Ruthenium PNN(O) Complexes: Cooperative Reactivity and Application as Catalysts for Acceptorless Dehydrogenative Coupling Reactions

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SUPPORTING INFORMATION FOR

Ruthenium PNN(O) Complexes: Cooperative Reactivity and Application as Catalysts for
Acceptorless Dehydrogenative Coupling Reactions

Sandra Y. de Boer, a,† Ties J. Korstanje, a,† Stefan R. La Rooij, a Rogier Kox, a Joost N. H. Reek, a

Jarl Ivar van der Vlugt*, a

†Homogeneous, Bioinspired and Supramolecular Catalysis, van ‘t Hoff Institute for Molecular
Sciences, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, the Netherlands

Corresponding author: j.i.vandervlugt@uva.nl
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Computational details S32
Spectra of relevant compounds

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Figure S24. CSI-MS of 1.
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Figure S26. 2D $[^1\text{H}-^1\text{H}]$-COSY NMR spectrum (CD$_3$OD) of 1'.
Figure S27. $^{31}$P NMR spectrum (CD$_3$OD) of 1'.
Crystallographic details of complex $1^{Me}$

Table S1. Selected bond lengths (Å), angles and torsion angles (°) for complexes 1 and 2

|                | Complex $1^{Me}$CN | Complex $1^{Me}$ |
|----------------|-------------------|-----------------|
| Ru1-P1         | 2.2711(6)         | 2.2779(12)      |
| Ru1-N1         | 2.0964(19)        | 2.0943(39)      |
| Ru1-N2         | 2.1598(18)        | 2.1740(40)      |
| Ru1-C20a       | 1.8524(25)        | 1.8404(53)      |
| Ru1-H1         | 1.7125(309)       | 1.9415(447)     |
| Ru1-Cl1b       | 2.1855(21)        | 2.5634(12)      |
| C20-O2a        | 1.1512(30)        | 1.1481(65)      |
| P1-Ru1-N1      | 82.72(5)          | 83.21(11)       |
| P1-Ru1-N2      | 157.27(7)         | 159.24(12)      |
| N1-Ru1-N2      | 76.24(7)          | 76.31(16)       |

Figure S28. ORTEP plot of $1^{Me}$. 
|                  |       |         |
|------------------|-------|---------|
| N1-Ru1-C20\(^a\) | (°)   | 171.49(9) 173.16(19) |
| H1-Ru1-Cl1\(^b\) | (°)   | 171.90(1.04) 172.13(1.30) |
| N2-C7-C6-N1      | (°)   | -1.00 -0.58 |
| N1-C2-C1-P1      | (°)   | 29.04 27.14 |

\(^a\) In complex 2, the corresponding bond lengths are between Ru1-C21 and C21-O2, and bond angle between N1-Ru1-C21.  
\(^b\) In complex 1\(\text{MeCN}\), the chloride ligand is replaced by an NCMe ligand, thus the bond length represents the Ru1-N3 bond and H1-Ru1-N3 bond angle.

**Details for complex 1\(\text{Me}\), [RuCl(CO)(H)(L\(\text{Me}\))]:** C\(_{21}\)H\(_{30}\)ClN\(_2\)O\(_2\)PRu, Fw = 509.96, orange-red rectangular block, 0.255×0.168×0.145 mm, triclinic \(P\overline{1}\) (No: 2)), a = 8.053(6), b = 8.281(5), c = 17.447(11) Å, \(\alpha = 103.250(17), \beta = 94.156(14), \gamma = 90.651(13)\)°, \(V = 1129.0(2)\) Å\(^3\), \(Z = 2, D_x = 1.459\) g/cm\(^3\), \(\mu = 0.905\) mm\(^-1\). 42825 Reflections were measured up to a resolution of \((\sin \theta/\lambda)_{\text{max}} = 0.75\) Å\(^-1\). 5605 Reflections were unique (\(R_{\text{int}} = 0.0664\)), of which 5035 were observed [\(I > 2\sigma(I)\)]. 264 Parameters were refined with 0 restraints. \(R_1/wR_2\) [\(I > 2\sigma(I)\): 0.0540/0.1349. \(R_1/wR_2\) [all refl.]: 0.0629/ 0.1387. \(S = 1.187\). Residual electron density between -1.49 and 1.64 e/Å\(^3\).
Computational details, energies and BP86-calculated structures

**Table S2.** Relative free energies of the calculated complexes using different functionals (BP86 was used in combination with disp3 dispersion corrections, TPSS and b3-lyp without).

| Complex  | **BP86 / disp3** | **TPSS** | **b3-lyp** |
|----------|-------------------|----------|------------|
| $1^{HH}$ | 0                 | 0        | 0          |
| TS''     | 22.5              | 24.4     | 28.1       |
| TS'PS'   | 22.3              | 25.0     | 28.3       |
| TS'      | 5.0               | 6.2      | 7.7        |
| Int''    | 4.7               | 4.6      | 4.7        |
| Int'     | 0.0               | -2.0     | -2.1       |
| $1''$    | 0.9               | -2.0     | -4.9       |
| $1'$     | -4.1              | -6.6     | -9.8       |

$1^{HH}$

![Image of the molecule $1^{HH}$]

Energy = -1476.645732639

| H       | 0.6777257 | -5.2287429 | -1.2097173 |
|---------|----------|------------|------------|
| C       | 0.7059704 | -4.1413941 | -1.1409273 |
| N       | 0.723217  | -1.363071  | -0.9690875 |
| C       | 0.4683446 | -3.5007987 | 0.0800503  |
| C       | 0.9963542 | -3.3724807 | -2.2615696 |
| C       | 1.0117247 | -1.9760763 | -2.1546206 |
| C       | 0.4949954 | -2.1106657 | 0.1447718  |
| H       | 0.2689409 | -4.0747679 | 0.9844525  |
| H       | 1.2058847 | -3.8489765 | -3.2176271 |
| C       | 0.3353654 | -1.3481377 | 1.4266346  |
| H       | 1.3430059 | -1.1886669 | 1.8457849  |
| H       | -0.2472089 | -1.9090638 | 2.1699962  |
| P       | -0.3196921 | 0.3733144  | 1.106949   |
| C       | -2.2198565 | 0.1551461  | 1.2360094  |
$1^\text{HH} + \text{tBuOH}$

Energy = -1710.459237659

H  2.7723603  -4.3151964  -1.4966799
C  2.2266819  -3.3717788  -1.5133307
N  0.8525453  -0.955686  -1.5316523
C  1.2367287  -3.108944  -0.5632311
C  2.4952096  -2.4217511  -2.4923879
C  1.7847885  -1.216125  -2.4913528
C  0.5520163  -1.8962809  -0.5979135
H  0.9801544  -3.8453494  0.1973571
H  3.245996  -2.6147176  -3.2562408
C  -0.5833758  -1.5797085  0.3281233
H  -0.4821488  -2.0957158  1.2923761
P  -0.8146841  0.2629988  0.5053284
C  -2.664862  0.4320891  0.9507544
C  -3.1585727  -0.6573454  1.9232175
H  -3.0573755  -1.6647398  1.4970701
H  -4.2324691  -0.495809  2.1099205
H  -2.6524905  -0.6385915  2.892873
C  -3.4831568  0.3058324  -0.3490287
H  -3.2208129  1.0853649  -1.0723772
H  -4.5503244  0.4056213  -0.0915534
H  -3.347966  -0.6652251  -0.8447564
C  -2.9204679  1.8293925  1.5456699
H  -2.5448153  2.6282558  0.8924411
H  -2.4736088  1.9520855  2.5405893
H  -4.0069896  1.9744558  1.6554697
C  0.2690091  0.7001271  2.0250382
C  -0.2817861  0.1987998  3.3691032
H  -0.464402  -0.8857097  3.3681379
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -1.207345 | 0.7083119 | 3.6647136 |
| H    | 0.4643187 | 0.4015923 | 4.1539037 |
| C    | 0.4671967 | 2.2266964 | 2.0739383 |
| H    | 0.9205119 | 2.5904136 | 1.143478  |
| H    | 1.144613  | 2.4723045 | 2.9075127 |
| H    | -0.470655 | 2.7713042 | 2.2355372 |
| C    | 1.6462502 | 0.0418358 | 1.7994332 |
| H    | 2.0622258 | 0.3124672 | 0.8193872 |
| H    | 1.144613  | 2.4723045 | 2.9075127 |
| H    | -0.470655 | 2.7713042 | 2.2355372 |
| C    | 1.8605377 | 1.8253161 | 5.4136076 |
| N    | 1.096208  | 0.9112383 | 3.3144427 |
| C    | 2.7527005 | -0.2615719 | 4.2753001 |
| C    | 2.7318707 | 0.755533  | -5.5745472 |
| C    | 1.044192  | 1.8618917 | -4.2753001 |
| H    | 3.4013834 | -1.125099 | -4.7480395 |
| H    | 3.3798142 | 0.702931  | -6.4494298 |
| H    | 1.7790698 | 2.6308649 | -6.1405202 |
| Ru   | -0.0061345 | 0.9527686 | 1.5027632 |
| O    | 0.1711433 | 2.859734  | 4.1258712 |
| H    | -0.3257676 | 2.662705  | -3.2822661 |
| H    | 1.3874715 | 1.4943087 | -0.7552199 |
| C    | -0.6853925 | 2.6506421 | 1.2467182 |
| O    | -1.1188995 | 3.7101475 | -0.9889319 |
| H    | -1.4024258 | 0.4394244 | 2.3341393 |
| H    | -1.7108599 | 1.0740695 | -2.3693792 |
| O    | -2.0146887 | -2.0243981 | 2.4290642 |
| H    | -1.4987753 | 1.9546342 | -0.1599153 |
| C    | -2.1812082 | -2.3242508 | -3.828477 |
| C    | -3.2723948 | -1.4161106 | 4.4149448 |
| H    | -4.2138434 | -1.558545 | -3.8663395 |
| H    | -3.4470918 | -1.6335668 | 5.4793897 |
| H    | -2.9755869 | -0.3614262 | 4.3193723 |
| C    | -2.597108 | -3.7933768 | -3.8885264 |
| H    | -3.5309369 | -3.9445911 | 3.3292553 |
| H    | -1.8184094 | -4.4252675 | 3.4384378 |
| H    | -2.7540953 | -4.114888 | 4.9278461 |
| C    | -0.8475794 | -2.1022546 | 4.5570585 |
| H    | -0.0628839 | -2.7216717 | -4.1001725 |
| H    | -0.5454165 | -1.0482638 | 4.4769366 |
| H    | -0.9244808 | -2.3590831 | 5.6237492 |
Energy = -1476.604590597

H  2.6646856  -4.6839751   -0.2639738
C  2.1547579  -3.7351918   -0.4344063
N  0.9139997  -1.2965242   -0.8390966
C  1.1509143  -3.3195929    0.4282095
C  2.4919326  -2.9518976   -1.5477411
C  1.8366742  -1.7369319   -1.735441
C  0.5081564  -2.0830199    0.2100765
H  0.8484677  -3.932896     1.2766153
H  3.2290615  -3.3009606   -2.2677854
C  -0.6516209  -1.5956088    0.9136981
H  -1.0047292  -2.2067534   1.7495515
P  -0.7304196   0.2318422   1.0071583
C  -2.5220679   0.5780709   1.5657515
C  -2.9516318  -0.3171025   2.7448291
H  -2.9554243  -1.3789454   2.4652565
H  -3.9836449  -0.0507769   3.0241956
H  -2.3292538  -0.1956867   3.6366147
C  -3.4857261   0.2904326    0.396401
H  -3.281979   0.9149385   -0.4791491
H  -4.5100932   0.5064381   0.7411833
H  -3.4537562  -0.7604671   0.0834305
C  -2.6630386   2.062109   1.9505409
H  -2.3189607   2.7285152   1.1483136
H  -2.1207278   2.3080087   2.8726968
H  -3.7272648   2.2815613   2.1307196
C  0.5190081   0.8711614   2.3019155
C  0.1291516   0.5591307   3.7548087
H  -0.0537057  -0.5142022   3.9085357
H  -0.7561781   1.1177812   4.0838038
H  0.9609464  0.8508593  4.4161278
C  0.7129728  2.3884818  2.1141116
H  1.0072098  2.6220034  1.0827946
H  1.5151297  2.7294948  2.78857
H  -0.1868059  2.9667242  2.3534036
C  1.8649305  0.1780977  2.0064554
H  2.1816965  0.334218  0.9676558
H  1.8258991  -0.9007376  2.2056965
H  2.6330025  0.6136049  2.6653364
C  1.9650386  -0.8744748  -2.9123415
C  1.9396933  0.7794451  -5.1230044
N  1.0503157  0.1502593  -2.965357
C  2.8939015  -1.0783648  -3.9331376
C  2.8794444  -0.2410951  -5.0488759
C  1.0450638  0.949162  -4.0582106
H  3.6187743  -1.8853518  -3.8529225
H  3.5971128  -0.3858209  -5.8564316
H  1.8753054  1.4581714  -5.9711691
Ru  -0.0879909  0.4963258  -1.1876031
O  0.1496624  1.9384609  -4.1144592
H  -0.3564084  1.8999904  -3.2569025
H  1.1337894  1.4751888  -0.8175515
C  -1.1095646  2.0199366  -1.3804046
O  -1.7778532  2.9868567  -1.4113346
H  -1.4775398  -0.8328635  -1.2754955
H  -1.3987059  -1.3660924  -0.3496814
TS'PS'

Energy = -1710.425535214

H  2.6821672 -4.22284 -1.8833048
C  2.1630379 -3.2641947 -1.8537873
N  0.8654135 -0.8227624 -1.761752
C  1.1226705 -3.0639149 -0.9587418
C  2.5385889 -2.2398664 -2.7320933
C  1.856504  -1.0248204 -2.6682206
C  0.45482  -1.8195987  -0.916038
H  0.8052837 -3.8561345 -0.2816256
H  3.3338588 -2.3960697 -3.4572313
C  -0.7327371 -1.5518405 -0.1322838
H  -0.941577  -2.2809633  0.6572369
P  -0.8787086  0.217809   0.2977374
C  -2.7100254  0.527263  0.7569948
C  -3.3188277 -0.7133317  1.4371869
C  -3.3170198 -1.5764779  0.758151
H  -4.3678411 -0.4959069  1.6945998
H  -2.8042122 -0.9955986  2.3638248
C  -3.5203696  0.8166832  0.522102
C  -3.1492921  1.7043778 -1.048539
H  -4.5634013  1.0125269 -0.2231715
H  -3.5172236 -0.0284444 -1.2189461
C  -2.845082  1.7649295  1.6645548
H  -2.4117957  2.6592247  1.1965401
H  -2.3938856  1.6317177  2.6546644
H  -3.9175922  1.9616411  1.8198733
C  0.2267937  0.4562373  1.8504314
C  -0.3461046 -0.2353381  3.0994636
Energy = -1476.63282645

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| H       | 1.6458733 | 0.8744884 | -5.1826559 |
| C       | 1.4210835 | 0.8825662 | -4.1160803 |
| N       | 0.8172319 | 0.8994929 | -1.3950262 |
| C       | 0.8668816 | -0.2435743 | -3.5000114 |
| C       | 1.7084478 | 2.0011236 | -3.3436203 |
| C       | 1.3855806 | 2.000935  | -1.981572  |
| C       | 0.6086551 | -0.2251893 | -2.1305302 |
| H       | 0.6644468 | -1.1505692 | -4.0692959 |
| H       | 2.1740218 | 2.8788733 | -3.7885603 |
| C       | 0.2158481 | -1.4721099 | -1.3865759 |
| H       | 1.1192416 | -2.1000712 | -1.324827  |
| H       | -0.5323233 | -2.0584406 | -1.9384043 |
| P       | -0.2715354 | -1.1397092 | 0.3901962  |
| C       | -2.1854616 | -1.159756  | 0.328775   |
| C       | -2.8066327 | -2.5287884 | 0.0139649  |
| H       | -2.4004392 | -2.9773953 | -0.9040692 |
| H       | -3.8906668 | -2.4017337 | -0.1378142 |
| H       | -2.6772211 | -3.2426834 | 0.8371435  |
| C       | -2.5848838 | -0.1703849 | -0.7872503 |
| H       | -2.1388367 | 0.8202281  | -0.626949  |
| H       | -3.6801424 | -0.0547914 | -0.7820583 |
| H       | -2.2976861 | -0.5267924 | -1.7865398 |
| C       | -2.7420896 | -0.6342013 | 1.6646124  |
| H       | -2.3135491 | 0.3449027  | 1.9146806  |
| H       | -2.5468408 | -1.3193328 | 2.4982775  |
| H       | -3.8340391 | -0.5182964 | 1.5771408  |
| C       | 0.3876635  | -2.6937512 | 1.2834342  |
| C       | 0.1321572  | -4.0151071 | 0.532602   |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 0.6068999 | -4.0310757| -0.4582757|
| H       | -0.9304601| -4.242692 | 0.4065473 |
| H       | 0.5769628 | -4.8395574| 1.1128782 |
| C       | -0.2362388| -2.7634586| 2.6884338 |
| H       | -0.1342324| -1.8132419| 3.229258 |
| H       | 0.2842977 | -3.5372452| 3.2746206 |
| H       | -1.2986534| -3.0369414| 2.6546434 |
| C       | 1.91241   | -2.5199154| 1.4347639 |
| H       | 2.1681526 | -1.6659311| 2.0700358 |
| H       | 2.4188103 | -2.3777094| 0.4696274 |
| H       | 2.3225283 | -3.4323788| 1.8964669 |
| C       | 1.5470894 | 3.1429949 | -1.0816102|
| C       | 1.2448611 | 5.2216375 | 0.7127705 |
| N       | 1.1846516 | 2.8723405 | 0.2061391 |
| C       | 1.8936072 | 4.4341298 | -1.4767381|
| C       | 1.7993509 | 5.4681776 | -0.5328756|
| C       | 0.833833  | 3.9037687 | 1.0466104 |
| H       | 2.1926565 | 4.6421016 | -2.5019446|
| H       | 2.0991558 | 6.4810981 | -0.8051027|
| H       | 1.0586851 | 6.0161347 | 1.4334975 |
| O       | 0.0994143 | 3.6110739 | 2.0661236 |
| C       | 0.9937767 | 0.7072447 | 2.5096067 |
| O       | 1.2934106 | 0.4959117 | 3.6174526 |
| Ru      | 0.6477531 | 0.903773  | 0.6996386 |
| H       | 2.1071493 | 0.2216444 | 0.5016997 |
| H       | -0.4674011| 2.5103434 | 1.6325127 |
| H       | -0.9280984| 1.7519736 | 1.1021958 |
Int""
H  0.8342715  -0.6747083  3.7733426
H  -0.6251009   0.200057   4.2973714
H   0.9768413  0.8576916   4.6569836
C  -0.1025544  2.5442081   2.799957
H  -0.0958281  3.1342515   1.87554
H   0.5411378  3.0626641   3.5290317
H  -1.1211546  2.5490148   3.2087912
C   1.9226514  1.2166739   2.1743666
H   2.0749059  1.9064747   1.3363527
H   2.3298272  0.2340717   1.8889807
H   2.5007229  1.5884028   3.0359973
C   1.6475728  -1.0767955  -3.0936941
C   2.0901446   0.8248171  -5.0650091
N   1.217447   0.2098816  -2.9016876
C   2.3022328  -1.4391635  -4.2721963
C   2.5245117  -0.4787992  -5.2599634
C   1.4314152   1.1304004  -3.8658631
H   2.6370317  -2.463571  -4.4130158
H   3.0377262  -0.7511607  -6.1825332
H   2.2356854   1.6130006  -5.800534
Ru  0.2141032   0.5914796  -1.0286026
O   0.987898   2.3761615  -3.6677873
H   0.5671521  2.3788535  -2.7644147
H   1.6593721   0.8605205  -0.4265976
C  -0.1029719  2.4042662  -0.8307598
O  -0.2755658   3.5411429  -0.600242
H  -1.2353195   0.3198496  -2.12829
H  -1.5021631   0.0498386  -1.3922403
Int'' + tBuOH

Energy = -1710.439259062

H  1.7326544  -4.8849035  -1.7135982
C  1.4416615  -3.8374957  -1.6228469
N  0.6261708  -1.1849254  -1.460415
C  0.6920891  -3.4239917  -0.5514304
C  1.8525687  -2.9099268  -2.6102748
C  1.413732  -1.5980411  -2.495295
C  0.3216943  -2.0412672  -0.3966012
H  0.386635  -4.1276046  0.2226455
H  2.4765002  -3.2243882  -3.4425031
C  -0.307053  -1.5262632  0.724455
H  -0.5920613  -2.1937704  1.5361121
P  -0.6490816   0.207479  0.7805196
C  -2.5474921   0.4050261  0.9994687
C  -3.027972   0.0680745  2.421942
H  -2.7202732  -0.9414739  2.7278165
H  -4.1297897   0.0923867  2.436374
H  -2.6787097   0.787486  3.1723713
C  -3.2264207  -0.5927681  0.043663
H  -2.9409576  -0.4722297  -1.0086014
H  -4.3173628  -0.4482166  0.103133
H  -2.9983664  -1.6322786  0.3126255
C  -2.9790628  1.8354682  0.6295704
H  -2.7510403  2.0656594  -0.4189298
H  -2.4981966  2.6001352  1.2511693
H  -4.0688866  1.9303218  0.7643281
C  0.2480192   0.8754728  2.33959
C  0.0961348  -0.0988149  3.5257745
H  0.5107513  -1.0863662  3.2825676
|    |        |        |        |
|----|--------|--------|--------|
| H  | -0.9383683 | -0.227618 | 3.8575937 |
| H  | 0.6672263  | 0.3001302 | 4.3792216 |
| C  | -0.2383287 | 2.2789316 | 2.7360314 |
| H  | -0.1632762 | 2.9914814 | 1.9047475 |
| H  | 0.3958498  | 2.2794485 | 3.1023485 |
| C  | 1.7505825  | 0.9484495 | 2.0096339 |
| H  | 2.1201379  | -0.0037637 | 1.6039692 |
| H  | 2.3038322  | 1.1652748 | 2.9377897 |
| C  | 1.7143687  | -0.5514011 | -3.4807646 |
| C  | 2.1186587  | 1.5398254 | -5.2557238 |
| N  | 1.2425961  | 0.6976717 | -3.1718782 |
| C  | 2.3976762  | -0.7801183 | -4.6758153 |
| C  | 2.6026079  | 0.2762877 | -5.5640832 |
| C  | 1.4336785  | 1.709972  | -4.0443759 |
| H  | 2.7529168  | -1.7792851 | -4.9138868 |
| H  | 3.133513   | 0.1085196 | -6.5014584 |
| H  | 2.2408733  | 2.3964724 | -5.9150499 |
| Ru | 0.1710736  | 0.8664538 | -1.3086221 |
| O  | 0.9367177  | 2.9134033 | -3.7420658 |
| H  | 0.5013298  | 2.8166408 | -2.8501552 |
| H  | 1.6044174  | 0.9673554 | -0.6249977 |
| C  | -0.0376925 | 2.6504222 | -0.8656884 |
| O  | -0.1305593 | 3.7540143 | -0.4818865 |
| H  | -1.2527504 | 0.8548887 | -2.4643383 |
| H  | -1.5522377 | 0.4724906 | -1.7949477 |
| O  | -2.1436925 | -1.9657938 | -2.7758148 |
| H  | -1.2185824 | -1.8468652 | -2.4815541 |
| C  | -2.156163  | -2.1359278 | -4.2107739 |
| C  | -3.6166289 | -2.4301576 | -4.5545737 |
| H  | -3.950803  | -3.3391502 | -4.035989 |
| H  | -3.7413712 | -2.5743097 | -5.6366516 |
| H  | -4.2569295 | -1.5960163 | -4.2348099 |
| C  | -1.2537045 | -3.3130546 | -4.6008147 |
| H  | -1.5724649 | -4.2218563 | -4.0723199 |
| H  | -0.2090188 | -3.1057999 | -4.3237468 |
| H  | -1.2917786 | -3.5019083 | -5.6838177 |
| C  | -1.6880863  | -0.8429493 | -4.8946883 |
| H  | -0.648529  | -0.6138268 | -4.6220642 |
| H  | -2.3228823  | -0.000433 | -4.5870865 |
| H  | -1.7357712  | -0.9325376 | -5.9899427 |
Energy = -1476.643496949

H  0.9494091  1.1431488  -5.2173308
C  0.899436   1.0874799  -4.1295365
N  0.7080339  0.9632258  -1.3727234
C  0.5637045  -0.116083   -3.5003718
C  1.2029862  2.2029565  -3.3587883
C  1.1168552  2.1242904  -1.9606044
C  0.4984795  -0.1576078  -2.1091831
H  0.3734819  -1.0199791  -4.0778823
H  1.5064681  3.1342016  -3.8323089
C  0.2997603  -1.4376777  -1.3439484
H  1.2960497  -1.8914465  -1.212905
H  -0.3085155  -2.1623168  -1.9023095
P  -0.3180356  -1.1250296   0.3958235
C  -2.2158844  -1.3253049   0.212331
C  -2.6939701  -2.7639203  -0.038915
H  -2.2047757  -3.2220382  -0.9100996
H  -3.7766023  -2.7492078  -0.2434894
H  -2.537876  -3.413329   0.8307413
C  -2.6437582  -0.4699987  -0.9989762
H  -2.2836755  0.5653381  -0.9369471
H  -3.743516  -0.4345335  -1.0379404
H  -2.2950327  -0.8917936  -1.9515931
C  -2.8982008  -0.7713234   1.4775141
H  -2.5945791  0.2620997   1.6870173
H  -2.6734407  -1.3702769   2.3679514
H  -3.9902804  -0.7821127   1.3344829
C  0.4107282  -2.5913492   1.3750574
C  0.3434786  -3.9404121   0.6329293
| Element | x     | y     | z     |
|---------|-------|-------|-------|
| H       | 0.8974877 | -3.9207874 | -0.3157295 |
| H       | -0.6781844 | -4.2724452 | 0.4265804 |
| H       | 0.8162341 | -4.7101646 | 1.2634374 |
| C       | -0.3124483 | -2.6942719 | 2.7304669 |
| H       | -0.3280919 | -1.7308223 | 3.2572482 |
| H       | 0.225016   | -3.413048  | 3.3687509 |
| H       | -1.3430151 | -3.0579146 | 2.6270164 |
| C       | 1.89528    | -2.272989  | 1.6455056 |
| H       | 2.0168954  | -1.3867937 | 2.2771903 |
| H       | 2.4659068  | -2.1043871 | 0.7211369 |
| H       | 2.3460278  | -3.1345971 | 2.1630841 |
| C       | 1.4669435  | 3.2012333  | -1.0245785 |
| C       | 2.153969   | 5.0935921  | 0.8535151 |
| N       | 1.3212684  | 2.8881706  | 0.2964955 |
| C       | 1.942795   | 4.4369304  | -1.455458 |
| C       | 2.3004699  | 5.3884723  | -0.4799793 |
| C       | 1.6099542  | 3.8257457  | 1.3082744 |
| H       | 2.0481153  | 4.6593411  | -2.5145429 |
| H       | 2.692974   | 6.35945    | -0.7895125 |
| H       | 2.4174127  | 5.8073159  | 1.6335739 |
| O       | 1.3947817  | 3.5654951  | 2.5034309 |
| C       | 0.501817   | 0.9440956  | 2.5733188 |
| O       | 0.5546821  | 0.7831398  | 3.7232176 |
| Ru      | 0.4616399  | 0.9960228  | 0.7083412 |
| H       | 1.9267074  | 0.3673909  | 0.7548379 |
| H       | -0.9467189 | 2.180961   | 0.8565257 |
| H       | -1.3034893 | 1.5479988  | 0.4777957 |
Energy = -1475.4448955
H  1.5041022  -5.1944942  -0.8767945
C  1.2869727  -4.1253091  -0.8790426
N  0.7291003  -1.3964981  -0.9154289
C  0.8151263  -3.5177242   0.2554282
C  1.4990738  -3.3709531  -2.0597208
C  1.2118501  -2.0149592  -2.0318433
C  0.523811   -2.1078225   0.2734195
H  0.6528406  -4.0878335  1.1701323
H  1.8824446  -3.8467957  -2.958598
C  0.0534529  -1.4274006  1.3854133
H -0.1353764  -1.9660304  2.3116601
P  -0.3787124   0.2766922  1.1569204
C  -2.2972314   0.3388790  1.1746303
C  -2.8805188  -0.1339870  2.5140662
H  -2.4734906  -1.1093238  2.8157996
H  -3.9733032  -0.2434870  2.417445
H  -2.6957899   0.5887001  3.3196826
C  -2.7269658  -0.6427998  0.0640726
H  -2.3763674  -0.3120679  -0.9274497
H  -3.8271738  -0.6855285  0.0221821
H  -2.3439058  -1.6562449  0.2424145
C  -2.8504858   1.7298019   0.822078
H  -2.4842014   2.0767844  -0.1523288
H  -2.6003699   2.4936564  1.5659426
H  -3.9499706   1.6702992  0.7658973
C  0.3605502   1.2129331  2.6365183
C  0.2293406   0.3998932  3.9388169
| Element | X    | Y    | Z    |
|---------|------|------|------|
| H       | 0.7730451 | -0.5514595 | 3.8734644 |
| H       | -0.8120867 | 0.1875818 | 4.207936  |
| H       | 0.672363  | 0.9813437 | 4.7633518 |
| C       | -0.2719666 | 2.6002695 | 2.8227216 |
| H       | -0.2728704 | 3.1850986 | 1.8942171 |
| H       | 0.312461  | 3.1602138 | 3.5703888 |
| H       | -1.3013917 | 2.5348995 | 3.1993486 |
| C       | 1.8615038  | 1.3791559 | 2.3262239 |
| H       | 2.0270899  | 2.080332  | 1.4989453 |
| H       | 2.3239847  | 0.4169285 | 2.0636075 |
| H       | 2.370628   | 1.7744925 | 3.220076  |
| C       | 1.4088697  | -1.1183681 | -3.1818056 |
| C       | 1.7517659  | 0.7383952  | -5.2129831 |
| N       | 1.1021087  | 0.2001441  | -2.9485886 |
| C       | 1.8763966  | -1.5348448 | -4.4275569 |
| C       | 2.0448712  | -0.5973517 | -5.4488968 |
| C       | 1.2838434  | 1.1011207  | -3.9423966 |
| H       | 2.1083004  | -2.5832073 | -4.5977146 |
| H       | 2.4093953  | -0.9124653 | -6.4268418 |
| H       | 1.8711575  | 1.5115679  | -5.9689907 |
| Ru      | 0.3722431  | 0.6492516  | -0.9860684 |
| O       | 1.0052565  | 2.3841582  | -3.6965988 |
| H       | 0.7071621  | 2.4248418  | -2.7453873 |
| H       | 1.7805082  | 0.9880353  | -0.4382291 |
| C       | 0.0251887  | 2.4553512  | -0.8346784 |
| O       | -0.1846296 | 3.5961349  | -0.6348579 |
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Energy = -1475.45404301

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | 0.9120119 | 1.1957997 | -5.1861796 |
| C       | 0.8817535 | 1.1319791 | -4.0981356 |
| N       | 0.777971  | 0.9753302 | -1.3363503 |
| C       | 0.6014572 | -0.0872836 | -3.4717763 |
| C       | 1.1291979 | 2.2611449 | -3.3260465 |
| C       | 1.0778498 | 2.1690481 | -1.9283278 |
| C       | 0.56555   | -0.142848 | -2.0807096 |
| H       | 0.4195857 | -0.9901936 | -4.0535379 |
| H       | 1.3540224 | 3.2136709 | -3.8013557 |
| C       | 0.3361536 | -1.4206866 | -1.3213596 |
| H       | 1.3119204 | -1.9168736 | -1.1919288 |
| H       | -0.3035139 | -2.1166779 | -1.8817796 |
| P       | -0.2655496 | -1.0721054 | 0.4216515 |
| C       | -2.1718386 | -1.0903946 | 0.252746 |
| C       | -2.7922538 | -2.4590881 | -0.0578142 |
| H       | -2.357739  | -2.9212592 | -0.9557746 |
| H       | -3.8713738 | -2.3334601 | -0.2444387 |
| H       | -2.687794  | -3.1611071 | 0.7789132 |
| C       | -2.510041  | -0.1225301 | -0.9013018 |
| H       | -2.0810014 | 0.877397  | -0.7409019 |
| H       | -3.6037066 | -0.0080185 | -0.9625522 |
| H       | -2.1618234 | -0.4882275 | -1.8771896 |
| C       | -2.779822  | -0.5161937 | 1.547229 |
| H       | -2.3636551 | 0.4738948  | 1.7799986 |
| H       | -2.6101559 | -1.1614014 | 2.4166607 |
| H       | -3.8685344 | -0.4077677 | 1.4183423 |
| C       | 0.3419803  | -2.5999315 | 1.3826735 |
|   | x-coordinates | y-coordinates | z-coordinates |
|---|---------------|---------------|---------------|
| C | 0.1794518     | -3.9277495    | 0.6195094     |
| H | 0.7557313     | -3.9423842    | -0.3156953    |
| H | -0.8634469    | -4.1630431    | 0.3827272     |
| H | 0.5653488     | -4.7466685    | 1.2475951     |
| C | -0.3904506    | -2.6723145    | 2.7343826     |
| H | -0.3467644    | -1.7161124    | 3.2729813     |
| H | 0.0959316     | -3.4333266    | 3.3651693     |
| H | -1.4419085    | -2.9665099    | 2.6212295     |
| C | 1.8426826     | -2.3779303    | 1.6606097     |
| H | 2.0102577     | -1.5069406    | 2.304928      |
| H | 2.4254627     | -2.2327049    | 0.7393286     |
| H | 2.243273      | -3.2691077    | 2.1694703     |
| C | 1.3164025     | 3.2764178     | -0.9898586    |
| C | 1.7631923     | 5.2595022     | 0.872896      |
| N | 1.1700065     | 2.9558687     | 0.3365917     |
| C | 1.6691905     | 4.546576      | -1.4249652    |
| C | 1.894875      | 5.5520615     | -0.4590842    |
| C | 1.3973656     | 3.9303327     | 1.3424862     |
| H | 1.7735875     | 4.7659394     | -2.4849624    |
| H | 2.1750923     | 6.5574586     | -0.7800141    |
| H | 1.9338576     | 6.0061127     | 1.6480386     |
| Ru| 0.5647669     | 0.9925625     | 0.7387346     |
| O | 1.2872751     | 3.6532679     | 2.5435845     |
| H | 1.948045      | 0.3190589     | 0.9345046     |
| C | 0.4196054     | 0.9896641     | 2.5918223     |
| O | 0.3305174     | 0.867753      | 3.7472356     |
tBuOH

Energy = -233.786168453
C  0.0058838  -0.009202  1.1341675
C  -0.7262433  -1.2685983  1.6159565
H  -0.2128871  -2.1761135  1.2609055
H  -1.7539638  -1.2792841  1.2287458
H  -0.7631432  -1.3132873  2.7142969
C  1.4620839  -0.0049546  1.616962
H  1.9853429  0.8800066  1.2301917
H  1.9914605  -0.9031148  1.2615535
H  1.5192859  0.0040821  2.7154246
C  -0.7241079  1.2541075  1.5891552
H  -0.2115429  2.1468471  1.205552
H  -0.7560219  1.3102177  2.6858795
H  -1.7532505  1.2556733  1.2056529
O  -0.0261879  0.0483643  -0.3136908
H  0.4259649  -0.7461275  -0.6486993

H₂

Energy =  -10.177530179
H  0  0  0.3754185
H  0  0  -0.3754185