Electronic Supplementary Material (ESI) for Dalton Transactions


# Proposing Late Transition Metal Complexes as Frustrated Lewis Pairs - A Computational Investigation

## Electronic Supplementary Information

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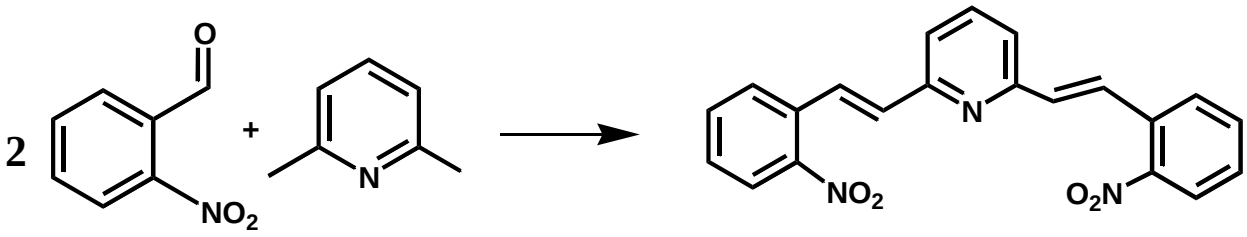
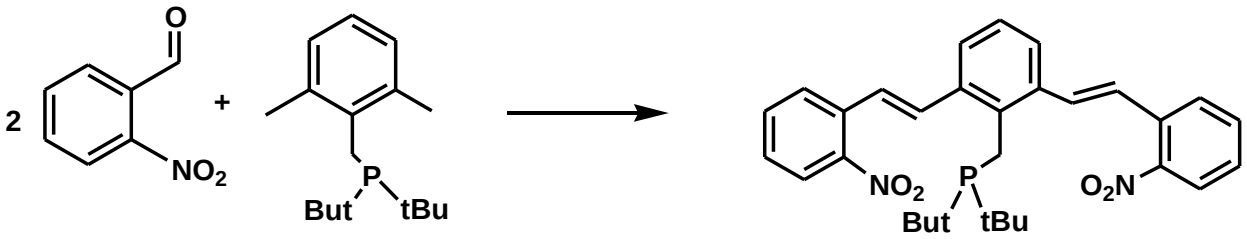
**Pune 411 008, India**

**I. Steps for formation of the proposed catalyst in compare to the existing Pd catalyst.**

**Step -1**

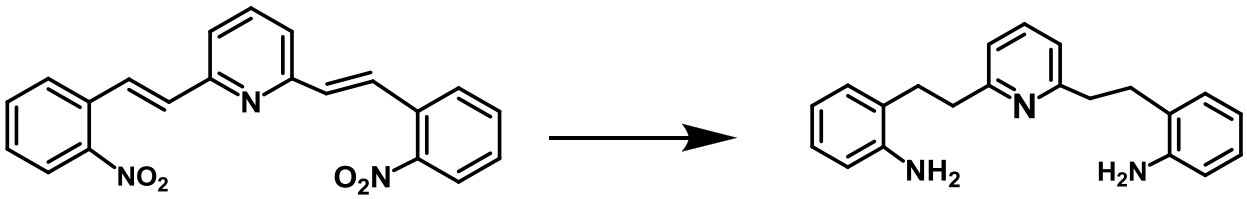



**ΔE= -10.8 kcal/mol.**

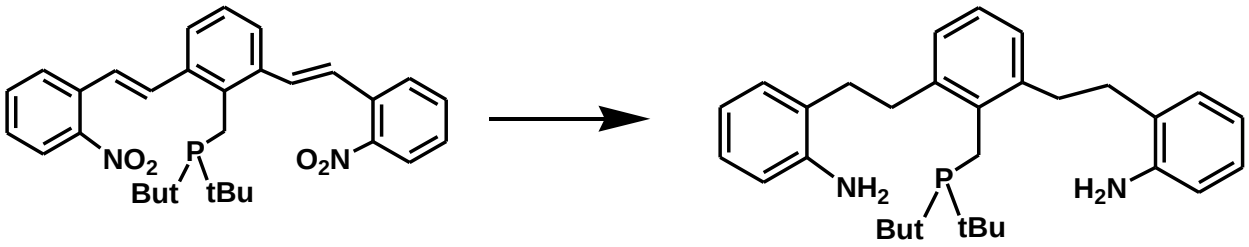



**ΔE= -9.8 kcal/mol.**

**Step -2**

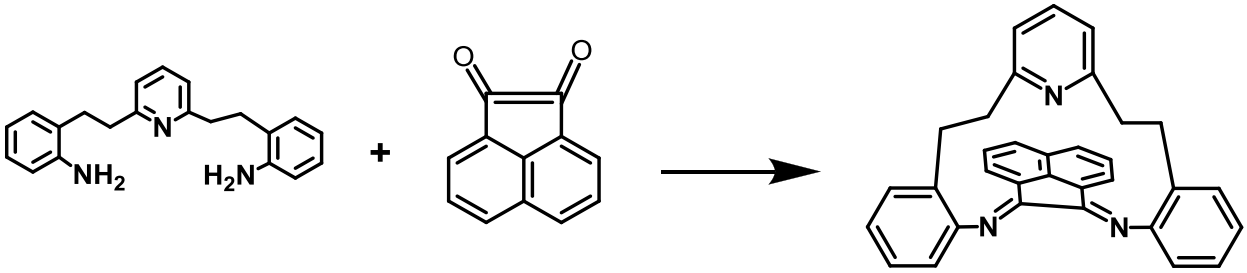



**ΔE= -1750.3 kcal/mol.**

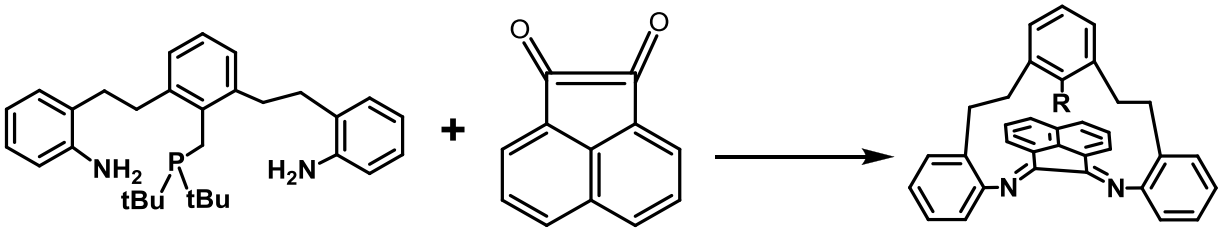



**ΔE= -1740.0 kcal/mol.**

**Step -3**

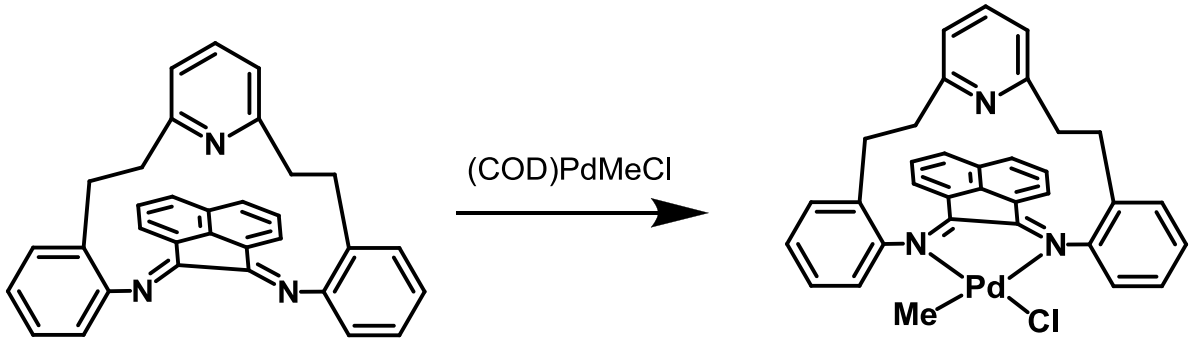



**ΔE= +21.8 kcal/mol.**

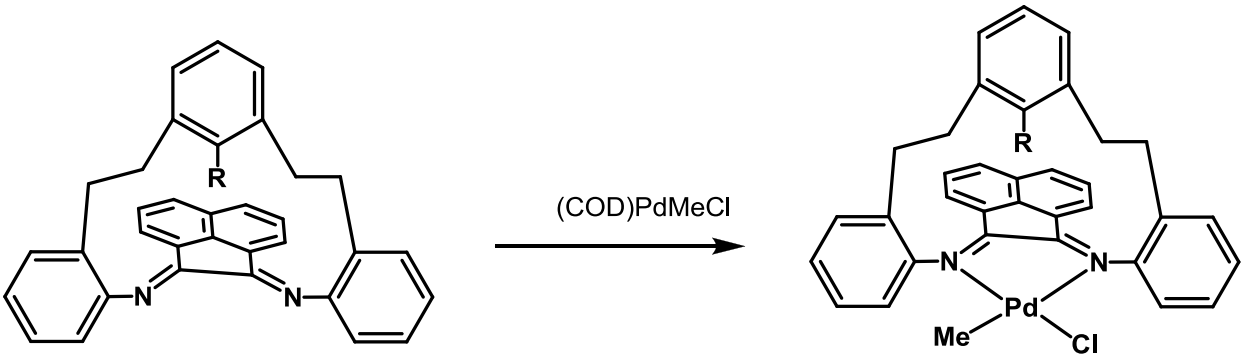



**ΔE= +22.1 kcal/mol.**

**Step -4**




**ΔE= -2.0 kcal/mol.**




**R=$CH_2P(tBU)_2$**

**ΔE= +5.0 kcal/mol.**

**Fig. S1** A comparison of the ΔE values for the corresponding steps leading to the formation of the existing palladium complex give formula here and the proposed palladium FLP complex respectively.

**II. The entropy (ΔG) values for all the reaction pathways in optimized 3D structure.**

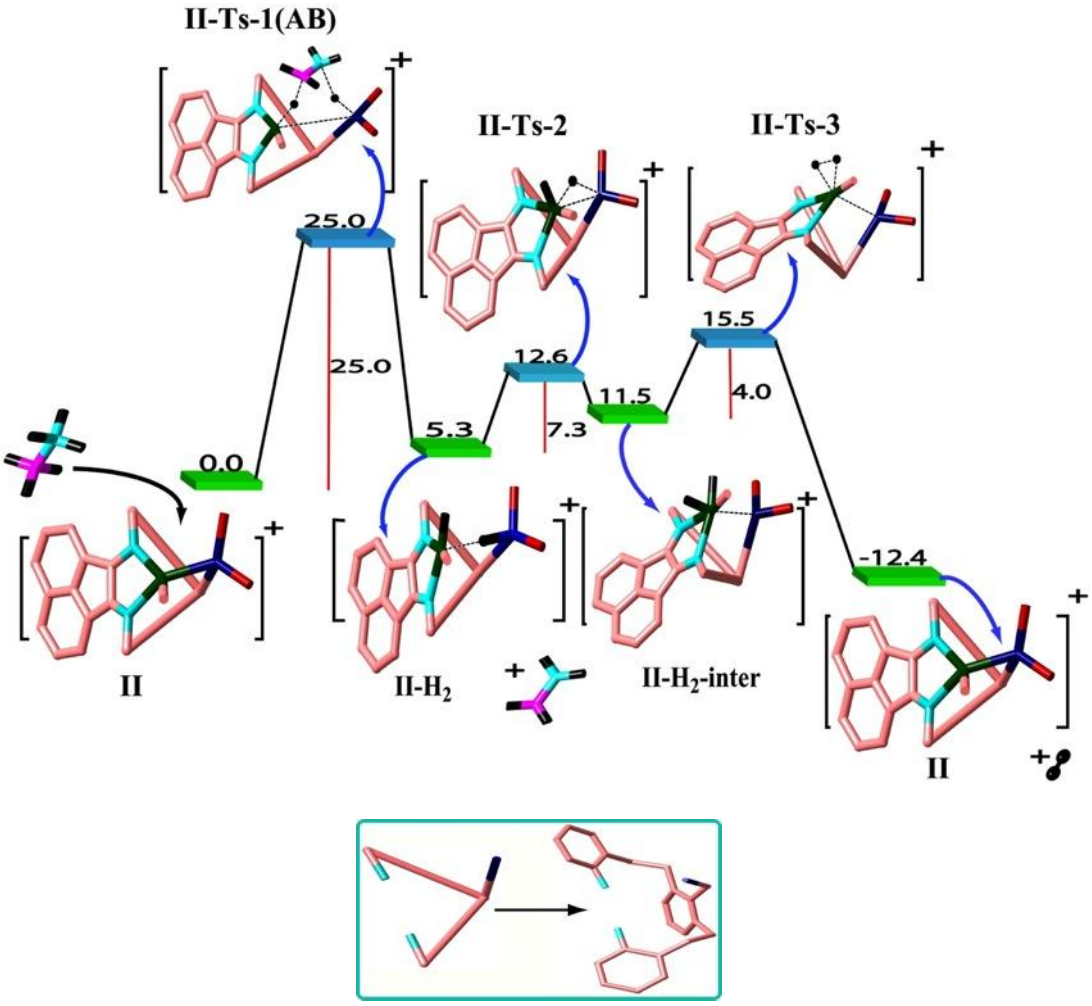



**Fig. S2** The free energy surface for the catalysis of the dehydrogenation of ammonia borane (AB) using the proposed palladium based FLP; all the structures shown are the optimized geometries obtained from the DFT/MP2 calculations; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1 and boron – magenta; all the values are in kcal/mol.

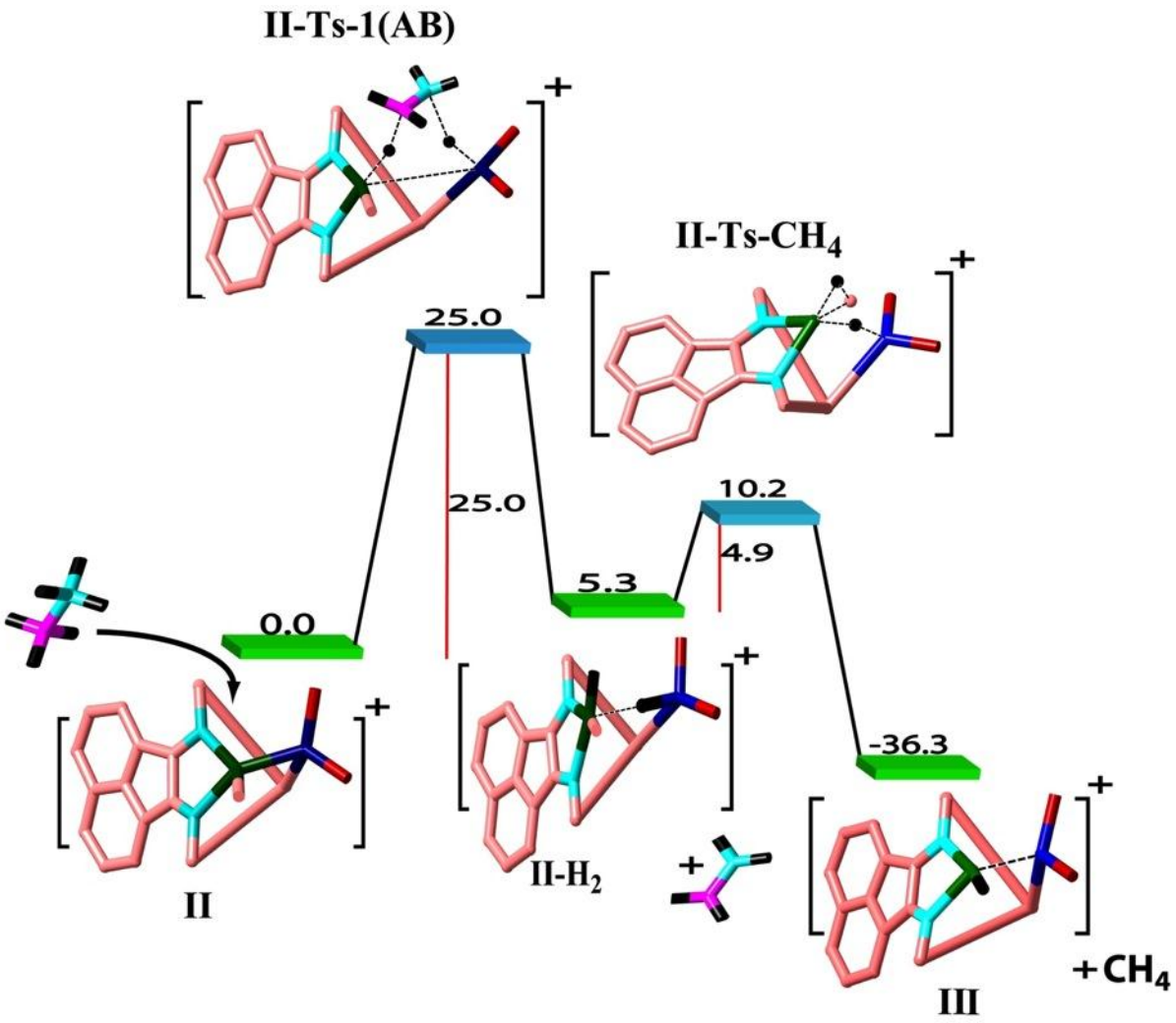



**Fig. S3** The free energy surface showing the possibility of dehydrogenation of ammonia borane followed by a reductive elimination step leading to the loss of methane from the palladium complex; all the structures shown are the optimized geometries obtained from the DFT/MP2 calculations; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

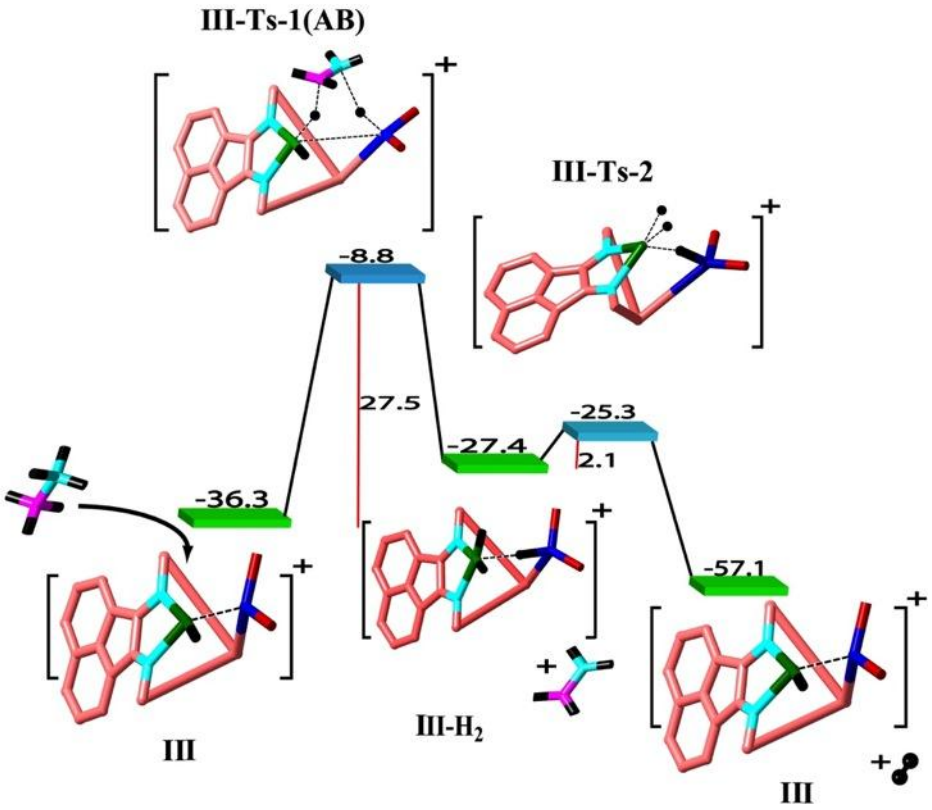



**Fig. S4** The free energy surface for the catalysis of the dehydrogenation of ammonia borane (AB) using FLP (**III**) formed during the catalysis; all the structures shown are the optimized geometries obtained from the DFT/MP2 calculations; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

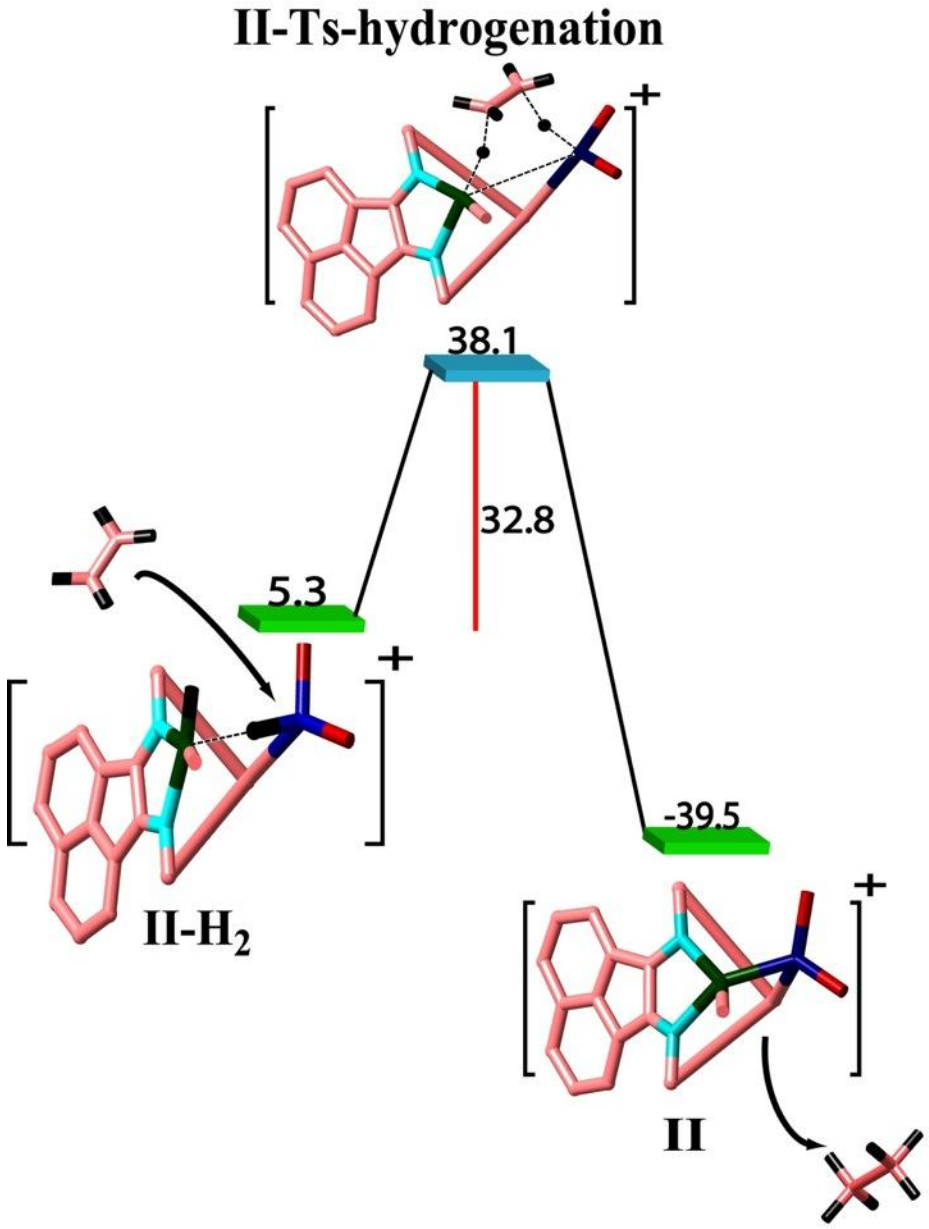



**Fig. S5** The free energy surface for the hydrogenation of ethylene with the hydrated palladium based FLP-**II-$H_2$**; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

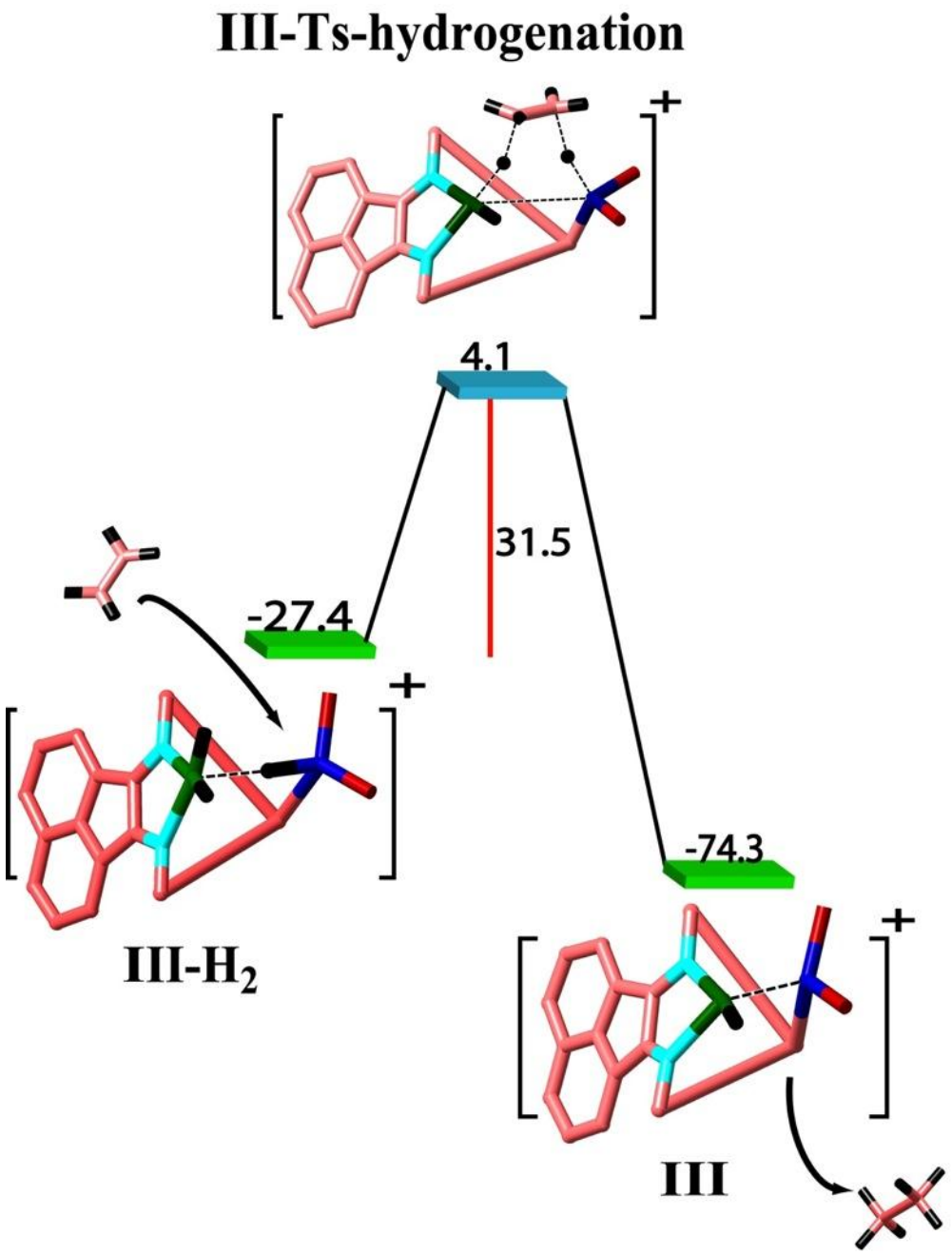



**Fig. S6** The free energy surface for the hydrogenation of ethylene with the hydrated palladium based FLP-**III-$H_2$** formed during the catalysis; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

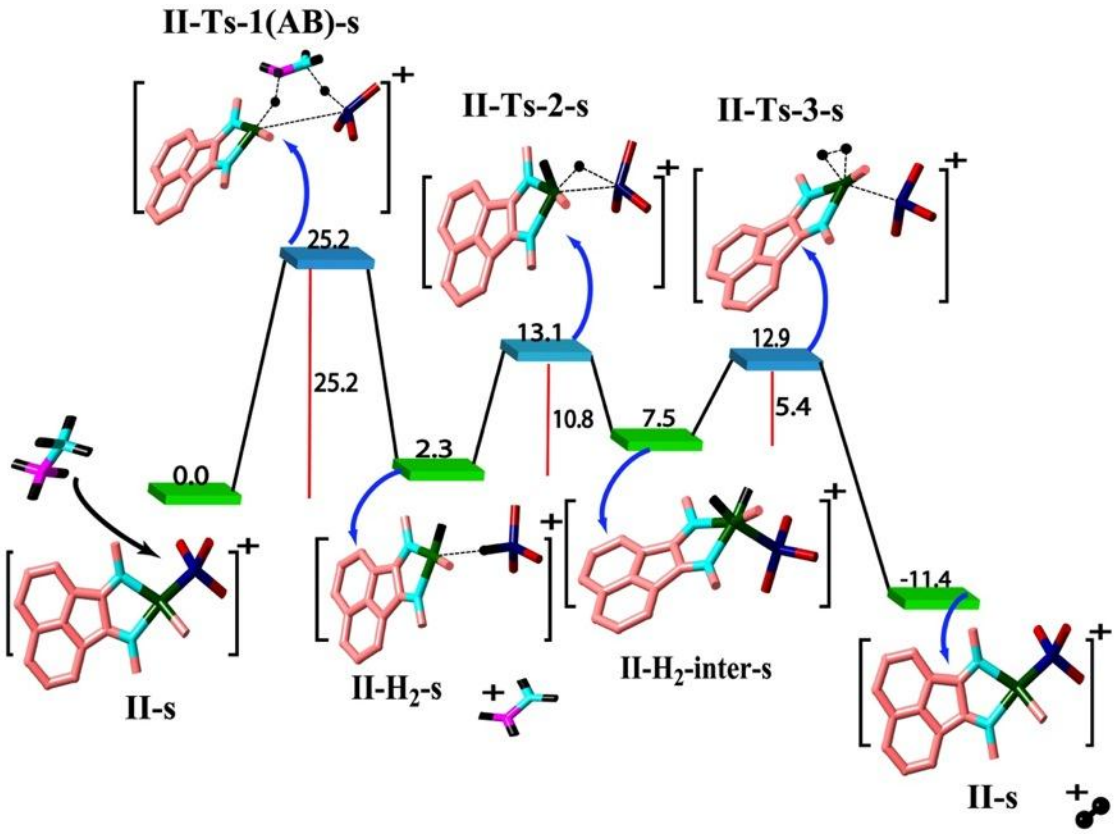



**Fig. S7** A simpler palladium based FLP system: no linkage between the phosphorus and the diimine ligand; shown above is the free energy surface for the catalysis of the dehydrogenation of ammonia borane; the colour scheme is as follows: carbon – light brown, nitrogen – light blue, palladium – green, phosphorus – blue, boron – magenta, the tertiary butyl groups – red; all the values are in kcal/mol.

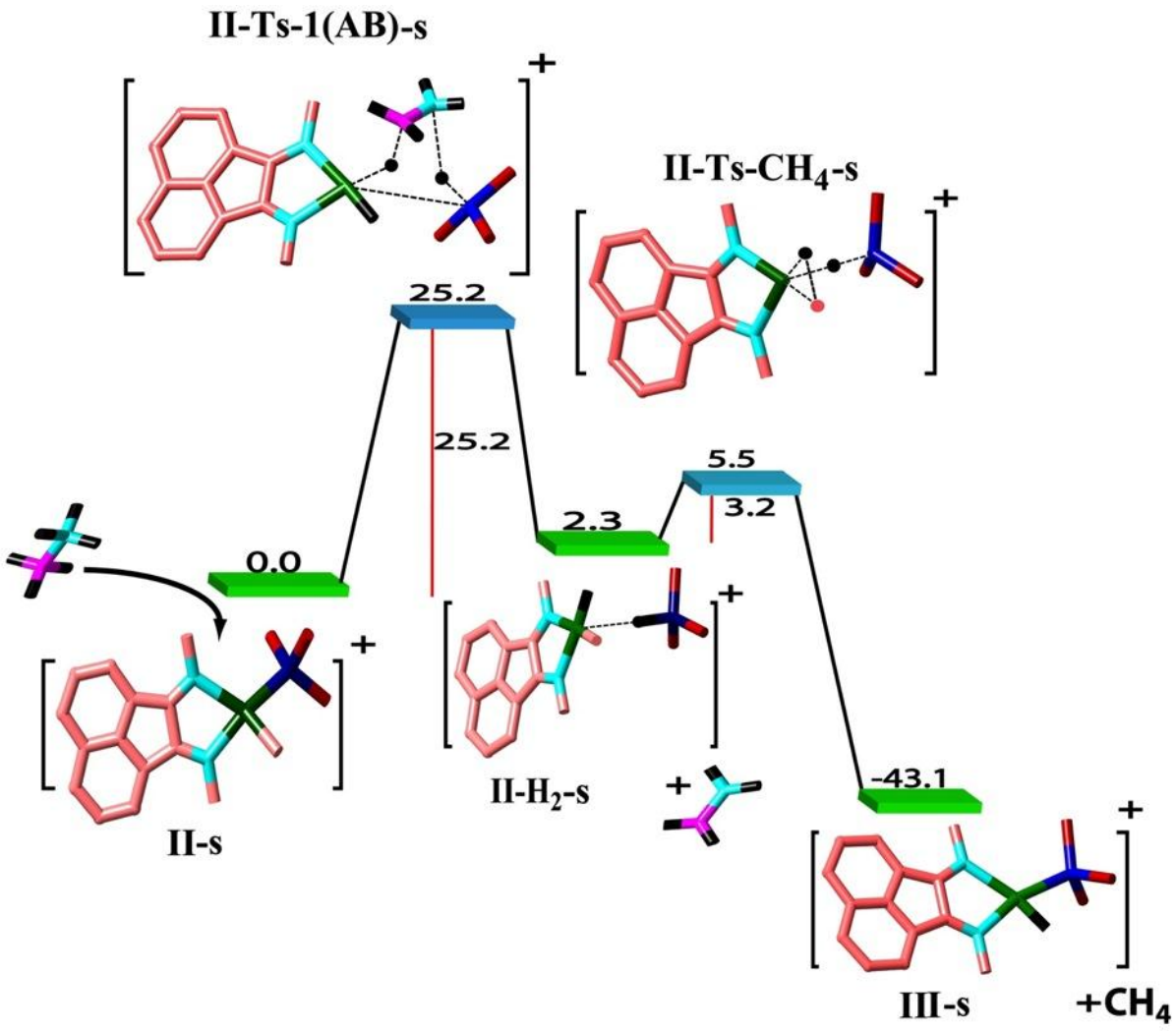



**Fig. S8** The free energy surface showing the possibility of dehydrogenation of ammonia borane followed by a reductive elimination step leading to the loss of methane from the simple palladium complex; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

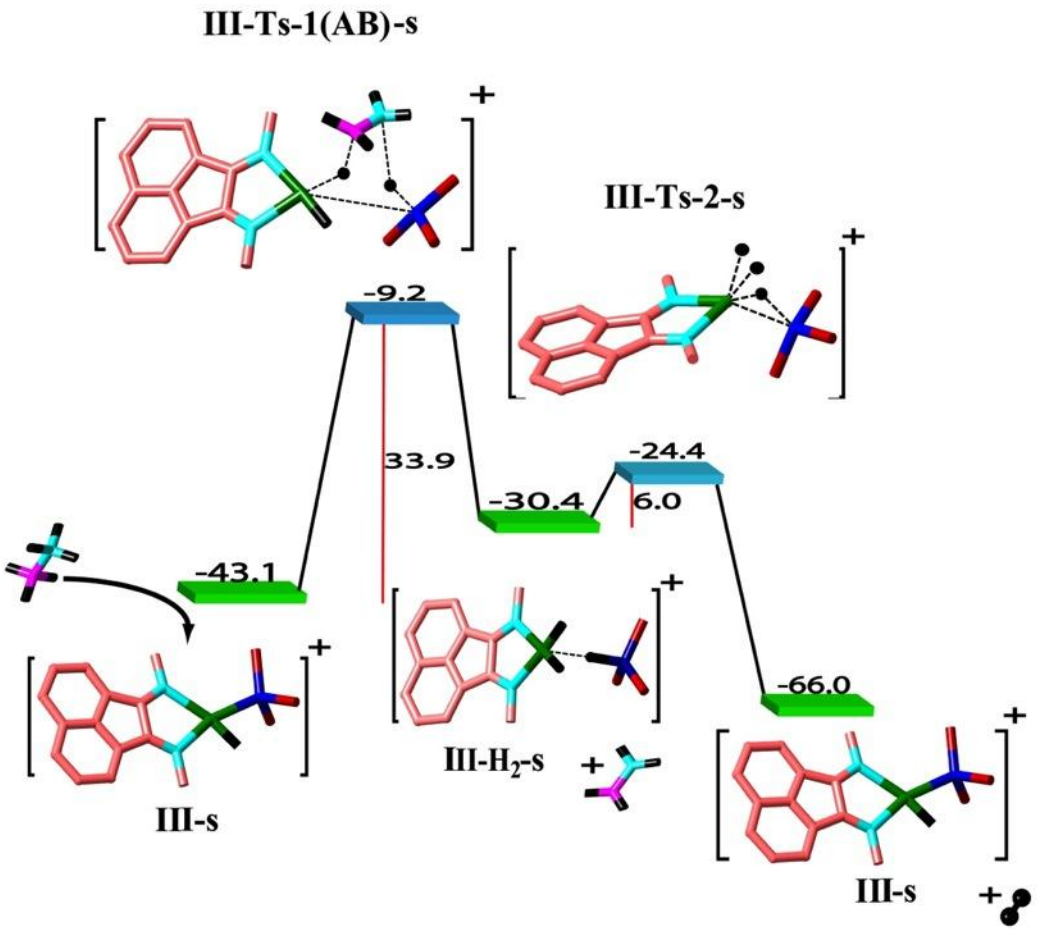



**Fig. S9** The free energy surface for the catalysis of the dehydrogenation of ammonia borane (AB) using FLP (**III-s**) formed during the catalysis; with the simple palladium based FLP; the colour scheme is as for Figure 3; all the values are in kcal/mol.

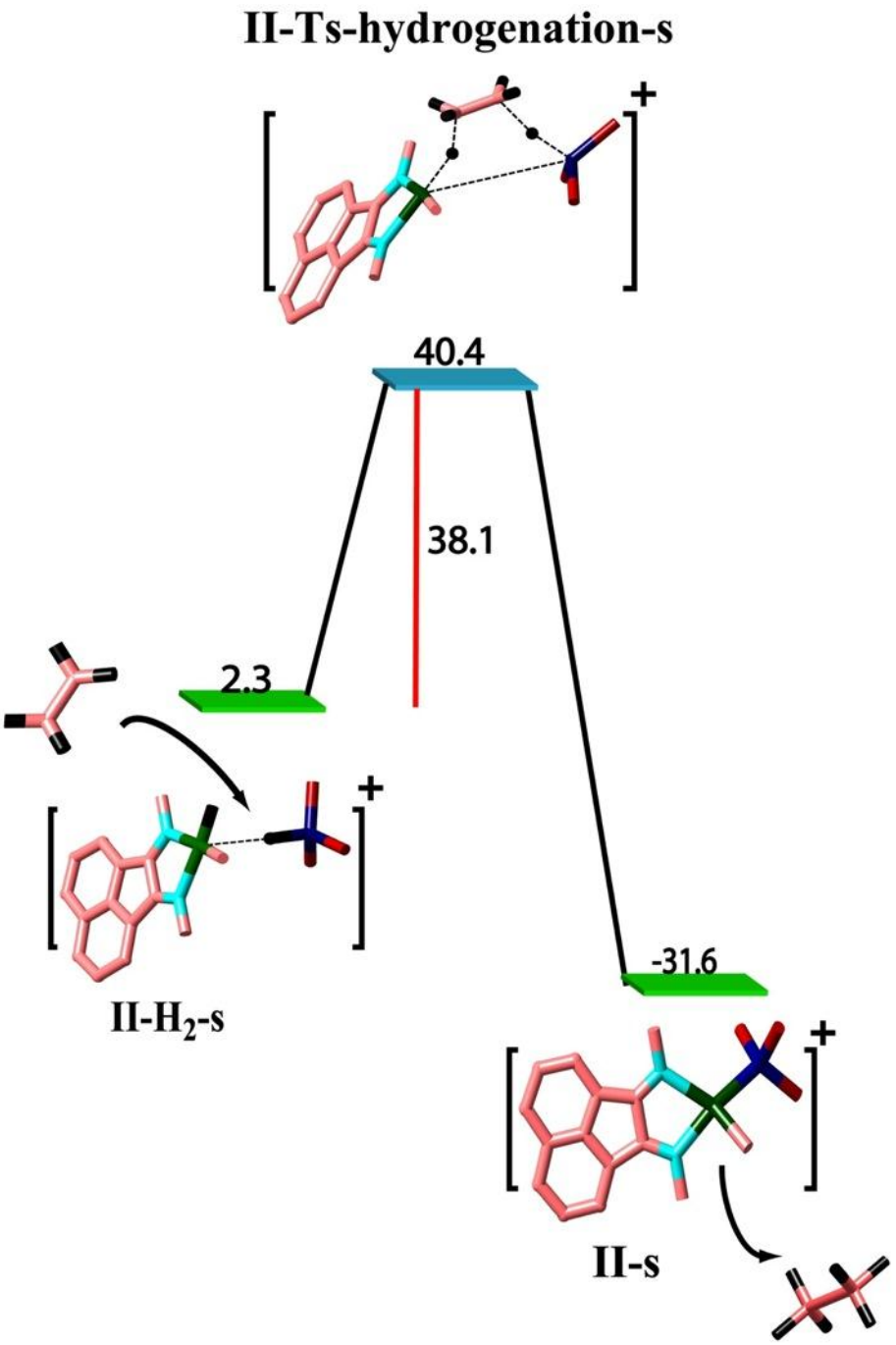



**Fig. S10** The free energy surface for the hydrogenation of ethylene to ethane with the hydrogenated simple palladium based FLP; the colour scheme is as for Figure 3; all the values are in kcal/mol.

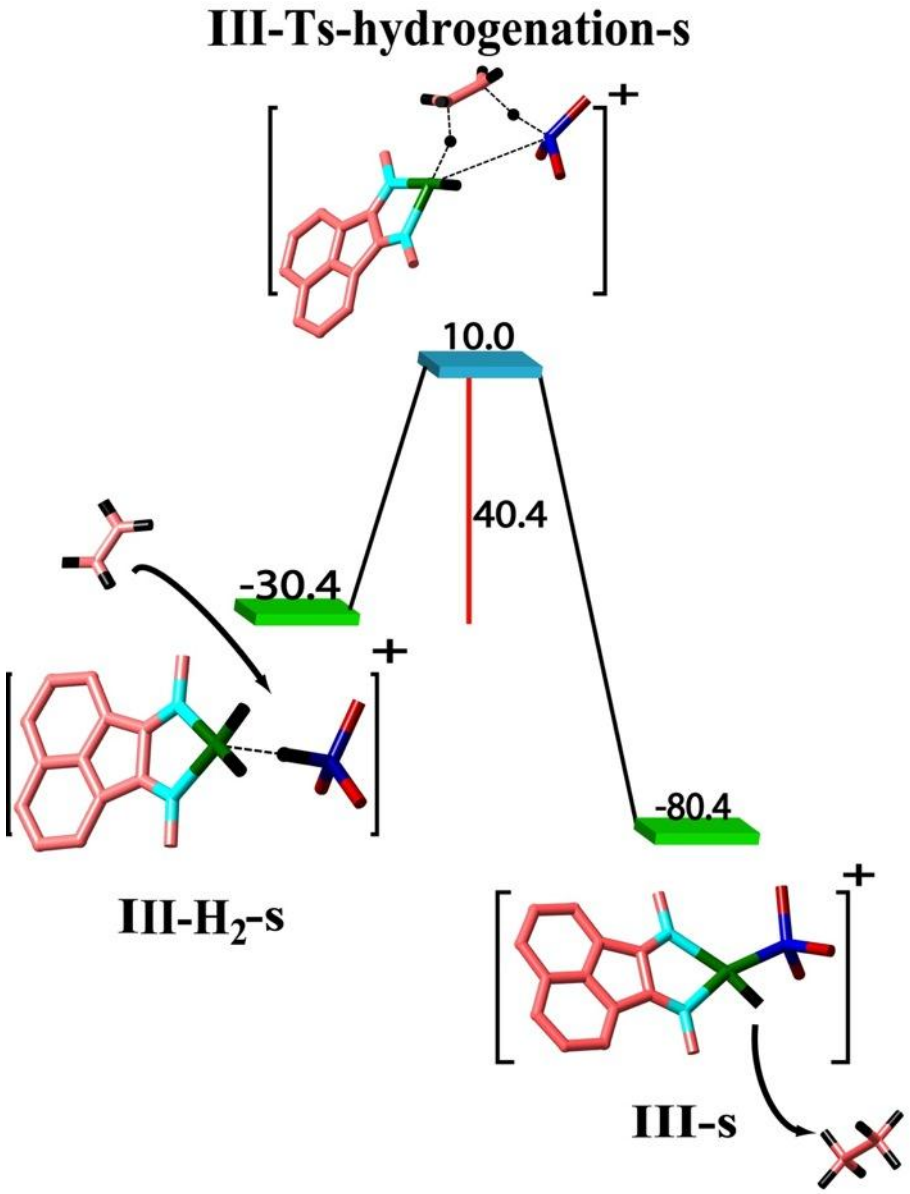



**Fig. S11** The free energy surface for the hydrogenation of ethylene with the hydrated simple palladium based FLP-**III-$H_2$-s** formed during the catalysis; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

**II. The enthalpy (ΔH) values for all the reaction pathways.**

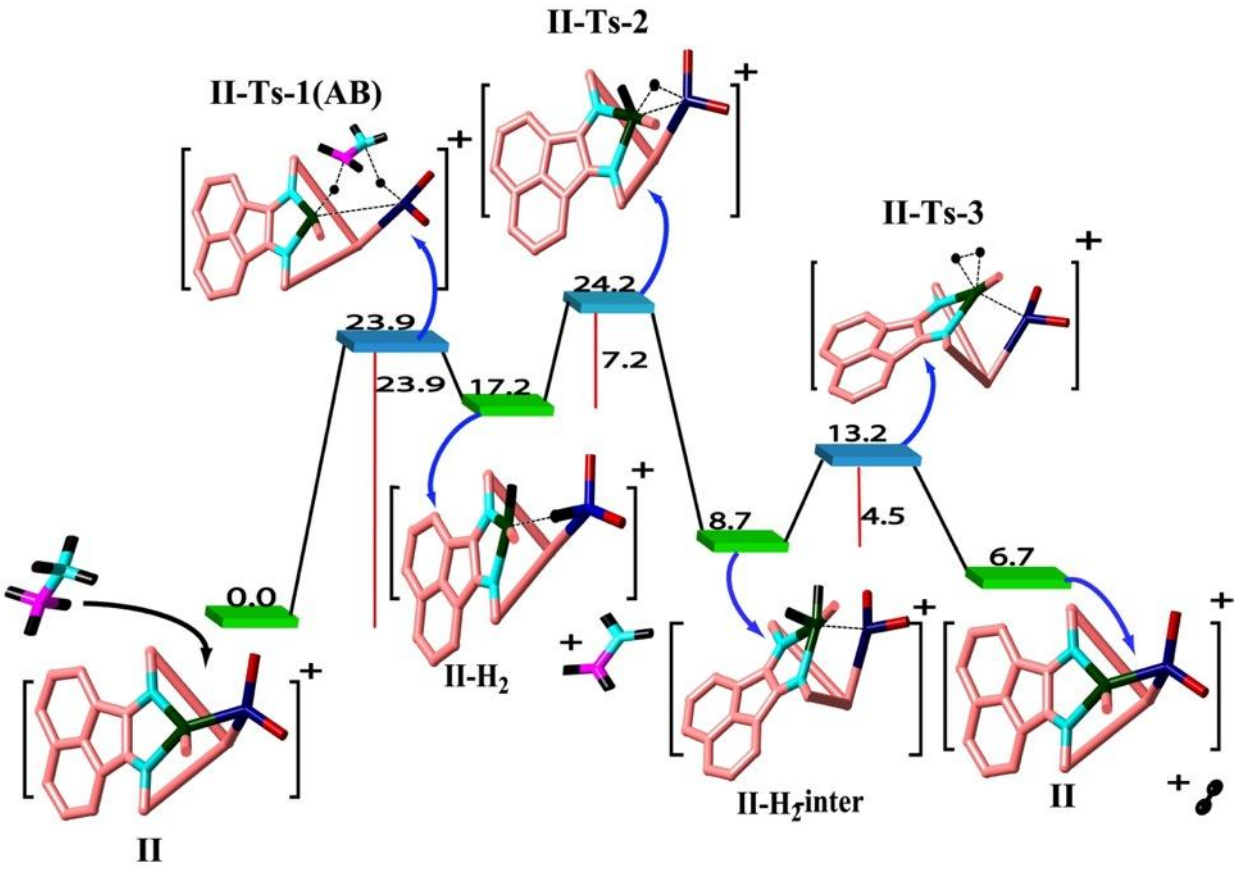



**Fig. S12a** The reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane (AB) using the proposed palladium based FLP; all the structures shown are the optimized geometries obtained from the DFT/MP2 calculations; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1and boron – magenta; all the values are in kcal/mol.

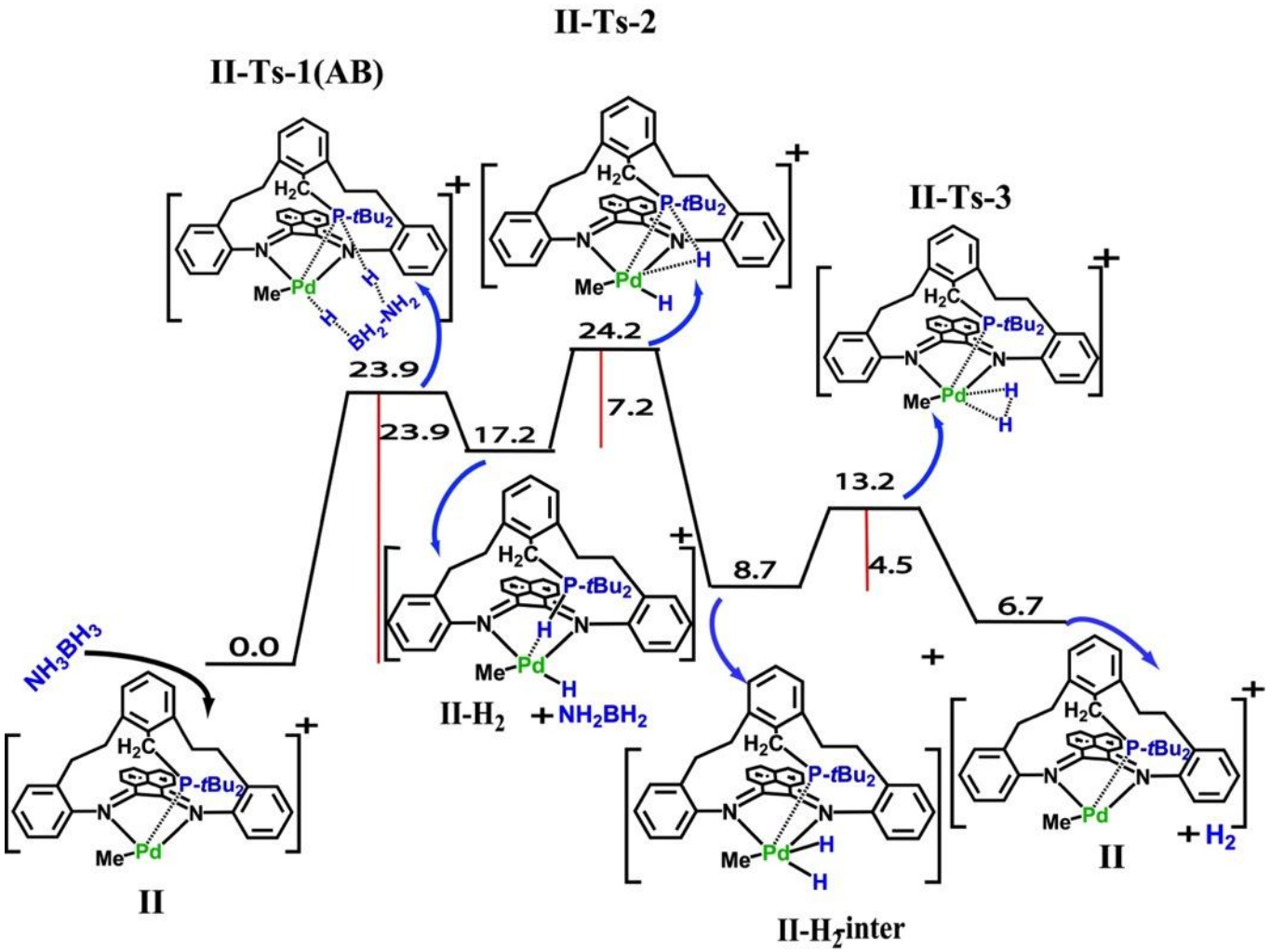



**Fig. S12b** The schematic representation of the reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane (AB) using the proposed palladium based FLP; all the values are in kcal/mol.

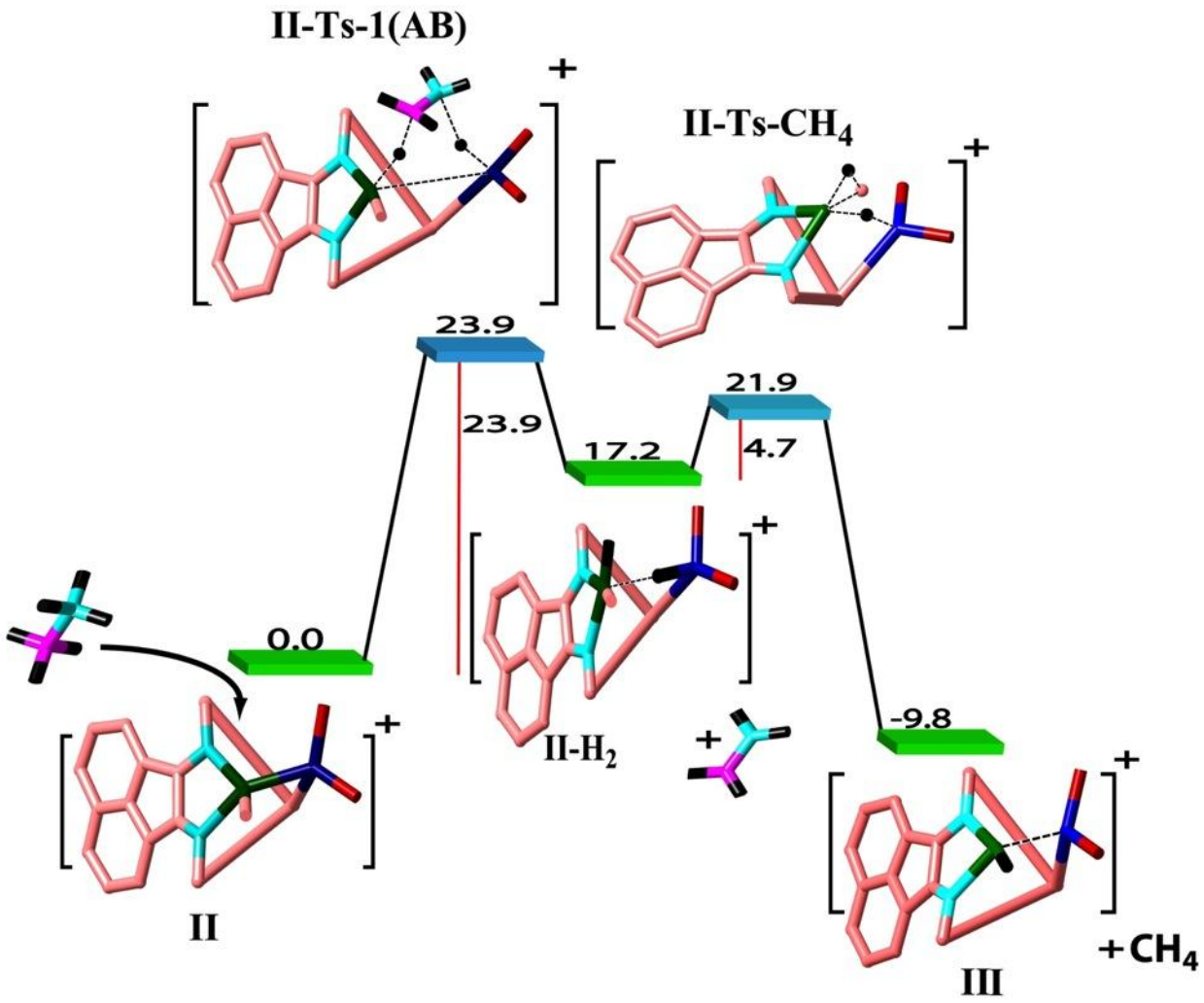



**Fig. S13a** The reaction enthalpy (ΔH) surface showing the possibility of dehydrogenation of ammonia borane followed by a reductive elimination step leading to the loss of methane from the palladium complex; all the structures shown are the optimized geometries obtained from the DFT/MP2 calculations; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

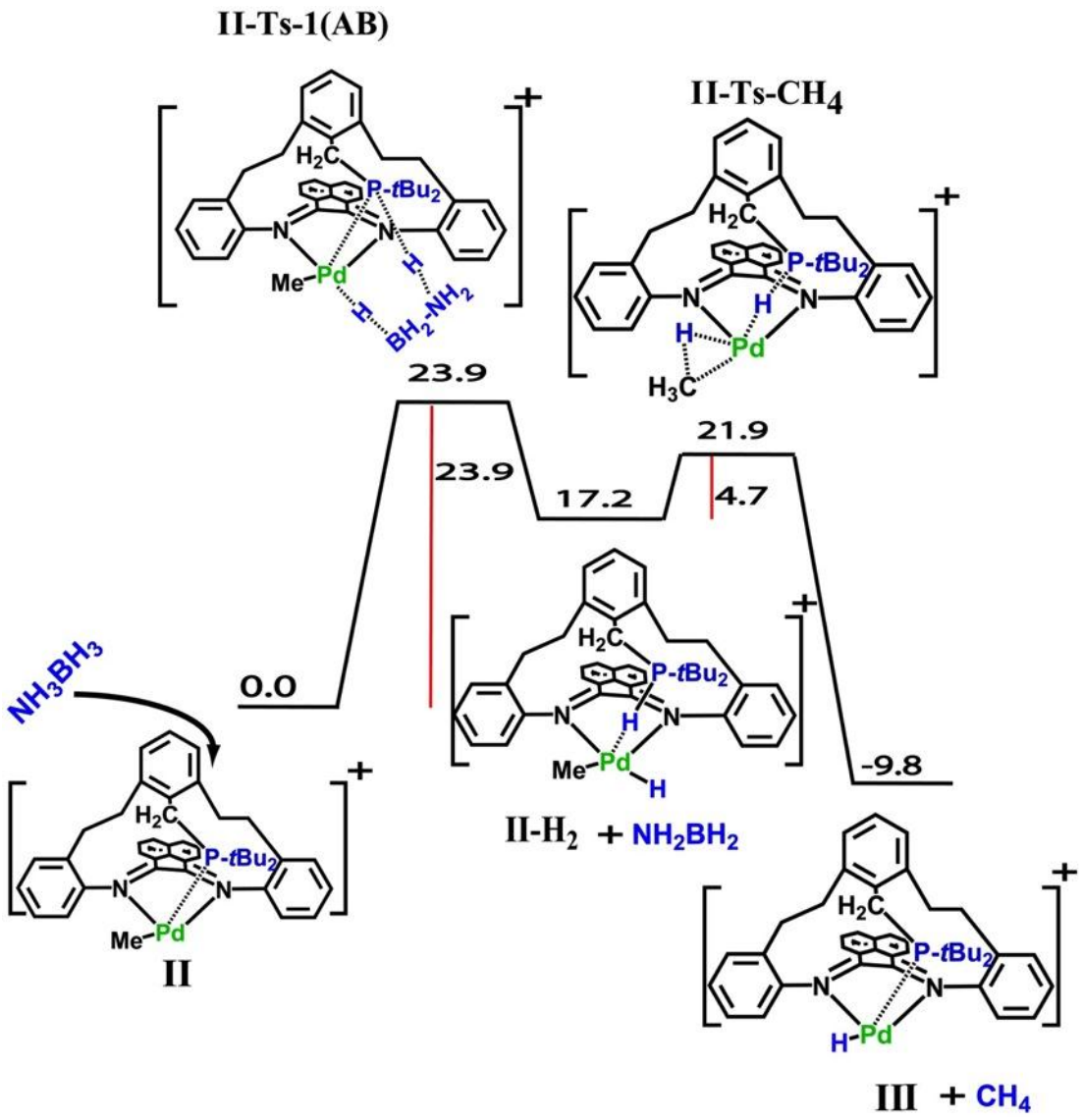



**Fig. S13b** The schematic representation of the reaction enthalpy (ΔH) surface showing the possibility of dehydrogenation of ammonia borane followed by a reductive elimination step leading to the loss of methane from the palladium complex; all the values are in kcal/mol.

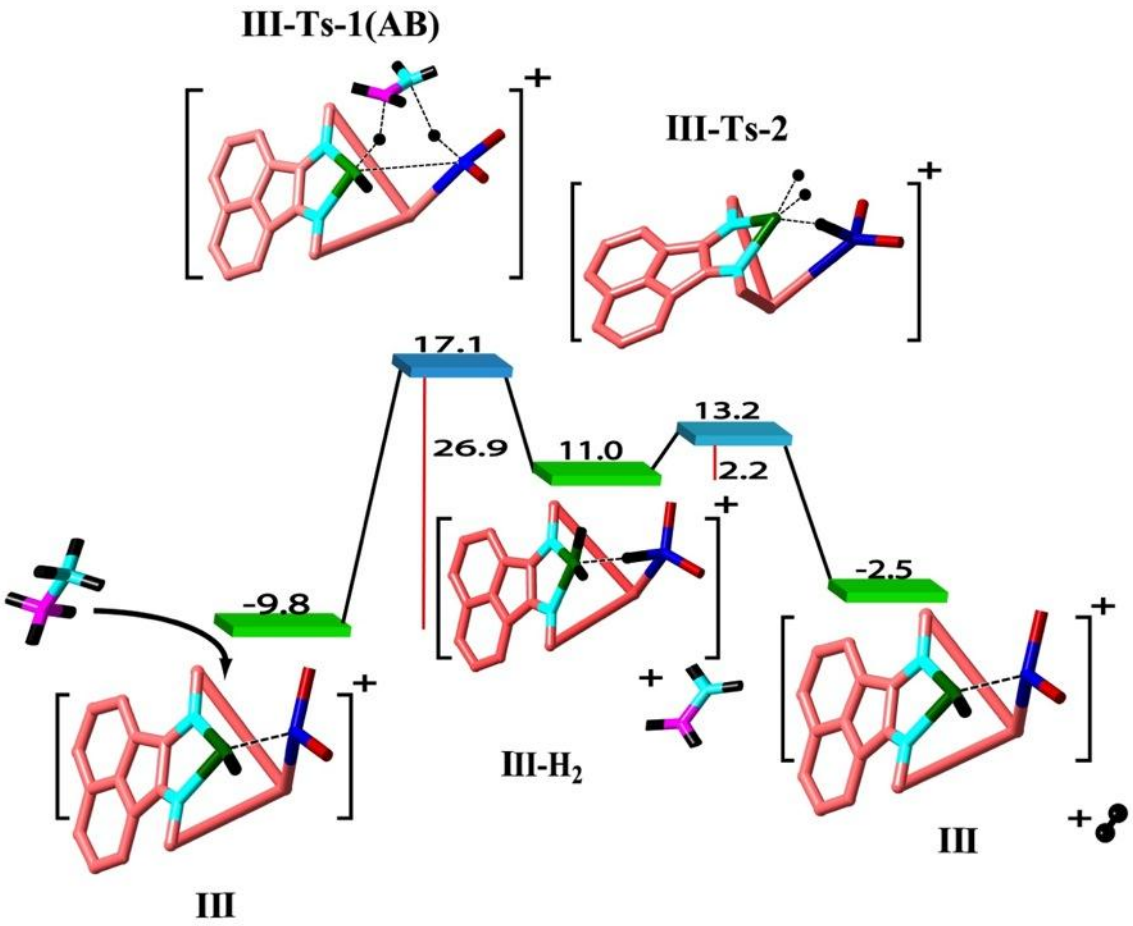



**Fig. S14a** The reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane (AB) using FLP (**III**) formed during the catalysis; all the structures shown are the optimized geometries obtained from the DFT/MP2 calculations; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

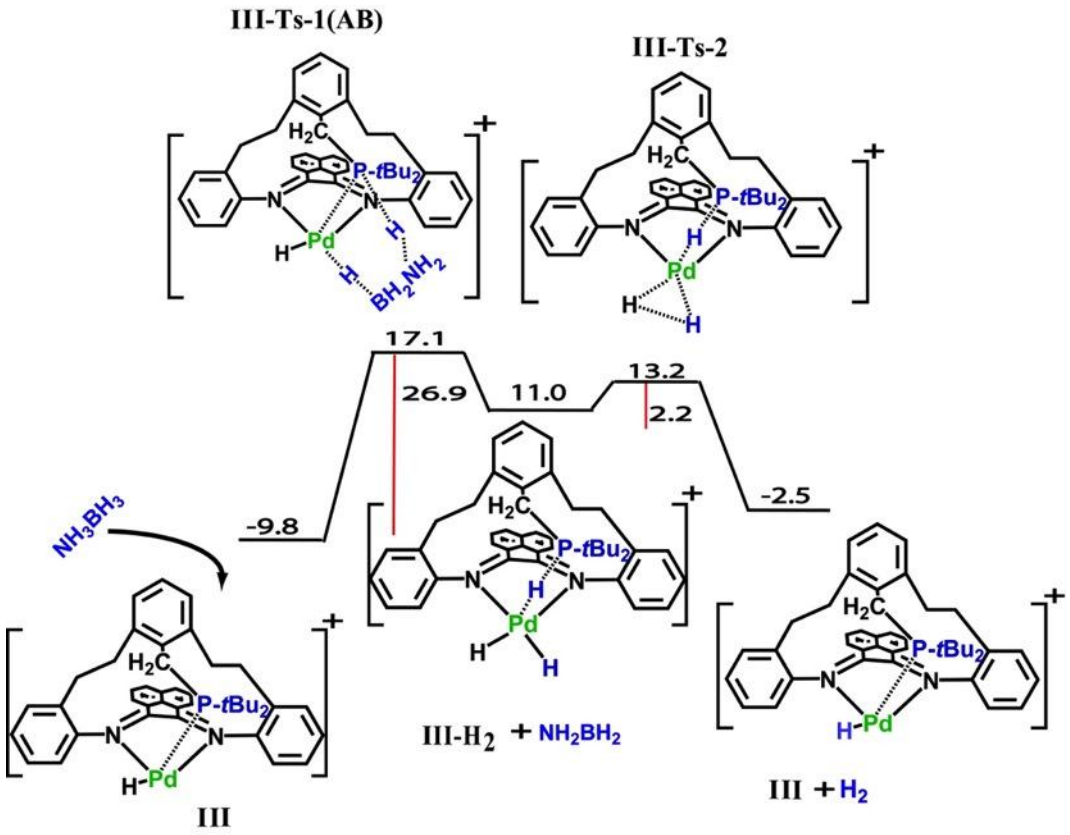



**Fig. S14b** The schematic representation of the reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane (AB) using FLP (**III**) formed during the catalysis; all the values are in kcal/mol.

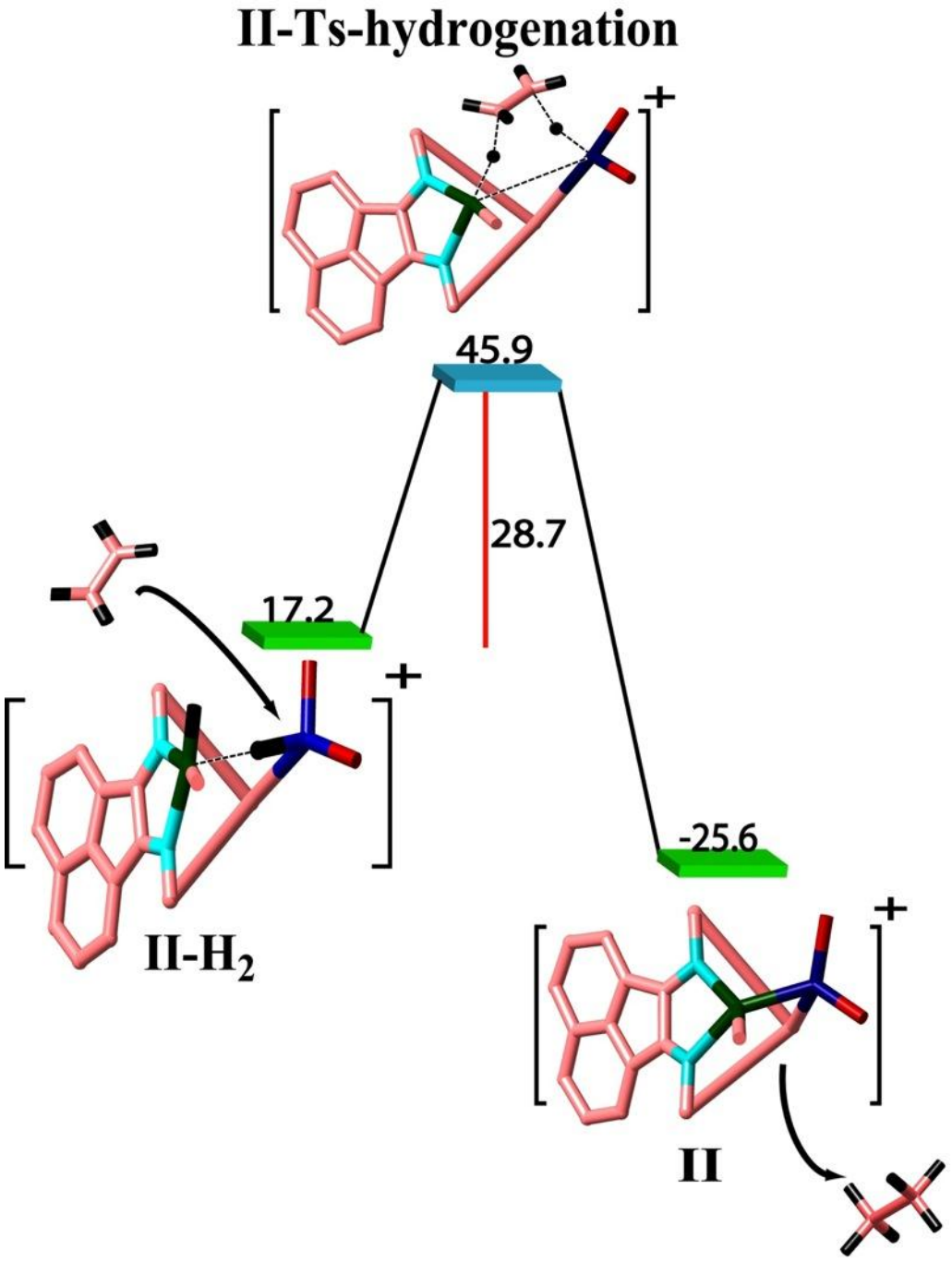



**Fig. S15a** The reaction enthalpy (ΔH) surface for the hydrogenation of ethylene with the hydrated palladium based FLP-**II-H$_2$**; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

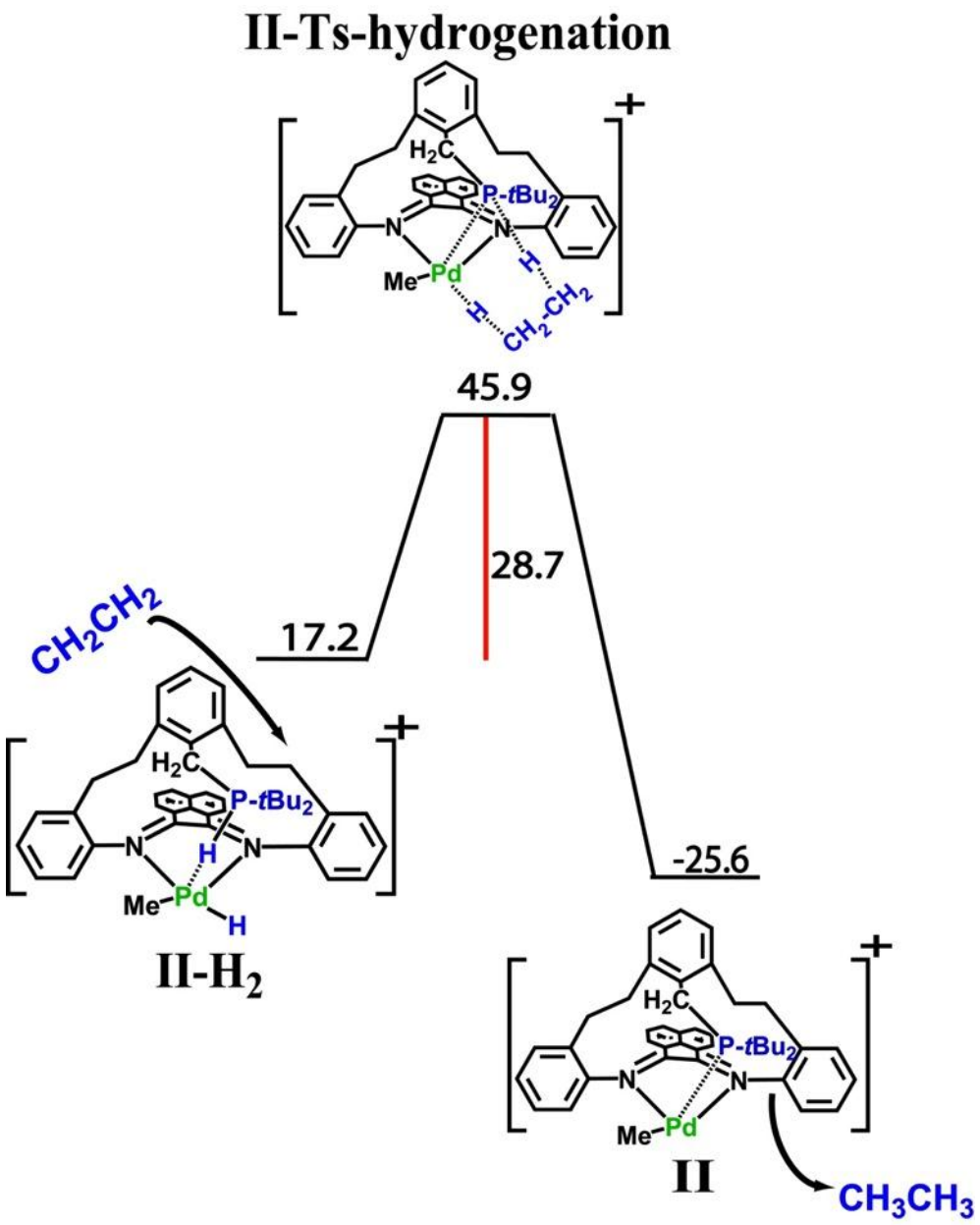



**Fig. S15b** The schematic representation of the reaction enthalpy (ΔH) surface for the hydrogenation of ethylene with the hydrated palladium based FLP-**II-H$_2$**; all the values are in kcal/mol.

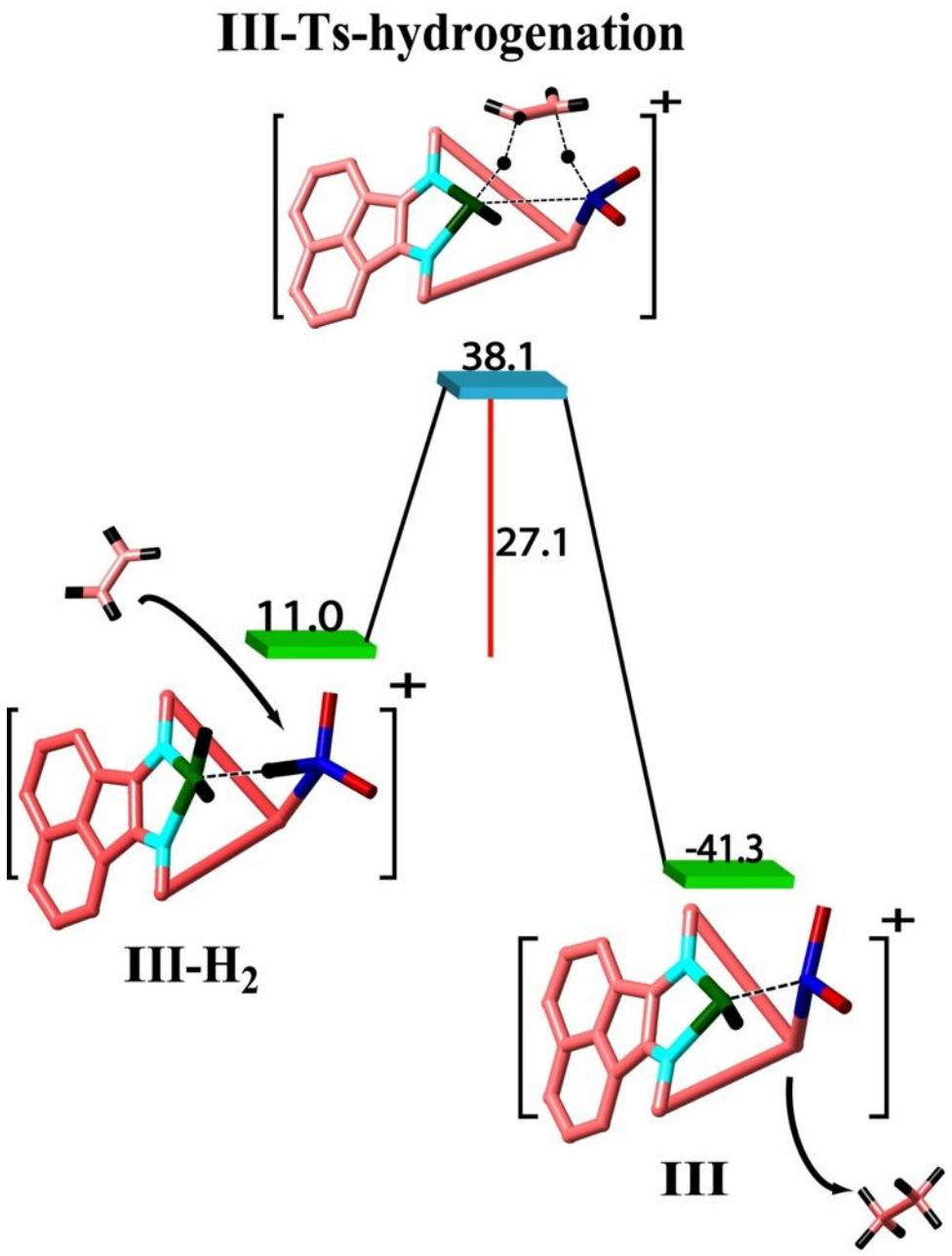



**Fig. S16a** The reaction enthalpy (ΔH) surface for the hydrogenation of ethylene with the hydrated palladium based FLP-**III-H$_2$** formed during the catalysis; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

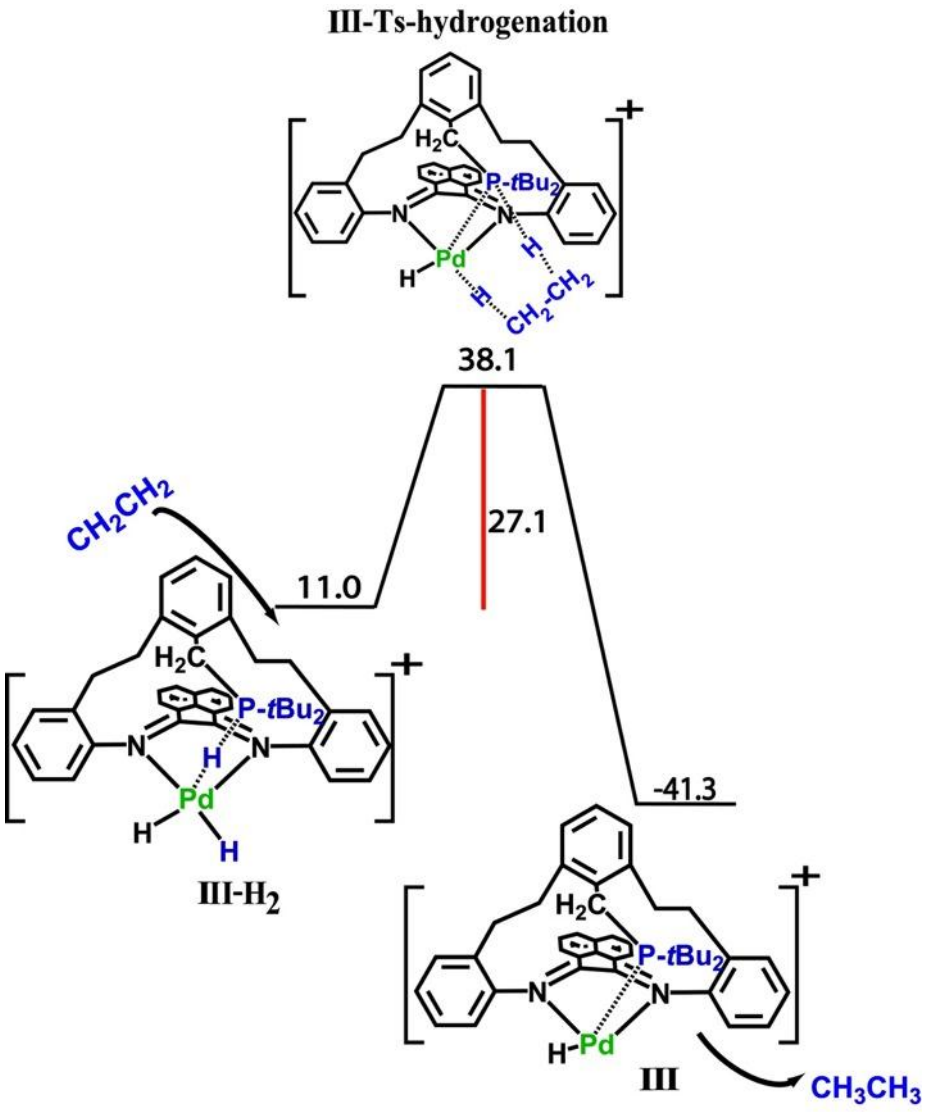



**Fig. S16b** The schematic representation of the reaction enthalpy (ΔH) surface for the hydrogenation of ethylene with the hydrated palladium based FLP-**III-H$_2$** formed during the catalysis; all the values are in kcal/mol.

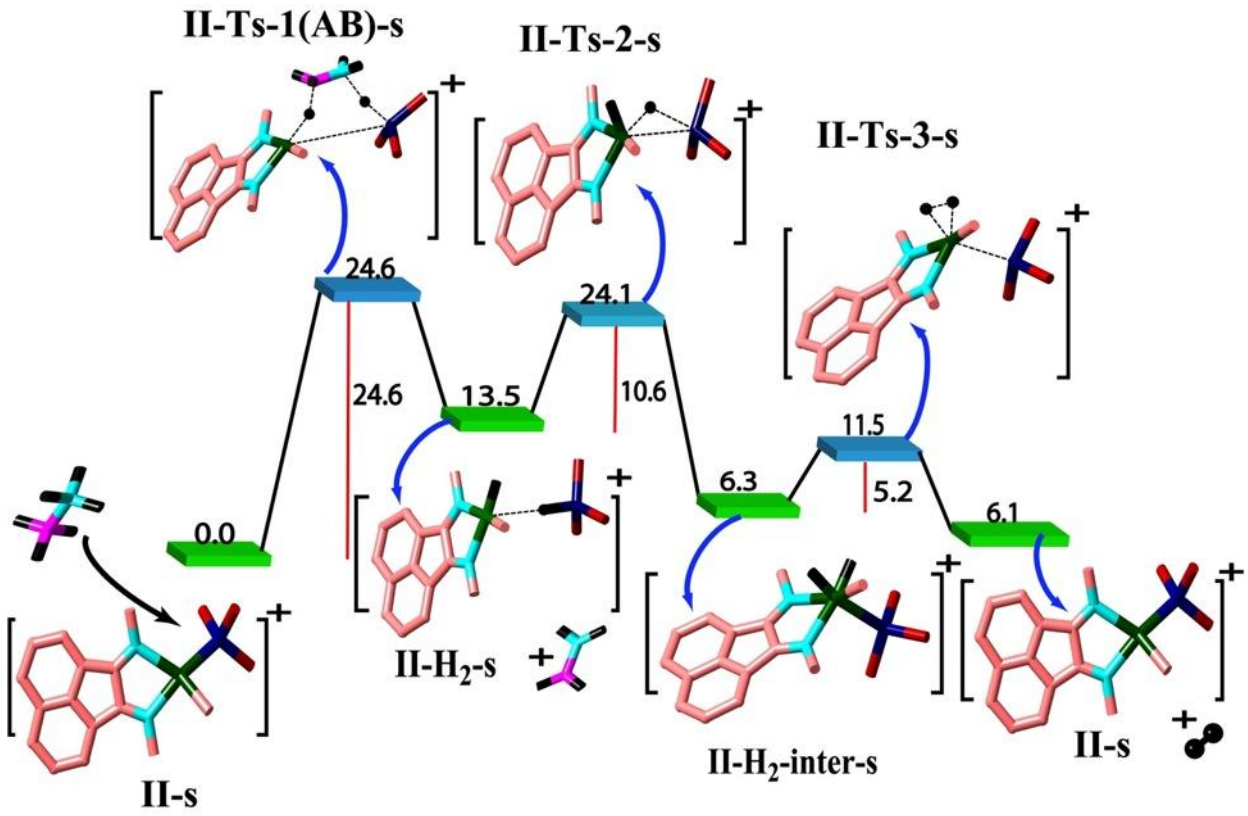



**Fig. S17a** A simpler palladium based FLP system: no linkage between the phosphorus and the diimine ligand; shown above is the reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane; the colour scheme is as follows: carbon – light brown, nitrogen – light blue, palladium – green, phosphorus – blue, boron – magenta, the tertiary butyl groups – red; all the values are in kcal/mol.

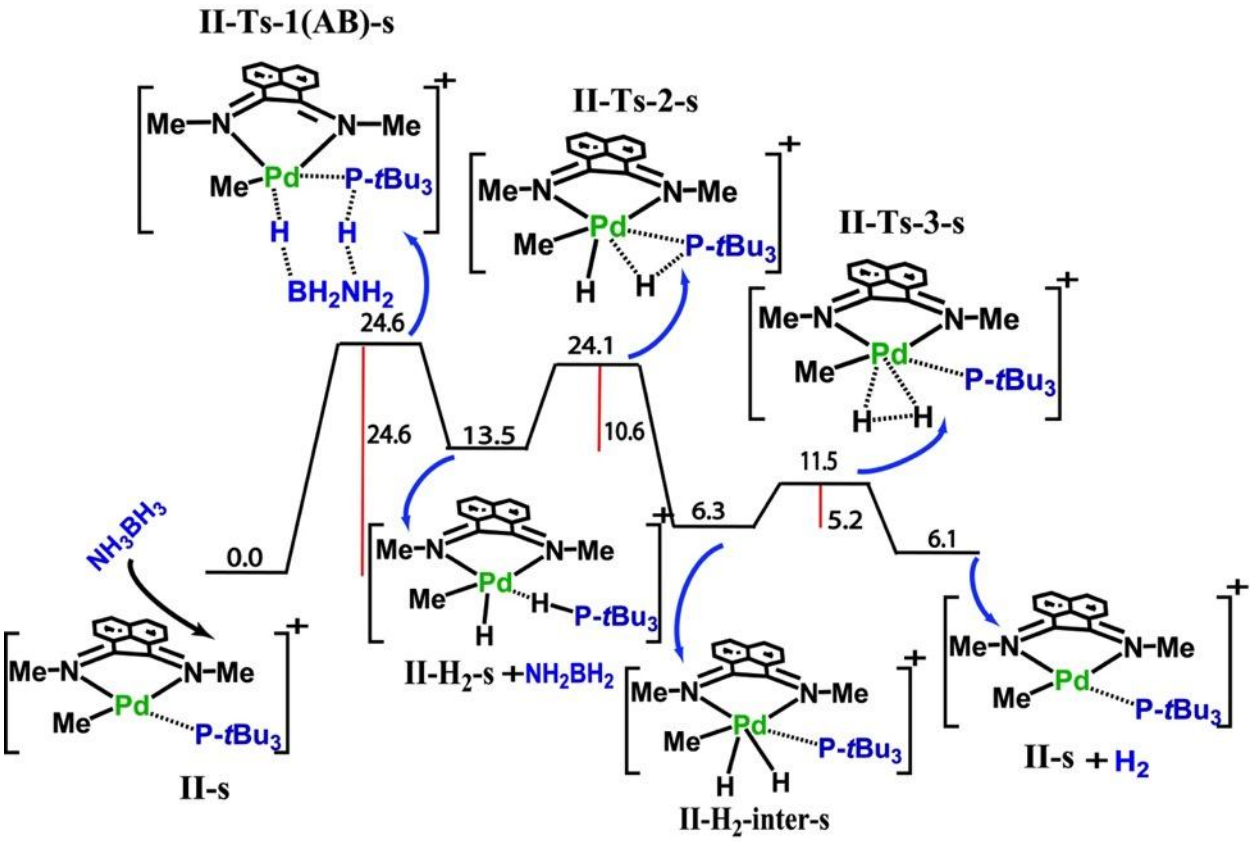



**Fig. S17b** A simpler palladium based FLP system: no linkage between the phosphorus and the diimine ligand; shown above is the schematic representation of the reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane; all the values are in kcal/mol.

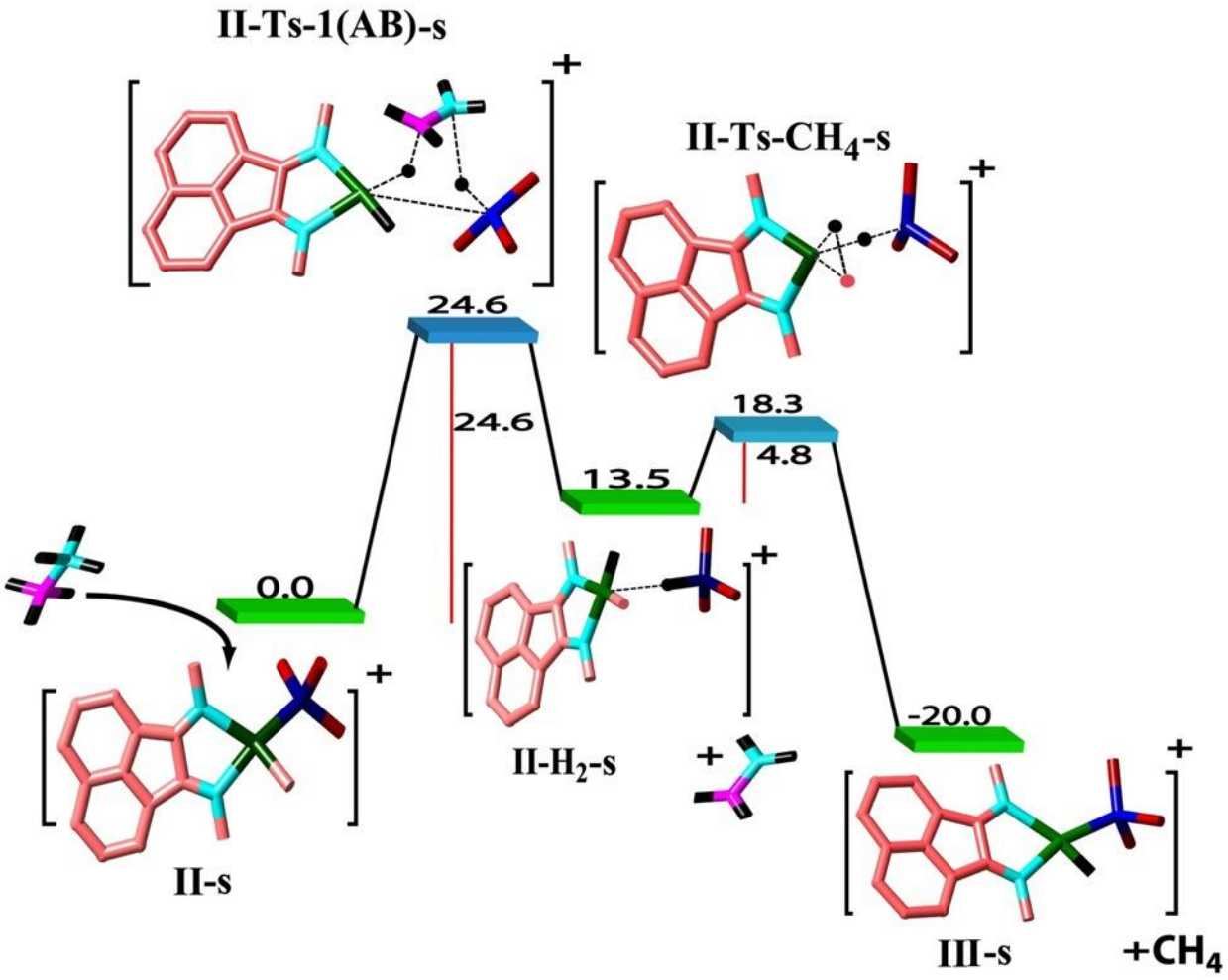



**Fig. S18a** The reaction enthalpy (ΔH) surface showing the possibility of dehydrogenation of ammonia borane followed by a reductive elimination step leading to the loss of methane from the simple palladium complex; only the hydrogens of AB are shown, the rest have been removed for the purpose of clarity; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

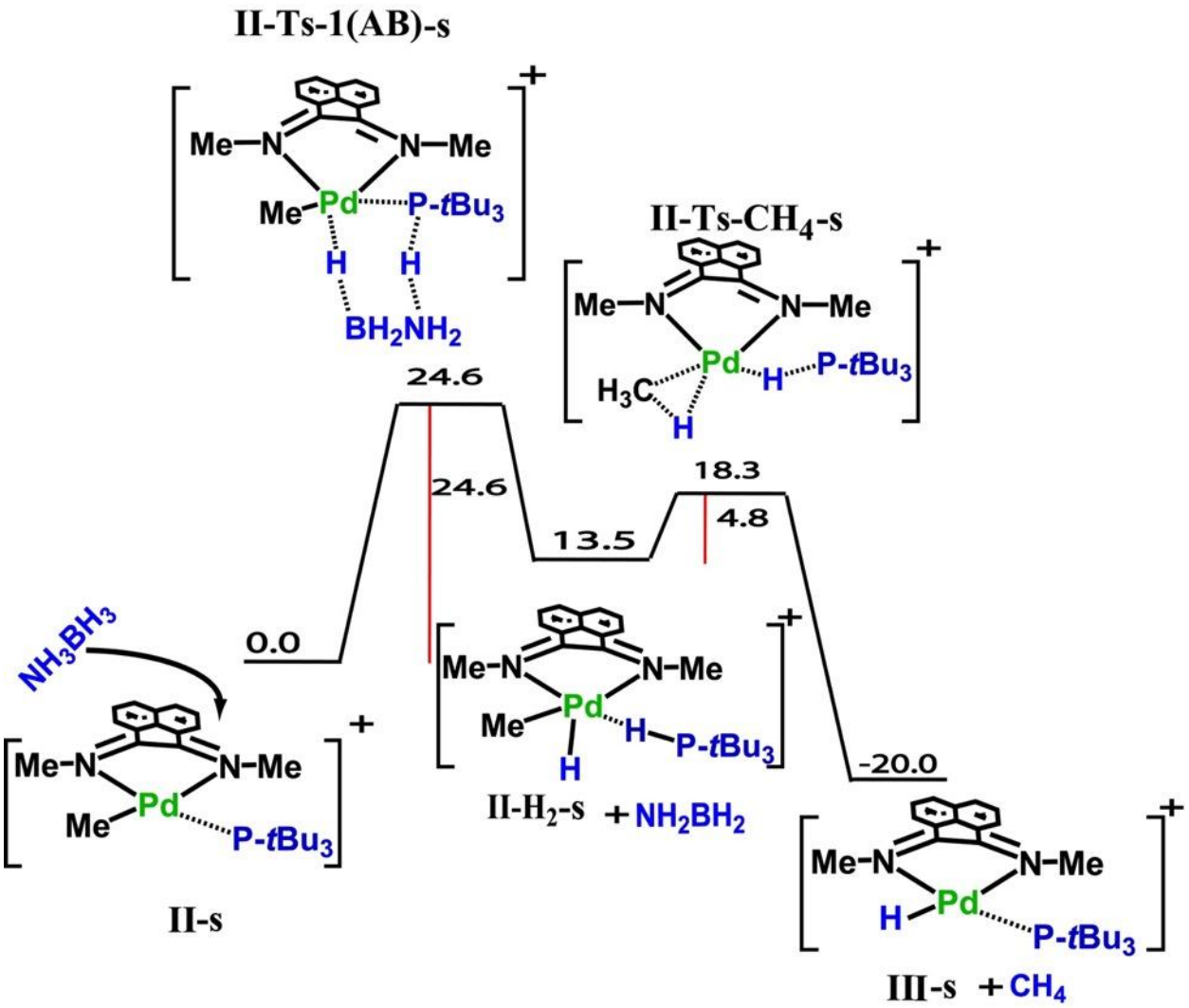



**Fig. S18b** The schematic representation of the reaction enthalpy (ΔH) surface showing the possibility of dehydrogenation of ammonia borane followed by a reductive elimination step leading to the loss of methane from the simple palladium complex; all the values are in kcal/mol.

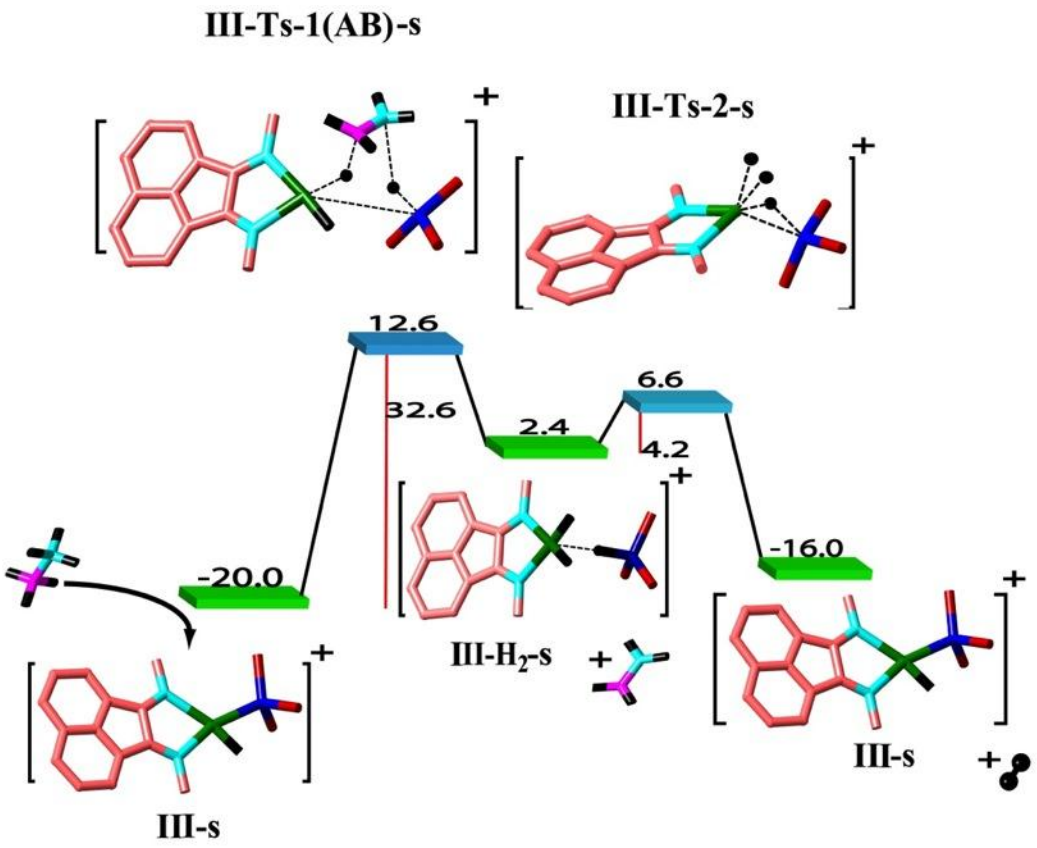



**Fig. S19a** The reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane (AB) using FLP (**III-s**) formed during the catalysis; with the simple palladium based FLP; the colour scheme is as for Figure 3; all the values are in kcal/mol.

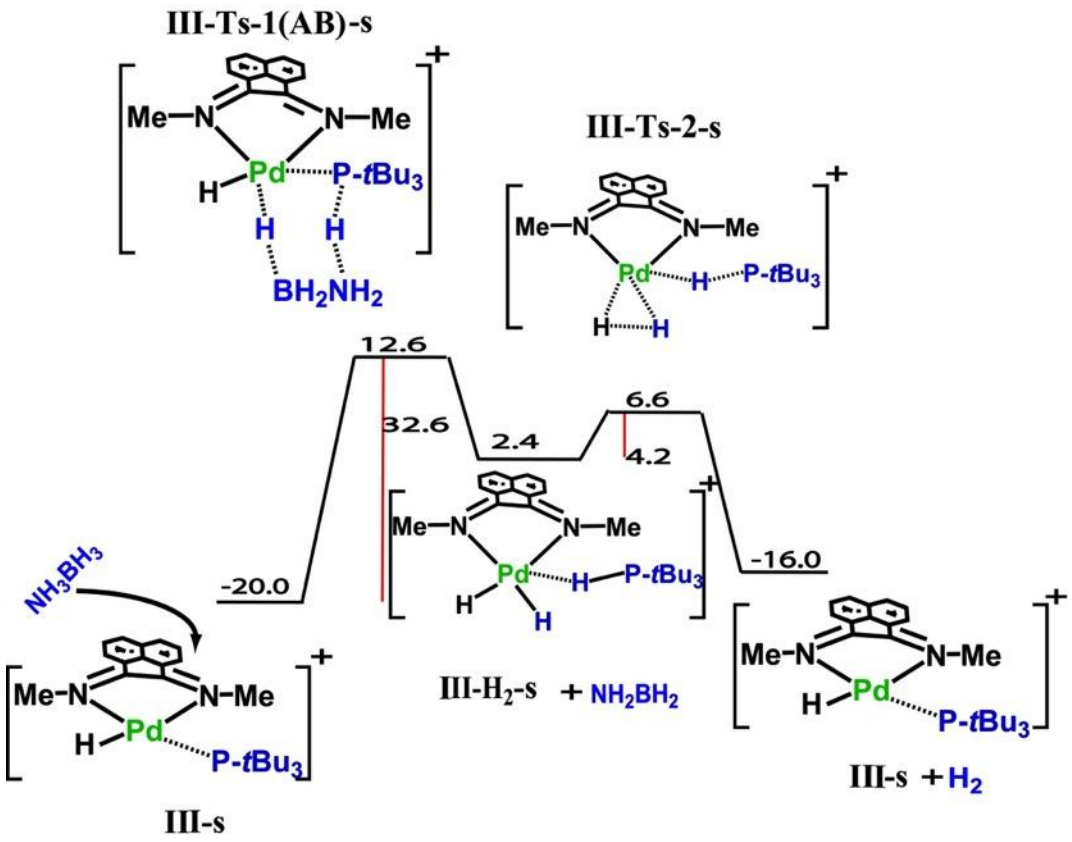



**Fig. S19b** The schematic representation of the reaction enthalpy (ΔH) surface for the catalysis of the dehydrogenation of ammonia borane (AB) using FLP (**III-s**) formed during the catalysis; with the simple palladium based FLP; all the values are in kcal/mol.

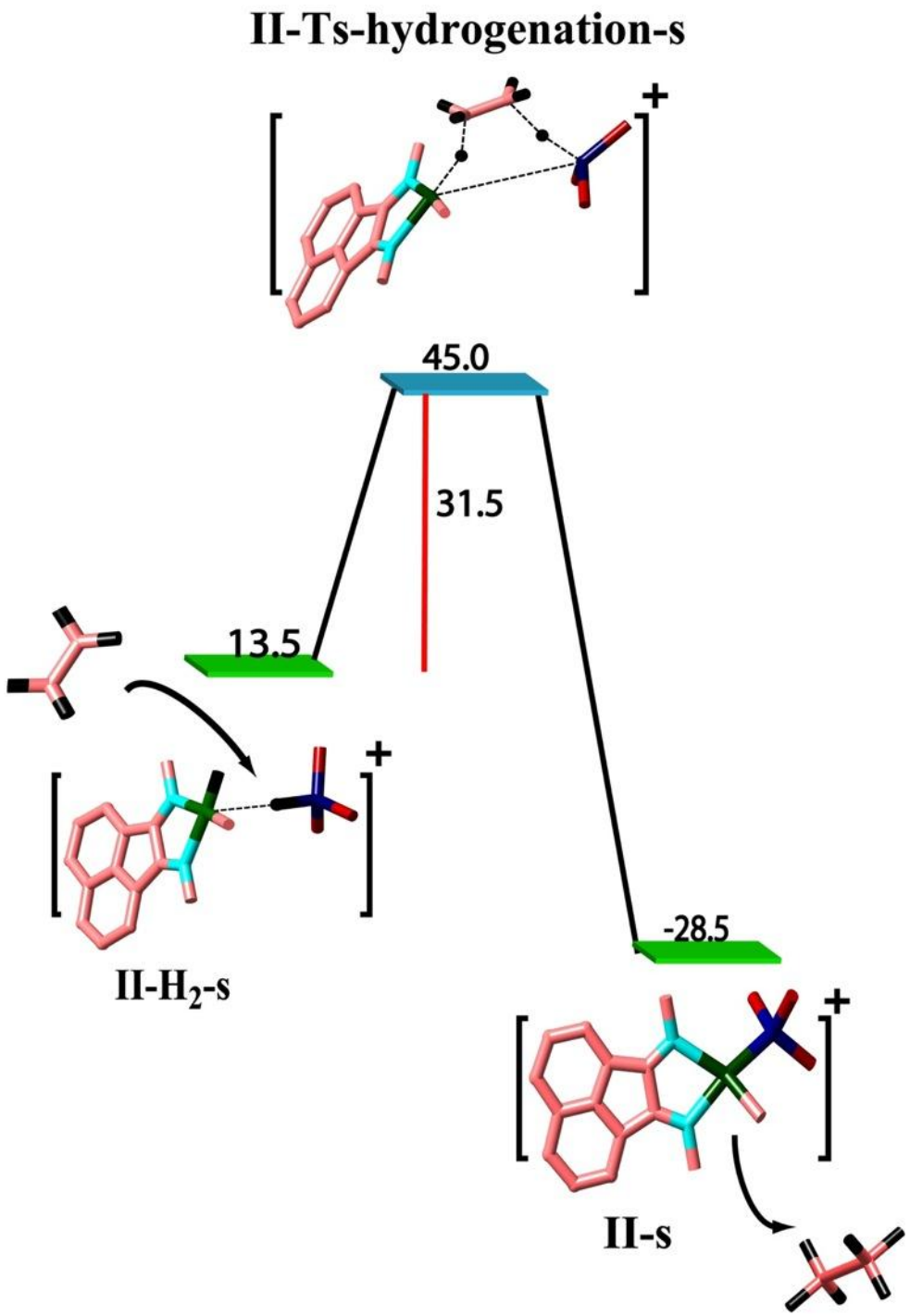



**Fig. S20a** The reaction enthalpy (ΔH) surface for the hydrogenation of ethylene to ethane with the hydrogenated simple palladium based FLP; the colour scheme is as for Figure 3; all the values are in kcal/mol.

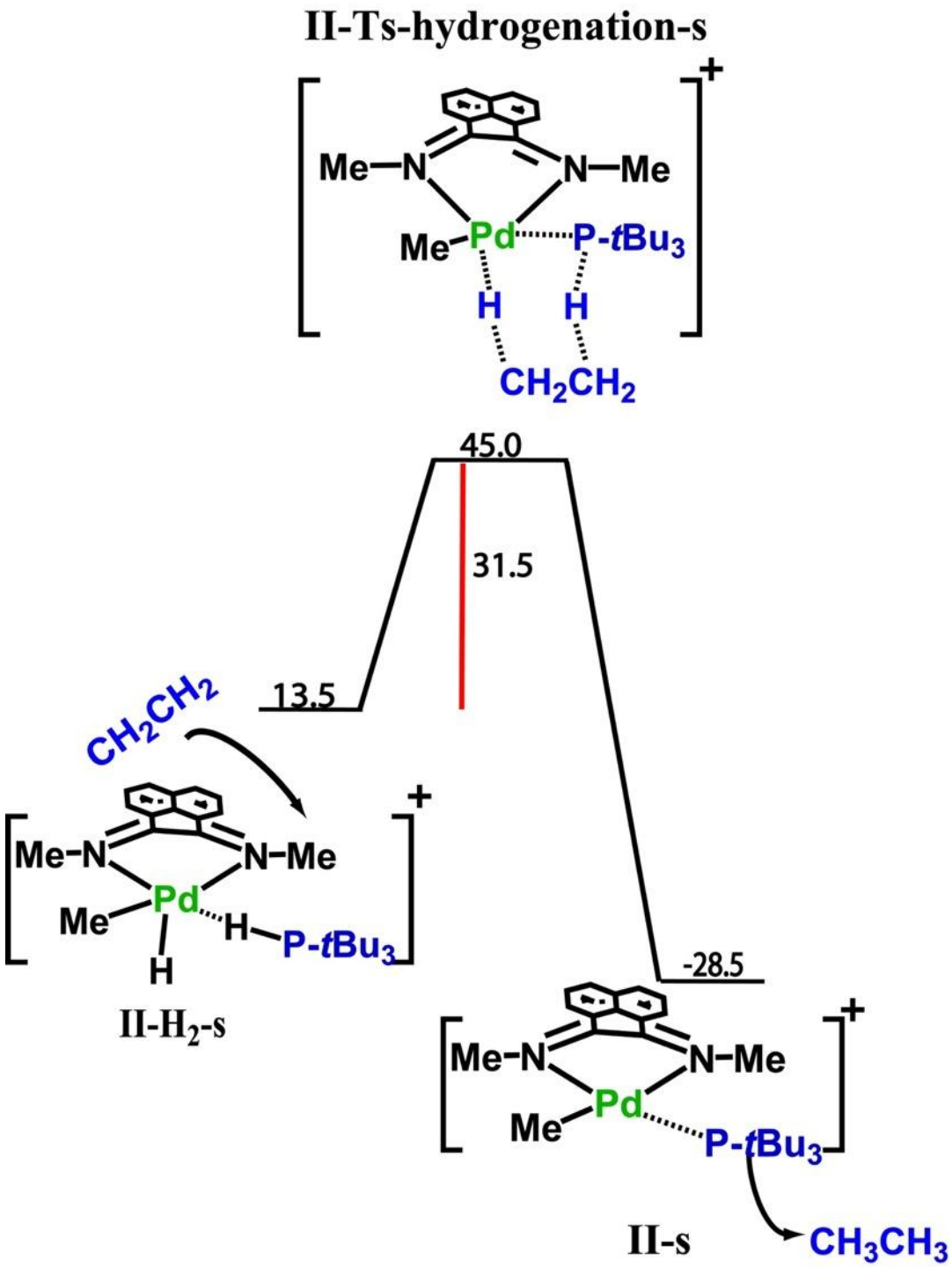



**Fig. S20b** The schematic representation of the reaction enthalpy (ΔH) surface for the hydrogenation of ethylene to ethane with the hydrogenated simple palladium based FLP; all the values are in kcal/mol.

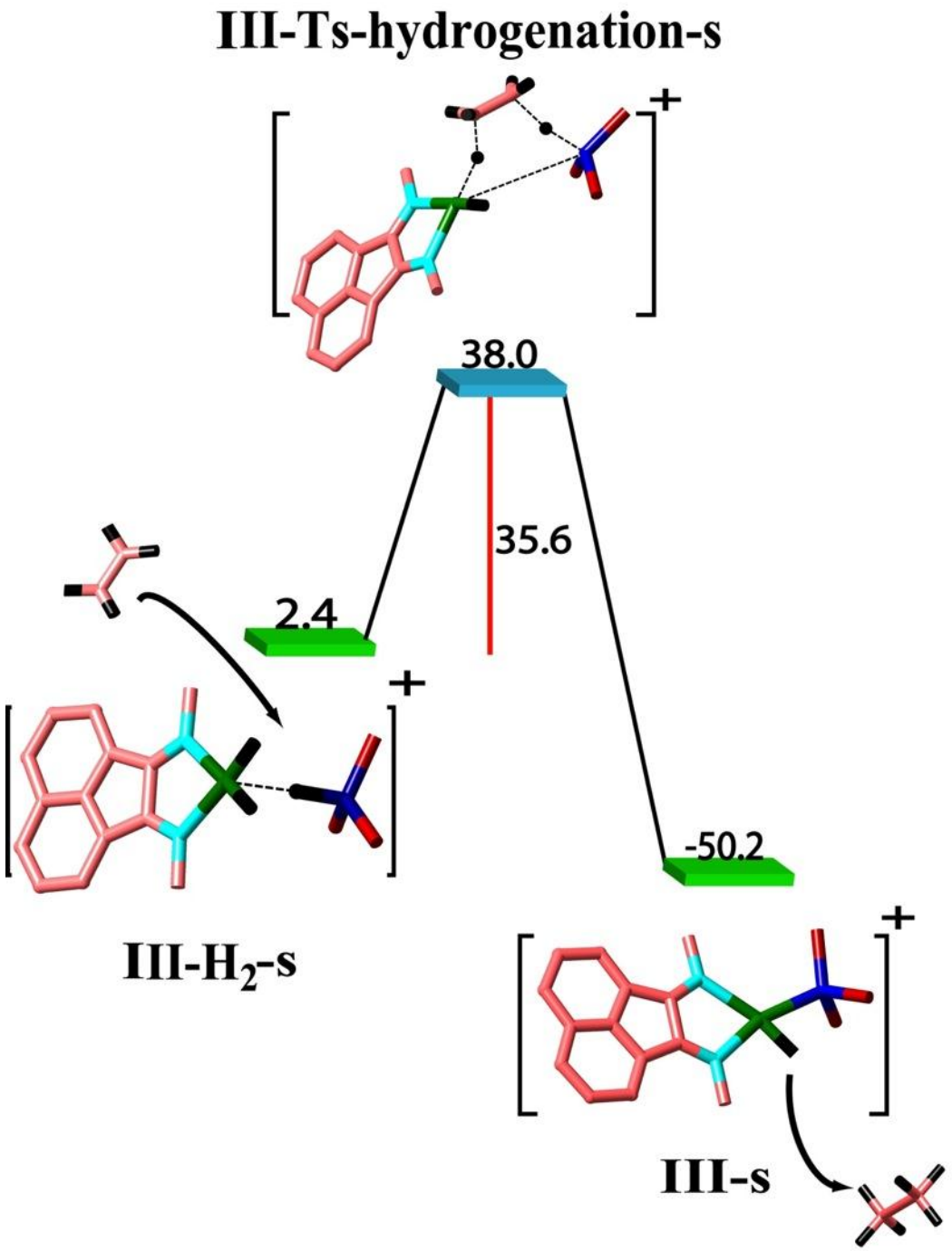



**Fig. S21a** The reaction enthalpy (ΔH) surface for the hydrogenation of ethylene with the hydrated simple palladium based FLP-**III-$H_2$-s** formed during the catalysis; the colour scheme is the same as used in Figure 1; all the values are in kcal/mol.

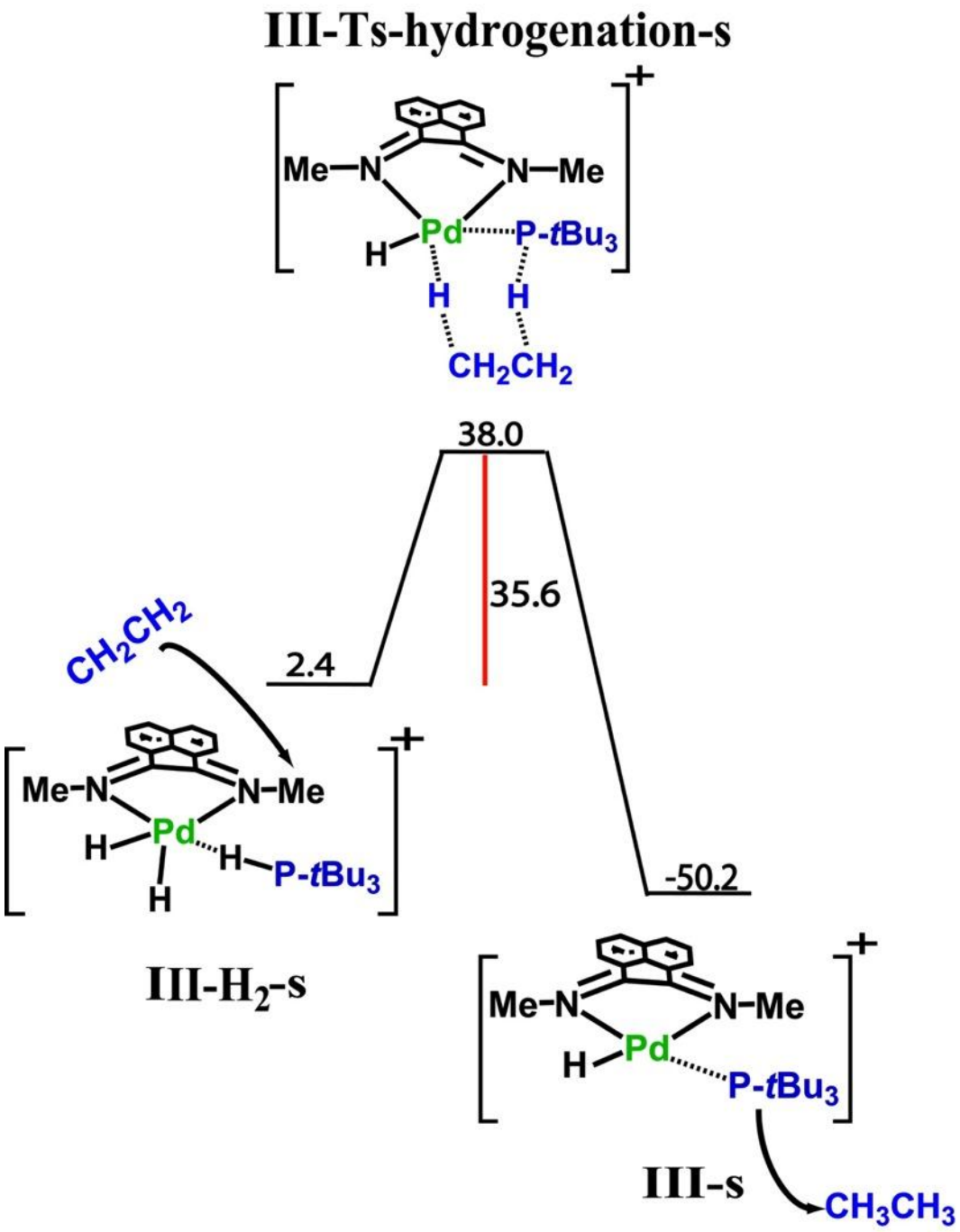



**Fig. S21b** The schematic representation of the reaction enthalpy (ΔH) surface for the hydrogenation of ethylene with the hydrated simple palladium based FLP-**III-$H_2$-s** formed during the catalysis; all the values are in kcal/mol.

## II. XYZ Coordinates of the optimized structures.

### II(Pd-P system)

| | | | |
|---|---|---|---|
| C | 11.466341 | 20.863540 | -3.234556 |
| C | 11.718748 | 19.646160 | -2.545060 |
| C | 11.876731 | 19.737081 | -1.143884 |
| C | 11.833176 | 20.967711 | -0.428254 |
| C | 11.571138 | 22.135228 | -1.132085 |
| C | 11.381246 | 22.059442 | -2.534473 |
| C | 12.091459 | 20.614702 | 0.977586 |
| C | 12.061446 | 19.116685 | 1.065163 |
| C | 12.071192 | 18.600334 | -0.309275 |
| C | 11.820813 | 18.345325 | -3.110498 |
| C | 12.048133 | 17.240395 | -2.300818 |
| C | 12.163861 | 17.343684 | -0.892052 |
| N | 11.963353 | 18.556547 | 2.231203 |
| Pd | 12.322826 | 20.086042 | 3.909660 |
| C | 13.658422 | 21.250129 | 4.933509 |
| N | 12.388184 | 21.290280 | 2.051189 |
| C | 12.517288 | 22.710679 | 1.971022 |
| C | 11.726337 | 23.578715 | 2.763755 |
| C | 11.887273 | 24.960356 | 2.551687 |
| C | 12.817427 | 25.478247 | 1.653013 |
| C | 13.654299 | 24.605506 | 0.950767 |
| C | 13.499844 | 23.232323 | 1.109036 |
| C | 10.872560 | 23.121797 | 3.923281 |
| C | 9.378619 | 22.759203 | 3.751626 |
| C | 9.081118 | 21.528805 | 2.928040 |
| C | 9.127846 | 20.178585 | 3.403753 |
| C | 8.815269 | 19.150164 | 2.471192 |
| C | 8.417171 | 19.475958 | 1.164224 |
| C | 8.358423 | 20.787753 | 0.718159 |
| C | 8.707923 | 21.798997 | 1.603262 |
| C | 8.810418 | 17.669016 | 2.793409 |
| C | 9.563310 | 16.766749 | 1.766457 |
| C | 10.947865 | 16.280348 | 2.141645 |
| C | 11.166948 | 14.900520 | 2.290950 |
| C | 12.419736 | 14.370031 | 2.603598 |
| C | 13.507069 | 15.228541 | 2.775416 |
| C | 13.325610 | 16.604163 | 2.634609 |
| C | 12.064445 | 17.129851 | 2.314642 |
| C | 9.288555 | 19.857758 | 4.902283 |
| P | 11.013082 | 19.597536 | 5.777973 |
| C | 11.248264 | 17.789449 | 6.506011 |
| C | 10.888522 | 20.756660 | 7.364919 |
| H | 11.511603 | 23.101488 | -0.633820 |
| H | 11.173691 | 22.980857 | -3.080992 |
| H | 11.333184 | 20.853927 | -4.318384 |
| H | 11.718699 | 18.217333 | -4.190380 |
| H | 12.131480 | 16.253858 | -2.759791 |
| H | 12.326190 | 16.446957 | -0.295109 |
| H | 14.162892 | 17.291854 | 2.768404 |
| H | 14.495234 | 14.833664 | 3.016484 |
| H | 12.544505 | 13.291369 | 2.709976 |
| H | 10.318651 | 14.225481 | 2.153520 |
| H | 8.954149 | 15.870546 | 1.581021 |
| H | 9.618922 | 17.290850 | 0.799964 |
| H | 7.759018 | 17.336234 | 2.810218 |

| | | | |
|---|---|---|---|
| H | 9.197907 | 17.478175 | 3.793627 |
| H | 8.119561 | 18.671604 | 0.488303 |
| H | 8.029014 | 21.019926 | -0.296151 |
| H | 8.660374 | 22.841385 | 1.280722 |
| H | 8.955113 | 22.657770 | 4.763603 |
| H | 8.851049 | 23.612339 | 3.299890 |
| H | 10.916724 | 23.929956 | 4.670071 |
| H | 11.369189 | 22.249170 | 4.370888 |
| H | 11.280089 | 25.646287 | 3.148125 |
| H | 12.917071 | 26.557800 | 1.530863 |
| H | 14.427750 | 24.991665 | 0.284991 |
| H | 14.143139 | 22.540567 | 0.562447 |
| H | 14.580114 | 20.712931 | 4.654165 |
| H | 13.644442 | 22.256383 | 4.495077 |
| H | 13.574438 | 21.298443 | 6.020767 |
| H | 8.854566 | 20.690725 | 5.471148 |
| H | 8.685204 | 18.975698 | 5.158601 |
| C | 12.774168 | 17.627717 | 6.668469 |
| C | 10.523828 | 17.461269 | 7.821979 |
| C | 10.773163 | 16.748412 | 5.494053 |
| C | 12.060814 | 20.493916 | 8.330130 |
| C | 10.952023 | 22.241225 | 6.985231 |
| C | 9.545756 | 20.549420 | 8.097704 |
| H | 12.979144 | 16.617701 | 7.058031 |
| H | 13.285243 | 17.728202 | 5.700449 |
| H | 13.219654 | 18.347961 | 7.365074 |
| H | 10.739565 | 16.406056 | 8.056487 |
| H | 10.849911 | 18.049408 | 8.685107 |
| H | 9.432512 | 17.546730 | 7.725160 |
| H | 11.143629 | 15.760668 | 5.811821 |
| H | 9.677312 | 16.680493 | 5.461940 |
| H | 11.163257 | 16.928274 | 4.489662 |
| H | 10.893241 | 22.827551 | 7.916112 |
| H | 11.883742 | 22.515672 | 6.480770 |
| H | 10.103327 | 22.548747 | 6.364558 |
| H | 9.542550 | 21.207491 | 8.981358 |
| H | 8.683847 | 20.845787 | 7.483699 |
| H | 9.378915 | 19.529607 | 8.451378 |
| H | 11.983160 | 21.215294 | 9.159444 |
| H | 12.055879 | 19.494505 | 8.775362 |
| H | 13.038334 | 20.652392 | 7.855324 |

**II(Pd-P system) with AB**

| | | | |
|---|---|---|---|
| C | 16.880671 | 24.051540 | -1.737176 |
| C | 16.468720 | 22.717159 | -2.004680 |
| C | 15.181460 | 22.352554 | -1.550040 |
| C | 14.326797 | 23.233881 | -0.828153 |
| C | 14.756384 | 24.533012 | -0.594665 |
| C | 16.034085 | 24.924481 | -1.066782 |
| C | 13.120474 | 22.449920 | -0.520763 |
| C | 13.232663 | 21.156015 | -1.271529 |
| C | 14.605234 | 21.073790 | -1.791164 |
| C | 17.206938 | 21.711549 | -2.687741 |
| C | 16.659063 | 20.452599 | -2.893055 |
| C | 15.351404 | 20.114750 | -2.462411 |
| N | 12.184290 | 20.405007 | -1.403285 |

| | | | |
|---|---|---|---|
| Pd | 10.448655 | 21.191861 | -0.043621 |
| C | 9.663187 | 21.418588 | 1.827271 |
| N | 12.099771 | 22.622865 | 0.269728 |
| C | 12.045402 | 23.800617 | 1.078782 |
| C | 10.990549 | 24.738423 | 0.969807 |
| C | 11.078069 | 25.893719 | 1.767439 |
| C | 12.117167 | 26.104093 | 2.671942 |
| C | 13.101463 | 25.123729 | 2.827804 |
| C | 13.063316 | 23.982158 | 2.033353 |
| C | 9.722852 | 24.500265 | 0.183553 |
| C | 9.594409 | 24.954310 | -1.289178 |
| C | 10.398668 | 24.172420 | -2.301592 |
| C | 10.066212 | 22.868348 | -2.783388 |
| C | 10.958262 | 22.260317 | -3.708027 |
| C | 12.059974 | 22.975956 | -4.200253 |
| C | 12.353891 | 24.258987 | -3.758241 |
| C | 11.535556 | 24.831253 | -2.792682 |
| C | 10.749213 | 20.857804 | -4.245376 |
| C | 12.040268 | 19.998315 | -4.391138 |
| C | 12.248515 | 18.889173 | -3.381422 |
| C | 12.396325 | 17.568299 | -3.835496 |
| C | 12.639725 | 16.503289 | -2.966879 |
| C | 12.747358 | 16.744094 | -1.596022 |
| C | 12.605864 | 18.044144 | -1.112048 |
| C | 12.362734 | 19.109899 | -1.990575 |
| C | 8.699269 | 22.225837 | -2.505497 |
| P | 8.351777 | 20.960121 | -1.067114 |
| C | 7.908496 | 19.201455 | -1.838617 |
| C | 9.193370 | 18.370225 | -1.823173 |
| C | 6.668260 | 21.649080 | -0.317612 |
| C | 5.560581 | 21.597425 | -1.386505 |
| C | 6.244033 | 20.857785 | 0.937902 |
| C | 6.801031 | 23.115028 | 0.120477 |
| C | 6.900981 | 18.421410 | -0.976784 |
| C | 7.370639 | 19.307236 | -3.276100 |
| N | 7.108357 | 14.106039 | 2.122137 |
| B | 7.328254 | 15.465270 | 1.219944 |
| H | 14.138139 | 25.251485 | -0.058632 |
| H | 16.364280 | 25.948024 | -0.882691 |
| H | 17.864829 | 24.390375 | -2.067338 |
| H | 18.212447 | 21.934552 | -3.051313 |
| H | 17.248680 | 19.694958 | -3.411841 |
| H | 14.957941 | 19.117866 | -2.656999 |
| H | 12.673216 | 18.248767 | -0.041729 |
| H | 12.935518 | 15.924764 | -0.900452 |
| H | 12.741845 | 15.491026 | -3.360693 |
| H | 12.315494 | 17.378235 | -4.908606 |
| H | 12.047719 | 19.531848 | -5.386249 |
| H | 12.922097 | 20.656493 | -4.369314 |
| H | 10.276535 | 20.933000 | -5.240000 |
| H | 10.031211 | 20.320279 | -3.619232 |
| H | 12.691658 | 22.524131 | -4.967251 |
| H | 13.205874 | 24.806852 | -4.164800 |
| H | 11.753486 | 25.836095 | -2.424253 |
| H | 8.523109 | 24.919433 | -1.543124 |
| H | 9.875878 | 26.015292 | -1.366249 |

| | | | |
|---|---|---|---|
| H | 8.919465 | 25.006185 | 0.740425 |
| H | 9.509751 | 23.421798 | 0.219990 |
| H | 10.275025 | 26.631728 | 1.692915 |
| H | 12.138048 | 27.010544 | 3.278849 |
| H | 13.894222 | 25.244596 | 3.567920 |
| H | 13.829653 | 23.212287 | 2.140551 |
| H | 10.504399 | 21.846240 | 2.389626 |
| H | 8.782550 | 22.058146 | 1.927632 |
| H | 9.433409 | 20.396404 | 2.159538 |
| H | 7.981742 | 23.030452 | -2.299435 |
| H | 8.340963 | 21.736620 | -3.420757 |
| H | 6.856967 | 17.395737 | -1.374653 |
| H | 7.221061 | 18.325879 | 0.068538 |
| H | 5.881710 | 18.820463 | -1.011985 |
| H | 7.095932 | 18.294078 | -3.610741 |
| H | 6.472055 | 19.931211 | -3.359664 |
| H | 8.118198 | 19.681932 | -3.987691 |
| H | 8.972044 | 17.367657 | -2.222737 |
| H | 9.988221 | 18.796703 | -2.438111 |
| H | 9.577839 | 18.243265 | -0.802111 |
| H | 5.807892 | 23.448328 | 0.460699 |
| H | 7.491197 | 23.244173 | 0.959166 |
| H | 7.097003 | 23.791745 | -0.689852 |
| H | 4.649122 | 22.045090 | -0.958444 |
| H | 5.814456 | 22.183419 | -2.282488 |
| H | 5.304000 | 20.580180 | -1.698794 |
| H | 5.426062 | 21.411374 | 1.426119 |
| H | 5.871286 | 19.855237 | 0.720530 |
| H | 7.057220 | 20.766949 | 1.668371 |
| H | 8.014977 | 15.124700 | 0.271828 |
| H | 7.891232 | 16.261853 | 1.952476 |
| H | 6.534589 | 14.294518 | 2.950281 |
| H | 7.999574 | 13.719207 | 2.448348 |
| H | 6.635471 | 13.373539 | 1.583208 |
| H | 6.209190 | 15.822264 | 0.895343 |

**II-$H_2$**

| | | | |
|---|---|---|---|
| C | 11.136342 | 20.792508 | -3.374796 |
| C | 11.458010 | 19.586736 | -2.694360 |
| C | 11.737104 | 19.696882 | -1.313071 |
| C | 11.758003 | 20.934803 | -0.610794 |
| C | 11.424031 | 22.089846 | -1.305821 |
| C | 11.107475 | 21.996195 | -2.684094 |
| C | 12.123035 | 20.603891 | 0.781428 |
| C | 12.175105 | 19.103057 | 0.871792 |
| C | 12.010657 | 18.572677 | -0.485371 |
| C | 11.530026 | 18.281530 | -3.254263 |
| C | 11.845206 | 17.189925 | -2.456249 |
| C | 12.077858 | 17.311912 | -1.063834 |
| N | 12.359893 | 18.551242 | 2.036372 |
| Pd | 13.149888 | 19.968325 | 3.503549 |
| C | 14.281679 | 21.278948 | 4.611306 |
| N | 12.388110 | 21.296170 | 1.853967 |
| C | 12.488447 | 22.710234 | 1.820788 |
| C | 11.850170 | 23.501138 | 2.807340 |
| C | 11.983999 | 24.896996 | 2.710304 |
| C | 12.764765 | 25.502990 | 1.728358 |

| | | | |
|---|---|---|---|
| C | 13.466381 | 24.704249 | 0.818995 |
| C | 13.326772 | 23.321984 | 0.867532 |
| C | 11.134698 | 22.925169 | 4.005414 |
| C | 9.605200 | 22.684971 | 3.915089 |
| C | 9.220564 | 21.530198 | 3.031495 |
| C | 9.234299 | 20.163900 | 3.446911 |
| C | 8.977686 | 19.174561 | 2.459281 |
| C | 8.603943 | 19.565162 | 1.161907 |
| C | 8.521256 | 20.897941 | 0.787308 |
| C | 8.859368 | 21.869017 | 1.721486 |
| C | 9.008871 | 17.677775 | 2.696842 |
| C | 9.829796 | 16.863548 | 1.644681 |
| C | 11.191595 | 16.340863 | 2.064370 |
| C | 11.319384 | 14.963432 | 2.318666 |
| C | 12.529781 | 14.374426 | 2.685052 |
| C | 13.668156 | 15.172972 | 2.817303 |
| C | 13.575146 | 16.544442 | 2.592769 |
| C | 12.361085 | 17.131864 | 2.198643 |
| C | 9.231068 | 19.794009 | 4.944239 |
| P | 10.771114 | 19.607468 | 6.069551 |
| C | 11.056789 | 17.806240 | 6.680428 |
| C | 10.601229 | 20.792802 | 7.597464 |
| H | 11.409115 | 23.064056 | -0.819618 |
| H | 10.849054 | 22.910632 | -3.220787 |
| H | 10.910459 | 20.768317 | -4.442919 |
| H | 11.337919 | 18.140590 | -4.320194 |
| H | 11.906144 | 16.199538 | -2.910619 |
| H | 12.299737 | 16.423679 | -0.472850 |
| H | 14.444698 | 17.191835 | 2.714739 |
| H | 14.625963 | 14.734169 | 3.101353 |
| H | 12.582506 | 13.299270 | 2.863238 |
| H | 10.430116 | 14.336644 | 2.215023 |
| H | 9.236053 | 15.983715 | 1.358089 |
| H | 9.928554 | 17.459768 | 0.727423 |
| H | 7.969934 | 17.309062 | 2.660851 |
| H | 9.375651 | 17.442680 | 3.694775 |
| H | 8.345050 | 18.791686 | 0.436135 |
| H | 8.200624 | 21.175784 | -0.218112 |
| H | 8.826952 | 22.925637 | 1.448213 |
| H | 9.217674 | 22.537777 | 4.934514 |
| H | 9.120738 | 23.599908 | 3.542872 |
| H | 11.308854 | 23.628890 | 4.832263 |
| H | 11.628509 | 21.978004 | 4.278224 |
| H | 11.486025 | 25.519441 | 3.458429 |
| H | 12.859224 | 26.589462 | 1.697147 |
| H | 14.130068 | 25.157263 | 0.080703 |
| H | 13.883874 | 22.690970 | 0.173616 |
| H | 15.335923 | 21.116639 | 4.345286 |
| H | 13.983211 | 22.293588 | 4.304647 |
| H | 14.184710 | 21.170678 | 5.700784 |
| H | 8.632599 | 20.551315 | 5.469709 |
| H | 8.682602 | 18.851561 | 5.076453 |
| H | 13.852502 | 19.005450 | 4.494260 |
| H | 11.956823 | 19.888114 | 5.165483 |
| C | 12.527455 | 17.708636 | 7.140885 |
| C | 10.079488 | 17.388193 | 7.790206 |

| | | | |
|---|---|---|---|
| C | 10.882411 | 16.836924 | 5.507039 |
| C | 11.605809 | 20.416996 | 8.702632 |
| C | 10.932700 | 22.234126 | 7.186023 |
| C | 9.165818 | 20.735063 | 8.150470 |
| H | 12.735860 | 16.652160 | 7.371786 |
| H | 13.218067 | 18.015062 | 6.341476 |
| H | 12.750586 | 18.288461 | 8.040336 |
| H | 10.259049 | 16.325241 | 8.016776 |
| H | 10.207612 | 17.943559 | 8.726049 |
| H | 9.029788 | 17.475558 | 7.471978 |
| H | 11.301432 | 15.863176 | 5.804768 |
| H | 9.824212 | 16.665074 | 5.275494 |
| H | 11.417529 | 17.153456 | 4.603958 |
| H | 10.905228 | 22.856773 | 8.093860 |
| H | 11.936575 | 22.321969 | 6.751127 |
| H | 10.200311 | 22.653066 | 6.490201 |
| H | 9.115702 | 21.388285 | 9.035737 |
| H | 8.421132 | 21.113186 | 7.436383 |
| H | 8.864023 | 19.729349 | 8.467044 |
| H | 11.503092 | 21.167716 | 9.501902 |
| H | 11.419983 | 19.439146 | 9.158595 |
| H | 12.645275 | 20.459163 | 8.350140 |

**II-Ts-1(AB)**

| | | | |
|---|---|---|---|
| C | 12.425636 | 17.339524 | -2.918786 |
| C | 12.402547 | 18.720940 | -2.579986 |
| C | 12.599050 | 19.039855 | -1.217203 |
| C | 12.759977 | 18.052960 | -0.204111 |
| C | 12.781627 | 16.712968 | -0.568696 |
| C | 12.621314 | 16.377868 | -1.936909 |
| C | 12.847681 | 18.790036 | 1.061445 |
| C | 12.873914 | 20.254783 | 0.728758 |
| C | 12.632744 | 20.374046 | -0.719822 |
| C | 12.199758 | 19.814885 | -3.465121 |
| C | 12.198673 | 21.115407 | -2.979360 |
| C | 12.421215 | 21.416608 | -1.612646 |
| N | 12.883260 | 18.441062 | 2.314818 |
| Pd | 13.502485 | 20.128568 | 3.589394 |
| C | 14.556918 | 21.629553 | 4.501284 |
| N | 13.096146 | 21.099425 | 1.697610 |
| C | 13.226374 | 22.494982 | 1.451049 |
| C | 12.479106 | 23.444707 | 2.190872 |
| C | 12.670408 | 24.802047 | 1.878166 |
| C | 13.593619 | 25.226034 | 0.924977 |
| C | 14.383303 | 24.279257 | 0.264567 |
| C | 14.197610 | 22.926454 | 0.527673 |
| C | 11.596163 | 23.088762 | 3.364105 |
| C | 10.063726 | 22.955844 | 3.136405 |
| C | 9.703617 | 21.663477 | 2.450468 |
| C | 9.602589 | 20.404343 | 3.109414 |
| C | 9.556625 | 19.232880 | 2.311466 |
| C | 9.397601 | 19.341985 | 0.924102 |
| C | 9.353272 | 20.581709 | 0.295260 |
| C | 9.558963 | 21.725463 | 1.056379 |
| C | 9.640678 | 17.858682 | 2.937629 |
| C | 10.369981 | 16.766330 | 2.103691 |
| C | 11.688911 | 16.277054 | 2.664582 |
| C | 12.865755 | 17.064637 | 2.701896 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 14.065857 | 16.525164 | 3.188963 | H | 10.147896 | 17.936651 | 3.906770 |
| C | 14.126098 | 15.203742 | 3.630289 | H | 9.283525 | 18.438115 | 0.324065 |
| C | 12.974648 | 14.413555 | 3.610647 | H | 9.191671 | 20.651032 | -0.781677 |
| C | 11.780375 | 14.954989 | 3.130974 | H | 9.600792 | 22.703630 | 0.572525 |
| C | 9.198465 | 20.331971 | 4.590319 | H | 9.565796 | 23.055951 | 4.113264 |
| P | 10.108196 | 19.629148 | 6.115065 | H | 9.705507 | 23.803296 | 2.532903 |
| C | 8.968417 | 18.316084 | 6.944455 | H | 11.751940 | 23.874165 | 4.120597 |
| C | 7.494196 | 18.756086 | 6.942585 | H | 11.965710 | 22.145101 | 3.796930 |
| C | 10.561234 | 21.048730 | 7.313087 | H | 12.097713 | 25.547223 | 2.436701 |
| C | 11.249240 | 22.144600 | 6.491489 | H | 13.725561 | 26.290653 | 0.726301 |
| C | 9.304586 | 21.630634 | 7.980725 | H | 15.151539 | 24.593667 | -0.443771 |
| C | 11.579244 | 20.547908 | 8.357202 | H | 14.819372 | 22.180302 | 0.030442 |
| C | 9.109776 | 16.986907 | 6.178781 | H | 15.603117 | 21.292543 | 4.440803 |
| C | 9.424358 | 18.062665 | 8.393678 | H | 14.422236 | 22.556845 | 3.927620 |
| N | 12.936442 | 17.677854 | 6.375500 | H | 14.302605 | 21.781614 | 5.557574 |
| B | 14.135516 | 18.497484 | 6.071908 | H | 8.924791 | 21.341986 | 4.926374 |
| H | 12.427910 | 22.455952 | -1.288023 | H | 8.261197 | 19.757193 | 4.619741 |
| H | 12.034492 | 21.941505 | -3.673499 | H | 8.815144 | 17.237076 | 8.792758 |
| H | 12.042752 | 19.628547 | -4.529830 | H | 10.474890 | 17.748041 | 8.453674 |
| H | 12.289251 | 17.037532 | -3.959366 | H | 9.271189 | 18.924580 | 9.052740 |
| H | 12.644433 | 15.324807 | -2.221843 | H | 6.909683 | 17.990199 | 7.475507 |
| H | 12.917759 | 15.922655 | 0.169818 | H | 7.328028 | 19.711873 | 7.455569 |
| H | 14.950057 | 17.161574 | 3.219574 | H | 7.071456 | 18.824027 | 5.930609 |
| H | 15.072031 | 14.799999 | 3.994630 | H | 8.598938 | 16.204798 | 6.761760 |
| H | 13.006392 | 13.379015 | 3.955958 | H | 8.635230 | 17.018730 | 5.193375 |
| H | 10.882705 | 14.332223 | 3.099080 | H | 10.159297 | 16.682158 | 6.059403 |
| H | 9.713341 | 15.890340 | 2.005840 | H | 11.623041 | 22.908106 | 7.190970 |
| H | 10.530711 | 17.127880 | 1.078915 | H | 12.107084 | 21.761057 | 5.923896 |
| H | 8.616953 | 17.503810 | 3.151184 | H | 10.558117 | 22.644882 | 5.804822 |

| | | | |
|---|---|---|---|
| H | 9.604223 | 22.512634 | 8.567723 |
| H | 8.557772 | 21.971718 | 7.247597 |
| H | 8.818355 | 20.931450 | 8.672739 |
| H | 11.879739 | 21.415484 | 8.965147 |
| H | 11.176945 | 19.797695 | 9.044467 |
| H | 12.488475 | 20.153051 | 7.881944 |
| H | 11.346774 | 18.900806 | 5.859012 |
| H | 13.767906 | 19.486210 | 5.049688 |
| H | 15.044878 | 17.980565 | 5.468749 |
| H | 14.407639 | 19.339684 | 6.901138 |
| H | 12.676160 | 17.627416 | 7.358722 |
| H | 12.909966 | 16.745308 | 5.962983 |

**II-Ts-2**

| | | | |
|---|---|---|---|
| C | 7.643002 | 19.431757 | 1.583529 |
| C | 6.395601 | 18.785136 | 1.800225 |
| C | 6.362094 | 17.389518 | 1.579067 |
| C | 7.479291 | 16.653915 | 1.095546 |
| C | 8.684982 | 17.314624 | 0.898721 |
| C | 8.748572 | 18.705252 | 1.161663 |
| C | 7.012696 | 15.271783 | 0.936215 |
| C | 5.616484 | 15.202220 | 1.492411 |
| C | 5.208847 | 16.586329 | 1.801217 |
| C | 5.178420 | 19.391297 | 2.214303 |
| C | 4.036873 | 18.619453 | 2.382529 |
| C | 4.033745 | 17.215261 | 2.191514 |
| N | 7.560608 | 14.194956 | 0.453906 |
| Pd | 6.488417 | 12.347316 | 1.105241 |
| N | 5.050977 | 14.033707 | 1.615970 |
| C | 3.788474 | 13.881172 | 2.245859 |
| C | 2.771285 | 13.104612 | 1.638651 |
| C | 1.537636 | 13.016211 | 2.307440 |
| C | 1.321824 | 13.603902 | 3.551779 |
| C | 2.369296 | 14.283704 | 4.182667 |
| C | 3.589918 | 14.420296 | 3.531747 |
| C | 2.977100 | 12.271849 | 0.397123 |
| C | 2.637268 | 12.859911 | -0.994429 |
| C | 3.577498 | 13.949900 | -1.435069 |
| C | 4.850620 | 13.719377 | -2.045184 |
| C | 5.660781 | 14.861194 | -2.299654 |
| C | 5.167209 | 16.150540 | -2.040170 |
| C | 3.907175 | 16.362631 | -1.499273 |
| C | 3.132486 | 15.254703 | -1.181539 |
| C | 7.043550 | 14.809163 | -2.915139 |
| C | 8.131291 | 15.645487 | -2.169969 |
| C | 9.146824 | 14.873607 | -1.350371 |
| C | 8.868676 | 14.222825 | -0.122044 |
| C | 9.877270 | 13.514622 | 0.551512 |
| C | 11.177395 | 13.470017 | 0.053077 |
| C | 11.475289 | 14.113678 | -1.149402 |
| C | 10.466320 | 14.796002 | -1.829367 |
| C | 5.218806 | 12.343014 | -2.620005 |
| P | 6.116147 | 10.926917 | -1.630055 |
| C | 7.791578 | 10.472143 | -2.537472 |
| C | 7.633991 | 9.707778 | -3.862112 |
| C | 4.969736 | 9.342765 | -1.842376 |
| C | 3.791257 | 9.437903 | -0.864027 |
| C | 4.394835 | 9.190604 | -3.261480 |
| C | 5.746659 | 8.073763 | -1.446070 |

| | | | |
|---|---|---|---|
| C | 8.591020 | 11.738636 | -2.850896 |
| C | 8.635443 | 9.662846 | -1.529491 |
| H | 3.115366 | 16.655539 | 2.359840 |
| H | 3.108417 | 19.103731 | 2.689651 |
| H | 5.143596 | 20.467352 | 2.396851 |
| H | 7.729691 | 20.507163 | 1.753457 |
| H | 9.698730 | 19.221129 | 1.013594 |
| H | 9.572482 | 16.791379 | 0.543882 |
| H | 9.624135 | 13.012361 | 1.486474 |
| H | 11.950515 | 12.930780 | 0.602596 |
| H | 12.486443 | 14.084018 | -1.558299 |
| H | 10.700729 | 15.293927 | -2.773580 |
| H | 8.702689 | 16.213968 | -2.917113 |
| H | 7.639947 | 16.400401 | -1.540653 |
| H | 6.970067 | 15.200774 | -3.943641 |
| H | 7.389669 | 13.782262 | -3.010350 |
| H | 5.784753 | 17.012128 | -2.303649 |
| H | 3.533660 | 17.374445 | -1.332790 |
| H | 2.140605 | 15.389766 | -0.744622 |
| H | 2.629315 | 12.028096 | -1.715541 |
| H | 1.610259 | 13.253542 | -0.978610 |
| H | 2.364344 | 11.368413 | 0.530540 |
| H | 4.024623 | 11.934058 | 0.363004 |
| H | 0.737886 | 12.431397 | 1.845547 |
| H | 0.355305 | 13.497638 | 4.046767 |
| H | 2.238302 | 14.697271 | 5.183961 |
| H | 4.416206 | 14.938963 | 4.020159 |
| H | 4.291017 | 11.864894 | -2.962087 |
| H | 5.824984 | 12.483588 | -3.525800 |
| H | 9.581952 | 9.379719 | -2.018035 |
| H | 8.891231 | 10.271715 | -0.649707 |
| H | 8.159227 | 8.741501 | -1.180538 |
| H | 8.634253 | 9.594722 | -4.311727 |
| H | 7.219526 | 8.700267 | -3.749277 |
| H | 7.017489 | 10.261077 | -4.585360 |
| H | 9.618509 | 11.441102 | -3.115280 |
| H | 8.188425 | 12.273960 | -3.720836 |
| H | 8.665071 | 12.418941 | -1.994545 |
| H | 3.227628 | 8.492231 | -0.909588 |
| H | 4.121270 | 9.578077 | 0.173429 |
| H | 3.093734 | 10.235908 | -1.133990 |
| H | 3.773615 | 8.280008 | -3.284638 |
| H | 3.735446 | 10.024961 | -3.539055 |
| H | 5.158950 | 9.084635 | -4.037851 |
| H | 5.038430 | 7.229497 | -1.452553 |
| H | 6.557530 | 7.815660 | -2.134479 |
| H | 6.155660 | 8.144078 | -0.427641 |
| C | 5.697616 | 10.862162 | 2.323573 |
| H | 6.090488 | 9.867396 | 2.090932 |
| H | 5.910460 | 11.111315 | 3.369814 |
| H | 4.616915 | 10.913558 | 2.141082 |
| H | 7.637093 | 11.935814 | 2.042732 |
| H | 7.175225 | 11.192905 | 0.344518 |

**II-$H_2$-inter**

| | | | |
|---|---|---|---|
| C | 10.459330 | 14.856124 | -2.091951 |
| C | 9.137184 | 14.876558 | -1.616127 |
| C | 8.861941 | 14.107264 | -0.457111 |
| C | 9.871369 | 13.349279 | 0.156996 |

| | | | |
|---|---|---|---|
| C | 11.175188 | 13.367071 | -0.334576 |
| C | 11.471338 | 14.122796 | -1.470493 |
| C | 8.115182 | 15.717077 | -2.358111 |
| C | 6.969055 | 14.963695 | -3.103931 |
| C | 5.599120 | 15.049942 | -2.461033 |
| C | 4.736835 | 13.936487 | -2.264358 |
| C | 3.469750 | 14.187837 | -1.652739 |
| C | 3.088092 | 15.495134 | -1.320253 |
| C | 3.919074 | 16.580776 | -1.565463 |
| C | 5.167424 | 16.343805 | -2.124156 |
| C | 2.459546 | 13.120300 | -1.317396 |
| C | 2.748881 | 12.340780 | -0.012587 |
| C | 2.676878 | 13.022425 | 1.326556 |
| C | 3.803257 | 13.616699 | 1.937297 |
| C | 3.759236 | 13.982470 | 3.296621 |
| C | 2.583403 | 13.857691 | 4.028233 |
| C | 1.429710 | 13.367735 | 3.405689 |
| C | 1.492237 | 12.945017 | 2.079265 |
| N | 5.020831 | 13.772269 | 1.217984 |
| Pd | 6.467949 | 12.070752 | 0.590243 |
| C | 5.632899 | 10.487419 | 1.648338 |
| C | 5.060931 | 12.563767 | -2.865784 |
| P | 5.907882 | 11.146932 | -1.852033 |
| C | 4.741080 | 9.568395 | -2.158571 |
| C | 5.486690 | 8.276543 | -1.770374 |
| N | 7.548185 | 14.011127 | 0.094442 |
| C | 7.000292 | 15.044793 | 0.659698 |
| C | 7.486794 | 16.397130 | 0.965327 |
| C | 6.387142 | 17.085534 | 1.548099 |
| C | 5.227424 | 16.276653 | 1.693059 |
| C | 5.609905 | 14.933867 | 1.212883 |
| C | 8.700994 | 17.060272 | 0.837308 |
| C | 8.787952 | 18.408613 | 1.262406 |
| C | 7.697674 | 19.095197 | 1.780116 |
| C | 6.443419 | 18.444466 | 1.933426 |
| C | 4.065389 | 16.868784 | 2.169351 |
| C | 4.090117 | 18.240492 | 2.524350 |
| C | 5.240225 | 19.012487 | 2.433129 |
| C | 7.581869 | 10.633530 | -2.767526 |
| C | 8.418629 | 9.795627 | -1.777441 |
| C | 7.412368 | 9.878286 | -4.098266 |
| C | 8.418850 | 11.868523 | -3.103721 |
| C | 3.483737 | 9.607663 | -1.279111 |
| C | 4.238614 | 9.475502 | -3.612644 |
| H | 3.141727 | 16.304335 | 2.283927 |
| H | 3.172215 | 18.696591 | 2.898955 |
| H | 5.223041 | 20.059433 | 2.742912 |
| H | 7.801946 | 20.141815 | 2.074536 |
| H | 9.744396 | 18.925018 | 1.165567 |
| H | 9.577996 | 16.572209 | 0.413357 |
| H | 9.616321 | 12.758186 | 1.037913 |
| H | 11.952287 | 12.787710 | 0.166310 |
| H | 12.484570 | 14.140246 | -1.874869 |
| H | 10.694277 | 15.440373 | -2.985076 |
| H | 8.677828 | 16.307371 | -3.094807 |
| H | 7.675931 | 16.453994 | -1.670089 |
| H | 6.890263 | 15.400784 | -4.113616 |
| H | 7.262975 | 13.927236 | -3.253186 |

| | | | |
|---|---|---|---|
| H | 5.823157 | 17.190475 | -2.339045 |
| H | 3.595132 | 17.596917 | -1.333981 |
| H | 2.100706 | 15.653764 | -0.880946 |
| H | 2.386696 | 12.378271 | -2.129896 |
| H | 1.463671 | 13.582238 | -1.247251 |
| H | 2.035563 | 11.505664 | 0.030334 |
| H | 3.751124 | 11.897943 | -0.103266 |
| H | 0.609098 | 12.499149 | 1.614497 |
| H | 0.497682 | 13.275981 | 3.965480 |
| H | 2.568537 | 14.134852 | 5.083440 |
| H | 4.664871 | 14.360898 | 3.773002 |
| H | 4.120995 | 12.117486 | -3.216133 |
| H | 5.673878 | 12.692994 | -3.768584 |
| H | 9.297218 | 9.402078 | -2.313835 |
| H | 8.793203 | 10.421834 | -0.955208 |
| H | 7.889618 | 8.942464 | -1.341269 |
| H | 8.416453 | 9.753481 | -4.535792 |
| H | 6.982337 | 8.876358 | -4.003862 |
| H | 6.818769 | 10.451149 | -4.824617 |
| H | 9.434700 | 11.533626 | -3.368471 |
| H | 8.029494 | 12.403033 | -3.980522 |
| H | 8.519843 | 12.556567 | -2.260429 |
| H | 2.945190 | 8.657338 | -1.423684 |
| H | 3.705271 | 9.699217 | -0.210011 |
| H | 2.798522 | 10.405529 | -1.580357 |
| H | 3.630508 | 8.560301 | -3.700291 |
| H | 3.577563 | 10.312428 | -3.877792 |
| H | 5.028542 | 9.412925 | -4.364340 |
| H | 4.778012 | 7.437930 | -1.862814 |
| H | 6.342315 | 8.042310 | -2.409958 |
| H | 5.829653 | 8.293382 | -0.726033 |
| H | 6.198062 | 10.261119 | 2.556172 |
| H | 4.632613 | 10.861275 | 1.905706 |
| H | 5.581771 | 9.600183 | 1.012144 |
| H | 7.080163 | 12.304639 | 1.994881 |
| H | 7.589368 | 11.040993 | 0.526702 |

**II-Ts-$CH_4$**

| | | | |
|---|---|---|---|
| C | 11.241924 | 21.224226 | -3.422142 |
| C | 11.767093 | 20.226491 | -2.560768 |
| C | 11.976985 | 20.586756 | -1.216884 |
| C | 11.681804 | 21.857649 | -0.722572 |
| C | 11.144340 | 22.818626 | -1.582446 |
| C | 10.913292 | 22.493923 | -2.917291 |
| C | 12.124880 | 18.814165 | -2.984495 |
| C | 10.942409 | 17.816146 | -3.209595 |
| C | 10.620780 | 17.529298 | -4.660697 |
| C | 9.328903 | 17.627866 | -5.244387 |
| C | 9.217758 | 17.364878 | -6.643424 |
| C | 10.331580 | 16.926041 | -7.372430 |
| C | 11.573424 | 16.759123 | -6.773980 |
| C | 11.706803 | 17.083647 | -5.432142 |
| C | 7.967507 | 17.575361 | -7.454063 |
| C | 7.810519 | 19.030318 | -7.970674 |
| C | 8.738734 | 19.522110 | -9.052091 |
| C | 9.923446 | 20.252335 | -8.778865 |
| C | 10.604264 | 20.888990 | -9.838062 |
| C | 10.190488 | 20.730458 | -11.155557 |
| C | 9.080915 | 19.927522 | -11.443389 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 8.365435 | 19.351540 | -10.395565 | H | 16.632873 | 19.320047 | -8.546442 |
| N | 10.337230 | 20.452962 | -7.444290 | H | 17.230290 | 20.345430 | -6.160189 |
| Pd | 9.058056 | 21.531799 | -5.752437 | H | 16.389083 | 21.302422 | -4.049268 |
| C | 7.505210 | 22.775017 | -6.539280 | H | 13.964856 | 21.545752 | -3.598226 |
| C | 8.068750 | 17.738739 | -4.362808 | H | 10.485029 | 23.223339 | -3.607207 |
| P | 7.159495 | 19.367759 | -3.909306 | H | 10.904075 | 23.818827 | -1.218297 |
| C | 5.321727 | 19.285912 | -4.512230 | H | 11.869684 | 22.094036 | 0.325908 |
| C | 4.668241 | 17.947831 | -4.124513 | H | 12.389248 | 19.833456 | -0.540886 |
| N | 10.961777 | 20.984091 | -4.799823 | H | 12.767150 | 18.405914 | -2.190831 |
| C | 11.921236 | 20.751374 | -5.648446 | H | 12.750070 | 18.836496 | -3.886584 |
| C | 11.579005 | 20.380061 | -7.070350 | H | 11.223077 | 16.861814 | -2.733655 |
| C | 12.850272 | 19.989665 | -7.720002 | H | 10.065519 | 18.171590 | -2.672627 |
| C | 13.877406 | 20.271804 | -6.777002 | H | 12.677683 | 16.961227 | -4.946626 |
| C | 13.384715 | 20.764474 | -5.536934 | H | 12.424352 | 16.383372 | -7.344604 |
| C | 13.213146 | 19.415528 | -8.931437 | H | 10.201614 | 16.700810 | -8.433044 |
| C | 14.583933 | 19.169207 | -9.194250 | H | 7.068314 | 17.314714 | -6.875794 |
| C | 15.586021 | 19.500388 | -8.292866 | H | 7.976503 | 16.890718 | -8.315311 |
| C | 15.253125 | 20.072198 | -7.035139 | H | 6.788844 | 19.129629 | -8.368484 |
| C | 14.292909 | 21.144606 | -4.556687 | H | 7.895400 | 19.716698 | -7.109067 |
| C | 15.677573 | 20.996354 | -4.818006 | H | 7.460849 | 18.778366 | -10.615407 |
| C | 16.155267 | 20.463649 | -6.007888 | H | 8.752165 | 19.787485 | -12.474235 |
| C | 7.167617 | 19.754043 | -2.010706 | H | 10.725740 | 21.241880 | -11.957458 |
| C | 8.514750 | 19.399671 | -1.377888 | H | 11.454884 | 21.531319 | -9.607526 |
| C | 6.986083 | 21.280779 | -1.874619 | H | 7.914248 | 23.744740 | -6.847270 |
| C | 6.088080 | 18.978780 | -1.235379 | H | 7.354612 | 22.147789 | -7.433376 |
| C | 4.519201 | 20.471468 | -3.942267 | H | 6.528008 | 22.940947 | -6.067459 |
| C | 5.277783 | 19.432381 | -6.038497 | H | 7.279500 | 17.125955 | -4.819854 |
| H | 12.471611 | 19.160580 | -9.687031 | H | 8.273758 | 17.267170 | -3.390750 |
| H | 14.856969 | 18.720095 | -10.150762 | H | 7.934299 | 20.508304 | -4.658129 |

| | | | |
|---|---|---|---|
| H | 7.014829 | 21.530167 | -0.802317 |
| H | 7.806245 | 21.823372 | -2.365632 |
| H | 6.036831 | 21.652310 | -2.272320 |
| H | 6.204150 | 19.223727 | -0.167537 |
| H | 5.061874 | 19.238898 | -1.513592 |
| H | 6.212907 | 17.890201 | -1.330765 |
| H | 8.498485 | 19.762857 | -0.338089 |
| H | 8.681267 | 18.315079 | -1.329829 |
| H | 9.360070 | 19.890722 | -1.872200 |
| H | 4.220568 | 19.491991 | -6.340917 |
| H | 5.776442 | 20.346050 | -6.385233 |
| H | 5.709805 | 18.569371 | -6.551022 |
| H | 3.637237 | 17.945967 | -4.512610 |
| H | 5.177555 | 17.085996 | -4.579192 |
| H | 4.612871 | 17.784975 | -3.042978 |
| H | 3.511684 | 20.427399 | -4.383647 |
| H | 4.394185 | 20.448503 | -2.855387 |
| H | 4.956894 | 21.437466 | -4.229948 |
| H | 8.138347 | 22.640798 | -5.123908 |

**III**

| | | | |
|---|---|---|---|
| C | 15.735629 | 20.132281 | -6.368683 |
| C | 14.783816 | 19.992817 | -7.414963 |
| C | 13.432721 | 20.241229 | -7.076525 |
| C | 13.011760 | 20.542708 | -5.752684 |
| C | 13.966766 | 20.668177 | -4.751064 |
| C | 15.328829 | 20.471759 | -5.084940 |
| C | 11.546074 | 20.614495 | -5.797234 |
| C | 11.125879 | 20.510176 | -7.253124 |
| C | 12.363214 | 20.183618 | -8.009319 |
| C | 15.043108 | 19.617415 | -8.760547 |
| C | 13.995142 | 19.501596 | -9.662326 |
| C | 12.652214 | 19.787604 | -9.308639 |
| N | 10.673962 | 20.701203 | -4.843787 |
| Pd | 8.549625 | 20.409497 | -5.022366 |
| C | 6.670584 | 24.005132 | -7.081437 |
| N | 9.884961 | 20.690423 | -7.565766 |
| C | 9.430547 | 20.810528 | -8.886292 |
| C | 8.152216 | 20.297767 | -9.239099 |
| C | 7.742035 | 20.413441 | -10.577318 |
| C | 8.503477 | 21.085786 | -11.531487 |
| C | 9.700189 | 21.700875 | -11.144431 |
| C | 10.156091 | 21.559986 | -9.840214 |
| C | 7.167123 | 19.784418 | -8.222160 |
| C | 7.116056 | 18.266067 | -7.892418 |
| C | 8.341821 | 17.794585 | -7.162655 |
| C | 8.491769 | 17.798431 | -5.734312 |
| C | 9.788780 | 17.481078 | -5.218038 |
| C | 10.813420 | 17.085590 | -6.093944 |
| C | 10.624165 | 17.002780 | -7.465505 |
| C | 9.395898 | 17.384643 | -7.988345 |
| C | 10.158355 | 17.452790 | -3.748734 |
| C | 11.488256 | 18.189241 | -3.381241 |
| C | 11.390221 | 19.566796 | -2.752777 |
| C | 11.067564 | 20.745114 | -3.466423 |
| C | 11.043115 | 21.991762 | -2.824428 |
| C | 11.363751 | 22.098741 | -1.472271 |
| C | 11.691677 | 20.950521 | -0.747128 |
| C | 11.701619 | 19.712161 | -1.389476 |

| | | | |
|---|---|---|---|
| C | 7.238016 | 17.816154 | -4.809681 |
| P | 6.636025 | 19.526246 | -4.177332 |
| C | 6.613794 | 19.554820 | -2.225275 |
| C | 5.452834 | 18.744248 | -1.621831 |
| C | 4.786600 | 19.825160 | -4.755826 |
| C | 4.755169 | 20.303251 | -6.211213 |
| C | 3.962772 | 18.529418 | -4.647348 |
| C | 4.133273 | 20.950829 | -3.932316 |
| C | 7.910503 | 18.961436 | -1.666286 |
| C | 6.580871 | 21.025364 | -1.763453 |
| H | 11.874232 | 19.702504 | -10.065964 |
| H | 14.208141 | 19.196079 | -10.688275 |
| H | 16.067307 | 19.412877 | -9.079295 |
| H | 16.794784 | 19.966822 | -6.578494 |
| H | 16.079344 | 20.578986 | -4.300117 |
| H | 13.692074 | 20.909404 | -3.725072 |
| H | 10.772985 | 22.875876 | -3.404506 |
| H | 11.354069 | 23.076918 | -0.988572 |
| H | 11.942902 | 21.018456 | 0.312378 |
| H | 11.967543 | 18.816719 | -0.821859 |
| H | 12.035433 | 17.559109 | -2.665860 |
| H | 12.129343 | 18.245545 | -4.272702 |
| H | 10.279661 | 16.395193 | -3.458828 |
| H | 9.350648 | 17.843373 | -3.133739 |
| H | 11.775927 | 16.789207 | -5.672792 |
| H | 11.424729 | 16.649876 | -8.117821 |
| H | 9.228358 | 17.357283 | -9.066799 |
| H | 6.203108 | 18.074294 | -7.310656 |
| H | 7.008691 | 17.697317 | -8.828113 |
| H | 6.170442 | 20.071070 | -8.588493 |
| H | 7.333779 | 20.329998 | -7.277473 |
| H | 6.768781 | 20.004379 | -10.861132 |
| H | 8.142567 | 21.175368 | -12.557203 |
| H | 10.271120 | 22.297754 | -11.857846 |
| H | 11.076398 | 22.056065 | -9.530426 |
| H | 7.171931 | 24.980381 | -7.086560 |
| H | 6.592460 | 23.632910 | -8.110577 |
| H | 5.665869 | 24.118184 | -6.654860 |
| H | 6.403589 | 17.339547 | -5.340927 |
| H | 7.432774 | 17.194092 | -3.925497 |
| H | 8.152797 | 21.681357 | -4.279694 |
| H | 6.590278 | 21.037938 | -0.661846 |
| H | 7.476000 | 21.561602 | -2.109077 |
| H | 5.698589 | 21.582775 | -2.089782 |
| H | 5.571418 | 18.743887 | -0.526622 |
| H | 4.461061 | 19.156482 | -1.834490 |
| H | 5.472404 | 17.693947 | -1.947424 |
| H | 7.919219 | 19.134648 | -0.578344 |
| H | 7.971762 | 17.873796 | -1.810519 |
| H | 8.802287 | 19.450449 | -2.079039 |
| H | 3.718925 | 20.587585 | -6.454930 |
| H | 5.391002 | 21.182741 | -6.374730 |
| H | 5.040058 | 19.515729 | -6.912345 |
| H | 2.929530 | 18.751185 | -4.959812 |
| H | 4.333786 | 17.743627 | -5.320936 |
| H | 3.918283 | 18.119795 | -3.632411 |
| H | 3.132668 | 21.130465 | -4.356619 |
| H | 3.992864 | 20.712347 | -2.873716 |

| | | | |
|---|---|---|---|
| H | 4.692505 | 21.893831 | -4.015367 |
| H | 7.255320 | 23.297962 | -6.478224 |

**III-Ts-1(AB)**

| | | | |
|---|---|---|---|
| C | 12.509183 | 17.242697 | -2.685911 |
| C | 12.494710 | 18.611225 | -2.370309 |
| C | 12.702068 | 18.970363 | -1.016589 |
| C | 12.934720 | 17.985232 | -0.045721 |
| C | 12.960260 | 16.635292 | -0.395640 |
| C | 12.731410 | 16.258127 | -1.720767 |
| C | 12.341675 | 19.622898 | -3.486096 |
| C | 11.011294 | 20.430777 | -3.516291 |
| C | 11.112320 | 21.911717 | -3.213742 |
| C | 10.060927 | 22.611737 | -2.565870 |
| C | 10.294904 | 23.958769 | -2.166275 |
| C | 11.463328 | 24.612413 | -2.585223 |
| C | 12.419808 | 23.964093 | -3.354613 |
| C | 12.255603 | 22.609332 | -3.624987 |
| C | 9.417749 | 24.725890 | -1.212976 |
| C | 9.739332 | 24.381516 | 0.268499 |
| C | 11.008941 | 24.908205 | 0.893193 |
| C | 12.207142 | 24.157770 | 1.012509 |
| C | 13.251413 | 24.632403 | 1.831269 |
| C | 13.168273 | 25.869555 | 2.459419 |
| C | 12.030967 | 26.662219 | 2.273341 |
| C | 10.972604 | 26.169957 | 1.512608 |
| N | 12.357418 | 22.878476 | 0.404538 |
| Pd | 11.049698 | 21.168195 | 0.735887 |
| H | 10.088003 | 21.757687 | 1.799785 |
| C | 8.624059 | 22.067883 | -2.624572 |
| P | 7.799172 | 20.615256 | -1.712035 |
| C | 6.550722 | 21.176378 | -0.375080 |
| C | 6.282060 | 19.990785 | 0.573253 |
| N | 12.614208 | 20.324932 | -0.572747 |
| C | 13.588706 | 21.161872 | -0.759854 |
| C | 14.911207 | 21.050590 | -1.383180 |
| C | 15.456635 | 22.364276 | -1.374794 |
| C | 14.611413 | 23.326016 | -0.749900 |
| C | 13.427900 | 22.579971 | -0.280452 |
| C | 15.652592 | 20.013570 | -1.933957 |
| C | 16.924143 | 20.308324 | -2.485795 |
| C | 17.439988 | 21.597106 | -2.511957 |
| C | 16.705709 | 22.680861 | -1.955895 |
| C | 15.015343 | 24.655218 | -0.754927 |
| C | 16.253530 | 24.996254 | -1.354302 |
| C | 17.090998 | 24.048793 | -1.927049 |
| C | 6.972795 | 19.518363 | -3.053459 |
| C | 6.072708 | 18.459418 | -2.391993 |
| C | 6.144774 | 20.361175 | -4.041711 |
| C | 8.078200 | 18.780400 | -3.828918 |
| C | 7.190277 | 22.299737 | 0.445516 |

| | | | |
|---|---|---|---|
| C | 5.248002 | 21.695320 | -1.004685 |
| B | 9.789907 | 18.469810 | 1.297387 |
| N | 9.407343 | 17.888645 | 0.011924 |
| H | 14.408334 | 25.437616 | -0.302090 |
| H | 16.561539 | 26.043262 | -1.349100 |
| H | 18.046481 | 24.352489 | -2.359991 |
| H | 18.417531 | 21.783867 | -2.961981 |
| H | 17.510408 | 19.492528 | -2.911819 |
| H | 15.278427 | 18.990093 | -1.948634 |
| H | 13.089503 | 18.294128 | 0.987712 |
| H | 13.148811 | 15.882928 | 0.371864 |
| H | 12.740668 | 15.204981 | -2.005857 |
| H | 12.357877 | 16.949598 | -3.727934 |
| H | 12.447957 | 19.077441 | -4.434212 |
| H | 13.195707 | 20.313505 | -3.450037 |
| H | 10.566684 | 20.308979 | -4.519010 |
| H | 10.312717 | 19.962049 | -2.811909 |
| H | 13.026536 | 22.087868 | -4.193799 |
| H | 13.300031 | 24.497830 | -3.716773 |
| H | 11.605299 | 25.657318 | -2.301004 |
| H | 8.347685 | 24.523556 | -1.377090 |
| H | 9.547252 | 25.805724 | -1.380210 |
| H | 8.907632 | 24.761319 | 0.882991 |
| H | 9.745355 | 23.284681 | 0.373952 |
| H | 10.058820 | 26.762732 | 1.421921 |
| H | 11.953415 | 27.639413 | 2.752339 |
| H | 13.982803 | 26.208279 | 3.101687 |
| H | 14.127009 | 24.000271 | 1.984671 |
| H | 7.926940 | 22.897340 | -2.439571 |
| H | 8.452911 | 21.778547 | -3.673100 |
| H | 5.710448 | 17.785920 | -3.183965 |
| H | 6.618645 | 17.842452 | -1.664990 |
| H | 5.189835 | 18.888022 | -1.903768 |
| H | 5.716421 | 19.678313 | -4.791619 |
| H | 5.311378 | 20.889309 | -3.565038 |
| H | 6.751525 | 21.093493 | -4.592446 |
| H | 7.590514 | 18.068799 | -4.513460 |
| H | 8.682170 | 19.457401 | -4.442936 |
| H | 8.745600 | 18.206948 | -3.169938 |
| H | 6.506311 | 22.542878 | 1.273849 |
| H | 8.151414 | 21.996684 | 0.882068 |
| H | 7.327698 | 23.214906 | -0.142120 |
| H | 4.622915 | 22.101848 | -0.194718 |
| H | 5.419331 | 22.513873 | -1.719577 |
| H | 4.663896 | 20.910288 | -1.500324 |
| H | 5.613178 | 20.351320 | 1.370315 |
| H | 5.782900 | 19.144466 | 0.090366 |
| H | 7.204174 | 19.637286 | 1.055855 |
| H | 8.739026 | 19.747290 | -1.042511 |
| H | 9.987856 | 20.018531 | 1.101033 |

| | | | |
|---|---|---|---|
| H | 10.886342 | 18.240856 | 1.736349 |
| H | 8.887276 | 18.686745 | 2.073513 |
| H | 8.480897 | 17.479440 | -0.072689 |
| H | 10.098771 | 17.347461 | -0.504279 |

**III-$H_2$**

| | | | |
|---|---|---|---|
| C | 11.042744 | 21.156477 | -3.550998 |
| C | 11.683466 | 20.190121 | -2.756805 |
| C | 11.874445 | 20.507391 | -1.391949 |
| C | 11.459927 | 21.742736 | -0.873355 |
| C | 10.826196 | 22.678370 | -1.691111 |
| C | 10.616199 | 22.383142 | -3.039418 |
| C | 12.087659 | 18.872374 | -3.386382 |
| C | 13.615768 | 18.567324 | -3.515857 |
| C | 14.149919 | 17.554788 | -2.522046 |
| C | 15.320787 | 17.732334 | -1.730965 |
| C | 15.666334 | 16.672356 | -0.830825 |
| C | 14.893772 | 15.501943 | -0.787107 |
| C | 13.786072 | 15.320315 | -1.604579 |
| C | 13.425788 | 16.352603 | -2.457902 |
| C | 16.839338 | 16.669586 | 0.119425 |
| C | 16.611265 | 17.363026 | 1.485999 |
| C | 15.606338 | 16.870817 | 2.498792 |
| C | 14.275416 | 17.349330 | 2.590861 |
| C | 13.509829 | 17.093682 | 3.744225 |
| C | 14.003947 | 16.295656 | 4.770202 |
| C | 15.277214 | 15.730305 | 4.649860 |
| C | 16.057961 | 16.035605 | 3.537157 |
| N | 13.675012 | 18.140184 | 1.561551 |
| Pd | 14.538199 | 19.874618 | 0.475068 |
| N | 12.537401 | 19.613959 | -0.489324 |
| C | 11.870024 | 18.633557 | 0.036147 |
| C | 10.516485 | 18.106935 | -0.169987 |
| C | 10.489026 | 16.853001 | 0.503187 |
| C | 11.693892 | 16.553922 | 1.201060 |
| C | 12.555878 | 17.736567 | 1.030044 |
| C | 9.385744 | 18.530689 | -0.856037 |
| C | 8.247801 | 17.686440 | -0.872285 |
| C | 8.235745 | 16.444780 | -0.250259 |
| C | 9.377413 | 15.981183 | 0.459532 |
| C | 11.809083 | 15.316572 | 1.820799 |
| C | 10.716023 | 14.416828 | 1.761371 |
| C | 9.525237 | 14.731972 | 1.121270 |
| C | 16.276731 | 18.915366 | -1.990555 |
| P | 16.177005 | 20.576751 | -0.979186 |
| C | 17.997175 | 20.893938 | -0.330228 |
| C | 18.072084 | 22.283313 | 0.331130 |
| C | 15.749733 | 22.149311 | -2.080016 |
| C | 15.143100 | 23.173319 | -1.099274 |
| C | 16.911890 | 22.777070 | -2.867455 |
| C | 14.679712 | 21.801120 | -3.114051 |
| C | 18.403392 | 19.890826 | 0.753586 |
| C | 19.026394 | 20.752594 | -1.470700 |

| | | | |
|---|---|---|---|
| H | 12.712451 | 15.026732 | 2.354355 |
| H | 10.814223 | 13.447192 | 2.252233 |
| H | 8.699580 | 14.017267 | 1.118660 |
| H | 7.344071 | 15.816606 | -0.305449 |
| H | 7.356122 | 18.023025 | -1.403312 |
| H | 9.356143 | 19.488385 | -1.374280 |
| H | 11.632840 | 21.954336 | 0.183729 |
| H | 10.497733 | 23.630932 | -1.272244 |
| H | 10.121137 | 23.103534 | -3.692194 |
| H | 10.876915 | 20.929484 | -4.607034 |
| H | 11.645065 | 18.857026 | -4.392546 |
| H | 11.604007 | 18.049251 | -2.839512 |
| H | 13.782858 | 18.160912 | -4.527496 |
| H | 14.178586 | 19.498073 | -3.475637 |
| H | 12.569214 | 16.219718 | -3.121900 |
| H | 13.223078 | 14.385605 | -1.587201 |
| H | 15.202291 | 14.704068 | -0.108527 |
| H | 17.717266 | 17.151174 | -0.339063 |
| H | 17.138586 | 15.625324 | 0.294979 |
| H | 17.585292 | 17.368179 | 1.999272 |
| H | 16.357728 | 18.410935 | 1.278726 |
| H | 17.079687 | 15.651499 | 3.479754 |
| H | 15.675685 | 15.090992 | 5.439091 |
| H | 13.398850 | 16.120666 | 5.661073 |
| H | 12.516282 | 17.537510 | 3.825266 |
| H | 17.305657 | 18.572977 | -1.812860 |
| H | 16.234766 | 19.200295 | -3.051089 |
| H | 14.846905 | 24.068543 | -1.670218 |
| H | 14.244071 | 22.769233 | -0.612898 |
| H | 15.838286 | 23.494097 | -0.315496 |
| H | 16.496851 | 23.624216 | -3.437775 |
| H | 17.719878 | 23.178558 | -2.248358 |
| H | 17.338307 | 22.080391 | -3.603172 |
| H | 14.336306 | 22.738104 | -3.580744 |
| H | 15.077010 | 21.171087 | -3.922547 |
| H | 13.801778 | 21.328552 | -2.667417 |
| H | 19.431037 | 20.135545 | 1.065851 |
| H | 17.767096 | 19.955796 | 1.645334 |
| H | 18.416974 | 18.857721 | 0.391076 |
| H | 20.024010 | 20.974275 | -1.059490 |
| H | 19.068212 | 19.725497 | -1.860559 |
| H | 18.863780 | 21.430358 | -2.311499 |
| H | 19.071001 | 22.392656 | 0.782100 |
| H | 17.938777 | 23.120380 | -0.360626 |
| H | 17.335468 | 22.379510 | 1.142458 |
| H | 15.733319 | 20.180066 | 1.393273 |

**III-Ts-2**

| | | | |
|---|---|---|---|
| C | 11.515581 | 19.553441 | -1.554944 |
| C | 11.482716 | 20.967648 | -1.669028 |
| C | 11.773336 | 21.709836 | -0.509820 |
| C | 12.093307 | 21.109773 | 0.708321 |
| C | 12.145325 | 19.716167 | 0.792795 |

| | | | |
|---|---|---|---|
| C | 11.874140 | 18.948657 | -0.337461 |
| C | 11.154290 | 21.729548 | -2.939402 |
| C | 12.263557 | 21.800305 | -4.039879 |
| C | 12.043015 | 20.881281 | -5.223799 |
| C | 12.997949 | 19.963983 | -5.741056 |
| C | 12.595011 | 19.142005 | -6.837207 |
| C | 11.341005 | 19.324235 | -7.435847 |
| C | 10.445654 | 20.278991 | -6.972329 |
| C | 10.799014 | 21.028301 | -5.860115 |
| C | 13.415436 | 18.017509 | -7.406958 |
| C | 13.200669 | 16.660514 | -6.683445 |
| C | 11.876335 | 15.957806 | -6.830066 |
| C | 10.820202 | 16.095535 | -5.894759 |
| C | 9.722998 | 15.212155 | -5.951032 |
| C | 9.609586 | 14.272333 | -6.968316 |
| C | 10.596774 | 14.199063 | -7.957091 |
| C | 11.715930 | 15.023845 | -7.866929 |
| N | 10.925377 | 17.024995 | -4.833660 |
| Pd | 12.611477 | 17.012100 | -3.255237 |
| C | 14.480830 | 20.048707 | -5.328019 |
| P | 15.321345 | 18.954298 | -3.996412 |
| C | 16.786219 | 17.950141 | -4.764227 |
| C | 16.232955 | 16.802763 | -5.620240 |
| N | 11.265632 | 18.681977 | -2.653565 |
| C | 10.095261 | 18.610749 | -3.213758 |
| C | 9.921921 | 17.757550 | -4.445988 |
| C | 8.551817 | 18.009888 | -4.943668 |
| C | 7.929942 | 18.847840 | -3.975862 |
| C | 8.791849 | 19.210363 | -2.904860 |
| C | 7.827369 | 17.675597 | -6.080635 |
| C | 6.497182 | 18.145748 | -6.214349 |
| C | 5.877256 | 18.914267 | -5.239114 |
| C | 6.591522 | 19.293963 | -4.070935 |
| C | 8.284273 | 19.972133 | -1.860063 |
| C | 6.930699 | 20.386620 | -1.916046 |
| C | 6.104864 | 20.077666 | -2.988806 |
| C | 15.974135 | 19.952946 | -2.475047 |
| C | 17.335810 | 20.618894 | -2.737300 |
| C | 14.994534 | 21.063431 | -2.091387 |
| C | 16.032087 | 18.965419 | -1.290247 |
| C | 17.666588 | 18.855828 | -5.643386 |
| C | 17.624651 | 17.288836 | -3.652948 |
| H | 8.252892 | 17.052472 | -6.865519 |
| H | 5.938004 | 17.873593 | -7.111316 |
| H | 4.840599 | 19.232545 | -5.368415 |
| H | 5.073296 | 20.436011 | -3.003828 |
| H | 6.531891 | 20.979568 | -1.091317 |
| H | 8.902157 | 20.259305 | -1.009639 |
| H | 11.918373 | 17.858542 | -0.300115 |
| H | 12.396146 | 19.225098 | 1.734491 |
| H | 12.301988 | 21.726857 | 1.583617 |
| H | 11.743609 | 22.800427 | -0.576307 |
| H | 10.918690 | 22.758426 | -2.631122 |
| H | 10.231462 | 21.338719 | -3.387397 |

| | | | |
|---|---|---|---|
| H | 12.281976 | 22.835145 | -4.419953 |
| H | 13.236485 | 21.634738 | -3.580534 |
| H | 10.103954 | 21.781828 | -5.482161 |
| H | 9.487159 | 20.436536 | -7.469791 |
| H | 11.081285 | 18.702845 | -8.295512 |
| H | 14.488751 | 18.256367 | -7.381652 |
| H | 13.163201 | 17.892960 | -8.470699 |
| H | 13.965204 | 15.964455 | -7.061103 |
| H | 13.392634 | 16.796343 | -5.602240 |
| H | 12.519642 | 14.917776 | -8.600509 |
| H | 10.514925 | 13.472613 | -8.767060 |
| H | 8.758879 | 13.588878 | -6.983212 |
| H | 8.969090 | 15.257049 | -5.164204 |
| H | 15.094537 | 19.881536 | -6.224015 |
| H | 14.704203 | 21.077159 | -5.011746 |
| H | 16.362276 | 19.524155 | -0.400382 |
| H | 15.039006 | 18.547535 | -1.071498 |
| H | 16.732273 | 18.137418 | -1.435575 |
| H | 17.598839 | 21.205228 | -1.842469 |
| H | 18.154751 | 19.913756 | -2.910942 |
| H | 17.294004 | 21.322973 | -3.581397 |
| H | 15.339548 | 21.497527 | -1.139940 |
| H | 14.982582 | 21.881215 | -2.824624 |
| H | 13.977251 | 20.693383 | -1.922207 |
| H | 17.084711 | 16.184474 | -5.944077 |
| H | 15.545050 | 16.158019 | -5.058380 |
| H | 15.734213 | 17.159350 | -6.524827 |
| H | 18.477866 | 18.240482 | -6.063468 |
| H | 17.114366 | 19.275850 | -6.496221 |
| H | 18.130924 | 19.681052 | -5.091882 |
| H | 18.393970 | 16.674944 | -4.147202 |
| H | 18.149128 | 17.996097 | -3.003404 |
| H | 17.020910 | 16.611990 | -3.032394 |
| H | 13.506630 | 15.695133 | -3.133456 |
| H | 13.597133 | 16.366618 | -2.187323 |
| H | 14.214346 | 17.996691 | -3.504795 |

**II-Ts-3**

| | | | |
|---|---|---|---|
| C | 10.446080 | 14.807927 | -2.040340 |
| C | 9.109530 | 14.837260 | -1.557729 |
| C | 8.838690 | 14.068924 | -0.402501 |
| C | 9.806611 | 13.249576 | 0.238728 |
| C | 11.105998 | 13.257349 | -0.250257 |
| C | 11.407492 | 14.051426 | -1.384645 |
| C | 9.104609 | 12.600175 | 1.363345 |
| C | 7.727858 | 13.192659 | 1.421969 |
| C | 7.568714 | 14.049060 | 0.238137 |
| C | 8.015218 | 15.555302 | -2.112341 |
| C | 6.761285 | 15.494978 | -1.518751 |
| C | 6.518669 | 14.756919 | -0.334006 |
| N | 6.923730 | 12.862661 | 2.389982 |
| Pd | 7.615644 | 10.993037 | 3.480054 |
| P | 7.822336 | 11.820916 | 5.986418 |
| C | 5.994496 | 12.172787 | 6.652418 |
| C | 5.371360 | 13.363931 | 5.922295 |
| N | 9.434062 | 11.664857 | 2.208674 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 10.655598 | 10.962288 | 2.008691 | C | 5.872084 | 12.496369 | 8.151596 |
| C | 11.598733 | 10.840503 | 3.053013 | H | 11.893852 | 12.663834 | 0.210016 |
| C | 12.804704 | 10.177923 | 2.766082 | H | 12.431216 | 14.049821 | -1.762706 |
| C | 13.052181 | 9.594568 | 1.524927 | H | 10.714235 | 15.385058 | -2.927839 |
| C | 12.064685 | 9.636261 | 0.534424 | H | 8.163992 | 16.154995 | -3.012823 |
| C | 10.877344 | 10.318272 | 0.775927 | H | 5.932787 | 16.044448 | -1.968535 |
| C | 11.294710 | 11.242442 | 4.472012 | H | 5.523343 | 14.762361 | 0.108550 |
| C | 11.636444 | 12.658075 | 4.991854 | H | 4.710212 | 11.548819 | 1.969321 |
| C | 10.822334 | 13.769850 | 4.380992 | H | 2.378007 | 12.401151 | 2.106541 |
| C | 9.478634 | 14.085612 | 4.752880 | H | 1.977123 | 14.798209 | 2.718146 |
| C | 8.832845 | 15.130750 | 4.037445 | H | 3.905922 | 16.291497 | 3.144592 |
| C | 9.534023 | 15.858588 | 3.061868 | H | 6.050229 | 16.787600 | 3.112118 |
| C | 10.851568 | 15.568302 | 2.735594 | H | 7.171829 | 15.851056 | 2.152923 |
| C | 11.476228 | 14.512287 | 3.387399 | H | 7.458897 | 16.538924 | 4.854277 |
| C | 7.412801 | 15.581600 | 4.308077 | H | 6.912582 | 14.884375 | 4.976137 |
| C | 6.527152 | 15.799954 | 3.042246 | H | 9.035844 | 16.695506 | 2.568073 |
| C | 5.413039 | 14.801518 | 2.795180 | H | 11.386049 | 16.160572 | 1.990871 |
| C | 4.083044 | 15.245728 | 2.881522 | H | 12.511757 | 14.261763 | 3.147172 |
| C | 2.993075 | 14.407838 | 2.642251 | H | 11.512690 | 12.640454 | 6.087667 |
| C | 3.215336 | 13.071865 | 2.305244 | H | 12.703496 | 12.860101 | 4.816723 |
| C | 4.521140 | 12.591318 | 2.228157 | H | 11.828752 | 10.525716 | 5.111803 |
| C | 5.615928 | 13.439771 | 2.456189 | H | 10.220459 | 11.083802 | 4.639444 |
| C | 8.839281 | 13.472828 | 6.005997 | H | 13.549554 | 10.086463 | 3.560989 |
| C | 8.297466 | 9.084596 | 3.931838 | H | 13.993297 | 9.073129 | 1.343905 |
| C | 8.632275 | 10.774873 | 7.470542 | H | 12.217460 | 9.133806 | -0.422061 |
| C | 8.952951 | 11.646086 | 8.701754 | H | 10.100656 | 10.358610 | 0.010432 |
| C | 7.705214 | 9.612613 | 7.874836 | H | 9.641670 | 13.274063 | 6.727553 |
| C | 9.959504 | 10.128638 | 7.051246 | H | 8.192830 | 14.218103 | 6.489890 |
| C | 5.134628 | 10.942659 | 6.294377 | H | 4.125123 | 11.095535 | 6.708947 |

| | | | |
|---|---|---|---|
| H | 5.033847 | 10.841011 | 5.204973 |
| H | 5.513604 | 9.994955 | 6.688236 |
| H | 4.819957 | 12.761272 | 8.348186 |
| H | 6.118840 | 11.664920 | 8.818809 |
| H | 6.476451 | 13.369849 | 8.436094 |
| H | 4.287216 | 13.360632 | 6.120325 |
| H | 5.753308 | 14.322105 | 6.298065 |
| H | 5.497777 | 13.310550 | 4.837330 |
| H | 10.303975 | 9.500335 | 7.888466 |
| H | 9.865585 | 9.481307 | 6.172536 |
| H | 10.741260 | 10.872982 | 6.874925 |
| H | 9.344263 | 10.982369 | 9.490294 |
| H | 9.743154 | 12.381236 | 8.496388 |
| H | 8.094459 | 12.176002 | 9.119992 |
| H | 8.237210 | 9.003301 | 8.622643 |
| H | 6.764086 | 9.929276 | 8.333484 |
| H | 7.474463 | 8.951168 | 7.028175 |
| H | 7.987777 | 8.400571 | 3.136448 |
| H | 9.388097 | 9.193925 | 3.938949 |
| H | 7.912372 | 8.746569 | 4.897179 |
| H | 6.777351 | 10.214898 | 2.368531 |
| H | 6.238384 | 10.236292 | 3.491878 |

**II(Pd-P system) with alkene**

| | | | |
|---|---|---|---|
| C | 10.808008 | 14.892132 | 2.857237 |
| C | 10.914636 | 16.232429 | 2.442835 |
| C | 12.166035 | 16.868015 | 2.639502 |
| C | 13.227425 | 16.176802 | 3.245745 |
| C | 13.089973 | 14.844608 | 3.627853 |
| C | 11.867725 | 14.196492 | 3.438741 |
| C | 9.705825 | 16.862038 | 1.771907 |
| C | 8.896846 | 17.958000 | 2.540865 |
| C | 9.149102 | 19.377672 | 2.065368 |
| C | 9.391571 | 20.485015 | 2.919885 |
| C | 9.699929 | 21.742452 | 2.318606 |
| C | 9.637626 | 21.886673 | 0.926937 |
| C | 9.292403 | 20.822973 | 0.101782 |
| C | 9.075291 | 19.578760 | 0.676618 |
| C | 10.121600 | 22.965857 | 3.089227 |
| C | 11.619165 | 22.980349 | 3.496153 |
| C | 12.647308 | 23.265070 | 2.427720 |
| C | 13.291884 | 22.255233 | 1.672839 |
| C | 14.382818 | 22.587093 | 0.845418 |
| C | 14.784723 | 23.908726 | 0.687125 |
| C | 14.097718 | 24.926010 | 1.357955 |
| C | 13.055325 | 24.593933 | 2.220873 |
| N | 12.931645 | 20.894746 | 1.839369 |
| Pd | 13.171089 | 19.743438 | 3.743282 |
| C | 14.318786 | 21.036420 | 4.851153 |
| C | 9.043010 | 20.389799 | 4.413672 |
| P | 10.279463 | 20.090541 | 5.830134 |
| C | 10.064261 | 21.455344 | 7.175146 |
| C | 11.345527 | 21.489389 | 8.031464 |
| N | 12.400076 | 18.242815 | 2.326839 |
| C | 12.493517 | 18.645192 | 1.092488 |
| C | 12.448901 | 17.958455 | -0.203292 |
| C | 12.527037 | 18.980925 | -1.189951 |
| C | 12.666838 | 20.287095 | -0.641516 |
| C | 12.726808 | 20.106514 | 0.822100 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 12.363047 | 16.634324 | -0.613930 | H | 8.813670 | 18.736327 | 0.033389 |
| C | 12.333521 | 16.352849 | -2.002707 | H | 9.201353 | 20.960017 | -0.977159 |
| C | 12.366027 | 17.354352 | -2.963582 | H | 9.845314 | 22.867905 | 0.495009 |
| C | 12.458063 | 18.720239 | -2.577603 | H | 9.525237 | 23.075869 | 4.003499 |
| C | 12.679218 | 21.368675 | -1.512735 | H | 9.910349 | 23.859665 | 2.483609 |
| C | 12.579991 | 21.130259 | -2.906217 | H | 11.746461 | 23.766480 | 4.257372 |
| C | 12.488372 | 19.851363 | -3.438108 | H | 11.874671 | 22.018685 | 3.973892 |
| C | 10.067318 | 18.338841 | 6.599272 | H | 12.557413 | 25.384677 | 2.788172 |
| C | 10.708652 | 18.249064 | 7.996786 | H | 14.398485 | 25.967909 | 1.238339 |
| C | 8.581463 | 17.947789 | 6.674545 | H | 15.640245 | 24.143348 | 0.051677 |
| C | 10.834977 | 17.357578 | 5.704668 | H | 14.924860 | 21.785584 | 0.341537 |
| C | 9.896167 | 22.843678 | 6.543478 | H | 15.357415 | 20.678444 | 4.804038 |
| C | 8.810649 | 21.182494 | 8.026969 | H | 14.252153 | 22.020606 | 4.362547 |
| C | 15.013507 | 18.493434 | 8.060461 | H | 14.034180 | 21.121841 | 5.908726 |
| C | 14.634294 | 17.263243 | 8.412958 | H | 8.557754 | 21.331478 | 4.706471 |
| H | 12.772190 | 22.391482 | -1.151082 | H | 8.275513 | 19.617049 | 4.548626 |
| H | 12.593206 | 21.986930 | -3.582164 | H | 10.633860 | 17.196570 | 8.313584 |
| H | 12.438031 | 19.710516 | -4.520000 | H | 11.778259 | 18.498118 | 7.982450 |
| H | 12.323358 | 17.095308 | -4.023629 | H | 10.204382 | 18.849150 | 8.762188 |
| H | 12.273211 | 15.311228 | -2.322105 | H | 8.514708 | 16.960244 | 7.156705 |
| H | 12.317296 | 15.815631 | 0.104118 | H | 7.978746 | 18.644834 | 7.271351 |
| H | 14.164963 | 16.711509 | 3.406897 | H | 8.117841 | 17.847263 | 5.683270 |
| H | 13.934505 | 14.319850 | 4.077578 | H | 10.683393 | 16.339663 | 6.096767 |
| H | 11.739511 | 13.154864 | 3.737369 | H | 10.495911 | 17.357518 | 4.666670 |
| H | 9.853264 | 14.381213 | 2.707514 | H | 11.911487 | 17.570038 | 5.699931 |
| H | 9.017152 | 16.035446 | 1.547164 | H | 9.860139 | 23.575436 | 7.365799 |
| H | 10.005764 | 17.265660 | 0.795437 | H | 10.739403 | 23.118005 | 5.900950 |
| H | 7.826389 | 17.736454 | 2.392461 | H | 8.955132 | 22.950369 | 5.988224 |
| H | 9.069066 | 17.857639 | 3.617418 | H | 8.700491 | 22.010453 | 8.745137 |

| | | | |
|---|---|---|---|
| H | 7.894288 | 21.162116 | 7.417952 |
| H | 8.864639 | 20.255214 | 8.606566 |
| H | 11.235588 | 22.293126 | 8.776414 |
| H | 11.537077 | 20.561155 | 8.577144 |
| H | 12.230584 | 21.721486 | 7.422035 |
| H | 11.640243 | 20.094582 | 5.189668 |
| H | 13.524184 | 18.868584 | 4.975506 |
| H | 14.955066 | 18.838135 | 7.025041 |
| H | 15.413411 | 19.200037 | 8.791396 |
| H | 14.706257 | 16.910787 | 9.444318 |
| H | 14.252436 | 16.548527 | 7.679402 |

**II-Ts-hydrogenation**

| | | | |
|---|---|---|---|
| C | 12.239370 | 14.848228 | 3.320605 |
| C | 11.983118 | 16.136127 | 2.820753 |
| C | 13.086597 | 17.009421 | 2.685010 |
| C | 14.381177 | 16.580075 | 3.018241 |
| C | 14.603090 | 15.288449 | 3.495784 |
| C | 13.523103 | 14.419928 | 3.662983 |
| C | 10.583263 | 16.479326 | 2.356521 |
| C | 9.827319 | 17.595360 | 3.132855 |
| C | 9.643065 | 18.917510 | 2.414413 |
| C | 9.592877 | 20.144704 | 3.127067 |
| C | 9.586452 | 21.357301 | 2.377439 |
| C | 9.431012 | 21.310971 | 0.984592 |
| C | 9.318878 | 20.102839 | 0.308937 |
| C | 9.469287 | 18.918886 | 1.023977 |
| C | 9.845524 | 22.717303 | 2.970245 |
| C | 11.365207 | 22.980272 | 3.169599 |
| C | 12.211864 | 23.340786 | 1.973040 |
| C | 13.007366 | 22.407599 | 1.262200 |
| C | 13.943005 | 22.863118 | 0.312229 |
| C | 14.040541 | 24.212469 | -0.007758 |
| C | 13.197195 | 25.134731 | 0.620752 |
| C | 12.313043 | 24.693223 | 1.602375 |
| N | 12.957629 | 21.019949 | 1.560291 |
| Pd | 13.363447 | 20.067563 | 3.537445 |
| C | 14.348058 | 21.582058 | 4.516216 |
| C | 9.196299 | 20.151240 | 4.608277 |
| P | 10.156399 | 19.646576 | 6.193566 |
| C | 10.567383 | 21.192927 | 7.260285 |
| C | 11.650398 | 20.814721 | 8.290235 |
| N | 12.935727 | 18.368098 | 2.268021 |
| C | 12.895076 | 18.677521 | 1.004267 |
| C | 12.889177 | 17.889015 | -0.230488 |
| C | 12.661115 | 18.820602 | -1.281966 |
| C | 12.579286 | 20.170350 | -0.835210 |
| C | 12.807833 | 20.126929 | 0.622527 |
| C | 13.013520 | 16.540601 | -0.539033 |
| C | 12.897553 | 16.141117 | -1.894493 |
| C | 12.644752 | 17.046548 | -2.915964 |
| C | 12.508722 | 18.434185 | -2.632705 |
| C | 12.292101 | 21.156631 | -1.769698 |
| C | 12.114506 | 20.786437 | -3.126387 |
| C | 12.230509 | 19.473304 | -3.561989 |
| C | 8.952775 | 18.474472 | 7.140220 |
| C | 9.472190 | 18.231565 | 8.569620 |
| C | 7.512201 | 19.014787 | 7.203714 |
| C | 8.933854 | 17.119384 | 6.408912 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 11.158358 | 22.261109 | 6.337186 | H | 15.412145 | 21.339512 | 4.360456 |
| C | 9.332171 | 21.778091 | 7.962379 | H | 14.122041 | 22.544880 | 4.034843 |
| C | 13.898616 | 18.304664 | 6.017049 | H | 14.163325 | 21.650689 | 5.596996 |
| C | 12.788838 | 17.812458 | 6.702465 | H | 8.824298 | 21.152218 | 4.869441 |
| H | 12.207162 | 22.204476 | -1.485718 | H | 8.322708 | 19.487176 | 4.685797 |
| H | 11.891404 | 21.569234 | -3.853524 | H | 8.826331 | 17.473122 | 9.039081 |
| H | 12.104579 | 19.234668 | -4.620280 | H | 10.497046 | 17.836861 | 8.582693 |
| H | 12.549248 | 16.694926 | -3.945463 | H | 9.427155 | 19.127192 | 9.199844 |
| H | 13.004867 | 15.082619 | -2.137165 | H | 6.894861 | 18.270622 | 7.731342 |
| H | 13.201409 | 15.793122 | 0.231951 | H | 7.428132 | 19.958267 | 7.753604 |
| H | 15.211238 | 17.277778 | 2.888338 | H | 7.060221 | 19.150272 | 6.211280 |
| H | 15.617241 | 14.967479 | 3.739214 | H | 8.347261 | 16.412399 | 7.016087 |
| H | 13.678861 | 13.409183 | 4.043020 | H | 8.449220 | 17.181921 | 5.427987 |
| H | 11.398868 | 14.156901 | 3.423505 | H | 9.938357 | 16.692425 | 6.281585 |
| H | 9.993366 | 15.553499 | 2.408054 | H | 11.554618 | 23.077409 | 6.961610 |
| H | 10.630085 | 16.734576 | 1.288306 | H | 11.984175 | 21.872239 | 5.728601 |
| H | 8.830191 | 17.200862 | 3.393466 | H | 10.399362 | 22.695973 | 5.677162 |
| H | 10.345242 | 17.767013 | 4.086174 | H | 9.631211 | 22.723775 | 8.441795 |
| H | 9.424391 | 17.971254 | 0.485939 | H | 8.520455 | 22.016381 | 7.259394 |
| H | 9.146615 | 20.080173 | -0.768345 | H | 8.934606 | 21.128264 | 8.751706 |
| H | 9.388782 | 22.252754 | 0.433763 | H | 11.868665 | 21.711046 | 8.891894 |
| H | 9.351282 | 22.841695 | 3.945849 | H | 11.347170 | 20.022215 | 8.982708 |
| H | 9.417733 | 23.492601 | 2.317263 | H | 12.584281 | 20.514452 | 7.796880 |
| H | 11.466558 | 23.812912 | 3.883548 | H | 11.459320 | 18.790989 | 6.185272 |
| H | 11.805402 | 22.088551 | 3.643852 | H | 13.557205 | 19.301846 | 4.984428 |
| H | 11.698226 | 25.422883 | 2.136180 | H | 14.383335 | 17.662459 | 5.280356 |
| H | 13.256990 | 26.195914 | 0.374459 | H | 14.571837 | 18.999328 | 6.528403 |
| H | 14.780703 | 24.544889 | -0.737549 | H | 12.609466 | 18.127730 | 7.731091 |
| H | 14.605629 | 22.138213 | -0.163006 | H | 12.355433 | 16.855998 | 6.401571 |

**II-with-alkane**

| | | | |
|---|---|---|---|
| C | 11.969662 | 15.490361 | 3.647385 |
| C | 11.894899 | 16.702147 | 2.907780 |
| C | 13.115274 | 17.376332 | 2.678459 |
| C | 14.368924 | 16.916108 | 3.172570 |
| C | 14.406494 | 15.723028 | 3.881508 |
| C | 13.195381 | 15.020535 | 4.099895 |
| C | 15.354812 | 17.920743 | 2.745809 |
| C | 14.647816 | 18.865290 | 1.817470 |
| C | 13.210744 | 18.570782 | 1.910539 |
| C | 10.726439 | 17.305854 | 2.366769 |
| C | 10.814671 | 18.487928 | 1.643870 |
| C | 12.051468 | 19.133821 | 1.393815 |
| N | 15.345252 | 19.678632 | 1.086678 |
| Pd | 17.596704 | 19.630789 | 1.762322 |
| C | 19.013603 | 20.127878 | 3.149589 |
| N | 16.595263 | 18.165470 | 3.057264 |
| C | 17.237349 | 17.343494 | 4.035111 |
| C | 18.390525 | 16.580030 | 3.733379 |
| C | 18.895674 | 15.756495 | 4.755990 |
| C | 18.338404 | 15.718831 | 6.032940 |
| C | 17.253887 | 16.547698 | 6.335016 |
| C | 16.708168 | 17.351390 | 5.338989 |
| C | 19.191599 | 16.721019 | 2.459201 |
| C | 18.901979 | 15.839143 | 1.222583 |
| C | 17.621734 | 16.131039 | 0.474764 |
| C | 17.417208 | 17.241469 | -0.402046 |
| C | 16.134330 | 17.383466 | -0.997628 |
| C | 15.154060 | 16.398420 | -0.804859 |
| C | 15.373805 | 15.301000 | 0.016920 |
| C | 16.595407 | 15.194729 | 0.669175 |
| C | 15.774525 | 18.548715 | -1.898666 |
| C | 14.338733 | 19.123698 | -1.714288 |
| C | 14.205899 | 20.449749 | -0.994170 |
| C | 13.558252 | 21.514402 | -1.642910 |
| C | 13.343104 | 22.747313 | -1.025445 |
| C | 13.778261 | 22.944005 | 0.286185 |
| C | 14.424899 | 21.908184 | 0.959356 |
| C | 14.635636 | 20.670714 | 0.333522 |
| C | 18.580619 | 18.127471 | -0.874740 |
| P | 19.066206 | 19.823486 | -0.053831 |
| C | 18.732257 | 21.282821 | -1.334854 |
| C | 17.359672 | 21.870756 | -0.997619 |
| C | 21.024397 | 19.672659 | 0.076066 |
| C | 21.638004 | 19.540367 | -1.330267 |
| C | 21.634692 | 20.880152 | 0.820404 |
| C | 21.439791 | 18.423268 | 0.866547 |
| C | 19.731234 | 22.441928 | -1.167479 |
| C | 18.752447 | 20.806650 | -2.797432 |
| C | 16.210500 | 25.030697 | 3.077091 |
| C | 17.446908 | 24.132383 | 3.127375 |
| H | 15.339032 | 15.319691 | 4.273330 |
| H | 13.231575 | 14.082304 | 4.656061 |
| H | 11.057989 | 14.925757 | 3.854226 |
| H | 9.753974 | 16.833998 | 2.523148 |
| H | 9.903050 | 18.936371 | 1.245584 |
| H | 12.072829 | 20.055103 | 0.812709 |
| H | 14.779538 | 22.048541 | 1.982489 |

| | | | |
|---|---|---|---|
| H | 13.618880 | 23.899359 | 0.788980 |
| H | 12.836908 | 23.548035 | -1.566656 |
| H | 13.210864 | 21.360586 | -2.667783 |
| H | 13.878407 | 19.250082 | -2.704041 |
| H | 13.712881 | 18.383824 | -1.193154 |
| H | 15.873904 | 18.219177 | -2.947717 |
| H | 16.501364 | 19.356455 | -1.773889 |
| H | 14.200638 | 16.482197 | -1.329554 |
| H | 14.605625 | 14.535964 | 0.142480 |
| H | 16.786414 | 14.343815 | 1.326428 |
| H | 19.768013 | 15.938494 | 0.548522 |
| H | 18.892335 | 14.782185 | 1.527597 |
| H | 20.240395 | 16.538606 | 2.738058 |
| H | 19.123025 | 17.771709 | 2.140819 |
| H | 19.781554 | 15.153237 | 4.541409 |
| H | 18.771794 | 15.074648 | 6.799423 |
| H | 16.835691 | 16.572089 | 7.342526 |
| H | 15.856377 | 17.997520 | 5.558425 |
| H | 19.054482 | 21.225777 | 3.122832 |
| H | 18.573207 | 19.764950 | 4.087732 |
| H | 20.014170 | 19.707074 | 3.018484 |
| H | 19.506714 | 17.544290 | -0.790873 |
| H | 18.459595 | 18.337484 | -1.945659 |
| H | 19.362168 | 23.278084 | -1.782781 |
| H | 19.780412 | 22.803572 | -0.131633 |
| H | 20.742997 | 22.212387 | -1.518573 |
| H | 18.615855 | 21.686810 | -3.446426 |
| H | 19.699227 | 20.333422 | -3.086793 |
| H | 17.935031 | 20.112958 | -3.031300 |
| H | 17.150979 | 22.705916 | -1.685195 |
| H | 16.544669 | 21.153493 | -1.108143 |
| H | 17.329387 | 22.260622 | 0.029049 |
| H | 22.539383 | 18.365055 | 0.836703 |
| H | 21.147067 | 18.473514 | 1.919105 |
| H | 21.065169 | 17.486297 | 0.438325 |
| H | 22.725605 | 19.401833 | -1.218831 |
| H | 21.256981 | 18.662532 | -1.873060 |
| H | 21.489279 | 20.425915 | -1.956139 |
| H | 22.672988 | 20.626085 | 1.086877 |
| H | 21.672795 | 21.790508 | 0.218971 |
| H | 21.105968 | 21.107339 | 1.754513 |
| H | 17.713666 | 23.873684 | 4.162736 |
| H | 18.319816 | 24.627134 | 2.676424 |
| H | 16.377487 | 25.972536 | 3.619017 |
| H | 15.337034 | 24.542721 | 3.535634 |
| H | 17.283629 | 23.188884 | 2.582544 |
| H | 15.943803 | 25.291046 | 2.041942 |

**III-with alkene**

| | | | |
|---|---|---|---|
| C | 10.799253 | 14.885578 | 2.860690 |
| C | 10.905871 | 16.240056 | 2.443450 |
| C | 12.155273 | 16.867721 | 2.649306 |
| C | 13.261152 | 16.231710 | 3.280993 |
| C | 13.123876 | 14.902899 | 3.661293 |
| C | 11.888895 | 14.245895 | 3.435077 |
| C | 14.346843 | 17.231392 | 3.302416 |
| C | 13.841214 | 18.439788 | 2.558882 |
| C | 12.433723 | 18.196259 | 2.224481 |
| C | 9.890158 | 17.030745 | 1.839352 |

| | | | |
|---|---|---|---|
| C | 10.146721 | 18.343613 | 1.467833 |
| C | 11.418240 | 18.943945 | 1.642083 |
| N | 14.647018 | 19.442011 | 2.368210 |
| Pd | 16.478664 | 19.282912 | 3.605549 |
| H | 17.627187 | 19.270278 | 4.653131 |
| N | 15.558385 | 17.266907 | 3.783939 |
| C | 16.057360 | 16.240579 | 4.626114 |
| C | 17.361068 | 15.721485 | 4.434831 |
| C | 17.791612 | 14.706574 | 5.305274 |
| C | 17.009097 | 14.253934 | 6.365703 |
| C | 15.760454 | 14.840235 | 6.596947 |
| C | 15.292008 | 15.822204 | 5.732098 |
| C | 18.335565 | 16.265639 | 3.420339 |
| C | 18.345196 | 15.639275 | 1.999432 |
| C | 17.163051 | 16.006611 | 1.141765 |
| C | 17.055535 | 17.223850 | 0.403788 |
| C | 15.824891 | 17.502863 | -0.247393 |
| C | 14.818669 | 16.522697 | -0.272619 |
| C | 14.962774 | 15.303740 | 0.374789 |
| C | 16.120944 | 15.071306 | 1.106300 |
| C | 15.510998 | 18.788138 | -0.992501 |
| C | 14.111341 | 19.404634 | -0.662646 |
| C | 14.038282 | 20.620357 | 0.245332 |
| C | 13.698870 | 21.855112 | -0.337846 |
| C | 13.560232 | 23.026977 | 0.406097 |
| C | 13.771720 | 22.991371 | 1.786261 |
| C | 14.127035 | 21.790261 | 2.395810 |
| C | 14.238683 | 20.605941 | 1.648997 |
| C | 18.302915 | 18.058764 | 0.074543 |
| P | 19.015262 | 19.456416 | 1.154219 |
| C | 18.752650 | 21.181982 | 0.344487 |
| C | 17.324369 | 21.627630 | 0.682780 |
| C | 20.883060 | 19.137773 | 1.502512 |
| C | 21.736487 | 19.489090 | 0.270653 |
| C | 21.276753 | 19.972213 | 2.738546 |
| C | 21.144885 | 17.664140 | 1.841010 |
| C | 19.693078 | 22.243984 | 0.945541 |
| C | 18.947058 | 21.108401 | -1.179482 |
| C | 18.580792 | 24.339992 | 4.254817 |
| C | 18.874450 | 23.307178 | 5.047836 |
| H | 13.938201 | 14.359172 | 4.137565 |
| H | 11.792212 | 13.202783 | 3.741411 |
| H | 9.857257 | 14.349480 | 2.726314 |
| H | 8.901743 | 16.598489 | 1.669747 |
| H | 9.348123 | 18.933890 | 1.015556 |
| H | 11.580407 | 19.971744 | 1.317332 |
| H | 14.322002 | 21.743419 | 3.468433 |
| H | 13.667515 | 23.895132 | 2.388806 |
| H | 13.286938 | 23.959834 | -0.089498 |
| H | 13.532167 | 21.886550 | -1.417607 |
| H | 13.645392 | 19.704831 | -1.611964 |
| H | 13.465054 | 18.613603 | -0.258189 |
| H | 15.521354 | 18.565407 | -2.073008 |
| H | 16.291716 | 19.540384 | -0.842113 |
| H | 13.907539 | 16.714919 | -0.842859 |
| H | 14.178430 | 14.547095 | 0.314799 |
| H | 16.244045 | 14.132999 | 1.651003 |
| H | 19.285371 | 15.928371 | 1.513326 |

| | | | |
|---|---|---|---|
| H | 18.384270 | 14.544462 | 2.099298 |
| H | 19.339094 | 16.114709 | 3.849840 |
| H | 18.174025 | 17.355774 | 3.343057 |
| H | 18.791709 | 14.288820 | 5.161269 |
| H | 17.386292 | 13.476619 | 7.031976 |
| H | 15.158286 | 14.542880 | 7.457071 |
| H | 14.329439 | 16.300831 | 5.918384 |
| H | 19.152601 | 17.368611 | -0.030052 |
| H | 18.175603 | 18.508720 | -0.918321 |
| H | 19.406985 | 23.209516 | 0.499198 |
| H | 19.565599 | 22.349165 | 2.031546 |
| H | 20.752773 | 22.087576 | 0.715868 |
| H | 18.821711 | 22.123411 | -1.587606 |
| H | 19.945404 | 20.758298 | -1.472482 |
| H | 18.196658 | 20.475250 | -1.672781 |
| H | 17.136586 | 22.593049 | 0.187077 |
| H | 16.557029 | 20.932032 | 0.336340 |
| H | 17.186408 | 21.761187 | 1.763070 |
| H | 22.210239 | 17.572563 | 2.104557 |
| H | 20.565699 | 17.322663 | 2.705625 |
| H | 20.972901 | 16.992736 | 0.989494 |
| H | 22.787468 | 19.256428 | 0.505083 |
| H | 21.461340 | 18.884569 | -0.606528 |
| H | 21.694339 | 20.547251 | -0.007926 |
| H | 22.326650 | 19.745635 | 2.981698 |
| H | 21.202306 | 21.052032 | 2.582668 |
| H | 20.667391 | 19.706944 | 3.614296 |
| H | 18.183165 | 19.455896 | 2.410057 |
| H | 16.991890 | 20.740944 | 3.758462 |
| H | 18.231383 | 22.425686 | 5.108718 |
| H | 19.764191 | 23.309276 | 5.681936 |
| H | 19.215598 | 25.227493 | 4.204816 |
| H | 17.680867 | 24.349650 | 3.634341 |

**III-Ts-hydrogenation**

| | | | |
|---|---|---|---|
| C | 12.258758 | 14.917216 | 3.614903 |
| C | 11.985858 | 16.210967 | 3.093534 |
| C | 13.096653 | 17.066413 | 2.915229 |
| C | 14.432761 | 16.705052 | 3.252208 |
| C | 14.661807 | 15.425834 | 3.742437 |
| C | 13.563219 | 14.546511 | 3.911017 |
| C | 15.269251 | 17.870421 | 2.901422 |
| C | 14.356146 | 18.880251 | 2.260869 |
| C | 12.987223 | 18.366683 | 2.348645 |
| C | 10.715925 | 16.734404 | 2.723455 |
| C | 10.605926 | 18.015323 | 2.198714 |
| C | 11.734311 | 18.847789 | 1.992407 |
| N | 14.874025 | 19.960736 | 1.762063 |
| Pd | 16.992076 | 20.172123 | 2.167646 |
| H | 18.459889 | 20.417825 | 2.637087 |
| N | 16.532048 | 18.173517 | 3.030581 |
| C | 17.408566 | 17.345035 | 3.782743 |
| C | 18.686613 | 16.968726 | 3.295034 |
| C | 19.466951 | 16.128801 | 4.109132 |
| C | 19.057246 | 15.721242 | 5.376821 |
| C | 17.836646 | 16.180353 | 5.883173 |
| C | 17.023938 | 16.980707 | 5.089712 |
| C | 19.306968 | 17.520957 | 2.035929 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 19.150064 | 16.747822 | 0.696645 | H | 11.439262 | 14.213733 | 3.777048 |
| C | 17.761124 | 16.874561 | 0.129037 | H | 9.822063 | 16.120220 | 2.852491 |
| C | 17.296281 | 18.005392 | -0.605064 | H | 9.619801 | 18.395505 | 1.927181 |
| C | 15.897793 | 18.131428 | -0.826986 | H | 11.604827 | 19.842218 | 1.565403 |
| C | 15.050880 | 17.061841 | -0.508420 | H | 14.085389 | 22.081018 | 3.045212 |
| C | 15.532488 | 15.898001 | 0.084189 | H | 12.775661 | 24.005479 | 2.147227 |
| C | 16.872048 | 15.836036 | 0.443200 | H | 12.055096 | 23.991832 | -0.252038 |
| C | 15.307818 | 19.380050 | -1.456231 | H | 12.595368 | 22.042004 | -1.682531 |
| C | 13.848441 | 19.748729 | -1.061221 | H | 13.275816 | 19.940987 | -1.979644 |
| C | 13.649793 | 20.949951 | -0.159558 | H | 13.357349 | 18.884784 | -0.591339 |
| C | 12.932176 | 22.057057 | -0.642715 | H | 15.328855 | 19.255221 | -2.552068 |
| C | 12.619192 | 23.154617 | 0.161555 | H | 15.957739 | 20.237987 | -1.235494 |
| C | 13.020987 | 23.163239 | 1.498360 | H | 13.990245 | 17.122233 | -0.755019 |
| C | 13.750749 | 22.087704 | 2.006038 | H | 14.860839 | 15.062431 | 0.287291 |
| C | 14.063408 | 20.987418 | 1.191974 | H | 17.258516 | 14.960792 | 0.969858 |
| C | 18.282915 | 18.837913 | -1.430885 | H | 19.916237 | 17.127879 | 0.003538 |
| P | 18.763293 | 20.696258 | -1.354261 | H | 19.388540 | 15.685109 | 0.852639 |
| C | 18.651971 | 21.267602 | -3.196225 | H | 20.385954 | 17.614709 | 2.235823 |
| C | 17.160450 | 21.358332 | -3.568852 | H | 18.913832 | 18.540209 | 1.889018 |
| C | 20.561634 | 20.927987 | -0.697896 | H | 20.449446 | 15.822707 | 3.741095 |
| C | 21.627531 | 20.528047 | -1.731366 | H | 19.703459 | 15.084447 | 5.982947 |
| C | 20.735057 | 22.401381 | -0.278691 | H | 17.524438 | 15.925472 | 6.897193 |
| C | 20.757293 | 20.063240 | 0.549425 | H | 16.078057 | 17.356472 | 5.482065 |
| C | 19.261178 | 22.673208 | -3.349987 | H | 19.263765 | 18.341980 | -1.414382 |
| C | 19.336281 | 20.300489 | -4.179922 | H | 17.936332 | 18.764540 | -2.472491 |
| C | 17.038908 | 23.104760 | 1.158715 | H | 19.083074 | 23.009107 | -4.383730 |
| C | 17.273634 | 23.295357 | -0.198692 | H | 18.790691 | 23.409336 | -2.684584 |
| H | 15.662174 | 15.087476 | 4.007480 | H | 20.345349 | 22.692115 | -3.188605 |
| H | 13.754972 | 13.545248 | 4.300766 | H | 19.169028 | 20.681191 | -5.199928 |

| | | | |
|---|---|---|---|
| H | 20.418743 | 20.226926 | -4.032499 |
| H | 18.913914 | 19.286637 | -4.149680 |
| H | 17.085641 | 21.805035 | -4.572625 |
| H | 16.682619 | 20.372716 | -3.618671 |
| H | 16.587790 | 21.993710 | -2.879664 |
| H | 21.735442 | 20.314068 | 0.990101 |
| H | 19.985869 | 20.252133 | 1.307229 |
| H | 20.775029 | 18.993686 | 0.308453 |
| H | 22.611513 | 20.588244 | -1.240060 |
| H | 21.506049 | 19.492549 | -2.081892 |
| H | 21.660028 | 21.192703 | -2.602486 |
| H | 21.767730 | 22.530195 | 0.082114 |
| H | 20.582891 | 23.114878 | -1.096419 |
| H | 20.062225 | 22.662609 | 0.548718 |
| H | 17.905692 | 21.827205 | -0.676108 |
| H | 17.321196 | 21.659156 | 1.576569 |
| H | 16.011860 | 23.041561 | 1.519097 |
| H | 17.760508 | 23.481104 | 1.887835 |
| H | 18.165450 | 23.836074 | -0.518919 |
| H | 16.428496 | 23.297692 | -0.891099 |

**III with alkane**

| | | | |
|---|---|---|---|
| C | 12.045225 | 15.498749 | 3.690614 |
| C | 11.898070 | 16.716496 | 2.988818 |
| C | 13.067263 | 17.448794 | 2.725571 |
| C | 14.329758 | 17.005269 | 3.123569 |
| C | 14.450872 | 15.794925 | 3.808666 |
| C | 13.309397 | 15.042331 | 4.085867 |
| C | 10.555850 | 17.280441 | 2.571624 |
| C | 9.720559 | 16.448508 | 1.546999 |
| C | 8.448752 | 15.840529 | 2.104131 |
| C | 8.014416 | 14.528649 | 1.769721 |
| C | 6.851900 | 14.027798 | 2.434669 |
| C | 6.140488 | 14.854387 | 3.317800 |
| C | 6.523004 | 16.166938 | 3.563230 |
| C | 7.680418 | 16.642497 | 2.961195 |
| C | 6.284520 | 12.638087 | 2.266702 |
| C | 7.041099 | 11.503912 | 2.998582 |
| C | 7.041903 | 11.371931 | 4.502383 |
| C | 8.057152 | 11.892277 | 5.339944 |
| C | 8.152928 | 11.480013 | 6.682073 |
| C | 7.208766 | 10.621580 | 7.234694 |
| C | 6.143684 | 10.172281 | 6.448204 |
| C | 6.084022 | 10.535866 | 5.104480 |
| N | 9.040743 | 12.819901 | 4.868749 |
| Pd | 10.301033 | 12.696339 | 3.059379 |
| P | 10.249937 | 12.687855 | 0.750485 |
| C | 9.779022 | 11.040683 | -0.194514 |
| C | 8.507714 | 10.406678 | 0.383079 |
| C | 8.654434 | 13.785596 | 0.585267 |
| N | 10.922147 | 14.658991 | 3.990487 |
| C | 10.233812 | 14.910793 | 5.060891 |
| C | 9.111981 | 13.986524 | 5.443960 |
| C | 8.339788 | 14.661378 | 6.498733 |
| C | 9.084264 | 15.828179 | 6.833219 |
| C | 10.255099 | 16.002493 | 6.042566 |
| C | 7.138543 | 14.430287 | 7.155613 |
| C | 6.713481 | 15.350556 | 8.145440 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 7.462512 | 16.464777 | 8.498156 | H | 5.927351 | 16.810713 | 4.212816 |
| C | 8.691122 | 16.740021 | 7.838650 | H | 5.242910 | 14.453964 | 3.793763 |
| C | 11.086911 | 17.085354 | 6.297481 | H | 6.248260 | 12.359958 | 1.200563 |
| C | 10.726909 | 17.987211 | 7.329875 | H | 5.235574 | 12.647164 | 2.598944 |
| C | 9.564247 | 17.837717 | 8.074713 | H | 6.637880 | 10.555904 | 2.610522 |
| H | 9.990851 | 11.238137 | 2.685902 | H | 8.090103 | 11.556420 | 2.683092 |
| C | 11.730950 | 13.496786 | -0.281233 | H | 5.288131 | 10.128816 | 4.475194 |
| C | 11.200164 | 14.428302 | -1.383321 | H | 5.386879 | 9.508618 | 6.868920 |
| C | 12.615667 | 14.278333 | 0.694372 | H | 7.306525 | 10.303190 | 8.273728 |
| C | 12.663523 | 12.444887 | -0.910313 | H | 8.985442 | 11.843542 | 7.287017 |
| C | 9.505888 | 11.333861 | -1.682170 | H | 7.914447 | 13.086959 | 0.173385 |
| C | 10.885708 | 9.983583 | -0.006500 | H | 8.863936 | 14.506034 | -0.216547 |
| C | 15.035076 | 11.351466 | 3.855122 | H | 13.502557 | 12.994772 | -1.365785 |
| C | 13.826270 | 10.640996 | 3.245974 | H | 13.093791 | 11.773530 | -0.155992 |
| H | 6.522774 | 13.560833 | 6.931957 | H | 12.206644 | 11.849049 | -1.706626 |
| H | 5.767758 | 15.163367 | 8.656828 | H | 12.060527 | 14.804012 | -1.959955 |
| H | 7.106829 | 17.137124 | 9.281864 | H | 10.529358 | 13.922591 | -2.090226 |
| H | 9.315785 | 18.566961 | 8.848712 | H | 10.680472 | 15.308730 | -0.981848 |
| H | 11.385325 | 18.832323 | 7.536456 | H | 13.467836 | 14.698110 | 0.136550 |
| H | 12.001097 | 17.250399 | 5.728770 | H | 12.106501 | 15.114626 | 1.174813 |
| H | 13.386439 | 14.089920 | 4.613726 | H | 13.016486 | 13.627658 | 1.482907 |
| H | 15.429063 | 15.432700 | 4.128958 | H | 8.263062 | 9.531455 | -0.239570 |
| H | 15.213792 | 17.603780 | 2.898512 | H | 8.661016 | 10.042824 | 1.405547 |
| H | 12.975223 | 18.398148 | 2.192081 | H | 7.632832 | 11.066942 | 0.360800 |
| H | 10.740501 | 18.281378 | 2.157276 | H | 9.232394 | 10.389080 | -2.178125 |
| H | 9.953868 | 17.443797 | 3.478038 | H | 8.658755 | 12.023158 | -1.815860 |
| H | 9.460309 | 17.108262 | 0.701619 | H | 10.366627 | 11.742907 | -2.220902 |
| H | 10.347113 | 15.659603 | 1.122276 | H | 10.493557 | 9.012784 | -0.347949 |
| H | 7.988339 | 17.673204 | 3.145933 | H | 11.796642 | 10.180779 | -0.574773 |

| | | | |
|---|---|---|---|
| H | 11.153468 | 9.872903 | 1.054944 |
| H | 13.559911 | 9.739213 | 3.816574 |
| H | 14.027319 | 10.325605 | 2.210660 |
| H | 15.918611 | 10.697320 | 3.868645 |
| H | 14.841228 | 11.656961 | 4.894482 |
| H | 12.934699 | 11.291100 | 3.227308 |
| H | 15.305070 | 12.253853 | 3.285423 |

## II-s (Pd-P system) with AB

| | | | |
|---|---|---|---|
| C | 12.360151 | 20.466841 | 1.078760 |
| C | 12.532022 | 21.011506 | -0.273792 |
| C | 12.107803 | 19.977886 | -1.159558 |
| C | 11.628381 | 18.816506 | -0.486387 |
| C | 11.691672 | 19.131432 | 0.949624 |
| C | 12.142769 | 20.100426 | -2.565547 |
| C | 11.682632 | 18.981499 | -3.313185 |
| C | 11.218342 | 17.847232 | -2.663858 |
| C | 11.174187 | 17.747632 | -1.250300 |
| C | 12.984035 | 22.208114 | -0.818101 |
| C | 13.021879 | 22.348857 | -2.228371 |
| C | 12.624334 | 21.333715 | -3.085748 |
| N | 11.301048 | 18.525985 | 2.026112 |
| C | 10.824641 | 17.151141 | 1.899651 |
| N | 12.752255 | 20.848741 | 2.256008 |
| C | 13.467421 | 22.113520 | 2.388773 |
| Pd | 11.913918 | 19.757453 | 3.933004 |
| C | 13.442763 | 20.443855 | 5.097486 |
| P | 10.503382 | 19.421004 | 5.836820 |
| C | 10.891899 | 17.748705 | 6.768804 |
| C | 10.212700 | 17.600914 | 8.141102 |
| C | 10.578404 | 20.901536 | 7.140556 |
| C | 10.687307 | 22.237588 | 6.376956 |
| C | 8.652600 | 19.370345 | 5.167023 |
| C | 8.586270 | 18.524477 | 3.884820 |
| C | 9.347420 | 20.970302 | 8.065105 |
| C | 11.816022 | 20.781351 | 8.053038 |
| C | 8.222706 | 20.790477 | 4.750433 |
| C | 7.633532 | 18.793473 | 6.166035 |
| C | 10.465147 | 16.566892 | 5.881340 |
| C | 12.418415 | 17.633630 | 6.937695 |
| H | 13.292727 | 23.047960 | -0.197637 |
| H | 13.375276 | 23.291936 | -2.648079 |
| H | 12.671284 | 21.482410 | -4.166609 |
| H | 11.691527 | 19.020446 | -4.404441 |
| H | 10.867556 | 17.001022 | -3.256599 |
| H | 10.788805 | 16.834508 | -0.799974 |
| H | 14.287501 | 20.275298 | 4.414299 |
| H | 13.345573 | 21.505284 | 5.354180 |
| H | 13.593055 | 19.838038 | 5.992227 |
| H | 12.638290 | 16.665683 | 7.416600 |
| H | 12.939950 | 17.648590 | 5.971087 |
| H | 12.853063 | 18.412957 | 7.572775 |
| H | 10.461046 | 16.602496 | 8.537497 |
| H | 10.572779 | 18.330980 | 8.875607 |
| H | 9.119966 | 17.668213 | 8.090356 |
| H | 10.835916 | 15.639943 | 6.346889 |
| H | 9.377649 | 16.467543 | 5.780660 |
| H | 10.919445 | 16.630062 | 4.882950 |

| | | | |
|---|---|---|---|
| H | 10.919751 | 23.031310 | 7.104545 |
| H | 11.484395 | 22.221546 | 5.624801 |
| H | 9.756576 | 22.518956 | 5.874211 |
| H | 9.512570 | 21.794990 | 8.777328 |
| H | 8.417044 | 21.196858 | 7.532298 |
| H | 9.201386 | 20.058397 | 8.656259 |
| H | 11.819053 | 21.661438 | 8.716609 |
| H | 11.787924 | 19.897226 | 8.700081 |
| H | 12.763281 | 20.786625 | 7.507364 |
| H | 10.705986 | 16.711944 | 2.893549 |
| H | 9.847610 | 17.112583 | 1.389980 |
| H | 11.538880 | 16.536478 | 1.329708 |
| H | 13.961652 | 22.159205 | 3.363453 |
| H | 14.229774 | 22.219046 | 1.602342 |
| H | 12.765569 | 22.960396 | 2.315444 |
| H | 7.541352 | 18.523364 | 3.533820 |
| H | 9.206131 | 18.958555 | 3.091408 |
| H | 8.880654 | 17.481799 | 4.036025 |
| H | 7.277622 | 20.709024 | 4.189836 |
| H | 8.033407 | 21.456261 | 5.599627 |
| H | 8.960742 | 21.263902 | 4.085837 |
| H | 6.629421 | 18.897589 | 5.722395 |
| H | 7.788928 | 17.722005 | 6.346947 |
| H | 7.618988 | 19.309133 | 7.130778 |
| B | 16.349901 | 18.487379 | 6.321901 |
| N | 17.800172 | 17.987859 | 6.916904 |
| H | 18.326638 | 17.451905 | 6.219805 |
| H | 18.384473 | 18.781904 | 7.197269 |
| H | 17.683871 | 17.388177 | 7.739810 |
| H | 15.817439 | 19.104187 | 7.229936 |
| H | 16.613538 | 19.188460 | 5.360627 |
| H | 15.748906 | 17.470417 | 6.020104 |

**II-Ts-1(AB)-s**

| | | | |
|---|---|---|---|
| C | 11.612247 | 21.718396 | 1.004579 |
| C | 11.087717 | 22.642069 | -0.005529 |
| C | 10.324879 | 21.838282 | -0.904174 |
| C | 10.316137 | 20.455143 | -0.558973 |
| C | 11.124414 | 20.343161 | 0.660142 |
| C | 9.647287 | 22.361002 | -2.026348 |
| C | 8.927804 | 21.428951 | -2.825326 |
| C | 8.913678 | 20.082453 | -2.491768 |
| C | 9.602316 | 19.573506 | -1.361375 |
| C | 11.172268 | 24.008923 | -0.243685 |
| C | 10.499334 | 24.549673 | -1.368175 |
| C | 9.757802 | 23.763456 | -2.238443 |
| N | 11.485277 | 19.364093 | 1.431012 |
| C | 11.092095 | 17.997385 | 1.110180 |
| N | 12.378333 | 21.853210 | 2.046093 |
| C | 12.908142 | 23.165606 | 2.395169 |
| Pd | 12.747912 | 20.029911 | 3.063753 |
| C | 14.014395 | 20.794222 | 4.477263 |
| P | 10.081281 | 19.189214 | 7.050029 |
| C | 10.311270 | 18.501984 | 8.831496 |
| C | 9.360993 | 19.160565 | 9.844180 |
| C | 10.052681 | 21.108482 | 6.974871 |
| C | 10.367088 | 21.553793 | 5.531428 |
| C | 8.640246 | 18.360531 | 6.088088 |
| C | 9.097014 | 16.945575 | 5.673454 |

| | | | |
|---|---|---|---|
| C | 8.694246 | 21.680627 | 7.415893 |
| C | 11.167382 | 21.666515 | 7.880371 |
| C | 8.360140 | 19.136091 | 4.787114 |
| C | 7.350441 | 18.298913 | 6.923621 |
| C | 10.085570 | 16.977709 | 8.841361 |
| C | 11.783328 | 18.735290 | 9.237104 |
| H | 11.738572 | 24.676215 | 0.404516 |
| H | 10.571265 | 25.622857 | -1.551557 |
| H | 9.256040 | 24.221499 | -3.093418 |
| H | 8.385076 | 21.778612 | -3.706106 |
| H | 8.356092 | 19.385407 | -3.119381 |
| H | 9.558468 | 18.505916 | -1.150185 |
| H | 14.938715 | 21.061349 | 3.940389 |
| H | 13.561911 | 21.699998 | 4.911452 |
| H | 14.255766 | 20.085939 | 5.279018 |
| H | 9.526689 | 18.694131 | 10.827963 |
| H | 9.548995 | 20.235389 | 9.962289 |
| H | 8.302871 | 19.017515 | 9.587388 |
| H | 10.314547 | 16.618913 | 9.856770 |
| H | 9.051814 | 16.687255 | 8.621535 |
| H | 10.604182 | 22.629249 | 5.560852 |
| H | 11.236355 | 21.034805 | 5.097077 |
| H | 9.519015 | 21.426897 | 4.852377 |
| H | 8.751352 | 22.779106 | 7.360685 |
| H | 7.872548 | 21.367615 | 6.758509 |
| H | 8.433224 | 21.418003 | 8.448939 |
| H | 11.197118 | 22.757279 | 7.732272 |
| H | 10.982256 | 21.493036 | 8.946969 |
| H | 12.158821 | 21.273754 | 7.615337 |
| H | 11.542547 | 17.315169 | 1.837425 |
| H | 9.995212 | 17.886414 | 1.152619 |
| H | 11.426974 | 17.721398 | 0.097247 |
| H | 13.564751 | 23.074295 | 3.265319 |
| H | 13.489261 | 23.586506 | 1.558984 |
| H | 12.091301 | 23.864880 | 2.638371 |
| H | 8.289550 | 16.498236 | 5.072334 |
| H | 9.999506 | 16.975894 | 5.046323 |
| H | 9.275445 | 16.275831 | 6.520309 |
| H | 7.628809 | 18.549736 | 4.208933 |
| H | 7.912086 | 20.121740 | 4.964745 |
| H | 9.258494 | 19.251955 | 4.165060 |
| H | 6.559689 | 17.848467 | 6.303342 |
| H | 7.449744 | 17.675785 | 7.820876 |
| H | 6.999210 | 19.293195 | 7.230376 |
| H | 11.310469 | 18.707300 | 6.391740 |
| H | 13.121277 | 18.649128 | 3.847526 |
| N | 12.763558 | 17.475627 | 5.853826 |
| B | 12.923440 | 17.367772 | 4.356332 |
| H | 12.480257 | 18.322555 | 8.494959 |
| H | 11.957311 | 18.209666 | 10.189034 |
| H | 12.030323 | 19.788563 | 9.397387 |
| H | 10.760271 | 16.449126 | 8.154341 |
| H | 12.272934 | 16.659610 | 6.224780 |
| H | 13.653263 | 17.540219 | 6.352867 |
| H | 13.990740 | 16.983427 | 3.920892 |
| H | 11.929199 | 16.937720 | 3.805974 |

**II-$H_2$-inter-s**

| | | | |
|---|---|---|---|
| C | 11.986476 | 17.306391 | -1.174937 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 12.028979 | 18.552326 | -0.560330 | H | 12.218236 | 16.387413 | -0.638280 |
| C | 11.722204 | 19.706614 | -1.339671 | H | 14.980771 | 21.502511 | 4.359515 |
| C | 11.374935 | 19.649563 | -2.706586 | H | 13.358144 | 22.195252 | 4.677074 |
| C | 11.338401 | 18.357241 | -3.300250 | H | 14.069477 | 20.982132 | 5.794639 |
| C | 11.638056 | 17.231346 | -2.547425 | H | 13.773944 | 18.910756 | 4.526565 |
| C | 11.813092 | 20.925445 | -0.605848 | H | 11.670776 | 19.795406 | 5.330833 |
| C | 11.545149 | 22.120071 | -1.263960 | H | 12.610010 | 16.582742 | 7.404683 |
| C | 11.190546 | 22.080132 | -2.636528 | H | 13.020372 | 17.954631 | 6.350738 |
| C | 11.104866 | 20.891110 | -3.346410 | H | 12.700402 | 18.209474 | 8.087737 |
| C | 12.330760 | 19.047317 | 0.787041 | H | 10.256808 | 16.379190 | 8.402202 |
| C | 12.213075 | 20.544535 | 0.755030 | H | 10.264634 | 18.050104 | 8.980843 |
| N | 12.489276 | 21.201692 | 1.838768 | H | 8.958720 | 17.481258 | 7.910614 |
| Pd | 13.204909 | 19.888568 | 3.454873 | H | 10.896928 | 15.765824 | 6.109078 |
| C | 13.971379 | 21.280294 | 4.742327 | H | 9.520520 | 16.699436 | 5.508205 |
| N | 12.664661 | 18.487379 | 1.911083 | H | 11.160800 | 16.978857 | 4.842314 |
| P | 10.564672 | 19.548439 | 6.258663 | H | 11.169109 | 22.967083 | 7.798183 |
| C | 10.675267 | 20.883939 | 7.636334 | H | 11.973685 | 22.184822 | 6.425067 |
| C | 9.352554 | 20.989483 | 8.415588 | H | 10.249600 | 22.626602 | 6.327914 |
| C | 10.890514 | 17.763845 | 6.882683 | H | 9.484392 | 21.735941 | 9.214572 |
| C | 10.587742 | 16.761115 | 5.753848 | H | 8.516778 | 21.330398 | 7.791571 |
| C | 12.396238 | 17.643892 | 7.202103 | H | 9.065251 | 20.044913 | 8.896279 |
| C | 10.036470 | 17.418661 | 8.113024 | H | 11.905008 | 21.386028 | 9.317262 |
| C | 11.817756 | 20.544242 | 8.612730 | H | 11.624781 | 19.644606 | 9.208820 |
| C | 11.031530 | 22.236688 | 6.985492 | H | 12.786539 | 20.444317 | 8.105136 |
| H | 11.599673 | 23.084281 | -0.760020 | C | 12.831338 | 17.039174 | 1.978837 |
| H | 10.981872 | 23.020926 | -3.148337 | C | 12.413422 | 22.655397 | 1.848337 |
| H | 10.832275 | 20.905366 | -4.403753 | C | 9.015064 | 19.717788 | 5.137430 |
| H | 11.078518 | 18.255402 | -4.356081 | H | 13.084545 | 16.756201 | 3.004542 |
| H | 11.609924 | 16.250540 | -3.024749 | H | 11.909311 | 16.517364 | 1.671922 |

| | | | |
|---|---|---|---|
| H | 13.648847 | 16.709429 | 1.316409 |
| H | 12.690893 | 23.025551 | 2.841035 |
| H | 13.106098 | 23.093285 | 1.111170 |
| H | 11.394260 | 23.003131 | 1.609568 |
| C | 8.749886 | 21.206742 | 4.844038 |
| C | 9.329302 | 19.045840 | 3.783672 |
| C | 7.767389 | 19.090699 | 5.780962 |
| H | 8.519364 | 19.307614 | 3.084798 |
| H | 10.277365 | 19.407419 | 3.356658 |
| H | 9.369665 | 17.954211 | 3.841854 |
| H | 7.922077 | 21.255524 | 4.119322 |
| H | 8.436357 | 21.773566 | 5.728597 |
| H | 9.617179 | 21.700888 | 4.384427 |
| H | 6.914828 | 19.243012 | 5.100955 |
| H | 7.870249 | 18.009061 | 5.934411 |
| H | 7.506383 | 19.554121 | 6.741713 |

**II-Ts-$CH_4$-s**

| | | | |
|---|---|---|---|
| C | 16.037185 | 19.857798 | -6.264929 |
| C | 15.046246 | 19.609306 | -7.254888 |
| C | 13.714823 | 19.929018 | -6.910450 |
| C | 13.341378 | 20.477264 | -5.648390 |
| C | 14.338827 | 20.714130 | -4.708982 |
| C | 15.680964 | 20.395364 | -5.036974 |
| C | 11.884467 | 20.656251 | -5.698083 |
| C | 11.424591 | 20.216772 | -7.068778 |
| C | 12.614773 | 19.752443 | -7.797357 |
| C | 15.256270 | 19.080103 | -8.558427 |
| C | 14.187985 | 18.905321 | -9.425829 |
| C | 12.857808 | 19.239178 | -9.065579 |
| N | 10.996416 | 21.081074 | -4.852903 |
| Pd | 9.042654 | 21.560280 | -5.745624 |
| C | 7.459771 | 22.809607 | -6.492238 |
| N | 10.170138 | 20.328588 | -7.358062 |
| C | 9.674636 | 19.924329 | -8.664544 |
| C | 11.418178 | 21.517211 | -3.525493 |
| P | 7.098605 | 19.146156 | -4.184047 |
| C | 7.129582 | 19.638648 | -2.324199 |
| C | 6.011906 | 18.956771 | -1.517461 |
| C | 7.956818 | 17.460545 | -4.539894 |
| C | 5.348028 | 19.282603 | -4.971265 |
| C | 5.517862 | 19.446091 | -6.496567 |
| C | 4.468778 | 18.059762 | -4.658797 |
| C | 4.651678 | 20.556769 | -4.457695 |
| C | 8.492463 | 19.265649 | -1.712074 |
| C | 7.003807 | 21.174792 | -2.239911 |
| H | 12.060517 | 19.088955 | -9.792501 |
| H | 14.372823 | 18.502064 | -10.422820 |
| H | 16.266611 | 18.815149 | -8.877168 |
| H | 17.083558 | 19.628856 | -6.477955 |
| H | 16.457545 | 20.585243 | -4.294232 |
| H | 14.124849 | 21.144835 | -3.731942 |
| H | 7.890134 | 23.750238 | -6.857206 |
| H | 7.248441 | 22.155850 | -7.354810 |
| H | 6.501935 | 23.036756 | -6.005286 |
| H | 7.959876 | 20.226933 | -4.885295 |

| | | | |
|---|---|---|---|
| H | 7.183876 | 21.470564 | -1.194564 |
| H | 7.749532 | 21.681439 | -2.871068 |
| H | 6.012061 | 21.545092 | -2.516592 |
| H | 6.109029 | 19.266322 | -0.464718 |
| H | 5.008783 | 19.250930 | -1.848569 |
| H | 6.079494 | 17.860989 | -1.544348 |
| H | 8.515026 | 19.668915 | -0.687590 |
| H | 8.649980 | 18.183493 | -1.635836 |
| H | 9.331280 | 19.714267 | -2.260098 |
| H | 4.529942 | 19.682535 | -6.921614 |
| H | 6.193791 | 20.275973 | -6.742424 |
| H | 5.877438 | 18.540075 | -6.992997 |
| H | 3.477455 | 18.224144 | -5.110278 |
| H | 4.867556 | 17.131063 | -5.085158 |
| H | 4.316974 | 17.910593 | -3.581613 |
| H | 3.708476 | 20.665164 | -5.015476 |
| H | 4.392417 | 20.507365 | -3.393863 |
| H | 5.247093 | 21.460892 | -4.642490 |
| H | 8.105016 | 22.686131 | -5.143337 |
| H | 11.999814 | 20.735293 | -3.008802 |
| H | 12.044645 | 22.422344 | -3.593392 |
| H | 10.535566 | 21.764572 | -2.927481 |
| H | 9.910206 | 18.868921 | -8.883708 |
| H | 8.586108 | 20.057025 | -8.696552 |
| H | 10.114886 | 20.542994 | -9.465007 |
| C | 7.690647 | 17.041522 | -5.997630 |
| C | 9.480572 | 17.659505 | -4.404278 |
| C | 7.470364 | 16.347659 | -3.595677 |
| H | 7.981324 | 15.411643 | -3.872953 |
| H | 7.711631 | 16.546771 | -2.543978 |
| H | 6.390210 | 16.167177 | -3.675128 |
| H | 8.291595 | 16.140210 | -6.196530 |
| H | 6.643427 | 16.777309 | -6.186134 |
| H | 8.004683 | 17.811585 | -6.715126 |
| H | 9.970996 | 16.734654 | -4.746569 |
| H | 9.839048 | 18.486258 | -5.032866 |
| H | 9.804893 | 17.838070 | -3.375010 |

**II-Ts-2-s**

| | | | |
|---|---|---|---|
| C | 13.365470 | 13.988672 | -0.515117 |
| C | 13.575736 | 14.119778 | 0.931892 |
| C | 14.966358 | 14.384484 | 1.100341 |
| C | 15.681856 | 14.459345 | -0.130394 |
| C | 14.687321 | 14.237916 | -1.184906 |
| C | 15.574688 | 14.562392 | 2.361175 |
| C | 16.974456 | 14.816964 | 2.361575 |
| C | 17.677331 | 14.881473 | 1.166906 |
| C | 17.049394 | 14.707110 | -0.091878 |
| C | 12.773708 | 14.037667 | 2.064469 |
| C | 13.367886 | 14.218181 | 3.339012 |
| C | 14.722728 | 14.471119 | 3.496846 |
| N | 14.730346 | 14.262057 | -2.483505 |
| C | 15.984972 | 14.542990 | -3.169402 |
| N | 12.328431 | 13.740908 | -1.257353 |
| C | 11.017516 | 13.581542 | -0.635645 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Pd | 12.746613 | 13.958958 | -3.417379 | H | 14.059380 | 14.080067 | -5.615042 |
| C | 13.274311 | 14.754663 | -5.243167 | H | 12.456641 | 14.825902 | -5.966602 |
| P | 12.030381 | 11.002520 | -4.412433 | H | 13.680906 | 15.755813 | -5.048769 |
| C | 12.819102 | 10.612052 | -6.154939 | H | 12.598682 | 9.393491 | -0.976961 |
| C | 10.119359 | 10.609618 | -4.480299 | H | 11.834767 | 10.927443 | -1.436838 |
| C | 12.873832 | 9.870233 | -3.058180 | H | 11.073194 | 9.370317 | -1.870288 |
| H | 11.663402 | 15.033455 | -3.633716 | H | 14.677329 | 9.915055 | -1.871000 |
| H | 17.653860 | 14.767152 | -0.995477 | H | 14.951588 | 10.488685 | -3.524061 |
| H | 18.750776 | 15.074689 | 1.191326 | H | 14.117628 | 11.533681 | -2.351213 |
| H | 17.496812 | 14.961225 | 3.309622 | H | 13.505775 | 7.852694 | -2.627094 |
| H | 15.140043 | 14.603748 | 4.497134 | H | 12.149907 | 7.907570 | -3.767257 |
| H | 12.732215 | 14.155651 | 4.223447 | H | 13.797017 | 8.305667 | -4.310486 |
| H | 11.703718 | 13.844850 | 2.005690 | H | 8.355454 | 11.168268 | -3.366305 |
| H | 10.272480 | 13.367048 | -1.405688 | H | 9.773945 | 10.990438 | -2.321025 |
| H | 11.019561 | 12.756106 | 0.095152 | H | 9.606166 | 12.426694 | -3.365164 |
| H | 10.723659 | 14.505016 | -0.110388 | H | 8.421104 | 11.159516 | -5.682942 |
| H | 15.804462 | 14.618620 | -4.246557 | H | 9.781319 | 12.277988 | -5.884603 |
| H | 16.423805 | 15.492132 | -2.822515 | H | 9.804816 | 10.672237 | -6.668292 |
| H | 16.716148 | 13.737417 | -2.991964 | H | 8.671024 | 9.010035 | -4.527565 |
| H | 11.540528 | 13.287744 | -4.119942 | H | 10.222155 | 8.541659 | -5.244030 |
| C | 9.764439 | 9.113270 | -4.427896 | H | 10.044180 | 8.642144 | -3.477365 |
| C | 9.442162 | 11.340424 | -3.303858 | H | 14.790036 | 10.598706 | -7.026471 |
| C | 9.518583 | 11.217300 | -5.760984 | H | 14.711313 | 11.561125 | -5.538674 |
| C | 12.392373 | 9.268613 | -6.770033 | H | 14.747677 | 9.777219 | -5.461880 |
| C | 12.445515 | 11.747887 | -7.130170 | H | 13.013042 | 11.597266 | -8.062803 |
| C | 14.352838 | 10.637360 | -6.016127 | H | 11.384835 | 11.759438 | -7.396912 |
| C | 13.084321 | 8.406353 | -3.482791 | H | 12.713140 | 12.733738 | -6.735143 |
| C | 14.234797 | 10.496268 | -2.696229 | H | 12.937562 | 9.134995 | -7.719410 |
| C | 12.028322 | 9.899517 | -1.772639 | H | 12.627554 | 8.408230 | -6.133205 |

| | | | |
|---|---|---|---|
| H | 11.322665 | 9.240038 | -7.010854 |

**II-$H_2$-inter-s**

| | | | |
|---|---|---|---|
| C | 5.122171 | 18.851984 | 2.243472 |
| C | 6.357506 | 18.339737 | 1.758698 |
| C | 6.391813 | 16.962692 | 1.450313 |
| C | 5.268021 | 16.099373 | 1.601975 |
| C | 4.077766 | 16.633871 | 2.081844 |
| C | 4.025723 | 18.015356 | 2.395466 |
| C | 5.726402 | 14.768111 | 1.186607 |
| C | 7.167829 | 14.896940 | 0.773584 |
| C | 7.556367 | 16.298921 | 0.966949 |
| C | 7.562730 | 19.067231 | 1.554679 |
| C | 8.697170 | 18.427410 | 1.076641 |
| C | 8.715030 | 17.042436 | 0.774998 |
| N | 7.794405 | 13.837378 | 0.369283 |
| Pd | 6.617708 | 11.962318 | 0.679172 |
| P | 5.960737 | 11.316315 | -1.846488 |
| C | 7.591922 | 10.755890 | -2.783289 |
| C | 8.443906 | 11.994992 | -3.112521 |
| N | 5.176760 | 13.593903 | 1.157826 |
| C | 5.775874 | 10.379314 | 1.752161 |
| C | 4.686275 | 9.829236 | -1.923290 |
| C | 4.041754 | 9.581145 | -3.299267 |
| C | 5.400226 | 8.530923 | -1.495051 |
| C | 3.550695 | 10.101068 | -0.913630 |
| C | 8.447678 | 9.877065 | -1.849379 |
| C | 7.346785 | 9.978483 | -4.089678 |
| H | 3.185034 | 16.027489 | 2.226478 |
| H | 3.088819 | 18.429361 | 2.771074 |
| H | 5.039540 | 19.910184 | 2.499770 |
| H | 7.592893 | 20.135729 | 1.777518 |
| H | 9.610675 | 19.004996 | 0.927474 |
| H | 9.636342 | 16.597337 | 0.402293 |
| H | 9.343775 | 9.556127 | -2.405139 |
| H | 8.790609 | 10.436675 | -0.967620 |
| H | 7.936965 | 8.973625 | -1.500598 |
| H | 8.322292 | 9.809572 | -4.574406 |
| H | 6.904691 | 8.989897 | -3.917586 |
| H | 6.718246 | 10.521606 | -4.803741 |
| H | 9.432050 | 11.649386 | -3.456233 |
| H | 8.020622 | 12.608821 | -3.916604 |
| H | 8.606459 | 12.629780 | -2.232362 |
| H | 2.956069 | 9.179561 | -0.805583 |
| H | 3.926405 | 10.369589 | 0.078980 |
| H | 2.867671 | 10.888116 | -1.248548 |
| H | 3.399752 | 8.688572 | -3.216192 |
| H | 3.394736 | 10.407068 | -3.618233 |
| H | 4.772104 | 9.382170 | -4.090839 |
| H | 4.635557 | 7.754222 | -1.336017 |
| H | 6.084665 | 8.154731 | -2.264836 |
| H | 5.963377 | 8.632205 | -0.558905 |
| H | 6.426481 | 10.051036 | 2.567378 |
| H | 4.846835 | 10.792248 | 2.166530 |
| H | 5.568977 | 9.537974 | 1.089508 |
| H | 7.233347 | 12.081139 | 2.093474 |
| H | 7.704001 | 10.894350 | 0.567323 |
| C | 9.220235 | 13.905381 | 0.067658 |
| C | 3.798483 | 13.423699 | 1.600161 |

| | | | |
|---|---|---|---|
| C | 5.178380 | 12.807493 | -2.854360 |
| C | 3.726812 | 13.023983 | -2.387569 |
| C | 5.938989 | 14.098983 | -2.501816 |
| C | 5.180095 | 12.637706 | -4.383885 |
| H | 3.492990 | 12.381353 | 1.460553 |
| H | 3.695304 | 13.676672 | 2.668158 |
| H | 3.114418 | 14.067492 | 1.025064 |
| H | 9.597401 | 12.901207 | -0.147040 |
| H | 9.405151 | 14.547148 | -0.809672 |
| H | 9.784177 | 14.316236 | 0.920624 |
| H | 3.379879 | 13.990939 | -2.786164 |
| H | 3.037746 | 12.257917 | -2.762071 |
| H | 3.645363 | 13.068579 | -1.293110 |
| H | 4.639242 | 13.492598 | -4.822887 |
| H | 6.190587 | 12.649710 | -4.809994 |
| H | 4.673103 | 11.726246 | -4.719396 |
| H | 5.479904 | 14.929938 | -3.062244 |
| H | 5.854196 | 14.328007 | -1.434965 |
| H | 6.999998 | 14.071113 | -2.767173 |

**II-Ts-3-s**

| | | | |
|---|---|---|---|
| C | 8.234658 | 17.356285 | 0.576187 |
| C | 7.221867 | 16.451588 | 0.873442 |
| C | 6.022588 | 16.939971 | 1.468769 |
| C | 5.806073 | 18.301857 | 1.767913 |
| C | 6.865100 | 19.198093 | 1.452887 |
| C | 8.036840 | 18.727140 | 0.877896 |
| C | 5.062987 | 15.918212 | 1.728145 |
| C | 3.844352 | 16.280524 | 2.290073 |
| C | 3.608337 | 17.645360 | 2.593407 |
| C | 4.551025 | 18.633348 | 2.349784 |
| C | 7.025136 | 15.007181 | 0.710078 |
| C | 5.684605 | 14.664174 | 1.282459 |
| N | 5.340978 | 13.411453 | 1.348816 |
| C | 4.092722 | 13.045489 | 2.006271 |
| N | 7.749127 | 14.050530 | 0.210632 |
| C | 9.095255 | 14.330106 | -0.280550 |
| Pd | 6.891516 | 12.056752 | 0.531557 |
| C | 6.195699 | 10.334368 | 1.458343 |
| P | 5.984625 | 11.319902 | -1.924142 |
| C | 5.651938 | 12.852355 | -3.110075 |
| C | 5.603992 | 12.522015 | -4.612947 |
| C | 7.401704 | 10.230557 | -2.730089 |
| C | 6.988735 | 9.458748 | -3.996865 |
| C | 4.337266 | 10.245892 | -1.917882 |
| C | 3.338960 | 10.894743 | -0.938720 |
| C | 8.590565 | 11.145151 | -3.076733 |
| C | 7.921739 | 9.216022 | -1.692805 |
| C | 3.645343 | 10.097885 | -3.285424 |
| C | 4.632371 | 8.826111 | -1.394546 |
| C | 4.326533 | 13.520053 | -2.695674 |
| C | 6.741917 | 13.917734 | -2.896466 |
| H | 3.061374 | 15.552905 | 2.498206 |
| H | 2.649735 | 17.922327 | 3.034607 |
| H | 4.329810 | 19.672597 | 2.601745 |
| H | 6.752341 | 20.263248 | 1.665419 |
| H | 8.836187 | 19.432360 | 0.645666 |
| H | 9.175459 | 17.047152 | 0.123237 |
| H | 8.737853 | 8.640405 | -2.158304 |

| | | | |
|---|---|---|---|
| H | 8.335514 | 9.717841 | -0.808106 |
| H | 7.164049 | 8.499443 | -1.361460 |
| H | 7.884140 | 8.958153 | -4.400410 |
| H | 6.252466 | 8.673185 | -3.790617 |
| H | 6.594058 | 10.105168 | -4.787962 |
| H | 9.450848 | 10.508988 | -3.339265 |
| H | 8.394548 | 11.794867 | -3.937829 |
| H | 8.892231 | 11.766441 | -2.220769 |
| H | 2.461827 | 10.234172 | -0.847371 |
| H | 3.766090 | 11.017629 | 0.062861 |
| H | 2.978829 | 11.871810 | -1.275709 |
| H | 2.781298 | 9.424682 | -3.156884 |
| H | 3.253583 | 11.045101 | -3.673629 |
| H | 4.293577 | 9.649338 | -4.047209 |
| H | 3.667672 | 8.315966 | -1.241149 |
| H | 5.200089 | 8.221531 | -2.111510 |
| H | 5.161206 | 8.819791 | -0.435282 |
| H | 6.325296 | 10.499800 | 2.534449 |
| H | 5.135787 | 10.238967 | 1.204609 |
| H | 6.751097 | 9.445263 | 1.144313 |
| H | 8.067457 | 11.847164 | 1.584128 |
| H | 8.262978 | 11.273313 | 0.523021 |
| H | 4.065372 | 11.962802 | 2.167421 |
| H | 3.999955 | 13.544734 | 2.983672 |
| H | 3.224569 | 13.325252 | 1.387298 |
| H | 9.552173 | 13.403951 | -0.641487 |
| H | 9.070030 | 15.054647 | -1.110237 |
| H | 9.726005 | 14.742827 | 0.523199 |
| H | 4.254327 | 14.489419 | -3.214637 |
| H | 3.441484 | 12.939203 | -2.978898 |
| H | 4.288425 | 13.721621 | -1.614988 |
| H | 5.300761 | 13.434664 | -5.152938 |
| H | 6.586839 | 12.233394 | -5.005759 |
| H | 4.883809 | 11.738419 | -4.868939 |
| H | 6.536495 | 14.756426 | -3.581548 |
| H | 6.715666 | 14.306963 | -1.874365 |
| H | 7.754394 | 13.561173 | -3.110652 |

**III+ AB**

| | | | |
|---|---|---|---|
| C | 22.637288 | 25.650348 | -0.055335 |
| C | 21.397712 | 25.122382 | -0.398831 |
| C | 20.742429 | 24.259766 | 0.527443 |
| C | 21.284216 | 23.926254 | 1.788061 |
| C | 22.543292 | 24.502023 | 2.113104 |
| C | 23.189973 | 25.332889 | 1.210163 |
| C | 19.500763 | 23.748048 | 0.047980 |
| C | 18.789811 | 22.869762 | 0.858625 |
| C | 19.314484 | 22.532798 | 2.131777 |
| C | 20.519904 | 23.038891 | 2.594794 |
| C | 20.517964 | 25.189820 | -1.569640 |
| C | 19.319767 | 24.320283 | -1.295259 |
| N | 18.384583 | 24.244947 | -2.189634 |
| C | 17.201229 | 23.452554 | -1.869325 |
| N | 20.559140 | 25.833514 | -2.692127 |
| C | 21.660293 | 26.748620 | -2.980300 |
| Pd | 19.026849 | 25.372848 | -4.092929 |
| P | 17.715939 | 25.158820 | -6.030660 |
| C | 18.492000 | 26.144923 | -7.539925 |
| C | 17.533127 | 26.261326 | -8.740604 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 15.904922 | 25.820359 | -5.724751 | H | 16.676575 | 26.912520 | -8.527634 |
| C | 15.456087 | 25.387828 | -4.317883 | H | 19.320785 | 28.072737 | -8.006177 |
| C | 15.918732 | 27.360098 | -5.718073 | H | 18.072744 | 28.182848 | -6.752337 |
| C | 14.876301 | 25.326475 | -6.756211 | H | 19.686210 | 27.565529 | -6.348643 |
| C | 18.901532 | 27.570927 | -7.119226 | H | 11.972886 | 26.244514 | -4.127274 |
| C | 19.785161 | 25.443150 | -7.994310 | H | 12.774233 | 28.111681 | -4.081872 |
| B | 12.005439 | 27.349028 | -4.642015 | H | 10.437029 | 28.922807 | -4.841849 |
| N | 10.507314 | 27.986558 | -4.430569 | H | 10.270041 | 28.069811 | -3.436910 |
| H | 19.750182 | 26.135642 | -5.194190 | H | 9.786962 | 27.404339 | -4.869659 |
| H | 23.202381 | 26.292390 | -0.729144 | H | 12.175597 | 27.305982 | -5.849043 |
| H | 24.160491 | 25.754655 | 1.476063 | H | 16.793374 | 23.727865 | -0.883608 |
| H | 23.005747 | 24.279129 | 3.076994 | H | 16.427247 | 23.625486 | -2.619169 |
| H | 20.890604 | 22.749754 | 3.580314 | H | 17.443958 | 22.376573 | -1.855702 |
| H | 18.747608 | 21.846689 | 2.762914 | H | 21.906366 | 27.366675 | -2.103904 |
| H | 17.846209 | 22.426025 | 0.546832 | H | 22.557663 | 26.180770 | -3.278169 |
| H | 14.932592 | 27.701399 | -5.366730 | H | 21.377451 | 27.401462 | -3.810104 |
| H | 16.676929 | 27.762117 | -5.030277 | C | 17.689419 | 23.259466 | -6.486708 |
| H | 16.072570 | 27.791238 | -6.714851 | C | 17.239679 | 22.943765 | -7.922650 |
| H | 13.906388 | 25.790786 | -6.514254 | C | 19.104604 | 22.692201 | -6.249236 |
| H | 15.130140 | 25.608998 | -7.784363 | C | 16.754386 | 22.520024 | -5.513808 |
| H | 14.731352 | 24.239090 | -6.721065 | H | 17.206995 | 21.847989 | -8.037044 |
| H | 14.477791 | 25.849956 | -4.111247 | H | 16.235363 | 23.324608 | -8.146929 |
| H | 15.327156 | 24.303152 | -4.230726 | H | 17.935060 | 23.321946 | -8.681379 |
| H | 16.165137 | 25.733023 | -3.550691 | H | 19.070569 | 21.600787 | -6.400911 |
| H | 20.288495 | 26.095395 | -8.725561 | H | 19.858100 | 23.096250 | -6.932934 |
| H | 20.484096 | 25.285645 | -7.159197 | H | 19.442162 | 22.883542 | -5.218996 |
| H | 19.604890 | 24.482242 | -8.490830 | H | 16.855068 | 21.438947 | -5.702540 |
| H | 18.084456 | 26.720602 | -9.576585 | H | 17.035590 | 22.696439 | -4.468210 |
| H | 17.155722 | 25.294642 | -9.091682 | H | 15.697084 | 22.776052 | -5.649902 |

**III-Ts-1(AB)-s**

| | | | |
|---|---|---|---|
| C | 14.557210 | 18.270724 | 0.462242 |
| C | 14.102143 | 17.685207 | -0.751982 |
| C | 13.833949 | 18.571295 | -1.817621 |
| C | 13.989891 | 19.984738 | -1.718043 |
| C | 14.426780 | 20.522393 | -0.513445 |
| C | 14.710425 | 19.645723 | 0.564501 |
| C | 13.369322 | 18.140579 | -3.095660 |
| C | 13.223390 | 19.359649 | -3.897709 |
| C | 13.592202 | 20.525075 | -3.024590 |
| C | 13.883185 | 16.302374 | -1.004266 |
| C | 13.421617 | 15.879287 | -2.242240 |
| C | 13.155786 | 16.782860 | -3.302033 |
| N | 13.513931 | 21.714414 | -3.533871 |
| Pd | 12.759233 | 21.666996 | -5.608301 |
| H | 12.177653 | 21.527672 | -7.044772 |
| N | 12.892283 | 19.606084 | -5.128667 |
| C | 12.572582 | 18.513791 | -6.041815 |
| C | 13.912853 | 22.872116 | -2.745408 |
| B | 13.484979 | 24.410424 | -6.122957 |
| N | 12.685467 | 25.503363 | -5.576026 |
| C | 9.058094 | 21.561015 | -5.177733 |
| C | 8.191701 | 22.836694 | -5.128953 |
| C | 8.128303 | 23.291805 | -3.658776 |
| C | 6.771132 | 22.541262 | -5.640341 |
| P | 9.041428 | 24.192803 | -6.188650 |
| C | 9.058462 | 23.840705 | -8.073593 |
| C | 9.254360 | 22.334459 | -8.326674 |
| C | 8.522875 | 25.983021 | -5.720479 |
| C | 6.992961 | 26.125306 | -5.653108 |
| C | 9.168855 | 26.325660 | -4.360883 |
| C | 9.082267 | 26.985219 | -6.747890 |
| C | 7.750729 | 24.303101 | -8.737953 |
| C | 10.280760 | 24.567044 | -8.673936 |
| H | 12.786955 | 16.391905 | -4.249457 |
| H | 13.255240 | 14.814264 | -2.411819 |
| H | 14.076613 | 15.572281 | -0.215599 |
| H | 14.784096 | 17.631420 | 1.317980 |
| H | 15.059151 | 20.073181 | 1.505947 |
| H | 14.558504 | 21.594273 | -0.372429 |
| H | 8.822214 | 27.994674 | -6.393543 |
| H | 10.175992 | 26.936719 | -6.822729 |
| H | 8.648515 | 26.873591 | -7.748355 |
| H | 6.755421 | 27.173965 | -5.416990 |
| H | 6.503311 | 25.885858 | -6.606750 |
| H | 6.542962 | 25.508088 | -4.865246 |
| H | 8.994254 | 27.395648 | -4.168470 |
| H | 8.740191 | 25.770498 | -3.521431 |
| H | 10.255891 | 26.160168 | -4.378701 |
| H | 9.374400 | 22.204224 | -9.413573 |
| H | 10.162996 | 21.945511 | -7.846005 |
| H | 8.387703 | 21.733848 | -8.024080 |
| H | 7.804990 | 24.048593 | -9.807594 |
| H | 6.866754 | 23.796322 | -8.326950 |
| H | 7.592397 | 25.386585 | -8.671706 |
| H | 10.341436 | 24.286479 | -9.736954 |
| H | 10.205605 | 25.657980 | -8.631934 |
| H | 11.220836 | 24.252657 | -8.198003 |

| | | | |
|---|---|---|---|
| H | 10.419853 | 24.139185 | -5.813027 |
| H | 12.478947 | 23.180749 | -6.072875 |
| H | 14.398010 | 23.986256 | -5.453817 |
| H | 13.578855 | 24.373560 | -7.326048 |
| H | 12.363163 | 26.237341 | -6.198748 |
| H | 12.868624 | 25.863893 | -4.644200 |
| H | 12.523482 | 18.905432 | -7.061075 |
| H | 13.332886 | 17.718325 | -5.994556 |
| H | 11.593318 | 18.074074 | -5.787136 |
| H | 13.913034 | 23.754825 | -3.392140 |
| H | 13.214464 | 23.033142 | -1.906646 |
| H | 14.926327 | 22.744595 | -2.331857 |
| H | 8.689741 | 20.882070 | -4.392577 |
| H | 8.984889 | 21.031553 | -6.131600 |
| H | 10.127381 | 21.754973 | -4.984940 |
| H | 6.331715 | 21.763214 | -4.997044 |
| H | 6.109827 | 23.416348 | -5.595563 |
| H | 6.766273 | 22.151759 | -6.666426 |
| H | 7.724438 | 22.450913 | -3.073946 |
| H | 9.121482 | 23.525591 | -3.250150 |
| H | 7.459910 | 24.145664 | -3.497912 |

**III-H2-s**

| | | | |
|---|---|---|---|
| C | 12.298276 | 19.922714 | -9.271266 |
| C | 12.169297 | 20.213645 | -7.918189 |
| C | 13.326597 | 20.130670 | -7.089310 |
| C | 14.599899 | 19.758178 | -7.572249 |
| C | 14.690938 | 19.457161 | -8.959709 |
| C | 13.569258 | 19.542670 | -9.771784 |
| C | 13.078294 | 20.481277 | -5.729801 |
| C | 14.139083 | 20.457261 | -4.831853 |
| C | 15.422514 | 20.076895 | -5.298789 |
| C | 15.658902 | 19.736020 | -6.622601 |
| C | 11.074238 | 20.636857 | -7.036782 |
| C | 11.651167 | 20.813455 | -5.655370 |
| N | 10.857601 | 21.211554 | -4.710050 |
| C | 11.366472 | 21.415538 | -3.358330 |
| N | 9.811411 | 20.880069 | -7.204436 |
| C | 9.203520 | 20.741983 | -8.522667 |
| Pd | 8.875605 | 21.761278 | -5.436812 |
| P | 6.555104 | 19.343179 | -4.134754 |
| C | 4.892207 | 19.768426 | -4.996518 |
| C | 4.301577 | 21.044835 | -4.367502 |
| C | 7.293671 | 17.650835 | -4.664380 |
| C | 6.535382 | 19.612903 | -2.230206 |
| C | 6.522901 | 21.133326 | -1.961112 |
| C | 5.325754 | 18.934806 | -1.566128 |
| C | 7.834703 | 19.060107 | -1.614680 |
| C | 5.193051 | 20.096577 | -6.474959 |
| C | 3.874431 | 18.621656 | -4.888675 |
| H | 11.457165 | 19.985635 | -9.959971 |
| H | 13.664166 | 19.315658 | -10.834786 |
| H | 15.652525 | 19.164839 | -9.386841 |
| H | 16.664528 | 19.454936 | -6.942278 |
| H | 16.251300 | 20.059029 | -4.589396 |
| H | 14.017378 | 20.727055 | -3.783604 |
| H | 7.520546 | 20.364753 | -4.660132 |
| H | 6.682084 | 21.282085 | -0.881503 |

| | | | |
|---|---|---|---|
| H | 7.327971 | 21.653196 | -2.499535 |
| H | 5.573555 | 21.612017 | -2.218129 |
| H | 5.387300 | 19.107660 | -0.479890 |
| H | 4.369776 | 19.353308 | -1.905362 |
| H | 5.306235 | 17.848247 | -1.725591 |
| H | 7.827910 | 19.322732 | -0.545354 |
| H | 7.915645 | 17.968319 | -1.677370 |
| H | 8.730695 | 19.515355 | -2.058333 |
| H | 4.270309 | 20.499029 | -6.920851 |
| H | 5.972726 | 20.868042 | -6.566973 |
| H | 5.484177 | 19.221431 | -7.064119 |
| H | 2.943056 | 18.941496 | -5.382224 |
| H | 4.209057 | 17.706420 | -5.393734 |
| H | 3.624892 | 18.373311 | -3.848624 |
| H | 3.415618 | 21.321834 | -4.960144 |
| H | 3.964942 | 20.898851 | -3.334448 |
| H | 5.000933 | 21.891081 | -4.408286 |
| H | 7.530443 | 22.338699 | -5.974880 |
| H | 8.264748 | 22.574768 | -4.256878 |
| H | 10.534407 | 21.677803 | -2.698404 |
| H | 11.865142 | 20.509649 | -2.975788 |
| H | 12.094143 | 22.243963 | -3.337804 |
| H | 8.119248 | 20.856332 | -8.431892 |
| H | 9.572894 | 21.528196 | -9.202230 |
| H | 9.431104 | 19.761788 | -8.973318 |
| C | 8.821430 | 17.714168 | -4.453063 |
| C | 6.680410 | 16.481552 | -3.875599 |
| C | 7.061928 | 17.421765 | -6.169833 |
| H | 9.258475 | 16.798014 | -4.879988 |
| H | 9.266999 | 18.574406 | -4.973714 |
| H | 9.113603 | 17.755073 | -3.399644 |
| H | 7.588776 | 16.494864 | -6.446389 |
| H | 6.005698 | 17.280881 | -6.427193 |
| H | 7.478174 | 18.232812 | -6.782615 |
| H | 7.126624 | 15.543464 | -4.241638 |
| H | 6.886343 | 16.539757 | -2.799591 |
| H | 5.593730 | 16.404027 | -4.016340 |

**III-s**

| | | | |
|---|---|---|---|
| C | 8.929125 | 15.766453 | 2.477371 |
| C | 8.914356 | 16.811880 | 1.513115 |
| C | 10.168932 | 17.251474 | 1.037698 |
| C | 11.406509 | 16.698220 | 1.478390 |
| C | 11.383382 | 15.687648 | 2.432797 |
| C | 10.131797 | 15.233027 | 2.917234 |
| C | 12.448008 | 17.426759 | 0.749288 |
| C | 11.769707 | 18.457895 | -0.111792 |
| C | 10.321609 | 18.299357 | 0.082760 |
| C | 7.768376 | 17.468600 | 0.985569 |
| C | 7.910131 | 18.492109 | 0.060255 |
| C | 9.178028 | 18.926570 | -0.400414 |
| N | 12.501586 | 19.236964 | -0.846264 |
| Pd | 14.719196 | 18.828928 | -0.471260 |
| P | 16.360763 | 20.246994 | -1.353610 |
| C | 15.585727 | 21.789222 | -2.265218 |
| C | 14.921532 | 21.284485 | -3.560350 |
| N | 13.736261 | 17.321941 | 0.671993 |
| C | 14.437631 | 16.293834 | 1.437011 |

| | | | |
|---|---|---|---|
| C | 11.814201 | 20.156562 | -1.749062 |
| C | 17.393935 | 19.182856 | -2.624385 |
| C | 17.533043 | 20.893757 | 0.071911 |
| C | 18.863652 | 21.460165 | -0.457949 |
| C | 16.801621 | 21.988629 | 0.870476 |
| C | 17.837100 | 19.762061 | 1.073707 |
| C | 14.486819 | 22.379543 | -1.354701 |
| C | 16.576965 | 22.908904 | -2.626548 |
| H | 12.294372 | 15.240774 | 2.827727 |
| H | 10.119734 | 14.438227 | 3.664517 |
| H | 7.986057 | 15.388652 | 2.878026 |
| H | 6.772582 | 17.166829 | 1.317024 |
| H | 7.018086 | 18.986651 | -0.327133 |
| H | 9.222435 | 19.742793 | -1.118896 |
| H | 13.818338 | 23.003555 | -1.968767 |
| H | 13.883376 | 21.601098 | -0.870151 |
| H | 14.894833 | 23.020818 | -0.567080 |
| H | 16.028047 | 23.683856 | -3.186804 |
| H | 16.999711 | 23.398050 | -1.740401 |
| H | 17.400797 | 22.568006 | -3.264548 |
| H | 14.291471 | 22.091784 | -3.966672 |
| H | 15.652500 | 21.026452 | -4.335409 |
| H | 14.282965 | 20.406568 | -3.392198 |
| H | 18.524915 | 20.164726 | 1.834885 |
| H | 16.926298 | 19.426713 | 1.588082 |
| H | 18.322588 | 18.890367 | 0.622808 |
| H | 19.415047 | 21.894489 | 0.391413 |
| H | 19.507857 | 20.686563 | -0.894473 |
| H | 18.728929 | 22.256116 | -1.199269 |
| H | 17.389013 | 22.195321 | 1.779460 |
| H | 16.717914 | 22.934067 | 0.322409 |
| H | 15.800205 | 21.668625 | 1.191706 |
| H | 16.104868 | 18.292935 | -0.102531 |
| H | 11.290871 | 20.944993 | -1.182430 |
| H | 12.535692 | 20.639491 | -2.410458 |
| H | 11.074617 | 19.622275 | -2.365972 |
| H | 14.471886 | 16.568535 | 2.504326 |
| H | 13.936944 | 15.318071 | 1.341142 |
| H | 15.463605 | 16.206673 | 1.071092 |
| C | 18.246963 | 20.016711 | -3.597173 |
| C | 18.324782 | 18.216037 | -1.870175 |
| C | 16.405562 | 18.307942 | -3.423402 |
| H | 18.815609 | 19.323116 | -4.237258 |
| H | 17.643073 | 20.642338 | -4.265376 |
| H | 18.974971 | 20.657070 | -3.084122 |
| H | 18.785184 | 17.545187 | -2.613272 |
| H | 19.142163 | 18.722603 | -1.343828 |
| H | 17.777016 | 17.583241 | -1.157699 |
| H | 16.988124 | 17.621663 | -4.058709 |
| H | 15.778782 | 17.699052 | -2.752994 |
| H | 15.746898 | 18.884505 | -4.080937 |

**II-Ts-hydrogenation-s**

| | | | |
|---|---|---|---|
| C | 11.573614 | 18.047286 | 2.590651 |
| C | 12.868735 | 17.933568 | 3.082038 |
| C | 13.137622 | 16.945584 | 4.074483 |
| C | 12.154792 | 16.068025 | 4.580462 |
| C | 10.842820 | 16.209128 | 4.048687 |
| C | 10.574454 | 17.172509 | 3.087010 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 14.494286 | 16.936698 | 4.513207 | H | 11.301100 | 18.788724 | 1.840768 |
| C | 14.873315 | 16.020204 | 5.486576 | H | 21.309084 | 23.538350 | -3.052905 |
| C | 13.899338 | 15.128137 | 6.001944 | H | 20.570199 | 23.379649 | -1.452931 |
| C | 12.580335 | 15.140910 | 5.572147 | H | 21.792316 | 22.200029 | -2.004433 |
| C | 14.144036 | 18.620168 | 2.844558 | H | 20.893233 | 21.956019 | -4.865004 |
| C | 15.166404 | 17.996244 | 3.754313 | H | 21.153055 | 20.486093 | -3.910105 |
| N | 16.375896 | 18.463759 | 3.723150 | H | 19.625096 | 20.726216 | -4.790998 |
| C | 17.411102 | 17.904610 | 4.585234 | H | 19.285137 | 23.708003 | -4.179350 |
| N | 14.530899 | 19.581167 | 2.064146 | H | 17.941732 | 22.569713 | -4.040874 |
| C | 13.576771 | 20.214777 | 1.164123 | H | 18.366307 | 23.619996 | -2.668448 |
| Pd | 16.640981 | 20.086714 | 2.357114 | H | 20.412003 | 18.415668 | 0.905554 |
| C | 16.650175 | 22.766411 | 0.996924 | H | 18.784915 | 19.103960 | 0.802804 |
| C | 17.243068 | 23.102762 | -0.231181 | H | 19.371064 | 17.945773 | -0.444302 |
| P | 18.985945 | 20.821550 | -1.707115 | H | 22.173448 | 18.928003 | -0.660644 |
| C | 20.285448 | 19.956975 | -0.571758 | H | 21.202299 | 18.682043 | -2.121822 |
| C | 19.651358 | 18.787397 | 0.200513 | H | 22.064833 | 20.218135 | -1.863447 |
| C | 17.765531 | 19.578832 | -2.526957 | H | 21.460556 | 20.504928 | 1.147845 |
| C | 19.818983 | 21.993132 | -2.997386 | H | 21.224793 | 21.873910 | 0.052576 |
| C | 20.400207 | 21.229669 | -4.199185 | H | 19.887050 | 21.320513 | 1.100382 |
| C | 18.773544 | 23.017825 | -3.489900 | H | 18.098573 | 21.844249 | -0.861062 |
| C | 20.936330 | 22.808353 | -2.317193 | H | 16.909353 | 21.401697 | 1.352818 |
| C | 21.491202 | 19.426133 | -1.367745 | H | 15.561314 | 22.680580 | 1.040416 |
| C | 20.733554 | 20.994353 | 0.480295 | H | 17.084374 | 23.169186 | 1.913871 |
| H | 18.145867 | 20.395989 | 2.643781 | H | 18.138632 | 23.729024 | -0.221916 |
| H | 15.892627 | 15.967980 | 5.866888 | H | 16.607463 | 23.190050 | -1.115462 |
| H | 14.202250 | 14.410331 | 6.765969 | H | 18.354898 | 18.419057 | 4.388441 |
| H | 11.861010 | 14.438448 | 5.998378 | H | 17.147582 | 18.041666 | 5.646976 |
| H | 10.042722 | 15.556862 | 4.404821 | H | 17.540840 | 16.826223 | 4.395236 |
| H | 9.559409 | 17.266128 | 2.697603 | H | 14.101912 | 20.934617 | 0.527396 |

| | | | |
|---|---|---|---|
| H | 13.078800 | 19.472516 | 0.518442 |
| H | 12.800152 | 20.755087 | 1.730326 |
| C | 16.924303 | 20.288304 | -3.603779 |
| C | 18.482046 | 18.376208 | -3.164688 |
| C | 16.787020 | 19.101804 | -1.433567 |
| H | 17.720361 | 17.714935 | -3.608411 |
| H | 19.167671 | 18.672227 | -3.968857 |
| H | 19.042691 | 17.779058 | -2.435388 |
| H | 16.024191 | 18.467864 | -1.913949 |
| H | 17.264866 | 18.509981 | -0.647633 |
| H | 16.272153 | 19.944551 | -0.951667 |
| H | 16.157766 | 19.576231 | -3.948784 |
| H | 16.397537 | 21.170169 | -3.213791 |
| H | 17.510117 | 20.580630 | -4.483439 |

**III-s with alkane**

| | | | |
|---|---|---|---|
| C | 10.124973 | 17.159576 | 8.607790 |
| C | 9.608610 | 15.839234 | 8.493783 |
| C | 9.673924 | 15.243598 | 7.215477 |
| C | 10.214467 | 15.901126 | 6.070918 |
| C | 10.705324 | 17.193751 | 6.220904 |
| C | 10.653611 | 17.803859 | 7.499348 |
| C | 10.079389 | 14.949231 | 4.958631 |
| C | 9.433490 | 13.708470 | 5.513655 |
| C | 9.191021 | 13.931033 | 6.941698 |
| C | 9.025945 | 15.059512 | 9.530901 |
| C | 8.547664 | 13.784416 | 9.267197 |
| C | 8.616242 | 13.202762 | 7.976819 |
| N | 10.405101 | 14.978500 | 3.703714 |
| Pd | 9.702623 | 13.048302 | 2.661995 |
| P | 9.945341 | 12.861698 | 0.332363 |
| C | 11.805329 | 13.096112 | -0.220506 |
| C | 12.601577 | 11.821695 | 0.113438 |
| N | 9.219677 | 12.716984 | 4.709678 |
| C | 8.637360 | 11.475558 | 5.215011 |
| C | 9.335972 | 11.110758 | -0.312939 |
| C | 9.912896 | 9.976133 | 0.558018 |
| C | 8.817089 | 14.244887 | -0.460731 |
| C | 7.804398 | 11.023606 | -0.177847 |
| C | 9.722466 | 10.835821 | -1.779631 |
| C | 11.050622 | 16.190468 | 3.205110 |
| C | 11.978912 | 13.427605 | -1.712523 |
| C | 12.426782 | 14.225018 | 0.619082 |
| C | 13.163393 | 11.508804 | 4.484990 |
| C | 13.882797 | 12.821261 | 4.795230 |
| H | 9.048756 | 11.734871 | 2.256433 |
| H | 8.212601 | 12.202247 | 7.829334 |
| H | 8.098117 | 13.206447 | 10.075854 |
| H | 8.950516 | 15.472435 | 10.539148 |
| H | 10.100108 | 17.668154 | 9.574003 |
| H | 11.042563 | 18.817104 | 7.608766 |
| H | 11.124738 | 17.756844 | 5.389824 |
| H | 13.670677 | 12.043173 | -0.033012 |
| H | 12.470240 | 11.513256 | 1.160917 |
| H | 12.357248 | 10.978768 | -0.542833 |
| H | 13.058339 | 13.488878 | -1.926566 |
| H | 11.559235 | 12.663065 | -2.376428 |
| H | 11.543876 | 14.397844 | -1.983603 |

| | | | |
|---|---|---|---|
| H | 13.501568 | 14.281846 | 0.382303 |
| H | 11.994829 | 15.206391 | 0.395539 |
| H | 12.330307 | 14.021675 | 1.695914 |
| H | 7.503520 | 9.985242 | -0.389696 |
| H | 7.464653 | 11.261401 | 0.840770 |
| H | 7.269185 | 11.664445 | -0.887786 |
| H | 9.241926 | 9.894315 | -2.089907 |
| H | 9.384889 | 11.615632 | -2.471303 |
| H | 10.803051 | 10.697251 | -1.909764 |
| H | 9.521865 | 9.023029 | 0.167960 |
| H | 11.005087 | 9.914850 | 0.542877 |
| H | 9.593018 | 10.057070 | 1.606672 |
| H | 13.060561 | 10.883423 | 5.384352 |
| H | 13.713964 | 10.915396 | 3.738937 |
| H | 14.894778 | 12.641995 | 5.185907 |
| H | 13.340666 | 13.411207 | 5.550240 |
| H | 12.151390 | 11.687238 | 4.084361 |
| H | 13.986325 | 13.447162 | 3.895077 |
| H | 11.967564 | 16.410314 | 3.776429 |
| H | 11.324992 | 16.061657 | 2.157523 |
| H | 10.375052 | 17.057638 | 3.288332 |
| H | 9.155912 | 11.137564 | 6.124851 |
| H | 7.571074 | 11.623579 | 5.451722 |
| H | 8.718237 | 10.699120 | 4.450694 |
| C | 8.502218 | 14.050645 | -1.952881 |
| C | 7.501627 | 14.298514 | 0.344352 |
| C | 9.494493 | 15.614607 | -0.277843 |
| H | 7.908684 | 14.914951 | -2.292171 |
| H | 9.403202 | 14.008915 | -2.577240 |
| H | 7.899604 | 13.155793 | -2.148173 |
| H | 6.901286 | 15.142882 | -0.031578 |
| H | 6.894499 | 13.393570 | 0.248476 |
| H | 7.696188 | 14.467931 | 1.414890 |
| H | 8.782261 | 16.391293 | -0.599255 |
| H | 9.734387 | 15.811353 | 0.775288 |
| H | 10.400221 | 15.736029 | -0.884121 |