

Mechanism and Kinetics for both Thermal and Electrochemical Reduction of N₂

Catalysed by Ru(0001) based on Quantum Mechanics

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William A. Goddard III,^{‡,*}

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[‡]*Materials and Process Simulation Center (139-74), California Institute of*

Technology, Pasadena, California 91125, United States

N₂TR

*vN₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N

27 2

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.000731438 | 1.558719332 | 12.070434974 |
| 1.324196048 | 0.746695684 | 14.150436942 |
| 2.695120330 | 1.562244564 | 12.074847845 |
| 4.059194680 | 0.753788483 | 14.152525163 |
| 5.391604685 | 1.557871290 | 12.071522405 |
| 6.741125009 | 0.773514261 | 14.147448526 |
| -1.358087749 | 3.897157334 | 12.088917634 |
| -0.037310843 | 3.112543164 | 14.150066878 |
| 1.353570272 | 3.887776505 | 12.076029995 |
| 2.679177024 | 3.092728066 | 14.305204625 |
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| 2.694737472 | 6.227600872 | 12.072373406 |
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| 2.459626364 | 2.917184772 | 16.267747129 |

2.269240544 2.794643829 17.377858060

*pN₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
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Ru N

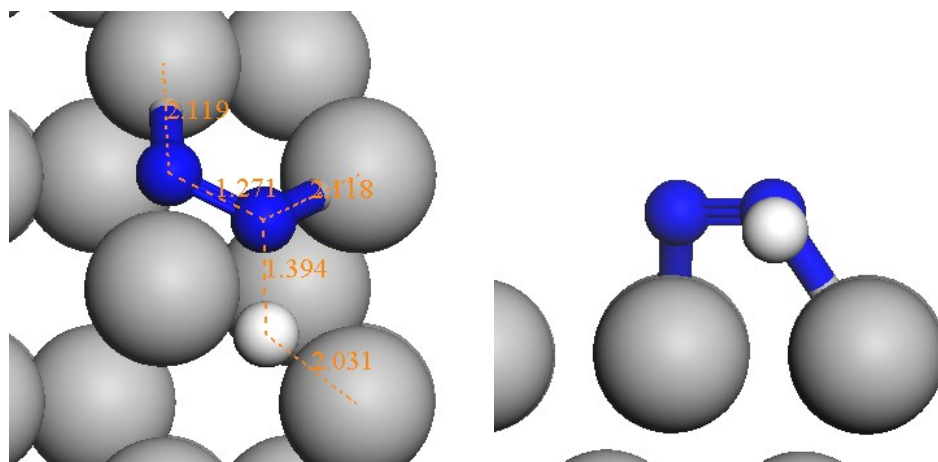
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Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
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| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.337643833 | 0.756088115 | 14.161083636 |
| 2.700444925 | 1.541849645 | 12.101236226 |
| 4.055317513 | 0.758194265 | 14.160361129 |
| 5.396382692 | 1.557977910 | 12.079985425 |
| 6.746034367 | 0.778176610 | 14.152359221 |
| -1.351123755 | 3.897216706 | 12.085680305 |
| -0.026553146 | 3.083656433 | 14.158278783 |
| 1.351306675 | 3.901838132 | 12.072370469 |
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| 4.048154214 | 3.900265183 | 12.079193164 |
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| -1.369638743 | 5.448864564 | 14.148523475 |
| -0.012678025 | 6.243016355 | 12.062346423 |
| 1.324768978 | 5.453794140 | 14.182697159 |
| 2.701234238 | 6.227609653 | 12.077538154 |
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| | 3.208971520 | 4.512247185 | 15.931891668 |
| TS *pN ₂ → *pNNH | | | |
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| | 0.0000000000 | 0.0000000000 | 69.2750015259 |
| Ru | N | | |
| 27 | 2 | | |
| Cartesian | | | |
| | 1.349986585 | 0.779415119 | 9.996419384 |
| | 4.050040625 | 0.779415119 | 9.996419384 |
| | 6.750014037 | 0.779415119 | 9.996419384 |
| | 0.000000000 | 3.117660474 | 9.996419384 |
| | 2.700054040 | 3.117660474 | 9.996419384 |
| | 5.400027452 | 3.117660474 | 9.996419384 |
| | -1.350027020 | 5.455975864 | 9.996419384 |
| | 1.350027020 | 5.455975864 | 9.996419384 |
| | 4.050000432 | 5.455975864 | 9.996419384 |
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| | 1.333455835 | 0.754504871 | 14.160933848 |
| | 2.699217110 | 1.537906089 | 12.093223304 |
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| | 5.394960672 | 1.558910620 | 12.075206895 |
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| | -0.034545861 | 3.087226718 | 14.159086463 |
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| | 2.688722779 | 3.107352266 | 14.190174809 |
| | 4.047717282 | 3.899974175 | 12.074042367 |
| | 5.410140614 | 3.078685464 | 14.173062268 |
| | -2.691418057 | 6.245749991 | 12.069434919 |
| | -1.354771231 | 5.455657260 | 14.155752947 |
| | -0.009648952 | 6.240246761 | 12.071338841 |
| | 1.345643459 | 5.455443604 | 14.218821023 |
| | 2.695434873 | 6.235302133 | 12.073584926 |
| | 4.053803912 | 5.471671066 | 14.191326120 |
| | 4.045406130 | 3.256321214 | 15.666781651 |

| | | |
|-------------|-------------|--------------|
| 2.063520106 | 4.348252437 | 15.877047244 |
| 3.331800794 | 4.433012297 | 15.889815934 |



*pNNH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
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| 27 | 1 | 2 |
|----|---|---|

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
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| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.341019283 | 0.750187519 | 14.161521252 |
| 2.696812415 | 1.544289242 | 12.097175063 |
| 4.068919039 | 0.754361562 | 14.160245117 |
| 5.395437977 | 1.555268315 | 12.075341264 |
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| -0.022784669 | 3.090477562 | 14.161641670 |

| | | |
|--------------|-------------|--------------|
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| 2.714069052 | 3.100608280 | 14.235388747 |
| 4.047432673 | 3.899755501 | 12.077154139 |
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| -2.695645433 | 6.246619671 | 12.074524038 |
| -1.353976546 | 5.452782301 | 14.149417797 |
| -0.010848463 | 6.247333811 | 12.053389984 |
| 1.363454105 | 5.449175641 | 14.198492447 |
| 2.698069741 | 6.232634141 | 12.068257908 |
| 4.071436406 | 5.444099307 | 14.204523615 |
| 3.689159403 | 3.986784889 | 16.692959923 |
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TS *pNNH → *HNNH

1.0

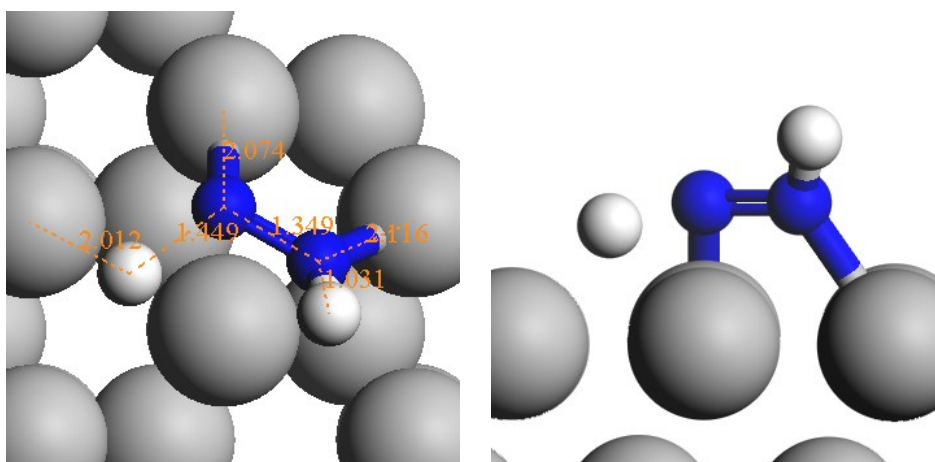
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| Ru | H | N |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
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| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.346492307 | 0.756014109 | 14.163625626 |
| 2.699464121 | 1.550931522 | 12.100919028 |
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| 5.397572607 | 1.550764067 | 12.076691558 |
| 6.752551984 | 0.786807601 | 14.145677503 |
| -1.349504572 | 3.909199047 | 12.075600456 |

| | | |
|--------------|-------------|--------------|
| -0.025623640 | 3.074614278 | 14.158079066 |
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| 4.051432893 | 3.903610940 | 12.076329571 |
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| 1.359287079 | 5.460937217 | 14.197919728 |
| 2.700339132 | 6.231753173 | 12.071475412 |
| 4.080080415 | 5.455538098 | 14.208933549 |
| 1.363411378 | 3.142159088 | 15.612794837 |
| 3.740558765 | 3.945646970 | 16.691858541 |
| 1.958756155 | 4.432652718 | 15.895905843 |
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TS *pNNH → *NNH₂

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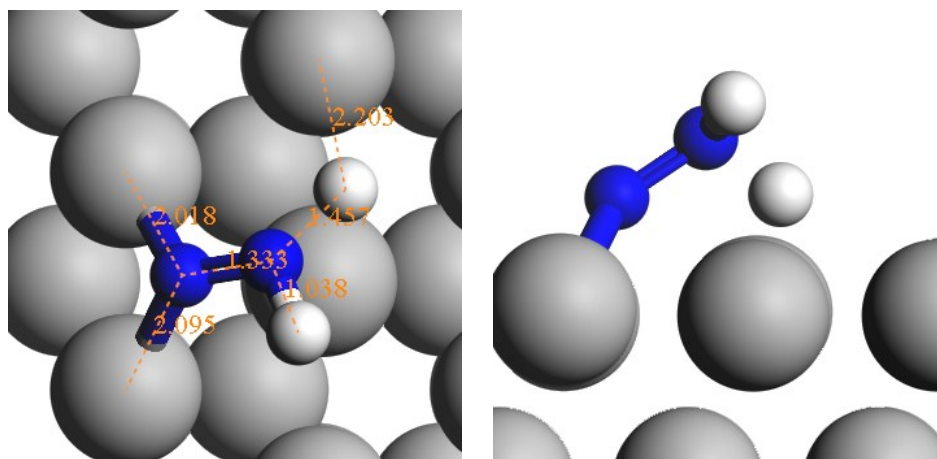
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.000971087 | 1.556029807 | 12.074035025 |
| 1.337760308 | 0.765546714 | 14.226392658 |
| 2.689948662 | 1.553508783 | 12.073231750 |
| 4.084534344 | 0.762197560 | 14.150287154 |
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*HNNH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
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| Ru | H | N |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.315681731 | 0.779062700 | 14.201300237 |
| 2.696905837 | 1.555591309 | 12.074052647 |
| 4.068110775 | 0.751284340 | 14.161513909 |
| 5.396414737 | 1.560870952 | 12.082697028 |
| 6.714841475 | 0.749981127 | 14.148289982 |
| -1.356584438 | 3.902854988 | 12.079405364 |
| 0.005015061 | 3.067484789 | 14.203771738 |
| 1.351588629 | 3.887934553 | 12.071390973 |
| 2.729044590 | 3.107772890 | 14.190267325 |
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| 1.339577106 | 5.467343993 | 14.163374511 |
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| 4.046377036 | 5.450726012 | 14.156193500 |
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| | | |
|-------------|-------------|--------------|
| 0.948826763 | 2.111661088 | 15.863937860 |
| 2.151516736 | 2.761917339 | 16.116130867 |

*pNNH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
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| 0.000000000 | 3.117660474 | 9.996419384 |
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| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 4.086418372 | 0.758674261 | 14.146300151 |
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| -1.334222760 | 5.471192742 | 14.153369556 |
| 0.000028726 | 6.236175575 | 12.081419424 |
| 1.350989235 | 5.498988193 | 14.142289652 |
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| | | |
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TS *HNNH → *HNNH₂

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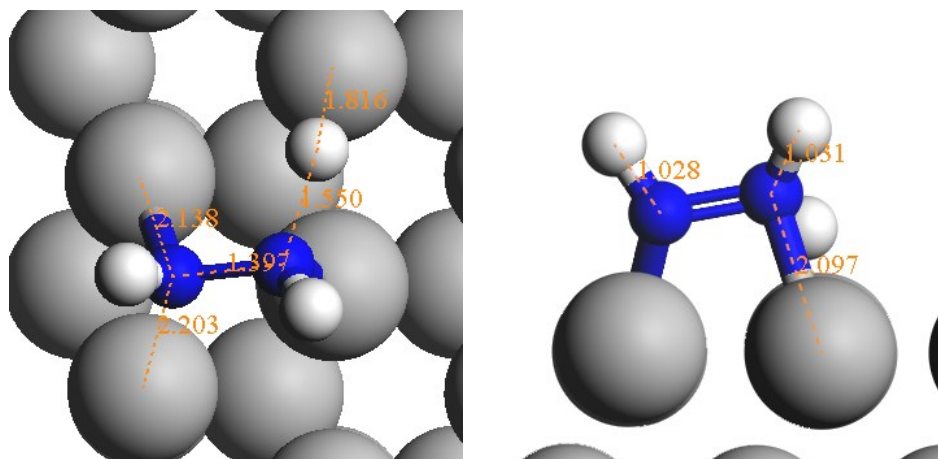
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Ru H N

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|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
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| 5.400027452 | 3.117660474 | 9.996419384 |
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| 1.350027020 | 5.455975864 | 9.996419384 |
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| | | |
|-------------|-------------|--------------|
| 4.060412205 | 5.459100438 | 14.165119100 |
| 1.717555520 | 4.463908070 | 15.700451637 |
| 2.644879563 | 2.705869647 | 16.918699201 |
| 0.440281278 | 1.938862301 | 16.736048928 |
| 0.947895326 | 2.207690611 | 15.883654069 |
| 2.062368271 | 3.014253729 | 16.125683522 |



TS *NNH₂ → *HNNH₂

1.0

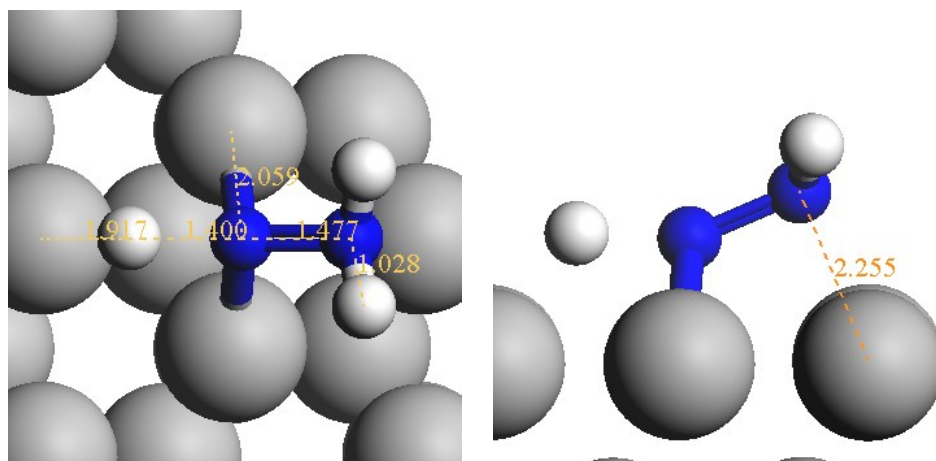
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 3 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.010356372 | 1.561499588 | 12.074090828 |
| 1.366942620 | 0.783391079 | 14.167208789 |
| 2.706323529 | 1.539754784 | 12.073757476 |

| | | |
|--------------|-------------|--------------|
| 4.073389896 | 0.793368924 | 14.163671150 |
| 5.401960936 | 1.560258309 | 12.084683187 |
| 6.760938088 | 0.822754779 | 14.155429875 |
| -1.342708833 | 3.904986120 | 12.074372047 |
| 0.001385267 | 3.119536347 | 14.215436109 |
| 1.349704994 | 3.897055732 | 12.060582009 |
| 2.716174653 | 3.144582901 | 14.164914977 |
| 4.057558388 | 3.901300854 | 12.079606549 |
| 5.442261745 | 3.106359452 | 14.155682458 |
| -2.693394570 | 6.239451925 | 12.100365400 |
| -1.338672102 | 5.469443767 | 14.167151517 |
| -0.013872949 | 6.250909531 | 12.073382272 |
| 1.380865478 | 5.457304215 | 14.163721079 |
| 2.707264622 | 6.240253869 | 12.079494209 |
| 4.073551060 | 5.470426337 | 14.222951941 |
| 3.891288431 | 4.395779154 | 16.876105083 |
| 3.043303371 | 5.860968350 | 16.868881485 |
| 0.945667577 | 3.672480298 | 15.789628343 |
| 2.159895206 | 4.366572565 | 15.726401668 |
| 3.333218046 | 5.047935320 | 16.310123907 |



*HNNH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |
| Ru | H | N |

27 3 2

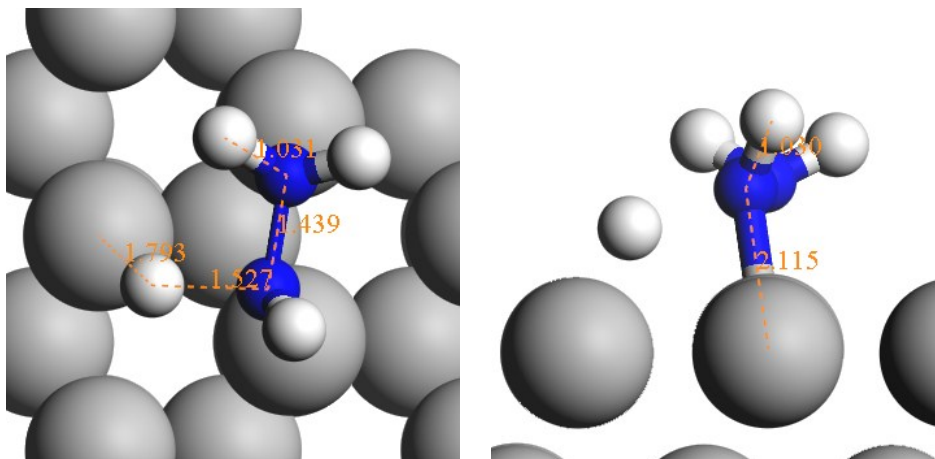
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|--------------|-------------|--------------|
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| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.004996533 | 1.557603906 | 12.065138060 |
| 1.310438820 | 0.807507849 | 14.196504085 |
| 2.690728260 | 1.561325652 | 12.073059200 |
| 4.057328727 | 0.762051167 | 14.152943688 |
| 5.391508125 | 1.565051161 | 12.077473539 |
| 6.699752509 | 0.753305299 | 14.140903379 |
| -1.363446139 | 3.908418008 | 12.083909282 |
| -0.005433043 | 3.076977673 | 14.187189329 |
| 1.344071952 | 3.891666229 | 12.071512859 |
| 2.716342546 | 3.134763260 | 14.180730824 |
| 4.057030449 | 3.903905293 | 12.085839638 |
| 5.395799834 | 3.108895529 | 14.162193829 |
| -2.698854167 | 6.224515602 | 12.086065788 |
| -1.345906100 | 5.462186963 | 14.168493735 |
| -0.011159143 | 6.231389831 | 12.083341703 |
| 1.332899049 | 5.477931502 | 14.150112402 |
| 2.699594658 | 6.228028604 | 12.076919177 |
| 4.038409185 | 5.464543459 | 14.162480189 |
| 1.818279179 | 3.669459835 | 16.771730772 |
| 2.683352259 | 2.214492925 | 16.840559811 |
| 0.309870875 | 1.773572860 | 16.670441799 |
| 0.871782518 | 2.084515179 | 15.867779481 |
| 2.058731115 | 2.799368529 | 16.271954409 |

TS HNNH₂ → H₂NNH₂

1.0

| | | |
|---------------|--------------|--------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |

| | 0.0000000000 | 0.0000000000 | 69.2750015259 |
|--------------|--------------|--------------|---------------|
| Ru | H | N | |
| 27 | 4 | 2 | |
| 1.349986585 | 0.779415119 | 9.996419384 | |
| 4.050040625 | 0.779415119 | 9.996419384 | |
| 6.750014037 | 0.779415119 | 9.996419384 | |
| 0.000000000 | 3.117660474 | 9.996419384 | |
| 2.700054040 | 3.117660474 | 9.996419384 | |
| 5.400027452 | 3.117660474 | 9.996419384 | |
| -1.350027020 | 5.455975864 | 9.996419384 | |
| 1.350027020 | 5.455975864 | 9.996419384 | |
| 4.050000432 | 5.455975864 | 9.996419384 | |
| 0.006350298 | 1.557588854 | 12.072421133 | |
| 1.353543537 | 0.763882877 | 14.160111483 | |
| 2.704431083 | 1.564021971 | 12.084480532 | |
| 4.066744186 | 0.787966877 | 14.162823820 | |
| 5.403012409 | 1.560461617 | 12.073374930 | |
| 6.754512927 | 0.786856416 | 14.155805813 | |
| -1.350780426 | 3.908091460 | 12.048647433 | |
| -0.008053065 | 3.073305160 | 14.166771173 | |
| 1.351245360 | 3.896628419 | 12.076701838 | |
| 2.716072300 | 3.147049779 | 14.205329827 | |
| 4.054687190 | 3.894787458 | 12.081146282 | |
| 5.420478760 | 3.111572719 | 14.158681155 | |
| -2.686013258 | 6.241013584 | 12.099928518 | |
| -1.345301759 | 5.451086845 | 14.155095054 | |
| 0.006153980 | 6.239806486 | 12.086045964 | |
| 1.368092342 | 5.461607037 | 14.202381060 | |
| 2.699488684 | 6.235588542 | 12.078826037 | |
| 4.101718682 | 5.479709745 | 14.142270561 | |
| 0.745690378 | 4.916012503 | 16.800607542 | |
| 2.685942347 | 3.283786772 | 17.042839650 | |
| 0.880619405 | 2.873389105 | 15.711687203 | |
| 2.318040161 | 5.535173540 | 16.747588476 | |
| 1.647298566 | 4.898803307 | 16.300950128 | |
| 2.154858661 | 3.555809063 | 16.203573265 | |



*H₂NNH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 4 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.010507789 | 1.556751056 | 12.074840502 |
| 1.351613402 | 0.775464088 | 14.154434225 |
| 2.709276138 | 1.559483437 | 12.084211061 |
| 4.069116171 | 0.786281038 | 14.168088426 |
| 5.404077943 | 1.560394719 | 12.078762891 |
| 6.758689579 | 0.788478755 | 14.161137971 |
| -1.342768821 | 3.904207590 | 12.076585091 |
| -0.030454513 | 3.092589461 | 14.136627079 |
| 1.358617438 | 3.900877722 | 12.071949741 |
| 2.711786505 | 3.127568964 | 14.193169100 |

| | | |
|--------------|-------------|--------------|
| 4.053413570 | 3.892468592 | 12.073428530 |
| 5.421386058 | 3.118748200 | 14.163044096 |
| -2.685634322 | 6.241018602 | 12.083081043 |
| -1.349481941 | 5.454652948 | 14.159227440 |
| 0.011358297 | 6.236918984 | 12.090511701 |
| 1.367952089 | 5.441328040 | 14.215005836 |
| 2.695559676 | 6.232579786 | 12.077921435 |
| 4.104929044 | 5.483229019 | 14.135766533 |
| 0.791204919 | 4.701765764 | 16.823197624 |
| 3.355241826 | 3.732196741 | 16.790621678 |
| 1.908307904 | 2.864968059 | 16.774864571 |
| 2.220342437 | 5.591249036 | 16.859682742 |
| 1.687128164 | 4.870752388 | 16.348714868 |
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TS *pN₂ Cleavage

1.0

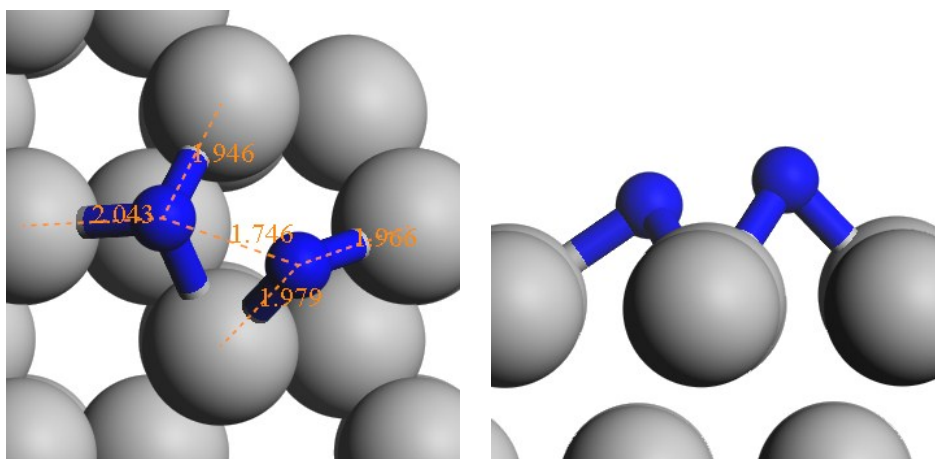
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | |
|----|---|
| Ru | N |
| 27 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.000701384 | 1.571708912 | 12.091421443 |
| 1.336336930 | 0.726072840 | 14.140725689 |
| 2.686798227 | 1.547282109 | 12.051251834 |
| 4.018379962 | 0.776611657 | 14.148113760 |
| 5.398576585 | 1.563844795 | 12.078542614 |
| 6.762116809 | 0.826502397 | 14.160452177 |

| | | |
|--------------|-------------|--------------|
| -1.346162526 | 3.894746901 | 12.100179633 |
| -0.002118999 | 3.128575994 | 14.226499859 |
| 1.355072738 | 3.899862120 | 12.046747181 |
| 2.776163467 | 3.063385381 | 14.239703228 |
| 4.047023260 | 3.891909991 | 12.101795728 |
| 5.455382375 | 3.107511568 | 14.164202750 |
| -2.717963358 | 6.233957057 | 12.056235221 |
| -1.417268179 | 5.481630148 | 14.143985780 |
| -0.009670920 | 6.244082549 | 12.083766103 |
| 1.332550952 | 5.586107058 | 14.191609543 |
| 2.711528691 | 6.249428985 | 12.092415623 |
| 4.015562959 | 5.445528006 | 14.315359368 |
| 3.097190830 | 4.375768587 | 15.686057307 |
| 1.409206665 | 4.048496995 | 15.382119899 |



*N + *N

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N

27 2

Cartesian

| | | |
|--------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.0000000000 | 3.117660474 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.015754532 | 1.549500523 | 12.082230042 |
| 1.358005522 | 0.726804071 | 14.164098486 |
| 2.699284641 | 1.579944732 | 12.109824069 |
| 4.039429487 | 0.726804071 | 14.164098486 |
| 5.414323754 | 1.549500523 | 12.082230042 |
| 6.748839451 | 0.763491521 | 14.183808820 |
| -1.350755984 | 3.875259396 | 12.110810173 |
| -0.055323058 | 3.084129740 | 14.209924793 |
| 1.341076676 | 3.879538385 | 12.062027757 |
| 2.698191165 | 3.117941029 | 14.289750031 |
| 4.057452172 | 3.879468560 | 12.062027757 |
| 5.452677259 | 3.084129740 | 14.209432842 |
| -2.704185037 | 6.239108652 | 12.083216146 |
| -1.351080122 | 5.517285325 | 14.148824519 |
| 0.002875543 | 6.239038827 | 12.083216146 |
| 1.317667508 | 5.524931394 | 14.210418212 |
| 2.699163278 | 6.243177330 | 12.094056683 |
| 4.079929541 | 5.525071881 | 14.209924793 |
| 4.168786516 | 3.943092705 | 15.322062267 |
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TS *pNNH Cleavage

1.0

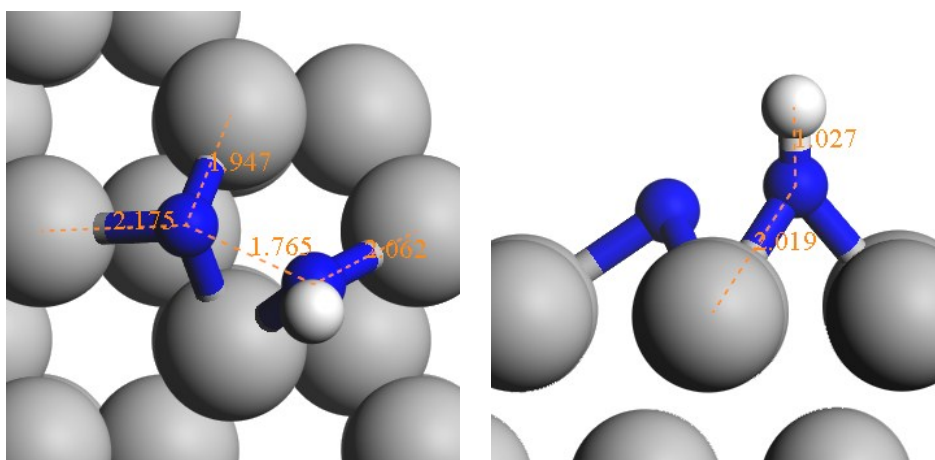
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| Ru | H | N |
|----|---|---|
| 27 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.0000000000 | 3.117660474 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.002225516 | 1.572828519 | 12.089535876 |
| 1.334742582 | 0.729747914 | 14.156017278 |
| 2.687534614 | 1.542632043 | 12.065760708 |
| 4.049394461 | 0.747483151 | 14.149184304 |
| 5.396508702 | 1.565153600 | 12.077783395 |
| 6.760030731 | 0.829923257 | 14.162748926 |
| -1.340211321 | 3.896231209 | 12.104720999 |
| 0.023975007 | 3.128710836 | 14.225078342 |
| 1.351351575 | 3.898540459 | 12.049784059 |
| 2.763934444 | 3.084927921 | 14.189746004 |
| 4.060446001 | 3.903601323 | 12.091159314 |
| 5.437643423 | 3.106482169 | 14.165343782 |
| -2.711023504 | 6.238540852 | 12.078128495 |
| -1.383266069 | 5.481240046 | 14.152582435 |
| -0.009515459 | 6.249498393 | 12.068978212 |
| 1.338573853 | 5.548096221 | 14.177610242 |
| 2.706035420 | 6.255717435 | 12.085294087 |
| 4.045156282 | 5.451942308 | 14.274549490 |
| 3.423894203 | 3.945580071 | 16.730129367 |
| 1.544061221 | 4.087759668 | 15.449364417 |
| 3.274329286 | 4.246780101 | 15.759691309 |



*N + *NH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.009128738 | 1.557804078 | 12.077578538 |
| 1.344692860 | 0.730123486 | 14.155550292 |
| 2.696229256 | 1.574170564 | 12.096555352 |
| 4.038144280 | 0.747978252 | 14.161383212 |
| 5.409053535 | 1.555802353 | 12.073530592 |
| 6.757031833 | 0.791052357 | 14.172223749 |
| -1.347104344 | 3.880133781 | 12.099967433 |
| -0.053890477 | 3.090027670 | 14.217663838 |
| 1.336391124 | 3.895067177 | 12.052265106 |
| 2.710825496 | 3.116997762 | 14.267104147 |
| 4.054437584 | 3.889881296 | 12.073627513 |
| 5.412755084 | 3.115588087 | 14.199398517 |
| -2.704532471 | 6.244612718 | 12.078785653 |
| -1.362764429 | 5.517147765 | 14.146620286 |
| 0.005660320 | 6.245735357 | 12.084760284 |
| 1.324285456 | 5.531878375 | 14.211827981 |
| 2.697146874 | 6.249899365 | 12.101283218 |
| 4.081930013 | 5.514943044 | 14.223236831 |
| 4.099554058 | 3.931365833 | 16.516597809 |
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TS *HNNH Cleavage

1.0

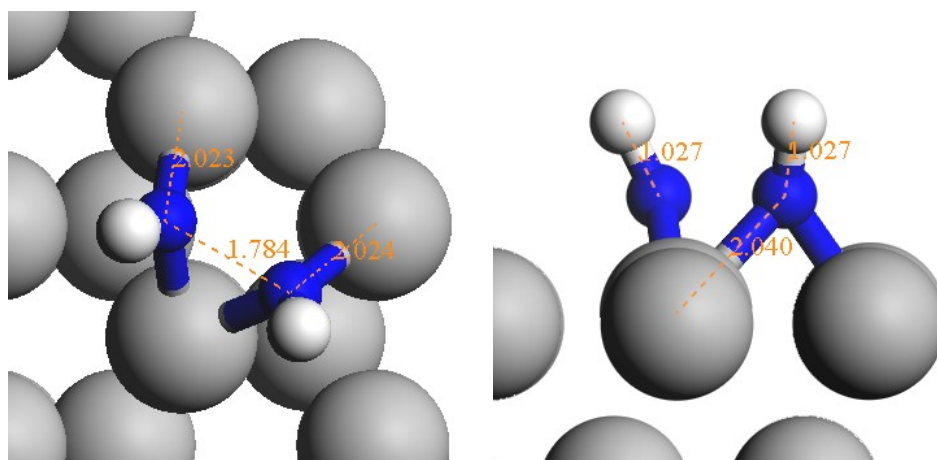
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.004760445 | 1.561218510 | 12.077579272 |
| 1.333466759 | 0.749888985 | 14.148350190 |
| 2.699409565 | 1.561464675 | 12.082459129 |
| 4.064383608 | 0.749939629 | 14.147874393 |
| 5.393868523 | 1.561425268 | 12.077862694 |
| 6.749116366 | 0.817556669 | 14.155563509 |
| -1.350861656 | 3.902866695 | 12.085970335 |
| -0.018966464 | 3.110452798 | 14.159459465 |
| 1.352257304 | 3.900306577 | 12.070316759 |
| 2.698992247 | 3.092531970 | 14.275941637 |
| 4.046709201 | 3.900427412 | 12.070897554 |
| 5.417229291 | 3.110682552 | 14.159271495 |
| -2.698356764 | 6.246919459 | 12.067670504 |
| -1.351196838 | 5.474968739 | 14.146699586 |
| -0.003105837 | 6.247566283 | 12.067580925 |
| 1.321650588 | 5.487222436 | 14.211626795 |
| 2.699452956 | 6.249426477 | 12.086963048 |
| 4.075021903 | 5.486603626 | 14.214092423 |
| 1.476877032 | 3.890396832 | 16.632831802 |
| 3.907971021 | 3.893594576 | 16.637290197 |

| | | |
|-------------|-------------|--------------|
| 1.801992966 | 4.223854854 | 15.717255791 |
| 3.586372267 | 4.226783750 | 15.720473295 |



*NH + *NH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.009051128 | 1.549219131 | 12.065653507 |
| 1.345296568 | 0.723984982 | 14.153332843 |
| 2.698165033 | 1.565839622 | 12.094465663 |
| 4.048147998 | 0.723749061 | 14.154144929 |
| 5.404894475 | 1.549789440 | 12.066044130 |
| 6.746107480 | 0.785138695 | 14.156009936 |
| -1.352528153 | 3.873591953 | 12.081499458 |

| | | |
|--------------|-------------|--------------|
| -0.031046423 | 3.083193998 | 14.189631460 |
| 1.339955619 | 3.883554798 | 12.065491971 |
| 2.694432102 | 3.101467297 | 14.277423363 |
| 4.055868113 | 3.883548526 | 12.064141676 |
| 5.420379304 | 3.086376272 | 14.191436259 |
| -2.707364018 | 6.236288048 | 12.075640840 |
| -1.353562306 | 5.492223510 | 14.142379231 |
| 0.004388631 | 6.235731119 | 12.077013896 |
| 1.316040238 | 5.498699275 | 14.213936761 |
| 2.696952789 | 6.243086599 | 12.094764504 |
| 4.075058596 | 5.502258689 | 14.208804320 |
| 1.222963853 | 3.890896898 | 16.502357672 |
| 4.144709156 | 3.931213639 | 16.496972648 |
| 1.247484904 | 3.898501992 | 15.475757938 |
| 4.137198515 | 3.907652439 | 15.473531678 |

TS *pNNH₂ Cleavage

1.0

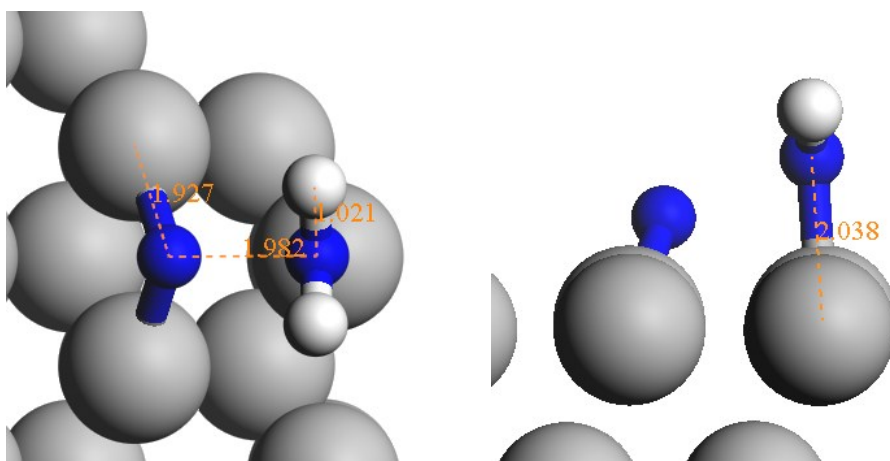
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.007835202 | 1.559231941 | 12.075570351 |
| 1.364500901 | 0.811485430 | 14.147301675 |
| 2.703483532 | 1.553351780 | 12.061977093 |
| 4.061461716 | 0.786099889 | 14.149817231 |
| 5.398533133 | 1.558273830 | 12.081491381 |
| 6.748867333 | 0.831289918 | 14.144092981 |

| | | |
|--------------|-------------|--------------|
| -1.345927102 | 3.903792401 | 12.075679021 |
| -0.031734048 | 3.099640971 | 14.155168480 |
| 1.363194119 | 3.904829745 | 12.069832885 |
| 2.722015418 | 3.101110018 | 14.252093043 |
| 4.035425737 | 3.906688266 | 12.084683187 |
| 5.443855581 | 3.092022079 | 14.144479199 |
| -2.694736627 | 6.238487751 | 12.084438680 |
| -1.315269693 | 5.452383838 | 14.147200347 |
| -0.003299681 | 6.241408285 | 12.061538743 |
| 1.346210504 | 5.483412572 | 14.251758223 |
| 2.700932248 | 6.218191612 | 12.084610496 |
| 4.103198215 | 5.487721247 | 14.257212267 |
| 3.530849090 | 6.149928062 | 16.853356403 |
| 4.393463160 | 4.686610767 | 16.861668166 |
| 2.402072540 | 4.505159717 | 15.532830091 |
| 3.983421913 | 5.427566202 | 16.291237407 |



*N + *NH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.016275109 | 1.551929562 | 12.081712392 |
| 1.343265107 | 0.728927468 | 14.154567860 |
| 2.697467512 | 1.554233794 | 12.096034765 |
| 4.043667274 | 0.777910636 | 14.156622304 |
| 5.384863381 | 1.552613076 | 12.074069534 |
| 6.714803122 | 0.798524648 | 14.148071174 |
| -1.365168218 | 3.887953786 | 12.082824054 |
| -0.050414454 | 3.090250944 | 14.205127172 |
| 1.338279346 | 3.891436684 | 12.043244786 |
| 2.713050469 | 3.085565965 | 14.203900967 |
| 4.038591200 | 3.901326777 | 12.088236980 |
| 5.396230490 | 3.085733629 | 14.152272579 |
| -2.701148602 | 6.235112727 | 12.067222609 |
| -1.399396459 | 5.476968583 | 14.153420954 |
| -0.006393931 | 6.238039532 | 12.095036913 |
| 1.325202530 | 5.486563487 | 14.203218110 |
| 2.697329371 | 6.225381100 | 12.087353671 |
| 4.076539336 | 5.477936938 | 14.225106244 |
| 3.498027299 | 6.190315883 | 16.727358289 |
| 4.375636581 | 4.749101821 | 16.767212168 |
| 1.311840381 | 3.877534360 | 15.298062417 |
| 4.090408181 | 5.546264459 | 16.197850483 |

TS *HNNH₂ Cleavage

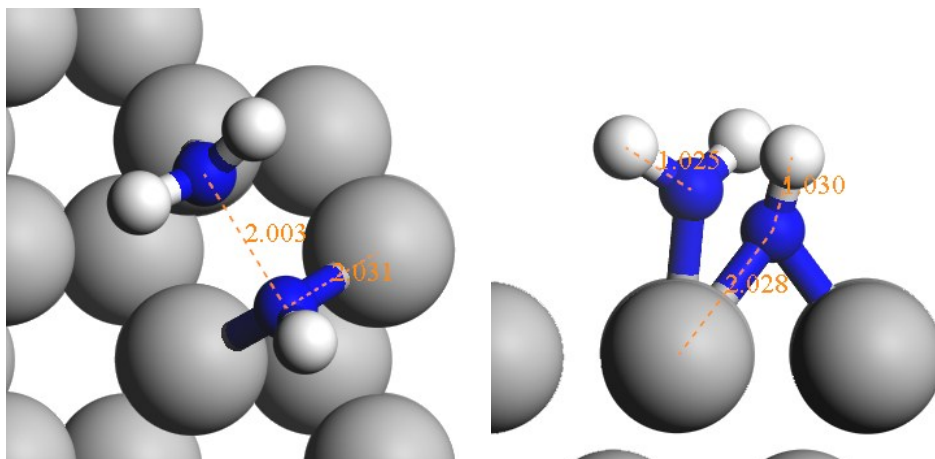
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| | | |
|---------------|--------------|---------------|
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | N | H |
| 27 | 2 | 3 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003361479 | 1.553428818 | 12.081244672 |
| 1.331761518 | 0.784886676 | 14.154736738 |
| 2.694384124 | 1.542555841 | 12.075824403 |
| 4.046962669 | 0.774925608 | 14.159665056 |
| 5.395734053 | 1.552516909 | 12.081737357 |
| 6.754063654 | 0.801441575 | 14.149316470 |
| -1.348812120 | 3.900933749 | 12.080751987 |
| -0.022518044 | 3.092126608 | 14.145866941 |
| 1.354117523 | 3.900302395 | 12.073360979 |
| 2.721519223 | 3.121308110 | 14.193172037 |
| 4.051903620 | 3.894550387 | 12.060549702 |
| 5.421006217 | 3.102508404 | 14.170997544 |
| -2.692602179 | 6.243598371 | 12.077795877 |
| -1.352497495 | 5.455905621 | 14.159665056 |
| -0.011542485 | 6.240020561 | 12.081244672 |
| 1.326699203 | 5.460325096 | 14.207954053 |
| 2.697219293 | 6.226903038 | 12.073853664 |
| 4.049716789 | 5.427986826 | 14.201054996 |
| 3.406535938 | 4.255321773 | 15.729072887 |
| 1.704523605 | 5.182608915 | 16.233156388 |
| 3.825589810 | 4.009452577 | 16.636718947 |
| 1.181992437 | 4.472430091 | 16.754979484 |
| 1.958823022 | 5.971143331 | 16.836282043 |



*NH + *NH₂

1.0

| | | |
|--------------|--------------|---------------|
| 8.100003815 | 0.000000000 | 0.000000000 |
| -4.050001907 | 7.0148061010 | 0.000000000 |
| 0.000000000 | 0.000000000 | 69.2750015259 |

| Ru | N | H |
|----|---|---|
| 27 | 2 | 3 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.008233571 | 1.566442439 | 12.079061732 |
| 1.352173448 | 0.754521752 | 14.150914208 |
| 2.715467716 | 1.555750611 | 12.073222939 |
| 4.053393443 | 0.798970724 | 14.159380165 |
| 5.408334408 | 1.558987135 | 12.071302863 |
| 6.757950778 | 0.817891683 | 14.169136942 |
| -1.363335458 | 3.885074228 | 12.082184518 |
| -0.001424012 | 3.121243302 | 14.202942030 |
| 1.347593720 | 3.911025791 | 12.061836116 |
| 2.663779763 | 3.103956754 | 14.164986934 |

| | | |
|--------------|-------------|--------------|
| 4.060418240 | 3.896442776 | 12.082481157 |
| 5.377987619 | 3.162741009 | 14.222794810 |
| -2.707387434 | 6.241867793 | 12.071839603 |
| -1.334456554 | 5.523584227 | 14.121765763 |
| 0.013891295 | 6.252874671 | 12.093279841 |
| 1.354405994 | 5.495452612 | 14.211055545 |
| 2.697818204 | 6.259774824 | 12.093789414 |
| 4.106012442 | 5.462032260 | 14.197288269 |
| 4.800109133 | 4.360088855 | 15.892078907 |
| 1.347368253 | 3.911320563 | 15.496054208 |
| 4.057672811 | 3.950348255 | 16.470913947 |
| 1.323315999 | 3.920135682 | 16.520062022 |
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TS *H₂NNH₂ Cleavage

1.0

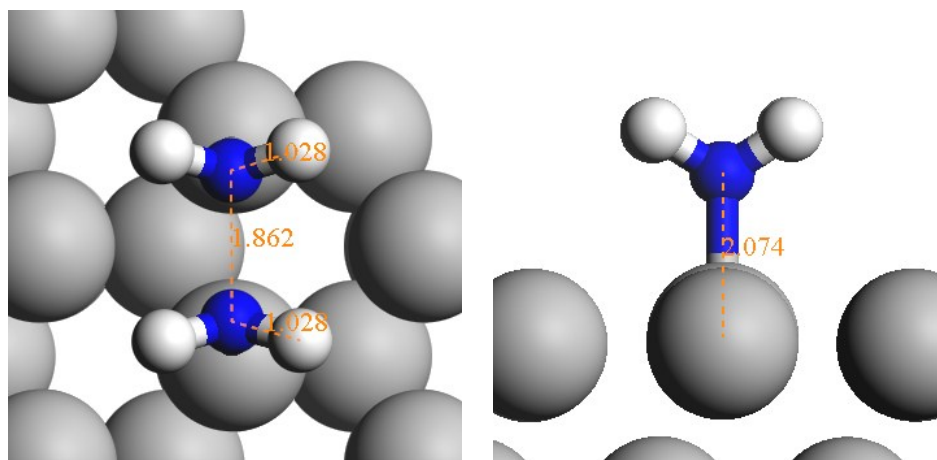
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 4 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.011767348 | 1.559028528 | 12.078589607 |
| 1.345823693 | 0.776957177 | 14.153692628 |
| 2.711598335 | 1.562786650 | 12.085054720 |
| 4.061038906 | 0.785401428 | 14.162936895 |
| 5.402895873 | 1.559914200 | 12.072837455 |
| 6.763371932 | 0.793823624 | 14.154453316 |
| -1.343396398 | 3.906258026 | 12.078412651 |

| | | |
|--------------|-------------|--------------|
| -0.026355079 | 3.101434057 | 14.132158405 |
| 1.360304333 | 3.902690668 | 12.057095033 |
| 2.711001838 | 3.130748520 | 14.234466523 |
| 4.045189112 | 3.889802691 | 12.076943408 |
| 5.420021068 | 3.120794664 | 14.154723522 |
| -2.689787046 | 6.240631009 | 12.086369770 |
| -1.354039189 | 5.452736727 | 14.153438576 |
| 0.008911479 | 6.243119212 | 12.084538539 |
| 1.365875577 | 5.458714099 | 14.232253480 |
| 2.691969110 | 6.234080819 | 12.076397122 |
| 4.097963964 | 5.483090623 | 14.139345290 |
| 0.704058013 | 4.870705559 | 16.789275054 |
| 3.347910061 | 3.711851263 | 16.803955744 |
| 1.893850167 | 2.858424768 | 16.804293501 |
| 2.154359448 | 5.729510477 | 16.813445252 |
| 1.558752512 | 5.096809203 | 16.264371026 |
| 2.500647508 | 3.490469392 | 16.265860094 |



*NH₂ + *NH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |
| Ru | H | N |
| 27 | 4 | 2 |
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.016750906 | 1.575971594 | 12.082651504 |
| 1.330333191 | 0.752705356 | 14.138144050 |
| 2.722360437 | 1.580814830 | 12.066992053 |
| 4.071703997 | 0.802468727 | 14.439132690 |
| 5.368599136 | 1.543506949 | 12.099185452 |
| 6.827074365 | 0.822476733 | 14.136442047 |
| -1.329039565 | 3.906511403 | 12.082785138 |
| 0.012372655 | 3.129029022 | 14.151638183 |
| 1.369871210 | 3.911852823 | 12.074737706 |
| 2.748642553 | 3.100964723 | 14.190180683 |
| 4.054561421 | 3.903777349 | 12.071150872 |
| 5.472459531 | 3.169899974 | 14.136891411 |
| -2.685868721 | 6.246011313 | 12.081711658 |
| -1.385842518 | 5.458536818 | 14.137983982 |
| 0.027666719 | 6.247783285 | 12.065419279 |
| 1.353265868 | 5.517123096 | 14.192192541 |
| 2.705411645 | 6.239612481 | 12.071182445 |
| 4.069067801 | 5.471474970 | 14.151227000 |
| 0.108429109 | 6.124838652 | 16.561970346 |
| 4.075524978 | 2.567626395 | 16.518053101 |
| 2.635320712 | 1.731809545 | 16.558639766 |
| 1.551593106 | 6.955207567 | 16.510898523 |
| 0.809946641 | 6.533358356 | 15.937494032 |
| 3.350310410 | 2.129628954 | 15.939219530 |

*N

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N

27 1

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.011299517 | 1.561285408 | 12.090607154 |
| 1.349986525 | 0.718666873 | 14.154244787 |
| 2.711272567 | 1.561285408 | 12.090607154 |
| 4.051012829 | 0.779836004 | 14.167548015 |
| 5.399986595 | 1.558760098 | 12.077795877 |
| 6.748879795 | 0.779836004 | 14.168041434 |
| -1.353429174 | 3.885922165 | 12.090607154 |
| -0.039689950 | 3.094651813 | 14.215838481 |
| 1.349945910 | 3.897005558 | 12.050694535 |
| 2.739501383 | 3.094651813 | 14.215838481 |
| 4.053402224 | 3.885922165 | 12.090607154 |
| 5.399946221 | 3.116257489 | 14.168041434 |
| -2.700013605 | 6.235250705 | 12.075331718 |
| -1.402555524 | 5.486069275 | 14.154244787 |
| 0.007857049 | 6.243738440 | 12.090607154 |
| 1.349986706 | 5.501361832 | 14.215838481 |
| 2.692116363 | 6.243738440 | 12.090607154 |
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TS *N → *NH

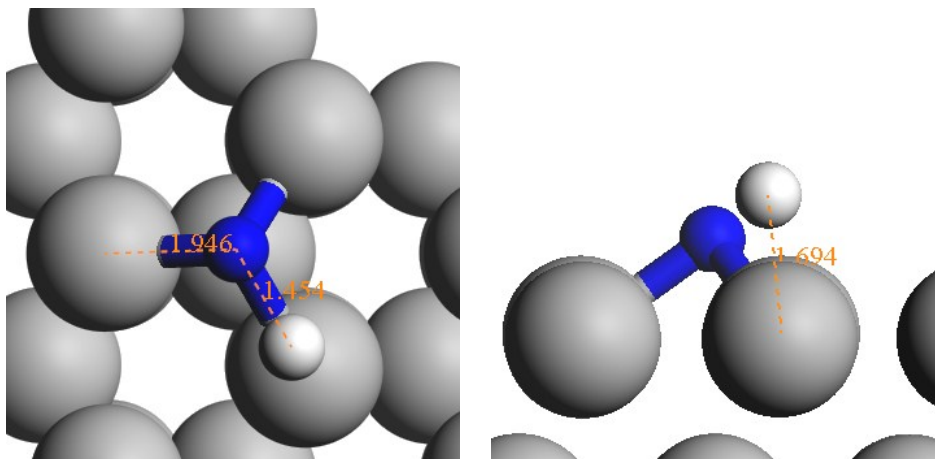
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| | | |
|---------------|--------------|---------------|
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | N | H |
| 27 | 1 | 1 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.006159291 | 1.560668584 | 12.090275271 |
| 1.358387385 | 0.724213482 | 14.156244897 |
| 2.702863318 | 1.568720539 | 12.087273637 |
| 4.065095070 | 0.761684794 | 14.162859064 |
| 5.402422551 | 1.557057952 | 12.075427906 |
| 6.758224585 | 0.773811384 | 14.170774330 |
| -1.347607178 | 3.885976938 | 12.094928977 |
| -0.038244453 | 3.087837793 | 14.227679073 |
| 1.338547299 | 3.903404391 | 12.020160551 |
| 2.746838580 | 3.089421821 | 14.224101783 |
| 4.042406508 | 3.889150013 | 12.086971859 |
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| -2.700305819 | 6.235125270 | 12.080721882 |
| -1.395145063 | 5.481343321 | 14.149818700 |
| 0.010604167 | 6.238268659 | 12.095042053 |
| 1.356226142 | 5.501921688 | 14.227936062 |
| 2.694973801 | 6.239224888 | 12.090243698 |
| 4.101312407 | 5.475071595 | 14.156145039 |
| 1.305333959 | 3.921023340 | 15.363016060 |
| 2.475867919 | 3.238561779 | 15.889585378 |



*NH

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| | | |
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
|----|---|---|

| | | |
|----|---|---|
| 27 | 1 | 1 |
|----|---|---|

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.008205206 | 1.560695239 | 12.080972998 |
| 1.351173393 | 0.736226815 | 14.148617459 |
| 2.709622365 | 1.561478578 | 12.081843089 |
| 4.058970088 | 0.788621802 | 14.157497536 |
| 5.400681039 | 1.560479074 | 12.070805038 |
| 6.743615430 | 0.788565305 | 14.157438796 |
| -1.353765624 | 3.891516544 | 12.083084714 |
| -0.020444790 | 3.108317276 | 14.209021660 |
| 1.350916092 | 3.899145053 | 12.062277403 |
| 2.719996721 | 3.109084517 | 14.212427133 |

| | | |
|--------------|-------------|--------------|
| 4.054561421 | 3.891282400 | 12.083622923 |
| 5.400696006 | 3.110244995 | 14.159697363 |
| -2.699282046 | 6.236390068 | 12.072204527 |
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| 2.696338187 | 6.244505681 | 12.082592764 |
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TS *NH → *NH₂

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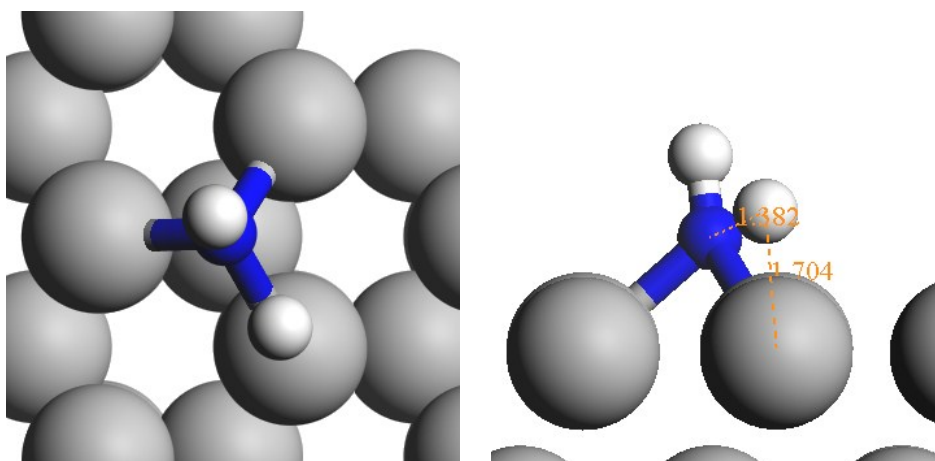
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| | | |
|----|---|---|
| Ru | N | H |
| 27 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.358223204 | 0.733171858 | 14.153203614 |
| 2.701999292 | 1.567271875 | 12.090814948 |
| 4.076823010 | 0.762100714 | 14.158991010 |
| 5.400704153 | 1.558716405 | 12.071061293 |
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| 2.726622756 | 3.103044218 | 14.217001540 |

| | | |
|--------------|-------------|--------------|
| 4.044017362 | 3.891421632 | 12.091182075 |
| 5.428966826 | 3.103881075 | 14.159151078 |
| -2.700849992 | 6.236180593 | 12.081892284 |
| -1.383604027 | 5.475781555 | 14.151392942 |
| 0.006608051 | 6.240222929 | 12.086681094 |
| 1.351646082 | 5.476283293 | 14.210943939 |
| 2.697788029 | 6.241676715 | 12.080890027 |
| 4.094694941 | 5.472937954 | 14.153224173 |
| 1.310818057 | 3.922539007 | 15.574099612 |
| 1.109528132 | 4.035398287 | 16.573874084 |
| 2.480750572 | 3.261012674 | 15.895399207 |



*NH₂

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| | | |
|---------------|--------------|---------------|
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
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| Ru | N | H |
|----|---|---|
| 27 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|-------------|
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| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003988452 | 1.554203063 | 12.079549278 |
| 1.344290086 | 0.772104952 | 14.155949727 |
| 2.710991458 | 1.553088472 | 12.079630046 |
| 4.065218546 | 0.786623892 | 14.166221951 |
| 5.400065955 | 1.558351704 | 12.080489124 |
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| -1.351418805 | 3.902189767 | 12.079506691 |
| -0.048266850 | 3.089015623 | 14.133245102 |
| 1.352532498 | 3.897783670 | 12.075090883 |
| 2.679090724 | 3.149775471 | 14.212450629 |
| 4.042629078 | 3.888407441 | 12.073673037 |
| 5.404854342 | 3.110471613 | 14.161723906 |
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| -1.358245925 | 5.453612260 | 14.156039306 |
| 0.001652375 | 6.246296050 | 12.080024340 |
| 1.368659147 | 5.418268578 | 14.214367034 |
| 2.689083670 | 6.232251566 | 12.073924886 |
| 4.100996658 | 5.484456605 | 14.129394670 |
| 2.016180831 | 4.275731222 | 15.897889799 |
| 1.287695913 | 3.848063104 | 16.477682307 |
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TS *NH₂ → *NH₃

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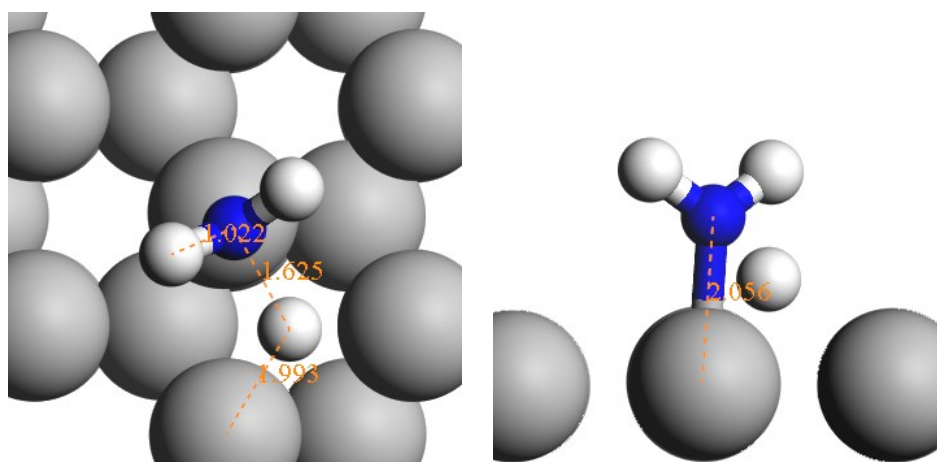
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| | | |
|----|---|---|
| Ru | N | H |
| 27 | 1 | 3 |

Cartesian

| | | |
|--------------|-------------|-------------|
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| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.0000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.326903396 | 0.762251967 | 14.147072587 |
| 2.697633775 | 1.569282695 | 12.075582834 |
| 4.059027843 | 0.788050135 | 14.178686659 |
| 5.394056331 | 1.562417873 | 12.075792096 |
| 6.751685664 | 0.779111253 | 14.161334751 |
| -1.352891217 | 3.905452736 | 12.081116911 |
| -0.028022903 | 3.120179199 | 14.155053936 |
| 1.342657114 | 3.901643290 | 12.079733576 |
| 2.664766842 | 3.140562307 | 14.203329717 |
| 4.039999762 | 3.894308716 | 12.074778825 |
| 5.399806089 | 3.107493171 | 14.177325351 |
| -2.698985850 | 6.235749098 | 12.080752721 |
| -1.362070769 | 5.464666385 | 14.154531147 |
| -0.008117760 | 6.234411966 | 12.080556675 |
| 1.333969411 | 5.480346534 | 14.155015755 |
| 2.694983699 | 6.239602446 | 12.074093765 |
| 4.056006435 | 5.486626204 | 14.145327998 |
| 2.873906213 | 3.046633393 | 16.246066055 |
| 2.362217473 | 2.375316270 | 16.821604291 |
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*NH₃

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|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
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| | | |
|----|---|---|
| Ru | N | H |
| 27 | 1 | 3 |

Cartesian

| | | |
|--------------|-------------|--------------|
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| 4.050040625 | 0.779415119 | 9.996419384 |
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| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
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| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.336155640 | 0.757579688 | 14.144808146 |
| 2.699513367 | 1.562941039 | 12.075355949 |
| 4.059350623 | 0.760934905 | 14.147933134 |
| 5.398671877 | 1.557714079 | 12.069572224 |
| 6.748221893 | 0.777135555 | 14.159393382 |
| -1.352092609 | 3.900501000 | 12.077707032 |
| -0.024189007 | 3.114659663 | 14.145217860 |
| 1.354170872 | 3.893294788 | 12.075503534 |
| 2.692762830 | 3.110856906 | 14.208249224 |
| 4.043052491 | 3.892373680 | 12.076584357 |
| 5.414819406 | 3.113439185 | 14.149113815 |
| -2.697632870 | 6.230695342 | 12.077673257 |
| -1.352200333 | 5.453443341 | 14.156360910 |
| -0.005030993 | 6.231688783 | 12.078044055 |
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| 2.699097376 | 6.233677338 | 12.069564882 |
| 4.054259432 | 5.468722101 | 14.149532341 |
| 2.611183666 | 3.063924958 | 16.405834012 |
| 1.783679848 | 2.532314699 | 16.699246612 |
| 3.453744133 | 2.615178198 | 16.782842983 |
| 2.541808904 | 4.023247446 | 16.763514461 |

N₂ER at 0.0V

*vN₂

1.0

| | | |
|---------------|--------------|---------------|
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N

27 2

Cartesian

| | | |
|--------------|-------------|--------------|
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| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 1.323983165 | 0.746861414 | 14.147353072 |
| 2.694998303 | 1.562700937 | 12.072588543 |
| 4.057061529 | 0.754308879 | 14.153845353 |
| 5.392829422 | 1.558156654 | 12.070907099 |
| 6.740105521 | 0.772687752 | 14.146272249 |
| -1.357284615 | 3.894481398 | 12.086861721 |
| -0.037142106 | 3.110158654 | 14.146301620 |
| 1.352849455 | 3.887894832 | 12.075040954 |
| 2.678107990 | 3.094696761 | 14.310886288 |
| 4.035030084 | 3.886757977 | 12.077304661 |
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| 2.694749783 | 6.227611325 | 12.071731667 |
| 4.043231368 | 5.462170238 | 14.154990790 |

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TS *vN₂ → *vN₂H

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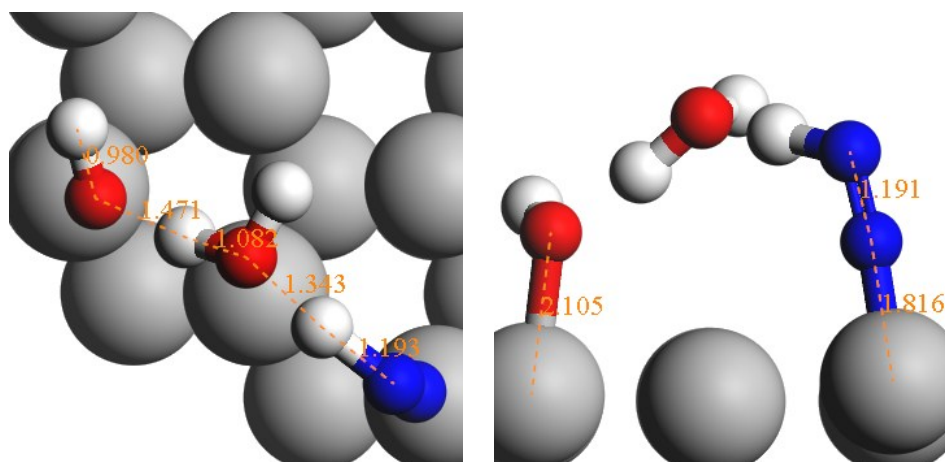
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| | | | |
|----|---|---|---|
| Ru | H | O | N |
| 27 | 4 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
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| 4.050040625 | 0.779415119 | 9.996419384 |
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| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
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| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
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| 5.396388365 | 1.559304379 | 12.089657028 |
| 6.732559545 | 0.798991107 | 14.139395220 |
| -1.352234431 | 3.920634493 | 12.077082916 |
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| 1.342881132 | 3.896584935 | 12.057868938 |
| 2.687426588 | 3.094922334 | 14.132412457 |
| 4.053254247 | 3.909129640 | 12.079450887 |
| 5.393111858 | 3.080911508 | 14.148729066 |
| -2.706489491 | 6.215631494 | 12.076751767 |
| -1.351242463 | 5.460407465 | 14.388683515 |
| -0.007993439 | 6.226669312 | 12.064455203 |
| 1.337770477 | 5.451276669 | 14.125990665 |
| 2.704235309 | 6.232026620 | 12.087083466 |
| 4.005427588 | 5.450519463 | 14.212064411 |

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| 4.379717187 | 4.780813337 | 16.628367534 |
| 2.484035165 | 5.289220721 | 17.069792673 |
| 1.690760975 | 4.163029571 | 17.922095016 |
| 0.380930722 | 5.411942916 | 17.555919240 |
| 3.728126001 | 5.434751509 | 16.298839880 |
| 1.674940421 | 5.121148933 | 17.767813410 |
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*vN₂H

1.0

| | | |
|---------------|--------------|---------------|
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| Ru | H | N |
|----|---|---|
| 27 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
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| 0.000000000 | 3.117660474 | 9.996419384 |
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| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003725327 | 1.552555794 | 12.083089120 |

| | | |
|--------------|-------------|--------------|
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| 2.709551997 | 1.548612969 | 12.063021938 |
| 4.066466880 | 0.783183119 | 14.156823490 |
| 5.400202044 | 1.554322016 | 12.076581420 |
| 6.745200575 | 0.783293501 | 14.152694041 |
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| 4.104137015 | 5.477768019 | 14.141875532 |
| 2.780376360 | 3.748101418 | 17.443399107 |
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*vN₂H₂

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| | | |
|----|---|---|
| Ru | H | N |
| 27 | 2 | 2 |

Cartesian

| | | |
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| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| -0.011047496 | 1.557455788 | 12.081390054 |
| 1.350129192 | 0.725250094 | 14.146429380 |
| 2.709948977 | 1.554088395 | 12.079505957 |
| 4.057936539 | 0.779740830 | 14.159284712 |
| 5.399652378 | 1.556898859 | 12.072242709 |
| 6.740045473 | 0.782909306 | 14.159579882 |
| -1.350889236 | 3.885075482 | 12.081785083 |
| -0.000857569 | 3.113942804 | 14.213597535 |
| 1.349943254 | 3.894870245 | 12.069324046 |
| 2.717549299 | 3.109450158 | 14.204204949 |
| 4.055037460 | 3.887444104 | 12.080778420 |
| 5.401866670 | 3.105146710 | 14.157979207 |
| -2.699306488 | 6.232897554 | 12.071441637 |
| -1.390551968 | 5.476501967 | 14.148043272 |
| 0.005208662 | 6.241595182 | 12.081417222 |
| 1.351448135 | 5.452714149 | 14.211894064 |
| 2.695062153 | 6.243139281 | 12.082219762 |
| 4.091739254 | 5.477571505 | 14.148012433 |
| 2.013171070 | 4.535676678 | 17.312364006 |
| 1.565356942 | 2.892561142 | 17.247331063 |
| 1.359240247 | 3.896855455 | 15.528170510 |
| 1.388679558 | 3.839873903 | 16.896557015 |

*pN₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N

27 2

Cartesian

| | | |
|--------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.0000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.004951874 | 1.563857652 | 12.081126457 |
| 1.341105825 | 0.759663260 | 14.157992424 |
| 2.701218970 | 1.547071275 | 12.101248708 |
| 4.059644013 | 0.763754098 | 14.157980676 |
| 5.398029877 | 1.564471445 | 12.080417901 |
| 6.752560644 | 0.784988017 | 14.148232710 |
| -1.349735108 | 3.900629779 | 12.087374230 |
| -0.022037057 | 3.087806016 | 14.155614907 |
| 1.354369302 | 3.905260403 | 12.069625825 |
| 2.700747216 | 3.112307138 | 14.198160563 |
| 4.049446422 | 3.903679929 | 12.077603503 |
| 5.433541092 | 3.085867426 | 14.156056928 |
| -2.691832660 | 6.244609792 | 12.057259506 |
| -1.359326185 | 5.457409162 | 14.142038537 |
| -0.012456421 | 6.248277079 | 12.053819523 |
| 1.333158553 | 5.465211189 | 14.180102302 |
| 2.702298807 | 6.231778260 | 12.071614921 |
| 4.059184450 | 5.450468035 | 14.200392698 |
| 2.012433114 | 4.508553975 | 15.906645053 |
| 3.246464137 | 4.500213834 | 15.914730666 |

TS *pN₂ → *pNNH

1.0

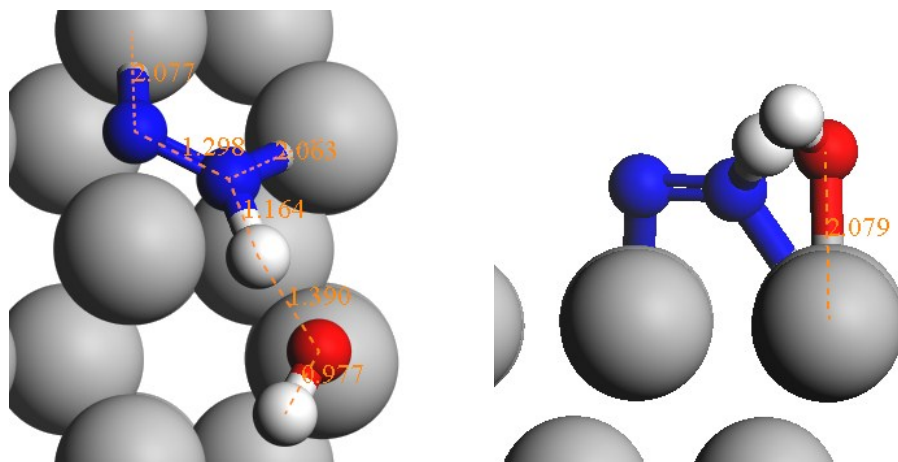
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | | |
|----|---|---|---|
| Ru | H | O | N |
| 27 | 2 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003817964 | 1.561517671 | 12.072091452 |
| 1.343110944 | 0.753503903 | 14.154418072 |
| 2.700250900 | 1.547900083 | 12.095882040 |
| 4.052641788 | 0.746818296 | 14.153535497 |
| 5.397293791 | 1.568042670 | 12.082400389 |
| 6.760508881 | 0.767928192 | 14.136293728 |
| -1.354621443 | 3.899138363 | 12.090410374 |
| -0.003357616 | 3.085934533 | 14.143634806 |
| 1.355463563 | 3.905913081 | 12.078864218 |
| 2.678805391 | 3.109117130 | 14.200425005 |
| 4.055356106 | 3.894473454 | 12.077078510 |
| 5.444120637 | 3.081737285 | 14.217901736 |
| -2.687524415 | 6.248901742 | 12.060477011 |
| -1.346245387 | 5.471357061 | 14.142091403 |
| -0.004311142 | 6.245059683 | 12.064771667 |
| 1.353107510 | 5.449076548 | 14.203924463 |
| 2.692415457 | 6.236616687 | 12.071052482 |
| 4.044890502 | 5.480173853 | 14.178832042 |
| 5.359849635 | 2.305435870 | 16.717670532 |
| 4.103600868 | 3.818241468 | 16.373216948 |
| 5.337246860 | 3.184042088 | 16.291858586 |
| 2.015155127 | 4.391557028 | 15.864431279 |
| 3.310591010 | 4.464378450 | 15.817903025 |



*pNNH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | N | H |
| 27 | 2 | 1 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.006300992 | 1.567486472 | 12.085483524 |
| 1.342008505 | 0.758643530 | 14.159475618 |
| 2.697504023 | 1.550372397 | 12.097039960 |
| 4.066980938 | 0.763858051 | 14.157709001 |
| 5.396257526 | 1.561454327 | 12.077259137 |
| 6.750409992 | 0.794621021 | 14.146335395 |
| -1.344232362 | 3.906762272 | 12.089383886 |
| -0.015640471 | 3.098564743 | 14.161935372 |
| 1.358492394 | 3.906506804 | 12.067532465 |
| 2.717749056 | 3.112664000 | 14.232721934 |
| 4.049127534 | 3.905238243 | 12.081818125 |
| 5.442859811 | 3.089351578 | 14.144750874 |
| -2.695875969 | 6.249861734 | 12.076690824 |
| -1.356173999 | 5.462113793 | 14.148057957 |
| -0.011787987 | 6.253651529 | 12.053775468 |
| 1.360224913 | 5.464876279 | 14.184161263 |
| 2.700307267 | 6.238815135 | 12.068310775 |
| 4.063744233 | 5.448031678 | 14.214914788 |
| 3.227943295 | 4.431364087 | 15.868425625 |
| 1.893394044 | 4.382218847 | 15.798711075 |
| 3.633872796 | 4.000342687 | 16.717736615 |

TS *pNNH → *pNNH₂

1.0

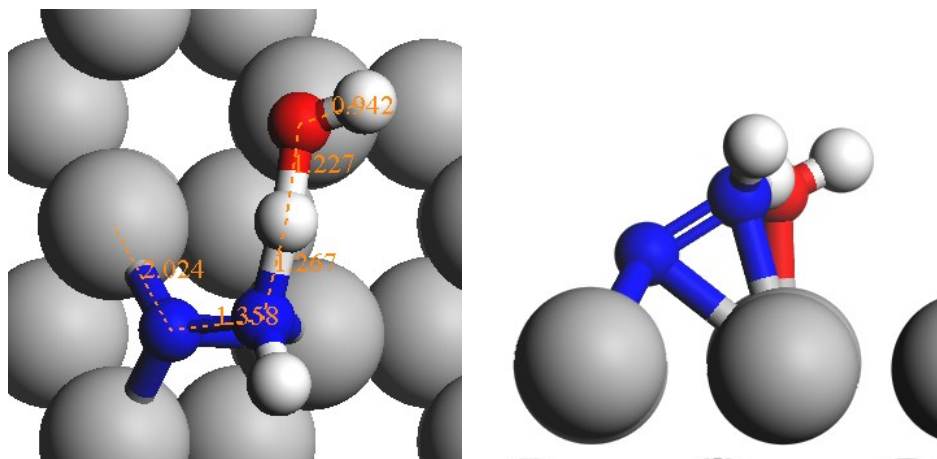
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N | O |
|----|---|---|---|
| 27 | 3 | 2 | 1 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996418649 |
| 4.050040625 | 0.779415119 | 9.996418649 |
| 6.750014037 | 0.779415119 | 9.996418649 |
| 0.000000000 | 3.117660474 | 9.996418649 |
| 2.700054040 | 3.117660474 | 9.996418649 |
| 5.400027452 | 3.117660474 | 9.996418649 |
| -1.350026899 | 5.455975864 | 9.996418649 |
| 1.350027020 | 5.455975864 | 9.996418649 |
| 4.050000915 | 5.455975864 | 9.996418649 |
| 0.002967817 | 1.554046792 | 12.074489528 |
| 1.340198738 | 0.764651007 | 14.213562291 |
| 2.685491837 | 1.558528881 | 12.076317088 |
| 4.082611693 | 0.782467201 | 14.139085364 |
| 5.400298724 | 1.563907512 | 12.069097161 |
| 6.717163098 | 0.774659374 | 14.137345180 |
| -1.358627577 | 3.910429978 | 12.058589242 |
| -0.018491633 | 3.090659651 | 14.184594473 |
| 1.353246073 | 3.894071645 | 12.075703986 |
| 2.763120206 | 3.124197703 | 14.208588449 |
| 4.058271721 | 3.899977520 | 12.082265286 |
| 5.440647873 | 3.115306905 | 14.146231131 |
| -2.694392573 | 6.231698400 | 12.080112451 |
| -1.354293985 | 5.462163548 | 14.142531956 |
| 0.005548552 | 6.233312742 | 12.088449914 |
| 1.349434386 | 5.490265059 | 14.210363877 |
| 2.695465289 | 6.226741646 | 12.082115498 |
| 4.086961489 | 5.482565471 | 14.144320600 |
| 2.748547804 | 2.406305283 | 16.891044230 |
| 1.944720020 | 5.983685946 | 16.732643455 |
| 1.818584790 | 4.195821914 | 16.489282064 |

| | | |
|-------------|-------------|--------------|
| 1.250117358 | 2.314235727 | 15.556997351 |
| 2.176557398 | 2.999176083 | 16.275035341 |
| 1.360355510 | 5.320805130 | 16.315417884 |



*pNNH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.001362515 | 1.555244483 | 12.074457955 |
| 1.359896882 | 0.816021455 | 14.147331045 |
| 2.701739607 | 1.553505751 | 12.073211925 |
| 4.061159576 | 0.792039475 | 14.147595377 |
| 5.396502305 | 1.561399136 | 12.083547295 |
| 6.742819417 | 0.824811487 | 14.140241081 |

| | | |
|--------------|-------------|--------------|
| -1.355916849 | 3.905411761 | 12.075866256 |
| -0.047050803 | 3.095841141 | 14.144768496 |
| 1.350569926 | 3.900442882 | 12.072911615 |
| 2.682261377 | 3.108046546 | 14.221737483 |
| 4.031859552 | 3.905773849 | 12.073772161 |
| 5.429139064 | 3.102347638 | 14.144474794 |
| -2.697331906 | 6.240321604 | 12.088128310 |
| -1.321501645 | 5.454596921 | 14.147557195 |
| -0.011712188 | 6.246502598 | 12.067645540 |
| 1.321227416 | 5.454506190 | 14.210622335 |
| 2.694901382 | 6.221194096 | 12.072200122 |
| 4.090587299 | 5.492546713 | 14.238430030 |
| 3.245947302 | 6.105317698 | 16.804215670 |
| 4.130070249 | 4.637700926 | 16.891781422 |
| 2.567639543 | 4.631457632 | 15.573939545 |
| 3.562500820 | 5.264903151 | 16.308349947 |

TS *pNNH → *HNNH

1.0

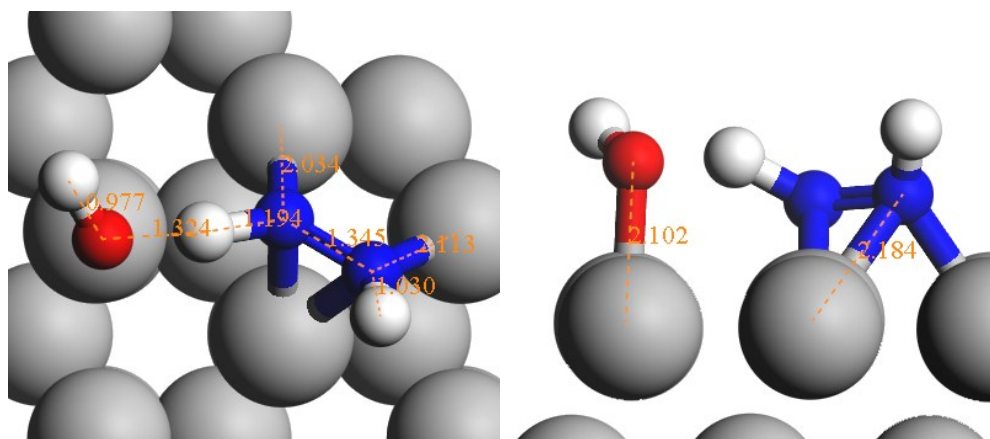
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | O | N |
|----|---|---|---|
| 27 | 3 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.005229724 | 1.564146674 | 12.082094939 |
| 1.353976606 | 0.750015047 | 14.152068456 |
| 2.697263348 | 1.557678539 | 12.098983532 |
| 4.062317113 | 0.761014869 | 14.153862975 |

| | | |
|--------------|-------------|--------------|
| 5.395719690 | 1.555700228 | 12.065220296 |
| 6.737102007 | 0.771488651 | 14.132590147 |
| -1.340119288 | 3.899281358 | 12.082743286 |
| -0.048912712 | 3.073129970 | 14.212453566 |
| 1.344530851 | 3.893427748 | 12.076767921 |
| 2.735507078 | 3.119880247 | 14.244365746 |
| 4.045117658 | 3.903988497 | 12.077715109 |
| 5.416524285 | 3.081372062 | 14.123824614 |
| -2.696562749 | 6.246954999 | 12.079650605 |
| -1.351274810 | 5.469641954 | 14.142885867 |
| -0.009876109 | 6.249442365 | 12.059034934 |
| 1.358435906 | 5.481311126 | 14.177989117 |
| 2.707264140 | 6.230868859 | 12.073750868 |
| 4.083619805 | 5.454764585 | 14.199748022 |
| 1.182767569 | 3.772605885 | 16.369121275 |
| 3.724230066 | 3.973795310 | 16.730072095 |
| -0.674394925 | 3.469156188 | 16.745119911 |
| 0.084604614 | 3.034471054 | 16.310120970 |
| 1.997266509 | 4.437854905 | 15.802752413 |
| 3.339238291 | 4.425533055 | 15.888344488 |



*HNNH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |
| Ru | N | H |
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.002440663 | 1.559343682 | 12.076162160 |
| 1.330580232 | 0.773577292 | 14.156822022 |
| 2.695352134 | 1.567725948 | 12.101804539 |
| 4.056943062 | 0.774275858 | 14.155102397 |
| 5.390441143 | 1.558873094 | 12.075703251 |
| 6.745050244 | 0.796221931 | 14.142714051 |
| -1.353969847 | 3.909416467 | 12.079143969 |
| -0.045364029 | 3.091791488 | 14.136793021 |
| 1.353216622 | 3.903857209 | 12.072109809 |
| 2.691455172 | 3.123608997 | 14.296687270 |
| 4.037682333 | 3.904521594 | 12.077571930 |
| 5.431900908 | 3.092064099 | 14.137232105 |
| -2.698276620 | 6.252022971 | 12.073012208 |
| -1.357808269 | 5.463010649 | 14.146972729 |
| -0.011819611 | 6.254237726 | 12.068486261 |
| 1.317581087 | 5.470226897 | 14.188086588 |
| 2.697233294 | 6.232038327 | 12.072052537 |
| 4.065883026 | 5.460500705 | 14.202331130 |
| 3.348123941 | 4.437635395 | 15.883151838 |
| 1.981438229 | 4.450982463 | 15.867211168 |
| 3.760198731 | 4.034030215 | 16.734633285 |
| 1.530767629 | 4.064101465 | 16.706254339 |

TS *pNNH₂ → *N + *NH₃

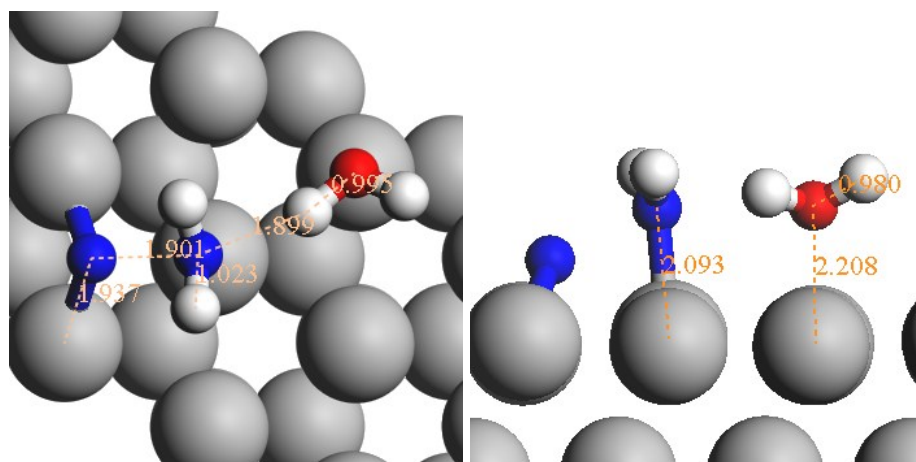
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru H O N
27 4 1 2

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.009583413 | 1.563927582 | 12.061338292 |
| 1.380066961 | 0.776007429 | 14.214111513 |
| 2.691098988 | 1.566768360 | 12.086753051 |
| 4.090351543 | 0.759045025 | 14.140409960 |
| 5.400784177 | 1.564143747 | 12.080798245 |
| 6.704184169 | 0.777991541 | 14.142111962 |
| -1.359587258 | 3.903827523 | 12.051994900 |
| -0.008317879 | 3.135669734 | 14.240331750 |
| 1.352409385 | 3.881965961 | 12.086191346 |
| 2.723292056 | 3.128932855 | 14.273070701 |
| 4.047059953 | 3.904424173 | 12.096016409 |
| 5.437665994 | 3.098598401 | 14.137243853 |
| -2.700981252 | 6.227125476 | 12.062936764 |
| -1.318348735 | 5.457413762 | 14.134869273 |
| -0.000833792 | 6.236486235 | 12.085238283 |
| 1.324731561 | 5.510709211 | 14.141824134 |
| 2.711408957 | 6.230014232 | 12.085427721 |
| 4.068965689 | 5.482513625 | 14.187361145 |
| 1.909657565 | 3.655568800 | 16.919587649 |
| 2.922669137 | 2.305823253 | 16.913888364 |
| -3.177769531 | 5.538522223 | 16.825227104 |
| 3.705326848 | 4.542662126 | 16.597276251 |
| 4.046170881 | 5.455639699 | 16.394704179 |
| 1.078199513 | 2.171445474 | 15.522922057 |
| 2.531031774 | 3.069482961 | 16.356700622 |



*N + *NH₃

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru H N

27 3 2

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.002366493 | 1.555861620 | 12.042147075 |
| 1.373173335 | 0.747089339 | 14.196020945 |
| 2.699144147 | 1.556669941 | 12.089820033 |
| 4.054329890 | 0.752299366 | 14.151253434 |
| 5.391277952 | 1.548978611 | 12.081871725 |
| 6.707170001 | 0.754810879 | 14.203577895 |
| -1.351241980 | 3.904021947 | 12.088746552 |
| -0.015608003 | 3.154075784 | 14.191179269 |
| 1.349814347 | 3.897225069 | 12.087749435 |
| 2.735595309 | 3.137061638 | 14.213145234 |

| | | |
|--------------|-------------|--------------|
| 4.045820612 | 3.893318202 | 12.069478974 |
| 5.359987233 | 3.144238165 | 14.139987029 |
| -2.693768738 | 6.230497573 | 12.088608513 |
| -1.352629420 | 5.453897832 | 14.159656245 |
| -0.007836771 | 6.230094510 | 12.078701948 |
| 1.329894358 | 5.471867580 | 14.150043382 |
| 2.685857375 | 6.232925149 | 12.079405364 |
| 4.052276099 | 5.409746140 | 14.135019061 |
| 1.776861418 | 3.382965747 | 16.741883317 |
| 2.974601628 | 2.241515699 | 16.784089748 |
| 3.363079322 | 3.847987425 | 16.757468608 |
| -0.015110661 | 1.551886078 | 15.298458914 |
| 2.709877282 | 3.149325579 | 16.391770097 |

TS *pNNH₂ → *HNNH₂

1.0

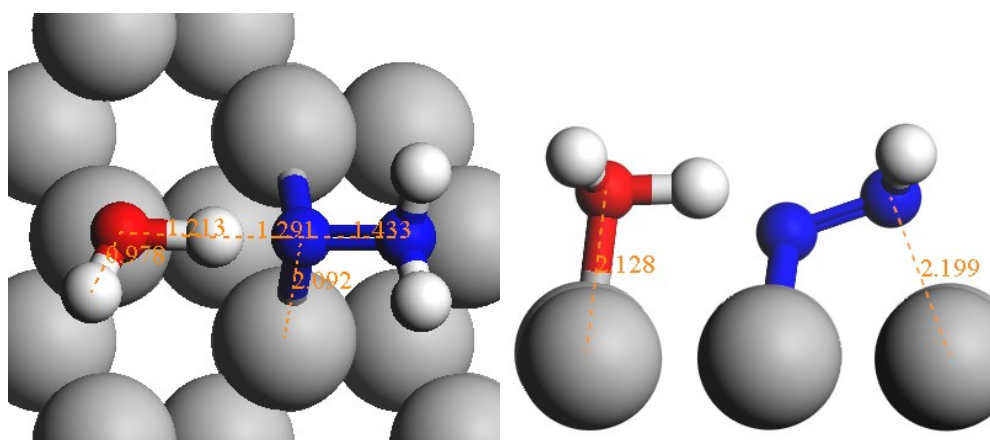
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | O | N |
|----|---|---|---|
| 27 | 4 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003795393 | 1.564155350 | 12.085460028 |
| 1.366270807 | 0.776133438 | 14.148477951 |
| 2.703871158 | 1.544515024 | 12.066354720 |
| 4.062502869 | 0.784807496 | 14.155011349 |
| 5.397287153 | 1.556234893 | 12.076582154 |
| 6.730184935 | 0.790194333 | 14.142225037 |
| -1.343654332 | 3.897484718 | 12.086222185 |

| | | |
|--------------|-------------|--------------|
| -0.029445346 | 3.100602844 | 14.219354092 |
| 1.345304293 | 3.892706082 | 12.065420014 |
| 2.705280565 | 3.153926517 | 14.176134390 |
| 4.051737055 | 3.901794648 | 12.078152725 |
| 5.400911213 | 3.091851488 | 14.143207470 |
| -2.690882091 | 6.239599937 | 12.091201900 |
| -1.344518057 | 5.471177272 | 14.149535278 |
| -0.010469708 | 6.244435020 | 12.066793070 |
| 1.388133997 | 5.437784097 | 14.176905357 |
| 2.704710623 | 6.232994556 | 12.076254677 |
| 4.078926529 | 5.471456573 | 14.191000111 |
| 3.165768132 | 5.910070524 | 16.809129303 |
| 4.005380998 | 4.458786161 | 16.806707731 |
| 1.238019173 | 3.831182128 | 16.367542628 |
| 0.220875578 | 2.406890853 | 16.770677850 |
| 0.159327689 | 3.278247375 | 16.331753583 |
| 2.237126897 | 4.405157056 | 15.786098047 |
| 3.411046958 | 5.084390769 | 16.249801943 |



TS *HNNH → *HNNH₂

1.0

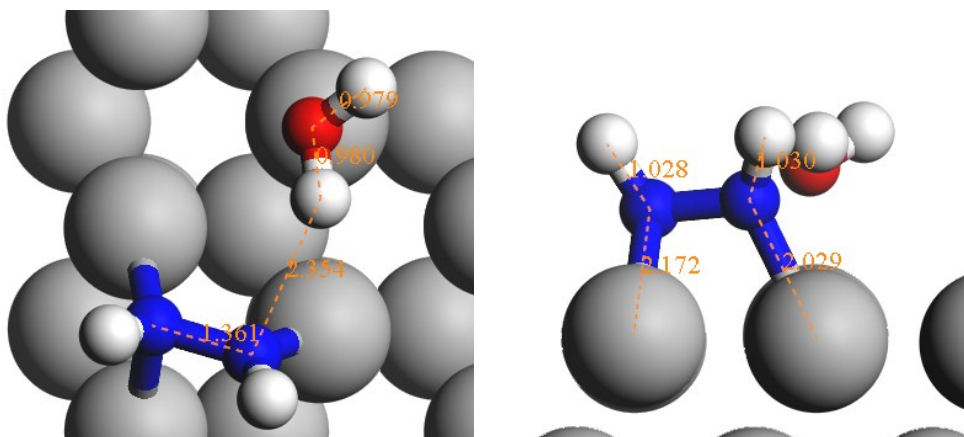
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | | |
|----|---|---|---|
| Ru | H | O | N |
| 27 | 4 | 1 | 2 |

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
|-------------|-------------|-------------|

| | | |
|--------------|-------------|--------------|
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.011974045 | 1.559641485 | 12.077503644 |
| 1.325353043 | 0.763960960 | 14.210857296 |
| 2.698218141 | 1.557097255 | 12.063949301 |
| 4.084079307 | 0.769034995 | 14.143953473 |
| 5.396289995 | 1.563243650 | 12.071280835 |
| 6.722179818 | 0.767994672 | 14.123784964 |
| -1.349221351 | 3.905266257 | 12.073915341 |
| -0.013446035 | 3.066713158 | 14.185907320 |
| 1.350334803 | 3.900423649 | 12.080489124 |
| 2.743529243 | 3.101739072 | 14.183758891 |
| 4.061288241 | 3.909562389 | 12.060597429 |
| 5.410330474 | 3.114189074 | 14.144985835 |
| -2.692287455 | 6.231870663 | 12.090567504 |
| -1.365657352 | 5.454802215 | 14.145009331 |
| 0.003406862 | 6.230102873 | 12.088671659 |
| 1.346626676 | 5.466250623 | 14.208688308 |
| 2.694838618 | 6.225158663 | 12.081818859 |
| 4.052724618 | 5.440552019 | 14.141733087 |
| 0.391609904 | 1.687985864 | 16.719751410 |
| 2.598398219 | 1.995331662 | 16.811078015 |
| 1.688702085 | 6.161999461 | 16.870831666 |
| 1.889767751 | 4.615880757 | 16.739545449 |
| 1.331927902 | 5.361915872 | 16.433881075 |
| 0.815335628 | 2.074537909 | 15.866087758 |
| 2.131973087 | 2.399141091 | 15.986715532 |



*HNNH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 3 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.010214308 | 1.559026124 | 12.075605595 |
| 1.357737328 | 0.801381993 | 14.154642754 |
| 2.711360074 | 1.556910044 | 12.084009875 |
| 4.069867223 | 0.797925018 | 14.162237885 |
| 5.398227281 | 1.562004671 | 12.082649301 |
| 6.748366822 | 0.813346669 | 14.141338058 |
| -1.347384849 | 3.909602946 | 12.076577014 |
| -0.028994292 | 3.104503021 | 14.138348172 |
| 1.356574721 | 3.903087878 | 12.067978157 |
| 2.679840147 | 3.169573009 | 14.206720505 |
| 4.050408396 | 3.905202285 | 12.070234522 |

| | | |
|--------------|-------------|--------------|
| 5.423146459 | 3.110940111 | 14.145972674 |
| -2.679511845 | 6.249791909 | 12.078667438 |
| -1.334417086 | 5.458796050 | 14.154178705 |
| -0.002877233 | 6.253087074 | 12.080809993 |
| 1.369819068 | 5.425437161 | 14.192213100 |
| 2.703547322 | 6.236410974 | 12.067171211 |
| 4.081075944 | 5.485089631 | 14.172367663 |
| 3.220197531 | 6.059400724 | 16.733357150 |
| 4.083839236 | 4.629822384 | 16.820366337 |
| 1.751531198 | 4.179676403 | 16.700863441 |
| 2.274380046 | 4.468433748 | 15.864830714 |
| 3.465979432 | 5.199342715 | 16.228085625 |

TS *HNNH₂ → *NH + *NH₃

1.0

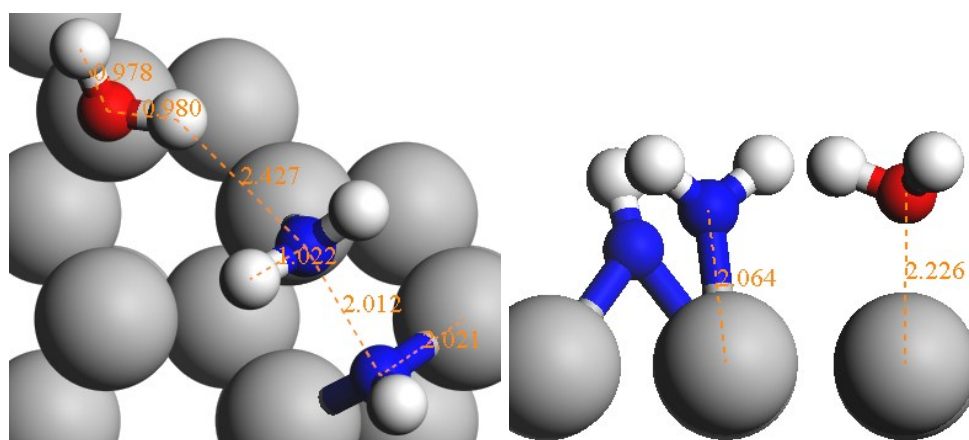
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | | |
|----|---|---|---|
| Ru | N | H | O |
| 27 | 2 | 5 | 1 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.002320205 | 1.555287444 | 12.086813260 |
| 1.330895197 | 0.804214357 | 14.140887225 |
| 2.695805662 | 1.540691989 | 12.066116821 |
| 4.060040692 | 0.786861956 | 14.149121158 |
| 5.399788890 | 1.551977018 | 12.087584961 |
| 6.758167916 | 0.801880596 | 14.142276435 |
| -1.344234353 | 3.907637387 | 12.091842170 |
| -0.010856067 | 3.079748312 | 14.145419045 |

| | | |
|--------------|-------------|--------------|
| 1.353045229 | 3.902788925 | 12.073287553 |
| 2.731459544 | 3.120739473 | 14.186459480 |
| 4.054875723 | 3.892918902 | 12.049965420 |
| 5.413111992 | 3.089794362 | 14.159049750 |
| -2.689357899 | 6.241431281 | 12.078304716 |
| -1.349785017 | 5.460539589 | 14.204457532 |
| -0.012635297 | 6.234015175 | 12.086388861 |
| 1.354181494 | 5.458943644 | 14.217190978 |
| 2.696629556 | 6.230558618 | 12.071036328 |
| 4.044000464 | 5.423558988 | 14.172078367 |
| 3.458460342 | 4.235893640 | 15.699435428 |
| 1.773163670 | 5.202048337 | 16.221458241 |
| 3.841640659 | 4.014625078 | 16.628016560 |
| 1.355962293 | 4.471490586 | 16.801418159 |
| 2.141650524 | 5.961772119 | 16.801921858 |
| -2.069376320 | 5.967079253 | 16.838772635 |
| -0.511017651 | 5.798404126 | 16.783437729 |
| -1.352850903 | 5.441335566 | 16.430265605 |



*NH + *NH₃

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | N | H |
|----|---|---|
| 27 | 2 | 4 |

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
|-------------|-------------|-------------|

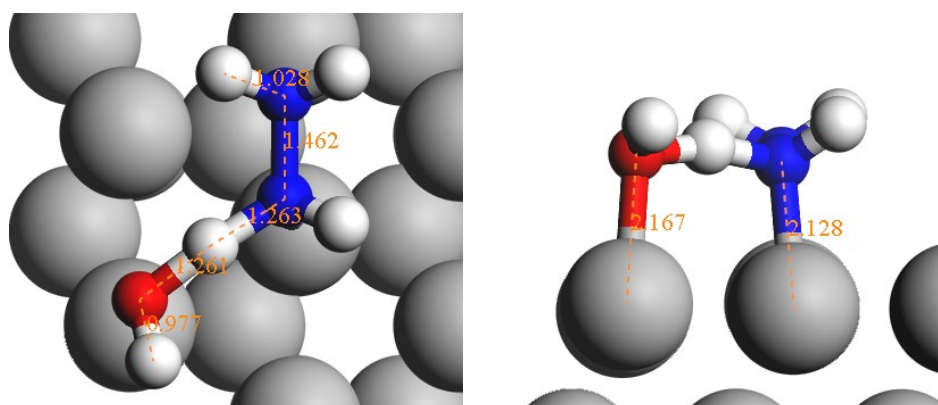
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|--------------|-------------|--------------|
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.008776899 | 1.556199039 | 12.075419095 |
| 1.347562609 | 0.783653707 | 14.152439989 |
| 2.694183099 | 1.557364117 | 12.085315380 |
| 4.043750828 | 0.749722941 | 14.134825218 |
| 5.412206566 | 1.556825271 | 12.074404355 |
| 6.775370992 | 0.801726677 | 14.146853779 |
| -1.339977345 | 3.888208418 | 12.071015035 |
| -0.001128298 | 3.091488355 | 14.145706873 |
| 1.350710903 | 3.899538081 | 12.083991519 |
| 2.702766276 | 3.104551105 | 14.196228005 |
| 4.052836386 | 3.898584361 | 12.055089784 |
| 5.430223548 | 3.105304339 | 14.195671440 |
| -2.698425322 | 6.245530481 | 12.081536905 |
| -1.326189490 | 5.477005377 | 14.128053921 |
| 0.005279634 | 6.234063258 | 12.067332013 |
| 1.323619920 | 5.478814143 | 14.210722194 |
| 2.700869002 | 6.238471863 | 12.082876920 |
| 4.069516079 | 5.471662703 | 14.193918040 |
| 4.081184573 | 3.894452130 | 15.472339248 |
| 1.280249966 | 5.516092860 | 16.391458773 |
| 4.133437038 | 3.881567079 | 16.499889108 |
| 1.695391970 | 4.664772619 | 16.782258516 |
| 1.794591437 | 6.317373095 | 16.770416456 |
| 0.317450798 | 5.575966514 | 16.732164721 |

TS *HNNH₂ → *H₂NNH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | O | N |
|--------------|---|-------------|--------------|
| 27 | 5 | 1 | 2 |
| Cartesian | | | |
| 1.349986585 | | 0.779415119 | 9.996419384 |
| 4.050040625 | | 0.779415119 | 9.996419384 |
| 6.750014037 | | 0.779415119 | 9.996419384 |
| 0.000000000 | | 3.117660474 | 9.996419384 |
| 2.700054040 | | 3.117660474 | 9.996419384 |
| 5.400027452 | | 3.117660474 | 9.996419384 |
| -1.350027020 | | 5.455975864 | 9.996419384 |
| 1.350027020 | | 5.455975864 | 9.996419384 |
| 4.050000432 | | 5.455975864 | 9.996419384 |
| 0.009468627 | | 1.549209828 | 12.083399709 |
| 1.344108102 | | 0.799255826 | 14.220078067 |
| 2.697234260 | | 1.552858718 | 12.089869962 |
| 4.079324445 | | 0.776174361 | 14.162669626 |
| 5.398407424 | | 1.559090305 | 12.082909962 |
| 6.729195863 | | 0.781431165 | 14.158910242 |
| -1.353432614 | | 3.904588074 | 12.079157920 |
| -0.065132661 | | 3.117205983 | 14.117222195 |
| 1.352188505 | | 3.897229668 | 12.060757496 |
| 2.720771128 | | 3.148798754 | 14.162978013 |
| 4.056201726 | | 3.902411368 | 12.067647008 |
| 5.409518047 | | 3.118602487 | 14.149579333 |
| -2.695098725 | | 6.249466616 | 12.094359196 |
| -1.357337662 | | 5.447492728 | 14.156006999 |
| 0.004922846 | | 6.238071309 | 12.087720064 |
| 1.353734423 | | 5.420540616 | 14.230281271 |
| 2.690453126 | | 6.232171706 | 12.077452980 |
| 4.082290421 | | 5.470690168 | 14.137900277 |
| 0.721544943 | | 4.537991363 | 16.794225400 |
| 3.230623064 | | 3.522813934 | 16.771481125 |
| 1.775683150 | | 2.331995581 | 16.455515157 |
| 2.165206221 | | 5.386404032 | 16.876193194 |
| 1.889051339 | | 0.514839979 | 16.752579940 |
| 1.287734476 | | 1.173872883 | 16.353239345 |
| 1.627415269 | | 4.697458762 | 16.335567302 |
| 2.356324083 | | 3.433154602 | 16.240541522 |



*H₂NNH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 4 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.008786314 | 1.556540117 | 12.073877894 |
| 1.351011444 | 0.772283958 | 14.144357313 |
| 2.710037872 | 1.559925176 | 12.081281385 |
| 4.070683876 | 0.784987285 | 14.157515158 |
| 5.402635283 | 1.558565988 | 12.072976963 |
| 6.757532645 | 0.789117896 | 14.149610172 |
| -1.344129345 | 3.902994220 | 12.074600401 |
| -0.034215748 | 3.091725008 | 14.126779255 |
| 1.359397639 | 3.900623090 | 12.073791986 |
| 2.708788694 | 3.129918143 | 14.205811498 |

| | | |
|--------------|-------------|--------------|
| 4.049845695 | 3.894103422 | 12.070187530 |
| 5.420365182 | 3.116098605 | 14.148209213 |
| -2.686105774 | 6.241395741 | 12.083317473 |
| -1.351621942 | 5.455315660 | 14.147121048 |
| 0.011984727 | 6.237440373 | 12.086572424 |
| 1.371557381 | 5.434534089 | 14.227439706 |
| 2.695769935 | 6.230909417 | 12.074766342 |
| 4.106006166 | 5.484489218 | 14.127582529 |
| 0.813861405 | 4.696064766 | 16.843047466 |
| 3.331683232 | 3.750115478 | 16.814677331 |
| 1.914205278 | 2.896478044 | 16.815045927 |
| 2.221234888 | 5.562180425 | 16.873046178 |
| 1.690865260 | 4.865916051 | 16.337972721 |
| 2.445955949 | 3.615638397 | 16.312257651 |

TS *H₂NNH₂ → *NH₂ + *NH₃

1.0

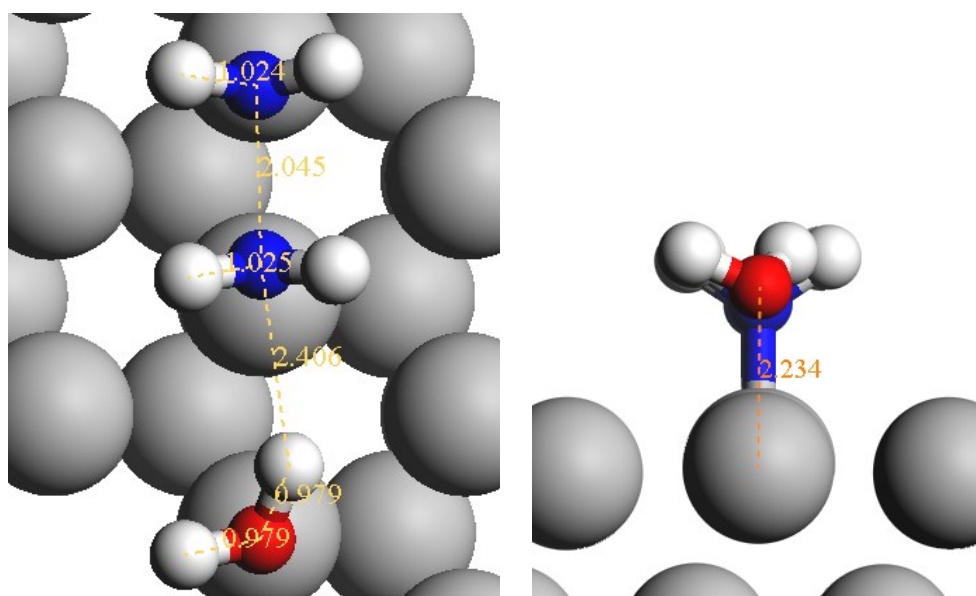
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | | |
|----|---|---|---|
| Ru | H | O | N |
| 27 | 6 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.012774162 | 1.560839489 | 12.081531031 |
| 1.334042193 | 0.777028936 | 14.140562685 |
| 2.721677098 | 1.566468362 | 12.089549093 |
| 4.061618263 | 0.789050736 | 14.203312095 |
| 5.398349127 | 1.556598130 | 12.075616609 |
| 6.779999875 | 0.796687868 | 14.140199963 |

| | | |
|--------------|-------------|--------------|
| -1.339402514 | 3.904974413 | 12.078805478 |
| -0.018663388 | 3.103187213 | 14.125351863 |
| 1.363521455 | 3.902872130 | 12.052977333 |
| 2.715908149 | 3.146119055 | 14.258610288 |
| 4.043031490 | 3.888792525 | 12.073474788 |
| 5.432796135 | 3.135247646 | 14.140044301 |
| -2.686525084 | 6.242643397 | 12.080729225 |
| -1.362112773 | 5.442313537 | 14.135528634 |
| 0.014059067 | 6.251499073 | 12.082177175 |
| 1.370760040 | 5.454381591 | 14.237844095 |
| 2.690695731 | 6.230823285 | 12.070534832 |
| 4.100257736 | 5.485371859 | 14.133698871 |
| 0.684994265 | 4.862908132 | 16.761818333 |
| 1.912707881 | 2.903076735 | 16.823680763 |
| 3.323384906 | 3.818389481 | 16.806076271 |
| 2.095280949 | 5.774338261 | 16.791684879 |
| 3.985654852 | 1.607712483 | 16.844433739 |
| 3.455328667 | 0.138656154 | 16.846519023 |
| 4.119701476 | 0.728345870 | 16.435825382 |
| 1.485750128 | 5.188959246 | 16.212976131 |
| 2.556451794 | 3.446271916 | 16.239586991 |



*NH₂ + *NH₃

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 5 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.016355434 | 1.563218563 | 12.081250546 |
| 1.337777086 | 0.752980685 | 14.147806842 |
| 2.708417664 | 1.572126504 | 12.088242854 |
| 4.091619309 | 0.717972018 | 14.200235567 |
| 5.391238724 | 1.554205258 | 12.066882649 |
| 6.809424913 | 0.804096083 | 14.122491207 |
| -1.345230425 | 3.892020791 | 12.084265396 |
| -0.022613397 | 3.107875746 | 14.144106198 |
| 1.371794676 | 3.885802166 | 12.084787451 |
| 2.716836448 | 3.112251947 | 14.247365911 |
| 4.045946380 | 3.889471126 | 12.083816032 |
| 5.421407542 | 3.118541233 | 14.150454564 |
| -2.697080308 | 6.236155088 | 12.085089964 |
| -1.390730603 | 5.424266439 | 14.130294866 |
| 0.001840666 | 6.230451163 | 12.077602034 |
| 1.335709656 | 5.497823324 | 14.189766563 |
| 2.697227259 | 6.223377074 | 12.062870681 |
| 4.068866233 | 5.462676575 | 14.147560132 |
| 0.037867751 | 6.186676192 | 16.495329386 |
| 1.773512009 | 3.132388994 | 16.825301998 |
| 3.269733052 | 3.836039788 | 16.833204047 |
| 1.468679852 | 7.013322211 | 16.491599372 |
| 3.129155776 | 2.191463149 | 16.778018929 |

| | | |
|-------------|-------------|--------------|
| 0.739431631 | 6.621177564 | 15.883360367 |
| 2.719854295 | 3.066944376 | 16.436221879 |

TS *N₂ Cleavage

1.0

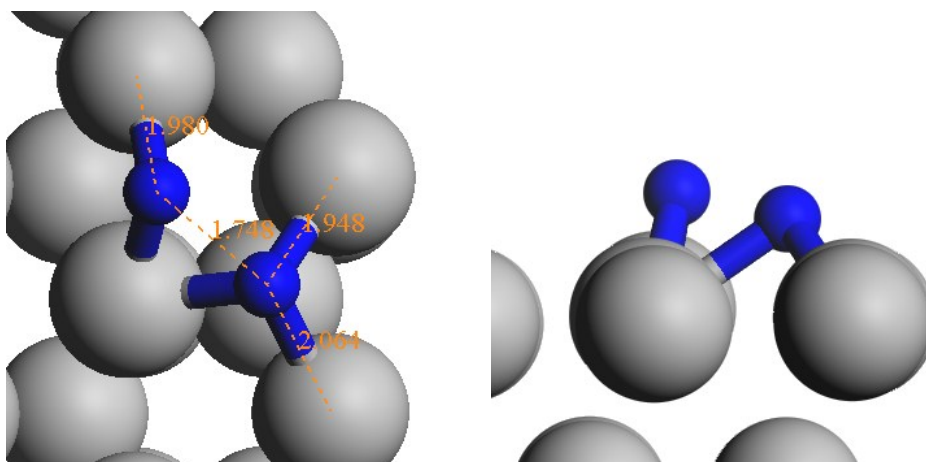
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| 0.0000000000 | 0.0000000000 | 69.2749977112 |

| | |
|----|---|
| Ru | N |
| 27 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419344 |
| 4.050040625 | 0.779415119 | 9.996419344 |
| 6.750014037 | 0.779415119 | 9.996419344 |
| 0.000000000 | 3.117660474 | 9.996419344 |
| 2.700054040 | 3.117660474 | 9.996419344 |
| 5.400027452 | 3.117660474 | 9.996419344 |
| -1.350027020 | 5.455975864 | 9.996419344 |
| 1.350027020 | 5.455975864 | 9.996419344 |
| 4.050000432 | 5.455975864 | 9.996419344 |
| 0.003769081 | 1.565328267 | 12.076256679 |
| 1.384342677 | 0.778588557 | 14.143749724 |
| 2.715630480 | 1.548161300 | 12.050676714 |
| 4.069027759 | 0.727933190 | 14.139151821 |
| 5.403384465 | 1.572456815 | 12.089179561 |
| 6.743213108 | 0.824509242 | 14.156484637 |
| -1.351541797 | 3.896386330 | 12.098455401 |
| -0.049639443 | 3.107550244 | 14.160540660 |
| 1.354329471 | 3.893196949 | 12.098779941 |
| 2.629871194 | 3.073746689 | 14.230761841 |
| 4.047351321 | 3.901006083 | 12.047060510 |
| 5.402990260 | 3.130371380 | 14.219358866 |
| -2.687909084 | 6.247029841 | 12.079327332 |
| -1.281016890 | 5.481912375 | 14.140588023 |
| 0.020019204 | 6.235347708 | 12.054112292 |
| 1.391197589 | 5.443944186 | 14.310100996 |
| 2.690993376 | 6.251779628 | 12.087145676 |
| 4.072347687 | 5.585260375 | 14.182798856 |

| | | |
|-------------|-------------|--------------|
| 3.983511230 | 4.061787617 | 15.393576019 |
| 2.288701273 | 4.357108113 | 15.700619300 |



*N + *N

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | |
|----|---|
| Ru | N |
| 27 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.014339995 | 1.550397380 | 12.081278448 |
| 1.356985371 | 0.727210478 | 14.160346444 |
| 2.699362553 | 1.576365772 | 12.107414979 |
| 4.041041247 | 0.727378247 | 14.160297984 |
| 5.413255806 | 1.550320865 | 12.081271839 |
| 6.748942106 | 0.767344347 | 14.179654407 |
| -1.350576625 | 3.876545936 | 12.108445139 |

| | | |
|--------------|-------------|--------------|
| -0.053596936 | 3.086689231 | 14.206525193 |
| 1.341842393 | 3.880302281 | 12.059045948 |
| 2.698978487 | 3.118401165 | 14.276344008 |
| 4.056867746 | 3.880245836 | 12.059042277 |
| 5.450404369 | 3.087189296 | 14.206868825 |
| -2.704048587 | 6.240124254 | 12.080986948 |
| -1.350969199 | 5.518957367 | 14.144037178 |
| 0.002959791 | 6.240037704 | 12.081014850 |
| 1.317253267 | 5.523078308 | 14.206605962 |
| 2.699325257 | 6.244757386 | 12.093078655 |
| 4.080806543 | 5.522483331 | 14.206788057 |
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TS *pNNH Cleavage

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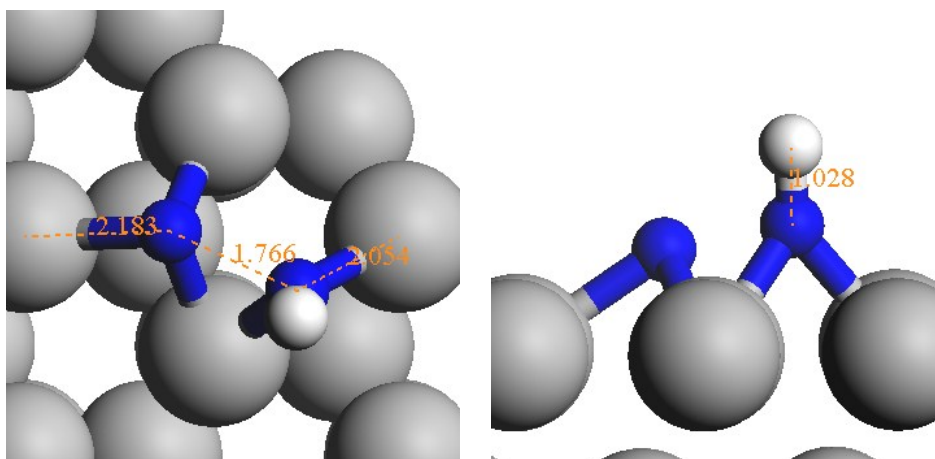
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | N | H |
|----|---|---|
| 27 | 2 | 1 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003364194 | 1.572807509 | 12.088140058 |
| 1.335355342 | 0.729180793 | 14.152141882 |
| 2.689170393 | 1.541586233 | 12.063684235 |
| 4.051335669 | 0.745938844 | 14.146159174 |
| 5.397004596 | 1.565596697 | 12.077258403 |
| 6.761808150 | 0.830560046 | 14.159139330 |
| -1.339839989 | 3.896676084 | 12.103875871 |

| | | |
|--------------|-------------|--------------|
| 0.026609030 | 3.128771672 | 14.218492077 |
| 1.352592606 | 3.898985333 | 12.048947009 |
| 2.764321165 | 3.084467158 | 14.184930762 |
| 4.061327348 | 3.904151144 | 12.090070414 |
| 5.439293384 | 3.107113104 | 14.163737233 |
| -2.710604677 | 6.238751582 | 12.075246545 |
| -1.381814537 | 5.480831966 | 14.148530817 |
| -0.008352882 | 6.249510518 | 12.067506766 |
| 1.340531114 | 5.546798392 | 14.174966925 |
| 2.706869935 | 6.256064889 | 12.084307983 |
| 4.043340239 | 5.449622188 | 14.274401170 |
| 3.284691089 | 4.239077586 | 15.750827386 |
| 1.550729139 | 4.088278549 | 15.452429196 |
| 3.437422917 | 3.941039760 | 16.722550389 |



*N + *NH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | N | H |
|----|---|---|
| 27 | 2 | 1 |

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.005759776 | 1.554367695 | 12.076832535 |
| 1.350111902 | 0.723742005 | 14.149317938 |
| 2.699682587 | 1.570690801 | 12.095000934 |
| 4.042582035 | 0.738770732 | 14.158778076 |
| 5.409336635 | 1.553355230 | 12.072203793 |
| 6.758675729 | 0.790189420 | 14.167777102 |
| -1.344383840 | 3.874055643 | 12.099266954 |
| -0.046634149 | 3.082742643 | 14.217337829 |
| 1.338668722 | 3.889520881 | 12.053098485 |
| 2.720001669 | 3.114647746 | 14.266117308 |
| 4.056854228 | 3.886124533 | 12.070597244 |
| 5.418287945 | 3.109732804 | 14.194863760 |
| -2.702416791 | 6.239226561 | 12.075034345 |
| -1.359417555 | 5.510055280 | 14.141528964 |
| 0.006886867 | 6.240406481 | 12.082437836 |
| 1.326870114 | 5.523460465 | 14.205973034 |
| 2.698176198 | 6.248868293 | 12.095484808 |
| 4.084874113 | 5.515254958 | 14.210175908 |
| 4.142442904 | 3.943079744 | 15.483445585 |
| 1.243596210 | 3.939623605 | 15.322554218 |
| 4.131595890 | 3.979285160 | 16.505172805 |

TS *HNNH Cleavage

1.0

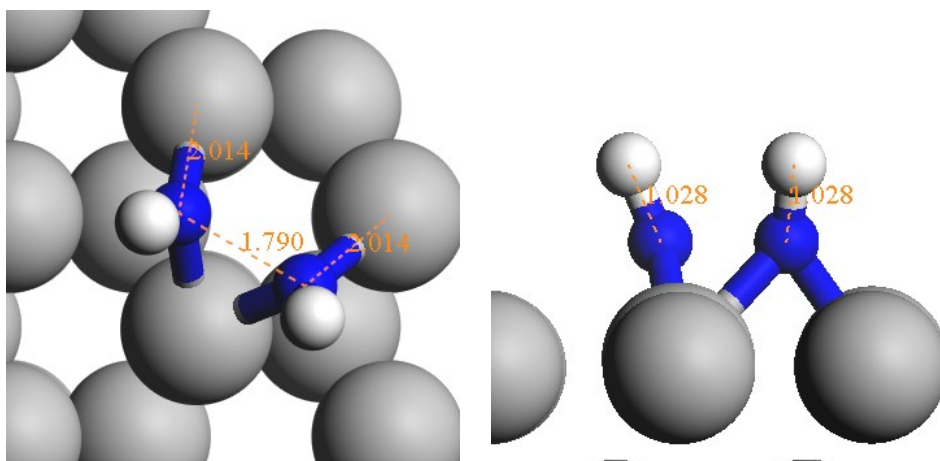
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.005756336 | 1.561517776 | 12.076955890 |
| 1.332869357 | 0.742469639 | 14.143590751 |
| 2.699672086 | 1.556453358 | 12.079568368 |
| 4.066358522 | 0.742508419 | 14.143439495 |
| 5.393720606 | 1.561537636 | 12.076946345 |
| 6.749690804 | 0.820987041 | 14.151058122 |
| -1.350294188 | 3.900724273 | 12.088214952 |
| -0.013334509 | 3.111617667 | 14.160579937 |
| 1.351137213 | 3.899318153 | 12.068619162 |
| 2.699810106 | 3.085185689 | 14.256856887 |
| 4.048363024 | 3.899417664 | 12.068984820 |
| 5.412675785 | 3.111476553 | 14.160472736 |
| -2.698480662 | 6.245537171 | 12.064844358 |
| -1.350632569 | 5.474005820 | 14.143257400 |
| -0.002222076 | 6.245706507 | 12.064622613 |
| 1.330757842 | 5.482950555 | 14.209233125 |
| 2.699774741 | 6.250366817 | 12.083907814 |
| 4.067783318 | 5.482341361 | 14.210573874 |
| 1.521200028 | 3.911346486 | 16.637100760 |
| 3.870488784 | 3.912770585 | 16.639732328 |
| 1.801778363 | 4.205688175 | 15.693474748 |
| 3.591873022 | 4.207327604 | 15.695564437 |



*NH *NH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | N | H |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.006116322 | 1.558739611 | 12.067345964 |
| 1.349605809 | 0.737807813 | 14.152548659 |
| 2.700058445 | 1.572792666 | 12.091991224 |
| 4.050151578 | 0.737946627 | 14.153049421 |
| 5.405407266 | 1.559681937 | 12.067377537 |
| 6.749393280 | 0.806231971 | 14.154625131 |
| -1.350660692 | 3.879092674 | 12.088918368 |
| -0.016126890 | 3.100883609 | 14.200673183 |
| 1.341323627 | 3.892291730 | 12.067761552 |
| 2.701328384 | 3.122122180 | 14.276301421 |
| 4.058433217 | 3.892723642 | 12.067690329 |
| 5.412394314 | 3.105239113 | 14.202062393 |
| -2.704811226 | 6.244248540 | 12.076061568 |
| -1.350578978 | 5.503768920 | 14.142661185 |
| 0.005057547 | 6.244080040 | 12.077349450 |
| 1.321635621 | 5.517458842 | 14.210435834 |
| 2.699212282 | 6.254305461 | 12.095641939 |
| 4.076991235 | 5.518871235 | 14.209271306 |
| 4.131173924 | 3.938796573 | 15.480922686 |
| 1.267039415 | 3.930377409 | 15.475897446 |

| | | |
|-------------|-------------|--------------|
| 4.099869567 | 3.992118364 | 16.504782181 |
| 1.304208075 | 3.962157496 | 16.500395743 |

TS *pNNH₂ Cleavage

1.0

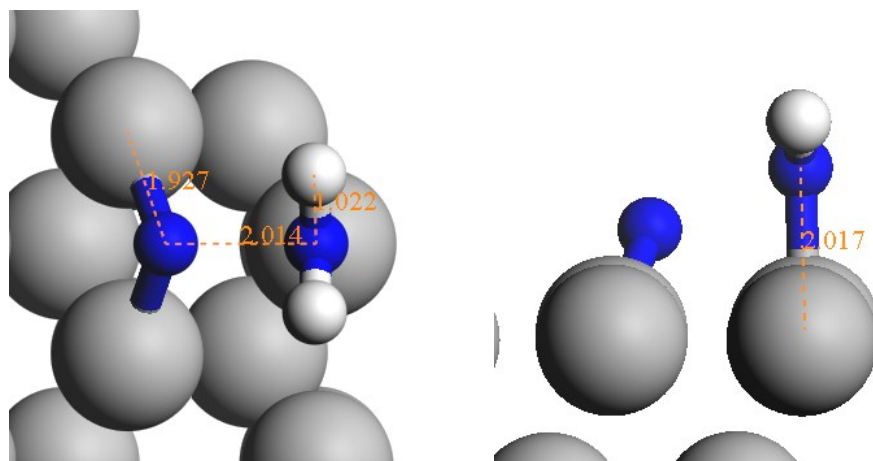
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.009269353 | 1.560042562 | 12.074314776 |
| 1.368690015 | 0.814800664 | 14.143965221 |
| 2.703779185 | 1.553578085 | 12.060644421 |
| 4.061474933 | 0.785990030 | 14.143266211 |
| 5.399433490 | 1.558552400 | 12.080606604 |
| 6.750800575 | 0.835358804 | 14.140191152 |
| -1.344362838 | 3.904551698 | 12.074354425 |
| -0.029363391 | 3.100806257 | 14.149641010 |
| 1.363911314 | 3.905112391 | 12.067975220 |
| 2.724964829 | 3.103035020 | 14.245964953 |
| 4.035962125 | 3.907599757 | 12.082890137 |
| 5.448770340 | 3.090824806 | 14.140357093 |
| -2.695724069 | 6.237888593 | 12.083181636 |
| -1.310084688 | 5.454373647 | 14.143896201 |
| -0.002741084 | 6.241330515 | 12.060399914 |
| 1.349729134 | 5.484768101 | 14.245756424 |
| 2.702117275 | 6.217965412 | 12.082853424 |
| 4.106022823 | 5.488653226 | 14.260400401 |

| | | |
|-------------|-------------|--------------|
| 3.608233586 | 6.187894161 | 16.841341058 |
| 4.464613049 | 4.718887575 | 16.844421991 |
| 2.445630543 | 4.529897911 | 15.510981606 |
| 4.056557307 | 5.463957680 | 16.276917971 |



*N + *NH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 2 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.016319767 | 1.551333121 | 12.082195532 |
| 1.343341811 | 0.729494745 | 14.152575092 |
| 2.697102034 | 1.553958674 | 12.096812341 |
| 4.043399412 | 0.777780027 | 14.152999491 |
| 5.384944733 | 1.552726385 | 12.074905116 |

| | | |
|--------------|-------------|--------------|
| 6.714798234 | 0.798669420 | 14.146630566 |
| -1.365709374 | 3.888267372 | 12.083310865 |
| -0.051102079 | 3.089806278 | 14.199797952 |
| 1.338854117 | 3.891811734 | 12.043475342 |
| 2.713263987 | 3.085350008 | 14.200323678 |
| 4.038311901 | 3.902246212 | 12.088846411 |
| 5.396291322 | 3.085655023 | 14.150639597 |
| -2.701185174 | 6.235085549 | 12.065576410 |
| -1.398912092 | 5.476790884 | 14.151472242 |
| -0.006824345 | 6.237818349 | 12.095755748 |
| 1.325140250 | 5.486758328 | 14.199552710 |
| 2.698034256 | 6.224621803 | 12.088074709 |
| 4.075816829 | 5.477934011 | 14.232401799 |
| 3.498625485 | 6.190030729 | 16.725621043 |
| 4.375333143 | 4.749719377 | 16.765134227 |
| 1.310942619 | 3.876979939 | 15.302096412 |
| 4.085683765 | 5.544088170 | 16.193466982 |

TS *HNNH₂ Cleavage

1.0

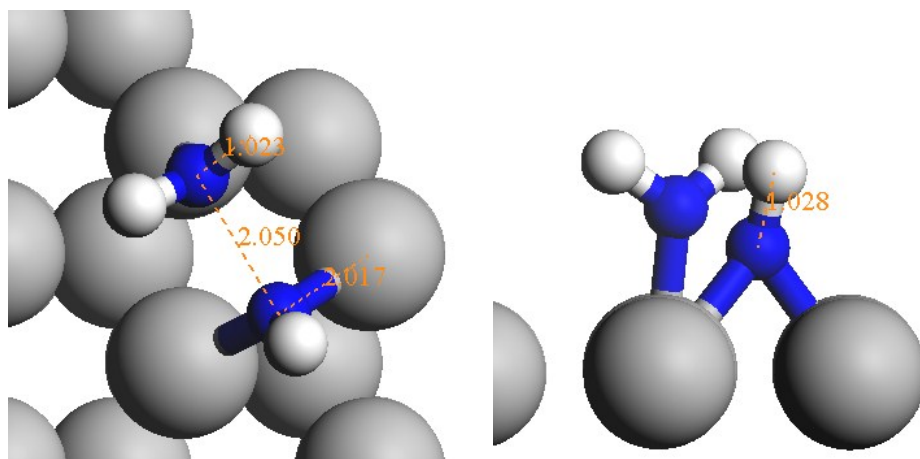
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| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | N | H |
| 27 | 2 | 3 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003533777 | 1.555331241 | 12.080944362 |
| 1.333654537 | 0.786928802 | 14.146438191 |
| 2.694317800 | 1.544317255 | 12.072656828 |

| | | |
|--------------|-------------|--------------|
| 4.046126253 | 0.774364028 | 14.155177291 |
| 5.395859279 | 1.553989197 | 12.082589826 |
| 6.754904084 | 0.806364670 | 14.145891906 |
| -1.348694679 | 3.901925100 | 12.082174973 |
| -0.023276881 | 3.095400030 | 14.144482136 |
| 1.353946612 | 3.902031719 | 12.072418930 |
| 2.722329357 | 3.124078540 | 14.190446483 |
| 4.051984730 | 3.895439299 | 12.057074474 |
| 5.415455613 | 3.107545644 | 14.170803700 |
| -2.691656016 | 6.245831524 | 12.073434404 |
| -1.349626660 | 5.459925797 | 14.155266870 |
| -0.010996199 | 6.240952958 | 12.077613048 |
| 1.334556735 | 5.460801748 | 14.213118801 |
| 2.696913441 | 6.228130206 | 12.072498964 |
| 4.052507118 | 5.430747640 | 14.193574408 |
| 3.451527609 | 4.237987979 | 15.705412262 |
| 1.720414889 | 5.215987038 | 16.204317799 |
| 3.816335786 | 4.026220244 | 16.643181857 |
| 1.233717929 | 4.511388377 | 16.765344224 |
| 2.053494812 | 5.985978053 | 16.790233991 |



*NH + *NH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N H

27 2 3

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.008514740 | 1.565562516 | 12.079778365 |
| 1.351412649 | 0.754717482 | 14.148950811 |
| 2.715686907 | 1.555973884 | 12.073855866 |
| 4.054001497 | 0.800192090 | 14.156424056 |
| 5.408810808 | 1.558326722 | 12.069552399 |
| 6.757767224 | 0.818395251 | 14.167512771 |
| -1.363787296 | 3.885522447 | 12.083498100 |
| -0.000803979 | 3.121418074 | 14.202840703 |
| 1.347892089 | 3.910934224 | 12.064432441 |
| 2.662689968 | 3.106429695 | 14.166687468 |
| 4.061433805 | 3.896378804 | 12.082479688 |
| 5.377125101 | 3.166083002 | 14.225580573 |
| -2.707603124 | 6.241533301 | 12.072545956 |
| -1.336253165 | 5.521495325 | 14.122038906 |
| 0.013861362 | 6.252862128 | 12.094592689 |
| 1.354855962 | 5.493020855 | 14.210394716 |
| 2.697324543 | 6.260179141 | 12.092815792 |
| 4.108225345 | 5.459170263 | 14.199422013 |
| 4.800766220 | 4.359778614 | 15.885119641 |
| 1.343670265 | 3.911461885 | 15.490205134 |
| 4.062433920 | 3.954397699 | 16.470596749 |
| 1.325261915 | 3.918916040 | 16.516274736 |
| -2.596316818 | 4.764105879 | 16.512735629 |

TS *H₂NNH₂ Cleavage

1.0

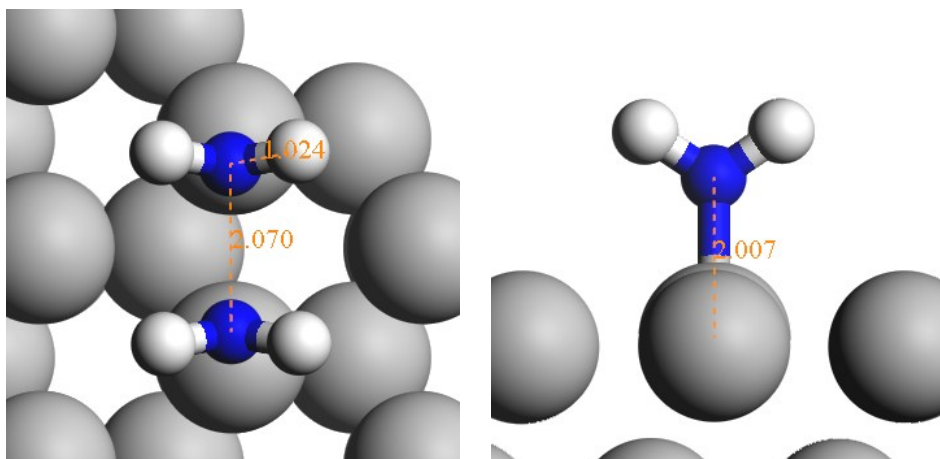
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| | | |
|----|---|---|
| Ru | H | N |
| 27 | 4 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.011543450 | 1.560421269 | 12.078626319 |
| 1.346110384 | 0.775600342 | 14.145098910 |
| 2.714145032 | 1.563158459 | 12.080799713 |
| 4.061763193 | 0.786659798 | 14.155080369 |
| 5.401893767 | 1.560038485 | 12.068674965 |
| 6.764321293 | 0.797537844 | 14.146329521 |
| -1.342799599 | 3.906542344 | 12.078676249 |
| -0.023524436 | 3.103908044 | 14.129316839 |
| 1.363624533 | 3.905093994 | 12.055719774 |
| 2.714706586 | 3.129251250 | 14.253125405 |
| 4.041572234 | 3.890289795 | 12.075290600 |
| 5.422893231 | 3.121374172 | 14.146461687 |
| -2.691395486 | 6.240467526 | 12.086921929 |
| -1.355856801 | 5.455203187 | 14.145140029 |
| 0.010291073 | 6.245883370 | 12.080744644 |
| 1.365811123 | 5.463230996 | 14.251984373 |
| 2.689846973 | 6.231472199 | 12.075065184 |
| 4.095965182 | 5.482925050 | 14.138149924 |
| 0.702851501 | 4.881932783 | 16.791772989 |
| 3.350795743 | 3.697586015 | 16.803830920 |
| 1.901443488 | 2.847292246 | 16.802619400 |
| 2.149827909 | 5.736374253 | 16.811471575 |
| 1.507443433 | 5.185443317 | 16.234413432 |
| 2.552945597 | 3.398599486 | 16.235356215 |



*NH₂ + *NH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | N |
|----|---|---|
| 27 | 4 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.015510780 | 1.574725089 | 12.083513519 |
| 1.330993236 | 0.751315228 | 14.135414090 |
| 2.721379272 | 1.580703402 | 12.066521396 |
| 4.073465514 | 0.802567768 | 14.447096417 |
| 5.369449463 | 1.543926527 | 12.100450573 |
| 6.826081070 | 0.820085428 | 14.134794379 |
| -1.330404373 | 3.906018446 | 12.083583273 |
| 0.013307955 | 3.129404907 | 14.148414805 |
| 1.370069398 | 3.911914704 | 12.073026159 |

| | | |
|--------------|-------------|--------------|
| 2.750771932 | 3.095031253 | 14.192797567 |
| 4.052759379 | 3.901238973 | 12.071341778 |
| 5.469799316 | 3.169908337 | 14.135086613 |
| -2.686464010 | 6.245485743 | 12.082949611 |
| -1.386567197 | 5.459426567 | 14.135521292 |
| 0.027398766 | 6.246664409 | 12.065685814 |
| 1.349629195 | 5.521376580 | 14.195341025 |
| 2.702470442 | 6.239073112 | 12.071896875 |
| 4.065575484 | 5.469030251 | 14.147032937 |
| 0.113182735 | 6.125369658 | 16.558635361 |
| 4.069874073 | 2.563820294 | 16.520035589 |
| 2.639970717 | 1.734258131 | 16.555046324 |
| 1.545912991 | 6.949793814 | 16.514130713 |
| 0.812530091 | 6.533713754 | 15.926439092 |
| 3.351024589 | 2.130294384 | 15.927578656 |

*N

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N

27 1

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.0000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.010353897 | 1.560819524 | 12.088933787 |
| 1.349951281 | 0.717947506 | 14.150867216 |
| 2.710321516 | 1.560820778 | 12.088929382 |
| 4.051165755 | 0.779927362 | 14.165568464 |
| 5.399982431 | 1.558769819 | 12.076991134 |

| | | |
|--------------|-------------|--------------|
| 6.748734201 | 0.779928459 | 14.165562590 |
| -1.353375885 | 3.886991285 | 12.088932319 |
| -0.041040455 | 3.093856140 | 14.212220073 |
| 1.349969084 | 3.897000123 | 12.047874997 |
| 2.740944465 | 3.093858231 | 14.212215668 |
| 4.053337288 | 3.886997975 | 12.088934522 |
| 5.399949601 | 3.116101114 | 14.165572870 |
| -2.700019761 | 6.235266175 | 12.074568828 |
| -1.403153228 | 5.486460630 | 14.150871621 |
| 0.006969667 | 6.243173985 | 12.088929382 |
| 1.349953152 | 5.503049762 | 14.212220073 |
| 2.692995779 | 6.243166877 | 12.088931585 |
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TS *N → *NH

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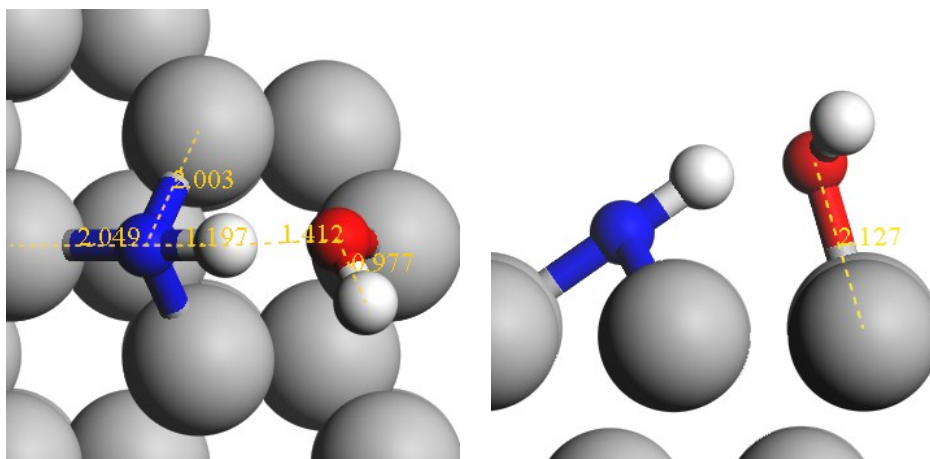
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| Ru | H | O | N |
|----|---|---|---|
| 27 | 2 | 1 | 1 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.006380412 | 1.566211849 | 12.089901535 |
| 1.348324313 | 0.736355543 | 14.153607454 |
| 2.701828502 | 1.545803550 | 12.072102466 |
| 4.048223073 | 0.779342889 | 14.144969682 |
| 5.398818949 | 1.557575578 | 12.075029205 |
| 6.739795836 | 0.814114119 | 14.152980401 |

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|--------------|-------------|--------------|
| -1.346782499 | 3.888241449 | 12.090555756 |
| 0.019461573 | 3.129009370 | 14.244841543 |
| 1.350677348 | 3.897517749 | 12.045488669 |
| 2.742023639 | 3.069247772 | 14.161096853 |
| 4.061754865 | 3.903794492 | 12.094818105 |
| 5.424587489 | 3.094187288 | 14.153907030 |
| -2.707777897 | 6.232156236 | 12.081916515 |
| -1.387427905 | 5.475463787 | 14.154896806 |
| -0.011579902 | 6.244911671 | 12.069245481 |
| 1.330055854 | 5.513385984 | 14.154686809 |
| 2.712289097 | 6.242765068 | 12.091524972 |
| 4.047907987 | 5.452217010 | 14.243845893 |
| 4.178715491 | 4.713949218 | 16.774143533 |
| 2.321241351 | 4.460249564 | 16.107995325 |
| 3.498908404 | 5.218368203 | 16.285877347 |
| 1.469809357 | 3.969981264 | 15.423593544 |



*NH

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N H

27 1 1

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.008710454 | 1.556371512 | 12.083759494 |
| 1.350058371 | 0.728488343 | 14.151442871 |
| 2.708787909 | 1.556591545 | 12.083803550 |
| 4.059279531 | 0.779859000 | 14.159287649 |
| 5.400022805 | 1.556596771 | 12.071526810 |
| 6.740797310 | 0.779657834 | 14.159277369 |
| -1.354468758 | 3.887517274 | 12.082827725 |
| -0.023248396 | 3.099154076 | 14.211150998 |
| 1.349926839 | 3.895043763 | 12.064548453 |
| 2.722526339 | 3.099343691 | 14.212062943 |
| 4.054267639 | 3.887492187 | 12.083241110 |
| 5.399905063 | 3.104293755 | 14.158819194 |
| -2.700002501 | 6.233436086 | 12.073398426 |
| -1.390665667 | 5.475530686 | 14.151849648 |
| 0.005391401 | 6.239958262 | 12.084305046 |
| 1.349774758 | 5.472446669 | 14.216446444 |
| 2.694589977 | 6.239839517 | 12.084291095 |
| 4.090697618 | 5.475529849 | 14.151886361 |
| 1.348772470 | 3.881870213 | 15.476123597 |
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TS *NH → *NH₂

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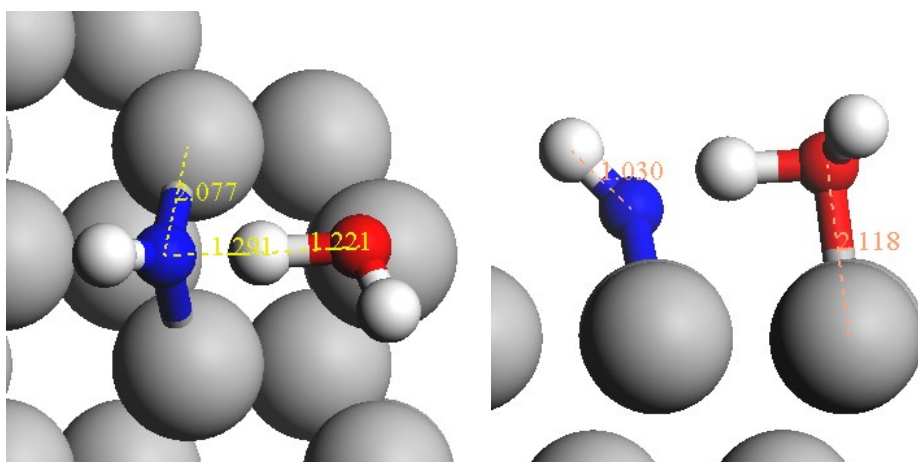
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| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | O | N |
|----|---|---|---|
| 27 | 3 | 1 | 1 |

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.001226004 | 1.556930322 | 12.081235127 |
| 1.356966602 | 0.772540733 | 14.146859653 |
| 2.707044708 | 1.552235727 | 12.077936120 |
| 4.057074957 | 0.782879672 | 14.147147481 |
| 5.397088059 | 1.555344621 | 12.077474274 |
| 6.730503973 | 0.802240384 | 14.147226781 |
| -1.350174756 | 3.898241925 | 12.081130128 |
| 0.000207120 | 3.117219363 | 14.160344976 |
| 1.356689627 | 3.899725815 | 12.057457021 |
| 2.687506612 | 3.111240736 | 14.186477102 |
| 4.053444711 | 3.898090985 | 12.083133909 |
| 5.411222684 | 3.091483756 | 14.147335450 |
| -2.694594383 | 6.237743507 | 12.083401178 |
| -1.352294600 | 5.460849831 | 14.146347143 |
| -0.001377422 | 6.244528259 | 12.075515282 |
| 1.339322430 | 5.445676018 | 14.183103936 |
| 2.705156004 | 6.235292098 | 12.080735099 |
| 4.078642644 | 5.468877639 | 14.193177911 |
| 4.496799478 | 4.926449490 | 16.753957401 |
| 1.121432232 | 3.761888761 | 16.456568078 |
| 2.778195321 | 4.748900289 | 16.229775879 |
| 3.793320098 | 5.425335559 | 16.291804251 |
| 1.757888918 | 4.130451303 | 15.735635655 |



*NH₂

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | N | H |
|----|---|---|
| 27 | 1 | 2 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.003958518 | 1.554364978 | 12.079862804 |
| 1.345106769 | 0.772082531 | 14.152118386 |
| 2.711119218 | 1.553818397 | 12.078036713 |
| 4.065087436 | 0.786812514 | 14.163938419 |
| 5.399517497 | 1.557994634 | 12.079910531 |
| 6.745371033 | 0.785348066 | 14.158067318 |
| -1.351292432 | 3.902013322 | 12.079714485 |
| -0.047588519 | 3.089443982 | 14.132356654 |
| 1.352814452 | 3.898096002 | 12.076697432 |
| 2.679322105 | 3.152386809 | 14.214002844 |

| | | |
|--------------|-------------|--------------|
| 4.042045134 | 3.888798379 | 12.073657618 |
| 5.403753805 | 3.109726114 | 14.157694316 |
| -2.691254087 | 6.239959516 | 12.085193494 |
| -1.357877913 | 5.454120269 | 14.152136008 |
| 0.002245492 | 6.246277652 | 12.078421462 |
| 1.370938193 | 5.417273047 | 14.216002954 |
| 2.689083187 | 6.231636100 | 12.074167925 |
| 4.101361170 | 5.484679042 | 14.128412237 |
| 2.017501765 | 4.276412749 | 15.890397464 |
| 1.293240602 | 3.852252617 | 16.475419334 |
| 2.717948693 | 4.678461705 | 16.522085628 |

TS *NH₂ → *NH₃

1.0

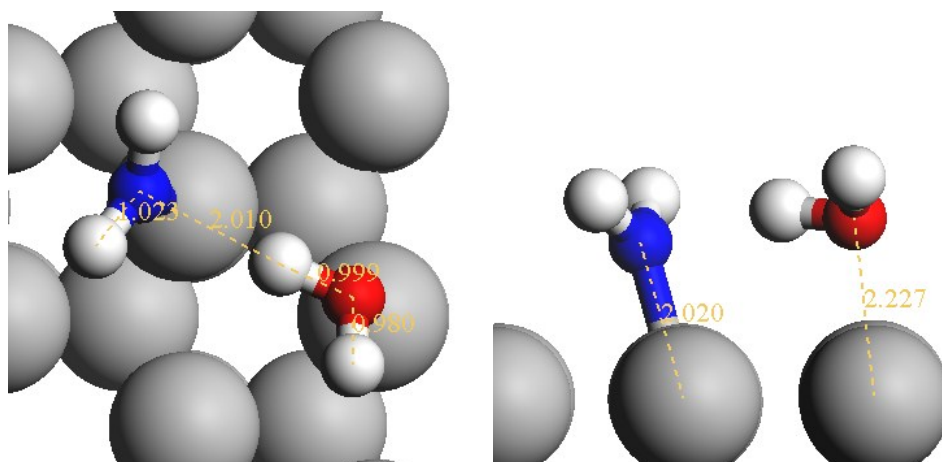
| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

| Ru | H | O | N |
|----|---|---|---|
| 27 | 4 | 1 | 1 |

Cartesian

| | | |
|--------------|-------------|--------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |
| 0.0000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| -0.000041883 | 1.563213860 | 12.067431872 |
| 1.342639492 | 0.738176224 | 14.131907290 |
| 2.701737857 | 1.567919535 | 12.063359695 |
| 4.047103133 | 0.746222064 | 14.142282309 |
| 5.401904207 | 1.565599728 | 12.084766158 |
| 6.752566015 | 0.766635171 | 14.152244678 |
| -1.356226262 | 3.884450400 | 12.112185432 |
| 0.016836361 | 3.120062127 | 14.174529309 |
| 1.346983946 | 3.898164991 | 12.076923583 |

| | | |
|--------------|-------------|--------------|
| 2.656501467 | 3.115406625 | 14.174563085 |
| 4.065126724 | 3.890842125 | 12.075386053 |
| 5.387171758 | 3.104948523 | 14.219060390 |
| -2.700621085 | 6.223413869 | 12.084068616 |
| -1.347727213 | 5.474094042 | 14.153451792 |
| -0.006110770 | 6.232131567 | 12.087022522 |
| 1.338957194 | 5.489197193 | 14.137550772 |
| 2.698821216 | 6.233574482 | 12.079008866 |
| 4.034259539 | 5.485936732 | 14.142630346 |
| 5.473042750 | 2.458368548 | 16.920881406 |
| 1.967857373 | 2.135113160 | 16.635873086 |
| 1.759190058 | 3.801197009 | 16.655653908 |
| 4.069778720 | 3.096923223 | 16.515063216 |
| 5.059706771 | 3.192241324 | 16.420347292 |
| 2.102093344 | 3.004251164 | 16.114038241 |



*NH₃

1.0

| | | |
|---------------|--------------|---------------|
| 8.1000003815 | 0.0000000000 | 0.0000000000 |
| -4.0500001907 | 7.0148061010 | 0.0000000000 |
| 0.0000000000 | 0.0000000000 | 69.2750015259 |

Ru N H

27 1 3

Cartesian

| | | |
|-------------|-------------|-------------|
| 1.349986585 | 0.779415119 | 9.996419384 |
| 4.050040625 | 0.779415119 | 9.996419384 |
| 6.750014037 | 0.779415119 | 9.996419384 |

| | | |
|--------------|-------------|--------------|
| 0.000000000 | 3.117660474 | 9.996419384 |
| 2.700054040 | 3.117660474 | 9.996419384 |
| 5.400027452 | 3.117660474 | 9.996419384 |
| -1.350027020 | 5.455975864 | 9.996419384 |
| 1.350027020 | 5.455975864 | 9.996419384 |
| 4.050000432 | 5.455975864 | 9.996419384 |
| 0.000172600 | 1.558357872 | 12.067776237 |
| 1.335608359 | 0.755967698 | 14.141260227 |
| 2.699591700 | 1.564319774 | 12.075426437 |
| 4.059947391 | 0.759713957 | 14.144548219 |
| 5.397516421 | 1.558400833 | 12.069488519 |
| 6.747945340 | 0.776999929 | 14.152824739 |
| -1.352096351 | 3.899295156 | 12.081050094 |
| -0.025880730 | 3.115080913 | 14.141769799 |
| 1.355356623 | 3.892736186 | 12.075493989 |
| 2.692029339 | 3.110486666 | 14.220001705 |
| 4.042123830 | 3.891821350 | 12.076012373 |
| 5.416174619 | 3.113569637 | 14.145709810 |
| -2.698724053 | 6.231262724 | 12.081049360 |
| -1.352328516 | 5.453355119 | 14.150663093 |
| -0.003902936 | 6.232365711 | 12.081582429 |
| 1.339028165 | 5.472323743 | 14.144336754 |
| 2.699006369 | 6.232405850 | 12.069471631 |
| 4.055022735 | 5.469825924 | 14.145908059 |
| 2.611451619 | 3.064363143 | 16.383950284 |
| 1.795291373 | 2.539776380 | 16.711110700 |
| 3.443277201 | 2.621438007 | 16.788805131 |
| 2.543369306 | 4.011089498 | 16.772124332 |