
N	2.79754400	1.30779200	0.53248800
O	5.02679300	2.16161400	0.47347600
C	3.74675000	-1.25594000	-0.98302200
O	4.22426900	-0.33733100	-1.63820500
C	4.45979400	-2.59124500	-0.83885700
H	4.65426600	-2.80273400	0.21733500
H	3.82632200	-3.40060000	-1.21675700
H	5.40046300	-2.57352800	-1.38961900
O	2.58585200	-1.20356400	-0.35508200
Ta	1.14444300	0.22727700	0.16562400

TS_TaN12

C	-0.71346981	2.29973999	-0.66486175
C	-0.79974620	2.66583746	-2.02448223
C	-1.91393885	2.19159304	0.05863744
C	-2.02510907	2.94180540	-2.63682806
H	0.11643327	2.72022463	-2.60438623
C	-3.15685844	2.45648337	-0.53223317
H	-1.85686103	1.90518872	1.10457610
C	-3.19933972	2.83540271	-1.87840248
H	-4.16007010	3.04734845	-2.34575577
C	-0.75848522	-0.60677237	2.30005862
C	-1.90387531	-1.24771236	1.79632771
C	-0.94366770	0.35802696	3.31505946
C	-3.18464571	-0.96449821	2.29092116
H	-1.77725331	-1.99224129	1.01659517
C	-2.20754855	0.65655915	3.82719630
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TS_TaN03

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H	-0.29562200	0.72092300	-4.26833600
H	-1.72382400	1.59940500	-4.84507000
H	-0.47796900	2.44653400	-3.91710700
H	-3.26556000	0.02337000	-3.88135800
H	-1.90592800	-0.95649800	-3.30441400
H	-3.19628800	-0.47647600	-2.18680900
N	-0.86121700	0.88674200	-1.57639400
N	-0.65086000	0.98038400	1.65213900
N	-0.80014600	-1.85763000	0.13635900
C	1.67914500	5.16188800	-1.03446300
H	2.69712300	5.56011000	-1.09062900
H	1.05355200	5.74807000	-1.71869600
H	1.30203500	5.34644200	-0.02193700
C	4.03858100	0.92973400	-2.50405400
H	4.57151000	1.47824700	-3.29019100
H	4.73338400	0.82179800	-1.66136700

H	3.81854700	-0.07475800	-2.87460200
C	4.14682600	-2.46265000	-0.00619900
H	4.44414200	-1.42724700	0.19671500
H	4.12245100	-2.97803400	0.96040400
H	4.92908800	-2.92444200	-0.61740900
C	1.34954900	-3.38201100	-4.12251300
H	1.99899000	-2.77753400	-4.76713200
H	1.65509000	-4.42817700	-4.25201000
H	0.32638300	-3.28636900	-4.49648800
C	2.04986100	-1.89462900	4.73685400
H	2.35512200	-2.85015100	4.29108600
H	2.78685800	-1.65071700	5.51055000
H	1.08597900	-2.05848300	5.22768000
C	4.30352900	1.51741400	1.75638800
H	4.54881000	2.36962800	2.40458900
H	5.17122000	0.84831200	1.76486500
H	4.17659000	1.90725000	0.74252300
C	-4.38227300	0.08586300	0.12137200
N	-2.87770800	0.04968400	0.18707700
O	-4.85702100	1.19435600	0.41414200
O	-4.87847500	-0.99708200	-0.22658200
V	-1.26665800	0.01611000	0.09699500
VNO			
C	-0.86987000	-1.28782500	1.79968200
C	-1.19343300	-0.74659900	3.05808800
C	-1.86338400	-1.96951800	1.08780300
C	-2.47228500	-0.88361600	3.60103100
H	-0.43138000	-0.21522600	3.61631100
C	-3.15726200	-2.12007400	1.60942900
H	-1.61503400	-2.40266800	0.12600200
C	-3.44565500	-1.57583700	2.86340200
H	-4.44325400	-1.69792200	3.28143900
C	-0.33007300	-1.04930200	-1.97977200
C	-1.66782200	-0.69534700	-2.20883700
C	0.05057900	-2.39035500	-2.14561000
C	-2.60977900	-1.64893200	-2.61343200
H	-1.96697300	0.33852400	-2.08231500
C	-0.87500600	-3.36571500	-2.53133600
H	1.08216200	-2.66906000	-1.96472400

C	-2.20107000	-2.97879700	-2.76530300
H	-2.92647100	-3.72745700	-3.07819600
C	-1.28481000	2.10516400	0.04755800
C	-2.50831700	1.59243400	0.50398100
C	-1.28468300	2.93609300	-1.08490200
C	-3.71225800	1.90938000	-0.13652800
H	-2.51488200	0.95648900	1.38108700
C	-2.47255000	3.25744800	-1.75121600
H	-0.34399200	3.32789500	-1.45397200
C	-3.67885200	2.73864200	-1.26388600
H	-4.60924800	2.99198500	-1.76857400
C	1.44202000	-2.21877700	1.85830800
C	0.70445200	-3.48455400	2.34769100
C	2.43427300	-2.66523400	0.77065000
C	2.20939000	-1.60360300	3.04543000
H	0.03739000	-3.28164000	3.18823900
H	0.11596100	-3.93945900	1.54620100
H	1.45016600	-4.21496800	2.67737300
H	2.96470000	-1.81745500	0.34086000
H	3.17318200	-3.34714700	1.20601700
H	1.91172000	-3.19905100	-0.02687200
H	2.90729300	-2.33814400	3.46302900
H	2.78320400	-0.73173700	2.72873300
H	1.52626200	-1.30440800	3.84514000
C	1.40337300	0.53273100	-2.80476500
C	2.40466700	-0.50390000	-3.35335700
C	0.41755600	0.92736900	-3.92771100
C	2.18700300	1.79272200	-2.39713300
H	3.10994600	-0.81128900	-2.57703000
H	1.89875100	-1.38641500	-3.75284600
H	2.98382200	-0.05401700	-4.16699300
H	-0.30349500	1.67028100	-3.57541500
H	0.98323700	1.36508000	-4.75627600
H	-0.13470300	0.06914200	-4.31571800
H	2.51112300	2.31393900	-3.30334600
H	1.57466400	2.48237300	-1.81319800
H	3.08255700	1.55592900	-1.82681300
C	0.34825700	2.90571100	1.74729800
C	1.14836300	4.00362400	1.01636500
C	-0.89129700	3.53882500	2.41653000
C	1.22103400	2.31515200	2.86726900
H	2.05156700	3.59122700	0.56130800
H	0.54371500	4.49313700	0.24808800
H	1.45364000	4.77462600	1.73302700

H	-1.49198200	2.78564600	2.93476700
H	-0.55472200	4.27279500	3.15549800
H	-1.53304300	4.05560200	1.69993000
H	1.46471200	3.10481800	3.58526600
H	0.69227100	1.52467200	3.40467200
H	2.15845300	1.91545600	2.48729600
N	-0.07259600	1.81968100	0.77178200
N	0.63152500	-0.03851200	-1.62638700
N	0.46540400	-1.21074800	1.27382700
C	-2.44812400	4.12930500	-2.98646700
H	-3.40268800	4.64411900	-3.13072500
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H	-2.25826700	3.53549600	-3.88954400
C	-5.02798300	1.40207800	0.40964000
H	-5.50963800	2.15977400	1.04082800
H	-5.73216400	1.16018600	-0.39324700
H	-4.88424700	0.50883200	1.02326600
C	-4.22068400	-2.84635200	0.81779300
H	-4.71963200	-2.16876400	0.11431300
H	-3.79135800	-3.66078700	0.22721800
H	-4.99083000	-3.26526800	1.47260000
C	-2.80634100	-0.31033600	4.95961800
H	-3.64408200	0.39391800	4.90090000
H	-3.09958600	-1.09838600	5.66311600
H	-1.95334800	0.22061300	5.39082900
C	-0.45614700	-4.81219400	-2.66921000
H	-0.58134600	-5.35494400	-1.72376100
H	-1.05573600	-5.33199800	-3.42272600
H	0.59635100	-4.89867400	-2.95534100
C	-4.03171400	-1.23735400	-2.92038100
H	-4.15536500	-1.01622000	-3.98823200
H	-4.74318500	-2.03123100	-2.67175700
H	-4.31167800	-0.33621700	-2.36799400
C	3.79125200	1.06406400	0.59801100
N	2.52724800	0.61560000	0.46525600
O	4.18160300	2.20822900	0.62162800
C	5.59414100	-0.27854600	-0.20109400
O	4.71646200	-0.00028400	0.81287700
C	6.64849300	-1.24761300	0.26988200
H	6.17775800	-2.13746000	0.69712000
H	7.28808100	-1.52379500	-0.56779000
H	7.24732200	-0.78288800	1.05901100
O	5.49851600	0.18758200	-1.31011800
V	0.89505000	0.29553300	0.20813800

VN3

C	0.61169500	1.11400000	1.87021100
C	1.35185000	0.40832100	2.83581800
C	1.19913800	2.23958300	1.27805600
C	2.63845600	0.80123700	3.20420600
H	0.91179000	-0.45319800	3.31647500
C	2.48403400	2.67122000	1.64712200
H	0.64328600	2.79554200	0.53376400
C	3.19454300	1.93770800	2.59875400
H	4.19224500	2.26283300	2.88792300
C	0.10092700	1.26226300	-1.72908800
C	1.46431500	1.33482100	-2.03950900
C	-0.66613500	2.43902100	-1.72569300
C	2.05914900	2.55851100	-2.37458800
H	2.06088000	0.43183100	-2.01917300
C	-0.09318900	3.66968400	-2.05644300
H	-1.71277900	2.36903200	-1.46029500
C	1.26928000	3.71246200	-2.38448600
H	1.72236900	4.66502400	-2.65170400
C	1.23856800	-2.10209700	-0.19302700
C	2.37614200	-1.28923200	-0.05645400
C	1.31250400	-3.20201600	-1.06332000
C	3.56125800	-1.56952100	-0.74355400
H	2.33748600	-0.44948500	0.62426500
C	2.48464700	-3.49772700	-1.77238300
H	0.44672400	-3.83616800	-1.20362700
C	3.60338900	-2.67849600	-1.59854200
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C	-1.75243000	1.54487900	2.48587400
C	-2.10096300	2.89860200	1.83688800
C	-3.02664200	0.72185400	2.74661800
C	-1.13575700	1.82628800	3.87695200
H	-1.21234700	3.53051300	1.75362500
H	-2.52893900	2.74771500	0.84804800
H	-2.82832300	3.42892300	2.46227900
H	-2.78923400	-0.21236600	3.26107700
H	-3.68858200	1.30221600	3.39735400
H	-3.56203900	0.48921700	1.83250100
H	-1.89580500	2.33164700	4.48086400

H	-0.85848100	0.90554300	4.39713900
H	-0.26014500	2.47576900	3.83101800
C	-0.96649200	-0.70432600	-2.79886700
C	-1.87348400	0.21681400	-3.64480200
C	0.28007900	-1.05457900	-3.64273800
C	-1.75546300	-1.98583000	-2.48788800
H	-2.79833800	0.45516100	-3.12075000
H	-1.36668200	1.13779800	-3.94032700
H	-2.14235600	-0.32465800	-4.55783600
H	0.99108200	-1.66338800	-3.08468100
H	-0.05237900	-1.62629200	-4.51509500
H	0.78877500	-0.16076500	-4.00944800
H	-1.93363800	-2.51788100	-3.42771200
H	-1.20498700	-2.65498700	-1.82736700
H	-2.72492800	-1.74693100	-2.04942900
C	-0.04616100	-2.91791800	1.73223800
C	-0.67421100	-4.22749400	1.19311800
C	1.34914600	-3.26502900	2.31154500
C	-0.92079200	-2.43490900	2.91151600
H	-1.57047900	-4.02296900	0.60673100
H	0.02828500	-4.80424000	0.58907700
H	-0.96215700	-4.85737100	2.04213900
H	1.84994900	-2.38499700	2.72138200
H	1.21717500	-3.98993600	3.12092200
H	2.00959100	-3.71365300	1.56830700
H	-0.71928200	-3.07152700	3.77882600
H	-0.70726800	-1.40501400	3.18980500
H	-1.98184200	-2.50055400	2.68721200
N	0.08535100	-1.85482900	0.63262300
N	-0.54069700	-0.00848000	-1.50499600
N	-0.76436600	0.78693400	1.57968400
C	2.51949800	-4.66734600	-2.72976200
H	3.54415100	-5.00474200	-2.91085900
H	1.94516000	-5.51689600	-2.34725600
H	2.08708600	-4.39663400	-3.70119400
C	4.78822300	-0.70764600	-0.54564800
H	5.60513500	-1.28111700	-0.09143400
H	5.16410300	-0.32033600	-1.49974200
H	4.57558100	0.14371300	0.10648300
C	3.06520400	3.93824300	1.06234600
H	2.72841100	4.09432300	0.03482200
H	2.75401700	4.81496200	1.64464300
H	4.15927500	3.91721600	1.07051300
C	3.41560300	0.03532800	4.25095400

H	4.36260700	-0.34213300	3.84835700
H	3.66314600	0.67315200	5.10739700
H	2.84809900	-0.82047400	4.62606100
C	-0.93829400	4.92274800	-2.09552400
H	-0.33936000	5.81639100	-1.89543600
H	-1.40252100	5.05592000	-3.08070300
H	-1.74604200	4.88248300	-1.35894100
C	3.53012500	2.61737400	-2.71942300
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H	3.83462800	3.62999700	-2.99814800
H	4.15050400	2.30169700	-1.87298400
C	-3.65926300	-2.20937600	0.58106800
N	-2.56881200	-1.69015400	0.59121400
O	-4.68849100	-2.79138300	0.64024800
C	-3.98744200	0.61027600	-0.80686500
O	-4.38833400	-0.37558800	-1.42164600
C	-4.88043700	1.83771700	-0.64313900
H	-5.07072800	2.02934000	0.41762900
H	-4.38885200	2.72811400	-1.04897500
H	-5.82701300	1.67488100	-1.15961000
O	-2.80447600	0.74341000	-0.25642400
V	-1.19962000	-0.44064200	0.19656000

TS_VN12

C	-0.49286960	2.21981932	-0.51647960
C	-0.48563346	2.64013062	-1.86378702
C	-1.73569720	2.14389640	0.13360071
C	-1.65966912	2.99497299	-2.53191162
H	0.46094937	2.66078526	-2.39271326
C	-2.92971939	2.48957697	-0.51361046
H	-1.75586945	1.80979465	1.16537325
C	-2.87996136	2.91593179	-1.84462510
H	-3.80258368	3.18524782	-2.35750474
C	-0.57885951	-0.67396311	2.17116979
C	-1.75072247	-1.29355818	1.70605428
C	-0.70923808	0.27897280	3.20329473
C	-3.00736150	-0.99720415	2.25018335
H	-1.66276232	-2.02867927	0.91297552
C	-1.94952229	0.59505538	3.76287682
H	0.18308656	0.78783667	3.55257128
C	-3.09492711	-0.05386878	3.27956399

H	-4.06662842	0.18007020	3.71279643
C	-0.37207942	-1.56457819	-1.68643140
C	-1.57779869	-0.93829907	-2.04500844
C	-0.41413572	-2.94355989	-1.39338750
C	-2.78130687	-1.65001909	-2.12984624
H	-1.55990532	0.12418698	-2.26320238
C	-1.59962746	-3.67870712	-1.47402893
H	0.50084964	-3.43230783	-1.07604512
C	-2.78071090	-3.01964639	-1.84333905
H	-3.71173128	-3.58203032	-1.90358561
C	1.53130121	3.07550442	0.61653796
C	0.62948490	4.28092332	0.97104174
C	2.30728736	2.69591307	1.89107869
C	2.54264016	3.50921707	-0.46710280
H	0.09559265	4.67025935	0.09971022
H	-0.11303774	4.00804252	1.72820303
H	1.24784648	5.09023373	1.37595516
H	2.97415047	1.85639608	1.69857206
H	2.90490513	3.54842177	2.23691416
H	1.61359363	2.41471436	2.68972831
H	3.14894859	4.35328902	-0.11205852
H	3.21636102	2.68463493	-0.70742265
H	2.03109030	3.83458541	-1.37870418
C	1.54089783	-1.91853247	2.48429253
C	2.51644972	-1.10231727	3.35965330
C	0.67584982	-2.81288737	3.40236383
C	2.35503901	-2.85482282	1.57247182
H	3.14749317	-0.47751727	2.72506453
H	1.97593512	-0.45978522	4.06247991
H	3.16362400	-1.76770166	3.94560716
H	-0.03714243	-3.40424242	2.81848113
H	1.32672332	-3.50611146	3.94703869
H	0.11023193	-2.23502431	4.13856309
H	2.96788266	-3.53377998	2.17883079
H	1.68081569	-3.45874217	0.95679965
H	3.01935446	-2.28856184	0.92074708
C	1.78023655	-1.04269142	-2.79404780
C	2.80615034	-2.15767994	-2.49227664
C	1.01064630	-1.41347561	-4.08323880
C	2.53493643	0.26952960	-3.08135729
H	3.37331407	-1.92014937	-1.59032292
H	2.30921994	-3.12234947	-2.34686759
H	3.51113224	-2.27226306	-3.32634030
H	0.26324225	-0.65202271	-4.32884959

H	1.71634294	-1.48066628	-4.91907590
H	0.49646586	-2.37486735	-3.99954837
H	3.22980683	0.13142613	-3.91932646
H	1.82734849	1.05995181	-3.35164867
H	3.10172971	0.59816830	-2.21071429
N	0.84423684	-0.82360612	-1.63819800
N	0.69134656	-1.02195258	1.62677840
N	0.71198290	1.89531570	0.17384876
C	-1.60500231	-5.16373830	-1.18289386
H	-0.82400710	-5.43177993	-0.46455339
H	-2.56735256	-5.48927123	-0.77328082
H	-1.42469798	-5.75276626	-2.09231273
C	-4.05080390	-0.95204182	-2.56651300
H	-4.16106030	-0.97448862	-3.65931800
H	-4.94032302	-1.43104860	-2.14284758
H	-4.04615736	0.09858544	-2.26306354
C	-4.24383693	2.43591460	0.23436476
H	-4.24853490	1.61940573	0.96209647
H	-4.42396341	3.36634734	0.78987156
H	-5.08989661	2.29700212	-0.44734713
C	-1.61660695	3.46807390	-3.96866005
H	-0.71176697	3.11894073	-4.47511903
H	-2.48171294	3.10808006	-4.53661987
H	-1.62350804	4.56459173	-4.03203576
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H	-1.15027336	1.70493739	5.44458258
H	-2.22248631	2.64787434	4.40963311
C	-4.23939007	-1.72743607	1.76232304
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H	-5.14892556	-1.14094952	1.93155240
H	-4.16600899	-1.95169505	0.69432167
C	4.85745822	0.02564369	0.06983132
N	2.83540238	0.04291946	0.14632049
O	5.15366839	-1.08025727	0.41057368
O	5.14568156	1.12452305	-0.29863040
V	1.25267237	0.02127757	0.07464824