

Electronic Supplementary Information (ESI) for the following manuscript:

## **On the inter-ring torsion potential of regioregular P3HT: a first principle reexamination with explicit side chains**

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MP2/6-311G(d,p) optimized structures for all conformational isomers of 3-hexyl-2,2'-bithiophene (HBT) discussed in the manuscript are provided in cartesian format, along with absolute energy (Hartree).

**I-A**

Absolute energy: -1338.090112

|   |           |          |           |
|---|-----------|----------|-----------|
| S | 7.991718  | 2.002460 | 1.120147  |
| C | 8.123815  | 3.660721 | 1.586163  |
| C | 9.001408  | 3.799306 | 2.654981  |
| C | 9.542579  | 2.565022 | 3.090636  |
| C | 9.068925  | 1.495837 | 2.354009  |
| C | 7.401056  | 4.717259 | 0.891101  |
| S | 8.252461  | 6.083560 | 0.269111  |
| C | 6.811334  | 6.803569 | -0.309073 |
| C | 5.710373  | 6.008918 | -0.051760 |
| C | 6.032517  | 4.808750 | 0.634323  |
| C | 5.020984  | 3.804469 | 1.120661  |
| C | 4.934422  | 3.774819 | 2.652882  |
| C | 3.952314  | 2.726042 | 3.172311  |
| C | 3.878031  | 2.689902 | 4.698745  |
| H | 10.233686 | 2.454990 | 3.918719  |
| H | 9.212658  | 4.764174 | 3.104036  |
| H | 4.699481  | 6.284012 | -0.335905 |
| H | 4.038735  | 4.059775 | 0.704150  |
| H | 5.265234  | 2.799970 | 0.756094  |
| H | 9.301051  | 0.445575 | 2.473369  |
| H | 6.843435  | 7.762734 | -0.809145 |
| H | 5.932424  | 3.573614 | 3.061686  |
| H | 4.640227  | 4.770714 | 3.009981  |
| H | 2.951609  | 2.925454 | 2.764080  |
| H | 4.254833  | 1.736840 | 2.801201  |
| H | 4.882551  | 2.500397 | 5.101539  |
| H | 3.573196  | 3.678456 | 5.068950  |
| C | 2.912359  | 1.632439 | 5.234309  |
| C | 2.851982  | 1.609322 | 6.761985  |
| H | 1.911334  | 1.823842 | 4.827544  |
| H | 3.219854  | 0.647247 | 4.861548  |
| H | 2.156921  | 0.846375 | 7.125116  |
| H | 3.839592  | 1.396259 | 7.183726  |
| H | 2.523478  | 2.578956 | 7.149977  |

**I-B**

Absolute energy: -1338.090028

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 7.228322  | 4.702049 | 0.485440  |
| C | 8.591716  | 4.626168 | 0.766525  |
| S | 9.539295  | 4.714989 | -0.676227 |
| C | 8.144732  | 4.836178 | -1.663055 |
| C | 6.988044  | 4.830136 | -0.909471 |
| C | 9.251668  | 4.475256 | 2.055885  |
| S | 8.947689  | 5.551384 | 3.374726  |
| C | 10.083230 | 4.754421 | 4.380932  |
| C | 10.702489 | 3.707469 | 3.724439  |
| C | 10.227184 | 3.546951 | 2.400538  |
| C | 6.143704  | 4.670676 | 1.523995  |
| C | 5.626427  | 6.074421 | 1.869599  |
| C | 4.560655  | 6.059164 | 2.964800  |
| C | 4.036075  | 7.454006 | 3.305611  |
| C | 2.977428  | 7.449759 | 4.408857  |
| C | 2.463658  | 8.851768 | 4.737966  |
| H | 11.449045 | 3.074229 | 4.190409  |
| H | 10.556441 | 2.776676 | 1.711127  |
| H | 5.995263  | 4.888283 | -1.345087 |
| H | 6.515129  | 4.184792 | 2.433780  |
| H | 5.307657  | 4.063827 | 1.152580  |
| H | 10.233021 | 5.087311 | 5.399789  |
| H | 8.242698  | 4.904645 | -2.738690 |
| H | 6.469867  | 6.698230 | 2.192066  |
| H | 5.220349  | 6.541400 | 0.962277  |
| H | 3.722626  | 5.422666 | 2.648421  |
| H | 4.983026  | 5.599778 | 3.869239  |
| H | 4.877488  | 8.089494 | 3.614506  |
| H | 3.613133  | 7.912112 | 2.400927  |
| H | 2.139978  | 6.812671 | 4.097630  |
| H | 3.403210  | 6.990844 | 5.310036  |
| H | 1.708199  | 8.827069 | 5.528941  |
| H | 3.284058  | 9.494626 | 5.073055  |
| H | 2.013562  | 9.315302 | 3.854136  |

I-C

Absolute energy: -1338.089749

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 6.673064  | 3.502049 | 0.986779  |
| C | 7.698928  | 4.110827 | 0.263057  |
| S | 7.847853  | 3.431430 | -1.316145 |
| C | 6.550285  | 2.348585 | -1.044511 |
| C | 6.026712  | 2.492652 | 0.226396  |
| C | 8.568449  | 5.185500 | 0.724507  |
| S | 8.618065  | 6.720037 | -0.069386 |
| C | 9.717155  | 7.358995 | 1.079376  |
| C | 10.031046 | 6.433091 | 2.056926  |
| C | 9.379655  | 5.191964 | 1.851915  |
| C | 6.258072  | 3.942075 | 2.365418  |
| C | 5.624395  | 5.339981 | 2.350973  |
| C | 5.240682  | 5.835162 | 3.744403  |
| C | 4.634696  | 7.238481 | 3.726150  |
| C | 4.261821  | 7.756842 | 5.115323  |
| C | 3.660052  | 9.161991 | 5.077818  |
| H | 10.716607 | 6.640393 | 2.870998  |
| H | 9.500435  | 4.315464 | 2.479250  |
| H | 5.197341  | 1.898876 | 0.597693  |
| H | 7.120408  | 3.950283 | 3.041834  |
| H | 5.540914  | 3.217996 | 2.771650  |
| H | 10.084379 | 8.371652 | 0.975418  |
| H | 6.246127  | 1.658398 | -1.820551 |
| H | 6.333981  | 6.043606 | 1.899111  |
| H | 4.737363  | 5.321550 | 1.703825  |
| H | 4.525951  | 5.135565 | 4.199973  |
| H | 6.135126  | 5.836255 | 4.382853  |
| H | 5.350380  | 7.930532 | 3.261268  |
| H | 3.740014  | 7.237498 | 3.088367  |
| H | 3.549246  | 7.061613 | 5.576904  |
| H | 5.157766  | 7.755201 | 5.748874  |
| H | 3.401185  | 9.515175 | 6.080474  |
| H | 4.368280  | 9.873112 | 4.640369  |
| H | 2.750637  | 9.176242 | 4.468391  |

I-D

Absolute energy: -1338.089602

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 7.078289  | 4.209555  | 0.632442  |
| C | 8.448586  | 4.034349  | 0.820343  |
| S | 9.264986  | 3.777134  | -0.681190 |
| C | 7.804671  | 3.895266  | -1.568790 |
| C | 6.726103  | 4.140521  | -0.743057 |
| C | 9.168733  | 4.039100  | 2.086188  |
| S | 10.137866 | 2.697533  | 2.584874  |
| C | 10.554567 | 3.456209  | 4.063093  |
| C | 9.954807  | 4.695152  | 4.189791  |
| C | 9.170944  | 5.031366  | 3.058968  |
| C | 6.099535  | 4.461276  | 1.742717  |
| C | 5.685649  | 5.937246  | 1.831721  |
| C | 4.722683  | 6.213478  | 2.986086  |
| C | 4.302885  | 7.680699  | 3.076109  |
| C | 3.344099  | 7.966118  | 4.232514  |
| C | 2.934874  | 9.437345  | 4.309348  |
| H | 10.095543 | 5.336457  | 5.052640  |
| H | 8.640146  | 5.967630  | 2.926953  |
| H | 5.709293  | 4.241249  | -1.110013 |
| H | 6.542256  | 4.150626  | 2.696678  |
| H | 5.202654  | 3.848585  | 1.581785  |
| H | 11.212092 | 2.957397  | 4.763004  |
| H | 7.813064  | 3.786221  | -2.645487 |
| H | 6.585730  | 6.554456  | 1.949551  |
| H | 5.222899  | 6.240597  | 0.883124  |
| H | 3.828037  | 5.586218  | 2.869919  |
| H | 5.197978  | 5.913167  | 3.930180  |
| H | 5.199282  | 8.306357  | 3.187497  |
| H | 3.828338  | 7.979336  | 2.131231  |
| H | 2.450763  | 7.339275  | 4.118379  |
| H | 3.820799  | 7.665076  | 5.173862  |
| H | 2.249576  | 9.620313  | 5.142305  |
| H | 3.813520  | 10.075778 | 4.447195  |
| H | 2.435821  | 9.747979  | 3.385741  |

### III-A

Absolute energy: -1338.092255

|   |          |          |           |
|---|----------|----------|-----------|
| C | 6.843011 | 4.335537 | 0.457142  |
| C | 8.044691 | 4.630000 | 1.101988  |
| S | 9.203389 | 5.292989 | 0.005790  |
| C | 8.108519 | 5.209821 | -1.307974 |
| C | 6.896433 | 4.671978 | -0.922668 |
| C | 8.390329 | 4.485998 | 2.510220  |
| S | 8.305812 | 2.967667 | 3.329430  |
| C | 8.858290 | 3.649498 | 4.801870  |
| C | 9.130242 | 4.998522 | 4.670484  |
| C | 8.864434 | 5.475194 | 3.363786  |
| C | 5.595809 | 3.842507 | 1.138533  |
| C | 4.668060 | 5.004913 | 1.534303  |
| C | 5.326068 | 5.969362 | 2.520371  |
| C | 4.387859 | 7.074558 | 3.002079  |
| C | 5.070796 | 8.055135 | 3.956209  |
| C | 4.129033 | 9.152234 | 4.453198  |
| H | 9.489194 | 5.613579 | 5.488034  |
| H | 8.984053 | 6.504241 | 3.041193  |
| H | 6.065046 | 4.530403 | -1.606598 |
| H | 5.852727 | 3.274277 | 2.038005  |
| H | 5.065834 | 3.158518 | 0.464366  |
| H | 8.954547 | 3.030145 | 5.684091  |
| H | 8.411785 | 5.540705 | -2.292793 |
| H | 4.368457 | 5.553748 | 0.631360  |
| H | 3.752972 | 4.592855 | 1.981155  |
| H | 5.698500 | 5.403736 | 3.385828  |
| H | 6.206366 | 6.423343 | 2.049032  |
| H | 3.997986 | 7.625096 | 2.134454  |
| H | 3.520202 | 6.625537 | 3.505220  |
| H | 5.474368 | 7.496475 | 4.810230  |
| H | 5.929818 | 8.507425 | 3.444382  |
| H | 4.639043 | 9.843346 | 5.131035  |
| H | 3.734274 | 9.732043 | 3.612491  |
| H | 3.279118 | 8.717688 | 4.989452  |

### III-B

Absolute energy: -1338.090794

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 6.628458  | 4.070146  | 1.329977  |
| C | 7.841052  | 4.615276  | 0.912629  |
| S | 7.892305  | 4.800139  | -0.805801 |
| C | 6.321824  | 4.144013  | -0.989862 |
| C | 5.766856  | 3.808911  | 0.228636  |
| C | 9.007827  | 4.995561  | 1.701249  |
| S | 8.947629  | 6.218955  | 2.921588  |
| C | 10.627063 | 6.088407  | 3.236349  |
| C | 11.231221 | 5.153222  | 2.417306  |
| C | 10.308351 | 4.531722  | 1.541914  |
| C | 6.254157  | 3.769327  | 2.755496  |
| C | 5.028216  | 4.579737  | 3.209275  |
| C | 5.249620  | 6.089532  | 3.137526  |
| C | 4.015967  | 6.896529  | 3.540727  |
| C | 4.243448  | 8.407201  | 3.478258  |
| C | 3.003567  | 9.208731  | 3.875609  |
| H | 12.288547 | 4.918054  | 2.464249  |
| H | 10.556719 | 3.758485  | 0.822596  |
| H | 4.780834  | 3.365659  | 0.327249  |
| H | 7.103270  | 3.982527  | 3.414291  |
| H | 6.035520  | 2.697570  | 2.850137  |
| H | 11.082375 | 6.692933  | 4.010110  |
| H | 5.886683  | 4.036634  | -1.975045 |
| H | 4.167823  | 4.313119  | 2.581333  |
| H | 4.769857  | 4.296693  | 4.238420  |
| H | 6.088571  | 6.362198  | 3.791355  |
| H | 5.544129  | 6.364459  | 2.115875  |
| H | 3.177992  | 6.629297  | 2.881938  |
| H | 3.715129  | 6.617954  | 4.560287  |
| H | 5.080553  | 8.668739  | 4.137876  |
| H | 4.550107  | 8.678538  | 2.460294  |
| H | 3.188496  | 10.285885 | 3.824903  |
| H | 2.165120  | 8.977534  | 3.210591  |
| H | 2.697783  | 8.965380  | 4.898365  |

### III-C

Absolute energy: -1338.092225

|   |          |          |           |
|---|----------|----------|-----------|
| C | 7.168516 | 4.822388 | 0.398084  |
| C | 8.302879 | 5.077131 | 1.169025  |
| S | 9.475015 | 5.989458 | 0.286356  |
| C | 8.475484 | 6.054610 | -1.102634 |
| C | 7.285425 | 5.383630 | -0.902558 |
| C | 8.539890 | 4.686973 | 2.552761  |
| S | 8.844009 | 5.862040 | 3.782570  |
| C | 8.944861 | 4.664265 | 5.002972  |
| C | 8.739321 | 3.395489 | 4.492828  |
| C | 8.517707 | 3.407356 | 3.093931  |
| C | 5.925261 | 4.141546 | 0.900036  |
| C | 4.858414 | 5.162444 | 1.332841  |
| C | 5.338640 | 6.051398 | 2.479049  |
| C | 4.267944 | 7.013674 | 2.990180  |
| C | 4.772518 | 7.915156 | 4.117555  |
| C | 3.699566 | 8.873485 | 4.635099  |
| H | 8.768669 | 2.499611 | 5.102921  |
| H | 8.363806 | 2.525987 | 2.480660  |
| H | 6.514453 | 5.303173 | -1.662897 |
| H | 6.166309 | 3.500112 | 1.754077  |
| H | 5.522936 | 3.496409 | 0.109098  |
| H | 9.154047 | 4.947613 | 6.026252  |
| H | 8.818559 | 6.558702 | -1.996774 |
| H | 4.583432 | 5.789368 | 0.474008  |
| H | 3.953047 | 4.623143 | 1.642964  |
| H | 5.683039 | 5.415314 | 3.306556  |
| H | 6.211824 | 6.627645 | 2.148762  |
| H | 3.913064 | 7.637880 | 2.158166  |
| H | 3.400158 | 6.440899 | 3.345845  |
| H | 5.136188 | 7.285561 | 4.939584  |
| H | 5.637176 | 8.485799 | 3.755709  |
| H | 4.082419 | 9.508996 | 5.439296  |
| H | 3.342647 | 9.524283 | 3.830197  |
| H | 2.839843 | 8.317534 | 5.023178  |

### IV-A

Absolute energy: -1338.091825

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 6.532493  | 3.816197  | 1.134546  |
| C | 7.774491  | 4.429689  | 0.970280  |
| S | 8.096037  | 4.772836  | -0.689759 |
| C | 6.587711  | 4.132893  | -1.184087 |
| C | 5.865353  | 3.653376  | -0.107773 |
| C | 8.743579  | 4.792724  | 1.995063  |
| S | 9.392880  | 3.621771  | 3.085002  |
| C | 10.339674 | 4.798471  | 3.896200  |
| C | 10.188732 | 6.052787  | 3.335112  |
| C | 9.276670  | 6.050282  | 2.251292  |
| C | 5.929871  | 3.479112  | 2.474880  |
| C | 5.745114  | 4.726741  | 3.354833  |
| C | 4.929298  | 5.821487  | 2.669312  |
| C | 4.745212  | 7.058579  | 3.547692  |
| C | 3.958489  | 8.174259  | 2.859490  |
| C | 3.788660  | 9.409633  | 3.744261  |
| H | 10.702999 | 6.933061  | 3.704087  |
| H | 8.987142  | 6.925474  | 1.678877  |
| H | 4.877822  | 3.212946  | -0.203675 |
| H | 6.547216  | 2.744573  | 3.004976  |
| H | 4.953189  | 3.008681  | 2.305754  |
| H | 10.960892 | 4.511395  | 4.734576  |
| H | 6.309217  | 4.137212  | -2.229841 |
| H | 5.253645  | 4.434181  | 4.292506  |
| H | 6.729334  | 5.130575  | 3.619817  |
| H | 5.429745  | 6.112947  | 1.736973  |
| H | 3.944127  | 5.422470  | 2.386783  |
| H | 4.232745  | 6.774875  | 4.477476  |
| H | 5.734535  | 7.439092  | 3.838110  |
| H | 4.473329  | 8.451355  | 1.930915  |
| H | 2.972924  | 7.789197  | 2.568577  |
| H | 3.224976  | 10.195913 | 3.233205  |
| H | 3.254738  | 9.154397  | 4.665412  |
| H | 4.764228  | 9.819890  | 4.024829  |

#### IV-B

Absolute energy: -1338.090434

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 6.868979  | 4.502155 | 1.269320  |
| C | 8.214301  | 4.766327 | 1.012365  |
| S | 8.471120  | 5.187921 | -0.643787 |
| C | 6.812273  | 4.993160 | -1.019620 |
| C | 6.078995  | 4.635581 | 0.094372  |
| C | 9.354869  | 4.687290 | 1.915583  |
| S | 9.439417  | 5.591988 | 3.385833  |
| C | 11.005011 | 4.996800 | 3.747269  |
| C | 11.469726 | 4.146656 | 2.761295  |
| C | 10.529364 | 3.969793 | 1.718172  |
| C | 6.327245  | 4.095223 | 2.611874  |
| C | 5.791925  | 5.277602 | 3.438672  |
| C | 4.665913  | 6.049453 | 2.752385  |
| C | 4.098198  | 7.166770 | 3.627789  |
| C | 2.989248  | 7.964711 | 2.941451  |
| C | 2.429418  | 9.078738 | 3.826492  |
| H | 12.437435 | 3.659812 | 2.805769  |
| H | 10.673214 | 3.331632 | 0.852708  |
| H | 5.010080  | 4.449509 | 0.066538  |
| H | 7.112012  | 3.581058 | 3.179235  |
| H | 5.513342  | 3.374408 | 2.459645  |
| H | 11.499526 | 5.292272 | 4.663498  |
| H | 6.459544  | 5.149842 | -2.030731 |
| H | 5.431981  | 4.895543 | 4.404036  |
| H | 6.616718  | 5.966032 | 3.658529  |
| H | 5.035718  | 6.480064 | 1.813845  |
| H | 3.857652  | 5.353214 | 2.484740  |
| H | 3.709497  | 6.736851 | 4.561324  |
| H | 4.911730  | 7.848776 | 3.911558  |
| H | 3.382569  | 8.393195 | 2.011075  |
| H | 2.181660  | 7.279198 | 2.654787  |
| H | 1.638672  | 9.637474 | 3.317029  |
| H | 2.010805  | 8.664981 | 4.749664  |
| H | 3.218916  | 9.785044 | 4.102987  |

#### IV-C

Absolute energy: -1338.091597

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 6.649824  | 3.571850 | 1.633039  |
| C | 7.056155  | 4.395949 | 0.583437  |
| S | 6.237318  | 4.005344 | -0.883871 |
| C | 5.345799  | 2.753735 | -0.130685 |
| C | 5.674700  | 2.632488 | 1.206190  |
| C | 8.015443  | 5.489458 | 0.656909  |
| S | 7.535295  | 7.129977 | 0.401747  |
| C | 9.096189  | 7.720261 | 0.790467  |
| C | 9.964866  | 6.694513 | 1.116622  |
| C | 9.349637  | 5.421380 | 1.034904  |
| C | 7.124335  | 3.717922 | 3.057609  |
| C | 6.883461  | 5.125016 | 3.632486  |
| C | 5.452102  | 5.620174 | 3.433946  |
| C | 5.227407  | 7.017256 | 4.010951  |
| C | 3.815602  | 7.549413 | 3.764709  |
| C | 3.604281  | 8.950470 | 4.339249  |
| H | 11.002397 | 6.860492 | 1.384417  |
| H | 9.842332  | 4.476188 | 1.236564  |
| H | 5.217523  | 1.901319 | 1.865548  |
| H | 8.191173  | 3.473833 | 3.133217  |
| H | 6.587467  | 2.983014 | 3.670402  |
| H | 9.303641  | 8.781411 | 0.743528  |
| H | 4.638795  | 2.167503 | -0.703083 |
| H | 7.122980  | 5.113916 | 4.704288  |
| H | 7.572672  | 5.833929 | 3.161021  |
| H | 5.223295  | 5.636102 | 2.360649  |
| H | 4.748236  | 4.912063 | 3.894966  |
| H | 5.428182  | 7.005886 | 5.091351  |
| H | 5.956149  | 7.706761 | 3.562047  |
| H | 3.624635  | 7.559315 | 2.684141  |
| H | 3.089234  | 6.854868 | 4.205512  |
| H | 2.590015  | 9.314365 | 4.149427  |
| H | 3.767847  | 8.952779 | 5.421857  |
| H | 4.308081  | 9.660123 | 3.892142  |

V-A

Absolute energy: -1338.088620

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 9.134204  | 6.277172  | 1.806248  |
| C | 8.111348  | 5.459831  | 2.271268  |
| S | 7.431167  | 6.103810  | 3.722280  |
| C | 8.475173  | 7.461497  | 3.696226  |
| C | 9.340913  | 7.419948  | 2.617196  |
| C | 7.580204  | 4.244419  | 1.661316  |
| C | 6.385114  | 4.121188  | 0.952946  |
| C | 6.189717  | 2.794517  | 0.488854  |
| C | 7.214700  | 1.937460  | 0.844818  |
| S | 8.422528  | 2.743152  | 1.750961  |
| C | 5.474027  | 5.288762  | 0.674522  |
| C | 6.148702  | 6.380108  | -0.200526 |
| C | 6.247612  | 7.735874  | 0.501825  |
| C | 7.094863  | 8.749006  | -0.263992 |
| C | 7.244367  | 10.076931 | 0.478505  |
| C | 8.146786  | 11.068259 | -0.256461 |
| H | 10.086118 | 8.184301  | 2.425562  |
| H | 9.689022  | 6.045643  | 0.902808  |
| H | 5.329389  | 2.480994  | -0.093918 |
| H | 5.157519  | 5.738421  | 1.624097  |
| H | 4.565515  | 4.913818  | 0.191044  |
| H | 8.415549  | 8.210434  | 4.475537  |
| H | 7.316524  | 0.884638  | 0.615895  |
| H | 7.159560  | 6.050853  | -0.467019 |
| H | 5.599410  | 6.499210  | -1.143017 |
| H | 5.239183  | 8.142714  | 0.662608  |
| H | 6.694283  | 7.591198  | 1.491229  |
| H | 8.092283  | 8.317477  | -0.428129 |
| H | 6.659434  | 8.928418  | -1.257228 |
| H | 6.250999  | 10.519243 | 0.627249  |
| H | 7.651403  | 9.871429  | 1.476611  |
| H | 8.238436  | 12.011538 | 0.290617  |
| H | 9.151512  | 10.651900 | -0.384600 |
| H | 7.747537  | 11.291508 | -1.251298 |

V-C

Absolute energy: -1338.088552

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 6.576483 | 3.403293  | 0.892288  |
| C | 7.570015 | 4.280051  | 0.457360  |
| S | 8.069867 | 3.923618  | -1.153686 |
| C | 6.973144 | 2.614808  | -1.272623 |
| C | 6.247155 | 2.451485  | -0.107219 |
| C | 8.137138 | 5.384078  | 1.225141  |
| S | 7.706809 | 7.026218  | 0.903504  |
| C | 8.621567 | 7.602913  | 2.231308  |
| C | 9.243040 | 6.569980  | 2.911397  |
| C | 8.967581 | 5.305343  | 2.336198  |
| C | 5.911536 | 3.530833  | 2.237299  |
| C | 5.035615 | 4.808177  | 2.351792  |
| C | 5.484375 | 5.734678  | 3.483754  |
| C | 4.725144 | 7.059197  | 3.516665  |
| C | 5.248053 | 8.014180  | 4.590114  |
| C | 4.514604 | 9.355603  | 4.597900  |
| H | 9.875098 | 6.727608  | 3.778336  |
| H | 9.349704 | 4.357545  | 2.700647  |
| H | 5.497124 | 1.677520  | 0.021257  |
| H | 6.679783 | 3.557267  | 3.019517  |
| H | 5.309914 | 2.633640  | 2.418869  |
| H | 8.678555 | 8.664793  | 2.433851  |
| H | 6.921462 | 2.028985  | -2.181109 |
| H | 5.081591 | 5.362734  | 1.407142  |
| H | 3.983842 | 4.532978  | 2.500995  |
| H | 5.367662 | 5.219392  | 4.447741  |
| H | 6.553732 | 5.943864  | 3.364560  |
| H | 4.815580 | 7.542071  | 2.533676  |
| H | 3.654362 | 6.872599  | 3.679958  |
| H | 5.155014 | 7.534881  | 5.573036  |
| H | 6.320087 | 8.176037  | 4.419357  |
| H | 4.905387 | 10.023640 | 5.371485  |
| H | 4.620610 | 9.858130  | 3.630760  |
| H | 3.445432 | 9.210929  | 4.784431  |

**I-P**

Absolute energy: -1338.086624

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 7.009202  | 4.252809 | 0.532761  |
| C | 8.368564  | 4.350354 | 0.851946  |
| S | 9.344849  | 4.175017 | -0.571825 |
| C | 7.975033  | 3.997475 | -1.583491 |
| C | 6.804038  | 4.065574 | -0.860920 |
| C | 9.036208  | 4.498591 | 2.136856  |
| S | 8.194944  | 4.682896 | 3.643361  |
| C | 9.651945  | 4.735777 | 4.543175  |
| C | 10.760372 | 4.619628 | 3.727646  |
| C | 10.411798 | 4.479612 | 2.365588  |
| C | 5.871261  | 4.404864 | 1.502171  |
| C | 5.584977  | 5.879795 | 1.827743  |
| C | 4.555773  | 6.050695 | 2.943506  |
| C | 4.237451  | 7.516044 | 3.239554  |
| C | 3.230115  | 7.699106 | 4.375074  |
| C | 2.921902  | 9.169725 | 4.658181  |
| H | 11.778392 | 4.630960 | 4.100270  |
| H | 11.135548 | 4.364425 | 1.565762  |
| H | 5.819694  | 3.972682 | -1.309018 |
| H | 6.069285  | 3.849975 | 2.427041  |
| H | 4.972442  | 3.955825 | 1.061732  |
| H | 9.615662  | 4.856750 | 5.617984  |
| H | 8.103104  | 3.859639 | -2.649168 |
| H | 6.517939  | 6.380473 | 2.112640  |
| H | 5.229526  | 6.376564 | 0.915404  |
| H | 3.629760  | 5.525331 | 2.670989  |
| H | 4.935560  | 5.571114 | 3.856333  |
| H | 5.168592  | 8.041285 | 3.493022  |
| H | 3.846737  | 7.992071 | 2.329691  |
| H | 2.303598  | 7.169690 | 4.119316  |
| H | 3.624112  | 7.222596 | 5.281612  |
| H | 2.200457  | 9.279047 | 5.473380  |
| H | 3.833315  | 9.707996 | 4.937760  |
| H | 2.504909  | 9.654685 | 3.769629  |

**II-P**

Absolute energy: -1338.083870

|   |           |           |           |
|---|-----------|-----------|-----------|
| S | 8.762136  | 4.629417  | 3.655487  |
| C | 8.778774  | 5.104257  | 1.985707  |
| C | 9.974409  | 5.759899  | 1.693297  |
| C | 10.843983 | 5.867456  | 2.801358  |
| C | 10.314288 | 5.294561  | 3.941011  |
| C | 7.685951  | 4.837388  | 1.064331  |
| S | 7.836164  | 5.368859  | -0.578721 |
| C | 6.297961  | 4.747630  | -0.997155 |
| C | 5.681407  | 4.150213  | 0.081367  |
| C | 6.460409  | 4.191547  | 1.270581  |
| C | 6.020485  | 3.610977  | 2.591810  |
| C | 4.639712  | 2.953359  | 2.571846  |
| C | 4.254055  | 2.385816  | 3.938182  |
| C | 2.876164  | 1.723802  | 3.943228  |
| H | 11.817589 | 6.343379  | 2.770543  |
| H | 10.203061 | 6.145823  | 0.705575  |
| H | 4.699322  | 3.697418  | 0.015070  |
| H | 6.755253  | 2.865734  | 2.927449  |
| H | 6.018161  | 4.400448  | 3.356442  |
| H | 10.753878 | 5.229623  | 4.927771  |
| H | 5.927533  | 4.852638  | -2.008520 |
| H | 3.886196  | 3.688469  | 2.261646  |
| H | 4.627627  | 2.144925  | 1.829766  |
| H | 5.009716  | 1.652386  | 4.251099  |
| H | 4.270890  | 3.193461  | 4.682688  |
| H | 2.121664  | 2.457930  | 3.628686  |
| H | 2.860083  | 0.917705  | 3.196834  |
| C | 2.484874  | 1.153829  | 5.307020  |
| C | 1.105007  | 0.495303  | 5.296620  |
| H | 3.241327  | 0.422542  | 5.618403  |
| H | 2.503773  | 1.961190  | 6.049835  |
| H | 0.844390  | 0.094450  | 6.280623  |
| H | 0.334300  | 1.218352  | 5.010608  |
| H | 1.076032  | -0.329005 | 4.576711  |



### III-P

Absolute energy:

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 6.880230  | 4.504163 | 0.638797  |
| C | 8.103815  | 4.788686 | 1.254657  |
| S | 9.188401  | 5.553995 | 0.132519  |
| C | 8.034404  | 5.516807 | -1.131047 |
| C | 6.856877  | 4.937284 | -0.716898 |
| C | 8.610678  | 4.500913 | 2.591265  |
| S | 7.684670  | 3.744552 | 3.846294  |
| C | 9.005498  | 3.746072 | 4.937666  |
| C | 10.130495 | 4.315010 | 4.375218  |
| C | 9.909165  | 4.735131 | 3.044423  |
| C | 5.651183  | 3.899529 | 1.262675  |
| C | 4.614866  | 4.980956 | 1.622579  |
| C | 5.118234  | 5.989627 | 2.653985  |
| C | 4.130005  | 7.128580 | 2.902579  |
| C | 4.620175  | 8.123694 | 3.954759  |
| C | 3.634692  | 9.268677 | 4.190097  |
| H | 11.073649 | 4.417506 | 4.899806  |
| H | 10.671814 | 5.192374 | 2.423293  |
| H | 5.995550  | 4.807835 | -1.365207 |
| H | 5.894757  | 3.303613 | 2.146234  |
| H | 5.205616  | 3.206188 | 0.537981  |
| H | 8.878800  | 3.344495 | 5.934599  |
| H | 8.281571  | 5.922002 | -2.103629 |
| H | 4.337682  | 5.516880 | 0.704860  |
| H | 3.704054  | 4.495461 | 1.998324  |
| H | 5.318507  | 5.473205 | 3.600967  |
| H | 6.075123  | 6.408332 | 2.315715  |
| H | 3.946865  | 7.660652 | 1.958681  |
| H | 3.164186  | 6.711956 | 3.221124  |
| H | 4.797549  | 7.588029 | 4.895865  |
| H | 5.589598  | 8.527465 | 3.636861  |
| H | 4.003819  | 9.967056 | 4.947126  |
| H | 3.466913  | 9.829804 | 3.265051  |
| H | 2.667622  | 8.882540 | 4.528481  |

### IV-P

Absolute energy:

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 6.721015  | 4.208399 | 1.297780  |
| C | 8.045680  | 4.619193 | 1.106857  |
| S | 8.328605  | 5.016746 | -0.559117 |
| C | 6.715054  | 4.654986 | -1.001050 |
| C | 5.976791  | 4.243389 | 0.086641  |
| C | 9.173012  | 4.673844 | 2.026836  |
| S | 9.056534  | 4.306783 | 3.717850  |
| C | 10.730987 | 4.564008 | 3.972087  |
| C | 11.374909 | 4.926072 | 2.805293  |
| C | 10.493912 | 4.982625 | 1.702249  |
| C | 6.091656  | 3.837471 | 2.612832  |
| C | 5.702876  | 5.075709 | 3.440665  |
| C | 4.683745  | 5.966415 | 2.731508  |
| C | 4.263437  | 7.170432 | 3.574029  |
| C | 3.265862  | 8.084287 | 2.861920  |
| C | 2.853689  | 9.285347 | 3.713568  |
| H | 12.437241 | 5.135276 | 2.750737  |
| H | 10.804629 | 5.234882 | 0.694028  |
| H | 4.929285  | 3.965222 | 0.026915  |
| H | 6.756193  | 3.188014 | 3.193963  |
| H | 5.186347  | 3.251705 | 2.408999  |
| H | 11.148666 | 4.443748 | 4.963169  |
| H | 6.394193  | 4.775190 | -2.027567 |
| H | 5.290959  | 4.747500 | 4.404928  |
| H | 6.600123  | 5.666133 | 3.660029  |
| H | 5.106424  | 6.318849 | 1.782440  |
| H | 3.793426  | 5.371666 | 2.480146  |
| H | 3.822327  | 6.819578 | 4.517342  |
| H | 5.157608  | 7.749866 | 3.842274  |
| H | 3.710940  | 8.432319 | 1.921372  |
| H | 2.376983  | 7.500236 | 2.591588  |
| H | 2.141022  | 9.926277 | 3.185974  |
| H | 2.385613  | 8.954835 | 4.646508  |
| H | 3.727325  | 9.892067 | 3.972909  |