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# Transition Metal Small Clusters Anchored on Biphenylene for Effective Electrocatalytic Nitrogen Reduction

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| $Ru_1$@BPN | | | | |
|---|---|---|---|---|
| Initial | $H_1$ | $H_2$ | $H_3$ | $T_1$ |
| | | | | |
| Final | | | | |
| Relative energy/eV | **0** | 0.26 | 0.50 | Move to $H_1$ |
| Initial | $T_2$ | $B_1$ | $B_2$ | $B_3$ |
| | | | | |
| Final | | | | |
| Relative energy/eV | Move to $H_2$ | Move to $H_1$ | Move to $H_1$ | Move to $H_2$ |

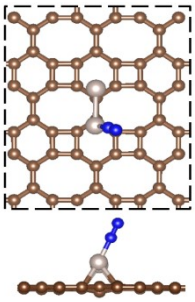
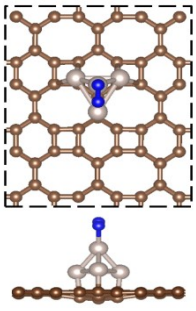
| $Ru_2$@BPN | | | | |
|---|---|---|---|---|
| Sites | | | | |
| Relative energy/eV | **0** | 0.28 | 0.10 | 0.37 |
| Sites | | | | |
| Relative energy/eV | 0.69 | 0.72 | 0.79 | 1.37 |
| $Ru_3$@BPN | | | | |
| Sites | | | | |
| Relative energy/eV | **0** | 0.05 | 0.06 | 0.11 |
| | | | | |
| | 0.56 | 0.65 | 0.84 | |

| $Ru_4$@BPN | | |
|---|---|---|
| Sites | | |
| Relative energy/eV | **0** | 0.10 |

**Fig. S1** The optimized structures and relative energies of $Ru_{1-4}$ clusters anchored on BPN sheet.

| | | | |
|---|---|---|---|
| $TM_1$@BPN | TM = V, Fe, Ni, Mo, Ru, Rh, W, Re, Ir | | |
| | | | |
| $TM_2$@BPN | Type 1 TM=V, Fe | Type 2<br>TM = Ni, Mo, Ru, Rh, W, Re, Ir | |
| | | | |
| $TM_3$@BPN | Type 1<br>TM = V, Fe, W | Type 2<br>TM=Ni, Ru, Rh, Ir | Type 3<br>TM = Mo, Re |
| | | | |
| $TM_4$@BPN | TM = V, Fe, Ni, Mo, Ru, Rh, W, Re, Ir | | |
| | | | |

**Fig. S2** The most stable structures for nine $TM_{1-4}$ clusters anchored on BPN sheet.

| **Structures of $N_2$ on $Ru_{2-4}$@BPN** | | | | |
|---|---|---|---|---|
| $Ru_2$@BPN | |  | | |
| Sites | Side on | End on-1 | End on-2 | |
| Relative energy/eV | / | 0 | 0.19 | |
| $Ru_3$@BPN | | | | |
| Sites | Side on-1 | Side on-2 | End on-1 | End on-2 |
| Energy/eV | **0** | 0.05 | **0** | 0.18 |
| $Ru_4$@BPN | | | |  |
| Sites | Side on-1 | Side on-2 | Side on-3 | Side on-4 |
| Relative energy/eV | **0** | 0.35 | 0.55 | 0.53 |
| $Ru_4$@BPN | | | | |
| Sites | End on-1 | End on-2 | | |
| Relative | **0** | 0.48 | | |

| | | | | |
|---|---|---|---|---|
| energy/eV | | | | |

**Fig. S3** Possible stable structures of $N_2$ adsorption on $Ru_n$@BPN (n=2-4) systems.

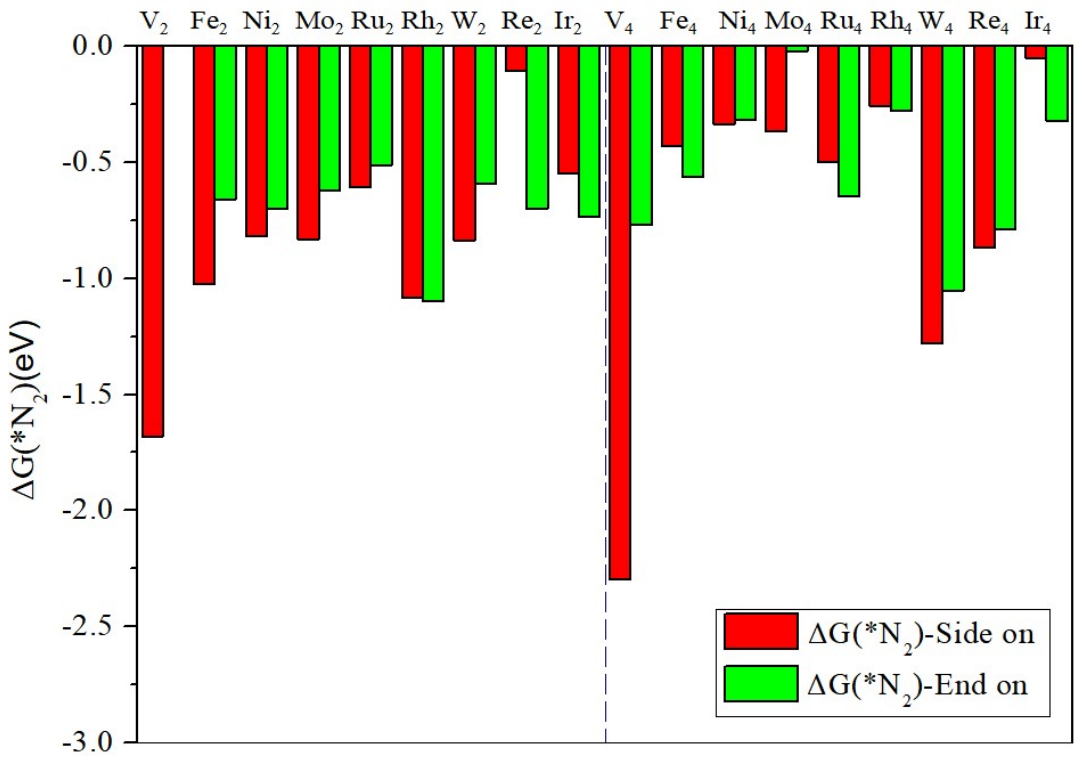
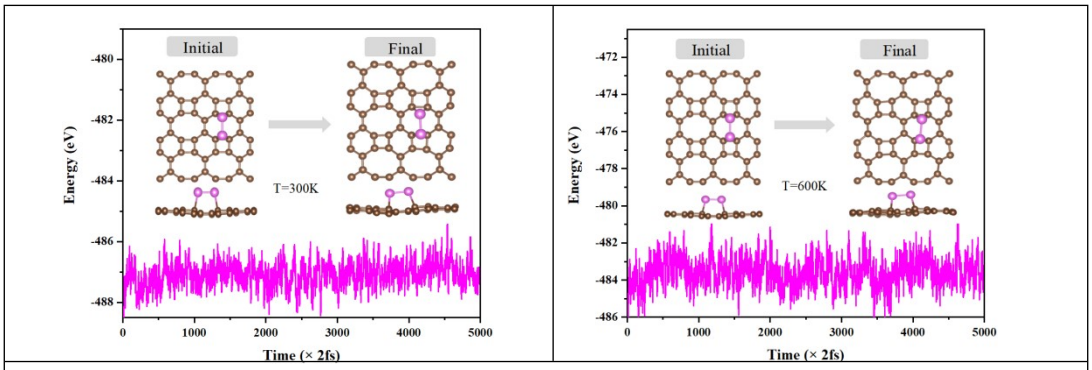
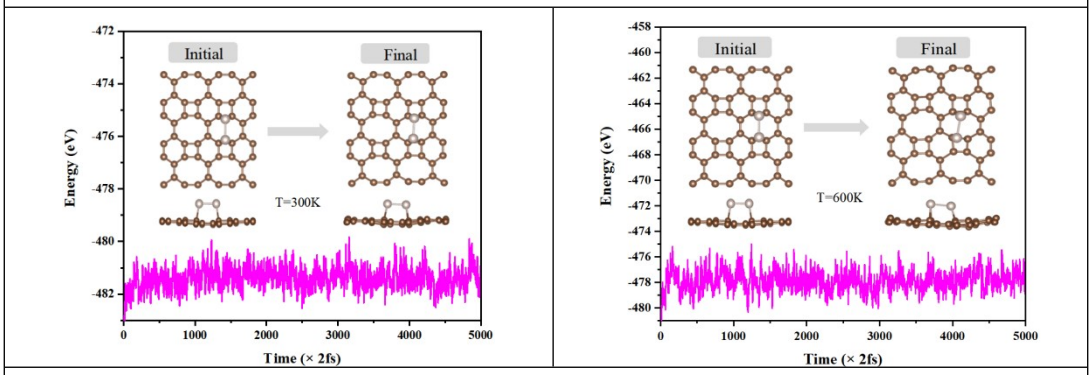


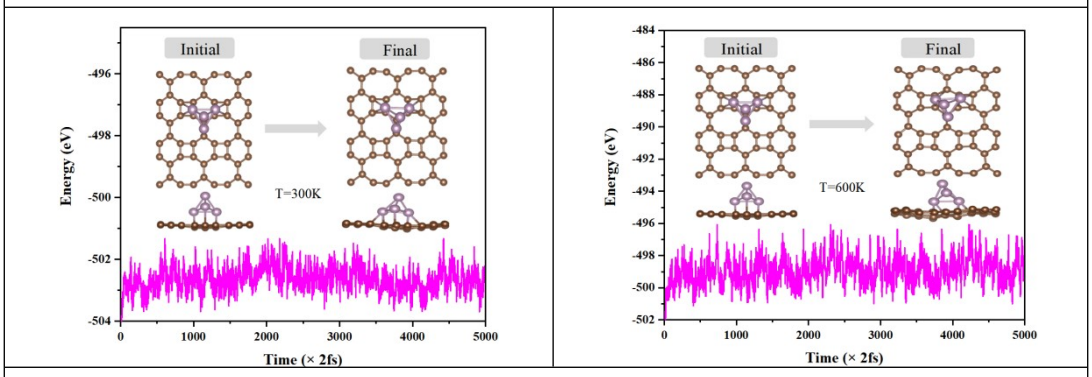

**Fig. S4.** The Gibbs free energy profile $\Delta G$ (*$N_2$) of $TM_2$ and $TM_4$ clusters anchored on BPN sheet. Note the end-on manner of $N_2$ adsorption over $V_2$@BPN can't be obtained.




$W_2$@BPN




$Ru_2$@BPN




$Mo_4$@BPN

**Figure S5.** Variation of energy with time for AIMD simulation of $W_2/Ru_2/Mo_4$ clusters anchored on BPN sheet at 300 and 600 K for a period of 10 ps.

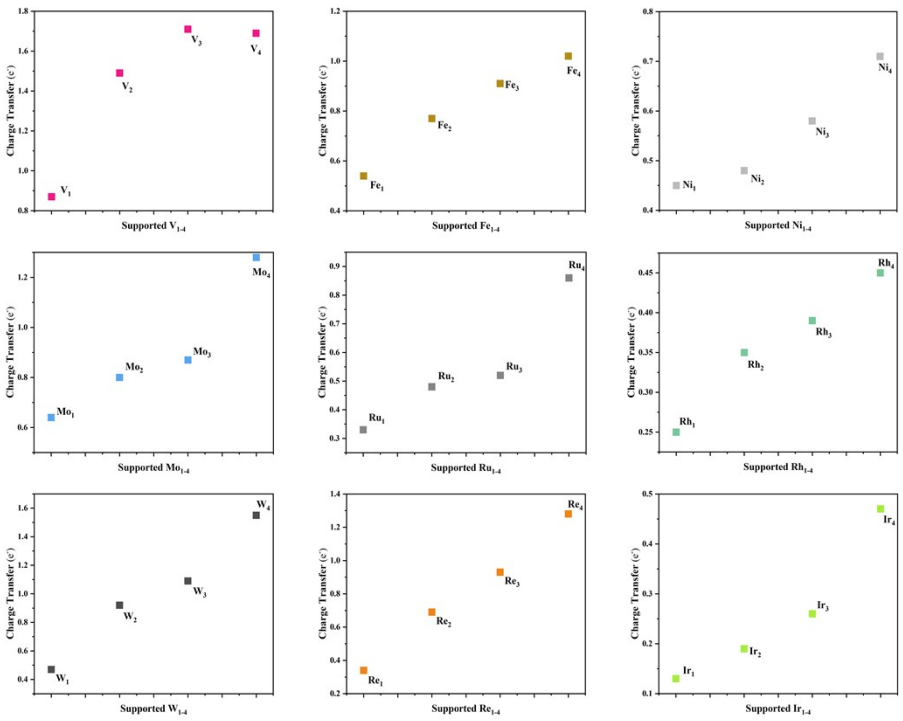



**Figure S6.** Bader charge transfers (|e|) of the $TM_{1-4}$@BPN with the number of TM atoms.

**Table S1** Bader charge dispersion (|e|) of the $Ru_{1-4}$@BPN and $Re_3$- and $Mo_3$@BPN catalysts.

| Atom | Charge of $Ru_1$@BPN | Charge of $Ru_2$@BPN | Charge of $Ru_3$@BPN | Charge of $Ru_4$@BPN | Charge of $Re_3$@BPN | Charge of $Mo_3$@BPN |
|---|---|---|---|---|---|---|
| 1 | +0.33 | +0.19 | +0.37 | −0.20 | −0.06 | −0.10 |
| 2 | | +0.19 | +0.37 | +0.35 | +0.47 | +0.47 |

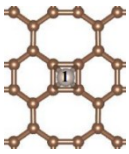
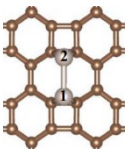
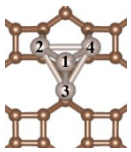
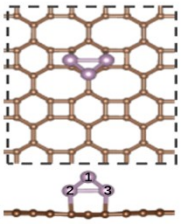
| | | | | | | |
|---|---|---|---|---|---|---|
| 3 | | | −0.22 | +0.38 | +0.48 | +0.50 |
| 1 | | | | +0.33 | | |
| Num. |  |  |  |  |  | |

**Table S2** Total Bader charge dispersion (|e|) of the $TM_{1-4}$@BPN catalysts.

| Atoms | Total Charge Transfers (\|e\|) | | | |
|---|---|---|---|---|
| | $TM_1$@BPN | $TM_2$@BPN | $TM_3$@BPN | $TM_4$@BPN |
| V | +0.87 | +1.49 | +1.71 | +1.69 |
| Fe | +0.54 | +0.77 | +0.91 | +1.02 |
| Ni | +0.45 | +0.46 | +0.46 | +0.71 |
| Mo | +0.64 | +0.80 | +0.87 | +1.28 |
| Ru | +0.33 | +0.38 | +0.52 | +0.86 |
| Rh | +0.25 | +0.35 | +0.26 | +0.45 |
| W | +0.47 | +0.92 | +1.09 | +1.55 |
| Re | +0.34 | +0.69 | +0.89 | +1.28 |
| Ir | +0.13 | +0.19 | +0.26 | +0.47 |

**Table S3** Bader charge dispersion (|e|) of the $TM_2$@BPN catalysts.

| DACs | Bader charge dispersion (\|e\|) of atom 1 | Bader charge dispersion (\|e\|) of atom 2 |
|---|---|---|
| $V_2$@BPN | +0.72 | +0.77 |
| $Fe_2$@BPN | +0.37 | +0.39 |
| $Ni_2$@BPN | +0.25 | +0.21 |
| $Mo_2$@BPN | +0.41 | +0.53 |

| | | |
|---|---|---|
| $Ru_2$@BPN | +0.19 | +0.27 |
| $Rh_2$@BPN | +0.17 | +0.18 |
| $W_2$@BPN | +0.52 | +0.37 |
| $Re_2$@BPN | +0.34 | +0.35 |
| $Ir_2$@BPN | +0.12 | +0.04 |

**Table S4** Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species for the screened three types of catalysts ($W_2$/$Ru_2$/$Mo_4$@BPN).

(a) Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species on $Ru_2$@BPN catalysts via the enzymatic pathway.

| Name | E /eV | $E_{ZPE}$/eV | TS/eV | G/eV |
|---|---|---|---|---|
| $H_2$ | -6.76565715 | 0.268608 | 0.4019062 | -6.89895535 |
| $N_2$ | -16.62627336 | 0.149570 | 0.59182775 | -17.06853111 |
| $NH_3$ | -19.54133424 | 0.909892 | 0.5951074 | -19.22654964 |
| $Ru_2$@BPN | -486.967 | 0.05684 | 0.2271903 | -487.1373503 |
| *N*N | -504.39840 | 0.263233 | 0.262526 | -504.397693 |
| *N*NH | -507.75419 | 0.580410 | 0.301215 | -507.474995 |
| *NH*NH | -510.81563 | 0.905457 | 0.332322 | -510.242495 |
| *NH*$NH_2$ | -495.90844 | 0.158166 | 0.252146 | -496.00282 |
| *$NH_2$*$NH_2$ | -499.72261 | 0.431923 | 0.264371 | -499.555058 |
| *$NH_2$ | -503.92511 | 0.777884 | 0.276249 | -503.423475 |
| *$NH_3$ | -507.30855 | 1.077951 | 0.399400 | -506.629999 |

(b) Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species on $W_2$@BPN catalysts via the consecutive pathway.

| Name | E /eV | $E_{ZPE}$/eV | TS/eV | G/eV |
|---|---|---|---|---|
| $W_2$@BPN | -492.703 | 0.051461 | 0.24060705 | -492.8921461 |
| *N*N | -510.754 | 0.248102 | 0.2927833 | -510.7986813 |
| *N*NH | -514.2436 | 0.551795 | 0.28652215 | -513.9783272 |
| *N*$NH_2$ | -517.69413 | 0.902867 | 0.38133385 | -517.1725969 |
| *N | -502.12865 | 0.139228 | 0.30142965 | -502.2908517 |
| *NH | -506.2148 | 0.431923 | 0.264371 | -506.047248 |
| *$NH_2$ | -509.80106 | 0.777884 | 0.276249 | -509.299425 |
| *$NH_3$ | -513.62218 | 1.077951 | 0.3994 | -512.943629 |

(c) Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species on $Mo_4$@BPN catalysts via the enzymatic pathway.

| Name | E /eV | $E_{ZPE}$/eV | TS/eV | G/eV |
|---|---|---|---|---|
| $Mo_4$@BPN | -508.80016 | 0.12636 | 0.430841 | -509.104641 |
| *N*N | -526.27272 | 0.318484 | 0.54814 | -526.502376 |

| | | | | |
|---|---|---|---|---|
| *N*NH | -529.88919 | 0.629341 | 0.520026 | -529.779875 |
| *NH*NH | -533.6458 | 0.970263 | 0.477964 | -533.153501 |
| *NH*$NH_2$ | -537.3689 | 1.330429 | 0.479917 | -536.518388 |
| *$NH_2$*$NH_2$ | -540.55188 | 1.628086 | 0.589149 | -539.512943 |
| *$NH_2$ | -525.99895 | 0.801735 | 0.54515 | -525.742365 |
| *$NH_3$ | -529.77104 | 1.157585 | 0.569335 | -529.18279 |

(d) Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species on $Mo_4$@BPN catalysts via the consecutive pathway.

| Name | E /eV | $E_{ZPE}$/eV | TS/eV | G/eV |
|---|---|---|---|---|
| $Mo_4$@BPN | -508.80016 | 0.12636 | 0.430841 | -509.104641 |
| *N*N | -526.27272 | 0.318484 | 0.54814 | -526.502376 |
| *N*NH | -529.88919 | 0.629341 | 0.520026 | -529.779875 |
| *N*$NH_2$ | -533.84784 | 0.989463 | 0.488202 | -533.346579 |
| *N | -518.5529 | 0.236008 | 0.430523 | -518.747415 |
| *NH | -522.43934 | 0.533874 | 0.428223 | -522.333689 |
| *$NH_2$ | -525.97361 | 0.801735 | 0.54515 | -525.717025 |
| *$NH_3$ | -529.7828 | 1.157585 | 0.569335 | -529.19455 |

(e) Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species on $Mo_4$@BPN catalysts via the enzymatic pathway using PBE+ U functional.

| Name | E /eV | $E_{ZPE}$/eV | TS/eV | G/eV |
|---|---|---|---|---|
| $Mo_4$@BPN | -494.574 | 0.090803 | 0.522202 | -495.005399 |
| *N*N | -512.941 | 0.280524 | 0.585392 | -513.245868 |
| *N*NH | -516.784 | 0.578571 | 0.505436 | -516.710865 |
| *N*$NH_2$ | -520.559 | 0.945462 | 0.561028 | -520.174566 |
| *N | -505.224 | 0.175477 | 0.483677 | -505.5322 |
| *NH | -509.165 | 0.466069 | 0.439419 | -509.13835 |
| *$NH_2$ | -512.657 | 0.803384 | 0.532326 | -512.385942 |
| *$NH_3$ | -517.076 | 1.098221 | 0.611879 | -516.589658 |

(f) Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species on the water solvation catalyst $Mo_4$@BPN via the enzymatic pathway.

| Name | E /eV | $E_{ZPE}$/eV | TS/eV | G/eV |
|---|---|---|---|---|
| $Mo_4$@BPN | -513.3199405 | 0.12636 | 0.430841 | -513.6244215 |
| *N*N | -531.0950405 | 0.318484 | 0.54814 | -531.3246965 |
| *N*NH | -534.8721405 | 0.629341 | 0.520026 | -534.7628255 |

| | | | | |
|---|---|---|---|---|
| *N*$NH_2$ | -538.8083405 | 0.989463 | 0.488202 | -538.3070795 |
| *N | -523.6277405 | 0.236008 | 0.430523 | -523.8222555 |
| *NH | -527.6133405 | 0.533874 | 0.428223 | -527.5076895 |
| *$NH_2$ | -531.0011405 | 0.801735 | 0.54515 | -530.7445555 |
| *$NH_3$ | -534.9187405 | 1.157585 | 0.569335 | -534.3304905 |

$Mo_4$@BPN

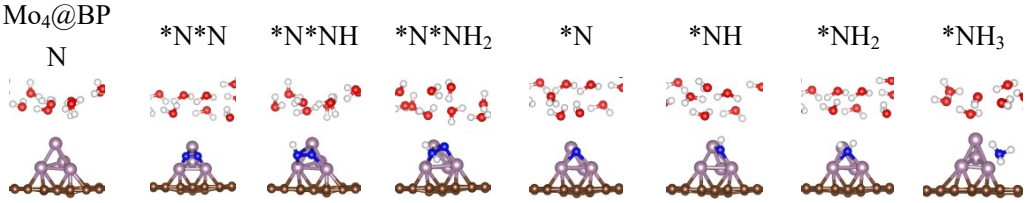



**Table S5** The optimized geometry of screened catalysts $W_2$@BPN, $Ru_2$@BPN and $Mo_4$@BPN.

$W_2$@BPN

1.00000000000000

| | | |
|---|---|---|
| 11.2750997542999993 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 13.5749998092999995 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 19.9498996734999992 |

C W

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Direct

| | | |
|---|---|---|
| 0.0589174744069909 | 0.0495851248695908 | 0.4002384903255636 |
| 0.2633317109073119 | 0.0495806496263571 | 0.4000857061860258 |
| 0.1611261756663091 | 0.1092192449380177 | 0.3989177742597703 |
| 0.1611301479008734 | 0.2157252855118958 | 0.3945943342205174 |
| 0.2630947273830969 | 0.2752648362371153 | 0.3913412752899832 |
| 0.0591622583865537 | 0.2752765854056121 | 0.3914789590181471 |
| 0.3928786734332452 | 0.0497484775005090 | 0.4021889436769226 |
| 0.5966614428488122 | 0.0500111267471929 | 0.4068076208994376 |
| 0.4947101049304376 | 0.1101504410715540 | 0.4047856932349537 |
| 0.4945782673025781 | 0.2169762708547752 | 0.4036731896001925 |
| 0.5974516717192008 | 0.2776196230431351 | 0.4080887547739839 |
| 0.3931766933982671 | 0.2756255724965028 | 0.3948429321713395 |
| 0.7255973299261240 | 0.0500144180927339 | 0.4068983121349877 |
| 0.9293705846550847 | 0.0497559857097074 | 0.4024258664652202 |
| 0.8275397397971801 | 0.1101683865092010 | 0.4049809051175812 |
| 0.8276768791960563 | 0.2169966979179701 | 0.4038797035925376 |
| 0.9290931213100785 | 0.2756458345542566 | 0.3950847146043651 |
| 0.7247843678645498 | 0.2776290140044043 | 0.4082094914421979 |
| 0.0596926398076315 | 0.3816575345608087 | 0.3860603910281712 |
| 0.2625607516402579 | 0.3816480245954263 | 0.3859185436716451 |
| 0.1611206648062264 | 0.4422326458999981 | 0.3839162685206366 |
| 0.1611187937974017 | 0.5498961896422832 | 0.3832606678953852 |
| 0.2625827749291758 | 0.6104951225032631 | 0.3846359507876160 |

| | | |
|---|---|---|
| 0.0596637465067064 | 0.6104984381681485 | 0.3847368668738010 |
| 0.3920740093799090 | 0.3822935464852133 | 0.3882138716211749 |
| 0.5945661057499491 | 0.3869350669524249 | 0.4065063668243079 |
| 0.4907557330380824 | 0.4433791140110371 | 0.3903298661144237 |
| 0.4907474716694654 | 0.5487427807611269 | 0.3899226997659695 |
| 0.5945489494768147 | 0.6053796984174608 | 0.4058281448728789 |
| 0.3921142057236590 | 0.6098196903524451 | 0.3871557070513979 |
| 0.7276700103539823 | 0.3869552076006705 | 0.4066660725882638 |
| 0.9301969133977538 | 0.3823201708881855 | 0.3884516458412848 |
| 0.8315132186842914 | 0.4433945970284379 | 0.3905368359112913 |
| 0.8315196492639357 | 0.5487485340414193 | 0.3901037765808522 |
| 0.9301460170804313 | 0.6098194405390510 | 0.3873362744751034 |
| 0.7276821450454155 | 0.6053759018668259 | 0.4059283752541211 |
| 0.0591276789099236 | 0.7169279282103712 | 0.3895111461692129 |
| 0.2631142099215002 | 0.7169258269979718 | 0.3894212136743899 |
| 0.1611224154490180 | 0.7764786952111886 | 0.3925582349868447 |
| 0.1611219282130049 | 0.8829445693674245 | 0.3975601119022108 |
| 0.2633399908683692 | 0.9425716923481026 | 0.3994756169194555 |
| 0.0589136032166025 | 0.9425746033699010 | 0.3996058449027370 |
| 0.3932120913705668 | 0.7165764063389618 | 0.3932150631853355 |
| 0.5974370811845560 | 0.7146721457288087 | 0.4068756683566779 |
| 0.4945577796432790 | 0.7752566741332914 | 0.4021739446470084 |
| 0.4947370294624417 | 0.8820728156031902 | 0.4036957810751731 |
| 0.5966724420481641 | 0.9421904971830229 | 0.4062648905283081 |
| 0.3929030116174536 | 0.9424685483113694 | 0.4016290747744376 |
| 0.7247829549214861 | 0.7146695879221815 | 0.4069481690087845 |
| 0.9290412746732026 | 0.7165762133593947 | 0.3933696855544330 |
| 0.8276826289970138 | 0.7752553969000413 | 0.4023027441175687 |
| 0.8275083854972705 | 0.8820720492085941 | 0.4038402673407552 |
| 0.9293442970523325 | 0.9424756216854481 | 0.4018362522791251 |
| 0.7255745348863480 | 0.9421923780590198 | 0.4063424683482124 |
| 0.6607884248779115 | 0.4194884207954490 | 0.5086704309903570 |
| 0.6607980891407257 | 0.5744860463010018 | 0.5081461766820001 |

$Ru_2$@BPN

1.00000000000000

| | | |
|---|---|---|
| 11.2750997542999993 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 13.5749998092999995 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 19.9498996734999992 |

C Ru

54 2

Direct

| | | |
|---|---|---|
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$Mo_4$@BPN

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| 54 | 4 |

Direct

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