

Supporting information for

Rate Constants of the CN + Toluene Reaction from 15 – 294 K and Interstellar Implications

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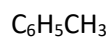
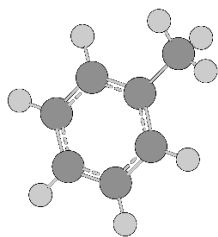
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(U)M06-2X/aug-cc-pVTZ XYZ Coordinates for the Optimized Structures of the CN channels included in Fig. 5 and Table 2 in the main text.

| | |
|-----------------|---------|
| Reactants | S2 |
| R1..... | S3—S4 |
| R2..... | S5—S6 |
| R3..... | S7—S8 |
| R4..... | S9 |
| R5..... | S10—S17 |
| R6..... | S18—S20 |
| R7..... | S21—S23 |
| R8..... | S24—S26 |

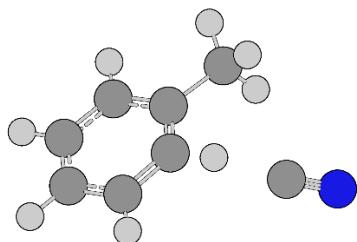
Reactants



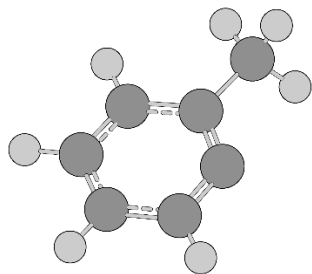
| | | | |
|---|-----------|-----------|-----------|
| C | -1.892906 | -0.001998 | 0.007632 |
| C | -1.191194 | -1.199697 | 0.001838 |
| C | 0.195619 | -1.194122 | -0.007874 |
| C | 0.907467 | 0.002748 | -0.010262 |
| C | 0.192202 | 1.196248 | -0.007847 |
| C | -1.195812 | 1.197115 | 0.001853 |
| H | -1.725511 | -2.14032 | 0.001347 |
| H | 0.737149 | -2.132354 | -0.016823 |
| H | 0.730163 | 2.136345 | -0.016771 |
| H | -1.732966 | 2.136108 | 0.001387 |
| C | 2.411091 | 0.001051 | 0.008269 |
| H | 2.785228 | -0.118345 | 1.026619 |
| H | 2.81037 | -0.82016 | -0.585733 |
| H | 2.810955 | 0.934643 | -0.384032 |
| H | -2.974186 | -0.003989 | 0.012347 |



| | | | |
|---|---|---|-----------|
| N | 0 | 0 | 0.531843 |
| C | 0 | 0 | -0.620484 |

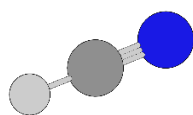
R1abs-*o*-TS

| | | | |
|---|-----------|-----------|-----------|
| C | -2.104947 | -1.253041 | -0.079800 |
| C | -0.77722 | -1.530348 | 0.216878 |
| C | 0.098254 | -0.469163 | 0.347791 |
| C | -0.247734 | 0.855647 | 0.123912 |
| C | -1.588099 | 1.103315 | -0.166104 |
| C | -2.502645 | 0.064079 | -0.267325 |
| H | -2.820729 | -2.058765 | -0.164470 |
| H | -0.439307 | -2.546532 | 0.364084 |
| H | 1.176000 | -0.683166 | 0.652109 |
| H | -1.911276 | 2.124693 | -0.323795 |
| H | -3.534888 | 0.284101 | -0.504393 |
| C | 0.771804 | 1.955481 | 0.179125 |
| H | 1.486361 | 1.787759 | 0.984730 |
| H | 1.339581 | 1.996293 | -0.751484 |
| H | 0.295768 | 2.922072 | 0.330179 |
| N | 3.750483 | -0.559347 | -0.427891 |
| C | 2.709771 | -0.711141 | 0.046902 |

*o*-C₆H₄CH₃

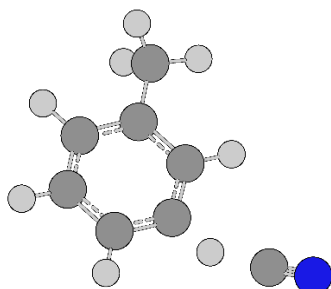
| | | | |
|---|-----------|-----------|-----------|
| C | 0.938171 | -0.061088 | -0.003928 |
| C | 0.150235 | -1.188993 | -0.002872 |
| C | -1.216947 | -1.22705 | -0.000114 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.882794 | -0.000556 | 0.00267 |
| C | -1.149962 | 1.177177 | 0.001239 |
| C | 0.23967 | 1.148056 | -0.002616 |
| H | -1.764283 | -2.160347 | -0.000858 |
| H | -2.964289 | 0.027362 | 0.004418 |
| H | -1.663273 | 2.12902 | 0.001313 |
| H | 0.798815 | 2.076522 | -0.006356 |
| C | 2.440307 | -0.121999 | 0.002446 |
| H | 2.868711 | 0.867651 | -0.145592 |
| H | 2.806606 | -0.514066 | 0.95167 |
| H | 2.805629 | -0.779428 | -0.785537 |

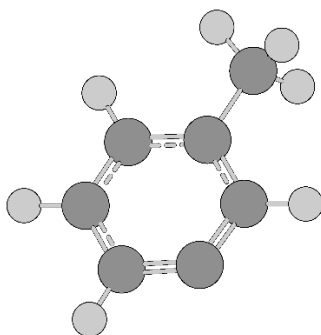


HCN

| | | | |
|---|---------|---------|-----------|
| N | 0.00000 | 0.00000 | 0.647167 |
| C | 0.00000 | 0.00000 | -0.49487 |
| H | 0.00000 | 0.00000 | -1.560946 |

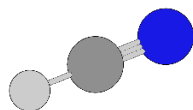
R2abs-*m*-TS

| | | | |
|---|-----------|-----------|-----------|
| C | -0.20767 | 1.622944 | -0.14558 |
| C | 1.138439 | 1.806662 | 0.143007 |
| C | 1.99185 | 0.715211 | 0.220099 |
| C | 1.535129 | -0.584874 | 0.011731 |
| C | 0.184959 | -0.77039 | -0.275023 |
| C | -0.642462 | 0.331965 | -0.379912 |
| H | -0.88919 | 2.459861 | -0.196107 |
| H | 1.52013 | 2.803669 | 0.316625 |
| H | 3.036224 | 0.873281 | 0.459526 |
| H | -0.21026 | -1.766988 | -0.424607 |
| H | -1.726129 | 0.161901 | -0.663879 |
| C | 2.476692 | -1.754312 | 0.07577 |
| H | 3.252888 | -1.591442 | 0.82191 |
| H | 1.947251 | -2.672423 | 0.323211 |
| H | 2.968596 | -1.902575 | -0.886934 |
| C | -3.211683 | -0.289229 | -0.039739 |
| N | -4.213003 | -0.690449 | 0.369734 |

*m*-C₆H₄CH₃

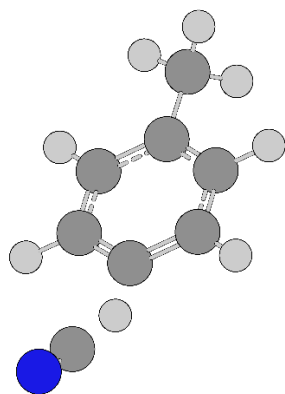
| | | | |
|---|----------|-----------|-----------|
| C | 0.875146 | 0.016561 | -0.002353 |
| C | 0.254736 | -1.239035 | -0.001823 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.111894 | -1.274628 | 0.000436 |
| C | -1.940832 | -0.182134 | 0.001723 |
| C | -1.315857 | 1.062332 | 0.000292 |
| C | 0.071127 | 1.152526 | -0.00183 |
| H | -3.018398 | -0.271193 | 0.0032 |
| H | -1.91416 | 1.964291 | 0.000412 |
| H | 0.539924 | 2.128274 | -0.003416 |
| C | 2.37538 | 0.11628 | 0.001898 |
| H | 2.700704 | 1.153526 | -0.048133 |
| H | 2.790221 | -0.325837 | 0.90844 |
| H | 2.80367 | -0.416851 | -0.847287 |
| H | 0.851213 | -2.143627 | -0.003278 |

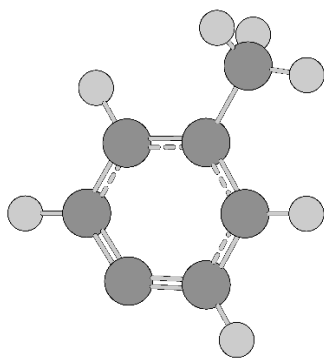


HCN

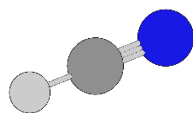
| | | | |
|---|---------|---------|-----------|
| N | 0.00000 | 0.00000 | 0.647167 |
| C | 0.00000 | 0.00000 | -0.49487 |
| H | 0.00000 | 0.00000 | -1.560946 |

R3abs-*p*-TS

| | | | |
|---|-----------|-----------|-----------|
| C | 0.795374 | -0.082912 | -0.397759 |
| C | 0.189184 | 1.153648 | -0.277609 |
| C | -1.1788 | 1.197321 | -0.051083 |
| C | -1.922381 | 0.026342 | 0.085866 |
| C | -1.266523 | -1.199608 | -0.001678 |
| C | 0.101644 | -1.265966 | -0.22713 |
| H | 1.909726 | -0.123292 | -0.632267 |
| H | 0.765318 | 2.064076 | -0.367395 |
| H | -1.675507 | 2.156158 | 0.031269 |
| H | -1.831059 | -2.116063 | 0.116359 |
| H | 0.607933 | -2.219566 | -0.281541 |
| C | -3.406832 | 0.087022 | 0.31056 |
| H | -3.766218 | -0.808813 | 0.813546 |
| H | -3.678731 | 0.953977 | 0.910443 |
| H | -3.933064 | 0.166858 | -0.642341 |
| C | 3.415593 | -0.036611 | 0.010549 |
| N | 4.462579 | 0.093036 | 0.477376 |

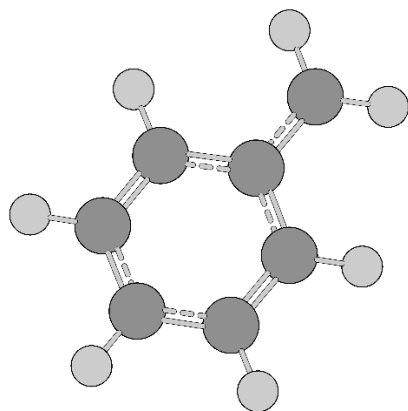
*p*-C₆H₄CH₃

| | | | |
|---|-----------|-----------|-----------|
| C | 0.837414 | 0.007814 | -0.004872 |
| C | 0.134946 | -1.196814 | -0.003618 |
| C | -1.25716 | -1.219196 | 0.001223 |
| C | -1.897447 | -0.006881 | 0.004051 |
| C | -1.271483 | 1.209787 | 0.001261 |
| C | 0.123979 | 1.202438 | -0.003644 |
| H | -1.821692 | 2.141204 | 0.001111 |
| H | 0.661252 | 2.143266 | -0.007886 |
| C | 2.342002 | 0.004078 | 0.003699 |
| H | 2.73979 | 1.005817 | -0.146768 |
| H | 2.724844 | -0.36984 | 0.954348 |
| H | 2.736305 | -0.639866 | -0.782416 |
| H | 0.683633 | -2.131663 | -0.007907 |
| H | -1.79764 | -2.156278 | 0.000921 |



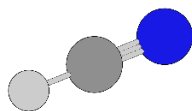
HCN

| | | | |
|---|---------|---------|-----------|
| N | 0.00000 | 0.00000 | 0.647167 |
| C | 0.00000 | 0.00000 | -0.49487 |
| H | 0.00000 | 0.00000 | -1.560946 |

R4

$C_6H_5CH_2$

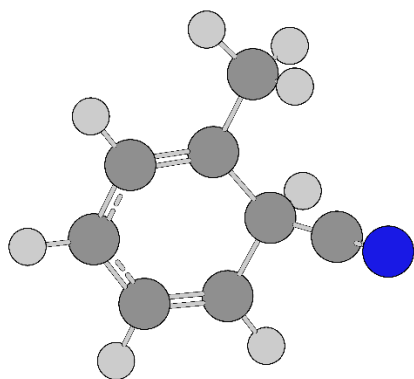
| | | | |
|---|---------|-----------|-----------|
| C | 0.00000 | 0.00000 | -1.828134 |
| C | 0.00000 | 1.204387 | -1.127307 |
| C | 0.00000 | 1.209828 | 0.251146 |
| C | 0.00000 | 0.00000 | 0.985399 |
| C | 0.00000 | -1.209828 | 0.251146 |
| C | 0.00000 | -1.204387 | -1.127307 |
| H | 0.00000 | 2.141081 | -1.6682 |
| H | 0.00000 | 2.147241 | 0.792459 |
| H | 0.00000 | -2.147241 | 0.792459 |
| H | 0.00000 | -2.141081 | -1.6682 |
| C | 0.00000 | 0.00000 | 2.390199 |
| H | 0.00000 | 0.926161 | 2.944764 |
| H | 0.00000 | -0.926161 | 2.944764 |
| H | 0.00000 | 0.00000 | -2.908897 |



HCN

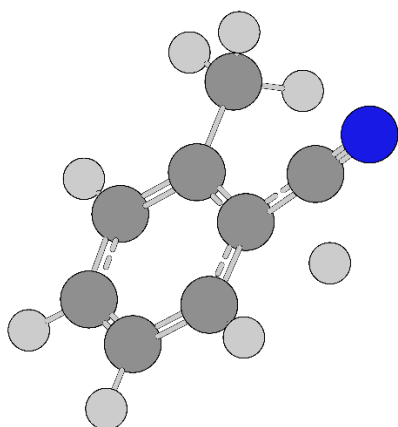
| | | | |
|---|---------|---------|-----------|
| N | 0.00000 | 0.00000 | 0.647167 |
| C | 0.00000 | 0.00000 | -0.49487 |
| H | 0.00000 | 0.00000 | -1.560946 |

R5



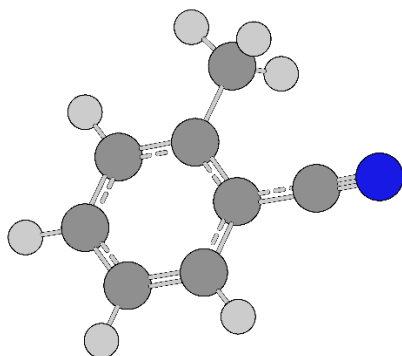
add-*o*-C₆H₅CH₃CN

| | | | |
|---|-----------|-----------|-----------|
| C | 1.83322 | -1.176204 | -0.012016 |
| C | 0.586381 | -1.467917 | 0.419887 |
| C | -0.466614 | -0.402565 | 0.568582 |
| C | -0.027091 | 0.976537 | 0.125712 |
| C | 1.247051 | 1.179317 | -0.292178 |
| C | 2.200525 | 0.140619 | -0.370077 |
| H | 0.301942 | -2.47783 | 0.679514 |
| H | 2.563654 | -1.970197 | -0.092311 |
| C | -1.702379 | -0.804155 | -0.132544 |
| N | -2.659976 | -1.113845 | -0.68093 |
| H | 1.539723 | 2.181553 | -0.580577 |
| H | 3.201566 | 0.350406 | -0.71442 |
| C | -1.047692 | 2.060695 | 0.213187 |
| H | -1.440571 | 2.143225 | 1.230688 |
| H | -0.624311 | 3.02082 | -0.073077 |
| H | -1.900672 | 1.847372 | -0.435697 |
| H | -0.761894 | -0.336393 | 1.629079 |



H-elim-o-TS (R5a)

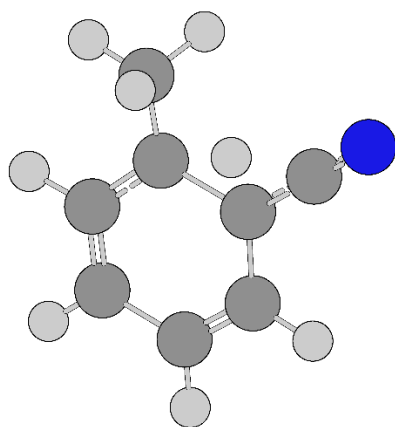
| | | | |
|---|-----------|-----------|-----------|
| C | 1.392258 | 1.137085 | -0.073482 |
| C | 0.029891 | 0.91952 | -0.011342 |
| C | -0.416727 | -0.423319 | 0.135017 |
| C | 0.496122 | -1.495601 | 0.024867 |
| C | 1.846949 | -1.235139 | -0.036529 |
| C | 2.298647 | 0.080619 | -0.066426 |
| H | 1.756016 | 2.154384 | -0.136667 |
| H | -0.644172 | -0.327388 | 1.850008 |
| H | 0.118339 | -2.507812 | 0.033035 |
| H | 2.551577 | -2.053608 | -0.077834 |
| H | 3.359134 | 0.285149 | -0.114443 |
| C | -0.965678 | 2.033006 | 0.015246 |
| H | -1.704626 | 1.920974 | -0.778948 |
| H | -1.513775 | 2.016336 | 0.961795 |
| H | -0.477206 | 2.998581 | -0.089558 |
| C | -1.824507 | -0.70146 | -0.035353 |
| N | -2.941003 | -0.910698 | -0.194196 |



o-C₆H₄CH₃CN (R5a)

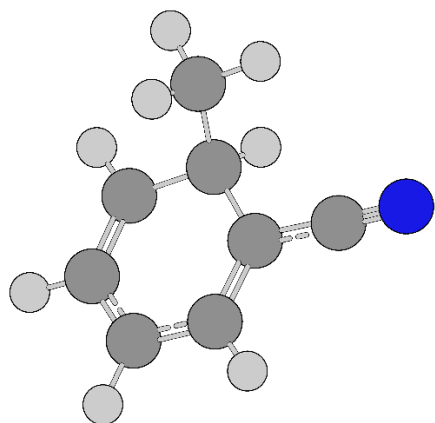
| | | | |
|---|-----------|-----------|---------|
| C | -0.617478 | -0.653649 | 0.00000 |
| C | 0.205421 | -1.772849 | 0.00000 |
| C | 1.587717 | -1.651108 | 0.00000 |
| C | 2.18265 | -0.397641 | 0.00000 |
| C | 1.386446 | 0.734366 | 0.00000 |
| H | 3.258991 | -0.301411 | 0.00000 |
| H | 1.825128 | 1.722298 | 0.00000 |
| C | 0.00000 | 0.603678 | 0.00000 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.819165 | 1.782963 | 0.00000 |
| N | -1.488311 | 2.715864 | 0.00000 |
| H | 2.202941 | -2.540677 | 0.00000 |
| H | -0.247407 | -2.755791 | 0.00000 |
| C | -2.112623 | -0.771681 | 0.00000 |
| H | -2.5401 | -0.282443 | 0.875946 |
| H | -2.5401 | -0.282443 | -0.875946 |
| H | -2.419088 | -1.815048 | 0.00000 |



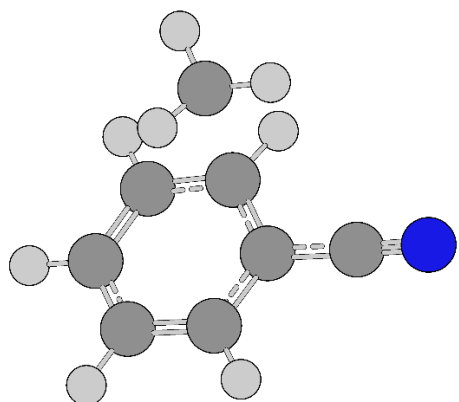
TS-bridge-H-o-tol-CN

| | | | |
|---|-----------|-----------|-----------|
| C | 1.451055 | 1.112778 | 0.002315 |
| C | 0.043883 | 0.960567 | 0.100799 |
| C | -0.479406 | -0.469495 | 0.115691 |
| C | 0.488979 | -1.546802 | -0.013263 |
| C | 1.809152 | -1.293271 | -0.058499 |
| C | 2.316559 | 0.063228 | -0.035129 |
| H | 1.829244 | 2.126961 | -0.044176 |
| H | -0.211031 | 0.240806 | 1.151458 |
| H | 0.106355 | -2.555454 | -0.080822 |
| H | 2.505876 | -2.115238 | -0.144411 |
| H | 3.380743 | 0.236702 | -0.082377 |
| C | -0.931922 | 2.077826 | -0.088681 |
| H | -0.458137 | 3.035061 | 0.120095 |
| H | -1.307048 | 2.089643 | -1.115653 |
| H | -1.799664 | 1.970863 | 0.562628 |
| C | -1.867944 | -0.703043 | 0.002062 |
| N | -3.004068 | -0.891439 | -0.074072 |



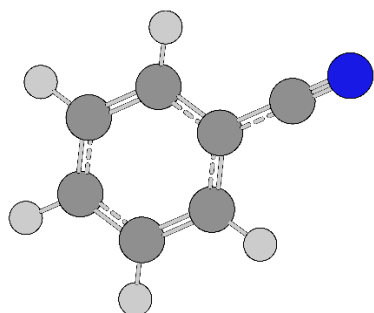
add-*o*-CN-*ipso*-H-C₆H₄CH₃

| | | | |
|---|-----------|-----------|-----------|
| C | -1.536739 | 0.917667 | -0.405996 |
| C | -0.042625 | 0.944352 | -0.393591 |
| C | 0.538472 | -0.411055 | -0.092727 |
| C | -0.237266 | -1.497034 | 0.225276 |
| C | -1.63057 | -1.404789 | 0.244582 |
| C | -2.261858 | -0.175831 | -0.088517 |
| H | -2.034162 | 1.846203 | -0.657829 |
| H | 0.245601 | -2.436824 | 0.456793 |
| H | -2.224083 | -2.269519 | 0.500186 |
| H | -3.342261 | -0.123179 | -0.090404 |
| C | 1.954948 | -0.530258 | -0.126776 |
| N | 3.104081 | -0.591253 | -0.167466 |
| H | 0.311936 | 1.259848 | -1.384481 |
| C | 0.470964 | 2.003392 | 0.604938 |
| H | 0.152648 | 1.747518 | 1.614798 |
| H | 1.558869 | 2.051979 | 0.580368 |
| H | 0.070927 | 2.984078 | 0.349705 |



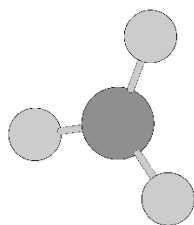
ipso-CH₃-elim-o-CN-TS (R5b)

| | | | |
|---|-----------|-----------|-----------|
| C | -1.486983 | 0.730408 | -0.763423 |
| C | -0.078243 | 0.748798 | -0.679613 |
| C | 0.568293 | -0.402895 | -0.166365 |
| C | -0.167408 | -1.418677 | 0.43121 |
| C | -1.551624 | -1.353116 | 0.44735 |
| C | -2.205707 | -0.286135 | -0.176416 |
| H | -1.996493 | 1.548455 | -1.253666 |
| H | 0.349896 | -2.261915 | 0.86725 |
| H | -2.122099 | -2.145295 | 0.910325 |
| H | -3.286534 | -0.267842 | -0.209964 |
| C | 1.996086 | -0.464581 | -0.196434 |
| N | 3.144718 | -0.488007 | -0.219891 |
| H | 0.489249 | 1.424684 | -1.303527 |
| C | 0.224867 | 2.158513 | 0.966083 |
| H | -0.305727 | 1.628744 | 1.744222 |
| H | 1.304737 | 2.159159 | 1.025162 |
| H | -0.241733 | 3.056168 | 0.585089 |



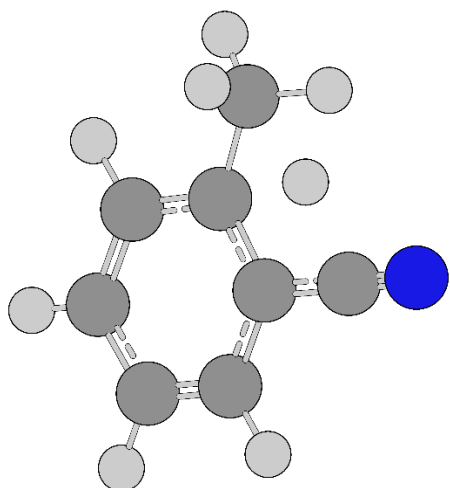
C₆H₅CN (R5b=R8)

| | | | |
|---|-----------|-----------|-----------|
| C | -2.165922 | 0.000052 | 0.000093 |
| C | -1.474492 | 1.204054 | 0.000011 |
| C | -0.089835 | 1.209847 | -0.000102 |
| C | 0.60112 | -0.000092 | -0.00014 |
| C | -0.089931 | -1.209919 | -0.000103 |
| C | -1.474623 | -1.20398 | 0.000012 |
| H | -3.247186 | 0.000095 | 0.000402 |
| H | -2.014715 | 2.140272 | 0.000113 |
| H | 0.461948 | 2.13907 | -0.000273 |
| H | 0.461691 | -2.139238 | -0.000273 |
| H | -2.014918 | -2.140159 | 0.000115 |
| C | 2.037163 | 0.000147 | 0.000046 |
| N | 3.184613 | -0.000098 | 0.000146 |



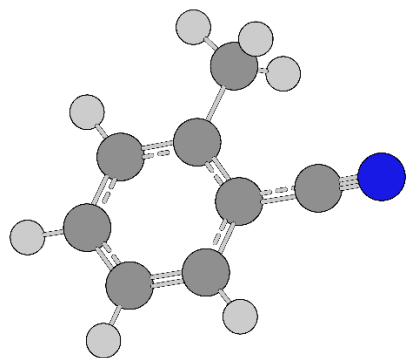
CH₃ (R5b=R8)

| | | | |
|---|-----------|-----------|----------|
| C | 0.00000 | 0.000023 | 0.00000 |
| H | 0.000043 | 1.076044 | 0.000001 |
| H | 0.93197 | -0.538129 | 0.000001 |
| H | -0.932013 | -0.538054 | 0.000001 |



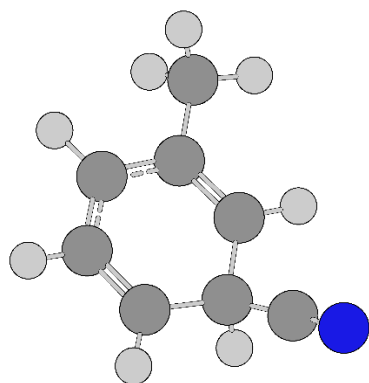
ipso-H-elim-o-CN-TS (R5c)

| | | | |
|---|-----------|-----------|-----------|
| C | 1.405224 | 1.100051 | -0.03232 |
| C | 0.015786 | 0.889054 | 0.072755 |
| C | -0.434492 | -0.451821 | -0.002471 |
| C | 0.463135 | -1.513386 | -0.009354 |
| C | 1.825741 | -1.269139 | -0.01589 |
| C | 2.291043 | 0.044099 | -0.051629 |
| H | 1.770795 | 2.118334 | -0.052801 |
| H | 0.082927 | -2.52521 | -0.020546 |
| H | 2.521587 | -2.095652 | -0.020369 |
| H | 3.354088 | 0.237057 | -0.097412 |
| C | -1.841507 | -0.716841 | -0.012544 |
| N | -2.972282 | -0.917911 | -0.020684 |
| H | -0.028268 | 1.028307 | 1.842733 |
| C | -0.94648 | 2.033776 | -0.113994 |
| H | -1.172276 | 2.151652 | -1.1754 |
| H | -1.88303 | 1.855123 | 0.409674 |
| H | -0.510546 | 2.961009 | 0.251589 |

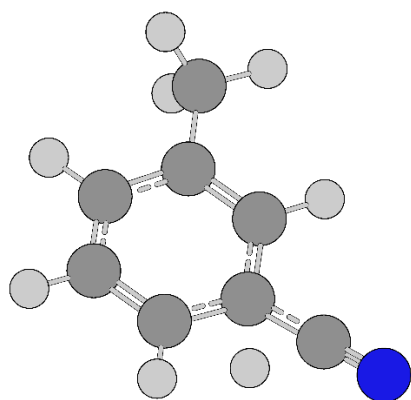


o-C₆H₄CH₃CN (R5c=R5a)

| | | | |
|---|-----------|-----------|-----------|
| C | -0.617478 | -0.653649 | 0.00000 |
| C | 0.205421 | -1.772849 | 0.00000 |
| C | 1.587717 | -1.651108 | 0.00000 |
| C | 2.18265 | -0.397641 | 0.00000 |
| C | 1.386446 | 0.734366 | 0.00000 |
| H | 3.258991 | -0.301411 | 0.00000 |
| H | 1.825128 | 1.722298 | 0.00000 |
| C | 0.00000 | 0.603678 | 0.00000 |
| C | -0.819165 | 1.782963 | 0.00000 |
| N | -1.488311 | 2.715864 | 0.00000 |
| H | 2.202941 | -2.540677 | 0.00000 |
| H | -0.247407 | -2.755791 | 0.00000 |
| C | -2.112623 | -0.771681 | 0.00000 |
| H | -2.5401 | -0.282443 | 0.875946 |
| H | -2.5401 | -0.282443 | -0.875946 |
| H | -2.419088 | -1.815048 | 0.00000 |

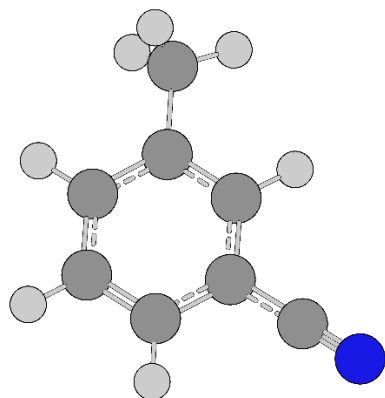
R6add-*m*-C₆H₅CH₃CN

| | | | |
|---|-----------|-----------|-----------|
| C | -0.18772 | -0.876519 | 0.429048 |
| C | -1.383636 | -0.399051 | 0.017555 |
| C | -1.532352 | 0.985154 | -0.281651 |
| C | -0.435165 | 1.864123 | -0.175671 |
| C | 0.783683 | 1.437263 | 0.229228 |
| C | 1.017765 | 0.004471 | 0.621666 |
| H | -0.058247 | -1.928834 | 0.645858 |
| H | -2.492187 | 1.355103 | -0.613639 |
| H | -0.5692 | 2.906589 | -0.432741 |
| H | 1.625611 | 2.111835 | 0.292126 |
| H | 1.309141 | -0.024694 | 1.683443 |
| C | -2.572557 | -1.303002 | -0.144669 |
| H | -3.392847 | -0.974667 | 0.494693 |
| H | -2.931624 | -1.27866 | -1.174167 |
| H | -2.327169 | -2.331704 | 0.109903 |
| C | 2.181911 | -0.546585 | -0.098014 |
| N | 3.08642 | -0.975727 | -0.655775 |



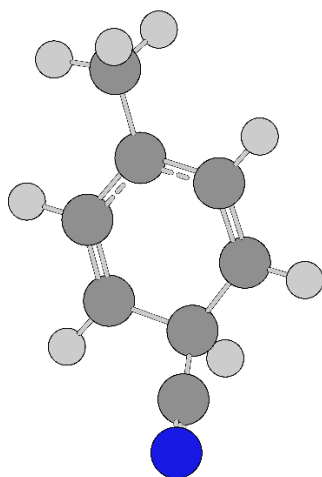
H-elim-*m*-TS

| | | | |
|---|-----------|-----------|-----------|
| C | -0.116785 | -0.883809 | 0.038418 |
| C | -1.418549 | -0.431202 | -0.011749 |
| C | -1.648547 | 0.949028 | -0.036208 |
| C | -0.594921 | 1.855014 | -0.063743 |
| C | 0.709948 | 1.41392 | -0.014872 |
| C | 0.957473 | 0.032419 | 0.143345 |
| H | 0.099235 | -1.943554 | 0.049383 |
| H | -2.667791 | 1.312231 | -0.074576 |
| H | -0.798116 | 2.914313 | -0.13818 |
| H | 1.54201 | 2.10188 | -0.044771 |
| H | 1.154798 | 0.003708 | 1.857661 |
| C | -2.573913 | -1.391213 | -0.047297 |
| H | -2.231243 | -2.416953 | -0.164129 |
| H | -3.15013 | -1.329436 | 0.876652 |
| H | -3.247572 | -1.156633 | -0.871008 |
| C | 2.304266 | -0.460888 | -0.032918 |
| N | 3.369283 | -0.855025 | -0.191556 |

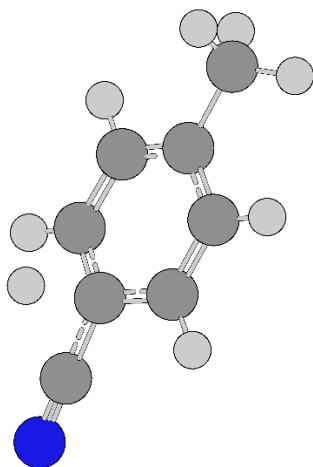
*m*-C₆H₄CH₃CN

| | | | |
|---|-----------|-----------|-----------|
| C | 0.090404 | -0.876097 | -0.006932 |
| C | 1.403295 | -0.426473 | -0.008492 |
| C | 1.631712 | 0.948555 | -0.006344 |
| C | 0.581328 | 1.85323 | 0.001721 |
| C | -0.728154 | 1.401776 | 0.006027 |
| C | -0.967701 | 0.030855 | 0.001064 |
| H | -0.121975 | -1.937074 | -0.014333 |
| H | 2.651477 | 1.313271 | -0.013927 |
| H | 0.782698 | 2.915377 | 0.001569 |
| C | 2.552531 | -1.39463 | 0.006835 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.237244 | -2.386207 | -0.311282 |
| H | 3.352812 | -1.059785 | -0.651673 |
| H | 2.967959 | -1.481468 | 1.011925 |
| C | -2.318358 | -0.457429 | 0.000415 |
| H | -1.558738 | 2.092698 | 0.009544 |
| N | -3.397403 | -0.847933 | 0.000345 |

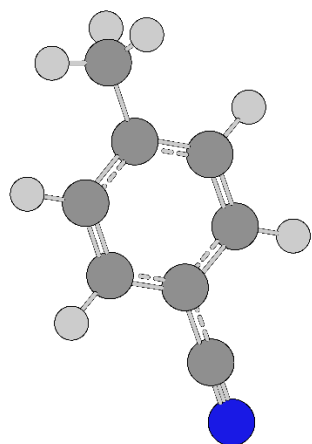
R7add-*p*-C₆H₅CH₂CN

| | | | |
|---|-----------|-----------|-----------|
| C | 0.927339 | 1.220768 | -0.077872 |
| C | -0.387929 | 1.257782 | -0.394073 |
| C | -1.184938 | 0.001622 | -0.625335 |
| C | -0.380721 | -1.251616 | -0.399772 |
| C | 0.929145 | -1.208763 | -0.08451 |
| C | 1.642635 | 0.011056 | 0.083043 |
| H | -0.910821 | 2.198114 | -0.496366 |
| H | 1.454507 | 2.156492 | 0.064712 |
| C | -2.400327 | -0.00478 | 0.211256 |
| N | -3.343831 | -0.009454 | 0.861921 |
| H | -1.560062 | 0.001673 | -1.660424 |
| H | -0.899126 | -2.19416 | -0.506831 |
| C | 3.093206 | -0.007858 | 0.438856 |
| H | 3.25611 | -0.506996 | 1.397241 |
| H | 3.673941 | -0.556233 | -0.306468 |
| H | 3.498361 | 0.999514 | 0.510665 |
| H | 1.463451 | -2.141491 | 0.054469 |



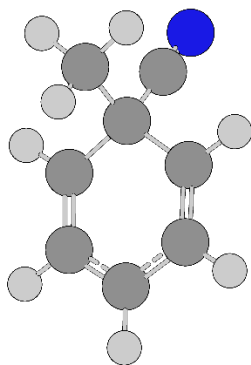
H-elim-*p*-TS

| | | | |
|---|-----------|-----------|-----------|
| C | 0.384803 | -1.216372 | 0.011252 |
| C | -0.989133 | -1.199157 | -0.037616 |
| C | -1.7043 | 0.00257 | -0.032016 |
| C | -0.988236 | 1.202043 | -0.03707 |
| C | 0.387119 | 1.217168 | 0.010815 |
| C | 1.094447 | 0.000421 | 0.147935 |
| H | 0.933862 | -2.146798 | -0.004515 |
| H | -1.526635 | 2.139236 | -0.097118 |
| H | 0.937116 | 2.147011 | -0.00546 |
| H | 1.296259 | -0.002698 | 1.859005 |
| C | 2.526507 | -0.000811 | -0.038085 |
| N | 3.661277 | -0.001892 | -0.202704 |
| C | -3.204146 | -0.001315 | -0.044549 |
| H | -3.589269 | -0.826243 | -0.642534 |
| H | -3.594881 | -0.120451 | 0.967956 |
| H | -3.598425 | 0.931332 | -0.443793 |
| H | -1.529341 | -2.135425 | -0.098611 |



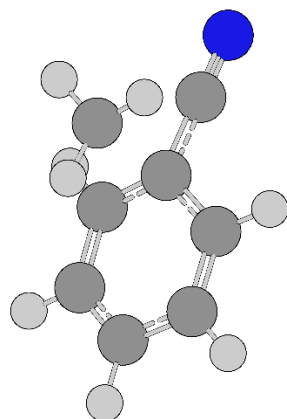
p-C₆H₄CH₃CN

| | | | |
|---|-----------|-----------|-----------|
| C | -0.970185 | 1.200727 | -0.005534 |
| C | -1.683515 | 0.006018 | -0.005797 |
| C | -0.972561 | -1.193559 | -0.005633 |
| C | 0.409234 | -1.205111 | -0.002056 |
| C | 1.108713 | 0.001037 | 0.00032 |
| C | 0.414648 | 1.207136 | -0.002045 |
| H | -1.506682 | 2.140644 | -0.009651 |
| H | -1.513668 | -2.13133 | -0.009831 |
| H | 0.954613 | -2.138283 | -0.002744 |
| C | -3.185219 | -0.003468 | 0.00808 |
| H | -3.589777 | 0.989393 | -0.176602 |
| H | -3.576971 | -0.682233 | -0.749052 |
| H | -3.556673 | -0.34503 | 0.975387 |
| H | 0.962436 | 2.138886 | -0.002737 |
| C | 2.543554 | -0.002042 | 0.002706 |
| N | 3.691244 | -0.005211 | 0.004998 |

R8

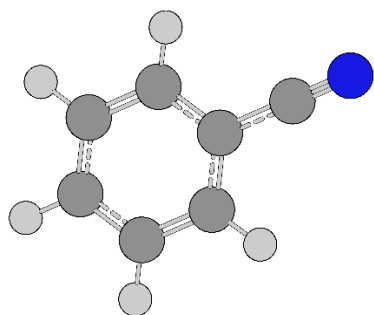
add-*ipso*-C₆H₅CH₃CN

| | | | |
|---|-----------|-----------|-----------|
| C | -0.087289 | 2.302058 | 0.00000 |
| C | -0.069144 | 1.589646 | 1.220585 |
| C | -0.069144 | 0.237394 | 1.252353 |
| C | -0.163471 | -0.596792 | 0.00000 |
| C | -0.069144 | 0.237394 | -1.252353 |
| C | -0.069144 | 1.589646 | -1.220585 |
| H | -0.086877 | 3.381132 | 0.00000 |
| H | -0.044298 | 2.138511 | 2.152569 |
| H | -0.039398 | -0.302662 | 2.189477 |
| H | -0.039398 | -0.302662 | -2.189477 |
| H | -0.044298 | 2.138511 | -2.152569 |
| C | -1.502656 | -1.381397 | 0.00000 |
| H | -1.5683 | -2.010355 | -0.886812 |
| H | -1.5683 | -2.010355 | 0.886812 |
| H | -2.32318 | -0.666554 | 0.00000 |
| C | 0.927105 | -1.594584 | 0.00000 |
| N | 1.761625 | -2.380822 | 0.00000 |



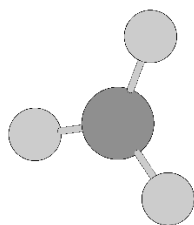
CH₃-elim-*ipso*-TS

| | | | |
|---|-----------|-----------|-----------|
| C | 0.285492 | -0.234545 | 1.222226 |
| C | 0.145646 | 0.482222 | 0.00000 |
| C | 0.285492 | -0.234545 | -1.222226 |
| C | 0.285492 | -1.609248 | -1.207761 |
| C | 0.251773 | -2.307517 | 0.00000 |
| C | 0.285492 | -1.609248 | 1.207761 |
| H | 0.331693 | 0.317192 | 2.15045 |
| H | 0.331693 | 0.317192 | -2.15045 |
| H | 0.332772 | -2.151409 | -2.142143 |
| H | 0.251681 | -3.388027 | 0.00000 |
| H | 0.332772 | -2.151409 | 2.142143 |
| C | -1.968547 | 0.83993 | 0.00000 |
| H | -2.104615 | 1.396675 | 0.917392 |
| H | -2.104615 | 1.396675 | -0.917392 |
| H | -2.305599 | -0.187677 | 0.00000 |
| C | 0.448703 | 1.894963 | 0.00000 |
| N | 0.688139 | 3.016961 | 0.00000 |



C_6H_5CN

| | | | |
|---|-----------|-----------|-----------|
| C | -2.165922 | 0.000052 | 0.000093 |
| C | -1.474492 | 1.204054 | 0.000011 |
| C | -0.089835 | 1.209847 | -0.000102 |
| C | 0.60112 | -0.000092 | -0.00014 |
| C | -0.089931 | -1.209919 | -0.000103 |
| C | -1.474623 | -1.20398 | 0.000012 |
| H | -3.247186 | 0.000095 | 0.000402 |
| H | -2.014715 | 2.140272 | 0.000113 |
| H | 0.461948 | 2.13907 | -0.000273 |
| H | 0.461691 | -2.139238 | -0.000273 |
| H | -2.014918 | -2.140159 | 0.000115 |
| C | 2.037163 | 0.000147 | 0.000046 |
| N | 3.184613 | -0.000098 | 0.000146 |



CH_3

| | | | |
|---|-----------|-----------|----------|
| C | 0.00000 | 0.000023 | 0.00000 |
| H | 0.000043 | 1.076044 | 0.000001 |
| H | 0.93197 | -0.538129 | 0.000001 |
| H | -0.932013 | -0.538054 | 0.000001 |