Electronic Supplementary Information for Dalton Transactions


# Supporting Information

**for**

# Hydrogentation of imines by phosphonium borate zwitterions: a theoretical study

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### Imaginary frequencies for transition states (in $cm^{-1}$):

TS1a: -875
TS1b: -887
TS2a: -69
TS2b: -70

### Summary of XYZ data, energies (B3LYP/6-31+G*), and negative eigenvalues (transition states only)

$A_a$ (Figure 1)

E = -3013.866072

| Atom | X | Y | Z |
|---|---|---|---|
| C | -1.010327 | -2.663888 | 4.183826 |
| C | -0.771054 | -1.850115 | 3.070387 |
| C | 0.357166 | -2.208845 | 2.332036 |
| C | 1.188094 | -3.282275 | 2.651640 |
| C | 0.893427 | -4.068258 | 3.760435 |
| C | -0.219047 | -3.754448 | 4.534791 |
| B | -1.868812 | -0.680463 | 2.716990 |
| C | -3.213178 | -1.422056 | 2.150596 |
| C | -4.434425 | -1.417905 | 2.826894 |
| C | -5.535280 | -2.174578 | 2.420969 |
| C | -5.434195 | -2.992258 | 1.300782 |
| C | -4.236696 | -3.028807 | 0.590665 |
| C | -3.174419 | -2.244095 | 1.023180 |
| F | -4.614621 | -0.659279 | 3.931099 |
| F | -6.691866 | -2.133291 | 3.110536 |
| F | -6.480916 | -3.735319 | 0.900403 |
| F | -4.123551 | -3.827922 | -0.489582 |
| F | -2.033845 | -2.298637 | 0.286613 |
| F | 0.706567 | -1.497278 | 1.224474 |
| F | 2.273048 | -3.573788 | 1.901962 |
| F | 1.671107 | -5.118413 | 4.078481 |
| F | -0.522342 | -4.511093 | 5.606341 |
| F | -2.084374 | -2.431318 | 4.971143 |
| C | -1.299555 | 0.544417 | 1.793816 |
| C | -0.097870 | 1.186661 | 2.137461 |
| C | 0.456798 | 2.229810 | 1.412714 |
| C | -0.201912 | 2.765107 | 0.293332 |
| C | -1.430057 | 2.174107 | -0.032142 |
| C | -1.950321 | 1.109736 | 0.685814 |
| P | 0.512097 | 3.989044 | -0.788266 |
| C | 0.552991 | 3.431759 | -2.518997 |
| F | 1.647467 | 2.751586 | 1.788850 |
| F | 0.586957 | 0.783744 | 3.224515 |

| | | | |
|---|---|---|---|
| F | -3.142133 | 0.647115 | 0.260715 |
| F | -2.112169 | 2.666201 | -1.101412 |
| C | -0.370233 | 5.575593 | -0.685259 |
| N | 4.010058 | 5.158663 | -0.086081 |
| C | 4.322906 | 6.419542 | 0.622934 |
| C | 3.010014 | 7.221373 | 0.697129 |
| C | 4.711134 | 4.755411 | -1.075975 |
| H | 5.530668 | 5.350098 | -1.499117 |
| C | 4.753382 | 6.003857 | 2.044955 |
| C | 5.418440 | 7.288349 | -0.019572 |
| H | -1.411338 | 5.433917 | -0.989713 |
| H | -0.344925 | 5.940764 | 0.345393 |
| H | 0.106649 | 6.311462 | -1.340574 |
| H | 1.024118 | 4.207367 | -3.131282 |
| H | 1.148994 | 2.517706 | -2.582636 |
| H | -0.459289 | 3.238611 | -2.880803 |
| H | 1.851162 | 4.203599 | -0.406457 |
| H | -2.146592 | -0.123881 | 3.756669 |
| H | 4.914723 | 6.890481 | 2.668806 |
| H | 3.986131 | 5.380282 | 2.514710 |
| H | 5.686065 | 5.429763 | 2.014517 |
| H | 5.545892 | 8.203641 | 0.567940 |
| H | 6.389318 | 6.780391 | -0.043540 |
| H | 5.157952 | 7.587359 | -1.042537 |
| H | 3.150001 | 8.136890 | 1.282263 |
| H | 2.670267 | 7.509533 | -0.305682 |
| H | 2.225479 | 6.627218 | 1.178651 |
| C | 4.485378 | 3.452911 | -1.737451 |
| C | 3.874999 | 2.377368 | -1.066797 |
| C | 3.681458 | 1.158637 | -1.717767 |
| C | 4.098677 | 0.995800 | -3.045098 |
| C | 4.715224 | 2.056280 | -3.715383 |
| C | 4.917909 | 3.273048 | -3.061453 |
| H | 3.590699 | 2.495433 | -0.025048 |
| H | 3.227993 | 0.327027 | -1.184476 |
| H | 3.955830 | 0.042346 | -3.546337 |
| H | 5.047277 | 1.932225 | -4.742630 |
| H | 5.406857 | 4.093413 | -3.583361 |

$A_b$ (Figure 1)

E = -3249.734045

| Atom | X | Y | Z |
|---|---|---|---|
| C | 5.714791 | 6.080054 | -3.557277 |
| C | 5.398494 | 5.094238 | -2.608868 |
| C | 5.463726 | 3.743144 | -2.986856 |
| C | 5.823650 | 3.387767 | -4.285100 |
| C | 6.123022 | 4.378343 | -5.228381 |
| C | 6.062180 | 5.725582 | -4.861857 |
| C | 5.038947 | 5.502658 | -1.232799 |
| N | 4.384483 | 4.754125 | -0.431153 |
| C | 4.111655 | 5.171882 | 0.965494 |
| C | 4.720416 | 6.519927 | 1.386658 |
| C | 2.579791 | 5.234447 | 1.130234 |
| C | 4.679174 | 4.049150 | 1.857368 |
| P | 1.343596 | 2.090800 | -1.824052 |
| C | 0.574765 | 3.507019 | -2.826775 |
| C | 0.346647 | 1.503302 | -0.451216 |
| C | 0.885235 | 1.328294 | 0.831695 |
| C | 0.135651 | 0.769502 | 1.854602 |
| C | -1.194692 | 0.351058 | 1.708463 |
| C | -1.736701 | 0.603281 | 0.441126 |
| C | -0.986565 | 1.120359 | -0.606665 |
| B | -1.959541 | -0.380339 | 2.963016 |
| C | -3.450717 | -0.962893 | 2.614380 |
| C | -4.585186 | -0.569544 | 3.328625 |
| C | -5.858581 | -1.087571 | 3.089978 |
| C | -6.038960 | -2.033720 | 2.088490 |
| C | -4.939904 | -2.453608 | 1.344010 |
| C | -3.688180 | -1.922989 | 1.631754 |
| F | -4.508591 | 0.381960 | 4.286445 |
| F | -6.915118 | -0.675242 | 3.817724 |
| F | -7.262636 | -2.531602 | 1.834552 |
| F | -5.106323 | -3.355778 | 0.355197 |
| F | -2.655121 | -2.342724 | 0.856579 |
| F | 0.757073 | 0.630868 | 3.044768 |

| | | | |
|---|---|---|---|
| F | 2.173862 | 1.682063 | 1.065600 |
| F | -1.574910 | 1.286493 | -1.821280 |
| F | -3.020813 | 0.316144 | 0.154398 |
| C | -1.079817 | -1.636843 | 3.562250 |
| C | -1.248412 | -2.028337 | 4.895722 |
| C | -0.610345 | -3.129079 | 5.465184 |
| C | 0.244997 | -3.904000 | 4.685981 |
| C | 0.452236 | -3.553891 | 3.356103 |
| C | -0.204184 | -2.442535 | 2.831714 |
| F | -2.081850 | -1.333836 | 5.700963 |
| F | 0.066184 | -2.162353 | 1.526119 |
| F | 1.285655 | -4.291621 | 2.591005 |
| F | 0.863477 | -4.977053 | 5.211576 |
| F | -0.810009 | -3.456795 | 6.757510 |
| C | 2.094168 | 0.614874 | -2.735273 |
| H | 5.372055 | 6.511755 | -0.958202 |
| C | -0.236773 | 3.029114 | -4.047400 |
| C | -0.325712 | 4.308233 | -1.861940 |
| C | 1.733509 | 4.419335 | -3.291687 |
| C | 3.060282 | 1.164988 | -3.796658 |
| C | 2.808044 | -0.227817 | -1.655272 |
| C | 1.007104 | -0.239367 | -3.410923 |
| H | 2.453795 | 2.697401 | -1.214581 |
| H | -2.082693 | 0.499297 | 3.781319 |
| H | 4.448308 | 4.246028 | 2.910291 |
| H | 4.245108 | 3.083207 | 1.585662 |
| H | 5.767769 | 3.980662 | 1.750405 |
| H | 4.491773 | 6.706421 | 2.441117 |
| H | 5.811777 | 6.524306 | 1.281005 |
| H | 4.311616 | 7.359372 | 0.811357 |
| H | 2.317532 | 5.479546 | 2.165294 |
| H | 2.146040 | 6.002817 | 0.478703 |
| H | 2.125010 | 4.269149 | 0.890744 |
| H | 5.190314 | 2.996526 | -2.249228 |
| H | 5.848010 | 2.340899 | -4.576273 |
| H | 6.386758 | 4.097142 | -6.244454 |
| H | 6.276747 | 6.497419 | -5.595395 |
| H | 5.673315 | 7.129268 | -3.271792 |
| H | 3.324871 | -1.058466 | -2.151054 |
| H | 3.558330 | 0.340401 | -1.093083 |
| H | 2.103790 | -0.664504 | -0.942805 |
| H | 1.486538 | -1.128326 | -3.838003 |
| H | 0.250577 | -0.585665 | -2.701072 |
| H | 0.509401 | 0.290731 | -4.226894 |
| H | 3.486614 | 0.321095 | -4.346605 |
| H | 2.555313 | 1.804920 | -4.527650 |
| H | 3.868728 | 1.752986 | -3.367685 |
| H | -0.660904 | 5.212543 | -2.383523 |
| H | -1.212048 | 3.747645 | -1.560079 |
| H | 0.211969 | 4.628072 | -0.963303 |
| H | 1.295295 | 5.267686 | -3.830641 |
| H | 2.309609 | 4.814792 | -2.450655 |
| H | 2.427276 | 3.922651 | -3.974200 |
| H | -0.699494 | 3.909463 | -4.509055 |
| H | 0.397318 | 2.563031 | -4.807580 |
| H | -1.034774 | 2.335945 | -3.778858 |

## $TS1_a$ (Figure 2)

E = -3013.855828

Negative eigenvalue: -875cm$^{-1}$

| Atom | X | Y | Z |
|---|---|---|---|
| C | -1.346784 | 0.069320 | -0.126729 |
| C | -0.928426 | -0.024043 | 1.203795 |
| C | 0.030235 | -1.009275 | 1.434675 |
| C | 0.547813 | -1.841507 | 0.445864 |
| C | 0.103305 | -1.701628 | -0.864284 |
| C | -0.858647 | -0.738492 | -1.151493 |
| B | -1.575058 | 0.973182 | 2.332759 |
| C | -0.939031 | 2.478499 | 2.272968 |
| C | -1.738232 | 3.604284 | 2.482059 |
| C | -1.266758 | 4.913301 | 2.425681 |
| C | 0.069132 | 5.147212 | 2.125176 |
| C | 0.907290 | 4.062367 | 1.888866 |
| C | 0.395729 | 2.769273 | 1.979712 |
| F | -3.042233 | 3.459474 | 2.824535 |

| | | | |
|---|---|---|---|
| F | -2.084498 | 5.955849 | 2.670501 |
| F | 0.544372 | 6.404360 | 2.068110 |
| F | 2.202635 | 4.275512 | 1.582994 |
| F | 1.288168 | 1.767021 | 1.786452 |
| F | 0.519438 | -1.208062 | 2.688889 |
| F | 1.484223 | -2.768565 | 0.738882 |
| F | 0.591708 | -2.488383 | -1.840556 |
| F | -1.308254 | -0.606320 | -2.415606 |
| F | -2.284627 | 0.978183 | -0.480893 |
| C | -1.615327 | 0.318963 | 3.834914 |
| C | -2.328061 | -0.872915 | 4.026910 |
| C | -2.559560 | -1.440554 | 5.268038 |
| C | -2.088950 | -0.853615 | 6.451200 |
| C | -1.365088 | 0.333209 | 6.275929 |
| C | -1.131173 | 0.882762 | 5.022994 |
| P | -2.384371 | -1.603987 | 8.066394 |
| C | -0.816745 | -1.580549 | 9.025990 |
| F | -3.269534 | -2.597958 | 5.335959 |
| F | -2.843953 | -1.526859 | 2.964809 |
| F | -0.402870 | 2.019672 | 5.011582 |
| F | -0.883233 | 0.975960 | 7.373967 |
| C | -3.506136 | -0.481281 | 8.997424 |
| N | -3.322268 | -4.529485 | 7.661014 |
| C | -2.172142 | -5.480837 | 7.600778 |
| C | -1.056132 | -4.799088 | 6.781633 |
| C | -4.490939 | -4.848484 | 7.234082 |
| H | -4.642950 | -5.813342 | 6.746680 |
| C | -1.722815 | -5.702971 | 9.057659 |
| C | -2.508175 | -6.832736 | 6.950147 |
| H | -3.006126 | 0.473712 | 9.184038 |
| H | -4.414169 | -0.306808 | 8.414863 |
| H | -3.777303 | -0.932707 | 9.958126 |
| H | -0.967892 | -2.091479 | 9.982955 |
| H | -0.025935 | -2.093635 | 8.471950 |
| H | -0.502769 | -0.551360 | 9.210475 |
| H | -2.958000 | -3.141067 | 7.881185 |
| H | -2.751071 | 1.071908 | 2.059184 |
| H | -0.821553 | -6.324930 | 9.081895 |
| H | -1.491400 | -4.751686 | 9.549619 |
| H | -2.505555 | -6.205410 | 9.636452 |
| H | -1.608150 | -7.454892 | 6.954994 |
| H | -3.289079 | -7.380307 | 7.489911 |
| H | -2.812179 | -6.719579 | 5.902862 |
| H | -0.217462 | -5.490094 | 6.651072 |
| H | -1.416689 | -4.516656 | 5.787724 |
| H | -0.671842 | -3.904105 | 7.279573 |
| C | -5.693932 | -4.014737 | 7.321712 |
| C | -6.690625 | -4.186026 | 6.345009 |
| C | -7.861630 | -3.432394 | 6.391772 |
| C | -8.069080 | -2.530843 | 7.439625 |
| C | -7.098986 | -2.382458 | 8.437016 |
| C | -5.916025 | -3.116013 | 8.378272 |
| H | -6.539440 | -4.902328 | 5.540771 |
| H | -8.617702 | -3.560531 | 5.622505 |
| H | -8.988145 | -1.953371 | 7.486173 |
| H | -7.276981 | -1.706262 | 9.268710 |
| H | -5.186450 | -3.039763 | 9.178666 |

## $TS1_b$ (Figure 2)

Negative eigenvalue: -887 $cm^{-1}$

E = -3249.706522

| Atom | X | Y | Z |
|---|---|---|---|
| C | -0.388758 | -0.078976 | -0.212160 |
| C | -0.310754 | 0.088772 | 1.182461 |
| C | 0.937034 | 0.319187 | 1.782260 |
| C | 2.093239 | 0.362319 | 1.001924 |
| C | 2.013661 | 0.156554 | -0.377475 |
| C | 0.771772 | -0.071479 | -0.983480 |
| C | -1.537082 | 0.198164 | 1.987010 |
| N | -1.717135 | -0.306950 | 3.157376 |
| C | -2.847288 | 0.182756 | 4.028305 |
| C | -4.010078 | 0.807443 | 3.234637 |
| C | -3.385716 | -0.989702 | 4.854075 |

| | | | |
|---|---|---|---|
| C | -2.225491 | 1.246776 | 4.955950 |
| P | -0.382101 | -3.154068 | 3.747742 |
| C | -1.652803 | -4.356214 | 2.947564 |
| C | -0.232199 | -3.469082 | 5.547281 |
| C | -0.066779 | -2.391349 | 6.432691 |
| C | 0.196530 | -2.561779 | 7.786130 |
| C | 0.335888 | -3.814977 | 8.401470 |
| C | 0.172328 | -4.881840 | 7.514841 |
| C | -0.093057 | -4.724514 | 6.157152 |
| B | 0.614640 | -3.882350 | 10.020479 |
| C | 0.372762 | -5.338780 | 10.733529 |
| C | -0.821460 | -5.668984 | 11.380408 |
| C | -1.019259 | -6.863119 | 12.076053 |
| C | 0.010780 | -7.794241 | 12.149502 |
| C | 1.214714 | -7.521462 | 11.509538 |
| C | 1.362046 | -6.322689 | 10.818645 |
| F | -1.875698 | -4.818864 | 11.357309 |
| F | -2.195391 | -7.127639 | 12.681991 |
| F | -0.154565 | -8.950800 | 12.818061 |
| F | 2.220583 | -8.416509 | 11.562734 |
| F | 2.551976 | -6.145419 | 10.193147 |
| F | 0.354731 | -1.435221 | 8.514405 |
| F | -0.112610 | -1.119629 | 5.938130 |
| F | -0.185792 | -5.848140 | 5.399285 |
| F | 0.300540 | -6.155778 | 7.944191 |
| C | 2.097456 | -3.287113 | 10.407962 |
| C | 2.336701 | -2.807656 | 11.701214 |
| C | 3.559930 | -2.292212 | 12.124132 |
| C | 4.624732 | -2.239294 | 11.228995 |
| C | 4.440609 | -2.707920 | 9.933549 |
| C | 3.200851 | -3.221298 | 9.561347 |
| F | 1.352748 | -2.840553 | 12.628512 |
| F | 3.111417 | -3.688404 | 8.285589 |
| F | 5.466602 | -2.668192 | 9.057138 |
| F | 5.815018 | -1.736246 | 11.607152 |
| F | 3.724863 | -1.836940 | 13.382331 |
| C | 1.406920 | -3.416576 | 3.100448 |
| H | -2.314998 | 0.826687 | 1.550340 |
| C | -1.102310 | -5.709476 | 2.453049 |
| C | -2.774943 | -4.640537 | 3.966702 |
| C | -2.240492 | -3.592073 | 1.738552 |
| C | 1.431067 | -3.287308 | 1.565417 |
| C | 2.270423 | -2.306042 | 3.732240 |
| C | 2.018185 | -4.769556 | 3.510694 |
| H | -1.027309 | -1.496305 | 3.489182 |
| H | -0.180876 | -3.101229 | 10.488597 |
| H | -2.989971 | 1.616859 | 5.647748 |
| H | -1.404613 | 0.831340 | 5.543110 |
| H | -1.848937 | 2.095318 | 4.373636 |
| H | -4.820217 | 1.039123 | 3.932488 |
| H | -3.739404 | 1.749478 | 2.746052 |
| H | -4.409380 | 0.117454 | 2.481480 |
| H | -4.126802 | -0.618323 | 5.568571 |
| H | -3.887421 | -1.720131 | 4.212191 |
| H | -2.596656 | -1.488055 | 5.422184 |
| H | 0.984984 | 0.487495 | 2.854331 |
| H | 3.054052 | 0.552912 | 1.471431 |
| H | 2.915449 | 0.182464 | -0.983006 |
| H | 0.709875 | -0.227554 | -2.056691 |
| H | -1.355684 | -0.228243 | -0.687130 |
| H | 3.296628 | -2.406547 | 3.356007 |
| H | 1.912242 | -1.311812 | 3.463034 |
| H | 2.312006 | -2.386943 | 4.822170 |
| H | 3.038186 | -4.812745 | 3.106975 |
| H | 2.097429 | -4.874442 | 4.594867 |
| H | 1.471261 | -5.626539 | 3.117623 |
| H | 2.475311 | -3.289507 | 1.228380 |
| H | 0.933567 | -4.127480 | 1.073659 |
| H | 0.975437 | -2.359630 | 1.211972 |
| H | -3.586857 | -5.167431 | 3.449198 |
| H | -2.431423 | -5.280578 | 4.782100 |
| H | -3.194558 | -3.731844 | 4.400207 |
| H | -2.969830 | -4.236572 | 1.232600 |
| H | -2.759989 | -2.677477 | 2.041968 |
| H | -1.473938 | -3.323700 | 1.003741 |
| H | -1.940713 | -6.272671 | 2.023262 |
| H | -0.353449 | -5.600574 | 1.664770 |

| | | | |
|---|---|---|---|
| H | -0.683835 | -6.310252 | 3.259855 |

## $B_{1a}$ (Figure 3)

E = -3013.877135

| Atom | X | Y | Z |
|---|---|---|---|
| C | -1.856953 | -0.873827 | 4.378566 |
| C | -1.191731 | -1.094311 | 3.168517 |
| C | -0.717427 | -2.396286 | 3.002980 |
| C | -0.897951 | -3.412572 | 3.940317 |
| C | -1.581504 | -3.142041 | 5.120910 |
| C | -2.059992 | -1.855202 | 5.345304 |
| B | -1.123840 | 0.117818 | 2.064472 |
| C | -2.616959 | 0.288239 | 1.395866 |
| C | -3.272236 | 1.518266 | 1.340007 |
| C | -4.587830 | 1.681961 | 0.907916 |
| C | -5.316489 | 0.572653 | 0.495310 |
| C | -4.704529 | -0.677589 | 0.506708 |
| C | -3.386059 | -0.786890 | 0.941088 |
| F | -2.632693 | 2.664457 | 1.708882 |
| F | -5.163242 | 2.904439 | 0.883649 |
| F | -6.589753 | 0.707505 | 0.082374 |
| F | -5.393413 | -1.758093 | 0.092151 |
| F | -2.842660 | -2.025128 | 0.895611 |
| F | -0.053653 | -2.743230 | 1.870874 |
| F | -0.439332 | -4.659779 | 3.710966 |
| F | -1.785147 | -4.114227 | 6.028733 |
| F | -2.724995 | -1.577732 | 6.484406 |
| F | -2.373626 | 0.348336 | 4.655312 |
| C | 0.116593 | 0.005913 | 1.001970 |
| C | 1.430218 | 0.130985 | 1.469517 |
| C | 2.533249 | 0.231165 | 0.636685 |
| C | 2.450378 | 0.206700 | -0.761387 |
| C | 1.145581 | 0.056593 | -1.237946 |
| C | 0.039977 | -0.046022 | -0.390291 |
| P | 3.963207 | 0.624275 | -1.733568 |
| C | 5.110332 | -0.770320 | -1.289536 |
| F | 3.762784 | 0.425750 | 1.213790 |
| F | 1.669672 | 0.205686 | 2.802267 |
| F | -1.158819 | -0.174505 | -1.007356 |
| F | 0.904661 | 0.045598 | -2.575604 |
| C | 3.581650 | 0.145141 | -3.485333 |
| N | 3.606452 | 3.594574 | 0.448199 |
| C | 4.695180 | 3.837758 | 1.467921 |
| C | 4.995025 | 5.347792 | 1.469592 |
| C | 2.354813 | 3.923166 | 0.588194 |
| C | 1.323587 | 3.862860 | -0.413277 |
| C | 1.595626 | 3.720607 | -1.793471 |
| C | 0.547551 | 3.686960 | -2.700913 |
| C | -0.777645 | 3.785425 | -2.249921 |
| C | -1.058649 | 3.925893 | -0.888840 |
| C | -0.013206 | 3.976926 | 0.027552 |
| C | 4.235138 | 3.357895 | 2.852899 |
| C | 5.922002 | 3.045107 | 0.999493 |
| H | 2.068318 | 4.291337 | 1.570549 |
| H | -0.889301 | 1.136712 | 2.674950 |
| H | 6.755823 | 3.238789 | 1.680591 |
| H | 5.722255 | 1.970773 | 0.997389 |
| H | 6.234639 | 3.348308 | -0.006798 |
| H | 5.801742 | 5.559179 | 2.178737 |
| H | 5.312879 | 5.690552 | 0.478725 |
| H | 4.117905 | 5.930286 | 1.773158 |
| H | 5.069163 | 3.458903 | 3.554515 |
| H | 3.410051 | 3.958197 | 3.251257 |
| H | 3.929191 | 2.308629 | 2.829307 |
| H | 2.618867 | 3.657081 | -2.153069 |
| H | 0.752913 | 3.583156 | -3.761833 |
| H | -1.592669 | 3.748104 | -2.967143 |
| H | -2.082795 | 3.983079 | -0.536530 |
| H | -0.232867 | 4.064493 | 1.088153 |
| H | 3.897236 | 3.117671 | -0.414537 |

| | | | |
|---|---|---|---|
| H | 6.019228 | -0.678490 | -1.894892 |
| H | 5.390726 | -0.719829 | -0.235282 |
| H | 4.650261 | -1.744957 | -1.485442 |
| H | 4.524329 | 0.211929 | -4.041125 |
| H | 3.191052 | -0.873180 | -3.569772 |
| H | 2.866184 | 0.833495 | -3.939640 |

$B_{2a}$ (Figure 3)

E = -3013.888336

| Atom | X | Y | Z |
|---|---|---|---|
| C | -1.772841 | -1.047270 | -3.241012 |
| C | -1.237912 | -0.333016 | -2.174132 |
| C | -0.255008 | 0.572372 | -2.585154 |
| C | 0.111689 | 0.772139 | -3.915754 |
| C | -0.474609 | 0.073297 | -4.977691 |
| C | -1.423760 | -0.867795 | -4.570724 |
| B | -1.725593 | -0.579960 | -0.624784 |
| C | -0.485143 | -0.496240 | 0.441703 |
| C | 0.306436 | -1.608942 | 0.725371 |
| C | 1.352308 | -1.611594 | 1.645642 |
| C | 1.657938 | -0.441946 | 2.333548 |
| C | 0.899557 | 0.699671 | 2.090901 |
| C | -0.137796 | 0.649488 | 1.162827 |
| F | 0.082589 | -2.791117 | 0.083778 |
| F | 2.067963 | -2.731145 | 1.878471 |
| F | 2.669408 | -0.414770 | 3.217585 |
| F | 1.177972 | 1.838871 | 2.751217 |
| F | -0.816045 | 1.804551 | 0.972843 |
| F | 0.369338 | 1.350207 | -1.672914 |
| F | 1.074699 | 1.693026 | -4.152756 |
| P | -0.047937 | 0.166737 | -6.787945 |
| C | 0.907018 | 1.754240 | -6.955571 |
| F | -2.039869 | -1.647526 | -5.505069 |
| F | -2.774444 | -1.984013 | -3.013424 |
| C | -2.993495 | 0.359472 | -0.161155 |
| C | -3.647964 | 0.052337 | 1.037404 |
| C | -4.743907 | 0.750519 | 1.535477 |
| C | -5.248112 | 1.829651 | 0.815347 |
| C | -4.638372 | 2.180023 | -0.385020 |
| C | -3.541014 | 1.447247 | -0.843592 |
| F | -3.214338 | -0.990906 | 1.788849 |
| F | -3.016612 | 1.860140 | -2.023601 |
| F | -5.115397 | 3.222160 | -1.092566 |
| F | -6.313617 | 2.514484 | 1.267349 |
| F | -5.329166 | 0.388133 | 2.696001 |
| C | -1.685048 | 0.759844 | -7.466887 |
| N | -2.811732 | -4.610243 | -1.982414 |
| C | -1.788792 | -5.405920 | -2.739802 |
| C | -2.167939 | -5.279456 | -4.228681 |
| C | -3.733049 | -5.047767 | -1.180809 |
| C | -4.796186 | -4.277331 | -0.578418 |
| C | -5.102257 | -2.947557 | -0.943132 |
| C | -6.166793 | -2.295557 | -0.335146 |
| C | -6.923547 | -2.942685 | 0.649441 |
| C | -6.627558 | -4.258592 | 1.019747 |
| C | -5.577993 | -4.927514 | 0.400861 |
| C | -0.423208 | -4.758446 | -2.462218 |
| C | -1.796758 | -6.870068 | -2.298895 |
| H | -3.706666 | -6.110074 | -0.955195 |
| H | -2.439010 | -0.026365 | -7.380953 |
| H | -2.046197 | 1.662247 | -6.961001 |
| H | -1.546965 | 0.982291 | -8.531519 |
| H | 1.006564 | 1.932335 | -8.033253 |
| H | 0.415354 | 2.618674 | -6.499655 |
| H | 1.910481 | 1.653186 | -6.536164 |
| H | -2.764805 | -3.603239 | -2.173733 |
| H | -1.013424 | -7.397239 | -2.851177 |
| H | -1.576683 | -6.978403 | -1.230904 |
| H | -2.744326 | -7.372028 | -2.527049 |
| H | 0.341296 | -5.264118 | -3.060702 |
| H | -0.418294 | -3.699362 | -2.737745 |
| H | -0.151710 | -4.833797 | -1.406069 |
| H | -1.425268 | -5.805894 | -4.837119 |
| H | -3.150810 | -5.722613 | -4.423362 |
| H | -2.186222 | -4.232731 | -4.548533 |

| | | | |
|---|---|---|---|
| H | -2.148454 | -1.719721 | -0.576758 |
| H | -5.347411 | -5.952724 | 0.680850 |
| H | -7.214822 | -4.757553 | 1.784422 |
| H | -7.745328 | -2.417783 | 1.128095 |
| H | -6.401116 | -1.274672 | -0.618768 |
| H | -4.520107 | -2.421795 | -1.690349 |

TS2a (Figure 4)

Negative eigenvalue: -69 $cm^{-1}$

E = -3013.871954

| Atom | X | Y | Z |
|---|---|---|---|
| C | -0.311468 | 0.315772 | -0.333036 |
| C | -0.188540 | 0.288999 | 1.064771 |
| C | 1.097034 | 0.214162 | 1.620122 |
| C | 2.229746 | 0.159464 | 0.804872 |
| C | 2.094272 | 0.178700 | -0.583879 |
| C | 0.818954 | 0.259827 | -1.148504 |
| C | -1.366694 | 0.408680 | 2.002953 |
| N | -2.387532 | 1.252191 | 1.600649 |
| C | -3.231419 | 2.129443 | 2.453464 |
| C | -2.420539 | 2.692598 | 3.635588 |
| C | -3.685638 | 3.287037 | 1.548790 |
| C | -4.464686 | 1.374754 | 2.985245 |
| F | -1.845833 | -0.445702 | 4.737454 |
| C | -2.051320 | -1.765390 | 4.999440 |
| C | -2.263602 | -2.658461 | 3.953018 |
| C | -2.459225 | -3.976629 | 4.382917 |
| C | -2.460157 | -4.363991 | 5.718030 |
| C | -2.266940 | -3.455907 | 6.761175 |
| C | -2.048739 | -2.141732 | 6.335760 |
| B | -2.307853 | -2.322094 | 2.373281 |
| C | -3.757502 | -2.138651 | 1.707231 |
| C | -4.962421 | -2.428311 | 2.366961 |
| C | -6.221820 | -2.247186 | 1.797325 |
| C | -6.331972 | -1.747803 | 0.505023 |
| C | -5.170551 | -1.443746 | -0.198682 |
| C | -3.936150 | -1.634180 | 0.410997 |
| F | -4.969775 | -2.918853 | 3.622087 |
| F | -7.329434 | -2.540107 | 2.495113 |
| F | -7.533528 | -1.550353 | -0.049421 |
| F | -5.258360 | -0.955138 | -1.447672 |
| F | -2.853593 | -1.308749 | -0.329514 |
| F | -1.828143 | -1.174929 | 7.260387 |
| P | -2.175606 | -3.802505 | 8.588335 |
| C | -2.767522 | -5.559147 | 8.755893 |
| F | -2.673701 | -5.676616 | 5.967470 |
| F | -2.714061 | -4.955872 | 3.481088 |
| C | -1.114544 | -3.037128 | 1.578655 |
| C | 0.181030 | -2.999611 | 2.114340 |
| C | 1.272804 | -3.654617 | 1.559739 |
| C | 1.098743 | -4.397707 | 0.395916 |
| C | -0.168330 | -4.477684 | -0.174985 |
| C | -1.239517 | -3.810025 | 0.417308 |
| F | 0.411094 | -2.306418 | 3.252677 |
| F | -2.438051 | -3.974320 | -0.178439 |
| F | -0.349474 | -5.205034 | -1.288618 |
| F | 2.140530 | -5.026651 | -0.161307 |
| F | 2.484591 | -3.579507 | 2.132904 |
| C | -3.722608 | -2.916020 | 9.139529 |
| H | -2.485724 | 1.398228 | 0.606224 |
| H | -3.609927 | -1.838311 | 8.995693 |
| H | -4.615870 | -3.259173 | 8.605282 |
| H | -3.855673 | -3.104219 | 10.210966 |
| H | -2.848521 | -5.746921 | 9.833052 |
| H | -3.738052 | -5.751894 | 8.289051 |
| H | -2.031859 | -6.257542 | 8.350204 |
| H | -4.345651 | 3.962949 | 2.101773 |
| H | -2.827264 | 3.864287 | 1.186106 |
| H | -4.247369 | 2.914464 | 0.682407 |
| H | -3.029245 | 3.420908 | 4.182095 |
| H | -2.136062 | 1.915947 | 4.350981 |
| H | -1.513988 | 3.197669 | 3.283176 |
| H | -5.083282 | 2.041803 | 3.597305 |
| H | -5.079834 | 1.006512 | 2.157996 |
| H | -4.168612 | 0.524655 | 3.605365 |

| | | | |
|---|---|---|---|
| H | -1.782985 | -0.800653 | 2.166570 |
| H | -1.059291 | 0.589313 | 3.028580 |
| H | 1.215736 | 0.199305 | 2.699606 |
| H | 3.215593 | 0.099435 | 1.257687 |
| H | 2.973024 | 0.129845 | -1.221491 |
| H | 0.700697 | 0.274392 | -2.228747 |
| H | -1.285671 | 0.363012 | -0.805665 |

## C (Figure 4)

E = -3013.902846

| Atom | X | Y | Z |
|---|---|---|---|
| C | -5.269294 | -4.483182 | 0.766329 |
| C | -5.137807 | -4.892043 | -0.566211 |
| C | -6.209704 | -4.674141 | -1.444849 |
| C | -7.384357 | -4.067821 | -0.996878 |
| C | -7.507927 | -3.668003 | 0.338081 |
| C | -6.445775 | -3.877682 | 1.219517 |
| C | -3.869154 | -5.576782 | -1.040957 |
| N | -3.425434 | -5.032915 | -2.326265 |
| C | -2.227011 | -5.626485 | -2.965993 |
| C | -2.541773 | -7.071503 | -3.391787 |
| C | -1.955049 | -4.784438 | -4.223718 |
| C | -0.977470 | -5.605806 | -2.056214 |
| F | -3.168313 | -0.794648 | -2.498165 |
| C | -2.007665 | -0.278514 | -2.960416 |
| C | -1.100934 | 0.305660 | -2.065038 |
| C | 0.082648 | 0.763621 | -2.658035 |
| C | 0.335971 | 0.668658 | -4.022156 |
| C | -0.573902 | 0.089275 | -4.914401 |
| C | -1.746919 | -0.396368 | -4.316918 |
| B | -1.380375 | 0.419298 | -0.528097 |
| C | -2.801110 | 0.839989 | -0.012549 |
| C | -3.384732 | 0.273178 | 1.130757 |
| C | -4.643390 | 0.631224 | 1.600254 |
| C | -5.368722 | 1.613586 | 0.927380 |
| C | -4.831393 | 2.210787 | -0.211779 |
| C | -3.577412 | 1.812738 | -0.662111 |
| F | 1.024018 | 1.365715 | -1.897713 |
| F | 1.518874 | 1.155194 | -4.458241 |
| P | -0.295226 | -0.264765 | -6.721661 |
| C | -1.745746 | 0.634551 | -7.477661 |
| F | -2.667310 | -1.026639 | -5.080621 |
| F | -2.734975 | -0.693061 | 1.807706 |
| F | -5.165189 | 0.045218 | 2.685412 |
| F | -6.572164 | 1.979972 | 1.372229 |
| F | -5.523700 | 3.156915 | -0.859952 |
| F | -3.102744 | 2.434461 | -1.758655 |
| C | -0.217303 | 0.119463 | 0.488028 |
| C | 0.673021 | -0.950084 | 0.309122 |
| C | 1.734053 | -1.208893 | 1.169929 |
| C | 1.951855 | -0.363380 | 2.256652 |
| C | 1.093757 | 0.712350 | 2.478936 |
| C | 0.028491 | 0.924420 | 1.609726 |
| F | 0.500966 | -1.805150 | -0.718386 |
| F | 2.545347 | -2.255716 | 0.966755 |
| F | 2.976395 | -0.586858 | 3.082482 |
| F | 1.302886 | 1.526616 | 3.522226 |
| F | -0.764962 | 1.983305 | 1.864117 |
| C | 1.060590 | 0.901412 | -7.231282 |
| H | -2.681653 | 0.126991 | -7.235066 |
| H | -1.806059 | 1.681409 | -7.160299 |
| H | -1.615598 | 0.603425 | -8.565339 |
| H | 1.101804 | 0.848316 | -8.325857 |
| H | 0.890221 | 1.941438 | -6.936830 |
| H | 2.027064 | 0.571878 | -6.843981 |
| H | -3.291864 | -4.025628 | -2.232298 |
| H | -1.710356 | -7.484540 | -3.974715 |
| H | -2.695498 | -7.732124 | -2.530858 |
| H | -3.446062 | -7.096781 | -4.009785 |
| H | -0.100702 | -5.995119 | -2.588144 |
| H | -0.746050 | -4.582692 | -1.732961 |
| H | -1.116167 | -6.220806 | -1.159609 |
| H | -1.094734 | -5.176458 | -4.777792 |
| H | -2.828917 | -4.786734 | -4.883998 |
| H | -1.733442 | -3.742150 | -3.959995 |

| | | | |
|---|---|---|---|
| H | -4.442903 | -4.637012 | 1.457886 |
| H | -6.527393 | -3.565322 | 2.257742 |
| H | -8.422855 | -3.194612 | 0.685879 |
| H | -8.205951 | -3.905564 | -1.690707 |
| H | -6.106416 | -4.973431 | -2.483939 |
| H | -4.070756 | -6.646532 | -1.181375 |
| H | -3.112191 | -5.505290 | -0.240340 |

Additional complexes:

E

| | | | |
|---|---|---|---|
| C | -0.109399 | 0.985905 | 1.339826 |
| C | -0.015451 | -0.109917 | 0.478890 |
| C | 1.239879 | -0.715368 | 0.464687 |
| C | 2.342430 | -0.262118 | 1.176147 |
| C | 2.195229 | 0.834093 | 2.018884 |
| C | 0.951778 | 1.449128 | 2.116415 |
| B | -1.204555 | -0.675148 | -0.487061 |
| C | -2.711477 | -0.317329 | 0.032735 |
| C | -3.304489 | -1.054067 | 1.057839 |
| C | -4.594408 | -0.833990 | 1.533789 |
| C | -5.362349 | 0.181336 | 0.973903 |
| C | -4.814513 | 0.961265 | -0.040995 |
| C | -3.516583 | 0.703053 | -0.480054 |
| F | -2.617267 | -2.075155 | 1.648383 |
| F | -5.113477 | -1.603552 | 2.515202 |
| F | -6.619693 | 0.395343 | 1.397547 |
| F | -5.543185 | 1.952336 | -0.585644 |
| F | -3.046900 | 1.517718 | -1.453413 |
| F | 1.454967 | -1.813668 | -0.317950 |
| F | 3.541950 | -0.857328 | 1.035296 |
| F | 3.238552 | 1.301473 | 2.720223 |
| F | 0.797665 | 2.496041 | 2.946543 |
| F | -1.269174 | 1.675526 | 1.448996 |
| C | -0.968410 | -0.325382 | -2.074291 |
| C | -1.675132 | -1.011633 | -3.062107 |
| C | -1.497857 | -0.831276 | -4.423966 |
| C | -0.562488 | 0.067960 | -4.949980 |
| C | 0.149999 | 0.770554 | -3.974476 |
| C | -0.060218 | 0.592466 | -2.605522 |
| F | -2.602469 | -1.957679 | -2.687556 |
| F | 0.681036 | 1.379264 | -1.789703 |
| F | 1.101727 | 1.665139 | -4.330884 |
| P | -0.322266 | 0.076423 | -6.797338 |
| C | 0.870324 | 1.467472 | -7.122073 |
| F | -2.250967 | -1.584594 | -5.272452 |
| C | -1.904727 | 0.924460 | -7.309517 |
| C | -6.042485 | -4.438488 | 0.479849 |
| C | -4.653763 | -4.467350 | 0.623898 |
| C | -3.841312 | -4.872663 | -0.439838 |
| C | -4.441852 | -5.257873 | -1.648066 |
| C | -5.827692 | -5.219613 | -1.796926 |
| C | -6.631527 | -4.808522 | -0.730959 |
| C | -2.344525 | -4.963941 | -0.242042 |
| N | -1.568882 | -4.297427 | -1.366474 |
| C | -0.271118 | -4.967669 | -1.865697 |
| C | 0.745980 | -4.960833 | -0.720307 |
| C | -0.596286 | -6.385700 | -2.351875 |
| C | 0.220629 | -4.105409 | -3.035850 |
| H | -2.761436 | 0.276538 | -7.103667 |
| H | -2.048524 | 1.883992 | -6.800251 |
| H | -1.863843 | 1.099235 | -8.390962 |
| H | 0.914738 | 1.577797 | -8.212427 |
| H | 0.573678 | 2.424058 | -6.683178 |
| H | 1.872973 | 1.210318 | -6.770224 |
| H | -1.356008 | -3.316001 | -1.073589 |
| H | 0.291319 | -6.796746 | -2.841473 |
| H | -0.862718 | -7.069159 | -1.540580 |
| H | -1.405625 | -6.387192 | -3.091971 |
| H | 1.620591 | -5.544808 | -1.023015 |
| H | 1.080454 | -3.940272 | -0.514456 |
| H | 0.350034 | -5.411861 | 0.194966 |
| H | 1.165512 | -4.513787 | -3.406778 |
| H | -0.491922 | -4.103541 | -3.869461 |

| | | | |
|---|---|---|---|
| H | 0.401220 | -3.071701 | -2.725997 |
| H | -4.204635 | -4.155127 | 1.562162 |
| H | -6.658050 | -4.108933 | 1.311635 |
| H | -7.710905 | -4.774418 | -0.846470 |
| H | -6.276613 | -5.512584 | -2.742325 |
| H | -3.839434 | -5.611864 | -2.483363 |
| H | -2.022655 | -6.005436 | -0.194320 |
| H | -2.043817 | -4.470852 | 0.682949 |
| H | -1.124297 | -1.902321 | -0.402341 |
| H | -2.193044 | -4.173679 | -2.170452 |

## $C_b$

E = -3249.767182

| | | | |
|---|---|---|---|
| C | -0.154023 | 1.030433 | 1.666178 |
| C | -0.315404 | 0.285818 | 0.486308 |
| C | 0.687931 | -0.665398 | 0.236190 |
| C | 1.763014 | -0.879139 | 1.092649 |
| C | 1.880317 | -0.107896 | 2.247195 |
| C | 0.918426 | 0.859940 | 2.533178 |
| B | -1.514263 | 0.515544 | -0.499892 |
| C | -2.944285 | 0.845972 | 0.050585 |
| C | -3.442808 | 0.261477 | 1.226399 |
| C | -4.671186 | 0.595472 | 1.780076 |
| C | -5.451319 | 1.575284 | 1.166607 |
| C | -5.010422 | 2.178688 | -0.007961 |
| C | -3.786396 | 1.796863 | -0.552784 |
| F | -2.720945 | -0.679104 | 1.863440 |
| F | -5.110666 | 0.002063 | 2.895484 |
| F | -6.612847 | 1.938832 | 1.709856 |
| F | -5.765458 | 3.123630 | -0.584171 |
| F | -3.398477 | 2.433491 | -1.673355 |
| F | 0.618859 | -1.454138 | -0.851770 |
| F | 2.678419 | -1.819245 | 0.824395 |
| F | 2.905146 | -0.300176 | 3.078242 |
| F | 1.034406 | 1.610593 | 3.635432 |
| F | -1.048066 | 1.982680 | 1.991822 |
| C | -1.250895 | 0.432784 | -2.050348 |
| C | -1.810708 | -0.537949 | -2.878463 |
| C | -1.542519 | -0.591698 | -4.241762 |
| C | -0.728284 | 0.342038 | -4.900147 |
| C | -0.207208 | 1.338418 | -4.068616 |
| C | -0.431722 | 1.359050 | -2.695645 |
| F | -2.585269 | -1.520760 | -2.355787 |
| F | 0.132252 | 2.353562 | -1.967001 |
| F | 0.545461 | 2.336378 | -4.579536 |
| P | -0.456724 | 0.029034 | -6.730927 |
| C | 1.353089 | 0.528471 | -7.142485 |
| F | -2.103685 | -1.601036 | -4.935104 |
| C | -1.715024 | 1.250782 | -7.505032 |
| C | -5.972267 | -4.260756 | 1.200576 |
| C | -4.836294 | -4.879367 | 0.671734 |
| C | -4.727178 | -5.136310 | -0.701163 |
| C | -5.779381 | -4.746605 | -1.543108 |
| C | -6.912696 | -4.122907 | -1.016454 |
| C | -7.016073 | -3.878432 | 0.355652 |
| C | -3.489878 | -5.825307 | -1.250318 |
| N | -3.144763 | -5.308543 | -2.573918 |
| C | -2.022566 | -5.938553 | -3.309850 |
| C | -0.685848 | -5.880613 | -2.535123 |
| C | -2.374105 | -7.401533 | -3.632749 |
| C | -1.882945 | -5.162408 | -4.629704 |
| C | -3.106364 | 0.651084 | -7.205895 |
| C | -1.680016 | 2.699922 | -6.991813 |
| C | -1.509822 | 1.230650 | -9.034143 |
| C | 1.665377 | -0.280425 | -8.427968 |
| C | 1.706893 | 2.001524 | -7.413562 |
| C | 2.255059 | -0.020406 | -6.019565 |
| H | -2.988486 | -4.300946 | -2.502988 |
| H | -1.609123 | -7.836171 | -4.286723 |
| H | -2.425182 | -8.026683 | -2.734212 |
| H | -3.340638 | -7.455885 | -4.145796 |
| H | 0.130550 | -6.308956 | -3.129776 |
| H | -0.418422 | -4.842734 | -2.297847 |
| H | -0.736517 | -6.440537 | -1.594135 |

| | | | |
|---|---|---|---|
| H | -1.056442 | -5.558070 | -5.231217 |
| H | -2.806815 | -5.233594 | -5.214116 |
| H | -1.684415 | -4.101353 | -4.444687 |
| H | -4.021254 | -5.164010 | 1.334860 |
| H | -6.035912 | -4.068884 | 2.268851 |
| H | -7.900436 | -3.393263 | 0.761546 |
| H | -7.720858 | -3.826519 | -1.681503 |
| H | -5.691681 | -4.929403 | -2.610035 |
| H | -3.696751 | -6.898139 | -1.352552 |
| H | -2.679189 | -5.735803 | -0.505182 |
| H | -2.456402 | 3.286134 | -7.503679 |
| H | -1.887669 | 2.754272 | -5.918321 |
| H | -0.721204 | 3.189449 | -7.174864 |
| H | -2.322914 | 1.789510 | -9.516470 |
| H | -0.569660 | 1.701057 | -9.337187 |
| H | -1.527305 | 0.209888 | -9.433804 |
| H | -3.875072 | 1.253294 | -7.708741 |
| H | -3.193633 | -0.379474 | -7.565805 |
| H | -3.336253 | 0.657132 | -6.134802 |
| H | 2.711506 | -0.111823 | -8.717238 |
| H | 1.524340 | -1.355421 | -8.274138 |
| H | 1.039114 | 0.022692 | -9.273469 |
| H | 2.779739 | 2.070692 | -7.643535 |
| H | 1.170786 | 2.399924 | -8.280534 |
| H | 1.511674 | 2.648463 | -6.558712 |
| H | 3.300814 | -0.004151 | -6.355604 |
| H | 2.194258 | 0.580241 | -5.108118 |
| H | 2.009788 | -1.059377 | -5.767421 |

## $B2_b$

E = -3249.752899

| | | | |
|---|---|---|---|
| C | -4.207165 | -5.388087 | 1.101704 |
| C | -3.891197 | -4.722001 | -0.102216 |
| C | -4.582664 | -3.540508 | -0.447828 |
| C | -5.559999 | -3.042934 | 0.403115 |
| C | -5.847052 | -3.695741 | 1.607907 |
| C | -5.170634 | -4.868572 | 1.958464 |
| C | -2.870628 | -5.318041 | -0.930612 |
| N | -2.290171 | -4.773757 | -1.955275 |
| C | -1.309932 | -5.396806 | -2.907236 |
| C | -0.989086 | -6.836757 | -2.503179 |
| C | -1.978411 | -5.357078 | -4.295815 |
| C | -0.043502 | -4.523662 | -2.879254 |
| F | -2.755967 | -2.206965 | -3.024012 |
| C | -1.913651 | -1.125569 | -3.261909 |
| C | -1.537430 | -0.298501 | -2.212386 |
| C | -0.699279 | 0.739486 | -2.626641 |
| C | -0.311355 | 0.939345 | -3.948062 |
| C | -0.710186 | 0.103427 | -4.998602 |
| C | -1.531383 | -0.953558 | -4.587447 |
| B | -2.060184 | -0.520357 | -0.673343 |
| C | -3.383266 | 0.380592 | -0.301339 |
| C | -4.045803 | 0.145301 | 0.907777 |
| C | -5.188692 | 0.822915 | 1.321922 |
| C | -5.733567 | 1.808714 | 0.503620 |
| C | -5.118759 | 2.082744 | -0.711618 |
| C | -3.977669 | 1.372560 | -1.084829 |
| F | -0.266855 | 1.646168 | -1.721057 |
| F | 0.478727 | 2.008850 | -4.199919 |
| P | -0.329677 | 0.220586 | -6.824918 |
| C | -1.481388 | 1.662524 | -7.363631 |
| F | -1.995564 | -1.858299 | -5.488736 |
| F | -3.569138 | -0.798796 | 1.760022 |
| F | -5.779605 | 0.527291 | 2.498952 |
| F | -6.838507 | 2.477064 | 0.877805 |
| F | -5.629202 | 3.029625 | -1.521201 |
| F | -3.459151 | 1.713922 | -2.290553 |
| C | -0.835084 | -0.328565 | 0.401065 |
| C | 0.044594 | -1.378085 | 0.670626 |
| C | 1.116090 | -1.293933 | 1.555547 |
| C | 1.356880 | -0.097969 | 2.222681 |
| C | 0.501211 | 0.977055 | 2.005998 |
| C | -0.561667 | 0.841124 | 1.115252 |
| F | -0.107687 | -2.582042 | 0.044682 |
| F | 1.920453 | -2.356191 | 1.771562 |
| F | 2.404990 | 0.019340 | 3.056609 |

| | | | |
|---|---|---|---|
| F | 0.716456 | 2.138721 | 2.650142 |
| F | -1.341634 | 1.934817 | 0.958876 |
| C | 1.534437 | 0.682723 | -6.996317 |
| H | -2.557637 | -6.327246 | -0.679456 |
| C | -2.912699 | 1.088963 | -7.257267 |
| C | -1.415456 | 2.965937 | -6.548576 |
| C | -1.195732 | 1.960853 | -8.850539 |
| C | 1.916639 | 0.165046 | -8.405615 |
| C | 1.965521 | 2.156663 | -6.891904 |
| C | 2.310015 | -0.158671 | -5.961870 |
| H | -2.502798 | -3.794707 | -2.178254 |
| H | -0.277452 | -7.243960 | -3.227062 |
| H | -0.518426 | -6.895854 | -1.515259 |
| H | -1.875385 | -7.481821 | -2.521728 |
| H | 0.679974 | -4.917804 | -3.600068 |
| H | -0.263723 | -3.488642 | -3.156258 |
| H | 0.414692 | -4.519834 | -1.885682 |
| H | -1.284353 | -5.758853 | -5.041135 |
| H | -2.889875 | -5.965022 | -4.311081 |
| H | -2.231109 | -4.334714 | -4.591639 |
| H | -2.412635 | -1.677256 | -0.581418 |
| H | -3.680320 | -6.302060 | 1.365460 |
| H | -5.396607 | -5.372758 | 2.892980 |
| H | -6.600003 | -3.285176 | 2.274570 |
| H | -6.089948 | -2.134127 | 0.137576 |
| H | -4.366470 | -3.013998 | -1.370684 |
| H | -2.134476 | 3.686873 | -6.963618 |
| H | -1.687328 | 2.805266 | -5.501241 |
| H | -0.427575 | 3.430671 | -6.574860 |
| H | -3.628822 | 1.830424 | -7.637291 |
| H | -3.029531 | 0.171439 | -7.844631 |
| H | -3.190294 | 0.869968 | -6.220563 |
| H | -1.960978 | 2.648972 | -9.234773 |
| H | -0.223911 | 2.441162 | -9.001124 |
| H | -1.229545 | 1.051973 | -9.463081 |
| H | 3.054313 | 2.218239 | -7.033167 |
| H | 1.508428 | 2.773992 | -7.671621 |
| H | 1.731591 | 2.595691 | -5.922274 |
| H | 3.383023 | -0.118463 | -6.194336 |
| H | 2.178030 | 0.213906 | -4.942424 |
| H | 2.007361 | -1.213153 | -5.985911 |
| H | 2.991680 | 0.319878 | -8.571442 |
| H | 1.705252 | -0.904262 | -8.514067 |
| H | 1.382296 | 0.694031 | -9.201874 |

## $TS2_b$

Negative eigenvalue: -70 cm-1
E = -3249.739119

| | | | |
|---|---|---|---|
| C | -0.039583 | -0.153405 | 0.194340 |
| C | -0.118321 | -0.008558 | 1.584496 |
| C | 1.115504 | -0.119766 | 2.240775 |
| C | 2.329292 | -0.323920 | 1.594420 |
| C | 2.352195 | -0.436548 | 0.207579 |
| C | 1.154710 | -0.356389 | -0.494947 |
| B | -1.468633 | 0.224683 | 2.446521 |
| C | -2.854823 | 0.555387 | 1.669820 |
| C | -4.052868 | -0.153709 | 1.844275 |
| C | -5.246012 | 0.170189 | 1.197797 |
| C | -5.289104 | 1.251456 | 0.325102 |
| C | -4.127723 | 1.986662 | 0.109217 |
| C | -2.962046 | 1.625325 | 0.773580 |
| F | -4.114433 | -1.229456 | 2.657567 |
| F | -6.356111 | -0.553278 | 1.414673 |
| F | -6.430290 | 1.585687 | -0.291528 |
| F | -4.145053 | 3.043453 | -0.723496 |
| F | -1.868935 | 2.385418 | 0.503688 |
| F | 1.168808 | -0.041577 | 3.592984 |
| F | 3.473331 | -0.412329 | 2.294864 |
| F | 3.511068 | -0.622163 | -0.441220 |
| F | 1.157696 | -0.479754 | -1.833238 |
| F | -1.155828 | -0.133437 | -0.567920 |
| C | -1.589886 | -0.789391 | 3.709513 |
| C | -2.042188 | -0.429877 | 4.974852 |
| C | -2.115955 | -1.301706 | 6.055764 |
| C | -1.754132 | -2.652478 | 5.960509 |
| C | -1.331401 | -3.031829 | 4.681320 |

| | | | |
|---|---|---|---|
| C | -1.248975 | -2.142412 | 3.613510 |
| F | -2.450540 | 0.853902 | 5.202640 |
| F | -0.840263 | -2.651964 | 2.423792 |
| F | -0.969722 | -4.312411 | 4.431676 |
| P | -1.855715 | -3.658688 | 7.543579 |
| C | -3.440110 | -4.711911 | 7.253228 |
| F | -2.561667 | -0.789829 | 7.225541 |
| C | -0.262305 | -4.748984 | 7.628127 |
| N | -1.861165 | 3.734749 | 3.221828 |
| C | -3.020392 | 4.171171 | 4.052342 |
| C | -4.258573 | 3.290559 | 3.799113 |
| C | -0.886460 | 2.843214 | 3.526584 |
| C | 0.490619 | 3.082445 | 2.994869 |
| C | 0.745807 | 3.557631 | 1.698314 |
| C | 2.050964 | 3.841013 | 1.297842 |
| C | 3.117946 | 3.657488 | 2.183506 |
| C | 2.872664 | 3.184418 | 3.474156 |
| C | 1.567453 | 2.892724 | 3.874111 |
| C | -2.646164 | 4.156850 | 5.543872 |
| C | -3.312479 | 5.618101 | 3.612042 |
| H | -1.805040 | 4.170514 | 2.309096 |
| C | -4.602342 | -3.694373 | 7.311239 |
| C | -3.537010 | -5.498159 | 5.935214 |
| C | -3.582612 | -5.672895 | 8.452253 |
| C | -0.085174 | -5.019274 | 9.143554 |
| C | -0.227846 | -6.097798 | 6.887174 |
| C | 0.921408 | -3.870958 | 7.169495 |
| H | -4.176814 | 6.008820 | 4.158612 |
| H | -2.455645 | 6.272253 | 3.809304 |
| H | -3.550807 | 5.668349 | 2.541554 |
| H | -3.459833 | 4.610037 | 6.119860 |
| H | -2.504586 | 3.144032 | 5.930506 |
| H | -1.736695 | 4.740667 | 5.727223 |
| H | -5.100782 | 3.650035 | 4.401950 |
| H | -4.557300 | 3.329182 | 2.746193 |
| H | -4.066547 | 2.249944 | 4.069367 |
| H | -1.196305 | 1.511581 | 3.012231 |
| H | -0.904389 | 2.521605 | 4.562696 |
| H | 1.384319 | 2.513806 | 4.876165 |
| H | 3.694707 | 3.032382 | 4.167903 |
| H | 4.133636 | 3.877172 | 1.865817 |
| H | 2.235340 | 4.200894 | 0.289148 |
| H | -0.062798 | 3.693827 | 0.987999 |
| H | -5.559099 | -4.230411 | 7.243005 |
| H | -4.599353 | -3.123841 | 8.246599 |
| H | -4.566291 | -2.982748 | 6.478700 |
| H | -4.498173 | -6.031934 | 5.901693 |
| H | -3.503130 | -4.836304 | 5.064417 |
| H | -2.742389 | -6.239848 | 5.827397 |
| H | -4.568876 | -6.155869 | 8.416207 |
| H | -2.830748 | -6.468587 | 8.441463 |
| H | -3.508586 | -5.143355 | 9.409674 |
| H | 1.864330 | -4.359325 | 7.451792 |
| H | 0.937638 | -3.727072 | 6.085719 |
| H | 0.908252 | -2.883352 | 7.647465 |
| H | 0.746145 | -6.576602 | 7.065204 |
| H | -0.993356 | -6.788857 | 7.254701 |
| H | -0.350224 | -5.987634 | 5.809386 |
| H | 0.847063 | -5.577433 | 9.307541 |
| H | -0.028259 | -4.087063 | 9.716017 |
| H | -0.903545 | -5.617612 | 9.558668 |