**Supporting Information**

**Fast-Tracking Transition State Localization via Reaction Directional Analysis**

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**S1.** Cartesian coordinates of initial states (IS), final states (FS) and transition states (TS) for gas-phase reaction.

Reaction: no. 1 HCN↔HNC

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.998532489 | 11.97628257 | 9.763853952 |
| C | 9.971797177 | 10.90373731 | 9.690665796 |
| N | 9.942974915 | 9.745350847 | 9.611515554 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.5434656 | 10.02606008 | 10.55561599 |
| C | 8.606585471 | 11.0192377 | 10.73220637 |
| N | 9.651475749 | 10.48358308 | 10.63711842 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.29760456 | 11.28765553 | 10.13818614 |
| C | 9.169440339 | 10.87386439 | 10.1721228 |
| N | 9.936653916 | 9.961252562 | 10.06616335 |

Reaction: no. 2 HCCH↔CCH2

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.204327346 | 10.28148466 | 8.0256249 |
| H | 9.402125238 | 10.84650588 | 11.32014174 |
| C | 9.267589173 | 10.46191999 | 9.079041959 |
| C | 9.338930808 | 10.66591666 | 10.26722562 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.509844322 | 10.85503811 | 9.410684564 |
| H | 9.177838725 | 11.3650614 | 11.18712982 |
| C | 9.790436064 | 10.8100389 | 10.46857107 |
| C | 10.81902362 | 10.11930428 | 10.85926295 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.250943032 | 10.79007 | 8.950559859 |
| H | 9.35252043 | 11.10965459 | 11.10113697 |
| C | 9.734708492 | 10.6070591 | 9.900864207 |
| C | 10.32507698 | 10.37086866 | 10.98959379 |

Reaction: no. 3 H2CO↔H2+CO

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.253831162 | 11.04970988 | 9.855417502 |
| H | 11.14538207 | 11.04970795 | 9.855413781 |
| C | 10.19964281 | 10.45450839 | 9.85525673 |
| O | 10.19974654 | 9.240022361 | 9.855691243 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.21710096 | 11.97324072 | 10.04503517 |
| H | 10.54588384 | 12.55183737 | 10.39407923 |
| C | 9.710428099 | 9.268754767 | 9.409278639 |
| O | 10.1634478 | 8.342565542 | 9.903499448 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.639956511 | 11.24959429 | 9.825989256 |
| H | 10.92552825 | 11.41288497 | 10.07752868 |
| C | 9.825062657 | 10.16362203 | 9.804300835 |
| O | 10.34245101 | 9.106748436 | 9.84785779 |

Reaction: no. 4 CH3O↔CH2OH

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.254900278 | 9.903256266 | 10.00688148 |
| H | 11.59854077 | 11.55865168 | 10.00684876 |
| H | 9.370013419 | 11.82046536 | 10.00666293 |
| C | 9.816845643 | 10.83060062 | 10.0067281 |
| O | 11.17523411 | 10.68175202 | 10.00707042 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.757315988 | 9.720682412 | 9.826723645 |
| H | 10.99735473 | 10.95105537 | 9.421201399 |
| H | 9.669249264 | 11.36067957 | 10.55566016 |
| C | 10.37583656 | 10.5458192 | 10.2591752 |
| O | 11.12478101 | 10.12482483 | 11.29484589 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.542592032 | 9.848005522 | 9.751110406 |
| H | 11.20976327 | 10.98526745 | 9.633873509 |
| H | 9.469487086 | 11.62633442 | 10.40539454 |
| C | 10.0583578 | 10.73665434 | 10.14037975 |
| O | 11.28981417 | 10.55269547 | 10.76510058 |

Reaction: no. 5 cyclopropyl ring opening

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.92687754 | 9.588152877 | 9.337786193 |
| H | 8.352827846 | 9.586992547 | 9.337811403 |
| H | 9.638611711 | 12.22118923 | 10.25484625 |
| H | 8.353118204 | 9.58784351 | 11.16594608 |
| H | 10.92657118 | 9.588934826 | 11.16592173 |
| C | 10.41179992 | 9.918468923 | 10.25163534 |
| C | 8.867524361 | 9.917913128 | 10.25166058 |
| C | 9.639188129 | 11.14015331 | 10.2509534 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.92687754 | 9.588152877 | 9.337786193 |
| H | 8.352827846 | 9.586992547 | 9.337811403 |
| H | 9.638611711 | 12.22118923 | 10.25484625 |
| H | 8.353118204 | 9.58784351 | 11.16594608 |
| H | 10.92657118 | 9.588934826 | 11.16592173 |
| C | 10.41179992 | 9.918468923 | 10.25163534 |
| C | 8.867524361 | 9.917913128 | 10.25166058 |
| C | 9.639188129 | 11.14015331 | 10.2509534 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.06700908 | 9.530437225 | 9.167512073 |
| H | 8.705245952 | 9.268866482 | 9.469397375 |
| H | 9.727525063 | 12.0012811 | 10.65967468 |
| H | 7.995901262 | 10.05577941 | 10.98690802 |
| H | 11.26786115 | 9.755225442 | 11.00667955 |
| C | 10.7833217 | 10.06331676 | 10.07798357 |
| C | 8.768548311 | 10.08064286 | 10.19954642 |
| C | 9.725003127 | 11.06950466 | 10.09694418 |

Reaction: no. 6 bicyclo[1.1.0] butane TS1

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.939496151 | -10.77453843 | -9.076805781 |
| H | 9.939396151 | -7.917438425 | -9.07650585 |
| H | 12.02359616 | -9.346138395 | -8.149305816 |
| H | 7.855296246 | -9.346138395 | -8.149005826 |
| H | 8.69379615 | -9.346238395 | -6.521105836 |
| H | 11.18529617 | -9.346238395 | -6.521205853 |
| C | 9.939496151 | -10.09273837 | -8.238005828 |
| C | 9.939496151 | -8.599538423 | -8.237905811 |
| C | 8.801996104 | -9.346138395 | -7.610005836 |
| C | 11.0769962 | -9.346138395 | -7.610105823 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.70348822 | -11.02204005 | -8.904691518 |
| H | 10.36468821 | -8.323840061 | -10.41729146 |
| H | 12.74478825 | -9.01714007 | -10.05099148 |
| H | 7.962288223 | -8.745240072 | -10.15719149 |
| H | 8.323388181 | -10.32874004 | -9.271091492 |
| H | 13.10588821 | -10.60064004 | -9.164791495 |
| C | 11.05068823 | -10.12264005 | -9.413391486 |
| C | 10.0174882 | -9.223240057 | -9.908591495 |
| C | 8.702488266 | -9.441040048 | -9.773491488 |
| C | 12.36568817 | -9.904840061 | -9.548491493 |

TS

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.01668369 | 8.78953964 | 11.16235314 |
| H | 10.09580975 | 11.93116399 | 10.47771452 |
| H | 12.13578487 | 11.07726081 | 11.50833444 |
| H | 7.831112512 | 11.13685604 | 11.55761293 |
| H | 8.877445537 | 10.20822986 | 12.80121191 |
| H | 11.28404742 | 10.38194333 | 12.98756833 |
| C | 10.55356282 | 9.718198324 | 10.95112367 |
| C | 9.992685414 | 11.1123316 | 11.19153268 |
| C | 8.820824594 | 10.84014462 | 11.91670212 |
| C | 11.27441153 | 10.52546824 | 11.89794012 |

Reaction: no. 7 1,2-migration-(formyloxy)ethyl

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.45965201 | 9.044619073 | 8.963339676 |
| H | 11.93218961 | 11.32771707 | 9.682243561 |
| H | 8.189418958 | 10.03784189 | 10.59680148 |
| H | 11.92211173 | 8.654161693 | 10.66312019 |
| H | 11.50094402 | 10.95479114 | 11.391233 |
| C | 11.25636784 | 9.249358972 | 10.02820979 |
| C | 9.133009487 | 9.98845854 | 10.03861601 |
| C | 11.2696181 | 10.74466779 | 10.33379 |
| O | 9.898357462 | 11.14049567 | 10.06777254 |
| O | 9.896699241 | 8.878091443 | 10.33661873 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.08679735 | 10.04928175 | 8.990951108 |
| H | 11.62079898 | 12.28402877 | 9.96750533 |
| H | 7.83711371 | 10.54696121 | 10.3997601 |
| H | 11.63627401 | 9.220494996 | 10.5061765 |
| H | 12.2851198 | 11.42226698 | 11.49297536 |
| C | 11.16688711 | 10.11690136 | 10.08514391 |
| C | 8.835228875 | 10.72348862 | 9.948186738 |
| C | 11.77430002 | 11.3662865 | 10.53253352 |
| O | 9.045418627 | 11.47007942 | 9.010380273 |
| O | 9.73974438 | 9.981565623 | 10.60687369 |

TS

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.55876534 | 9.166623373 | 8.962976185 |
| H | 11.9758749 | 11.46903313 | 9.696886471 |
| H | 8.213845591 | 10.12747422 | 10.7965051 |
| H | 11.79409655 | 8.709982031 | 10.69583452 |
| H | 11.40560889 | 11.09096406 | 11.39963703 |
| C | 11.27498618 | 9.380866905 | 10.00239652 |
| C | 9.095781782 | 10.12970259 | 10.13313678 |
| C | 11.3813131 | 10.82370747 | 10.34112852 |
| O | 9.72814111 | 11.21567913 | 9.833093484 |
| O | 9.824396259 | 8.995940846 | 10.13821862 |

Reaction: no. 8 parent Diels-Alder

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 7.5496 | 12.59160042 | 10.19940018 |
| H | 9.20480012 | 11.83019996 | 9.43799972 |
| H | 8.93440008 | 14.7420001 | 10.92939972 |
| H | 11.01519942 | 11.62099958 | 9.83060002 |
| H | 11.37159944 | 14.5886004 | 11.19600058 |
| H | 12.66499996 | 12.38800048 | 10.59780002 |
| H | 8.70100022 | 10.56759954 | 11.02699996 |
| H | 11.36219978 | 10.42680026 | 11.4093995 |
| H | 8.8274002 | 9.17439998 | 9.6337998 |
| H | 11.48859978 | 9.03339982 | 10.01600028 |
| C | 8.67680014 | 12.64420032 | 10.03659964 |
| C | 9.46560026 | 13.78479958 | 10.61079978 |
| C | 10.79460024 | 13.70700002 | 10.76060056 |
| C | 11.55240058 | 12.47300028 | 10.36460042 |
| C | 9.3276 | 9.84120012 | 10.4113996 |
| C | 10.86199998 | 9.7600001 | 10.6317997 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 7.62279988 | 12.70879984 | 10.35159946 |
| H | 8.6581999 | 12.7520001 | 8.93559992 |
| H | 8.93679976 | 14.71019984 | 10.8596003 |
| H | 11.80619956 | 12.54220008 | 9.28939998 |
| H | 11.35660052 | 14.56760048 | 11.13479972 |
| H | 12.52079964 | 12.43020058 | 10.88840008 |
| H | 8.7371999 | 10.93219996 | 11.33960008 |
| H | 10.95420002 | 10.87839962 | 11.67680026 |
| H | 8.9222002 | 10.52940012 | 9.64100004 |
| H | 11.1995995 | 10.36520004 | 10.01520038 |
| C | 8.67680014 | 12.64420032 | 10.03659964 |
| C | 9.46560026 | 13.78479958 | 10.61079978 |
| C | 10.79460024 | 13.70700002 | 10.76060056 |
| C | 11.55240058 | 12.47300028 | 10.36460042 |
| C | 9.23479974 | 11.25120044 | 10.4113996 |
| C | 10.76920032 | 11.16999984 | 10.6317997 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.876447175 | 12.85896465 | 8.844366416 |
| H | 11.39262283 | 9.597930156 | 8.392696881 |
| H | 11.49937115 | 8.653114602 | 9.964998559 |
| H | 11.25787647 | 12.97069156 | 8.941151956 |
| H | 8.912317452 | 9.498868628 | 8.522835378 |
| H | 9.054209979 | 8.560666195 | 10.1077467 |
| H | 7.550605914 | 11.16019979 | 9.971759644 |
| H | 12.6416115 | 11.3026874 | 10.03344401 |
| H | 11.25237135 | 10.8004229 | 11.14374412 |
| H | 8.895753129 | 10.86110102 | 11.20141146 |
| C | 10.90318066 | 9.30359436 | 9.31854371 |
| C | 9.520828453 | 9.228916122 | 9.380911526 |
| C | 9.36730121 | 12.20911303 | 9.577499643 |
| C | 10.77838984 | 12.24607188 | 9.604268223 |
| C | 8.609533071 | 11.2529917 | 10.2263271 |
| C | 11.56465015 | 11.28458591 | 10.220599 |

Reaction: no. 9 s-tetrazine↔2HCN+N2

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 7.693242262 | 10.84799737 | 9.990689224 |
| H | 12.40353207 | 10.73073923 | 10.08524139 |
| C | 8.783810616 | 10.82088988 | 10.01257559 |
| C | 11.31295206 | 10.75802064 | 10.06351765 |
| N | 9.414856608 | 12.00538955 | 9.947484617 |
| N | 10.74475446 | 11.97230499 | 9.974365847 |
| N | 9.352004254 | 9.606433099 | 10.10173177 |
| N | 10.68194992 | 9.573492298 | 10.12843915 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 7.437102491 | 10.50547029 | 10.60072763 |
| H | 12.87098672 | 10.67813859 | 10.49360676 |
| C | 7.234819615 | 9.450085094 | 10.54699684 |
| C | 13.09562912 | 9.626633044 | 10.46529637 |
| N | 9.520769729 | 12.18934248 | 10.37963637 |
| N | 10.63251373 | 12.24600238 | 10.33049884 |
| N | 7.024102135 | 8.309066713 | 10.48561483 |
| N | 13.32873004 | 8.488740192 | 10.43284444 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 7.547902796 | 10.84482347 | 10.09014116 |
| H | 12.5823368 | 10.78707232 | 10.14855183 |
| C | 8.584466712 | 10.52646563 | 10.10498224 |
| C | 11.53844393 | 10.49241079 | 10.13849602 |
| N | 9.493091627 | 12.04112365 | 10.01564693 |
| N | 10.66782276 | 12.0275908 | 10.03070689 |
| N | 9.077019589 | 9.417403772 | 10.1577483 |
| N | 11.01911387 | 9.394875844 | 10.17530978 |

Reaction: no. 10 trans-butadiene↔cis-butadiene

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.82719209 | 9.743149567 | 9.036725599 |
| H | 9.950067343 | 12.0516117 | 9.036727122 |
| H | 10.30367261 | 8.286349216 | 10.07004577 |
| H | 10.47364063 | 13.50840229 | 10.07003332 |
| H | 10.0031876 | 9.726169794 | 12.00939155 |
| H | 10.77413949 | 12.06860483 | 12.00940434 |
| C | 10.48070011 | 9.359997155 | 9.99900763 |
| C | 10.29653269 | 12.43479358 | 9.999011682 |
| C | 10.29556017 | 10.17098448 | 11.05294654 |
| C | 10.48187403 | 11.62383585 | 11.05299003 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.25791493 | 8.696209712 | 10.09981316 |
| H | 9.188706135 | 12.23676697 | 10.09982051 |
| H | 10.69614113 | 7.684018853 | 10.0998116 |
| H | 10.75044189 | 13.24893585 | 10.09992336 |
| H | 9.345216801 | 9.734940543 | 10.09945281 |
| H | 12.10117294 | 11.19806186 | 10.09952354 |
| C | 11.16568922 | 8.667888169 | 10.0997611 |
| C | 10.28088036 | 12.26503948 | 10.09997334 |
| C | 10.43846431 | 9.799007158 | 10.09961275 |
| C | 11.00790195 | 11.13390673 | 10.09970285 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.66371722 | 9.213773533 | 9.299799964 |
| H | 9.39494667 | 12.21894455 | 9.299496792 |
| H | 10.4594277 | 8.005464583 | 10.05487364 |
| H | 10.59895436 | 13.42707229 | 10.05447169 |
| H | 9.475217894 | 9.772951456 | 11.40225146 |
| H | 11.58313733 | 11.65992814 | 11.40238001 |
| C | 10.83697479 | 9.028050374 | 9.989707674 |
| C | 10.22118833 | 12.4049585 | 9.989311165 |
| C | 10.30140571 | 10.01111302 | 10.7207147 |
| C | 10.75705159 | 11.4216166 | 10.72079321 |

Reaction: no. 11 CH3CH3↔CH2CH2+H2

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.049000395 | 10.54958443 | 9.160492129 |
| H | 10.82137949 | 10.54956788 | 9.160478189 |
| H | 9.935216572 | 12.08450595 | 9.160471429 |
| H | 9.935206472 | 10.03789212 | 11.49022832 |
| H | 10.82139905 | 11.57278983 | 11.49025893 |
| H | 9.048979678 | 11.57278571 | 11.49024558 |
| C | 9.935200607 | 11.06131032 | 9.562136751 |
| C | 9.935204882 | 11.06119854 | 11.08859167 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.205167265 | 10.18582788 | 9.146179025 |
| H | 11.06093207 | 10.15532343 | 9.114073103 |
| H | 9.97641677 | 13.38411642 | 8.90946672 |
| H | 9.246306816 | 10.31156987 | 11.62268278 |
| H | 11.10413247 | 10.28202991 | 11.5943352 |
| H | 9.949135053 | 13.43122082 | 9.657859327 |
| C | 10.14348129 | 10.19128897 | 9.706117782 |
| C | 10.16651971 | 10.26174007 | 11.03722255 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.14995938 | 10.50720635 | 9.129982082 |
| H | 10.95636455 | 10.80963062 | 9.055899162 |
| H | 9.773591064 | 12.3509825 | 9.153727677 |
| H | 9.221006696 | 10.49549145 | 11.652864 |
| H | 11.06536418 | 10.8164255 | 11.59741135 |
| H | 9.895191872 | 11.88895149 | 10.28771257 |
| C | 10.04314975 | 10.85662388 | 9.647149822 |
| C | 10.13534509 | 10.60577505 | 11.07382225 |

Reaction: no. 12 CH3CH2F↔CH2CH2+HF

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.54064167 | 8.708990979 | 9.72121498 |
| H | 9.055249728 | 8.719296472 | 9.721401088 |
| H | 10.22088878 | 10.8382753 | 10.65079476 |
| H | 11.5406505 | 8.708993233 | 11.58039063 |
| H | 9.055246157 | 8.719295999 | 11.58020515 |
| C | 10.96701208 | 8.7185936 | 10.6508388 |
| C | 9.629022995 | 8.722708494 | 10.65080155 |
| F | 10.08918587 | 11.78152952 | 10.6510428 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.46915855 | 10.02258335 | 8.695657523 |
| H | 9.068706407 | 9.273230023 | 8.839124192 |
| H | 11.33800748 | 10.76181177 | 10.31522232 |
| H | 11.22114531 | 8.991371708 | 10.13012924 |
| H | 8.937015015 | 10.01559177 | 10.46554733 |
| C | 10.96450767 | 9.956679396 | 9.668735149 |
| C | 9.46719103 | 10.05949366 | 9.500484511 |
| F | 9.137901883 | 11.30450854 | 8.905693436 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.5393408 | 9.144881747 | 9.211990999 |
| H | 9.034747804 | 9.328689622 | 9.158681083 |
| H | 10.67284853 | 10.63428817 | 10.13867035 |
| H | 11.48241275 | 9.102673034 | 11.07375555 |
| H | 8.993833658 | 9.324290604 | 11.00662892 |
| C | 10.98985247 | 9.348840747 | 10.13213389 |
| C | 9.586483014 | 9.400835527 | 10.09499057 |
| F | 9.553676786 | 11.34009385 | 10.08949908 |

Reaction: no. 13 vinyl alcohol↔acetaldehyde

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.49142086 | 10.77602582 | 9.708843775 |
| H | 10.93247624 | 9.306651746 | 10.59109173 |
| H | 9.475358559 | 12.07273536 | 10.5914065 |
| H | 11.49136142 | 10.77571863 | 11.47400023 |
| C | 10.94604246 | 10.40178991 | 10.59136862 |
| C | 9.548587802 | 10.95313917 | 10.59115911 |
| O | 8.535755103 | 10.27365259 | 10.5906661 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.88533494 | 11.90700069 | 9.4556462 |
| H | 8.728246311 | 9.278300614 | 10.52111017 |
| H | 8.416859772 | 11.83667291 | 9.341058661 |
| H | 10.91996568 | 10.20774878 | 10.22925475 |
| C | 10.34083223 | 11.03777576 | 9.817952378 |
| C | 9.005147338 | 11.01283229 | 9.75028082 |
| O | 8.180203934 | 10.00058926 | 10.16038486 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.34452446 | 11.23003197 | 9.46076538 |
| H | 9.759488667 | 9.513335308 | 10.30970974 |
| H | 8.763766046 | 11.98245813 | 9.967929756 |
| H | 11.08116872 | 10.43840612 | 11.08837901 |
| C | 10.64626711 | 10.70099126 | 10.11448982 |
| C | 9.278835877 | 11.03851205 | 10.19846324 |
| O | 8.570425455 | 10.01710606 | 10.56384102 |

Reaction: no. 14 HCOCl↔HCl+CO

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.29532036 | 11.58398288 | 9.891275906 |
| C | 10.22776455 | 10.48197706 | 9.891892232 |
| O | 11.1478144 | 9.717677941 | 9.89181412 |
| Cl | 8.52392642 | 9.981401457 | 9.891997781 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 7.976801311 | 11.01497951 | 9.653483336 |
| C | 10.13615248 | 10.51758925 | 9.700904997 |
| O | 11.23841257 | 10.22429145 | 9.723140829 |
| Cl | 6.703737399 | 11.25214313 | 9.619080398 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.461674268 | 11.41894965 | 9.810304891 |
| C | 10.30269232 | 10.6594955 | 9.822729586 |
| O | 11.02143847 | 9.759185168 | 9.834126219 |
| Cl | 7.970417771 | 10.3597014 | 9.797355191 |

Reaction: no. 15 H2PO4-↔H2O+PO3-

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.682542395 | 11.76819146 | 10.32822584 |
| H | 12.57636563 | 10.45518837 | 10.32621934 |
| O | 11.19971145 | 12.18018547 | 8.7600185 |
| O | 10.05374006 | 10.03900571 | 8.765693924 |
| O | 9.559355021 | 11.64083247 | 10.7366616 |
| O | 11.70168378 | 10.58921312 | 10.73697746 |
| P | 10.62890065 | 11.11171394 | 9.675711184 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.971687924 | 10.42029207 | 11.60838054 |
| H | 10.30301888 | 10.41569782 | 12.23261617 |
| O | 11.43523959 | 10.33566608 | 8.083264834 |
| O | 9.301835287 | 10.38386511 | 9.585967855 |
| O | 9.371917858 | 10.4300643 | 12.48677912 |
| O | 11.64590241 | 10.37577032 | 10.68432296 |
| P | 10.79959344 | 10.36486434 | 9.440426689 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.632751669 | 10.79152455 | 11.51368742 |
| H | 11.00077996 | 10.40089649 | 11.44575103 |
| O | 11.58990959 | 11.23692497 | 8.303974062 |
| O | 9.476367785 | 10.09476793 | 9.400062805 |
| O | 9.528101907 | 11.18560196 | 11.46127068 |
| O | 11.71792745 | 10.34366211 | 10.71676281 |
| P | 10.87718102 | 10.62646393 | 9.429312102 |

Reaction: no. 16 claisen rearrangement

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.479725 | 14.102608 | 12.138174 |
| H | 10.78885 | 13.609544 | 11.97936 |
| H | 10.7005 | 13.16289 | 14.501943 |
| H | 11.937975 | 14.845974 | 15.755796 |
| H | 12.940625 | 15.269332 | 14.245659 |
| H | 12.2006 | 11.767106 | 11.246499 |
| H | 11.395375 | 11.257142 | 12.75372 |
| H | 14.299275 | 12.36404 | 12.618936 |
| C | 11.712575 | 13.42835 | 12.55311 |
| C | 11.479425 | 13.74919 | 14.000607 |
| C | 12.1517 | 14.665846 | 14.701905 |
| C | 13.48305 | 11.655618 | 12.925143 |
| C | 12.129575 | 11.958414 | 12.332466 |
| O | 13.725125 | 10.72669 | 13.675905 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.65283322 | 15.95862714 | 12.93234719 |
| H | 10.81465923 | 15.70492272 | 13.07872427 |
| H | 11.18485736 | 13.73124014 | 14.49692841 |
| H | 13.51307832 | 13.88089344 | 15.6108568 |
| H | 14.18331064 | 14.41661353 | 14.04264026 |
| H | 13.91144988 | 10.67835797 | 11.39072432 |
| H | 13.46174087 | 10.03645866 | 13.09595745 |
| H | 13.99416854 | 12.97878605 | 12.25744961 |
| C | 11.82162966 | 15.37363538 | 13.33429553 |
| C | 12.0314222 | 14.30843582 | 14.11148795 |
| C | 13.38630546 | 13.81842781 | 14.52015495 |
| C | 13.76281284 | 12.12337457 | 12.90248585 |
| C | 13.70456668 | 10.87161248 | 12.44008713 |
| O | 13.5709651 | 12.41818229 | 14.22517828 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.4578993 | 14.39586851 | 12.07930335 |
| H | 10.74250313 | 13.71850756 | 12.06534193 |
| H | 10.76606792 | 13.52962808 | 14.53791164 |
| H | 12.84220206 | 13.94376818 | 15.81799884 |
| H | 13.67036246 | 14.6190079 | 14.32250737 |
| H | 12.65983805 | 11.67472443 | 11.26230412 |
| H | 11.74536297 | 11.34362144 | 12.85156742 |
| H | 14.58869858 | 12.5638256 | 12.51759492 |
| C | 11.65271311 | 13.91288164 | 12.63375516 |
| C | 11.64180754 | 13.92683445 | 14.01757489 |
| C | 12.84609874 | 14.03158346 | 14.73189163 |
| C | 13.69925041 | 12.19682406 | 13.07083321 |
| C | 12.58778395 | 11.81120342 | 12.34376202 |
| O | 13.66794036 | 12.35963225 | 14.35710115 |

Reaction: no. 17 SiH3CH2CH3↔SiH2+CH3CH3

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.345093903 | 9.262708822 | 8.757885683 |
| H | 10.48796092 | 10.5024885 | 9.195470645 |
| H | 9.166220137 | 11.63602597 | 9.239934851 |
| H | 7.641890065 | 9.855377424 | 10.272051 |
| H | 9.00632519 | 8.724267363 | 10.31637075 |
| H | 12.53220799 | 11.15901584 | 10.54895125 |
| H | 9.825697465 | 11.08466663 | 10.80009297 |
| H | 11.79452757 | 9.103161497 | 10.84171967 |
| C | 8.586908016 | 9.584653618 | 9.779443143 |
| C | 9.547732037 | 10.76422561 | 9.790904843 |
| Si | 12.28696748 | 9.938420484 | 9.653296504 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.806265872 | 9.802297785 | 9.060633257 |
| H | 11.73262849 | 10.37802938 | 8.614544471 |
| H | 9.549106651 | 12.09318169 | 9.891414854 |
| H | 7.752262888 | 10.38142164 | 10.36326939 |
| H | 8.987335734 | 9.154711456 | 10.69986123 |
| H | 12.52149347 | 11.81071798 | 10.39964222 |
| H | 9.729104824 | 11.44982693 | 11.51765111 |
| H | 11.9820637 | 9.493676655 | 10.84850616 |
| C | 8.780658528 | 10.07027948 | 10.12697578 |
| C | 9.793513567 | 11.17611311 | 10.45189085 |
| Si | 11.57807102 | 10.70169645 | 10.06614784 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.629282586 | 9.498875202 | 8.885135198 |
| H | 10.74220144 | 10.4997814 | 8.934515778 |
| H | 9.5162974 | 11.81212062 | 9.525111707 |
| H | 7.755137679 | 10.12280422 | 10.29673275 |
| H | 9.028597749 | 8.90274485 | 10.50657891 |
| H | 12.36068653 | 11.54083918 | 10.47946763 |
| H | 9.91612824 | 11.20168332 | 11.14570847 |
| H | 11.69728235 | 9.249540603 | 10.86194921 |
| C | 8.745065168 | 9.798053064 | 9.937131635 |
| C | 9.758284194 | 10.91193228 | 10.10367384 |
| Si | 11.96374473 | 10.26855038 | 9.793301493 |

Reaction: no. 18 HNCCS↔HNC+CS

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.517549902 | 12.55650912 | 10.09680912 |
| C | 10.545472 | 9.467213215 | 9.720142368 |
| C | 9.942982501 | 10.59727012 | 9.854658505 |
| N | 9.218573174 | 11.59230979 | 9.97052822 |
| S | 11.32200674 | 8.103636886 | 9.558829177 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.541771335 | 10.90990681 | 9.895616459 |
| C | 11.22922371 | 9.814561268 | 9.980699763 |
| C | 7.800516939 | 12.25878855 | 9.789604291 |
| N | 8.731706286 | 11.54058164 | 9.847363455 |
| S | 12.62050707 | 9.178231866 | 10.0372524 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 9.339254526 | 12.62967978 | 10.14593978 |
| C | 11.21448382 | 9.539016825 | 9.933609692 |
| C | 9.36061429 | 10.52630879 | 9.671659146 |
| N | 9.152562412 | 11.67674203 | 9.875123674 |
| S | 11.40227488 | 8.046431532 | 9.5302948 |

Reaction: no. 19 HCONH3+↔NH4++CO

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.24003846 | 10.26649392 | 9.119150173 |
| H | 11.32782092 | 9.066796632 | 9.777499061 |
| H | 9.407700832 | 11.78770787 | 9.895925861 |
| H | 12.0983874 | 10.14338132 | 10.75738959 |
| C | 9.083295879 | 10.76976306 | 9.518535841 |
| N | 11.58926984 | 10.04918612 | 9.876143887 |
| O | 8.40486369 | 10.01299228 | 10.14775131 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.21951446 | 10.06946747 | 9.425934567 |
| H | 12.2462398 | 8.647613149 | 10.3544082 |
| H | 10.74955866 | 9.585693091 | 10.25694568 |
| H | 12.17106237 | 10.16436927 | 11.10597274 |
| C | 8.829596417 | 9.388522769 | 10.1732309 |
| N | 11.84283794 | 9.611828502 | 10.28525617 |
| O | 7.976414298 | 10.17928563 | 10.2560791 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.38529939 | 10.16172182 | 9.246571319 |
| H | 11.66981716 | 8.886420833 | 9.988243359 |
| H | 9.640227764 | 11.22296229 | 9.876306092 |
| H | 12.35558726 | 10.07452618 | 10.88580181 |
| C | 8.759824942 | 10.58115027 | 9.55820192 |
| N | 11.80267703 | 9.898478973 | 10.04446837 |
| O | 8.100018615 | 9.943470706 | 10.31791256 |

Reaction: no. 20 rotational TS in acrolein

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.08112194 | 9.245743203 | 9.823052877 |
| H | 7.82950061 | 10.351708 | 9.823042538 |
| H | 8.669524005 | 12.01207137 | 9.822950932 |
| H | 11.03731847 | 12.24021008 | 9.823120734 |
| C | 9.96257139 | 10.33121241 | 9.823043364 |
| C | 8.758849473 | 10.9224238 | 9.823013106 |
| C | 11.19672888 | 11.12991642 | 9.82305652 |
| O | 12.32667785 | 10.65667851 | 9.823217404 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.21261817 | 10.05837495 | 11.03364254 |
| H | 8.190997623 | 10.61721485 | 9.68528002 |
| H | 9.224180599 | 11.82678789 | 8.69702045 |
| H | 12.38973017 | 11.11748869 | 10.62218093 |
| C | 10.24535936 | 10.7914026 | 10.22271944 |
| C | 9.155486901 | 11.0891467 | 9.499850309 |
| C | 11.55108458 | 11.44279475 | 9.958270162 |
| O | 11.74275884 | 12.28178346 | 9.085484162 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 10.18665489 | 9.533015582 | 10.45133974 |
| H | 8.008665932 | 10.44336432 | 9.725072464 |
| H | 8.836211029 | 12.03058633 | 9.211238582 |
| H | 11.66942227 | 11.92695172 | 10.79306692 |
| C | 10.10434538 | 10.5388846 | 10.02355845 |
| C | 8.924882074 | 11.029006 | 9.63728073 |
| C | 11.39174957 | 11.29357881 | 9.909812907 |
| O | 12.12938221 | 11.23264385 | 8.940329105 |

Reaction: no. 21 OCHNHOH↔HOCHNOH

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.71831398 | 10.12036491 | 9.512056389 |
| H | 10.02077084 | 12.16170332 | 9.512198041 |
| H | 8.59554605 | 9.694791547 | 9.512330838 |
| C | 9.889599134 | 11.07573453 | 9.512268522 |
| N | 10.83902033 | 10.21887432 | 9.512171638 |
| O | 8.594954612 | 10.67442284 | 9.511251443 |
| O | 12.10368048 | 10.87529675 | 9.511904264 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.69653246 | 10.09543074 | 9.969046608 |
| H | 9.553855364 | 12.13007919 | 9.879469119 |
| H | 9.355863601 | 9.203589961 | 9.508781664 |
| C | 8.972127409 | 11.18333983 | 9.897948737 |
| N | 9.789103719 | 10.0788352 | 9.811433839 |
| O | 7.758348909 | 11.10848635 | 10.0434 |
| O | 11.07134447 | 10.2718931 | 9.239318906 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 12.1555532 | 9.89943582 | 9.903351789 |
| H | 9.645640703 | 12.28686935 | 9.759980944 |
| H | 9.129420883 | 9.61426467 | 9.581962933 |
| C | 9.447233277 | 11.21415065 | 9.707038481 |
| N | 10.30644931 | 10.22766348 | 9.600471735 |
| O | 8.271764807 | 10.66786884 | 9.755497651 |
| O | 11.66244741 | 10.42685493 | 9.245532645 |

Reaction: no. 22 H2CNH↔HNC+H2

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.21688927 | 9.568674233 | 9.716125203 |
| H | 8.80092543 | 11.17231262 | 9.716108107 |
| H | 11.06021626 | 11.4325204 | 9.716136076 |
| C | 10.55739171 | 10.44821199 | 9.716080199 |
| N | 9.295629783 | 10.26821939 | 9.71603885 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 13.27673966 | 9.803490089 | 10.10147626 |
| H | 7.666943863 | 10.75290949 | 9.777957782 |
| H | 12.53923869 | 9.947487844 | 10.05401652 |
| C | 9.821925011 | 10.42917229 | 9.894991123 |
| N | 8.65842245 | 10.59657545 | 9.832463664 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.44799726 | 9.711768999 | 9.785312552 |
| H | 8.499925331 | 10.93597734 | 9.718671482 |
| H | 11.49484752 | 10.84007058 | 9.768770651 |
| C | 10.36996513 | 10.89722224 | 9.747850536 |
| N | 9.292419611 | 10.27545929 | 9.742115392 |

Reaction: no. 23 H2CNH↔HCNH2

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.34261044 | 9.940352189 | 9.772341041 |
| H | 8.934800334 | 11.54346022 | 9.772546156 |
| H | 11.18957089 | 11.64958228 | 9.772471567 |
| C | 9.410251068 | 10.53312935 | 9.772237496 |
| N | 10.70551702 | 10.73861839 | 9.772195522 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.34261044 | 9.940352189 | 9.772341041 |
| H | 8.934800334 | 11.54346022 | 9.772546156 |
| H | 11.18957089 | 11.64958228 | 9.772471567 |
| C | 9.410251068 | 10.53312935 | 9.772237496 |
| N | 10.70551702 | 10.73861839 | 9.772195522 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 11.34261044 | 9.940352189 | 9.772341041 |
| H | 8.934800334 | 11.54346022 | 9.772546156 |
| H | 11.18957089 | 11.64958228 | 9.772471567 |
| C | 9.410251068 | 10.53312935 | 9.772237496 |
| N | 10.70551702 | 10.73861839 | 9.772195522 |

Reaction: no. 24 HCNH2↔HCN+H2

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.960065821 | 9.764346075 | 10.04591519 |
| H | 11.36798332 | 11.3672932 | 10.04589116 |
| H | 9.11314565 | 11.47396313 | 10.0459178 |
| C | 10.89227146 | 10.35711106 | 10.0463177 |
| N | 9.59697353 | 10.56280418 | 10.04627721 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.12694295 | 10.18288591 | 9.646453529 |
| H | 12.35284022 | 11.18614751 | 9.597694404 |
| H | 7.442723343 | 10.22311959 | 9.956963736 |
| C | 11.61462531 | 10.65295096 | 9.027110838 |
| N | 10.81697276 | 10.07901788 | 8.40747323 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 8.886557017 | 9.968463165 | 9.807736929 |
| H | 11.57395774 | 11.38215619 | 9.967540988 |
| H | 8.603450592 | 11.32935533 | 10.14042009 |
| C | 11.06568206 | 10.43023511 | 9.776928017 |
| N | 9.889409237 | 10.16401499 | 9.785814943 |

**S2.** Cartesian coordinates of initial states (IS), final states (FS) and transition states (TS) for heterogeneous catalysis Reactions.

Reaction: no. 1 CO + O ↔ CO2 on Pt(111)

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 4.703009362 | 2.86546483 | 10.4956231 |
| O | 6.395859325 | -0.030493258 | 9.657986461 |
| O | 4.674848555 | 2.870250665 | 11.65252864 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.70610164 | 4.218513714 | 6.184636733 |
| Pt | 3.144530976 | 5.627735967 | 6.180144565 |
| Pt | 5.583529963 | -1.390490328 | 6.184559743 |
| Pt | 0.704897163 | 1.42477159 | 6.20179658 |
| Pt | 3.165860748 | 0.006160187 | 6.218514934 |
| Pt | 0.700907211 | 7.00624654 | 6.220228014 |
| Pt | 5.572425169 | 4.204895467 | 6.215899466 |
| Pt | 3.161667374 | 2.814545787 | 6.21615283 |
| Pt | 5.570696207 | 1.422384383 | 6.234995094 |
| Pt | 2.317215608 | 4.225676573 | 8.447549211 |
| Pt | 4.761138119 | 5.636649614 | 8.445735712 |
| Pt | 2.312574636 | 1.372235664 | 8.491288674 |
| Pt | 7.233929858 | 4.209261148 | 8.493975053 |
| Pt | 2.329334794 | 7.016322262 | 8.509565352 |
| Pt | 4.671867877 | -0.025890059 | 8.538506995 |
| Pt | 7.259447029 | 1.465571122 | 8.541195345 |
| Pt | 7.259037973 | -1.515547506 | 8.54694521 |
| Pt | 4.752729997 | 2.831658032 | 8.653633482 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 5.566835757 | -0.317692901 | 10.52500174 |
| O | 6.676328992 | -0.995061447 | 10.50112399 |
| O | 4.942063677 | 0.135604449 | 11.45652224 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.709403624 | 4.224287148 | 6.192574945 |
| Pt | 3.140503105 | 5.634096329 | 6.175792674 |
| Pt | 5.564283555 | -1.385408393 | 6.197969802 |
| Pt | 0.703320235 | 1.447268558 | 6.237965323 |
| Pt | 3.157787915 | 0.017826395 | 6.205457037 |
| Pt | 0.718087844 | 7.047321991 | 6.161980024 |
| Pt | 5.579411679 | 4.226452866 | 6.173817891 |
| Pt | 3.143959422 | 2.818920129 | 6.187955636 |
| Pt | 5.570756639 | 1.405454341 | 6.194274548 |
| Pt | 2.346198062 | 4.217180723 | 8.451917981 |
| Pt | 4.752056388 | 5.590199308 | 8.435638079 |
| Pt | 2.374180509 | 1.389805207 | 8.485188438 |
| Pt | 7.208029907 | 4.200950014 | 8.461063772 |
| Pt | 2.347054647 | 7.030084004 | 8.462505566 |
| Pt | 4.798785837 | -0.007598387 | 8.617512278 |
| Pt | 7.223367513 | 1.448736342 | 8.422381694 |
| Pt | 7.217499281 | -1.435236736 | 8.540834188 |
| Pt | 4.77484651 | 2.810170292 | 8.453172029 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 5.124504358 | 0.144479725 | 10.41592338 |
| O | 7.120344134 | 0.050999957 | 9.989785168 |
| O | 4.993512387 | 0.242562187 | 11.5665631 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.710717987 | 4.243139154 | 6.179865545 |
| Pt | 3.146540262 | 5.651594972 | 6.176426214 |
| Pt | 5.574359442 | -1.366400802 | 6.20904567 |
| Pt | 0.688097793 | 1.455640022 | 6.224007911 |
| Pt | 3.156840854 | 0.027524969 | 6.203430237 |
| Pt | 0.690003473 | 7.034465207 | 6.225991668 |
| Pt | 5.575578957 | 4.241431741 | 6.179895915 |
| Pt | 3.14627009 | 2.82853587 | 6.177933271 |
| Pt | 5.576605256 | 1.423736334 | 6.204016204 |
| Pt | 2.407712032 | 4.255789506 | 8.43062745 |
| Pt | 4.79464254 | 5.649640728 | 8.459255359 |
| Pt | 2.328256518 | 1.455540041 | 8.481354641 |
| Pt | 7.20939948 | 4.256507899 | 8.501791909 |
| Pt | 2.332971089 | 7.05787074 | 8.482942527 |
| Pt | 4.661221615 | 0.046597676 | 8.573322581 |
| Pt | 7.272356977 | 1.477680141 | 8.538616639 |
| Pt | 7.264553712 | -1.387708288 | 8.545953078 |
| Pt | 4.796190088 | 2.862950421 | 8.455134745 |

Reaction: no. 2 C + O ↔ CO on Pt(111)

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 3.15404878 | 5.597848156 | 9.439557832 |
| O | 3.996059167 | 1.384228056 | 9.689922254 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.728985639 | 7.025582916 | 6.190040042 |
| Pt | 5.577233232 | 4.20187034 | 6.241697289 |
| Pt | 3.159586166 | 5.615980151 | 6.195289723 |
| Pt | 3.155480966 | 2.806735158 | 6.207138844 |
| Pt | 0.728495087 | 4.205268761 | 6.188130056 |
| Pt | 5.578596013 | -1.397925803 | 6.237124321 |
| Pt | 5.589133679 | 1.402903128 | 6.161440341 |
| Pt | 3.156228467 | -0.000471228 | 6.206714004 |
| Pt | 0.74479344 | 1.401609343 | 6.230222149 |
| Pt | 7.208575523 | 1.386031954 | 8.447096243 |
| Pt | 4.875250677 | 5.599526968 | 8.624663573 |
| Pt | 2.297211528 | 4.141448538 | 8.540237862 |
| Pt | 7.22226302 | 4.200932506 | 8.526484523 |
| Pt | 4.861865074 | 2.832570449 | 8.510943963 |
| Pt | 2.299065572 | 7.055634333 | 8.536260641 |
| Pt | 2.272837367 | 1.386133757 | 8.581675191 |
| Pt | 7.219294094 | -1.429006766 | 8.522556481 |
| Pt | 4.862936591 | -0.060387772 | 8.508524473 |

FS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 3.157652076 | 5.594225575 | 9.89831798 |
| O | 3.147098186 | 5.588535162 | 11.09320787 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.729741831 | 7.021018251 | 6.195733285 |
| Pt | 5.582994354 | 4.220165537 | 6.198565835 |
| Pt | 3.154311853 | 5.615476641 | 6.209557405 |
| Pt | 3.150698764 | 2.814700967 | 6.195292647 |
| Pt | 0.728293293 | 4.211414463 | 6.194305111 |
| Pt | 5.583385249 | -1.413483659 | 6.199338271 |
| Pt | 5.584673481 | 1.403293263 | 6.16463727 |
| Pt | 3.151712258 | -0.00968469 | 6.19672624 |
| Pt | 0.721890748 | 1.402625748 | 6.193839501 |
| Pt | 7.191421661 | 1.385565455 | 8.45668779 |
| Pt | 4.800982312 | 5.59950888 | 8.577455161 |
| Pt | 2.338455716 | 4.179424853 | 8.567331653 |
| Pt | 7.215878478 | 4.192661986 | 8.482646887 |
| Pt | 4.791121443 | 2.771239354 | 8.457489966 |
| Pt | 2.344381351 | 7.016812654 | 8.570085506 |
| Pt | 2.350547296 | 1.383950561 | 8.480035069 |
| Pt | 7.216292185 | -1.422703947 | 8.485434188 |
| Pt | 4.794743654 | 0.000409212 | 8.463460125 |

TS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 3.29169422 | 5.4591277 | 9.429999695 |
| O | 3.58349052 | 3.640522389 | 10.07178412 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.741588605 | 7.029570461 | 6.219887276 |
| Pt | 5.594625362 | 4.216558247 | 6.193176386 |
| Pt | 3.153037935 | 5.623700344 | 6.20871833 |
| Pt | 3.160363202 | 2.816895049 | 6.205186042 |
| Pt | 0.737035567 | 4.232822059 | 6.231475467 |
| Pt | 5.586524452 | -1.370248101 | 6.162091087 |
| Pt | 5.557466228 | 1.458525425 | 6.217778672 |
| Pt | 3.143967986 | -0.006234357 | 6.202334308 |
| Pt | 0.714961406 | 1.416311579 | 6.186179335 |
| Pt | 7.113332227 | 1.412596901 | 8.485221485 |
| Pt | 4.887565818 | 5.650395004 | 8.436029024 |
| Pt | 2.165776687 | 4.082829594 | 8.552263524 |
| Pt | 7.215250426 | 4.18545223 | 8.505450509 |
| Pt | 4.785327001 | 2.778780643 | 8.688664737 |
| Pt | 2.299977327 | 6.985094469 | 8.674002367 |
| Pt | 2.302067167 | 1.330749715 | 8.463861767 |
| Pt | 7.147254231 | -1.414454645 | 8.500591192 |
| Pt | 4.749972677 | 0.011723461 | 8.479617865 |

Reaction: no. 3 C + N ↔ CNon Pt(111)

IS:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 3.143159667 | 5.591487806 | 9.458340219 |
| N | 4.009759308 | 1.381110367 | 9.625299923 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.733526496 | 7.025531243 | 6.194966575 |
| Pt | 5.586890892 | 4.20687528 | 6.239755889 |
| Pt | 3.165262186 | 5.613818022 | 6.194035604 |
| Pt | 3.164663199 | 2.800446925 | 6.218568597 |
| Pt | 0.733553032 | 4.202785632 | 6.191879404 |
| Pt | 5.585947616 | -1.404916123 | 6.236482142 |
| Pt | 5.588896829 | 1.40289715 | 6.179644114 |
| Pt | 3.16447559 | 0.000766936 | 6.218899405 |
| Pt | 0.749008537 | 1.400301339 | 6.22913637 |
| Pt | 7.22181124 | 1.380539921 | 8.450011585 |
| Pt | 4.871185665 | 5.593986154 | 8.626104325 |
| Pt | 2.301629183 | 4.138188968 | 8.541396631 |
| Pt | 7.225284909 | 4.20114856 | 8.533096795 |
| Pt | 4.853877423 | 2.809347864 | 8.589747904 |
| Pt | 2.303886833 | 7.045811994 | 8.54199789 |
| Pt | 2.311339562 | 1.380951521 | 8.647197469 |
| Pt | 7.223206211 | -1.438618808 | 8.527735147 |
| Pt | 4.852279606 | -0.047671419 | 8.588367434 |

FS:

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 3.166586321 | 5.582303216 | 9.925483633 |
| N | 3.160798708 | 5.563485748 | 11.12948302 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.737177813 | 7.020106821 | 6.190930836 |
| Pt | 5.593620484 | 4.217248268 | 6.193940597 |
| Pt | 3.162501183 | 5.612268833 | 6.202649918 |
| Pt | 3.156864978 | 2.809631359 | 6.191809725 |
| Pt | 0.736328728 | 4.20673557 | 6.191038118 |
| Pt | 5.590901098 | -1.415875534 | 6.191850819 |
| Pt | 5.594348827 | 1.401976784 | 6.172230415 |
| Pt | 3.155133575 | -0.010654143 | 6.191150969 |
| Pt | 0.729671773 | 1.399882424 | 6.194298486 |
| Pt | 7.213633654 | 1.379679994 | 8.455201979 |
| Pt | 4.833274196 | 5.592317035 | 8.539096713 |
| Pt | 2.353101813 | 4.155957644 | 8.530873555 |
| Pt | 7.235848806 | 4.187389894 | 8.481607169 |
| Pt | 4.813702712 | 2.767603207 | 8.458368857 |
| Pt | 2.356252424 | 7.020696726 | 8.53747539 |
| Pt | 2.368895885 | 1.376833812 | 8.477355171 |
| Pt | 7.23137606 | -1.43091061 | 8.475167997 |
| Pt | 4.809711083 | -0.006395384 | 8.453772468 |

TS:

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 3.303977967 | 5.550217661 | 9.500956831 |
| N | 3.650598603 | 3.574742145 | 9.999885849 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.742409968 | 7.022264468 | 6.214989758 |
| Pt | 5.587906152 | 4.204247325 | 6.208009564 |
| Pt | 3.152255282 | 5.613442241 | 6.211862173 |
| Pt | 3.16345763 | 2.810562083 | 6.217584448 |
| Pt | 0.746188873 | 4.223982045 | 6.229355233 |
| Pt | 5.591979997 | -1.389410834 | 6.166262778 |
| Pt | 5.575306627 | 1.445869269 | 6.209410648 |
| Pt | 3.150236312 | -0.010250523 | 6.198221967 |
| Pt | 0.720638828 | 1.409012621 | 6.186247519 |
| Pt | 7.157058568 | 1.392384183 | 8.480859023 |
| Pt | 4.898894464 | -2.767921252 | 8.463651149 |
| Pt | 2.222686863 | 4.070863199 | 8.627010052 |
| Pt | 7.220247889 | 4.180237671 | 8.501899121 |
| Pt | 4.796655297 | 2.77989642 | 8.73823211 |
| Pt | 2.313803677 | 6.987080897 | 8.640009632 |
| Pt | 2.30711984 | 1.325201586 | 8.473696475 |
| Pt | 7.187230383 | -1.41358405 | 8.493909012 |
| Pt | 4.77784333 | 0.020769015 | 8.463590713 |

Reaction: no. 4 N + N ↔ N2 on Pt(111)

IS:

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| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| N | 3.948401904 | 4.314060867 | 9.62116538 |
| N | 3.939506533 | 1.238135176 | 9.634810167 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.728045008 | 7.01281672 | 6.170458037 |
| Pt | 5.589762742 | 4.19132486 | 6.222980586 |
| Pt | 3.177135123 | 5.604211252 | 6.187107779 |
| Pt | 3.174484737 | 2.801164321 | 6.228460702 |
| Pt | 0.756169692 | 4.202476627 | 6.211095172 |
| Pt | 5.599848525 | -1.409824222 | 6.220776662 |
| Pt | 5.590107552 | 1.410830101 | 6.22785493 |
| Pt | 3.176326116 | -0.000731848 | 6.190353073 |
| Pt | 0.756146982 | 1.399054504 | 6.213128638 |
| Pt | 7.256012312 | 1.373774293 | 8.478282783 |
| Pt | 4.866436233 | -2.77146411 | 8.565056283 |
| Pt | 2.305326579 | 4.205833045 | 8.596176444 |
| Pt | 7.256067071 | 4.179313659 | 8.474893283 |
| Pt | 4.835046793 | 2.769768683 | 8.721928355 |
| Pt | 2.341374084 | 6.991537689 | 8.420197209 |
| Pt | 2.303252255 | 1.350983074 | 8.597722393 |
| Pt | 7.245281446 | -1.434026344 | 8.506577871 |
| Pt | 4.863932119 | -0.101436878 | 8.580284173 |

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| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| N | 2.882374439 | 3.472437215 | 10.42124819 |
| N | 3.335747663 | 2.391216844 | 10.45419574 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.73243116 | 7.00632952 | 6.19782872 |
| Pt | 5.597771282 | 4.212431894 | 6.183083499 |
| Pt | 3.165572241 | 5.600318273 | 6.203616708 |
| Pt | 3.166796074 | 2.807308932 | 6.23090425 |
| Pt | 0.757925592 | 4.205974551 | 6.199133978 |
| Pt | 5.611852006 | -1.420508194 | 6.140701423 |
| Pt | 5.609207314 | 1.397570519 | 6.154433344 |
| Pt | 3.163132442 | 0.001855983 | 6.183208693 |
| Pt | 0.75381392 | 1.393448489 | 6.189736816 |
| Pt | 7.236474328 | 1.366762712 | 8.484009513 |
| Pt | 4.829760573 | 5.602702702 | 8.458837972 |
| Pt | 2.35954894 | 4.242796289 | 8.59767759 |
| Pt | 7.255219153 | 4.200758747 | 8.462240396 |
| Pt | 4.888197401 | 2.758687092 | 8.428510033 |
| Pt | 2.378601297 | 7.018003724 | 8.459423772 |
| Pt | 2.380073374 | 1.368912971 | 8.531829956 |
| Pt | 7.237255333 | -1.429750556 | 8.437566868 |
| Pt | 4.820482417 | -0.052242966 | 8.405802369 |

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| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| N | 3.583420798 | 3.395699019 | 9.971548979 |
| N | 3.754497387 | 1.556246593 | 9.656947706 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.731359724 | 7.025490444 | 6.180094173 |
| Pt | 5.593985543 | 4.220817129 | 6.188258657 |
| Pt | 3.155624313 | 5.602403309 | 6.210874296 |
| Pt | 3.15835359 | 2.81896928 | 6.214640159 |
| Pt | 0.756574763 | 4.218561173 | 6.226258761 |
| Pt | 5.580994913 | -1.363669076 | 6.191946981 |
| Pt | 5.585034076 | 1.424555255 | 6.218293822 |
| Pt | 3.158746488 | 0.008364408 | 6.186369162 |
| Pt | 0.727001269 | 1.422599999 | 6.188343178 |
| Pt | 7.24983386 | 1.376651457 | 8.460847048 |
| Pt | 4.803508197 | 5.684418033 | 8.478953562 |
| Pt | 2.308551063 | 4.113974014 | 8.736351403 |
| Pt | 7.229436635 | 4.223700961 | 8.462142057 |
| Pt | 4.910138289 | 2.918044975 | 8.545912098 |
| Pt | 2.339279425 | 6.969138901 | 8.450540593 |
| Pt | 2.228815828 | 1.349606227 | 8.486470386 |
| Pt | 7.164586917 | -1.397384285 | 8.504544585 |
| Pt | 4.785028075 | -0.004331911 | 8.59388718 |

Reaction: no. 5 C + H ↔ CHon Pt(111)

IS:

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| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 3.143043304 | 5.619544551 | 9.403809286 |
| C | 3.986198131 | 1.389501724 | 9.332683566 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.727133723 | 7.025757289 | 6.185754405 |
| Pt | 5.583569883 | 4.206705924 | 6.211141243 |
| Pt | 3.162249654 | 5.618764833 | 6.199878293 |
| Pt | 3.161723262 | 2.804214551 | 6.217516408 |
| Pt | 0.727798566 | 4.210815915 | 6.184050656 |
| Pt | 5.584612204 | -1.396775102 | 6.211485184 |
| Pt | 5.583188494 | 1.40506372 | 6.206368536 |
| Pt | 3.162287518 | 0.007004494 | 6.218452419 |
| Pt | 0.740395103 | 1.405080368 | 6.206884064 |
| Pt | 7.24161317 | 1.392087774 | 8.458813473 |
| Pt | 4.82788596 | 5.604926251 | 8.559371814 |
| Pt | 2.343251218 | 4.200345466 | 8.508617868 |
| Pt | 7.233602778 | 4.194088713 | 8.503038399 |
| Pt | 4.869300245 | 2.897275904 | 8.598277311 |
| Pt | 2.343677101 | 7.011814453 | 8.507634048 |
| Pt | 2.230327403 | 1.391435407 | 8.615863864 |
| Pt | 7.23585737 | -1.409400498 | 8.501487809 |
| Pt | 4.873355198 | -0.115851446 | 8.6012926 |

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 4.011677819 | 1.368020562 | 10.81665878 |
| C | 4.002008117 | 1.373872915 | 9.717988416 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.730623941 | 7.019510603 | 6.193141767 |
| Pt | 5.593294446 | 4.199166565 | 6.209903052 |
| Pt | 3.167517725 | 5.609842465 | 6.192417184 |
| Pt | 3.168592489 | 2.796228398 | 6.209521488 |
| Pt | 0.732287156 | 4.203898491 | 6.191515184 |
| Pt | 5.593776171 | -1.405451837 | 6.207920236 |
| Pt | 5.592844722 | 1.39813643 | 6.210286359 |
| Pt | 3.166929465 | -0.002479296 | 6.210124889 |
| Pt | 0.740971037 | 1.397111158 | 6.209199352 |
| Pt | 7.25863506 | 1.376956622 | 8.4792482 |
| Pt | 4.804938354 | 5.590757314 | 8.500941311 |
| Pt | 2.363483783 | 4.202831042 | 8.479968019 |
| Pt | 7.238757721 | 4.18398334 | 8.503766059 |
| Pt | 4.827288755 | 2.817630228 | 8.611610114 |
| Pt | 2.361707334 | 6.975860669 | 8.480180895 |
| Pt | 2.335433299 | 1.375998308 | 8.613500632 |
| Pt | 7.23875127 | -1.43029951 | 8.49762607 |
| Pt | 4.82625026 | -0.061684702 | 8.609090387 |

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| --- | --- | --- | --- |
|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 4.57542911 | 2.565734157 | 10.19942059 |
| C | 3.920385028 | 1.400524756 | 9.383753148 |
| Pt | 7.200306949 | -1.388457762 | 1.627319733 |
| Pt | 2.33566777 | 1.420142976 | 1.627319733 |
| Pt | 4.767991008 | 0.0158405 | 1.627319733 |
| Pt | 7.200306949 | 1.420147188 | 1.627319733 |
| Pt | 2.33566777 | 4.228747926 | 1.627319733 |
| Pt | 4.767991008 | 2.824445451 | 1.627319733 |
| Pt | 2.33566777 | 7.037344451 | 1.627319733 |
| Pt | 4.767991008 | 5.633041976 | 1.627319733 |
| Pt | 7.200306949 | 4.228743713 | 1.627319733 |
| Pt | 1.52489579 | 0.015844713 | 3.920524277 |
| Pt | 3.957219028 | -1.388457762 | 3.920524277 |
| Pt | 6.389534969 | -2.792756024 | 3.920524277 |
| Pt | 1.52489579 | 2.824449664 | 3.920524277 |
| Pt | 3.957219028 | 1.420147188 | 3.920524277 |
| Pt | 6.389534969 | 0.015848926 | 3.920524277 |
| Pt | 1.52489579 | 5.633046188 | 3.920524277 |
| Pt | 3.957219028 | 4.228743713 | 3.920524277 |
| Pt | 6.389534969 | 2.824445451 | 3.920524277 |
| Pt | 0.699825342 | 7.047797246 | 6.176606183 |
| Pt | 5.555534732 | 4.215894602 | 6.229524854 |
| Pt | 3.139790829 | 5.637259524 | 6.177525629 |
| Pt | 3.13968182 | 2.825098717 | 6.210104303 |
| Pt | 0.703424492 | 4.234693274 | 6.179047373 |
| Pt | 5.564801765 | -1.366778901 | 6.196543018 |
| Pt | 5.559032776 | 1.427443686 | 6.206627767 |
| Pt | 3.139317332 | 0.031453644 | 6.202772802 |
| Pt | 0.719819471 | 1.431876172 | 6.199489141 |
| Pt | 7.202369814 | 1.442788056 | 8.451415298 |
| Pt | 4.747855334 | 5.681054463 | 8.487883181 |
| Pt | 2.309427059 | 4.267766644 | 8.455051319 |
| Pt | 7.207206161 | 4.26387669 | 8.486032576 |
| Pt | 4.837071167 | 2.991532955 | 8.638315675 |
| Pt | 2.304236822 | 7.035465158 | 8.442969938 |
| Pt | 2.198897886 | 1.446070167 | 8.590680885 |
| Pt | 7.186480929 | -1.361739528 | 8.495705913 |
| Pt | 4.812544608 | -0.062628304 | 8.578147513 |

Reaction: no. 6 C + O ↔ CO on Pt(211)

IS:

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 5.318440427 | 2.728031508 | 10.10381282 |
| O | 0.627808302 | 4.361265462 | 11.18056673 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.286900186 | 1.39248636 | 5.893621764 |
| Pt | 2.293377358 | 4.193542623 | 5.898840275 |
| Pt | 4.590723308 | -0.029412834 | 6.692025002 |
| Pt | 4.606547154 | 2.774652918 | 6.65472131 |
| Pt | 0.023102683 | 1.390131193 | 7.514859565 |
| Pt | 0.014485767 | 4.172808179 | 7.473121512 |
| Pt | 2.306341102 | -0.038910517 | 8.330738738 |
| Pt | 2.300203571 | 2.770047353 | 8.350989732 |
| Pt | 4.54957855 | 1.275778221 | 9.149688932 |
| Pt | 4.562310839 | 4.190712017 | 9.12532323 |
| Pt | 0.095398439 | 0.034640529 | 9.846361175 |
| Pt | 0.326820134 | 2.668459406 | 10.21890239 |

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 6.846646995 | 4.206224213 | 11.28001926 |
| O | 0.066305373 | 4.205121582 | 12.45878669 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.267359648 | 1.402330802 | 5.918811968 |
| Pt | 2.282434011 | 4.211391709 | 5.910603579 |
| Pt | 4.571458505 | 6.11E-05 | 6.648285052 |
| Pt | 4.570879759 | 2.801427967 | 6.647542389 |
| Pt | 0.00404298 | 1.399784918 | 7.486371536 |
| Pt | 9.90E-06 | 4.20957 | 7.42540789 |
| Pt | 2.231696801 | -0.003798687 | 8.426004124 |
| Pt | 2.232350366 | 2.801259603 | 8.426069185 |
| Pt | 4.469843628 | 1.398409427 | 9.062836859 |
| Pt | 4.441872647 | 4.208012775 | 9.050224311 |
| Pt | 6.720060308 | -0.004507621 | 9.843475971 |
| Pt | 6.719030832 | 2.800752921 | 9.841279117 |

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 5.362475342 | 2.987660881 | 10.21075007 |
| O | -0.273582752 | 3.976663164 | 11.21307578 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.310929521 | 1.401618075 | 5.894235061 |
| Pt | 2.320141279 | 4.21441284 | 5.900128172 |
| Pt | 4.605018167 | 5.622892245 | 6.72319118 |
| Pt | 4.62920165 | 2.779352032 | 6.667240673 |
| Pt | 0.053308332 | 1.291506136 | 7.485906171 |
| Pt | 0.050592892 | 4.106118551 | 7.43335832 |
| Pt | 2.312318241 | 5.634820341 | 8.38273859 |
| Pt | 2.357037568 | 2.81923474 | 8.332551538 |
| Pt | 4.521669103 | 1.416468548 | 9.293427549 |
| Pt | 4.534098771 | 4.297343791 | 9.103182875 |
| Pt | 0.006174971 | 5.388614881 | 9.825273989 |
| Pt | 0.292263948 | 2.37436121 | 9.934838627 |

Reaction: no. 7 C + N ↔ CNon Pt(211)

IS:

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 5.214036403 | 2.848222958 | 10.11526548 |
| N | 0.582541036 | 1.20785168 | 11.15246901 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.300295975 | 1.413850002 | 5.896774783 |
| Pt | 2.282503624 | 4.213624986 | 5.891738946 |
| Pt | 4.598045023 | 0.011602103 | 6.697270509 |
| Pt | 4.618804084 | 2.829538187 | 6.649373279 |
| Pt | 0.019344814 | 1.415470492 | 7.463128053 |
| Pt | 0.032198326 | 4.208003716 | 7.540552833 |
| Pt | 2.298757433 | 0.001674147 | 8.331708553 |
| Pt | 2.3111476 | 2.826060417 | 8.340372295 |
| Pt | 4.516004118 | 1.392746416 | 9.112661803 |
| Pt | 4.561995342 | 4.328071437 | 9.140632175 |
| Pt | 0.104747086 | -0.071648249 | 9.917222855 |
| Pt | 0.278886964 | 2.774532173 | 10.11633616 |

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 6.76742243 | 1.613562182 | 11.26043267 |
| N | 6.784640652 | 0.613387145 | 11.93783888 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.268467239 | 1.406389518 | 5.904802633 |
| Pt | 2.258187252 | 4.214244253 | 5.907271768 |
| Pt | 4.562506567 | 5.611756637 | 6.63325223 |
| Pt | 4.56381121 | 2.809744158 | 6.635873358 |
| Pt | 6.858951266 | 1.397269976 | 7.444540876 |
| Pt | 6.853047892 | 4.210804578 | 7.496476399 |
| Pt | 2.224299456 | 0.006374501 | 8.397454403 |
| Pt | 2.22576462 | 2.81063991 | 8.402711037 |
| Pt | 4.433510584 | 1.403793903 | 9.024320614 |
| Pt | 4.418115989 | 4.215025486 | 9.041498386 |
| Pt | 6.724484639 | -0.110203551 | 9.810591217 |
| Pt | 6.725114746 | 2.86609903 | 9.807550349 |

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| C | 5.337079692 | 2.720017149 | 10.17853364 |
| N | -0.20009782 | 1.662820464 | 11.16681682 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.314144214 | 1.408207502 | 5.905389352 |
| Pt | 2.293726115 | 4.219652197 | 5.895806961 |
| Pt | 4.586089381 | -0.001282143 | 6.714163483 |
| Pt | 4.620591285 | 2.838045936 | 6.661667137 |
| Pt | 6.914350189 | 1.480214251 | 7.43238329 |
| Pt | 0.038151678 | 4.290728693 | 7.515732077 |
| Pt | 2.285126805 | 0.007590806 | 8.400211969 |
| Pt | 2.349258102 | 2.831194065 | 8.332520796 |
| Pt | 4.546045063 | 1.359823035 | 9.092646363 |
| Pt | 4.569287773 | 4.242738163 | 9.232444147 |
| Pt | 6.913726439 | 5.890202033 | 9.910153607 |
| Pt | 0.395899636 | 3.175549316 | 10.02324977 |

Reaction: no. 8 C + H ↔ CHon Pt(211)

IS:

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 0.637598854 | 4.273853709 | 10.81807241 |
| C | 5.289420881 | 2.789898375 | 10.13787982 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.300217839 | 1.399429175 | 5.90357229 |
| Pt | 2.307033478 | 4.209173607 | 5.90028639 |
| Pt | 4.594664274 | -0.010505233 | 6.708748317 |
| Pt | 4.622460098 | 2.798019794 | 6.663820434 |
| Pt | 0.023259636 | 1.403235191 | 7.476858965 |
| Pt | 0.021118157 | 4.194089274 | 7.457385639 |
| Pt | 2.286375058 | -0.004925705 | 8.367720498 |
| Pt | 2.303507539 | 2.803623602 | 8.327126414 |
| Pt | 4.522531679 | 1.331528404 | 9.173718678 |
| Pt | 4.519664668 | 4.246496747 | 9.169458916 |
| Pt | 0.039500975 | -0.035275263 | 9.825746763 |
| Pt | 0.290172141 | 2.706358987 | 10.07470998 |

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 4.605208216 | 2.826581588 | 11.63723115 |
| C | 4.856336063 | 2.820361768 | 10.56765141 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.31792086 | 1.406234677 | 5.915644271 |
| Pt | 2.318154589 | 4.221802462 | 5.916991812 |
| Pt | 4.578259484 | 0.007941523 | 6.741752344 |
| Pt | 4.572657457 | 2.816868808 | 6.701407981 |
| Pt | -0.001199445 | 1.409122909 | 7.396800659 |
| Pt | -0.000819772 | 4.221109792 | 7.395248982 |
| Pt | 2.221495345 | 0.010023059 | 8.44084102 |
| Pt | 2.182501212 | 2.819619344 | 8.411236354 |
| Pt | 4.36297429 | 1.386541579 | 9.258400873 |
| Pt | 4.361864527 | 4.252949033 | 9.25373584 |
| Pt | 6.720337602 | 0.011555304 | 9.709138285 |
| Pt | 6.681512161 | 2.818668219 | 9.750759837 |

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|  | Coordinates (Angstroms) | | |
|  | X | Y | Z |
| H | 6.105802059 | 2.884024206 | 11.39795232 |
| C | 5.235918529 | 2.852966491 | 10.13813246 |
| Pt | 2.550136593 | 1.404322219 | 1.230415528 |
| Pt | 2.550136593 | 4.212921719 | 1.230415528 |
| Pt | 4.784890033 | 3.37E-05 | 1.839667586 |
| Pt | 4.784890033 | 2.808633203 | 1.839667586 |
| Pt | 0.114029967 | 1.404305367 | 2.484486454 |
| Pt | 0.114029967 | 4.212904867 | 2.484486454 |
| Pt | 2.323707133 | 5.617165297 | 3.533288805 |
| Pt | 2.323707133 | 2.808565797 | 3.533288805 |
| Pt | 4.635966552 | 1.40429975 | 4.257875874 |
| Pt | 4.635966552 | 4.21289925 | 4.257875874 |
| Pt | 0.013009392 | 5.617193383 | 5.009873545 |
| Pt | 0.013009392 | 2.808593883 | 5.009873545 |
| Pt | 2.27763701 | 1.416417269 | 5.904225565 |
| Pt | 2.276907445 | 4.228266787 | 5.906320101 |
| Pt | 4.541529949 | 0.023152267 | 6.719512908 |
| Pt | 4.555263525 | 2.831062183 | 6.671194259 |
| Pt | 6.845640195 | 1.447395517 | 7.437574105 |
| Pt | 6.843487808 | 4.2237888 | 7.440132386 |
| Pt | 2.20621429 | 0.031865258 | 8.376607314 |
| Pt | 2.212348183 | 2.841149251 | 8.365662744 |
| Pt | 4.452303245 | 1.396104782 | 9.172630837 |
| Pt | 4.449320576 | 4.304941382 | 9.173237891 |
| Pt | 6.806821104 | 5.660722053 | 9.753990638 |
| Pt | 0.26765507 | 2.85529635 | 10.09692712 |