# SUPPORTING INFORMATION

## Kinetics and Mechanism of the Oxidation of Hydroxylamine by a $\{Mn_3O_4\}^{4+}$ Core in Aqueous Acidic Media

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**Table S1** Stoichiometry of reduction of the $Mn^{IV}_3$ complex (**1**) by hydroxylamine, T = 25 °C, $C_{phen}$ = 5.0 mM

| $Mn^{IV}_3$ (mM) | pH | $T_R$ (mM)[a] | $\Delta[Mn^{IV}_3]/\Delta T_R$ |
|---|---|---|---|
| 0.10 | 2.3 | 0.50 | 0.30 |
| 0.15 | 3.0 | 0.80 | 0.35 |
| 0.20 | 3.5 | 1.0 | 0.34 |
| 0.30 | 4.0 | 1.20 | 0.31 |
| | | | Average = 0.32 ± 0.02 |

[a] $T_R$ = analytical concentration of hydroxylamine ≈ $[NH_3OH^+]$ (see text)

**Stoichiometric Results**

The stoichiometric experiments were carried out in absence of any externally added $NaNO_3$ and using hydroxylamine sulfate. However, the trinuclear Mn oxidant is a nitrate salt and so proper spectrophotometric blank correction was made for the detection of nitrate following Griess-Ilsovey reaction. No red coloration was observed when the product solution of the redox reaction was tested for nitrite and nitrate. These observations along with the observed value for $\Delta[Mn^{IV}_3]/\Delta T_R$ (Table S1) clearly suggest $N_2O$ as the sole oxidation product of hydroxylamine. The results of EDTA titration of the product solutions revealed quantitative formation of $Mn^{II}$ as the only reduction product of **1**. The likely $Mn^{II}$ species under the specified reaction condition is expected to be $Mn^{II}$–phen complexes.[1] Optical spectra for the product solutions were superimposable on those of mixtures of $Mn(NO_3)_2$ and 1,10-phenanthroline under similar experimental condition (see Figure below).

**Reference**

1. The stability constants (25.0 ºC, $I$ = 0.1 M) for the formation of 1 : 1, 1 : 2, 1 : 3 complexes of $Mn^{2+}$ and phen are, respectively, $1 \times 10^4$ $M^{-1}$, $2 \times 10^7$ $M^{-2}$ and $2 \times 10^{10}$ $M^{-3}$, and the p$K_a$ (25.0 ºC, $I$ = 1.0 M) of $Hphen^+$ is 5.12. See: R. M. Smith, A. E. Martell, *Critical Stability Constants*, Plenum, New York, 1975, **2**, p. 251.

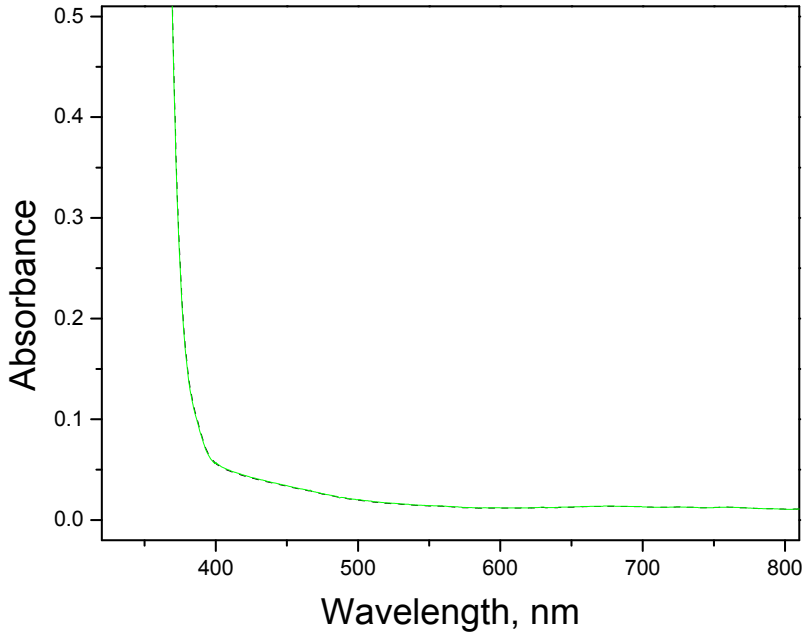
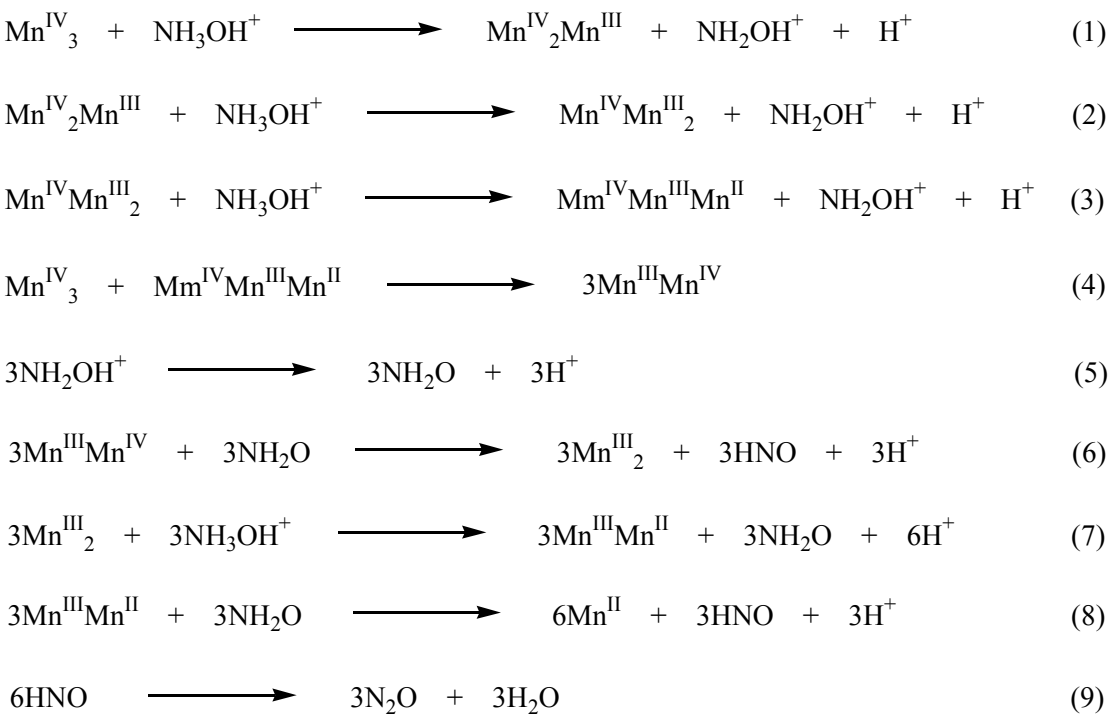



**Figure.** Optical spectrum (shown in black) of product solution when 0.10 mM of $[Mn^{IV}_3(\mu\text{-}O)_4(phen)_4(H_2O)_2]^{4+}$ (**1**) is reacted with 2.0 mM N(-I) in aqueous acidic media at pH 3.65 in presence 5.0 mM phen. The spectrum shown in green is that of a mixture of 0.30 mM $Mn(NO_3)_2$ and 5.0 mM phen at pH 3.65. Both at $I$ = 1.0 M ($NaNO_3$), T = 25.0 °C.

**Table S2** Some representative first-order rate constants ($k_0$, $s^{-1}$) for the oxidation of hydroxylamine in $H_2O$ solvent by the title complex (**1**) (0.10 mM) at T = 25.0 °C, $I$ = 1.0 M ($NaNO_3$)

| pH | $T_R$ (mM) | $C_{phen}$ (mM) | $10^3 k_0$ ($s^{-1}$) |
|---|---|---|---|
| 2.00 | 2.0 | 5.0 | 3.35 |
| 2.26 | 2.0 | 5.0 | 3.44 |
| 2.40 | 2.0 | 5.0 | 3.45 |
| 2.60 | 2.0 | 5.0 | 3.60 |
| 2.76 | 2.0 | 5.0 | 3.70 |
| 2.94 | 2.0 | 5.0 | 3.90 |
| 3.15 | 2.0 | 5.0 | 4.10 |
| 3.45 | 2.0 | 5.0 | 4.80 |
| 3.75 | 2.0 | 5.0 | 5.70 |
| 4.07 | 2.0 | 5.0 | 7.25 |
| 3.42 | 4.0 | 5.0 | 9.20 |
| 3.43 | 6.0 | 5.0 | 14.6 |
| 3.42 | 8.0 | 5.0 | 19.0 |
| 3.26 | 8.0 | 5.0 | 18.0 |
| 3.15 | 2.0 | 2.0 | 4.18 |
| 3.13 | 2.0 | 10.0 | 4.11 |
| 3.14 | 2.0 | 15.0 | 3.95 |
| 3.15 | 2.0 | 20.0 | 4.00 |
| 3.09 | 5.0 | 5.0 | 10.0 |
| 3.09 | 5.0 | 5.0 | 7.50[a] |
| 3.07 | 5.0 | 5.0 | 12.0[b] |
| 4.05 | 2.0 | 5.0 | 7.44[c] |
| 4.05 | 2.0 | 5.0 | 7.33[d] |

[a] $I$ = 0.5 M ($NaNO_3$). [b] $I$ = 1.5 M ($NaNO_3$). [c] [**1**] = 0.20 mM. [d] kinetics measured at 450 nm.



$$Mn^{IV}{}_3 + NH_3OH^+ \longrightarrow Mn^{IV}{}_2Mn^{III} + NH_2OH^+ + H^+ \quad (1)$$

$$Mn^{IV}{}_2Mn^{III} + NH_3OH^+ \longrightarrow Mn^{IV}Mn^{III}{}_2 + NH_2OH^+ + H^+ \quad (2)$$

$$Mn^{IV}Mn^{III}{}_2 + NH_3OH^+ \longrightarrow Mm^{IV}Mn^{III}Mn^{II} + NH_2OH^+ + H^+ \quad (3)$$

$$Mn^{IV}{}_3 + Mm^{IV}Mn^{III}Mn^{II} \longrightarrow 3Mn^{III}Mn^{IV} \quad (4)$$

$$3NH_2OH^+ \longrightarrow 3NH_2O + 3H^+ \quad (5)$$

$$3Mn^{III}Mn^{IV} + 3NH_2O \longrightarrow 3Mn^{III}{}_2 + 3HNO + 3H^+ \quad (6)$$

$$3Mn^{III}{}_2 + 3NH_3OH^+ \longrightarrow 3Mn^{III}Mn^{II} + 3NH_2O + 6H^+ \quad (7)$$

$$3Mn^{III}Mn^{II} + 3NH_2O \longrightarrow 6Mn^{II} + 3HNO + 3H^+ \quad (8)$$

$$6HNO \longrightarrow 3N_2O + 3H_2O \quad (9)$$

Adding equations (1) to (9), the stoichiometric equation (10) results

$$2Mn^{IV}{}_3 + 6NH_3OH^+ \longrightarrow 6Mn^{II} + 3N_2O + 3H_2O + 18H^+ \quad (10)$$

**Proposed scheme for the generation of $N_2O$**

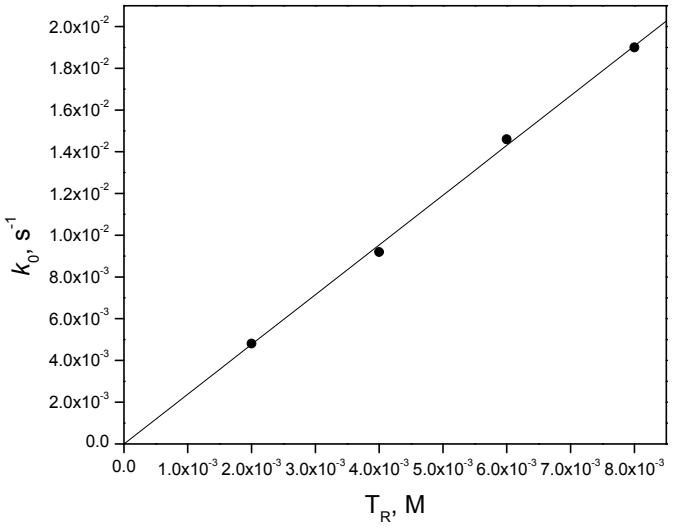



**Fig. S1** Plot of $k_0$ *versus* $T_R$ at [**1**] = 0.10 mM, $C_{phen}$ = 5.0 mM, T = 25.0 °C, $I$ = 1.0 M ($NaNO_3$), pH = 3.40 ± 0.05.

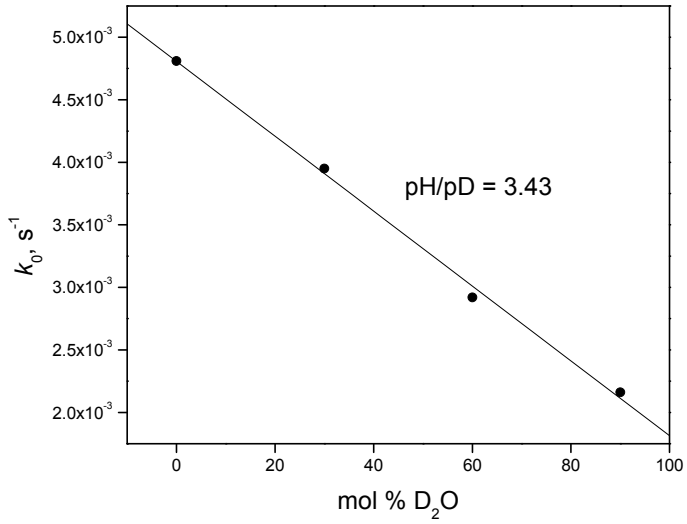



**Fig. S2** Effect of the amount of $D_2O$ (mol %) on $k_0$ at [**1**] = 0.1 mM, T = 25.0 °C, $I$ = 1.0 M ($NaNO_3$), $C_{phen}$ = 5.0 mM, $T_R$ = 2.0 mM.

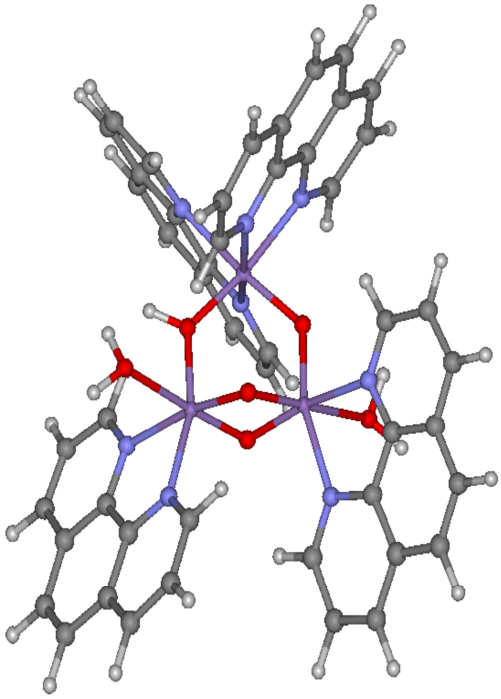


**Fig. S3.** Optimized geometry (RI-BP86/def2-TZVP) of protonated species **1B (1A + $H^+$ → 1B)**.

## Cartesian coordinates

### 1

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101
Energy = -6194.199028237 Hartrees
Mn     0.1810513   -2.2527834    0.0676140
O      0.6288143   -1.1340345   -1.2637974
O     -1.0788204   -1.2087392    0.8082018
N     -1.1128854   -3.3368875   -1.0925492
N      1.5047428   -3.7245415   -0.7278560
N     -0.0672285   -3.6614742    1.6540344
N      1.6457941   -1.6324982    1.3595773
Mn    -1.7046213    0.4671271    0.3508680
O     -0.1023650    1.1899329    0.0033007
O     -1.7370631    0.1857638   -1.4614886
O     -3.6471900   -0.4793284    0.6448923
N     -1.7545475    1.1322256    2.3385227
N     -2.8605436    2.2069760    0.1747686
Mn     0.0009344    0.5442435   -1.7122271
O      2.1279013    0.9829113   -1.8876780
N     -0.2021035    2.4632580   -2.5276313
N     -0.0599247    0.1156147   -3.7637722
C     -2.4169059   -3.0922736   -1.2712725
C     -3.2277922   -3.9345580   -2.0513115
C     -2.6793353   -5.0505648   -2.6619995
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C      0.7138726   -6.6394635   -2.9189185
C      1.4941397   -5.7352116   -2.1237181
C      2.8859623   -5.8707395   -1.9071024
C      3.5447501   -4.9339965   -1.1292201
C      2.8217232   -3.8738932   -0.5535665
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C     -0.9710684   -5.5086812    2.9016755
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C      2.8193265   -3.0081594    4.6229753
C      2.7572954   -2.1491460    3.4753061
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C     -0.2620591   -0.1373394   -6.5493027
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```

| | | | |
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| H | -4.2854925 | -3.6977023 | -2.1612847 |
| H | -3.3002916 | -5.7184146 | -3.2620120 |
| H | -1.2104747 | -7.1387632 | -3.7067183 |
| H | 1.2120865 | -7.4936421 | -3.3797993 |
| H | 3.4286979 | -6.7061436 | -2.3529437 |
| H | 4.6170031 | -5.0053830 | -0.9489948 |
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| H | -0.6310324 | 4.5013324 | -6.6469076 |
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## 1A

101
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| N | -1.0843353 | -3.2900255 | -1.1432259 |
| N | 1.5047935 | -3.6989787 | -0.7227003 |
| N | -0.0818486 | -3.6510975 | 1.6277917 |
| N | 1.5922717 | -1.6042823 | 1.3780413 |
| Mn | -1.7067563 | 0.4607976 | 0.3418443 |
| O | -0.1033919 | 1.1930834 | 0.0082363 |
| O | -1.7397165 | 0.1824215 | -1.4650198 |
| O | -3.6423729 | -0.5228896 | 0.6659288 |
| N | -1.7470707 | 1.1279922 | 2.3479359 |
| N | -2.8710553 | 2.2108588 | 0.1964018 |
| Mn | 0.0006576 | 0.5491677 | -1.7004435 |
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| C | 2.8929508 | -5.8796985 | -1.8320846 |
| C | 3.5485761 | -4.9159136 | -1.0842935 |

| | | | |
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| C | -0.9801067 | -4.6323803 | 1.7553769 |
| C | -0.9876996 | -5.5161445 | 2.8485707 |
| C | -0.0321861 | -5.3850199 | 3.8423155 |
| C | 0.9223427 | -4.3470180 | 3.7499107 |
| C | 1.9384593 | -4.0977173 | 4.7318576 |
| C | 2.8018207 | -3.0436270 | 4.6029306 |
| C | 2.7205366 | -2.1496140 | 3.4829639 |
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| C | -3.0265803 | 2.8800686 | 1.3743153 |
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| H | -0.6539995 | -0.3887380 | 3.2005705 |
| H | -0.7145544 | 0.6191386 | 5.5142855 |
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| H | -3.3205807 | 2.1061382 | -1.8095509 |
| H | -0.1264218 | 3.5716151 | -0.8144373 |
| H | -0.3394363 | 5.7875383 | -2.0009955 |
| H | -0.5698117 | 5.8212834 | -4.4932494 |
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| H | -0.6124512 | 2.2704471 | -7.8064374 |
| H | -0.3633098 | -0.2857518 | -7.6307724 |
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| H | 0.1776400 | -1.9295721 | -3.6577418 |

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H    -3.4281980   -1.2383764    1.2952287
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## 1B

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102
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Mn    0.2165122   -2.3400181    0.1359046
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N    -1.0637982   -3.3663696   -1.0651960
N     1.5298936   -3.8016680   -0.6490122
N    -0.1167634   -3.6547091    1.6821114
N     1.6806162   -1.7244836    1.4259894
Mn   -1.6003468    0.4795128    0.2969988
O    -0.0085855    1.2385460   -0.1031462
O    -1.6522688    0.1675889   -1.5242618
O    -3.5145179   -0.4853827    0.6537150
N    -1.6038626    1.1831246    2.2675992
N    -2.8179479    2.1770304    0.1238459
Mn    0.0230968    0.6515808   -1.8255673
O     2.1526941    1.1399501   -1.9918914
N    -0.3131752    2.5101216   -2.5926749
N    -0.0143208    0.2054264   -3.8742931
C    -2.3526757   -3.0845769   -1.3000558
C    -3.1628833   -3.9108915   -2.0974296
C    -2.6351655   -5.0587667   -2.6663423
C    -1.2710996   -5.3700432   -2.4586163
C    -0.6154259   -6.5192078   -3.0141620
C     0.7162912   -6.7476702   -2.7951894
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C     3.5526992   -5.0649696   -0.9925842
C     2.8434350   -3.9810689   -0.4488814
C     0.8677699   -4.7138800   -1.4244043
C    -0.5180598   -4.4783852   -1.6500257
C    -1.0769093   -4.5798085    1.8076324
C    -1.1497209   -5.4422306    2.9144316
C    -0.2026281   -5.3543976    3.9212403
C     0.8149976   -4.3769433    3.8286632
C     1.8341573   -4.1772679    4.8196323
C     2.7684410   -3.1855279    4.6850442
C     2.7584189   -2.3086227    3.5492306
C     3.6644788   -1.2389253    3.3602875
C     3.5406864   -0.4353581    2.2374606
C     2.5365195   -0.7028984    1.2909465
C     1.7746817   -2.5074274    2.5450674
C     0.8080693   -3.5405701    2.6830578
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C    -1.7592832    2.4019671    4.7901891
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C    -4.3297726    3.7126656   -0.9340342
C    -3.4826956    2.5905998   -0.9621212
C    -2.9830081    2.8582544    1.2961802
C    -2.3161421    2.3350957    2.4416387
C    -0.3797022    3.6594871   -1.9082010
C    -0.5527601    4.8964554   -2.5521493
C    -0.6759581    4.9463283   -3.9322256
C    -0.6055824    3.7479499   -4.6819299
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C    -0.2420064   -0.0110094   -6.6655101
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H    -2.7401772   -2.1774503   -0.8415351
H    -4.2066800   -3.6385673   -2.2502522
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H    -1.2004440   -7.2120339   -3.6206686
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H     3.4175764   -6.8608236   -2.1803037
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H     3.3548748   -3.2433019    0.1686044
H    -1.8121040   -4.6434886    1.0073373
H    -1.9529391   -6.1771663    2.9601026
H    -0.2391143   -6.0257818    4.7809444
H     1.8487596   -4.8313166    5.6927539
H     3.5345918   -3.0437158    5.4484653
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H    -5.1389365    5.3030747    0.2788614
H    -4.8615367    4.0010717   -1.8402376
H    -3.3352937    2.0000788   -1.8670450
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H    -0.8691741    4.6014803   -6.6699368
H    -0.6934016    2.4449361   -7.8576686
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H     0.1000579   -2.1130810   -6.3199013
H     0.2883855   -1.8365072   -3.8310432
H    -3.4474690   -1.1112254    1.3993749
H    -4.3489852    0.0084314    0.7645256
H     2.5534779    1.3085865   -2.8666742
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**2**

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O    -0.5323464   -0.5939725    1.2623082
N    -0.7141452   -2.6768367   -0.6068165
N     1.9150916   -3.1365273   -0.3921751
N     0.4534689   -3.0403294    2.0966234
N     2.1677609   -1.0195990    1.7331292
Mn   -1.3660950    0.9988918    0.7047163
O     0.3421010    1.8072531    0.3691101
O    -1.2684562    0.7525688   -1.1366059
O    -2.9918271    0.1410161    0.9062016
N    -1.4035023    1.6995071    2.6813347
N    -2.4347184    2.7823993    0.4900384
Mn    0.4545135    1.1568081   -1.2713303
O     2.6491989    1.6146010   -1.4639218
N     0.2498210    3.0720264   -2.1229640
N     0.4797793    0.7345017   -3.3800736
C    -2.0270343   -2.4236550   -0.6629444
C    -2.8937455   -3.2280591   -1.4275813
C    -2.3965987   -4.3039355   -2.1404427
C    -1.0115491   -4.5916947   -2.0913397
C    -0.3937228   -5.6886342   -2.7795422
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| C | 3.1849581 | -5.2518660 | -1.7344389 |
| C | 3.9017861 | -4.3755857 | -0.9384073 |
| C | 3.2309023 | -3.3284425 | -0.2807432 |
| C | 1.2006446 | -3.9833191 | -1.1873084 |
| C | -0.2013364 | -3.7393622 | -1.2991866 |
| C | -0.4496616 | -4.0058303 | 2.2771324 |
| C | -0.4505630 | -4.8397472 | 3.4102157 |
| C | 0.5139932 | -4.6668271 | 4.3866363 |
| C | 1.4756526 | -3.6406495 | 4.2358569 |
| C | 2.5029523 | -3.3571803 | 5.1964414 |
| C | 3.3827475 | -2.3262428 | 5.0067599 |
| C | 3.3055736 | -1.4917155 | 3.8421842 |
| C | 4.1573498 | -0.3883238 | 3.6011958 |
| C | 3.9803886 | 0.3713645 | 2.4577037 |
| C | 2.9696383 | 0.0321982 | 1.5401180 |
| C | 2.3112578 | -1.7681851 | 2.8675710 |
| C | 1.3957567 | -2.8458035 | 3.0626256 |
| C | -0.8955962 | 1.1012546 | 3.7566107 |
| C | -1.0181102 | 1.6545686 | 5.0443680 |
| C | -1.6905190 | 2.8526319 | 5.2171900 |
| C | -2.2518426 | 3.5013251 | 4.0929678 |
| C | -2.9999842 | 4.7249413 | 4.1502966 |
| C | -3.5536047 | 5.2709775 | 3.0238003 |
| C | -3.3987775 | 4.6431266 | 1.7427506 |
| C | -3.9780802 | 5.1174858 | 0.5431645 |
| C | -3.7828973 | 4.4133928 | -0.6343628 |
| C | -2.9985934 | 3.2462961 | -0.6279439 |
| C | -2.6359637 | 3.4503496 | 1.6598801 |
| C | -2.0719847 | 2.8738264 | 2.8354683 |
| C | 0.2058939 | 4.2278328 | -1.4543752 |
| C | 0.0822003 | 5.4642751 | -2.1132592 |
| C | -0.0144531 | 5.4989856 | -3.4949676 |
| C | 0.0316126 | 4.2899480 | -4.2287770 |
| C | -0.0504931 | 4.2077719 | -5.6590639 |
| C | 0.0244707 | 3.0023734 | -6.3031681 |
| C | 0.2020942 | 1.7802351 | -5.5723153 |
| C | 0.3137381 | 0.5031383 | -6.1703891 |
| C | 0.5024423 | -0.6100281 | -5.3681981 |
| C | 0.5829532 | -0.4556431 | -3.9721276 |
| C | 0.2844567 | 1.8353534 | -4.1578261 |
| C | 0.1806507 | 3.0915341 | -3.4846545 |
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| H | -3.9561667 | -2.9878457 | -1.4388191 |
| H | -3.0598149 | -4.9363676 | -2.7333004 |
| H | -1.0217154 | -6.3444353 | -3.3841555 |
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| H | 3.6839996 | -6.0768483 | -2.2453655 |
| H | 4.9776592 | -4.4853386 | -0.8069672 |
| H | 3.7779835 | -2.6304534 | 0.3526279 |
| H | -1.2076181 | -4.1239573 | 1.5037448 |
| H | -1.2141171 | -5.6111992 | 3.5023007 |
| H | 0.5348956 | -5.3059135 | 5.2706725 |
| H | 2.5672850 | -3.9784513 | 6.0906193 |
| H | 4.1560629 | -2.1180820 | 5.7470911 |
| H | 4.9389253 | -0.1400437 | 4.3210811 |
| H | 4.6117776 | 1.2350798 | 2.2535385 |
| H | 2.7892767 | 0.6167487 | 0.6401823 |
| H | -0.3941392 | 0.1509226 | 3.5748478 |
| H | -0.5898207 | 1.1265130 | 5.8952768 |
| H | -1.8009781 | 3.2919745 | 6.2097979 |
| H | -3.1345224 | 5.2095627 | 5.1181411 |
| H | -4.1341867 | 6.1920835 | 3.0874546 |
| H | -4.5864953 | 6.0233611 | 0.5555009 |
| H | -4.2354436 | 4.7451946 | -1.5680362 |
| H | -2.8206442 | 2.6585869 | -1.5292901 |
| H | 0.2744671 | 4.1451633 | -0.3688163 |
| H | 0.0642489 | 6.3816215 | -1.5260548 |
| H | -0.1177097 | 6.4491350 | -4.0219442 |
| H | -0.1722481 | 5.1294728 | -6.2293063 |

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| H | 0.2541236 | 0.4044693 | -7.2555175 |
| H | 0.5947056 | -1.6039163 | -5.8043804 |
| H | 0.7406077 | -1.3034067 | -3.3044675 |
| H | -3.7430027 | 0.5885875 | 0.4749900 |
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## 2A

100
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| O | 1.0746477 | -0.5005752 | -0.8475835 |
| O | -0.6495655 | -0.5916936 | 1.2383862 |
| N | -0.7177853 | -2.6767778 | -0.5498631 |
| N | 1.8930491 | -3.0732981 | -0.3564817 |
| N | 0.4711657 | -3.0111941 | 2.1160841 |
| N | 2.0801316 | -0.9497223 | 1.7692424 |
| Mn | -1.4207248 | 0.9858824 | 0.6949068 |
| O | 0.2779549 | 1.8095604 | 0.3759699 |
| O | -1.3252398 | 0.7298573 | -1.1356429 |
| O | -3.1012216 | 0.1830028 | 0.8862631 |
| N | -1.4986999 | 1.6933767 | 2.6745509 |
| N | -2.4650966 | 2.8200623 | 0.4657643 |
| Mn | 0.4001530 | 1.1443156 | -1.2664007 |
| O | 2.6618246 | 1.4121956 | -1.4682291 |
| N | 0.2833223 | 3.0705203 | -2.1257739 |
| N | 0.3992482 | 0.7359443 | -3.3888038 |
| C | -2.0344051 | -2.4309558 | -0.6250630 |
| C | -2.8907057 | -3.2506423 | -1.3819850 |
| C | -2.3896520 | -4.3415522 | -2.0743277 |
| C | -1.0057705 | -4.6184721 | -2.0134575 |
| C | -0.3676470 | -5.7143472 | -2.6855636 |
| C | 0.9832790 | -5.9147035 | -2.5946111 |
| C | 1.8123858 | -5.0367508 | -1.8198995 |
| C | 3.2136016 | -5.1643081 | -1.6993373 |
| C | 3.9136467 | -4.2450316 | -0.9334374 |
| C | 3.2197060 | -3.2157780 | -0.2754225 |
| C | 1.1989401 | -3.9584440 | -1.1289927 |
| C | -0.2055882 | -3.7461915 | -1.2323258 |
| C | -0.4258581 | -3.9819209 | 2.3180465 |
| C | -0.3347872 | -4.8853419 | 3.3900243 |
| C | 0.7166761 | -4.7854118 | 4.2880879 |
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| C | 3.5839434 | -2.4276991 | 4.8502004 |
| C | 3.3881215 | -1.5035698 | 3.7688824 |
| C | 4.1370721 | -0.3199557 | 3.5868233 |
| C | 3.8035842 | 0.5335307 | 2.5459368 |
| C | 2.7683856 | 0.1962602 | 1.6587297 |
| C | 2.3527459 | -1.7664820 | 2.8351422 |
| C | 1.4888519 | -2.8819616 | 3.0172769 |
| C | -1.0231762 | 1.0786580 | 3.7536958 |
| C | -1.1663387 | 1.6199997 | 5.0449065 |
| C | -1.8253696 | 2.8256729 | 5.2130192 |
| C | -2.3508556 | 3.4928719 | 4.0827853 |
| C | -3.0753906 | 4.7304029 | 4.1370328 |
| C | -3.5859444 | 5.3032273 | 3.0040452 |
| C | -3.4110489 | 4.6891076 | 1.7191264 |
| C | -3.9371828 | 5.2025576 | 0.5116011 |
| C | -3.7228363 | 4.5154204 | -0.6716381 |
| C | -2.9757697 | 3.3230488 | -0.6577287 |
| C | -2.6793843 | 3.4764374 | 1.6374956 |
| C | -2.1535034 | 2.8739584 | 2.8230109 |
| C | 0.2948771 | 4.2221368 | -1.4525206 |
| C | 0.2523021 | 5.4679967 | -2.1045795 |
| C | 0.1816220 | 5.5177836 | -3.4873268 |
| C | 0.1723785 | 4.3122174 | -4.2268763 |

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| C | 0.1035355 | 4.2381527 | -5.6585742 |
| C | 0.1085556 | 3.0327797 | -6.3072061 |
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| C | 0.2266428 | 0.5177108 | -6.1782292 |
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| H | 4.3972892 | -2.2408535 | 5.5525335 |
| H | 4.9482014 | -0.0772224 | 4.2746950 |
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| H | -0.7627814 | 1.0783824 | 5.8995317 |
| H | -1.9518954 | 3.2596047 | 6.2061574 |
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| H | -4.1452351 | 6.2378592 | 3.0639703 |
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| H | -4.1297400 | 4.8800918 | -1.6141436 |
| H | -2.7822263 | 2.7437119 | -1.5620226 |
| H | 0.3399003 | 4.1231621 | -0.3667254 |
| H | 0.2741409 | 6.3812035 | -1.5110998 |
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| H | 0.0454633 | 5.1675339 | -6.2266790 |
| H | 0.0506954 | 2.9944088 | -7.3958482 |
| H | 0.1657956 | 0.4244210 | -7.2637637 |
| H | 0.3548497 | -1.6047043 | -5.8113006 |
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| H | -3.7706480 | 0.6093602 | 0.3214156 |
| H | 2.6530627 | 0.4264461 | -1.3768071 |
| H | 3.0596710 | 1.6197945 | -2.3323762 |