

Cartesian coordinates for all the species calculated in this study

coumarin

E= -803.035008 a.u.

G= -802.860386 a.u.

6 4.232066 -1.293417 -0.000075
6 3.902012 0.052082 -0.000089
6 2.557359 0.416090 -0.000012
6 1.546942 -0.549658 0.000059
6 1.900591 -1.906504 0.000059
6 3.234118 -2.275023 0.000001
1 5.277686 -1.584575 -0.000127
1 4.658791 0.828564 -0.000144
6 0.178577 -0.069104 0.000058
1 1.118102 -2.656977 0.000099
1 3.504869 -3.325477 0.000002
6 -0.084478 1.260294 0.000057
6 0.985564 2.229243 0.000225
1 -1.090105 1.658937 -0.000035
8 2.277980 1.749140 0.000013
8 -0.749471 -1.042722 0.000033
8 0.849465 3.434370 -0.000234
6 -2.097293 -0.684909 0.000017
6 -2.752300 -0.537502 -1.214598
6 -2.752329 -0.537501 1.214616
6 -4.110836 -0.232772 -1.207022
1 -2.203837 -0.661432 -2.142431
6 -4.110863 -0.232770 1.207008
1 -2.203887 -0.661428 2.142463
6 -4.789470 -0.080325 -0.000015
1 -4.637231 -0.114494 -2.148775
1 -4.637281 -0.114488 2.148749
1 -5.848867 0.155706 -0.000027

IM1

E= -1386.634278 a.u.

G= -1386.371933 a.u.

6 4.165007 -2.577089 -0.643924
6 3.832400 -1.895487 0.514769
6 2.510932 -1.507782 0.711927
6 1.527013 -1.804913 -0.238952
6 1.881477 -2.507491 -1.402425
6 3.193165 -2.887180 -1.604977
1 5.196370 -2.873307 -0.806166
1 4.570743 -1.649571 1.269023
6 0.179286 -1.363980 0.036821
1 1.114824 -2.734169 -2.134876
1 3.471359 -3.422885 -2.505722
6 -0.065646 -0.510890 1.129443
6 0.972432 -0.394736 2.170593
1 -1.073352 -0.330884 1.494886
8 2.229641 -0.860364 1.875104
8 -0.731332 -1.847605 -0.783145
8 0.801332 0.090125 3.260107
6 -2.107884 -1.661606 -0.586025
6 -2.807725 -1.067681 -1.623228
6 -2.727129 -2.145571 0.556018
6 -4.186610 -0.933870 -1.496073
1 -2.276458 -0.705865 -2.496051
6 -4.104782 -1.989445 0.673285
1 -2.148113 -2.624291 1.338514

6 -4.833521 -1.386529 -0.348276
1 -4.752638 -0.466621 -2.295139
1 -4.605973 -2.346346 1.566562
1 -5.907559 -1.268600 -0.249316
46 0.281688 1.249709 -0.069407
8 -1.631806 1.605226 -0.468894
6 -2.620465 1.573020 0.380412
8 -2.579099 1.110454 1.517781
6 -3.877424 2.219280 -0.161943
6 2.330487 2.467514 -0.695988
8 1.203402 2.948361 -1.020609
8 2.339134 1.362747 -0.045953
6 3.606029 3.135973 -1.078541
1 4.439359 2.730455 -0.504068
1 3.517847 4.212973 -0.921097
1 3.784888 2.963375 -2.144464
1 -3.952075 2.102888 -1.244140
1 -3.835603 3.290641 0.062069
1 -4.753703 1.794821 0.330095

IM2

E= -1386.640548 a.u.

G= -1386.375971 a.u.

6 -5.956092 -0.288036 -0.217247
6 -5.194568 0.801836 0.172072
6 -3.806119 0.697261 0.146008
6 -3.169470 -0.474762 -0.265765
6 -3.958328 -1.567007 -0.656208
6 -5.339249 -1.473925 -0.630965
1 -7.038986 -0.216303 -0.199225
1 -5.646292 1.732184 0.498246
6 -1.713820 -0.484346 -0.266613
1 -3.471824 -2.480842 -0.977457
1 -5.943281 -2.323043 -0.933496
6 -1.010654 0.607178 0.128698
6 -1.719945 1.793519 0.567496
1 3.162807 0.046210 1.228375
8 -3.095919 1.789394 0.540218
8 -1.210682 -1.674065 -0.678250
8 -1.198015 2.816930 0.970758
6 0.142392 -1.838064 -0.937155
6 0.906557 -2.560222 -0.027927
6 0.679957 -1.359069 -2.125693
6 2.257660 -2.761400 -0.295528
1 0.441941 -2.933939 0.878414
6 2.032175 -1.568212 -2.381583
1 0.052925 -0.801720 -2.813125
6 2.823676 -2.257296 -1.465522
1 2.869363 -3.312433 0.411923
1 2.468063 -1.180268 -3.296936
1 3.878863 -2.412135 -1.666679
46 0.936837 0.808113 0.224465
8 0.929622 -0.160021 2.103138
6 1.971007 -0.622550 2.585017
8 3.162163 -0.490848 2.050612
6 1.963457 -1.398667 3.857880
6 2.684188 1.617713 -1.361191
8 3.059617 1.176481 -0.226558
8 1.441539 1.687536 -1.622751

6 3.688089 2.081249 -2.366717
1 3.294118 1.965459 -3.377582
1 4.622972 1.531175 -2.248010
1 3.887558 3.143823 -2.193229
1 0.943986 -1.512421 4.222571
1 2.571656 -0.875612 4.601196
1 2.419577 -2.377819 3.687956

IM3-2

E= -1386.648735 a.u.

G= -1386.383172 a.u.

46 0.898512 0.037489 0.227109
6 -1.031614 0.349299 -0.056139
6 -1.862088 -0.705406 0.124559
6 -3.298272 -0.600023 0.039470
6 -3.800781 0.667092 -0.269054
6 -1.593150 1.613674 -0.485041
8 2.935746 -0.369112 0.663451
6 3.762702 0.039258 -0.208959
8 3.488516 0.870157 -1.114041
6 5.157774 -0.536267 -0.165637
1 -0.072783 -1.345121 -1.863284
6 0.536372 -1.797853 -1.087855
6 -0.038677 -2.160572 0.154730
6 1.810880 -2.321464 -1.416682
8 -1.375003 -1.936779 0.430736
1 5.888934 0.273729 -0.094838
1 5.349546 -1.060902 -1.106872
1 5.281801 -1.225517 0.669969
6 0.650876 -2.995534 1.052665
6 1.898967 -3.466047 0.704629
1 2.583069 2.037314 -0.773969
8 1.057218 1.948735 1.120828
6 1.409395 2.964365 0.490958
8 2.174771 2.955488 -0.552088
6 0.991287 4.317464 0.967921
1 0.950188 5.018192 0.133650
1 1.732835 4.677768 1.688675
1 0.022584 4.249386 1.461822
6 -4.193143 -1.657105 0.259052
6 -5.556094 -1.434847 0.175657
6 -6.041978 -0.157290 -0.129359
6 -5.171626 0.897281 -0.354549
1 -3.801665 -2.640465 0.496367
1 -6.250057 -2.250794 0.347437
1 -7.111863 0.012728 -0.194708
1 -5.527130 1.892682 -0.596922
8 -2.972009 1.719296 -0.514114
8 -0.980163 2.601977 -0.836578
6 2.481807 -3.136013 -0.533108
1 0.174205 -3.260888 1.989417
1 2.437523 -4.104941 1.396714
1 3.460510 -3.528319 -0.787016
1 2.242305 -2.067497 -2.378545

IM3

E= -1386.630182 a.u.

G= -1386.369956 a.u.

46 0.957505 0.007571 0.041958
6 -0.993152 0.297977 0.204858
6 -1.914749 -0.580826 -0.262887
6 -3.312085 -0.243762 -0.410786

6 -3.689582 1.030596 0.018844
6 -1.479392 1.511602 0.844355
8 3.100110 -0.027902 -0.021034
6 3.731496 -0.312146 -1.130049
8 3.210745 -0.880243 -2.086717
6 5.183593 0.110816 -1.141546
1 0.901605 -1.972563 -1.590713
6 0.798468 -2.268281 -0.548949
6 -0.464198 -2.324963 0.054382
6 1.886324 -2.855188 0.136282
8 -1.567926 -1.843150 -0.629015
1 5.248910 1.197615 -1.026052
1 5.663360 -0.186745 -2.074180
1 5.709020 -0.337840 -0.293649
6 -0.660009 -2.919082 1.301946
6 0.427302 -3.480732 1.950102
1 3.232778 1.396816 0.525239
8 1.142523 2.104122 -0.276651
6 2.023326 2.835959 0.205436
8 3.144560 2.398017 0.699585
6 1.805741 4.310225 0.267085
1 1.324011 4.646377 -0.652517
1 2.739858 4.845056 0.436399
1 1.113637 4.504637 1.093259
6 -4.276944 -1.090255 -0.974490
6 -5.581543 -0.649828 -1.114732
6 -5.938539 0.636166 -0.691484
6 -4.999548 1.481270 -0.120931
1 -3.984556 -2.082283 -1.301881
1 -6.328433 -1.302998 -1.553445
1 -6.962502 0.977872 -0.804614
1 -5.257127 2.476329 0.224838
8 -2.798502 1.862933 0.624497
8 -0.853432 2.244470 1.581492
6 1.703014 -3.446858 1.371843
1 -1.655202 -2.937201 1.732366
1 0.285862 -3.952219 2.917485
1 2.543799 -3.897780 1.887660
1 2.858005 -2.845442 -0.343200

IM4

E= -1386.649330 a.u.

G= -1386.383946 a.u.

46 0.943277 -0.192373 -0.112182
6 -1.008004 -0.378999 -0.244573
6 -1.909076 0.543058 0.165911
6 -3.321832 0.239531 0.304799
6 -3.729945 -1.043609 -0.064108
6 -1.505342 -1.654562 -0.738776
8 3.191522 -0.124649 0.034321
6 3.875690 0.552753 0.808121
8 3.392092 1.585872 1.455367
6 5.312542 0.257239 1.069422
1 2.458634 1.732122 1.207056
6 0.633342 1.718748 -0.490200
6 -0.486952 2.424890 -0.051840
6 1.651691 2.475685 -1.096796
8 -1.601651 1.819616 0.499062
1 5.394655 -0.758416 1.466080
1 5.744825 0.968449 1.771885
1 5.854175 0.288022 0.120428
6 -0.579474 3.812826 -0.138278

6 0.457500 4.534112 -0.714446
1 3.287482 -1.840675 -0.434127
8 1.261432 -2.310714 0.596669
6 2.013339 -3.137183 0.086942
8 3.146412 -2.810534 -0.509715
6 1.698366 -4.595588 0.071032
1 2.576670 -5.199557 -0.156141
1 0.935671 -4.753785 -0.698707
1 1.263457 -4.882690 1.029613
6 -4.280994 1.139742 0.789534
6 -5.604330 0.750199 0.908166
6 -5.991040 -0.543385 0.539962
6 -5.058874 -1.444657 0.050487
1 -3.969770 2.139860 1.069990
1 -6.342268 1.450755 1.285188
1 -7.029324 -0.846021 0.633018
1 -5.334551 -2.449963 -0.249092
8 -2.846783 -1.945583 -0.573799
8 -0.854581 -2.510593 -1.307671
6 1.572585 3.861675 -1.209134
1 -1.472429 4.304200 0.235331
1 0.385332 5.614556 -0.790752
1 2.380876 4.412506 -1.680848
1 2.533159 1.967628 -1.479782

IM5

E= -1386.651534 a.u.

G= -1386.385152 a.u.

46 -1.111908 0.043728 0.009358
6 -0.727949 1.970165 -0.086830
6 0.464881 2.559417 0.321475
6 0.622014 3.940360 0.430913
6 -0.430455 4.776710 0.089120
6 -1.626643 4.223957 -0.364403
6 -1.768025 2.842193 -0.446092
8 -1.702170 -2.134100 0.381259
6 -0.992663 -3.017288 0.865596
8 0.061422 -2.738089 1.601976
6 -1.229266 -4.468384 0.644453
1 1.574094 4.336385 0.770453
1 -0.311816 5.853002 0.166423
1 -2.452740 4.868682 -0.650245
1 -2.714292 2.429041 -0.779708
1 0.176900 -1.771229 1.655517
6 0.830787 -0.216799 -0.290800
6 1.814643 0.619036 0.128629
6 1.227012 -1.446932 -0.959735
8 0.475919 -2.259006 -1.473700
8 1.605083 1.843660 0.650801
1 -2.288244 -4.652202 0.463996
1 -0.863261 -5.061964 1.482346
1 -0.668251 -4.746533 -0.254865
6 3.221454 0.263894 0.064791
6 3.537600 -0.960301 -0.524589
6 5.869840 -0.594144 -0.138723
6 4.855396 -1.398505 -0.632357
6 4.263080 1.068457 0.549386
6 5.575697 0.640248 0.452195
1 6.900286 -0.926055 -0.217245
1 5.057497 -2.355225 -1.101349
1 4.023284 2.024690 1.000641
1 6.377530 1.265337 0.831156

8 2.566762 -1.768441 -1.030837
1 -3.256569 -1.931797 -0.282313
8 -3.322254 0.358141 0.234856
6 -4.270283 -0.331513 -0.138413
8 -4.170499 -1.605053 -0.457762
6 -5.656272 0.211110 -0.271189
1 -6.004134 0.065148 -1.297751
1 -5.671898 1.269781 -0.017016
1 -6.329778 -0.345543 0.386197

IM6

E= -1386.627304 a.u.

G= -1386.360049 a.u.

6 -4.950539 0.107341 0.244069
6 -4.193070 1.267871 0.212007
6 -2.867422 1.216993 0.635135
6 -2.302314 0.023615 1.096106
6 -3.078152 -1.144266 1.103936
6 -4.395722 -1.099867 0.685485
1 -5.983345 0.138038 -0.088057
1 -4.599403 2.209071 -0.140983
6 -0.907973 0.067049 1.475281
1 -2.624980 -2.074633 1.425941
1 -4.994105 -2.004458 0.689128
6 -0.211472 1.226229 1.415212
6 -0.824906 2.436967 0.918746
1 0.835697 1.303885 1.675310
8 -2.149995 2.374773 0.565003
8 -0.379752 -1.126952 1.842644
8 -0.261891 3.503824 0.789414
6 0.958591 -1.365324 1.581888
6 1.259482 -2.080270 0.400632
6 1.943640 -0.967890 2.466418
6 2.610965 -2.377827 0.127490
1 0.444405 -2.554793 -0.151333
6 3.272733 -1.264444 2.156508
1 1.680926 -0.435721 3.373940
6 3.612189 -1.953626 0.994205
1 2.851907 -2.963358 -0.753844
1 4.053172 -0.948021 2.841031
1 4.652152 -2.169542 0.776780
46 1.210288 -0.201113 -0.928766
8 -0.492602 -0.609058 -1.874594
6 -1.351296 -1.582656 -1.796038
8 -1.187007 -2.656455 -1.217572
6 -2.641047 -1.259806 -2.519493
6 2.436830 1.919777 -0.897438
8 1.477828 1.768610 -1.712822
8 2.778094 0.890234 -0.207283
6 3.104003 3.231942 -0.696918
1 4.066729 3.101094 -0.200965
1 2.449607 3.844585 -0.067435
1 3.226887 3.738775 -1.656029
1 -2.435912 -1.072458 -3.577232
1 -3.074945 -0.346844 -2.101499
1 -3.346544 -2.085113 -2.419197

IM7

E= -1386.644469 a.u.

G= -1386.377878 a.u.

6 4.248581 -1.279031 -0.602608
6 3.807954 -0.031341 -1.012425

6 2.468587 0.130180 -1.360065
6 1.571428 -0.938427 -1.291842
6 2.032983 -2.192408 -0.867347
6 3.364894 -2.363219 -0.533860
1 5.291739 -1.413734 -0.335458
1 4.475667 0.821126 -1.069806
6 0.183733 -0.653607 -1.596836
1 1.328685 -3.014458 -0.803705
1 3.723548 -3.336070 -0.214437
6 -0.183690 0.570849 -2.046847
6 0.772677 1.649584 -2.119102
1 -1.213324 0.825347 -2.261681
8 2.072616 1.373478 -1.749399
8 -0.660816 -1.678811 -1.378302
8 0.531024 2.791609 -2.449645
6 -1.974924 -1.422265 -0.982008
6 -2.258299 -0.594167 0.108408
6 -2.972840 -2.095958 -1.672249
6 -3.590846 -0.450532 0.488148
1 1.550944 0.558538 1.861516
6 -4.296959 -1.950859 -1.268170
1 -2.699716 -2.726237 -2.512860
6 -4.605759 -1.127521 -0.190248
1 -3.845131 0.199050 1.321451
1 -5.083378 -2.475701 -1.801178
1 -5.637434 -1.005105 0.125294
46 -0.853263 0.435807 0.999080
8 0.050332 -1.324041 1.723822
6 1.228888 -1.325881 2.106430
8 2.005766 -0.270159 2.128884
6 1.865404 -2.566209 2.634533
6 -0.246827 2.865220 0.885915
8 0.544920 2.094281 1.519620
8 -1.337311 2.395277 0.422001
6 0.101727 4.297373 0.644829
1 -0.798452 4.914219 0.671177
1 0.537244 4.372567 -0.357369
1 0.830599 4.642481 1.379160
1 2.938669 -2.559098 2.443695
1 1.392382 -3.443612 2.194718
1 1.705521 -2.590197 3.718002

IM8

E= -1386.652837 a.u.

G= -1386.387161 a.u.

46 0.584462 -0.251027 0.057145
6 1.723411 1.336376 -0.242665
6 1.078851 2.573775 -0.299096
6 1.738929 3.766247 -0.538263
6 3.118343 3.723475 -0.734421
6 3.792488 2.506840 -0.698231
6 3.096661 1.318560 -0.460718
8 -0.797540 -1.865474 0.322271
6 -0.605196 -2.915035 -0.368209
8 0.511319 -3.262298 -0.835642
6 -1.815624 -3.755201 -0.682116
1 1.186053 4.699173 -0.572440
1 3.660069 4.645124 -0.920865
1 4.866600 2.477525 -0.854029
1 3.635674 0.375549 -0.438781
1 0.012814 0.988506 -2.187474
6 -0.677690 0.669683 -1.412996

6 -0.994885 1.526387 -0.346476
6 -1.684050 -0.301303 -1.875315
8 -1.560205 -0.992857 -2.856760
8 -0.292713 2.621003 -0.040642
1 -2.559168 -3.675513 0.112786
1 -1.537227 -4.796748 -0.849110
1 -2.259380 -3.362108 -1.604004
6 -2.221123 1.335150 0.394406
6 -3.096525 0.338310 -0.052399
6 -4.595155 0.828740 1.745204
6 -4.287354 0.082820 0.617825
6 -2.547290 2.077770 1.538781
6 -3.729526 1.826650 2.208809
1 -5.521861 0.631045 2.274354
1 -4.946367 -0.694330 0.248133
1 -1.857041 2.838125 1.886594
1 -3.982789 2.396431 3.096085
8 -2.843861 -0.411863 -1.163413
1 1.715930 -2.868474 -0.187777
8 2.035557 -0.996264 1.418480
6 2.788322 -1.972452 1.240959
8 2.644899 -2.861359 0.316995
6 3.971262 -2.173647 2.137344
1 3.885595 -3.143532 2.634591
1 4.030942 -1.376163 2.876513
1 4.882141 -2.193319 1.531898

IM8-2

E= -1386.657933 a.u.

G= -1386.392157 a.u.

46 0.584462 -0.251027 0.057145
6 1.723411 1.336376 -0.242665
6 1.078851 2.573775 -0.299096
6 1.738929 3.766247 -0.538263
6 3.118343 3.723475 -0.734421
6 3.792488 2.506840 -0.698231
6 3.096661 1.318560 -0.460718
8 -0.797540 -1.865474 0.322271
6 -0.605196 -2.915035 -0.368209
8 0.511319 -3.262298 -0.835642
6 -1.815624 -3.755201 -0.682116
1 1.186053 4.699173 -0.572440
1 3.660069 4.645124 -0.920865
1 4.866600 2.477525 -0.854029
1 3.635674 0.375549 -0.438781
1 0.012814 0.988506 -2.187474
6 -0.677690 0.669683 -1.412996
6 -0.994885 1.526387 -0.346476
6 -1.684050 -0.301303 -1.875315
8 -1.560205 -0.992857 -2.856760
8 -0.292713 2.621003 -0.040642
1 -2.559168 -3.675513 0.112786
1 -1.537227 -4.796748 -0.849110
1 -2.259380 -3.362108 -1.604004
6 -2.221123 1.335150 0.394406
6 -3.096525 0.338310 -0.052399
6 -4.595155 0.828740 1.745204
6 -4.287354 0.082820 0.617825
6 -2.547290 2.077770 1.538781
6 -3.729526 1.826650 2.208809
1 -5.521861 0.631045 2.274354
1 -4.946367 -0.694330 0.248133

1 -1.8570412.838125 1.886594
1 -3.9827892.396431 3.096085
8 -2.843861-0.411863-1.163413
1 1.715930 -2.868474-0.187777
8 2.035557 -0.996264 1.418480
6 2.788322 -1.972452 1.240959
8 2.644899 -2.861359 0.316995
6 3.971262 -2.173647 2.137344
1 3.885595 -3.143532 2.634591
1 4.030942 -1.376163 2.876513
1 4.882141 -2.193319 1.531898

Pd(HOAc)₂

E= -584.793105 a.u.

G= -584.705649 a.u.

46 0.000004 0.531433 0.000003
8 2.083642 0.536139 0.490612
6 2.811068 -0.316683 -0.017535
8 2.338448 -1.255968 -0.816516
6 4.283905 -0.376838 0.207136
1 1.363070 -1.099306 -0.890098
1 4.587079 0.408305 0.897889
1 4.798959 -0.254451 -0.749803
1 4.555063 -1.357688 0.606289
1 -1.363086 -1.099359 0.890082
8 -2.083636 0.536132 -0.490619
6 -2.811068 -0.316689 0.017523
8 -2.338464 -1.255999 0.816482
6 -4.283910 -0.376813 -0.207114
1 -4.798924 -0.253989 0.749795
1 -4.555180 -1.357804 -0.605842
1 -4.587041 0.408091 -0.898155

PC

E= -801.846274 a.u.

G= -801.690707 a.u.

6 4.379902 -0.491942 0.000334
6 3.652879 0.688516 0.000280
6 2.262394 0.623433 0.000012
6 1.602953 -0.615378 -0.000162
6 2.352997 -1.798965 -0.000065
6 3.734831 -1.734847 0.000165
1 5.464304 -0.446884 0.000523
1 4.136244 1.659063 0.000402
6 0.176108 -0.518742 -0.000243
1 1.836080 -2.752877 -0.000151
1 4.318323 -2.649347 0.000240
6 -0.495098 0.670988 -0.000386
6 0.212496 1.925086 -0.000730
8 1.588633 1.815487 -0.000129
8 -0.657215 -1.577969 -0.000186
8 -0.267224 3.036509 0.000271
6 -1.936760 -1.055159 -0.000057
6 -1.900055 0.344325 -0.000081
6 -3.105688 -1.795601 0.000112
6 -3.098456 1.060586 0.000062
6 -4.289561 -1.064934 0.000264
1 -3.092453 -2.879674 0.000133
6 -4.284985 0.338779 0.000238
1 -3.090819 2.144881 0.000008
1 -5.237247 -1.593777 0.000398
1 -5.231712 0.869524 0.000341

Pd(OAc)₂

E= -583.579026 a.u.

G= -583.512283 a.u.

46 -0.000002 0.000005 0.000022
8 -1.747715 1.082779 -0.019641
6 -2.423608 -0.000004 -0.019668
8 -1.747704 -1.082779 -0.019670
6 -3.910101 -0.000011 0.015394
6 2.423604 -0.000004 0.019402
8 1.747716 1.082781 0.019480
8 1.747702 -1.082780 0.019509
6 3.910109 -0.000014 -0.015086
1 4.297383 -0.899434 0.468221
1 4.297395 0.899219 0.468562
1 4.234213 0.000196 -1.062084
1 -4.297558 0.899285 -0.467996
1 -4.233831 0.000049 1.062509
1 -4.297549 -0.899364 -0.467896

TS0

E= -1386.622722 a.u.

G= -1386.359592 a.u.

Frequency= -121.57 cm⁻¹

6 4.279882 -2.069259 -0.297956
6 3.804607 -1.471982 0.857754
6 2.435423 -1.255281 0.990329
6 1.545333 -1.642366 -0.016530
6 2.044440 -2.245415 -1.180462
6 3.403687 -2.455553 -1.321021
1 5.346471 -2.234973 -0.411152
1 4.467315 -1.157237 1.655883
6 0.142381 -1.346970 0.191275
1 1.351672 -2.533057 -1.963280
1 3.791331 -2.918619 -2.221856
6 -0.246398 -0.589153 1.273480
6 0.701549 -0.302580 2.343335
1 -1.286447 -0.418710 1.518050
8 2.013875 -0.658405 2.137091
8 -0.669732 -1.855681 -0.734480
8 0.424282 0.209644 3.402082
6 -2.059629 -1.780102 -0.607618
6 -2.751486 -1.114004 -1.606792
6 -2.704422 -2.437399 0.431773
6 -4.142027 -1.095446 -1.552613
1 -2.204846 -0.614559 -2.398092
6 -4.095195 -2.399371 0.478679
1 -2.130271 -2.964348 1.186861
6 -4.813783 -1.732458 -0.511382
1 -4.698449 -0.575514 -2.325728
1 -4.615043 -2.901698 1.288014
1 -5.898231 -1.711623 -0.472153
46 0.141250 1.485605 -0.135673
8 -1.743811 1.607004 -0.713382
6 -2.402702 1.973476 0.346494
8 -1.805313 2.196385 1.408812
6 -3.893730 2.052224 0.209744
6 2.423930 1.668846 -1.076038
8 1.459705 1.862768 -1.869890
8 2.143545 1.491495 0.164866
6 3.836348 1.586545 -1.541028
1 4.522823 1.713814 -0.703229
1 4.022493 2.336070 -2.312691

1 3.991530 0.595585 -1.981084
1 -4.179040 2.292896 -0.815819
1 -4.293473 2.792457 0.904796
1 -4.314972 1.073510 0.463089

TS1

E= -1386.619736 a.u.

G= -1386.359282 a.u.

Frequency= -906.53 cm⁻¹

6 -5.590009 -0.202639 0.458656
6 -4.853200 -0.108084 -0.709803
6 -3.468730 -0.247845 -0.646725
6 -2.823340 -0.478176 0.573289
6 -3.590528 -0.570320 1.748133
6 -4.962995 -0.433049 1.690767
1 -6.669020 -0.093663 0.414836
1 -5.321448 0.068826 -1.671440
6 -1.384962 -0.593501 0.551747
1 -3.087843 -0.746018 2.692508
1 -5.553670 -0.502590 2.597616
6 -0.663607 -0.491681 -0.636041
6 -1.413405 -0.252030 -1.873038
1 0.140960 -1.445378 -0.896462
8 -2.788954 -0.154190 -1.818146
8 -0.858418 -0.808777 1.749305
8 -0.916665 -0.152974 -2.972092
6 0.522704 -0.948154 1.928806
6 1.227322 0.148908 2.406682
6 1.122061 -2.172781 1.685913
6 2.599036 0.020195 2.601547
1 0.707609 1.083300 2.590156
6 2.495995 -2.284146 1.885172
1 0.532218 -3.006725 1.322801
6 3.233222 -1.190691 2.332416
1 3.171179 0.871833 2.954126
1 2.988428 -3.230825 1.687409
1 4.304368 -1.284595 2.478167
46 1.020852 0.755010 -0.603146
8 2.348185 -0.609522 -1.295048
6 2.100539 -1.833061 -1.521052
8 0.978375 -2.381988 -1.346918
6 3.231421 -2.671554 -2.047389
6 1.134298 3.128641 0.065412
8 2.196639 2.577162 -0.340019
8 0.061846 2.422182 0.109743
6 1.084550 4.564889 0.468738
1 2.092087 4.960917 0.599231
1 0.507121 4.672000 1.389912
1 0.573632 5.130991 -0.316513
1 4.186768 -2.164521 -1.913819
1 3.062162 -2.848355 -3.114058
1 3.235942 -3.640333 -1.543744

TS2

E= -1386.612422 a.u.

G= -1386.353230 a.u.

Frequency= -1011.78 cm⁻¹

46 1.052367 -0.180682 -0.220842
6 -0.899901 -0.402800 -0.361624
6 -1.783022 0.401224 0.272663
6 -3.168810 0.030758 0.476795
6 -3.578003 -1.184744 -0.076080

6 -1.414818 -1.576416 -1.054543
8 3.173006 0.044749 0.170238
6 3.418548 0.803059 1.171374
8 2.561338 1.591076 1.645096
6 4.786170 0.721143 1.784653
1 1.457813 1.586448 0.755959
6 0.719974 1.885450 -0.268350
6 -0.561942 2.372545 0.025812
6 1.528835 2.682176 -1.110202
8 -1.458831 1.635323 0.768911
1 4.901020 -0.261769 2.252680
1 4.927300 1.498383 2.535023
1 5.545093 0.803784 1.002790
6 -1.005351 3.611567 -0.413356
6 -0.171965 4.373696 -1.225085
1 3.528402 -1.531328 0.005484
8 1.300213 -2.317685 -0.013907
6 2.321817 -3.009905 -0.041099
8 3.539505 -2.527513 -0.057419
6 2.224321 -4.500736 -0.040991
1 3.189894 -4.966010 -0.236909
1 1.488415 -4.803348 -0.788627
1 1.855407 -4.824277 0.937099
6 -4.097385 0.793947 1.198584
6 -5.391739 0.332679 1.367690
6 -5.779260 -0.892759 0.813503
6 -4.878032 -1.655842 0.087725
1 -3.784022 1.740456 1.624915
1 -6.106309 0.923458 1.931224
1 -6.794900 -1.251472 0.947427
1 -5.156807 -2.603444 -0.359919
8 -2.728204 -1.940948 -0.823564
8 -0.808143 -2.268889 -1.844749
6 1.091586 3.905948 -1.590612
1 -2.001829 3.947920 -0.148336
1 -0.519312 5.336325 -1.588200
1 1.730242 4.504573 -2.231447
1 2.533494 2.336820 -1.338436

TS3

E= -1386.627239 a.u.

G= -1386.363256 a.u.

Frequency= -279.29 cm⁻¹

46 0.955675 0.120243 -0.015350
6 -0.990956 0.014023 -0.484292
6 -1.966535 0.519256 0.343898
6 -3.192666 -0.165903 0.642419
6 -3.420720 -1.346841 -0.067586
6 -1.313713 -1.199573 -1.211859
8 3.104280 0.779052 0.616803
6 3.825061 0.318886 1.495519
8 3.678610 -0.896375 1.997339
6 4.956691 1.078327 2.113261
1 2.953770 -1.370969 1.515897
6 -0.070515 1.670995 -0.773883
6 -0.909364 2.459935 0.023216
6 0.627092 2.332934 -1.806074
8 -1.831929 1.780634 0.790958
1 5.067099 2.047701 1.629384
1 5.882371 0.503685 2.024641
1 4.755618 1.217504 3.179585
6 -0.969321 3.843656 -0.049418

6 -0.202525 4.474568 -1.020883
1 0.955590 -2.215800 -1.803006
8 1.906436 -2.028518 0.363498
6 2.395423 -2.641734 -0.596335
8 1.836335 -2.690377 -1.772465
6 3.671244 -3.411910 -0.476380
1 4.119367 -3.589579 -1.453892
1 3.448904 -4.375791 -0.007187
1 4.363588 -2.873460 0.173527
6 -4.162514 0.277227 1.554336
6 -5.312841 -0.465240 1.750894
6 -5.518403 -1.651444 1.034554
6 -4.577567 -2.096976 0.119325
1 -3.993246 1.200983 2.097336
1 -6.059786 -0.126633 2.461093
1 -6.424646 -2.227429 1.191418
1 -4.717209 -3.008265 -0.451793
8 -2.519512 -1.801760 -0.988927
8 -0.601546 -1.768505 -2.035707
6 0.566627 3.716942 -1.911524
1 -1.635901 4.395256 0.605467
1 -0.237012 5.555273 -1.114755
1 1.132164 4.217583 -2.691992
1 1.239898 1.762795 -2.496722

TS_{IM2-3}

E= -1386.634650 a.u.

G= -1386.370603 a.u.

Frequency= -51.36 cm⁻¹

6 -6.000564 0.101330 -0.262946
6 -5.075396 1.036348 -0.698995
6 -3.718417 0.763484 -0.547401
6 -3.279161 -0.430638 0.030844
6 -4.229932 -1.364074 0.467566
6 -5.580373 -1.098930 0.321720
1 -7.060180 0.305226 -0.379603
1 -5.377120 1.972849 -1.154950
6 -1.846082 -0.621896 0.139437
1 -3.890346 -2.290084 0.918135
1 -6.313256 -1.823612 0.660285
6 -0.979023 0.316562 -0.311265
6 -1.477893 1.542494 -0.892081
1 3.106720 1.626249 0.436645
8 -2.841180 1.708869 -0.989460
8 -1.482066 -1.781256 0.732000
8 -0.786627 2.455186 -1.305042
6 -0.142965 -2.148142 0.727306
6 0.508684 -2.257937 1.954694
6 0.476228 -2.529601 -0.466009
6 1.808997 -2.747757 1.981787
1 -0.011872 -1.962743 2.859249
6 1.781862 -3.023473 -0.415808
1 -0.067984 -2.475029 -1.403376
6 2.446607 -3.128636 0.800015
1 2.326754 -2.833814 2.931624
1 2.271540 -3.315107 -1.338646
1 3.461368 -3.511472 0.831911
46 0.957637 0.202432 -0.193051
8 0.879047 1.770498 1.311920
6 1.800946 2.577753 1.487068
8 2.995144 2.465674 0.965487
6 1.611640 3.794176 2.332995

6 3.210453 -0.148850 -1.537947
8 3.107767 0.149006 -0.281845
8 2.191434 -0.354834 -2.225353
6 4.592875 -0.259183 -2.112719
1 5.142341 -1.042634 -1.582355
1 5.128622 0.681800 -1.957959
1 4.551960 -0.490772 -3.177253
1 0.647625 3.752230 2.837425
1 1.649938 4.677703 1.688438
1 2.423513 3.873981 3.059544

TS4

E= -1386.619837 a.u.

G= -1386.357481 a.u.

Frequency= -118.93 cm⁻¹

6 -4.338162 -2.446615 -1.195652
6 -4.771343 -1.312685 -0.528057
6 -3.906541 -0.226649 -0.417977
6 -2.623207 -0.263112 -0.968970
6 -2.199814 -1.422475 -1.634287
6 -3.052896 -2.504980 -1.748691
1 -5.005227 -3.298047 -1.285193
1 -5.758954 -1.248309 -0.085327
6 -1.787502 0.903026 -0.766330
1 -1.195870 -1.459855 -2.040509
1 -2.722336 -3.401708 -2.261440
6 -2.257936 1.979612 -0.093672
6 -3.597228 1.988296 0.450824
1 -1.676729 2.878147 0.064300
8 -4.362408 0.858314 0.270534
8 -0.570007 0.811610 -1.339374
8 -4.104624 2.907735 1.056143
6 0.517462 1.548403 -0.913981
6 0.771478 1.804581 0.440177
6 1.409651 1.951064 -1.901809
6 1.930124 2.510625 0.784967
1 0.054423 1.539258 1.207740
6 2.562513 2.635192 -1.532668
1 1.190053 1.724897 -2.939479
6 2.826230 2.920495 -0.193268
1 2.119303 2.720334 1.832445
1 3.260427 2.951584 -2.301171
1 3.727655 3.456441 0.082958
46 1.788163 -0.651506 0.569408
8 -0.012865 -1.455457 0.695145
6 -0.484374 -1.094521 1.848814
8 0.204621 -0.409406 2.621941
6 -1.890098 -1.509011 2.168884
6 3.966953 -1.197089 -0.426694
8 3.008118 -2.016033 -0.567455
8 3.731622 -0.137725 0.254969
6 5.315756 -1.443691 -1.004389
1 5.716410 -0.514072 -1.414356
1 5.264150 -2.213954 -1.774698
1 5.985691 -1.778774 -0.206315
1 -2.280083 -2.209667 1.429183
1 -2.520715 -0.614471 2.195535
1 -1.915749 -1.957639 3.164999

TS5

E= -1386.612008 a.u.

G= -1386.351296 a.u.

Frequency= -1000.58 cm⁻¹

6 -4.725962 -0.017282 0.203130
6 -4.005179 1.145392 0.423354
6 -2.697268 1.047184 0.891058
6 -2.112024 -0.196908 1.141985
6 -2.851883 -1.363918 0.902668
6 -4.152471 -1.272701 0.439987
1 -5.744864 0.051083 -0.164541
1 -4.428451 2.126067 0.237540
6 -0.731174 -0.191129 1.569850
1 -2.385383 -2.328328 1.069311
1 -4.724539 -2.175298 0.253590
6 -0.068305 0.972660 1.765626
6 -0.702771 2.240808 1.485886
1 0.972203 1.006597 2.062652
8 -2.013767 2.212245 1.072739
8 -0.173779 -1.411383 1.741455
8 -0.175433 3.329674 1.581314
6 1.157897 -1.608337 1.404611
6 1.538644 -1.546141 0.049701
6 2.030437 -1.978573 2.412426
6 2.867881 -1.899556 -0.252875
1 0.599548 -2.013196 -0.694519
6 3.345487 -2.290597 2.072126
1 1.682266 -2.025449 3.438562
6 3.766841 -2.256652 0.743562
1 3.189733 -1.893308 -1.290129
1 4.043503 -2.572827 2.854156
1 4.790076 -2.514582 0.491779
46 0.928223 0.201878 -1.029307
8 -0.740181 -0.491269 -1.932193
6 -1.110712 -1.706315 -1.868390
8 -0.465510 -2.606344 -1.268219
6 -2.379285 -2.061447 -2.589586
6 1.921045 2.439306 -0.900185
8 0.889879 2.243982 -1.617761
8 2.446181 1.416785 -0.334396
6 2.476882 3.800949 -0.676945
1 3.555959 3.749724 -0.522233
1 2.010427 4.204451 0.227923
1 2.232527 4.452308 -1.517249
1 -2.137167 -2.241733 -3.642065
1 -3.087202 -1.233177 -2.537586
1 -2.814495 -2.968719 -2.170535

1 -2.104774 4.965029 -0.562196
1 -2.485011 2.581996 -1.004727
1 0.406149 -1.093200 0.831305
6 0.858970 -0.489244 -0.144177
6 1.850582 0.408437 0.258168
6 1.286310 -1.591967 -1.029682
8 0.551562 -2.340582 -1.625811
8 1.605566 1.563937 0.832806
1 -2.873975 -3.725276 1.908146
1 -1.304308 -4.259361 2.584122
1 -1.772748 -4.682526 0.915185
6 3.251860 0.103525 0.118529
6 3.585009 -1.052866 -0.595223
6 5.911266 -0.619815 -0.248997
6 4.915262 -1.419063 -0.785073
6 4.278911 0.912179 0.636778
6 5.598394 0.547448 0.461779
1 6.950107 -0.900467 -0.390357
1 5.140928 -2.318179 -1.347167
1 4.016106 1.814746 1.176914
1 6.391768 1.165039 0.868072
8 2.638462 -1.842836 -1.163152
1 -3.297786 -1.847809 0.009290
8 -3.262463 0.496161 -0.342432
6 -4.267103 -0.225315 -0.317663
8 -4.244256 -1.515604 -0.121150
6 -5.634579 0.343654 -0.524257
1 -6.073835 -0.097954 -1.423424
1 -5.580260 1.426014 -0.631342
1 -6.275236 0.077453 0.320467

TS6

E= -1386.619256 a.u.

G= -1386.357911 a.u.

Frequency= -383.14 cm⁻¹

46 -1.140523 0.000962 -0.209903
6 -0.639732 1.904306 -0.133023
6 0.508854 2.373483 0.494809
6 0.732440 3.713487 0.797271
6 -0.216115 4.654316 0.425445
6 -1.363414 4.237114 -0.246360
6 -1.569952 2.886624 -0.509308
8 -1.784877 -2.058420 0.198810
6 -1.182947 -2.654544 1.157478
8 -0.101615 -2.250129 1.648197
6 -1.818779 -3.910441 1.689140
1 1.649331 3.997747 1.303596
1 -0.052862 5.704393 0.645710