

Supplementary Information

Novel Two-Dimensional Molybdenene as a Promising Electrocatalyst for Nitrogen Reduction Reaction: A First- Principles Prediction

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Coordinates of various adsorbed species

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1.000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

Mo

72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1250000000000000 | 0.0416666666666643 | 0.4476023543301935 | T | T | T |
| 0.2916666666666643 | 0.0416666666666643 | 0.4476023543301935 | T | T | T |
| 0.4583333333333357 | 0.0416666666666643 | 0.4476023543301935 | T | T | T |
| 0.6250000000000000 | 0.0416666666666643 | 0.4476023543301935 | T | T | T |
| 0.7916666666666643 | 0.0416666666666643 | 0.4476023543301935 | T | T | T |
| 0.9583333333333357 | 0.0416666666666643 | 0.4476023543301935 | T | T | T |
| 0.1250000000000000 | 0.2083333333333357 | 0.4476023543301935 | T | T | T |
| 0.2916666666666643 | 0.2083333333333357 | 0.4476023543301935 | T | T | T |
| 0.4583333333333357 | 0.2083333333333357 | 0.4476023543301935 | T | T | T |
| 0.6250000000000000 | 0.2083333333333357 | 0.4476023543301935 | T | T | T |
| 0.7916666666666643 | 0.2083333333333357 | 0.4476023543301935 | T | T | T |
| 0.9583333333333357 | 0.2083333333333357 | 0.4476023543301935 | T | T | T |
| 0.1250000000000000 | 0.3750000000000000 | 0.4476023543301935 | T | T | T |
| 0.2916666666666643 | 0.3750000000000000 | 0.4476023543301935 | T | T | T |
| 0.4583333333333357 | 0.3750000000000000 | 0.4476023543301935 | T | T | T |
| 0.6250000000000000 | 0.3750000000000000 | 0.4476023543301935 | T | T | T |
| 0.7916666666666643 | 0.3750000000000000 | 0.4476023543301935 | T | T | T |
| 0.9583333333333357 | 0.3750000000000000 | 0.4476023543301935 | T | T | T |
| 0.1250000000000000 | 0.5416666666666643 | 0.4476023543301935 | T | T | T |
| 0.2916666666666643 | 0.5416666666666643 | 0.4476023543301935 | T | T | T |
| 0.4583333333333357 | 0.5416666666666643 | 0.4476023543301935 | T | T | T |
| 0.6250000000000000 | 0.5416666666666643 | 0.4476023543301935 | T | T | T |
| 0.7916666666666643 | 0.5416666666666643 | 0.4476023543301935 | T | T | T |
| 0.9583333333333357 | 0.5416666666666643 | 0.4476023543301935 | T | T | T |
| 0.1250000000000000 | 0.7083333333333357 | 0.4476023543301935 | T | T | T |
| 0.2916666666666643 | 0.7083333333333357 | 0.4476023543301935 | T | T | T |
| 0.4583333333333357 | 0.7083333333333357 | 0.4476023543301935 | T | T | T |
| 0.6250000000000000 | 0.7083333333333357 | 0.4476023543301935 | T | T | T |
| 0.7916666666666643 | 0.7083333333333357 | 0.4476023543301935 | T | T | T |
| 0.9583333333333357 | 0.7083333333333357 | 0.4476023543301935 | T | T | T |
| 0.1250000000000000 | 0.8750000000000000 | 0.4476023543301935 | T | T | T |
| 0.2916666666666643 | 0.8750000000000000 | 0.4476023543301935 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.4583333333333357 | 0.8750000000000000 | 0.4476023543301935 | T | T | T |
| 0.6250000000000000 | 0.8750000000000000 | 0.4476023543301935 | T | T | T |
| 0.7916666666666643 | 0.8750000000000000 | 0.4476023543301935 | T | T | T |
| 0.9583333333333357 | 0.8750000000000000 | 0.4476023543301935 | T | T | T |
| 0.0416666666666643 | 0.1250000000000000 | 0.5523976456698065 | T | T | T |
| 0.2083333333333357 | 0.1250000000000000 | 0.5523976456698065 | T | T | T |
| 0.3750000000000000 | 0.1250000000000000 | 0.5523976456698065 | T | T | T |
| 0.5416666666666643 | 0.1250000000000000 | 0.5523976456698065 | T | T | T |
| 0.7083333333333357 | 0.1250000000000000 | 0.5523976456698065 | T | T | T |
| 0.8750000000000000 | 0.1250000000000000 | 0.5523976456698065 | T | T | T |
| 0.0416666666666643 | 0.2916666666666643 | 0.5523976456698065 | T | T | T |
| 0.2083333333333357 | 0.2916666666666643 | 0.5523976456698065 | T | T | T |
| 0.3750000000000000 | 0.2916666666666643 | 0.5523976456698065 | T | T | T |
| 0.5416666666666643 | 0.2916666666666643 | 0.5523976456698065 | T | T | T |
| 0.7083333333333357 | 0.2916666666666643 | 0.5523976456698065 | T | T | T |
| 0.8750000000000000 | 0.2916666666666643 | 0.5523976456698065 | T | T | T |
| 0.0416666666666643 | 0.4583333333333357 | 0.5523976456698065 | T | T | T |
| 0.2083333333333357 | 0.4583333333333357 | 0.5523976456698065 | T | T | T |
| 0.3750000000000000 | 0.4583333333333357 | 0.5523976456698065 | T | T | T |
| 0.5416666666666643 | 0.4583333333333357 | 0.5523976456698065 | T | T | T |
| 0.7083333333333357 | 0.4583333333333357 | 0.5523976456698065 | T | T | T |
| 0.8750000000000000 | 0.4583333333333357 | 0.5523976456698065 | T | T | T |
| 0.0416666666666643 | 0.6250000000000000 | 0.5523976456698065 | T | T | T |
| 0.2083333333333357 | 0.6250000000000000 | 0.5523976456698065 | T | T | T |
| 0.3750000000000000 | 0.6250000000000000 | 0.5523976456698065 | T | T | T |
| 0.5416666666666643 | 0.6250000000000000 | 0.5523976456698065 | T | T | T |
| 0.7083333333333357 | 0.6250000000000000 | 0.5523976456698065 | T | T | T |
| 0.8750000000000000 | 0.6250000000000000 | 0.5523976456698065 | T | T | T |
| 0.0416666666666643 | 0.7916666666666643 | 0.5523976456698065 | T | T | T |
| 0.2083333333333357 | 0.7916666666666643 | 0.5523976456698065 | T | T | T |
| 0.3750000000000000 | 0.7916666666666643 | 0.5523976456698065 | T | T | T |
| 0.5416666666666643 | 0.7916666666666643 | 0.5523976456698065 | T | T | T |
| 0.7083333333333357 | 0.7916666666666643 | 0.5523976456698065 | T | T | T |
| 0.8750000000000000 | 0.7916666666666643 | 0.5523976456698065 | T | T | T |
| 0.0416666666666643 | 0.9583333333333357 | 0.5523976456698065 | T | T | T |
| 0.2083333333333357 | 0.9583333333333357 | 0.5523976456698065 | T | T | T |
| 0.3750000000000000 | 0.9583333333333357 | 0.5523976456698065 | T | T | T |
| 0.5416666666666643 | 0.9583333333333357 | 0.5523976456698065 | T | T | T |
| 0.7083333333333357 | 0.9583333333333357 | 0.5523976456698065 | T | T | T |
| 0.8750000000000000 | 0.9583333333333357 | 0.5523976456698065 | T | T | T |

*N₂ end-on

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000566999999982

N Mo
2 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5423289317127171 | 0.4576680108266373 | 0.7199879438518337 | T | T | T |
| 0.5420784012710271 | 0.4579196692289997 | 0.6632756835520155 | T | T | T |
| 0.1253267657677029 | 0.0419965111174392 | 0.4479363672052088 | T | T | T |
| 0.2921944646909935 | 0.0421863751263984 | 0.4469974650054809 | T | T | T |
| 0.4582523017687592 | 0.0419210514717534 | 0.4483163284217895 | T | T | T |
| 0.6248776583860831 | 0.0418442717710050 | 0.4470764119964130 | T | T | T |
| 0.7917350147181992 | 0.0422048493737250 | 0.4473037446313626 | T | T | T |
| 0.9580331624026499 | 0.0419671203682768 | 0.4485601870345235 | T | T | T |
| 0.1255272716675506 | 0.2088628254381462 | 0.4469989342878051 | T | T | T |
| 0.2917931257897379 | 0.2084602154265625 | 0.4457597519526360 | T | T | T |
| 0.4586152966473378 | 0.2084067689155091 | 0.4469203882071042 | T | T | T |
| 0.6252875142679031 | 0.2089830939363964 | 0.4472514607704099 | T | T | T |
| 0.7914085867071847 | 0.2085913505855359 | 0.4466042679337647 | T | T | T |
| 0.9577951908828055 | 0.2082650592031285 | 0.4473037444715686 | T | T | T |
| 0.1252645128370844 | 0.3749122675736203 | 0.4482779173830949 | T | T | T |
| 0.2917375469905963 | 0.3752722862856288 | 0.4469299298851581 | T | T | T |
| 0.4579223262100456 | 0.3746037845267480 | 0.4469950584406277 | T | T | T |
| 0.6242412374364719 | 0.3757586260583494 | 0.4497921770929096 | T | T | T |
| 0.7910167995116169 | 0.3747124277091132 | 0.4472514186596328 | T | T | T |
| 0.9581556573561514 | 0.3751224169196732 | 0.4470763945695850 | T | T | T |
| 0.1251892256963814 | 0.5415395300210477 | 0.4470849098949969 | T | T | T |
| 0.2923219536660611 | 0.5419378745087187 | 0.4472823051881463 | T | T | T |
| 0.4591024626766185 | 0.5408973373901986 | 0.4498559813695593 | T | T | T |
| 0.6253960830269278 | 0.5420775143570893 | 0.4469951011419724 | T | T | T |
| 0.7915931400702476 | 0.5413847021896601 | 0.4469204631882633 | T | T | T |
| 0.9580788304147561 | 0.5417477972098013 | 0.4483162540370245 | T | T | T |
| 0.1255524344600758 | 0.7084014657657320 | 0.4473235350121598 | T | T | T |
| 0.2919355642504868 | 0.7080644386141017 | 0.4466270673698531 | T | T | T |
| 0.4580620592986975 | 0.7076779653417731 | 0.4472822969104513 | T | T | T |
| 0.6247277471486612 | 0.7082624213227930 | 0.4469300276918204 | T | T | T |
| 0.7915397888856930 | 0.7082069061378249 | 0.4457597187572730 | T | T | T |
| 0.9578135809131894 | 0.7078055729067074 | 0.4469973322478538 | T | T | T |
| 0.1253053389680687 | 0.8746949136096944 | 0.4485292350067880 | T | T | T |
| 0.2915986275076392 | 0.8744475503895828 | 0.4473235304560248 | T | T | T |
| 0.4584605586255819 | 0.8748107146621322 | 0.4470849320028947 | T | T | T |
| 0.6250878831735704 | 0.8747353635380080 | 0.4482779040447653 | T | T | T |
| 0.7911372049209788 | 0.8744726864626529 | 0.4469988108416629 | T | T | T |
| 0.9580037177195280 | 0.8746734556886580 | 0.4479361084317830 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.0414330728699213 | 0.1251887396051927 | 0.5523312479917095 | T | T | T |
| 0.2078921560563103 | 0.1245567185026744 | 0.5511582194490288 | T | T | T |
| 0.3747009552214067 | 0.1253562157630057 | 0.5514923152571001 | T | T | T |
| 0.5415975317003117 | 0.1251219308372811 | 0.5524283149163907 | T | T | T |
| 0.7078417215039252 | 0.1245677625680273 | 0.5509709689578344 | T | T | T |
| 0.8747533141482862 | 0.1252468224517571 | 0.5524203561464631 | T | T | T |
| 0.0415448759845702 | 0.2917537652978055 | 0.5523781632285534 | T | T | T |
| 0.2086967736840180 | 0.2913674342965749 | 0.5514924515972126 | T | T | T |
| 0.3754581722803536 | 0.2921281710509618 | 0.5498765598098601 | T | T | T |
| 0.5416936429929251 | 0.2904794253664846 | 0.5532522641862130 | T | T | T |
| 0.7085089839885867 | 0.2914908377360916 | 0.5527876188101359 | T | T | T |
| 0.8754321596710284 | 0.2921582850482309 | 0.5509709380301118 | T | T | T |
| 0.0416726013393287 | 0.4583298126524298 | 0.5528659811737242 | T | T | T |
| 0.2084720316719242 | 0.4582631480963073 | 0.5524214144396211 | T | T | T |
| 0.3738402486331651 | 0.4583628337680707 | 0.5533286484211430 | T | T | T |
| 0.5416618232436505 | 0.4583379255215050 | 0.5589816298182626 | T | T | T |
| 0.7095203883554717 | 0.4583061462030074 | 0.5532520745895440 | T | T | T |
| 0.8748778769544145 | 0.4584023838713733 | 0.5524280468459324 | T | T | T |
| 0.0417914024253889 | 0.6249040413919573 | 0.5524092164989369 | T | T | T |
| 0.2079117617658639 | 0.6245023160979102 | 0.5509885467295348 | T | T | T |
| 0.3748305998585906 | 0.6251692340258899 | 0.5528389023664673 | T | T | T |
| 0.5416369398302336 | 0.6261595100322026 | 0.5533285259241012 | T | T | T |
| 0.7078716723338374 | 0.6245416708840423 | 0.5498762994594202 | T | T | T |
| 0.8746436935962834 | 0.6252990695895733 | 0.5514918860868860 | T | T | T |
| 0.0418960814264508 | 0.7914704865044300 | 0.5523042184070661 | T | T | T |
| 0.2085836910490073 | 0.7914164399105985 | 0.5524269334636998 | T | T | T |
| 0.3754977214486743 | 0.7920881744022665 | 0.5509885543409396 | T | T | T |
| 0.5417367794980592 | 0.7915277528352718 | 0.5524212472796464 | T | T | T |
| 0.7086326117166166 | 0.7913031256681720 | 0.5514920556692431 | T | T | T |
| 0.8754433766679171 | 0.7921079378693676 | 0.5511578067621770 | T | T | T |
| 0.0416664832112517 | 0.9583338923265501 | 0.5535656673867422 | T | T | T |
| 0.2085297724450115 | 0.9581041241324542 | 0.5523045217842082 | T | T | T |
| 0.3750961337169656 | 0.9582086026973968 | 0.5524094592755731 | T | T | T |
| 0.5416702797573407 | 0.9583272501054552 | 0.5528660579587026 | T | T | T |
| 0.7082463824565934 | 0.9584550718978377 | 0.5523780048160916 | T | T | T |
| 0.8748115310340125 | 0.9585670710593064 | 0.5523310464820739 | T | T | T |

*N_{Li, 2020 #53} side-on

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9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

N Mo

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Selective dynamics

Direct

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|--------------------|--------------------|--------------------|---|---|---|
| 0.4333039900987501 | 0.5666997263632823 | 0.6268806583234721 | T | T | T |
| 0.4833637178237566 | 0.5166329521499264 | 0.6268796090733062 | T | T | T |
| 0.1254193570196307 | 0.0416511769920973 | 0.4469752772951949 | T | T | T |
| 0.2920767605857009 | 0.0417361726218104 | 0.4470683214114928 | T | T | T |
| 0.4583280822522227 | 0.0416631547774031 | 0.4475674711663657 | T | T | T |
| 0.6245846464902556 | 0.0415904621559733 | 0.4470652454664545 | T | T | T |
| 0.7912492265916384 | 0.0416778955402322 | 0.4469758480573347 | T | T | T |
| 0.9583362049618174 | 0.0416640009914957 | 0.4480185546858380 | T | T | T |
| 0.1249690446702090 | 0.2083001148571668 | 0.4452234710309781 | T | T | T |
| 0.2922763172927958 | 0.2087932469207630 | 0.4463124475238871 | T | T | T |
| 0.4596931319780850 | 0.2090036611550943 | 0.4476006972234856 | T | T | T |
| 0.6250620522638641 | 0.2085899815943080 | 0.4474577600694971 | T | T | T |
| 0.7909358983937267 | 0.2090660725447364 | 0.4466536328767106 | T | T | T |
| 0.9583229534413817 | 0.2087533105305042 | 0.4469737218849303 | T | T | T |
| 0.1254641491098880 | 0.3756141334174643 | 0.4463109561288050 | T | T | T |
| 0.2899335288295575 | 0.3732680916390265 | 0.4453904076848119 | T | T | T |
| 0.4593955033727610 | 0.3754824132212207 | 0.4497062464686721 | T | T | T |
| 0.6248024690555170 | 0.3751990415508644 | 0.4491294147657499 | T | T | T |
| 0.7914127625045921 | 0.3749416012928535 | 0.4474556486334578 | T | T | T |
| 0.9584105749508183 | 0.3754184987008102 | 0.4470610738600413 | T | T | T |
| 0.1256748503826230 | 0.5430364518117941 | 0.4475984489586224 | T | T | T |
| 0.2921481612329870 | 0.5427348862074837 | 0.4497077540108450 | T | T | T |
| 0.4583318389065241 | 0.5416683433956351 | 0.4500974917575604 | T | T | T |
| 0.6245195532543946 | 0.5406044257890770 | 0.4497052198003217 | T | T | T |
| 0.7909983596900574 | 0.5403070942810118 | 0.4475971920178523 | T | T | T |
| 0.9583371696503349 | 0.5416722420969791 | 0.4475677335953208 | T | T | T |
| 0.1252561207723559 | 0.7083974162505129 | 0.4474609836058221 | T | T | T |
| 0.2918620418615845 | 0.7081369782882661 | 0.4491350074663885 | T | T | T |
| 0.4572647284543692 | 0.7078500451747942 | 0.4497080470190440 | T | T | T |
| 0.6267329927549454 | 0.7100654312692356 | 0.4453901575198813 | T | T | T |
| 0.7912073909426525 | 0.7077212869095462 | 0.4463114737151344 | T | T | T |
| 0.9582621265785178 | 0.7079200522120246 | 0.4470654172297870 | T | T | T |
| 0.1257312758180902 | 0.8742660203589239 | 0.4466603117522681 | T | T | T |
| 0.2915999197573598 | 0.8747409879930998 | 0.4474617613505885 | T | T | T |
| 0.4569640772467238 | 0.8743237459789768 | 0.4476025091941125 | T | T | T |
| 0.6243880271402276 | 0.8745360286131287 | 0.4463134831607363 | T | T | T |
| 0.7917014953382377 | 0.8750299413897267 | 0.4452241852762384 | T | T | T |
| 0.9583481574011543 | 0.8745781532309422 | 0.4469742831401788 | T | T | T |
| 0.0421970488010146 | 0.1255280968180372 | 0.5516081952328165 | T | T | T |
| 0.2086013703310741 | 0.1249620174409287 | 0.5506084491408672 | T | T | T |
| 0.3747785597501547 | 0.1239356071151008 | 0.5523898830879119 | T | T | T |
| 0.5414545653994125 | 0.1247930589295763 | 0.5527530582869602 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.7082913139404710 | 0.1250487850226349 | 0.5520564747985617 | T | T | T |
| 0.8750238951364082 | 0.1249776730671428 | 0.5516654861640191 | T | T | T |
| 0.0416339131588614 | 0.2919390361707102 | 0.5506116766387379 | T | T | T |
| 0.2099269418863230 | 0.2932610480206463 | 0.5496443582929942 | T | T | T |
| 0.3747742172768866 | 0.2900347553762757 | 0.5515640382456510 | T | T | T |
| 0.5417625527810443 | 0.2900922641540831 | 0.5544586438119197 | T | T | T |
| 0.7089880461733813 | 0.2910137069059502 | 0.5525710462275910 | T | T | T |
| 0.8749528974418865 | 0.2917119435139455 | 0.5520558864753724 | T | T | T |
| 0.0406059811586132 | 0.4581187265451234 | 0.5523922821679150 | T | T | T |
| 0.2067008851465744 | 0.4581106540364388 | 0.5515660775265445 | T | T | T |
| 0.3745549514613771 | 0.4578897635302965 | 0.5554456015250366 | T | T | T |
| 0.5435289793119367 | 0.4564728153539122 | 0.5565862361930769 | T | T | T |
| 0.7099105712088232 | 0.4582403986721957 | 0.5544577330431224 | T | T | T |
| 0.8752084045029775 | 0.4585440568218218 | 0.5527581158329440 | T | T | T |
| 0.0414632285362657 | 0.6247979623608728 | 0.5527563630713388 | T | T | T |
| 0.2067569643600535 | 0.6250983949408422 | 0.5544563140208183 | T | T | T |
| 0.3731376736053775 | 0.6268607527005088 | 0.5565845175270212 | T | T | T |
| 0.5421103306875565 | 0.6254446418237904 | 0.5554454426782769 | T | T | T |
| 0.7099667842853705 | 0.6252255045516861 | 0.5515652508565481 | T | T | T |
| 0.8760658301824336 | 0.6252205511687094 | 0.5523927234615229 | T | T | T |
| 0.0417180293758719 | 0.7916232380665278 | 0.5520534852601386 | T | T | T |
| 0.2076781583951899 | 0.7923192209125887 | 0.5525660967943153 | T | T | T |
| 0.3748990670426764 | 0.7932407486034592 | 0.5544561510456987 | T | T | T |
| 0.5418884043952588 | 0.7932968444420396 | 0.5515653661775133 | T | T | T |
| 0.7067401844299113 | 0.7900711902506359 | 0.5496447470504151 | T | T | T |
| 0.8750380425716671 | 0.7913967489566787 | 0.5506095450557638 | T | T | T |
| 0.0416475462662689 | 0.9583512718147560 | 0.5516597983788358 | T | T | T |
| 0.2083740731174970 | 0.9582804232330133 | 0.5520521232441453 | T | T | T |
| 0.3752025061874562 | 0.9585356194635892 | 0.5527505247940994 | T | T | T |
| 0.5418814392006439 | 0.9593925912404657 | 0.5523907609415559 | T | T | T |
| 0.7080622729309383 | 0.9583660052312908 | 0.5506122340923483 | T | T | T |
| 0.8744728921006484 | 0.9578014921213409 | 0.5516087084050127 | T | T | T |

*N-NH

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

H N Mo

1 2 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4948405143520205 | 0.5051579166577085 | 0.6848761210201246 | T | T | T |
| 0.4341338953200093 | 0.5658670729585893 | 0.6231448647679585 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4864770593034464 | 0.5135220778826906 | 0.6347131795599736 | T | T | T |
| 0.1254118670810982 | 0.0413762643724596 | 0.4469472950846409 | T | T | T |
| 0.2924051333412336 | 0.0415953063444263 | 0.4448641859919746 | T | T | T |
| 0.4586187556545838 | 0.0414735755742086 | 0.4467162547531913 | T | T | T |
| 0.6248986356331585 | 0.0412774449321631 | 0.4463515114352177 | T | T | T |
| 0.7915737930913664 | 0.0412554174357496 | 0.4444734873084855 | T | T | T |
| 0.9584443577173900 | 0.0415560419108871 | 0.4465801142732602 | T | T | T |
| 0.1256093456077210 | 0.2079845572609997 | 0.4449222452273531 | T | T | T |
| 0.2929088146490599 | 0.2085092414886986 | 0.4476073835356118 | T | T | T |
| 0.4594167427963356 | 0.2088036173515562 | 0.4462780351617752 | T | T | T |
| 0.6252771263962060 | 0.2082851029616748 | 0.4456472206235418 | T | T | T |
| 0.7912074136012279 | 0.2087912702845429 | 0.4464062580844512 | T | T | T |
| 0.9587441297294177 | 0.2084256239205970 | 0.4444736523529187 | T | T | T |
| 0.1263947199865783 | 0.3754167003553164 | 0.4458752759163147 | T | T | T |
| 0.2910664360206923 | 0.3742612589499927 | 0.4459541027949072 | T | T | T |
| 0.4593455919100009 | 0.3769324215323806 | 0.4505656209378159 | T | T | T |
| 0.6249743057468606 | 0.3750254264318755 | 0.4486911026428615 | T | T | T |
| 0.7917140683186616 | 0.3747219175118914 | 0.4456478186957042 | T | T | T |
| 0.9587214230029986 | 0.3751003275210607 | 0.4463525520655907 | T | T | T |
| 0.1258177366785702 | 0.5426137464861469 | 0.4471378528299823 | T | T | T |
| 0.2923062765685387 | 0.5433293190022823 | 0.4510167902571993 | T | T | T |
| 0.4590524262422662 | 0.5409470375670935 | 0.4512538426018580 | T | T | T |
| 0.6230674306199120 | 0.5406540907501451 | 0.4505659566726621 | T | T | T |
| 0.7911966263317041 | 0.5405826384604779 | 0.4462777350942702 | T | T | T |
| 0.9585263792634393 | 0.5413810081387780 | 0.4467159378145524 | T | T | T |
| 0.1252550240136188 | 0.7083368626987578 | 0.4484507141465528 | T | T | T |
| 0.2915351524423997 | 0.7084660129625178 | 0.4486203165757132 | T | T | T |
| 0.4566717339714543 | 0.7076943919329537 | 0.4510172646124460 | T | T | T |
| 0.6257387658398983 | 0.7089333093919947 | 0.4459546363980280 | T | T | T |
| 0.7914913805255068 | 0.7070911605508030 | 0.4476081515027772 | T | T | T |
| 0.9584048736531159 | 0.7075946053548421 | 0.4448641050233704 | T | T | T |
| 0.1255902001281015 | 0.8744108481387514 | 0.4444876493457954 | T | T | T |
| 0.2916639577363114 | 0.8747456430081471 | 0.4484508877442366 | T | T | T |
| 0.4573867417990556 | 0.8741829491204243 | 0.4471374488780882 | T | T | T |
| 0.6245837021806437 | 0.8736050622557414 | 0.4458751195574280 | T | T | T |
| 0.7920161803267476 | 0.8743904970577745 | 0.4449219418898380 | T | T | T |
| 0.9586246704952543 | 0.8745884848243506 | 0.4469463359334398 | T | T | T |
| 0.0423019733102024 | 0.1253662730235447 | 0.5510871581702830 | T | T | T |
| 0.2089248449092693 | 0.1245617435900783 | 0.5510394571577137 | T | T | T |
| 0.3750893530402024 | 0.1232878561111050 | 0.5512699042935196 | T | T | T |
| 0.5418337730572986 | 0.1245338131232714 | 0.5511135938810270 | T | T | T |
| 0.7085317901024268 | 0.1246468441133288 | 0.5520174892920053 | T | T | T |
| 0.8750769100742914 | 0.1249222756222395 | 0.5490293514210407 | T | T | T |
| 0.0418608507964535 | 0.2915624893982809 | 0.5487869312541989 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2104415934141883 | 0.2927221818221568 | 0.5506022312250352 | T | T | T |
| 0.3743196612748676 | 0.2898866130193269 | 0.5523827951646680 | T | T | T |
| 0.5413103757786857 | 0.2897134769395038 | 0.5539477152320913 | T | T | T |
| 0.7094518906676299 | 0.2905467966811983 | 0.5509174800897014 | T | T | T |
| 0.8753516731310214 | 0.2914676970962802 | 0.5520174512393936 | T | T | T |
| 0.0407826607343154 | 0.4581212258323930 | 0.5524424316850940 | T | T | T |
| 0.2074836274747938 | 0.4573131363739336 | 0.5517290150375729 | T | T | T |
| 0.3748392284068203 | 0.4584452728435551 | 0.5586621772771636 | T | T | T |
| 0.5450735132615208 | 0.4549265941747578 | 0.5570996052438559 | T | T | T |
| 0.7102857857680789 | 0.4586882938334469 | 0.5539474589274391 | T | T | T |
| 0.8754653819777687 | 0.4581661571458113 | 0.5511130824291470 | T | T | T |
| 0.0416793984074673 | 0.6246796623665603 | 0.5527463644613206 | T | T | T |
| 0.2067486927015381 | 0.6252983680644135 | 0.5548413556929219 | T | T | T |
| 0.3708755951148603 | 0.6291243480712936 | 0.5570326912270147 | T | T | T |
| 0.5415555895995823 | 0.6251617693126832 | 0.5586627543669707 | T | T | T |
| 0.7101134473371360 | 0.6256792586837889 | 0.5523826736715804 | T | T | T |
| 0.8767123475804581 | 0.6249099136071408 | 0.5512693833966296 | T | T | T |
| 0.0415796220420148 | 0.7916548794973437 | 0.5504285282713610 | T | T | T |
| 0.2074522089776920 | 0.7925480857852989 | 0.5542513876995088 | T | T | T |
| 0.3747020570686956 | 0.7932519554631057 | 0.5548420560479954 | T | T | T |
| 0.5426878653574008 | 0.7925167596487839 | 0.5517299722864379 | T | T | T |
| 0.7072788008341178 | 0.7895582171512103 | 0.5506022459679798 | T | T | T |
| 0.8754391803444577 | 0.7910753783913265 | 0.5510384132531172 | T | T | T |
| 0.0416863744285081 | 0.9583142074407789 | 0.5517319659621478 | T | T | T |
| 0.2083459985277116 | 0.9584209257196790 | 0.5504300230440933 | T | T | T |
| 0.3753205509340987 | 0.9583210042079031 | 0.5527483254598025 | T | T | T |
| 0.5418796171181413 | 0.9592170438510408 | 0.5524429019849606 | T | T | T |
| 0.7084375149103863 | 0.9581381905809394 | 0.5487874255799809 | T | T | T |
| 0.8746340448676833 | 0.9576978897168615 | 0.5510865532419160 | T | T | T |

*N-NH₂

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

H N Mo
2 2 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5722388053467924 | 0.5209282976642555 | 0.6936757494857346 | T | T | T |
| 0.4791103230627627 | 0.4277298468597763 | 0.6937314510363919 | T | T | T |
| 0.4788191841210718 | 0.5210427500683537 | 0.6240234302678331 | T | T | T |
| 0.5222738385247325 | 0.4776913238335041 | 0.6657588288282312 | T | T | T |
| 0.1230476976608230 | 0.0434571595168336 | 0.4447401117084198 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2899448109081604 | 0.0440706371915809 | 0.4449565493222138 | T | T | T |
| 0.4566678478148987 | 0.0434625134902973 | 0.4471256607577274 | T | T | T |
| 0.6234520253326536 | 0.0428376427217785 | 0.4450916962222848 | T | T | T |
| 0.7899565144133334 | 0.0431279028639295 | 0.4444658720852530 | T | T | T |
| 0.9563878899589682 | 0.0433972161892768 | 0.4429607400767281 | T | T | T |
| 0.1229823821165397 | 0.2099738209718467 | 0.4433506259958904 | T | T | T |
| 0.2895233770112853 | 0.2099738780342832 | 0.4457018148557381 | T | T | T |
| 0.4581052531513663 | 0.2106573833082876 | 0.4461287807520193 | T | T | T |
| 0.6241902151818195 | 0.2101657114806628 | 0.4452654493174535 | T | T | T |
| 0.7897729261361519 | 0.2099927856167696 | 0.4440617294276663 | T | T | T |
| 0.9566445207976457 | 0.2098134665776996 | 0.4445218034970040 | T | T | T |
| 0.1234252972213454 | 0.3761510674180997 | 0.4459735453539793 | T | T | T |
| 0.2881113370227695 | 0.3757429890400985 | 0.4449444075778786 | T | T | T |
| 0.4562675815559203 | 0.3763037890499845 | 0.4468725824389637 | T | T | T |
| 0.6225469355845661 | 0.3772099296456091 | 0.4474068647607012 | T | T | T |
| 0.7896287762172705 | 0.3755912423845942 | 0.4452713596909277 | T | T | T |
| 0.9569387370084357 | 0.3763030277598034 | 0.4451451655116685 | T | T | T |
| 0.1242338903366758 | 0.5424606665588101 | 0.4476417717574250 | T | T | T |
| 0.2910937877071618 | 0.5425114241536093 | 0.4494450147214053 | T | T | T |
| 0.4576164917750560 | 0.5421533256468578 | 0.4519753244525120 | T | T | T |
| 0.6234653887205397 | 0.5435002194703813 | 0.4468261672998963 | T | T | T |
| 0.7891259541662166 | 0.5416674003734343 | 0.4460874477464785 | T | T | T |
| 0.9563268207557698 | 0.5431020896591008 | 0.4471385074469083 | T | T | T |
| 0.1240441079787331 | 0.7096815993514838 | 0.4470442419293335 | T | T | T |
| 0.2907962167597589 | 0.7089664447169355 | 0.4496845423664695 | T | T | T |
| 0.4572497658018122 | 0.7086773473490595 | 0.4494043602407984 | T | T | T |
| 0.6240388719967953 | 0.7116702475879464 | 0.4448558614339291 | T | T | T |
| 0.7898043429448336 | 0.7102655507661524 | 0.4456234069269485 | T | T | T |
| 0.9557187532823193 | 0.7098291722005996 | 0.4449243766751536 | T | T | T |
| 0.1243307685831283 | 0.8754418638255146 | 0.4433325243357800 | T | T | T |
| 0.2901030306556223 | 0.8757448779091348 | 0.4470398460571374 | T | T | T |
| 0.4572954100378723 | 0.8755533385860659 | 0.4476110308629728 | T | T | T |
| 0.6236247666731884 | 0.8763628174274842 | 0.4458859657752896 | T | T | T |
| 0.7898125898718291 | 0.8768002670233557 | 0.4432753250312444 | T | T | T |
| 0.9563253694888090 | 0.8767415482985044 | 0.4447017981717565 | T | T | T |
| 0.0401185016366696 | 0.1269716855283036 | 0.5487881794826777 | T | T | T |
| 0.2067272837552139 | 0.1273396312643982 | 0.5501330681438859 | T | T | T |
| 0.3724794579868060 | 0.1256023065349154 | 0.5509981729601208 | T | T | T |
| 0.5399548478216616 | 0.1255278337163830 | 0.5511546434204462 | T | T | T |
| 0.7066069492854723 | 0.1255377946227441 | 0.5496244667645129 | T | T | T |
| 0.8732780841012229 | 0.1264827819143832 | 0.5503187299953254 | T | T | T |
| 0.0406406148888223 | 0.2931938774525094 | 0.5505667282171274 | T | T | T |
| 0.2075542124741006 | 0.2946689818574981 | 0.5500309313199239 | T | T | T |
| 0.3727177853350554 | 0.2927894125469876 | 0.5504473579357381 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.5392839344152023 | 0.2904639392634607 | 0.5518379587170017 | T | T | T |
| 0.7074136528130097 | 0.2923535338202896 | 0.5502878134240277 | T | T | T |
| 0.8742472519898712 | 0.2931827128150815 | 0.5496644348832760 | T | T | T |
| 0.0401988584248443 | 0.4597141852041844 | 0.5520489103967279 | T | T | T |
| 0.2076531129666748 | 0.4595333050589403 | 0.5535930116793111 | T | T | T |
| 0.3727409874877665 | 0.4601399100825674 | 0.5580447191289366 | T | T | T |
| 0.5417363835419167 | 0.4580891260588444 | 0.5549722945925737 | T | T | T |
| 0.7093215927672318 | 0.4605108276480010 | 0.5518011947862647 | T | T | T |
| 0.8742475903954556 | 0.4598263749411586 | 0.5511647999151350 | T | T | T |
| 0.0396567669834980 | 0.6264623684498360 | 0.5519283537401449 | T | T | T |
| 0.2058848391701602 | 0.6265654294586795 | 0.5545572781766168 | T | T | T |
| 0.3703941868143517 | 0.6294024164062009 | 0.5559345756519249 | T | T | T |
| 0.5396569881332454 | 0.6270859649922684 | 0.5579830996719366 | T | T | T |
| 0.7070073099852223 | 0.6270887274007606 | 0.5503763100906127 | T | T | T |
| 0.8741727599562523 | 0.6273085073676228 | 0.5509570595180477 | T | T | T |
| 0.0395471876752325 | 0.7933821657531368 | 0.5486886609672439 | T | T | T |
| 0.2064430760152334 | 0.7933331032453097 | 0.5516471725922756 | T | T | T |
| 0.3731861327938120 | 0.7938654636061315 | 0.5545359246258883 | T | T | T |
| 0.5402536192391167 | 0.7921412142718012 | 0.5535224045383416 | T | T | T |
| 0.7051082558465254 | 0.7922315970508578 | 0.5499462370757442 | T | T | T |
| 0.8724343619242774 | 0.7930575076461963 | 0.5500679528188783 | T | T | T |
| 0.0397691802948685 | 0.9600017154930285 | 0.5494971663905019 | T | T | T |
| 0.2064000138887536 | 0.9602238605493341 | 0.5486981087698126 | T | T | T |
| 0.3733259487646592 | 0.9601250625514979 | 0.5519319713684183 | T | T | T |
| 0.5400719080337169 | 0.9595805144810257 | 0.5520031906357019 | T | T | T |
| 0.7065841993451656 | 0.9591246386907244 | 0.5504867395509621 | T | T | T |
| 0.8728067407718711 | 0.9596697893089896 | 0.5487399656004115 | T | T | T |

*HN-NH

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

H N Mo

2 2 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.3830908075690189 | 0.5276791874468785 | 0.6846775267129317 | T | T | T |
| 0.5302210928043039 | 0.5534185200303909 | 0.6850719529966369 | T | T | T |
| 0.4105791645920647 | 0.5391066306238486 | 0.6378799252093614 | T | T | T |
| 0.5036562125947768 | 0.5439981418006070 | 0.6379682270817426 | T | T | T |
| 0.1249769496563218 | 0.0413009299978171 | 0.4436242318533772 | T | T | T |
| 0.2909499125667594 | 0.0412159709927025 | 0.4473329193951514 | T | T | T |
| 0.4583517038904716 | 0.0416640941551591 | 0.4454456719871303 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6257079574393671 | 0.0421171925757022 | 0.4472980005505960 | T | T | T |
| 0.7917042823279061 | 0.0419739669518862 | 0.4435916796593489 | T | T | T |
| 0.9583713493836115 | 0.0416510080392811 | 0.4442357799533454 | T | T | T |
| 0.1250442409618273 | 0.2077639685404691 | 0.4432560597847726 | T | T | T |
| 0.2905530905864850 | 0.2077306403198165 | 0.4447893384063093 | T | T | T |
| 0.4577885730766624 | 0.2088230342581454 | 0.4482824364784577 | T | T | T |
| 0.6246060426430873 | 0.2094509246856191 | 0.4458068416370651 | T | T | T |
| 0.7913039414909804 | 0.2087976104110822 | 0.4473901345837206 | T | T | T |
| 0.9588834825214931 | 0.2084156190458089 | 0.4437391588301551 | T | T | T |
| 0.1251073502888076 | 0.3751444593962958 | 0.4446376464441855 | T | T | T |
| 0.2908697301747836 | 0.3742024818819942 | 0.4425906152488324 | T | T | T |
| 0.4567432403181400 | 0.3759811399502553 | 0.4489348109867848 | T | T | T |
| 0.6225867950641870 | 0.3765099838860735 | 0.4513917747219551 | T | T | T |
| 0.7905079559050634 | 0.3751364594211211 | 0.4464447892693215 | T | T | T |
| 0.9583437764229288 | 0.3744161673513489 | 0.4479232071638819 | T | T | T |
| 0.1262068558643179 | 0.5422949505910921 | 0.4478574235131987 | T | T | T |
| 0.2943033899658971 | 0.5420397946932098 | 0.4500446127791875 | T | T | T |
| 0.4583346260329790 | 0.5416870547283708 | 0.4498579844174273 | T | T | T |
| 0.6223534636438401 | 0.5414476717601033 | 0.4501991994393535 | T | T | T |
| 0.7904058481648875 | 0.5410720073258659 | 0.4478924336705816 | T | T | T |
| 0.9582904088551913 | 0.5416697501578511 | 0.4455301382391710 | T | T | T |
| 0.1261303103510940 | 0.7082211468667268 | 0.4462298004598750 | T | T | T |
| 0.2940554762043561 | 0.7069012430801038 | 0.4512008531287108 | T | T | T |
| 0.4599605104877043 | 0.7072399589396952 | 0.4489868260857008 | T | T | T |
| 0.6259338337151164 | 0.7091910753753865 | 0.4424179508229216 | T | T | T |
| 0.7915791263935219 | 0.7082537127263677 | 0.4446051370202824 | T | T | T |
| 0.9582888097230793 | 0.7089391966302756 | 0.4476730946384038 | T | T | T |
| 0.1253769064128605 | 0.8745490986383118 | 0.4471913076141618 | T | T | T |
| 0.2920754809187187 | 0.8739553501807791 | 0.4456584497605292 | T | T | T |
| 0.4588905032912436 | 0.8744656133686206 | 0.4482049521391644 | T | T | T |
| 0.6261252266738779 | 0.8755660081553884 | 0.4447237127332073 | T | T | T |
| 0.7916863712617896 | 0.8755610781059815 | 0.4429372413520909 | T | T | T |
| 0.9578142463630712 | 0.8749085322470265 | 0.4435255990703482 | T | T | T |
| 0.0413298035923972 | 0.1244566893864345 | 0.5500625669826604 | T | T | T |
| 0.2080137649245515 | 0.1255465744212927 | 0.5497487355537913 | T | T | T |
| 0.3748279075065213 | 0.1248238238319104 | 0.5520661825662856 | T | T | T |
| 0.5415017002205644 | 0.1246872864714277 | 0.5500720434387816 | T | T | T |
| 0.7084336897928765 | 0.1250117162797508 | 0.5520128571217882 | T | T | T |
| 0.8753761301895437 | 0.1245749378750887 | 0.5486945530322132 | T | T | T |
| 0.0424386749323489 | 0.2909371656598765 | 0.5494898793554199 | T | T | T |
| 0.2083998438630417 | 0.2914419951848402 | 0.5487385212489428 | T | T | T |
| 0.3745300735194803 | 0.2925153405956067 | 0.5527645257859817 | T | T | T |
| 0.5400002608148569 | 0.2922472873994835 | 0.5552971142050254 | T | T | T |
| 0.7078943808985159 | 0.2918546606133745 | 0.5509611140855242 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.8756484014032893 | 0.2918401964764215 | 0.5524518870720385 | T | T | T |
| 0.0415494478424847 | 0.4583749254602054 | 0.5522357706729011 | T | T | T |
| 0.2068830848224650 | 0.4565641681249986 | 0.5514495781600246 | T | T | T |
| 0.3719992548716817 | 0.4538678614572049 | 0.5546520239409958 | T | T | T |
| 0.5412316650018099 | 0.4599936114191223 | 0.5617313078075412 | T | T | T |
| 0.7078424174016362 | 0.4601357752224260 | 0.5548060364571583 | T | T | T |
| 0.8750098280054033 | 0.4589504847929433 | 0.5503173024088781 | T | T | T |
| 0.0416230191850744 | 0.6244650650431112 | 0.5501656827252148 | T | T | T |
| 0.2086878387342352 | 0.6232830853317921 | 0.5546617192313548 | T | T | T |
| 0.3750792902231765 | 0.6232575430219001 | 0.5615596350642349 | T | T | T |
| 0.5446576868841717 | 0.6291322627948048 | 0.5549085384490766 | T | T | T |
| 0.7095462399570778 | 0.6266214465711144 | 0.5516863781328354 | T | T | T |
| 0.8750103913995986 | 0.6249860400708229 | 0.5521431294477637 | T | T | T |
| 0.0409722050670851 | 0.7914948899006475 | 0.5522185596361950 | T | T | T |
| 0.2087510945314435 | 0.7915016200956018 | 0.5507458123981195 | T | T | T |
| 0.3766447167875029 | 0.7910469042019983 | 0.5551688136297344 | T | T | T |
| 0.5421552670878000 | 0.7906945044837386 | 0.5527569527432306 | T | T | T |
| 0.7081679672506098 | 0.7917538885204252 | 0.5485382483623198 | T | T | T |
| 0.8740986222010392 | 0.7922811382002948 | 0.5493876315589290 | T | T | T |
| 0.0413018602647881 | 0.9586818915692561 | 0.5486729035854410 | T | T | T |
| 0.2082168102172233 | 0.9582793902237867 | 0.5520029178828665 | T | T | T |
| 0.3751989312784900 | 0.9586377085214082 | 0.5499978867143795 | T | T | T |
| 0.5419022109366765 | 0.9584539630435458 | 0.5519418802104425 | T | T | T |
| 0.7086657247796424 | 0.9577352698215407 | 0.5496288689778908 | T | T | T |
| 0.8753179284167132 | 0.9587403622241553 | 0.5498643152632141 | T | T | T |

*HN-NH₂

1.0000000000000000

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| 9.1482180682119907 | -13.2029053235859699 | 0.0000000000000000 |
| 9.1482180682119907 | 13.2029053235859699 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 20.0000566999999982 |

H N Mo
3 2 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4353193899712113 | 0.5644898964493180 | 0.6746869714593151 | T | T | T |
| 0.6015502366182862 | 0.4899684887346867 | 0.6986797530015754 | T | T | T |
| 0.5097078811803927 | 0.3990296662472537 | 0.6988547244474655 | T | T | T |
| 0.4313083459201917 | 0.5683285547222539 | 0.6237467847444146 | T | T | T |
| 0.5515079132096867 | 0.4485512155529506 | 0.6700991543968418 | T | T | T |
| 0.1221490863986116 | 0.0448542852417404 | 0.4428938172883339 | T | T | T |
| 0.2884623300071406 | 0.0453733435008007 | 0.4439104512801444 | T | T | T |
| 0.4558049383856991 | 0.0441910220185707 | 0.4474787431258052 | T | T | T |
| 0.6229459136634327 | 0.0434555953700351 | 0.4439578875508559 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7892143226941387 | 0.0433265947536201 | 0.4416243736442306 | T | T | T |
| 0.9555180814356827 | 0.0441272839570880 | 0.4442834487406739 | T | T | T |
| 0.1237761134026502 | 0.2109808449355933 | 0.4429889972213333 | T | T | T |
| 0.2888243006537481 | 0.2113323174738111 | 0.4445603655968184 | T | T | T |
| 0.4562806691265013 | 0.2119804290537036 | 0.4459554604458186 | T | T | T |
| 0.6227726750651669 | 0.2117981110489625 | 0.4451891391316405 | T | T | T |
| 0.7886383493593705 | 0.2109971368685906 | 0.4426355758607033 | T | T | T |
| 0.9563232263566255 | 0.2104318660185466 | 0.4415895112418387 | T | T | T |
| 0.1228476515803747 | 0.3769587140661892 | 0.4442338668053258 | T | T | T |
| 0.2888759432088792 | 0.3772312276989147 | 0.4446806075659843 | T | T | T |
| 0.4552991152952204 | 0.3795910924654609 | 0.4515068750948845 | T | T | T |
| 0.6211155699648397 | 0.3784848548333560 | 0.4485423584697422 | T | T | T |
| 0.7878124786018492 | 0.3768530018320055 | 0.4451829275456325 | T | T | T |
| 0.9561880428634215 | 0.3766977199554031 | 0.4439280493021271 | T | T | T |
| 0.1228707390774482 | 0.5444754098457780 | 0.4455716956045537 | T | T | T |
| 0.2904982901722833 | 0.5442126569036930 | 0.4498605389924702 | T | T | T |
| 0.4568949933782723 | 0.5427420319905111 | 0.4556025429133394 | T | T | T |
| 0.6200223777424875 | 0.5443279591654835 | 0.4515305587789850 | T | T | T |
| 0.7876271829478334 | 0.5433352834269581 | 0.4459665070083567 | T | T | T |
| 0.9554428734618823 | 0.5438267672069587 | 0.4474757615482780 | T | T | T |
| 0.1225816490301392 | 0.7111694181190334 | 0.4456796152697204 | T | T | T |
| 0.2892145613788787 | 0.7104385324872956 | 0.4460252187386154 | T | T | T |
| 0.4554349115590740 | 0.7091497671698005 | 0.4498885586431276 | T | T | T |
| 0.6224035834179866 | 0.7107619024303736 | 0.4447107312822637 | T | T | T |
| 0.7882832157130597 | 0.7108085535306022 | 0.4446151168927424 | T | T | T |
| 0.9542604507915207 | 0.7111666592636166 | 0.4439584461927838 | T | T | T |
| 0.1226242718165994 | 0.8770112432899499 | 0.4439149281460875 | T | T | T |
| 0.2884724623069092 | 0.8770566229169132 | 0.4456818567459897 | T | T | T |
| 0.4551732437624652 | 0.8767788404456591 | 0.4455933689536062 | T | T | T |
| 0.6226877338343614 | 0.8768034018712483 | 0.4442937582533444 | T | T | T |
| 0.7886538390978262 | 0.8758692908484152 | 0.4430590338188328 | T | T | T |
| 0.9547866453599380 | 0.8774789375064616 | 0.4429392202188359 | T | T | T |
| 0.0392453599306633 | 0.1273449264071258 | 0.5496895278416016 | T | T | T |
| 0.2060989620488792 | 0.1283563726855475 | 0.5493146355810904 | T | T | T |
| 0.3722664712860282 | 0.1271376554977322 | 0.5502053786858407 | T | T | T |
| 0.5393071408407965 | 0.1269616586937046 | 0.5508869870689985 | T | T | T |
| 0.7061658229790680 | 0.1260026093476045 | 0.5477422686345684 | T | T | T |
| 0.8726201686716607 | 0.1270287220236013 | 0.5465713273140558 | T | T | T |
| 0.0404469839937954 | 0.2940013963222388 | 0.5479341726307848 | T | T | T |
| 0.2081924521198880 | 0.2958252574703489 | 0.5498242638472354 | T | T | T |
| 0.3720292800255013 | 0.2964686807305764 | 0.5522746484725438 | T | T | T |
| 0.5386355920464152 | 0.2925269597692156 | 0.5525270139301431 | T | T | T |
| 0.7066038934028078 | 0.2930406484581861 | 0.5498812869919606 | T | T | T |
| 0.8736464880943162 | 0.2934835411575847 | 0.5477185708552458 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.0382117416716130 | 0.4602605651920256 | 0.5503524979251084 | T | T | T |
| 0.2063391080514622 | 0.4602648652484395 | 0.5507925335889055 | T | T | T |
| 0.3729997756382058 | 0.4608255127137614 | 0.5614129319921994 | T | T | T |
| 0.5439519940423456 | 0.4557336776113824 | 0.5713123264955815 | T | T | T |
| 0.7071290823854103 | 0.4610196274655348 | 0.5525151115345636 | T | T | T |
| 0.8726768841259429 | 0.4603326903207819 | 0.5508734250131284 | T | T | T |
| 0.0378727311763240 | 0.6274390004285787 | 0.5513759505637383 | T | T | T |
| 0.2038995298969843 | 0.6268196086302539 | 0.5507671384471823 | T | T | T |
| 0.3688094052873591 | 0.6308346459776881 | 0.5583391972644259 | T | T | T |
| 0.5388236791274020 | 0.6266970465114886 | 0.5614122586931922 | T | T | T |
| 0.7031989323360691 | 0.6276471418500236 | 0.5522883116220375 | T | T | T |
| 0.8725100524273995 | 0.6273732748274137 | 0.5502297551099609 | T | T | T |
| 0.0377804023425495 | 0.7942166621819616 | 0.5485262440396476 | T | T | T |
| 0.2045212669153245 | 0.7951103852263954 | 0.5504796613641112 | T | T | T |
| 0.3728183539132952 | 0.7957418754529998 | 0.5507831960338226 | T | T | T |
| 0.5393917145165781 | 0.7933265113602338 | 0.5508329927982303 | T | T | T |
| 0.7038381495755750 | 0.7914687988252642 | 0.5498814990361941 | T | T | T |
| 0.8712996206732042 | 0.7935488803456987 | 0.5493775603724435 | T | T | T |
| 0.0382636910629744 | 0.9613737439153311 | 0.5489833488466113 | T | T | T |
| 0.2054027974770087 | 0.9618615200208970 | 0.5484932800537299 | T | T | T |
| 0.3721763925512931 | 0.9617662150695075 | 0.5513694692249382 | T | T | T |
| 0.5393683060229703 | 0.9614374306697234 | 0.5503832889334666 | T | T | T |
| 0.7056477045335864 | 0.9592038588808282 | 0.5479906870385046 | T | T | T |
| 0.8723016504056444 | 0.9604043411384966 | 0.5497312699393377 | T | T | T |

HN₂-NH₂

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

H N Mo

4 2 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4329841527128385 | 0.5575591730767678 | 0.6706198803733689 | T | T | T |
| 0.3237150145638947 | 0.5300886615199748 | 0.6736927311483180 | T | T | T |
| 0.6036427895814166 | 0.5293488166743705 | 0.6884493708392618 | T | T | T |
| 0.5027747251455792 | 0.4512138527755821 | 0.6962780950714350 | T | T | T |
| 0.3767853411482912 | 0.5436849883666914 | 0.6420486751468728 | T | T | T |
| 0.5505919323550078 | 0.4867410175684778 | 0.6633016528975570 | T | T | T |
| 0.1253853733327773 | 0.0441099423454647 | 0.4454753949409205 | T | T | T |
| 0.2911192565955444 | 0.0440297054612838 | 0.4427186009838837 | T | T | T |
| 0.4574823970190757 | 0.0433349635138257 | 0.4454333464918911 | T | T | T |
| 0.6239120416636224 | 0.0438259135506948 | 0.4453306516586472 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7901227034132454 | 0.0432543825520602 | 0.4461585865101328 | T | T | T |
| 0.9581113069705806 | 0.0437643165883666 | 0.4458672000518624 | T | T | T |
| 0.1250542874070147 | 0.2102461361750226 | 0.4433601106029074 | T | T | T |
| 0.2908389918756494 | 0.2097634336056205 | 0.4440829557818095 | T | T | T |
| 0.4575981076499918 | 0.2104058486853158 | 0.4442443169904358 | T | T | T |
| 0.6236631601324747 | 0.2105482211791093 | 0.4452936820491983 | T | T | T |
| 0.7899715606722665 | 0.2104854193243866 | 0.4458802787591689 | T | T | T |
| 0.9578572196408499 | 0.2108062497297106 | 0.4451285434041815 | T | T | T |
| 0.1249627959555606 | 0.3775139424446847 | 0.4439550204479408 | T | T | T |
| 0.2909204587581861 | 0.3767042834420218 | 0.4434543510325413 | T | T | T |
| 0.4557432467056118 | 0.3774128035561461 | 0.4476056949597007 | T | T | T |
| 0.6216902758206347 | 0.3777357068150059 | 0.4484534606370912 | T | T | T |
| 0.7895689921318484 | 0.3758862952447063 | 0.4461905236835629 | T | T | T |
| 0.9573236117743191 | 0.3767922182188032 | 0.4474091213329160 | T | T | T |
| 0.1258192702570798 | 0.5448150256161992 | 0.4456022348506861 | T | T | T |
| 0.2939027216668251 | 0.5441684992817408 | 0.4471748013300753 | T | T | T |
| 0.4566854195025953 | 0.5411255128972187 | 0.4498891182527635 | T | T | T |
| 0.6216038106543160 | 0.5407794718486761 | 0.4477258380810508 | T | T | T |
| 0.7898656402150497 | 0.5413807906996934 | 0.4460496504240255 | T | T | T |
| 0.9578204134214896 | 0.5429391436623558 | 0.4463067824952435 | T | T | T |
| 0.1255072395142284 | 0.7102195792721797 | 0.4460967250526587 | T | T | T |
| 0.2930788363933493 | 0.7100034383391045 | 0.4453702403916305 | T | T | T |
| 0.4572237651169906 | 0.7094740353092420 | 0.4469647008826761 | T | T | T |
| 0.6222465092040000 | 0.7085415047207362 | 0.4447495659253199 | T | T | T |
| 0.7897944185539603 | 0.7091585113628603 | 0.4464662742863111 | T | T | T |
| 0.9573708436646957 | 0.7098417533340879 | 0.4462840038995176 | T | T | T |
| 0.1255122023699177 | 0.8759306728313212 | 0.4442181466157144 | T | T | T |
| 0.2919923208310168 | 0.8764209675698142 | 0.4454501482048708 | T | T | T |
| 0.4576868715519359 | 0.8765110243627060 | 0.4454181626920193 | T | T | T |
| 0.6234568861678231 | 0.8768471180790584 | 0.4465058034602676 | T | T | T |
| 0.7900428108331279 | 0.8761134567407861 | 0.4459500405496158 | T | T | T |
| 0.9576358213275928 | 0.8760567322101954 | 0.4480353749322958 | T | T | T |
| 0.0402566823377201 | 0.1261263029358577 | 0.5495514807226285 | T | T | T |
| 0.2074948256751764 | 0.1270597679700803 | 0.5497977990018266 | T | T | T |
| 0.3746457535094779 | 0.1266093682765521 | 0.5479783533204965 | T | T | T |
| 0.5407246306909477 | 0.1269768204800465 | 0.5503390035128197 | T | T | T |
| 0.7075454213077570 | 0.1265185682216395 | 0.5507879700127242 | T | T | T |
| 0.8742865845307060 | 0.1269555340876512 | 0.5502324324202430 | T | T | T |
| 0.0409051266812426 | 0.2932785455134975 | 0.5497417372615058 | T | T | T |
| 0.2082417706032110 | 0.2936886476441071 | 0.5476400518315002 | T | T | T |
| 0.3744495578548948 | 0.2944479833491155 | 0.5509851743747102 | T | T | T |
| 0.5398141167259867 | 0.2930918952695943 | 0.5517108651661405 | T | T | T |
| 0.7078561170922925 | 0.2937475747223389 | 0.5512264140631037 | T | T | T |
| 0.8744246489611701 | 0.2937192223883782 | 0.5518146116259213 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.0404190256119035 | 0.4595574991467504 | 0.5515917672086987 | T | T | T |
| 0.2052395485349249 | 0.4578785448372045 | 0.5483662181741186 | T | T | T |
| 0.3741734355892313 | 0.4588023919034211 | 0.5563313453792250 | T | T | T |
| 0.5429806797203468 | 0.4614241530244730 | 0.5651474092644387 | T | T | T |
| 0.7098776122885422 | 0.4615610578510983 | 0.5517851737780974 | T | T | T |
| 0.8744890019367405 | 0.4600481927246539 | 0.5515522427151958 | T | T | T |
| 0.0404808618134442 | 0.6253232368744538 | 0.5513944333928987 | T | T | T |
| 0.2060084891378466 | 0.6251861289669746 | 0.5510203292144392 | T | T | T |
| 0.3716068839520407 | 0.6266719506312676 | 0.5573996797565036 | T | T | T |
| 0.5441406024853496 | 0.6296063046216054 | 0.5508191069564402 | T | T | T |
| 0.7094896053288168 | 0.6283620588166323 | 0.5492955632810834 | T | T | T |
| 0.8749422893139746 | 0.6267423967329292 | 0.5507121071567744 | T | T | T |
| 0.0409556473785381 | 0.7927869612565824 | 0.5505565489184958 | T | T | T |
| 0.2072326101451668 | 0.7931545731946333 | 0.5508014119667023 | T | T | T |
| 0.3741462947182351 | 0.7928205082002444 | 0.5513031443324437 | T | T | T |
| 0.5408297088961397 | 0.7930144037130643 | 0.5511939392793964 | T | T | T |
| 0.7082108072043342 | 0.7943543192184230 | 0.5495417847887027 | T | T | T |
| 0.8746538568793946 | 0.7936460524453939 | 0.5525416046963102 | T | T | T |
| 0.0408298596285857 | 0.9597530077393970 | 0.5515582069664275 | T | T | T |
| 0.2073632338333565 | 0.9594452143905293 | 0.5478844329025147 | T | T | T |
| 0.3740823836506280 | 0.9605627660279329 | 0.5507939899949021 | T | T | T |
| 0.5405680576743751 | 0.9603478991057902 | 0.5502212396772845 | T | T | T |
| 0.7076703428805066 | 0.9603585573473659 | 0.5512742013870018 | T | T | T |
| 0.8745655625631320 | 0.9601209094640661 | 0.5510696871245275 | T | T | T |

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9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

N Mo

1 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4820141841928773 | 0.5179858016164758 | 0.6151160722200615 | T | T | T |
| 0.1249123938911438 | 0.0421833707491288 | 0.4448493565962011 | T | T | T |
| 0.2915466677030309 | 0.0424685295963414 | 0.4472843149847634 | T | T | T |
| 0.4586975369551851 | 0.0418592232844617 | 0.4471143232024630 | T | T | T |
| 0.6255643503879327 | 0.0415805035227947 | 0.4463935833901260 | T | T | T |
| 0.7920314599134102 | 0.0416685731062927 | 0.4457648025869290 | T | T | T |
| 0.9582722131462944 | 0.0417275462453688 | 0.4470948953746898 | T | T | T |
| 0.1247824987586199 | 0.2096108995329899 | 0.4463856382297422 | T | T | T |
| 0.2915135821721364 | 0.2098568743676452 | 0.4458042529196504 | T | T | T |
| 0.4596632416999142 | 0.2091346003739716 | 0.4481073415980106 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.6259211128677862 | 0.2080948618999230 | 0.4468430385192192 | T | T | T |
| 0.7922874062191667 | 0.2077119580668381 | 0.4454676887495950 | T | T | T |
| 0.9583312730457934 | 0.2079680345753729 | 0.4457648098539053 | T | T | T |
| 0.1254395181297809 | 0.3753659987683804 | 0.4477182229109715 | T | T | T |
| 0.2914831728639484 | 0.3745440665683475 | 0.4473058554091480 | T | T | T |
| 0.4591145205490150 | 0.3745828350932285 | 0.4493012862320072 | T | T | T |
| 0.6258456770470602 | 0.3741537018146985 | 0.4482689012225478 | T | T | T |
| 0.7919048024983297 | 0.3740784490524192 | 0.4468433256434139 | T | T | T |
| 0.9584191619107472 | 0.3744350197165787 | 0.4463933526128514 | T | T | T |
| 0.1257841756210709 | 0.5409122366550392 | 0.4480338914347755 | T | T | T |
| 0.2930168486927158 | 0.5417249599145180 | 0.4506187738041234 | T | T | T |
| 0.4575023849803799 | 0.5424978995847596 | 0.4516029763783322 | T | T | T |
| 0.6254168467375578 | 0.5408851412680917 | 0.4493013863212241 | T | T | T |
| 0.7908647479030790 | 0.5403365129336422 | 0.4481074192398893 | T | T | T |
| 0.9581409644204797 | 0.5413026545988515 | 0.4471145182441560 | T | T | T |
| 0.1253522281912254 | 0.7083407028241524 | 0.4461429467543283 | T | T | T |
| 0.2914108297788545 | 0.7085895726971358 | 0.4491060249260741 | T | T | T |
| 0.4582751493495749 | 0.7069833851514034 | 0.4506186687311384 | T | T | T |
| 0.6254557812221151 | 0.7085171076880812 | 0.4473059251997711 | T | T | T |
| 0.7901427696242465 | 0.7084865543075267 | 0.4458045550067666 | T | T | T |
| 0.9575313649294444 | 0.7084536232438055 | 0.4472846428278032 | T | T | T |
| 0.1251234190577364 | 0.8748769930788995 | 0.4472441768233111 | T | T | T |
| 0.2916596379559380 | 0.8746480982208027 | 0.4461426462056721 | T | T | T |
| 0.4590879021127350 | 0.8742161677897826 | 0.4480339635530441 | T | T | T |
| 0.6246337757640035 | 0.8745604443813164 | 0.4477182593585880 | T | T | T |
| 0.7903887525397124 | 0.8752174072603580 | 0.4463860475379349 | T | T | T |
| 0.9578166338329197 | 0.8750877866272972 | 0.4448495296542916 | T | T | T |
| 0.0418753846763309 | 0.1257802503981367 | 0.5527065699763867 | T | T | T |
| 0.2082350307110730 | 0.1262267484779329 | 0.5491834940943576 | T | T | T |
| 0.3744049233552360 | 0.1241663594902391 | 0.5526562546009117 | T | T | T |
| 0.5415962418491489 | 0.1242444152259026 | 0.5517317157129895 | T | T | T |
| 0.7085706143480337 | 0.1235643563240814 | 0.5513789407110181 | T | T | T |
| 0.8758368236613592 | 0.1241626509887297 | 0.5520401708982163 | T | T | T |
| 0.0419737671974687 | 0.2924236913460732 | 0.5518410422166795 | T | T | T |
| 0.2094176058716712 | 0.2944822837789900 | 0.5526575183005917 | T | T | T |
| 0.3752021812058288 | 0.2918098846376722 | 0.5512263098586772 | T | T | T |
| 0.5420836378231400 | 0.2892993634787615 | 0.5540454317051697 | T | T | T |
| 0.7101582074906929 | 0.2898413841572776 | 0.5518799421017917 | T | T | T |
| 0.8764355420414276 | 0.2914290147946375 | 0.5513788677220575 | T | T | T |
| 0.0416836347332961 | 0.4583335007246845 | 0.5532526908356274 | T | T | T |
| 0.2088253050449680 | 0.4575638744891037 | 0.5547964692252307 | T | T | T |
| 0.3766248047131953 | 0.4618326251014153 | 0.5609615874739831 | T | T | T |
| 0.5460616518887207 | 0.4539383624958617 | 0.5550296364817839 | T | T | T |
| 0.7107003625186579 | 0.4579160953057340 | 0.5540456686495858 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.8757551496490663 | 0.4584035042687447 | 0.5517317431048241 | T | T | T |
| 0.0412139566059579 | 0.6246555184129789 | 0.5512979864708427 | T | T | T |
| 0.2064464313545784 | 0.6254952042246913 | 0.5548435329550685 | T | T | T |
| 0.3695040801623151 | 0.6304962213733631 | 0.5558157267804447 | T | T | T |
| 0.5381673718651356 | 0.6233754317376281 | 0.5609616460687619 | T | T | T |
| 0.7081899392011550 | 0.6247979464377167 | 0.5512266089192437 | T | T | T |
| 0.8758333532164642 | 0.6255953284100144 | 0.5526567073397572 | T | T | T |
| 0.0412146319676410 | 0.7919557595688858 | 0.5521910765024813 | T | T | T |
| 0.2074489543954527 | 0.7925516170946096 | 0.5505986403375758 | T | T | T |
| 0.3745051437451750 | 0.7935540467424005 | 0.5548437001019977 | T | T | T |
| 0.5424362442599744 | 0.7911749617273642 | 0.5547960799364446 | T | T | T |
| 0.7055174234432968 | 0.7905823972258474 | 0.5526577267112316 | T | T | T |
| 0.8737729484845147 | 0.7917651433541550 | 0.5491839648068293 | T | T | T |
| 0.0414717377653773 | 0.9585281896860778 | 0.5496273902660960 | T | T | T |
| 0.2080444760047655 | 0.9587854604044281 | 0.5521908864028049 | T | T | T |
| 0.3753447788215638 | 0.9587865880803932 | 0.5512974672061048 | T | T | T |
| 0.5416665607476503 | 0.9583164424851915 | 0.5532523476356346 | T | T | T |
| 0.7075759478111081 | 0.9580258754014395 | 0.5518409578507786 | T | T | T |
| 0.8742193560122544 | 0.9581245292546399 | 0.5527067472056331 | T | T | T |

*NH

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

H N Mo
1 1 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4835820628061905 | 0.5164179087734961 | 0.6734802009315378 | T | T | T |
| 0.4849389000450877 | 0.5150602308802736 | 0.6222941999096269 | T | T | T |
| 0.1252298028903751 | 0.0418560912336850 | 0.4448076726579718 | T | T | T |
| 0.2918653375341984 | 0.0417837286267441 | 0.4474934678846590 | T | T | T |
| 0.4588605709531945 | 0.0414427553564565 | 0.4470128213569479 | T | T | T |
| 0.6259923588751671 | 0.0416929191419010 | 0.4453322000149014 | T | T | T |
| 0.7924459698959075 | 0.0415377919542869 | 0.4448118207684095 | T | T | T |
| 0.9583885104828147 | 0.0416129989909474 | 0.4464861225905301 | T | T | T |
| 0.1251170198451500 | 0.2087284182060042 | 0.4460189875626790 | T | T | T |
| 0.2919876474000056 | 0.2092102253394156 | 0.4455221278635997 | T | T | T |
| 0.4598114931980384 | 0.2084536361643320 | 0.4477640247743933 | T | T | T |
| 0.6261749575548410 | 0.2077535468199127 | 0.4459422177568115 | T | T | T |
| 0.7924082352075419 | 0.2075951074778684 | 0.4434829449946245 | T | T | T |
| 0.9584635006392042 | 0.2075559550537217 | 0.4448120789031618 | T | T | T |
| 0.1249992191314492 | 0.3746876908217356 | 0.4471053210194066 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.2914854831876877 | 0.3742863635883803 | 0.4472955054739367 | T | T | T |
| 0.4591173832394046 | 0.3751449557716576 | 0.4499084026771569 | T | T | T |
| 0.6261243573411331 | 0.3738776804825016 | 0.4476328600302772 | T | T | T |
| 0.7922486329930728 | 0.3738264887978054 | 0.4459422291198177 | T | T | T |
| 0.9583086240219023 | 0.3740092701193299 | 0.4453328645156873 | T | T | T |
| 0.1257229600728602 | 0.5405276842958151 | 0.4481943017154275 | T | T | T |
| 0.2926532771982436 | 0.5409602060372283 | 0.4505617768903973 | T | T | T |
| 0.4584700316626792 | 0.5415283177829724 | 0.4537531585869761 | T | T | T |
| 0.6248557248644384 | 0.5408820502309171 | 0.4499086369484815 | T | T | T |
| 0.7915485987578158 | 0.5401889338954027 | 0.4477642633914141 | T | T | T |
| 0.9585573477881095 | 0.5411390685685403 | 0.4470133706793513 | T | T | T |
| 0.1258595392466031 | 0.7080318505183636 | 0.4469070007766363 | T | T | T |
| 0.2917195232818843 | 0.7082773463913384 | 0.4496784882121105 | T | T | T |
| 0.4590375216383172 | 0.7073443149181354 | 0.4505612616485514 | T | T | T |
| 0.6257142925695739 | 0.7085128665841663 | 0.4472948955101562 | T | T | T |
| 0.7907911185170486 | 0.7080113583879002 | 0.4455223055283686 | T | T | T |
| 0.9582160689155543 | 0.7081327967959911 | 0.4474938250026159 | T | T | T |
| 0.1256539842056606 | 0.8743443129667349 | 0.4480036581004609 | T | T | T |
| 0.2919658791852103 | 0.8741387807105032 | 0.4469071690481548 | T | T | T |
| 0.4594710340339764 | 0.8742757289504273 | 0.4481936279674208 | T | T | T |
| 0.6253128609270845 | 0.8749994972168454 | 0.4471049893215694 | T | T | T |
| 0.7912727879261754 | 0.8748827653678783 | 0.4460190025551205 | T | T | T |
| 0.9581444191682729 | 0.8747695866366237 | 0.4448078268706231 | T | T | T |
| 0.0419408665442261 | 0.1255202892188171 | 0.5521494080445525 | T | T | T |
| 0.2085488409698794 | 0.1254267773445814 | 0.5491943720857373 | T | T | T |
| 0.3751717956315703 | 0.1238983359922550 | 0.5526495911780279 | T | T | T |
| 0.5420766831786505 | 0.1238195145287831 | 0.5516354429142635 | T | T | T |
| 0.7087843234182657 | 0.1235114609801330 | 0.5499367872503559 | T | T | T |
| 0.8760701698834339 | 0.1239318251573009 | 0.5508638680112075 | T | T | T |
| 0.0423976370134714 | 0.2922023550660252 | 0.5511495402074114 | T | T | T |
| 0.2098342273898922 | 0.2936329706073050 | 0.5525543726142761 | T | T | T |
| 0.3753062836499197 | 0.2911610978156954 | 0.5511107245542336 | T | T | T |
| 0.5424255758198500 | 0.2895988756995622 | 0.5534058109615004 | T | T | T |
| 0.7102339288009326 | 0.2897693957174037 | 0.5513480299524186 | T | T | T |
| 0.8764898208014834 | 0.2912175712177563 | 0.5499358837045409 | T | T | T |
| 0.0416560789569330 | 0.4583259511987037 | 0.5532100589831545 | T | T | T |
| 0.2102453712115370 | 0.4574030773755455 | 0.5543387945870528 | T | T | T |
| 0.3747614513917945 | 0.4603325624691739 | 0.5608956985252650 | T | T | T |
| 0.5459312965899807 | 0.4540689898047550 | 0.5556927714995871 | T | T | T |
| 0.7104031453068977 | 0.4575749188331658 | 0.5534052925074174 | T | T | T |
| 0.8761821607798372 | 0.4579245434708513 | 0.5516346364096564 | T | T | T |
| 0.0417421708325182 | 0.6242584222659424 | 0.5519288141787291 | T | T | T |
| 0.2071143945965214 | 0.6249598222188805 | 0.5554708079760989 | T | T | T |
| 0.3707444509595740 | 0.6292534823491762 | 0.5553867916035944 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.5396671999414413 | 0.6252368298529564 | 0.5608959184951605 | T | T | T |
| 0.7088397597645661 | 0.6246926416306687 | 0.5511107199372792 | T | T | T |
| 0.8761022787881667 | 0.6248267430673258 | 0.5526487822425008 | T | T | T |
| 0.0416760739864471 | 0.7916568749536278 | 0.5529162984077961 | T | T | T |
| 0.2081007812343618 | 0.7918960621923661 | 0.5519319862309656 | T | T | T |
| 0.3750379458025653 | 0.7928827961428888 | 0.5554712730295693 | T | T | T |
| 0.5425960677555537 | 0.7897531840874150 | 0.5543396439983479 | T | T | T |
| 0.7063679879476669 | 0.7901648257540530 | 0.5525547928176026 | T | T | T |
| 0.8745742521794979 | 0.7914500750121700 | 0.5491943199054378 | T | T | T |
| 0.0417866269812062 | 0.9582130745144023 | 0.5492842017299040 | T | T | T |
| 0.2083411829892929 | 0.9583232552606508 | 0.5529164507306893 | T | T | T |
| 0.3757399625321403 | 0.9582567643920299 | 0.5519294729280311 | T | T | T |
| 0.5416742612858763 | 0.9583436647034858 | 0.5532112123890351 | T | T | T |
| 0.7078002532598634 | 0.9576034452971245 | 0.5511508633290779 | T | T | T |
| 0.8744808459319579 | 0.9580594172333183 | 0.5521495979446573 | T | T | T |

*NH₂

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

H N Mo
2 1 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.5950360448388565 | 0.5553421510571042 | 0.6736744335647700 | T | T | T |
| 0.4857899342606018 | 0.5247595964926219 | 0.6739018481001935 | T | T | T |
| 0.5402988425352646 | 0.5398724659716976 | 0.6435477202279998 | T | T | T |
| 0.1243127209753609 | 0.0400827923731057 | 0.4476770978429556 | T | T | T |
| 0.2905110047834540 | 0.0395062628592626 | 0.4465780129799128 | T | T | T |
| 0.4565905275169868 | 0.0395773104129944 | 0.4455075939172204 | T | T | T |
| 0.6233801794916474 | 0.0399090120805212 | 0.4455230466072564 | T | T | T |
| 0.7894946519681838 | 0.0399445038749278 | 0.4463418294489685 | T | T | T |
| 0.9557817284821510 | 0.0394844142284612 | 0.4476526681086739 | T | T | T |
| 0.1238954154202858 | 0.2064499752529585 | 0.4474983816843690 | T | T | T |
| 0.2903517586521076 | 0.2067735751176514 | 0.4460226696497713 | T | T | T |
| 0.4564791766387231 | 0.2063489999627350 | 0.4462836687621348 | T | T | T |
| 0.6230844364881918 | 0.2067217706006019 | 0.4460349649446940 | T | T | T |
| 0.7894757414344511 | 0.2067149850847230 | 0.4451583835421431 | T | T | T |
| 0.9563113604448716 | 0.2063247803932171 | 0.4479479471594274 | T | T | T |
| 0.1234204330203070 | 0.3734730055468845 | 0.4481366393724073 | T | T | T |
| 0.2905908486886162 | 0.3741426278331446 | 0.4463331223618852 | T | T | T |
| 0.4569942242229246 | 0.3727324765485847 | 0.4468009060075033 | T | T | T |
| 0.6217078005699790 | 0.3732360681145650 | 0.4470232736314159 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.7890161381711351 | 0.3726636327780639 | 0.4470758320591059 | T | T | T |
| 0.9564560862993332 | 0.3728733775942317 | 0.4472080078481540 | T | T | T |
| 0.1235398446016660 | 0.5399187236493361 | 0.4478925126813280 | T | T | T |
| 0.2908944044223674 | 0.5415136670948542 | 0.4467091230923756 | T | T | T |
| 0.4591351364590821 | 0.5400902732404660 | 0.4497617300080492 | T | T | T |
| 0.6209042513781924 | 0.5396297408931972 | 0.4496417982801759 | T | T | T |
| 0.7890775578914742 | 0.5380588355904834 | 0.4463255950634490 | T | T | T |
| 0.9564501975483068 | 0.5394777013206991 | 0.4478528521419278 | T | T | T |
| 0.1235385342267890 | 0.7064691990191179 | 0.4474292957050849 | T | T | T |
| 0.2909782277844997 | 0.7067651898972969 | 0.4474582736473636 | T | T | T |
| 0.4582384961670343 | 0.7063434471656649 | 0.4474682428428096 | T | T | T |
| 0.6229873827911661 | 0.7069428593843838 | 0.4469901780044054 | T | T | T |
| 0.7894749172651174 | 0.7055057357867298 | 0.4463005214608700 | T | T | T |
| 0.9566055589813800 | 0.7060288679131901 | 0.4480084129967068 | T | T | T |
| 0.1237323616029826 | 0.8731334680290104 | 0.4480049639283123 | T | T | T |
| 0.2905268782084818 | 0.8726696342371127 | 0.4454511634534626 | T | T | T |
| 0.4568975911701898 | 0.8727816592498669 | 0.4465235323158936 | T | T | T |
| 0.6234863758074241 | 0.8731506539506029 | 0.4463951573722227 | T | T | T |
| 0.7896600385667725 | 0.8728028032021768 | 0.4460158691197762 | T | T | T |
| 0.9561225819814254 | 0.8731075875018206 | 0.4474124214771251 | T | T | T |
| 0.0400220921702754 | 0.1233718988239687 | 0.5526036114907953 | T | T | T |
| 0.2065767598941690 | 0.1223931258001585 | 0.5518607310089365 | T | T | T |
| 0.3735637820395397 | 0.1233592398032286 | 0.5510851336017950 | T | T | T |
| 0.5401104556330267 | 0.1226844929531339 | 0.5509008559463169 | T | T | T |
| 0.7062054006182450 | 0.1231621331655504 | 0.5502692674595622 | T | T | T |
| 0.8734265313914520 | 0.1232182698100246 | 0.5521833031409074 | T | T | T |
| 0.0400113757380041 | 0.2897576019642045 | 0.5533077086672264 | T | T | T |
| 0.2063807306179513 | 0.2893869503552082 | 0.5516236964404442 | T | T | T |
| 0.3735441984613601 | 0.2902853322415027 | 0.5507572938831871 | T | T | T |
| 0.5402871339287643 | 0.2904989615823368 | 0.5522469027697596 | T | T | T |
| 0.7066335078317820 | 0.2895148405419263 | 0.5520360730416556 | T | T | T |
| 0.8735290197663730 | 0.2899589095812303 | 0.5510995570602546 | T | T | T |
| 0.0397204864034606 | 0.4564815935266466 | 0.5531518422452351 | T | T | T |
| 0.2057962738193027 | 0.4561205856856958 | 0.5523289562125342 | T | T | T |
| 0.3705124016760095 | 0.4545400436009004 | 0.5507342512519031 | T | T | T |
| 0.5423165094608464 | 0.4561947060268920 | 0.5582716928179323 | T | T | T |
| 0.7081434138547280 | 0.4575024848726486 | 0.5520535441705690 | T | T | T |
| 0.8736615036280924 | 0.4569784631123639 | 0.5524642880736295 | T | T | T |
| 0.0401764240231515 | 0.6228608339162207 | 0.5532433437061712 | T | T | T |
| 0.2062217682293195 | 0.6223838533899695 | 0.5526982751196599 | T | T | T |
| 0.3718272162231528 | 0.6220548138222952 | 0.5526275465933281 | T | T | T |
| 0.5378184973644053 | 0.6234329442872806 | 0.5584415335581667 | T | T | T |
| 0.7095490987863684 | 0.6250987314809109 | 0.5506570115587408 | T | T | T |
| 0.8741596488516663 | 0.6233507216296843 | 0.5519953265217623 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.0400005535741386 | 0.7896882632272764 | 0.5532409620042671 | T | T | T |
| 0.2063880455741511 | 0.7894357958582177 | 0.5513236423328607 | T | T | T |
| 0.3732488110152659 | 0.7899292058307381 | 0.5525545231764326 | T | T | T |
| 0.5397156395969560 | 0.7890885574311071 | 0.5526727190481608 | T | T | T |
| 0.7065679904776587 | 0.7893439867839049 | 0.5508974281749985 | T | T | T |
| 0.8737488522130761 | 0.7902104236248135 | 0.5515529439749756 | T | T | T |
| 0.0400982394717104 | 0.9562093023734448 | 0.5525462636569927 | T | T | T |
| 0.2065977967405317 | 0.9562640571708414 | 0.5523529107199394 | T | T | T |
| 0.3737213243319175 | 0.9562809725307275 | 0.5504740078555130 | T | T | T |
| 0.5398027521374900 | 0.9568405707658201 | 0.5511764349055994 | T | T | T |
| 0.7064929306572267 | 0.9561926843852717 | 0.5509758680534986 | T | T | T |
| 0.8735566333503115 | 0.9572339400222845 | 0.5517915197691252 | T | T | T |

*NH₃

1.0000000000000000

9.1482180682119907 -13.2029053235859699 0.0000000000000000

9.1482180682119907 13.2029053235859699 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000566999999982

H N Mo
3 1 72

Selective dynamics

Direct

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.4950438199295277 | 0.5022189019814576 | 0.6905381130602137 | T | T | T |
| 0.5959769364034457 | 0.4967021160362535 | 0.6948945976762317 | T | T | T |
| 0.5070441493121081 | 0.4041080030771056 | 0.6950286244932187 | T | T | T |
| 0.533662223809044 | 0.4667401321727311 | 0.6755032179043994 | T | T | T |
| 0.1228531847308929 | 0.0446719754495319 | 0.4448136747664080 | T | T | T |
| 0.2892576388574284 | 0.0449804466486015 | 0.4453823255848093 | T | T | T |
| 0.4555175627674046 | 0.0445834657010593 | 0.4462588670565424 | T | T | T |
| 0.6221365822662577 | 0.0448412865178653 | 0.4452159779046312 | T | T | T |
| 0.7892028998597453 | 0.0449587200330086 | 0.4455694608087981 | T | T | T |
| 0.9555981126569861 | 0.0446057977190293 | 0.4461335527625394 | T | T | T |
| 0.1229051598966961 | 0.2111466935672581 | 0.4453783716279816 | T | T | T |
| 0.2895171245408434 | 0.2114322804721738 | 0.4445525908050314 | T | T | T |
| 0.4557947574641616 | 0.2113036800932093 | 0.4452667725284130 | T | T | T |
| 0.6223028718154353 | 0.2121839383321813 | 0.4466736550224155 | T | T | T |
| 0.7886913674056544 | 0.2114920761975512 | 0.4447695313749733 | T | T | T |
| 0.9552206587551595 | 0.2109855778075627 | 0.4455550687315650 | T | T | T |
| 0.1223805636632775 | 0.3776790977008702 | 0.4471731781185255 | T | T | T |
| 0.2893065360276523 | 0.3779332876866093 | 0.4448895232438375 | T | T | T |
| 0.4558606261439024 | 0.3777936363212930 | 0.4473469083148132 | T | T | T |
| 0.6214161359783290 | 0.3788163288283215 | 0.4474510255244653 | T | T | T |
| 0.7880043500736775 | 0.3779033627526331 | 0.4466982586652293 | T | T | T |
| 0.9553524625845995 | 0.3780508483970735 | 0.4452081661793201 | T | T | T |

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 0.1225822662014622 | 0.5444243988689763 | 0.4450947294881473 | T | T | T |
| 0.2900530163244284 | 0.5447595584529950 | 0.4461735493352350 | T | T | T |
| 0.4564842814379588 | 0.5437256104315153 | 0.4464139978889392 | T | T | T |
| 0.6224418303791595 | 0.5443681541076302 | 0.4473819193935924 | T | T | T |
| 0.7889192896757322 | 0.5444139558096381 | 0.4453192290401091 | T | T | T |
| 0.9556339014505824 | 0.5446791313819475 | 0.4462667245262608 | T | T | T |
| 0.1226504096820449 | 0.7112511660913157 | 0.4446808930102080 | T | T | T |
| 0.2892404031505862 | 0.7109662536587606 | 0.4444773078719138 | T | T | T |
| 0.4554335158854741 | 0.7101543302915232 | 0.4461922287292523 | T | T | T |
| 0.6222719850957006 | 0.7109030266083849 | 0.4449223069974408 | T | T | T |
| 0.7887893781696178 | 0.7106930923194099 | 0.4445944814154856 | T | T | T |
| 0.9552381902989566 | 0.7109513403028771 | 0.4454197967587916 | T | T | T |
| 0.1226133012091424 | 0.8776090434468600 | 0.4465880630120864 | T | T | T |
| 0.2889619537337467 | 0.8775566934165653 | 0.4446944295833291 | T | T | T |
| 0.4557655324049605 | 0.8776206689002848 | 0.4451184612187191 | T | T | T |
| 0.6225083423940134 | 0.8778188836860679 | 0.4471997636086513 | T | T | T |
| 0.7890642970843942 | 0.8773041432216502 | 0.4454235338908958 | T | T | T |
| 0.9555497344491783 | 0.8773540563785929 | 0.4448377211670334 | T | T | T |
| 0.0390605756839619 | 0.1278600915032655 | 0.5504626195332847 | T | T | T |
| 0.2054687327444853 | 0.1273927440704909 | 0.5497010685249322 | T | T | T |
| 0.3723763387850312 | 0.1283122191790369 | 0.5505424117738968 | T | T | T |
| 0.5388277020601890 | 0.1281615713317450 | 0.5514216057576320 | T | T | T |
| 0.7050724725698032 | 0.1277011992942931 | 0.5493618518300352 | T | T | T |
| 0.8723701724948612 | 0.1278357105602765 | 0.5502960427227208 | T | T | T |
| 0.0390740248743384 | 0.2945751429139420 | 0.5511976229631657 | T | T | T |
| 0.2062027717058115 | 0.2943517323427400 | 0.5503129275141347 | T | T | T |
| 0.3726921544146009 | 0.2946449360809069 | 0.5504153209662590 | T | T | T |
| 0.5388450998667551 | 0.2942469053855987 | 0.5518813758049106 | T | T | T |
| 0.7054577421881731 | 0.2947461583171105 | 0.5527958590357116 | T | T | T |
| 0.8724967798786096 | 0.2951267400079232 | 0.5493557012518053 | T | T | T |
| 0.0388908101963139 | 0.4612073883820287 | 0.5507791023136903 | T | T | T |
| 0.2058531945098494 | 0.4609744898695425 | 0.5514224902497489 | T | T | T |
| 0.3717032179539430 | 0.4607555653555266 | 0.5504016320225702 | T | T | T |
| 0.5392200890100014 | 0.4610272930231076 | 0.5599432768908486 | T | T | T |
| 0.7059680530143169 | 0.4613694067234633 | 0.5519295679438727 | T | T | T |
| 0.8720512251447161 | 0.4613680528265220 | 0.5514367727169542 | T | T | T |
| 0.0389738030633850 | 0.6278374066545780 | 0.5504373108150560 | T | T | T |
| 0.2054070797961813 | 0.6272874524047793 | 0.5491627500905452 | T | T | T |
| 0.3725548413208770 | 0.6276503705875953 | 0.5519347827288925 | T | T | T |
| 0.5394772455768475 | 0.6285205733283803 | 0.5504413578313674 | T | T | T |
| 0.7056068789748338 | 0.6275567305317722 | 0.5504379962736365 | T | T | T |
| 0.8719205927563394 | 0.6278312067534344 | 0.5505803754659766 | T | T | T |
| 0.0392496370898172 | 0.7943997917291483 | 0.5511029118872486 | T | T | T |
| 0.2057300832971904 | 0.7944581795118211 | 0.5498011461780337 | T | T | T |

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|--------------------|--------------------|--------------------|---|---|---|
| 0.3729055196353599 | 0.7947847170744566 | 0.5491839862989423 | T | T | T |
| 0.5392262465857272 | 0.7943683016981922 | 0.5514535239677940 | T | T | T |
| 0.7058798688078127 | 0.7940325723565707 | 0.5503542251622093 | T | T | T |
| 0.8728463261415840 | 0.7947598411606478 | 0.5497390379102498 | T | T | T |
| 0.0392204522213362 | 0.9610007521822652 | 0.5503721332577243 | T | T | T |
| 0.2058158939912929 | 0.9609781976472149 | 0.5510833851145449 | T | T | T |
| 0.3723475987623033 | 0.9612307828342281 | 0.5504444377478137 | T | T | T |
| 0.5389701564695599 | 0.9613202059194492 | 0.5507968607592701 | T | T | T |
| 0.7056356714680874 | 0.9611310465434357 | 0.5512097913226484 | T | T | T |
| 0.8723567857141532 | 0.9611524863286576 | 0.5504767997065514 | T | T | T |