Electronic Supplementary Material (ESI) for RSC Advances.

Vibronic Spectra for Organic Electronic Chromophores: Electronic Supporting Information

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[‡]CINam, Marseille
[¶]MolTech, Angers
[§]IUF, Paris

S1 Stick spectra of 5 and 6

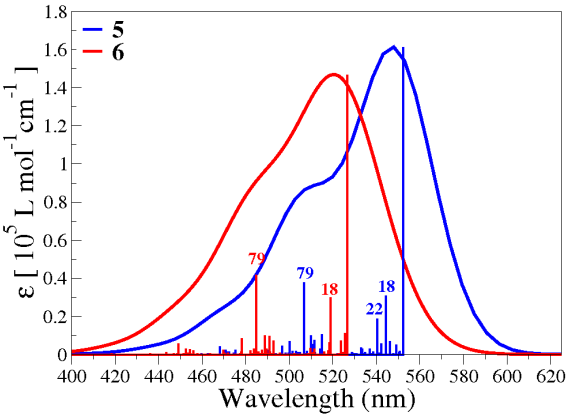
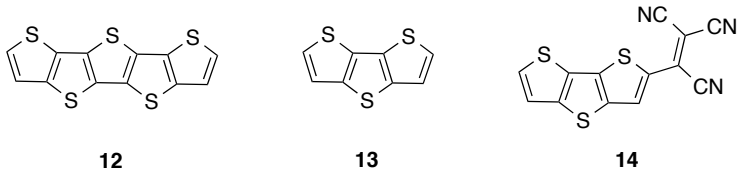


Figure S-1: Stick and convoluted absorption spectra for molecules: **5** and **6**. The numbering of the vibrational modes leading to the main contributions is indicated. Movies of modes 79 for the two systems can be found in the SI.

S2 Additional molecules

We have also treated with the same computational approach, three molecules, shown in Figure S-2 for which experimental data are also available (**12**,[?] **13**[?] and **14**[?]) For **12** the main structure is due to mode 53 (1609 cm^{-1}) that corresponds to an in-phase stretching of the C-C bonds affecting the full structure (see movie).



12 **13** **14**

Figure S-2: Representation of three additional molecules.

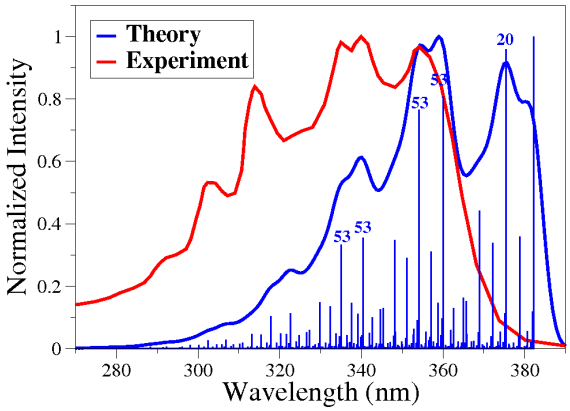


Figure S-3: Comparison between experimental (red) and theoretical (blue) band shapes for the absorption spectra of **12** in chloroform. Intensities have been normalized to 1, but no offset was applied on the energy scale. Experimental spectra adapted, with permission from, Xiao *et al. J. Am. Chem. Soc.* **127** (2005) 13281–13286, Copyright 2005 American Chemical Society.

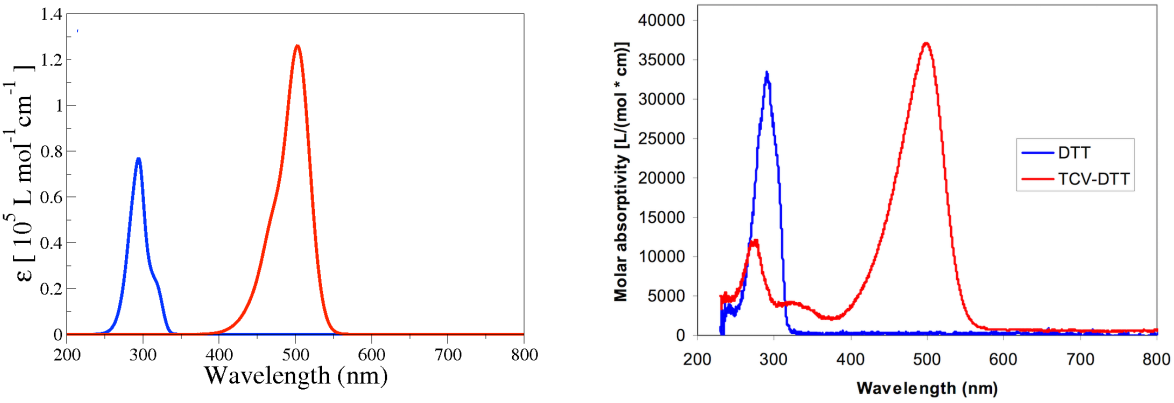


Figure S-4: Comparison between theoretical (left) and experimental (right) band shapes for the absorption spectra of **13** (DTT) and **14** (TCV-DTT) in dichloromethane. No normalisation not offset applied. Experimental spectra reproduced, with permission from, Pappenfus *et al. Org. Lett.* **10** (2008) 1553–1556, Copyright 2008 American Chemical Society.

S3 Cartesian Coordinates

S3.1 Molecule 1

Ground-state

SCF[PCM-M06/6-31G(d)]= -1843,00243779 au.

6 -0.002792 -4.317552 -0.989036
6 0.000000 -5.055761 0.161712
6 -0.002816 -2.928345 -0.693957
6 0.003648 -2.633687 0.672128
6 0.006034 -1.228009 0.785315
6 0.000924 -0.712948 -0.520549
6 -0.000924 0.712948 -0.520549
6 -0.006034 1.228009 0.785315
6 0.002816 2.928345 -0.693957
6 -0.003648 2.633687 0.672128
6 0.002792 4.317552 -0.989036
6 0.000000 5.055761 0.161712
1 0.002840 4.759192 -1.982210
1 -0.001275 6.136623 0.254245
7 0.011841 1.757138 -1.425725
6 -0.005104 1.679507 -2.868964
1 -0.971394 1.314955 -3.241001
1 0.165196 2.679902 -3.276634
1 0.796933 1.026870 -3.232028
16 -0.004283 4.086708 1.619962
16 0.000000 0.000000 2.032304
16 0.004283 -4.086708 1.619962
1 0.001275 -6.136623 0.254245
1 -0.002840 -4.759192 -1.982210
7 -0.011841 -1.757138 -1.425725
6 0.005104 -1.679507 -2.868964
1 -0.165196 -2.679902 -3.276634
1 -0.796933 -1.026870 -3.232028
1 0.971394 -1.314955 -3.241001

Excited-state

SCF[PCM-M06/6-31G(d)]= -1842,99438959 au.

6 -0.001886 4.294988 -0.981800
6 0.000000 5.032576 0.195631
6 -0.000639 2.922250 -0.714623
6 0.002335 2.599402 0.674867
6 0.001818 1.228176 0.781279
6 -0.000446 0.690891 -0.562962

6 0.000446 -0.690891 -0.562962
6 -0.001818 -1.228176 0.781279
6 0.000639 -2.922250 -0.714623
6 -0.002335 -2.599402 0.674867
6 0.001886 -4.294988 -0.981800
6 0.000000 -5.032576 0.195631
1 0.003910 -4.754085 -1.966838
1 0.000574 -6.112855 0.295862
7 -0.000955 -1.755476 -1.460780
6 0.047459 -1.677945 -2.898064
1 0.963289 -1.174320 -3.237994
1 0.044263 -2.692195 -3.306893
1 -0.827719 -1.146921 -3.296007
16 -0.004767 -4.048900 1.651457
16 0.000000 0.000000 2.043507
16 0.004767 4.048900 1.651457
1 -0.000574 6.112855 0.295862
1 -0.003910 4.754085 -1.966838
7 0.000955 1.755476 -1.460780
6 -0.047459 1.677945 -2.898064
1 -0.044263 2.692195 -3.306893
1 0.827719 1.146921 -3.296007
1 -0.963289 1.174320 -3.237994

S3.2 Molecule 2

Ground-state

SCF[PCM-M06/6-31G(d)]= -2317,20326026

6 -0.011240 3.651984 0.000147
6 -1.410258 3.714286 -0.001240
6 -1.933938 5.033620 0.009027
6 -0.923041 5.954111 0.014993
16 0.677254 5.244429 0.008898
1 -2.987701 5.299950 0.013212
1 -1.012725 7.035203 0.023933
6 0.335854 2.283271 -0.007728
6 -0.868433 1.568429 -0.014909
16 1.736434 1.235496 -0.012850
6 -0.677114 0.165347 -0.020104
6 0.677114 -0.165347 -0.020104
7 -1.933938 2.436841 -0.018888
6 -3.331199 2.064466 0.029059
1 -3.598758 1.648316 1.008734
1 -3.943959 2.951280 -0.155118
1 -3.555325 1.326886 -0.750786
6 0.868433 -1.568429 -0.014909

6 -0.335854 -2.283271 -0.007728
6 1.410258 -3.714286 -0.001240
6 0.011240 -3.651984 0.000147
6 1.933938 -5.033620 0.009027
6 0.923041 -5.954111 0.014993
1 2.987701 -5.299950 0.013212
1 1.012725 -7.035203 0.023933
7 1.933938 -2.436841 -0.018888
6 3.331199 -2.064466 0.029059
1 3.598758 -1.648316 1.008734
1 3.943959 -2.951280 -0.155118
1 3.555325 -1.326886 -0.750786
16 -0.677254 -5.244429 0.008898
16 -1.736434 -1.235496 -0.012850

Excited-state

SCF[PCM-M06/6-31G(d)]= -2317,3183692 au.

6 -0.001011 3.619121 0.001169
6 -1.420860 3.695836 0.011356
6 -1.927340 5.000346 0.081718
6 -0.901155 5.928067 0.117432
16 0.701016 5.214315 0.065982
1 -2.979212 5.272611 0.110464
1 -0.989011 7.007812 0.176152
6 0.340419 2.279886 -0.055570
6 -0.889642 1.535521 -0.076027
16 1.764859 1.249438 -0.090695
6 -0.701016 0.172155 -0.101757
6 0.701016 -0.172155 -0.101757
7 -1.952422 2.419588 -0.064827
6 -3.347945 2.071326 0.069927
1 -3.628849 1.913235 1.120275
1 -3.962063 2.876552 -0.346539
1 -3.557857 1.159843 -0.500644
6 0.889642 -1.535521 -0.076027
6 -0.340419 -2.279886 -0.055570
6 1.420860 -3.695836 0.011356
6 0.001011 -3.619121 0.001169
6 1.927340 -5.000346 0.081718
6 0.901155 -5.928067 0.117432
1 2.979212 -5.272611 0.110464
1 0.989011 -7.007812 0.176152
7 1.952422 -2.419588 -0.064827
6 3.347945 -2.071326 0.069927
1 3.628849 -1.913235 1.120275
1 3.962063 -2.876552 -0.346539
1 3.557857 -1.159843 -0.500644
16 -0.701016 -5.214315 0.065982
16 -1.764859 -1.249438 -0.090695

S3.3 Molecule 3

Ground-state

SCF[PCM-M06/6-31G(d)]= -2543,79373074 au.

6 -0.433581 3.612513 0.011796
6 0.958612 3.842800 0.013344
6 1.310097 5.198520 0.012306
6 0.181220 6.000535 0.013247
16 -1.329932 5.091607 0.015026
1 2.319373 5.604938 0.009809
6 -0.610264 2.219574 0.009398
6 0.677242 1.654769 0.009400
16 -1.877194 1.015640 0.007136
6 0.654729 0.242499 0.001276
6 -0.654729 -0.242499 -0.001276
7 1.631808 2.636463 0.019728
6 3.065394 2.431442 -0.022270
1 3.367180 1.717706 0.752950
1 3.382400 2.061009 -1.004801
1 3.568005 3.381787 0.175588
6 -0.677242 -1.654769 -0.009400
6 0.610264 -2.219574 -0.009398
6 -0.958612 -3.842800 -0.013344
6 0.433581 -3.612513 -0.011796
6 -1.310097 -5.198520 -0.012306
6 -0.181220 -6.000535 -0.013247
1 -2.319373 -5.604938 -0.009809
7 -1.631808 -2.636463 -0.019728
6 -3.065394 -2.431442 0.022270
1 -3.382400 -2.061009 1.004801
1 -3.367180 -1.717706 -0.752950
1 -3.568005 -3.381787 -0.175588
16 1.329932 -5.091607 -0.015026
16 1.877194 -1.015640 -0.007136
6 0.167897 7.438049 0.011930
8 -0.839509 8.136242 0.013194
1 1.180592 7.898520 0.009733
6 -0.167897 -7.438049 -0.011930
8 0.839509 -8.136242 -0.013194
1 -1.180592 -7.898520 -0.009733

Excited-state

SCF[PCM-M06/6-31G(d)]= -2543,89152287 au.

6 -0.431412 3.586573 0.018912
6 0.976576 3.824331 0.018795

6 1.326753 5.169787 0.012069
6 0.184569 5.980230 0.012301
16 -1.335064 5.074886 0.018827
1 2.335073 5.576866 0.005916
6 -0.609243 2.217468 0.017147
6 0.700755 1.626967 0.016099
16 -1.893128 1.027549 0.011225
6 0.671143 0.249020 0.002281
6 -0.671143 -0.249020 -0.002281
7 1.652095 2.620021 0.029371
6 3.085546 2.420016 -0.020634
1 3.391673 1.698568 0.745704
1 3.400556 2.062580 -1.008868
1 3.585086 3.369610 0.188096
6 -0.700755 -1.626967 -0.016099
6 0.609243 -2.217468 -0.017147
6 -0.976576 -3.824331 -0.018795
6 0.431412 -3.586573 -0.018912
6 -1.326753 -5.169787 -0.012069
6 -0.184569 -5.980230 -0.012301
1 -2.335073 -5.576866 -0.005916
7 -1.652095 -2.620021 -0.029371
6 -3.085546 -2.420016 0.020634
1 -3.400556 -2.062580 1.008868
1 -3.391673 -1.698568 -0.745704
1 -3.585086 -3.369610 -0.188096
16 1.335064 -5.074886 -0.018827
16 1.893128 -1.027549 -0.011225
6 0.147607 7.411540 0.006997
8 -0.884295 8.089528 0.007776
1 1.148131 7.895940 0.002017
6 -0.147607 -7.411540 -0.006997
8 0.884295 -8.089528 -0.007776
1 -1.148131 -7.895940 -0.002017

S3.4 Molecule 4

Ground-state

SCF[PCM-M06/6-31G(d)]= -2840,71057116

6 -0.167350 3.624883 0.007144
6 1.241507 3.755665 0.008652
6 1.684446 5.074209 0.006056
6 0.616342 5.975720 0.006412
16 -0.960704 5.157256 0.008924
1 2.720345 5.405583 0.002984
6 -0.445491 2.254205 0.005993

6 0.800832 1.595753 0.006887
16 -1.799718 1.151450 0.005098
6 0.672665 0.191766 0.001034
6 -0.672665 -0.191766 -0.001034
7 1.824450 2.503936 0.016074
6 3.241004 2.196557 -0.022194
1 3.488780 1.466051 0.756025
1 3.531056 1.802823 -1.003551
1 3.808933 3.109363 0.174477
6 -0.800832 -1.595753 -0.006887
6 0.445491 -2.254205 -0.005993
6 -1.241507 -3.755665 -0.008652
6 0.167350 -3.624883 -0.007144
6 -1.684446 -5.074209 -0.006056
6 -0.616342 -5.975720 -0.006412
1 -2.720345 -5.405583 -0.002984
7 -1.824450 -2.503936 -0.016074
6 -3.241004 -2.196557 0.022194
1 -3.531056 -1.802823 1.003551
1 -3.488780 -1.466051 -0.756025
1 -3.808933 -3.109363 -0.174477
16 0.960704 -5.157256 -0.008924
16 1.799718 -1.151450 -0.005098
6 0.800771 7.372046 0.004598
1 1.847056 7.683715 0.001317
6 -0.800771 -7.372046 -0.004598
1 -1.847056 -7.683715 -0.001317
6 0.120176 -8.398523 -0.006915
6 -0.120176 8.398523 0.006915
6 1.528338 -8.201995 -0.011970
7 2.683227 -8.044128 -0.016224
6 -1.528338 8.201995 0.011970
7 -2.683227 8.044128 0.016224
6 -0.332728 -9.748045 -0.004607
7 -0.707832 -10.851449 -0.002673
6 0.332728 9.748045 0.004607
7 0.707832 10.851449 0.002673

Excited-state

SCF[PCM-M06/6-31G(d)]= -2840,79146313 au.

6 -0.160275 3.602715 0.011785
6 1.261365 3.735422 0.011009
6 1.707537 5.045406 0.004629
6 0.631747 5.957698 0.006094
16 -0.953584 5.147109 0.012675
1 2.742938 5.376051 -0.002094
6 -0.440896 2.252528 0.010912
6 0.820962 1.569188 0.010243
16 -1.808503 1.164821 0.008760
6 0.686414 0.195117 0.001235

6 -0.686414 -0.195117 -0.001235
7 1.843864 2.486080 0.020252
6 3.260727 2.180676 -0.019629
1 3.507715 1.444036 0.752966
1 3.552165 1.796412 -1.004374
1 3.826647 3.092419 0.186955
6 -0.820962 -1.569188 -0.010243
6 0.440896 -2.252528 -0.010912
6 -1.261365 -3.735422 -0.011009
6 0.160275 -3.602715 -0.011785
6 -1.707537 -5.045406 -0.004629
6 -0.631747 -5.957698 -0.006094
1 -2.742938 -5.376051 0.002094
7 -1.843864 -2.486080 -0.020252
6 -3.260727 -2.180676 0.019629
1 -3.552165 -1.796412 1.004374
1 -3.507715 -1.444036 -0.752966
1 -3.826647 -3.092419 -0.186955
16 0.953584 -5.147109 -0.012675
16 1.808503 -1.164821 -0.008760
6 0.807044 7.349182 0.002485
1 1.848643 7.674439 -0.003025
6 -0.807044 -7.349182 -0.002485
1 -1.848643 -7.674439 0.003025
6 0.137654 -8.372663 -0.005698
6 -0.137654 8.372663 0.005698
6 1.540739 -8.170055 -0.014020
7 2.698145 -8.013910 -0.021005
6 -1.540739 8.170055 0.014020
7 -2.698145 8.013910 0.021005
6 -0.299000 -9.723159 -0.001202
7 -0.667002 -10.831069 0.002497
6 0.299000 9.723159 0.001202
7 0.667002 10.831069 -0.002497

S3.5 Molecule 5

Ground-state

SCF[PCM-M06/6-31G(d)]= -1780,23698364 au.

6 2.493695 0.689613 0.000000
6 1.280141 1.373875 0.000000
6 -0.006291 0.728084 0.000000
6 0.006291 -0.728084 0.000000
6 1.190543 -1.406689 0.000000
6 2.474144 -0.760379 0.000000
1 -1.176756 2.495864 0.000000

6 -1.190543 1.406689 0.000000
6 -1.280141 -1.373875 0.000000
1 1.176756 -2.495864 0.000000
6 -2.493695 -0.689613 0.000000
6 -2.474144 0.760379 0.000000
6 -3.607730 1.567259 0.000000
6 3.607730 -1.567259 0.000000
6 -4.950037 1.100919 0.000000
7 -6.067908 0.772717 0.000000
6 -3.502152 2.988384 0.000000
7 -3.428019 4.150832 0.000000
6 3.502152 -2.988384 0.000000
7 3.428019 -4.150832 0.000000
6 4.950037 -1.100919 0.000000
7 6.067908 -0.772717 0.000000
6 3.224993 2.890984 0.000000
1 3.861283 3.769099 0.000000
6 -3.224993 -2.890984 0.000000
1 -3.861283 -3.769099 0.000000
6 -3.607730 -1.584124 0.000000
6 3.607730 1.584124 0.000000
1 -4.650890 -1.290804 0.000000
1 4.650890 1.290804 0.000000
16 -1.511131 -3.085405 0.000000
16 1.511131 3.085405 0.000000

Excited-state

SCF[PCM-M06/6-31G(d)]= -1780,31928921 au.

6 2.497320 0.642830 0.000000
6 1.284643 1.346872 0.000000
6 0.007154 0.718966 0.000000
6 -0.007154 -0.718966 0.000000
6 1.193108 -1.429315 0.000000
6 2.460196 -0.801983 0.000000
1 -1.156421 2.518175 0.000000
6 -1.193108 1.429315 0.000000
6 -1.284643 -1.346872 0.000000
1 1.156421 -2.518175 0.000000
6 -2.497320 -0.642830 0.000000
6 -2.460196 0.801983 0.000000
6 -3.614352 1.631782 0.000000
6 3.614352 -1.631782 0.000000
6 -4.947898 1.168936 0.000000
7 -6.065594 0.827603 0.000000
6 -3.495006 3.042104 0.000000
7 -3.395555 4.205934 0.000000
6 3.495006 -3.042104 0.000000
7 3.395555 -4.205934 0.000000
6 4.947898 -1.168936 0.000000
7 6.065594 -0.827603 0.000000

6 3.243032 2.844538 0.000000
1 3.893928 3.712103 0.000000
6 -3.243032 -2.844538 0.000000
1 -3.893928 -3.712103 0.000000
6 -3.614352 -1.529552 0.000000
6 3.614352 1.529552 0.000000
1 -4.656030 -1.230356 0.000000
1 4.656030 1.230356 0.000000
16 -1.535546 -3.065442 0.000000
16 1.535546 3.065442 0.000000

S3.6 Molecule 6

Ground-state

SCF[PCM-M06/6-31G(d)]= -1780,23600928 au.

6 2.470318 0.667197 0.000000
6 1.283723 1.399058 0.000000
6 -0.001189 0.726497 0.000000
6 0.001189 -0.726497 0.000000
6 1.180110 -1.410035 0.000000
6 2.470318 -0.767753 0.000000
1 -1.166929 2.497828 0.000000
6 -1.180110 1.410035 0.000000
6 -1.283723 -1.399058 0.000000
1 1.166929 -2.497828 0.000000
6 -2.470318 -0.667197 0.000000
6 -2.470318 0.767753 0.000000
6 -3.606192 1.574402 0.000000
6 3.606192 -1.574402 0.000000
6 -4.937073 1.080310 0.000000
7 -6.042367 0.710406 0.000000
6 -3.506936 2.994034 0.000000
7 -3.434759 4.156875 0.000000
6 3.506936 -2.994034 0.000000
7 3.434759 -4.156875 0.000000
6 4.937073 -1.080310 0.000000
7 6.042367 -0.710406 0.000000
6 1.509251 2.799623 0.000000
6 2.838608 3.109183 0.000000
1 0.730606 3.556677 0.000000
1 3.289237 4.096040 0.000000
6 -1.509251 -2.799623 0.000000
6 -2.838608 -3.109183 0.000000
1 -0.730606 -3.556677 0.000000
1 -3.289237 -4.096040 0.000000
16 -3.855822 -1.723567 0.000000

16 3.855822 1.723567 0.000000

Excited-state

SCF[PCM-M06/6-31G(d)]= -1780,32198134 au.

6 2.466851 0.660861 0.000000
6 1.268992 1.393299 0.000000
6 0.001542 0.717356 0.000000
6 -0.001542 -0.717356 0.000000
6 1.204851 -1.411680 0.000000
6 2.466851 -0.767296 0.000000
1 -1.187323 2.499511 0.000000
6 -1.204851 1.411680 0.000000
6 -1.268992 -1.393299 0.000000
1 1.187323 -2.499511 0.000000
6 -2.466851 -0.660861 0.000000
6 -2.466851 0.767296 0.000000
6 -3.638893 1.579445 0.000000
6 3.638893 -1.579445 0.000000
6 -4.955195 1.073386 0.000000
7 -6.058900 0.687360 0.000000
6 -3.547141 2.989477 0.000000
7 -3.468839 4.155363 0.000000
6 3.547141 -2.989477 0.000000
7 3.468839 -4.155363 0.000000
6 4.955195 -1.073386 0.000000
7 6.058900 -0.687360 0.000000
6 1.493461 2.798165 0.000000
6 2.818796 3.111694 0.000000
1 0.712315 3.552667 0.000000
1 3.267945 4.099201 0.000000
6 -1.493461 -2.798165 0.000000
6 -2.818796 -3.111694 0.000000
1 -0.712315 -3.552667 0.000000
1 -3.267945 -4.099201 0.000000
16 -3.845532 -1.724881 0.000000
16 3.845532 1.724881 0.000000

S3.7 Molecule 7

Ground-state

SCF[PCM-M06/6-31G(d)]= -1334,25319991 au.

6 2.444687 0.745265 0.000000

6 1.248730 1.411677 0.000000
6 0.009271 0.712449 0.000000
6 -0.009271 -0.712449 0.000000
6 1.248730 -1.369974 0.000000
6 2.462846 -0.672454 0.000000
1 3.385340 1.294606 0.000000
1 1.239443 2.501743 0.000000
6 -1.248730 1.369974 0.000000
6 -1.248730 -1.411677 0.000000
6 -2.444687 -0.745265 0.000000
6 -2.462846 0.672454 0.000000
1 -1.239443 -2.501743 0.000000
1 -3.385340 -1.294606 0.000000
6 3.595205 -1.550346 0.000000
6 3.240705 -2.861265 0.000000
1 4.626011 -1.203442 0.000000
1 3.890016 -3.730578 0.000000
6 -3.595205 1.550346 0.000000
6 -3.240705 2.861265 0.000000
1 -4.626011 1.203442 0.000000
16 1.514555 -3.096058 0.000000
16 -1.514555 3.096058 0.000000
1 -3.890016 3.730578 0.000000

Excited-state

SCF[PCM-M06/6-31G(d)]= -1334,24507909 au.

6 2.451958 0.799574 0.000000
6 1.243838 1.453091 0.000000
6 -0.004958 0.728835 0.000000
6 0.004958 -0.728835 0.000000
6 1.243838 -1.339316 0.000000
6 2.489302 -0.614035 0.000000
1 3.386199 1.359682 0.000000
1 1.213218 2.542336 0.000000
6 -1.243838 1.339316 0.000000
6 -1.243838 -1.453091 0.000000
6 -2.451958 -0.799574 0.000000
6 -2.489302 0.614035 0.000000
1 -1.213218 -2.542336 0.000000
1 -3.386199 -1.359682 0.000000
6 3.596178 -1.479812 0.000000
6 3.244154 -2.814907 0.000000
1 4.630319 -1.142753 0.000000
1 3.918084 -3.665869 0.000000
6 -3.596178 1.479812 0.000000
6 -3.244154 2.814907 0.000000
1 -4.630319 1.142753 0.000000
16 1.528635 -3.093951 0.000000
16 -1.528635 3.093951 0.000000
1 -3.918084 3.665869 0.000000

S3.8 Molecule 8

Ground-state

SCF[PCM-M06/6-31G(d)]=-5336,45254197 au.

6 2.440437 0.739409 0.000000
6 1.246280 1.408310 0.000000
6 0.006317 0.712225 0.000000
6 -0.006317 -0.712225 0.000000
6 1.246280 -1.373256 0.000000
6 2.459925 -0.678697 0.000000
1 3.381960 1.287662 0.000000
1 1.239522 2.498918 0.000000
6 -1.246280 1.373256 0.000000
6 -1.246280 -1.408310 0.000000
6 -2.440437 -0.739409 0.000000
6 -2.459925 0.678697 0.000000
1 -1.239522 -2.498918 0.000000
1 -3.381960 -1.287662 0.000000
6 3.622959 -1.521814 0.000000
6 3.364640 -2.852261 0.000000
1 4.633165 -1.114828 0.000000
1 4.085738 -3.662922 0.000000
6 -3.622959 1.521814 0.000000
6 -3.364640 2.852261 0.000000
1 -4.633165 1.114828 0.000000
1 -4.085738 3.662922 0.000000
34 1.527125 -3.221017 0.000000
34 -1.527125 3.221017 0.000000

Excited-state

SCF[PCM-M06/6-31G(d)]= -5336,44453298 au.

6 2.444772 0.791215 0.000000
6 1.242064 1.448275 0.000000
6 -0.008023 0.729795 0.000000
6 0.008023 -0.729795 0.000000
6 1.242064 -1.344008 0.000000
6 2.485323 -0.625778 0.000000
1 3.380163 1.350119 0.000000
1 1.216223 2.538152 0.000000
6 -1.242064 1.344008 0.000000
6 -1.242064 -1.448275 0.000000

6 -2.444772 -0.791215 0.000000
6 -2.485323 0.625778 0.000000
1 -1.216223 -2.538152 0.000000
1 -3.380163 -1.350119 0.000000
6 3.619545 -1.456865 0.000000
6 3.362956 -2.814638 0.000000
1 4.634442 -1.061530 0.000000
1 4.103927 -3.607511 0.000000
6 -3.619545 1.456865 0.000000
6 -3.362956 2.814638 0.000000
1 -4.634442 1.061530 0.000000
1 -4.103927 3.607511 0.000000
34 1.542733 -3.220247 0.000000
34 -1.542733 3.220247 0.000000

S3.9 Molecule 9

Ground-state

SCF[PCM-M06/6-31G(d)]= -1334,25371776 au.

6 -0.833625 2.155854 0.000000
6 0.521655 1.747496 0.000000
6 0.608018 0.319470 0.000000
6 -0.608018 -0.319470 0.000000
6 0.833625 -2.155854 0.000000
6 -0.521655 -1.747496 0.000000
16 1.955332 -0.794506 0.000000
16 -1.955332 0.794506 0.000000
6 -1.182264 3.505756 0.000000
6 -0.165451 4.452209 0.000000
1 -2.227436 3.811115 0.000000
1 -0.420259 5.510499 0.000000
6 1.182264 -3.505756 0.000000
6 0.165451 -4.452209 0.000000
1 2.227436 -3.811115 0.000000
1 0.420259 -5.510499 0.000000
6 1.530996 2.720166 0.000000
6 1.182264 4.061384 0.000000
1 2.578005 2.417291 0.000000
1 1.961664 4.821149 0.000000
6 -1.530996 -2.720166 0.000000
6 -1.182264 -4.061384 0.000000
1 -2.578005 -2.417291 0.000000
1 -1.961664 -4.821149 0.000000

Excited-state

SCF[PCM-M06/6-31G(d)]= -1334,24449429 au.

6 -0.826745 2.160347 0.000000
6 0.541359 1.737050 0.000000
6 0.635690 0.346469 0.000000
6 -0.635690 -0.346469 0.000000
6 0.826745 -2.160347 0.000000
6 -0.541359 -1.737050 0.000000
16 1.962707 -0.765513 0.000000
16 -1.962707 0.765513 0.000000
6 -1.184548 3.484311 0.000000
6 -0.158201 4.464021 0.000000
1 -2.230905 3.785250 0.000000
1 -0.426576 5.518512 0.000000
6 1.184548 -3.484311 0.000000
6 0.158201 -4.464021 0.000000
1 2.230905 -3.785250 0.000000
1 0.426576 -5.518512 0.000000
6 1.552494 2.738628 0.000000
6 1.184548 4.078095 0.000000
1 2.602762 2.447842 0.000000
1 1.960291 4.842330 0.000000
6 -1.552494 -2.738628 0.000000
6 -1.184548 -4.078095 0.000000
1 -2.602762 -2.447842 0.000000
1 -1.960291 -4.842330 0.000000

S3.10 Molecule 10

Ground-state

SCF[PCM-M06/6-31G(d)]= -1302,82190959 au.

6 0.000000 0.699330 -0.647602
6 0.000000 1.405531 0.540985
6 0.000000 0.715401 1.797155
6 0.000000 -0.715401 1.797155
6 0.000000 -1.405531 0.540985
6 0.000000 -0.699330 -0.647602
1 0.000000 2.479055 3.047209
6 0.000000 1.395750 3.036679
6 0.000000 -1.395750 3.036679
6 0.000000 -0.704475 4.225940
6 0.000000 0.704475 4.225940
1 0.000000 -2.479055 3.047209

1 0.000000 -1.245665 5.166477
1 0.000000 1.245665 5.166477
6 0.000000 -2.806224 0.134411
6 0.000000 -2.776955 -1.291684
6 0.000000 -4.033699 0.764695
6 0.000000 -3.886770 -2.085733
6 0.000000 -5.218275 -0.011044
1 0.000000 -4.128486 1.844983
6 0.000000 -6.500310 0.610808
6 0.000000 -5.148513 -1.441012
6 0.000000 -7.646839 -0.136685
1 0.000000 -6.547859 1.696537
6 0.000000 -6.360464 -2.187207
6 0.000000 -7.575165 -1.554816
1 0.000000 -8.616293 0.351157
1 0.000000 -6.300912 -3.272161
1 0.000000 -8.491046 -2.137276
6 0.000000 2.806224 0.134411
6 0.000000 2.776955 -1.291684
6 0.000000 4.033699 0.764695
6 0.000000 3.886770 -2.085733
6 0.000000 5.218275 -0.011044
1 0.000000 4.128486 1.844983
6 0.000000 6.500310 0.610808
6 0.000000 5.148513 -1.441012
6 0.000000 7.646839 -0.136685
1 0.000000 6.547859 1.696537
6 0.000000 6.360464 -2.187207
6 0.000000 7.575165 -1.554816
1 0.000000 8.616293 0.351157
1 0.000000 6.300912 -3.272161
1 0.000000 8.491046 -2.137276
8 0.000000 1.485551 -1.757308
8 0.000000 -1.485551 -1.757308
1 0.000000 -3.808950 -3.167816
1 0.000000 3.808950 -3.167816

Excited-state

SCF[PCM-M06/6-31G(d)]= -1302,81191116 au.

6 0.000000 0.679102 -0.731591
6 0.000000 1.416275 0.498081
6 0.000000 0.717675 1.762674
6 0.000000 -0.717675 1.762674
6 0.000000 -1.416275 0.498081
6 0.000000 -0.679102 -0.731591
1 0.000000 2.472849 3.006655
6 0.000000 1.390276 2.990454
6 0.000000 -1.390276 2.990454
6 0.000000 -0.694793 4.200003
6 0.000000 0.694793 4.200003

1 0.000000 -2.472849 3.006655
1 0.000000 -1.244640 5.135177
1 0.000000 1.244640 5.135177
6 0.000000 -2.778496 0.112614
6 0.000000 -2.781948 -1.326093
6 0.000000 -4.022204 0.765963
6 0.000000 -3.898522 -2.095027
6 0.000000 -5.209631 0.011260
1 0.000000 -4.100436 1.846838
6 0.000000 -6.485907 0.649134
6 0.000000 -5.165282 -1.426533
6 0.000000 -7.646667 -0.084365
1 0.000000 -6.519206 1.735336
6 0.000000 -6.375244 -2.147210
6 0.000000 -7.593873 -1.495791
1 0.000000 -8.608387 0.418665
1 0.000000 -6.334580 -3.233095
1 0.000000 -8.514672 -2.070267
6 0.000000 2.778496 0.112614
6 0.000000 2.781948 -1.326093
6 0.000000 4.022204 0.765963
6 0.000000 3.898522 -2.095027
6 0.000000 5.209631 0.011260
1 0.000000 4.100436 1.846838
6 0.000000 6.485907 0.649134
6 0.000000 5.165282 -1.426533
6 0.000000 7.646667 -0.084365
1 0.000000 6.519206 1.735336
6 0.000000 6.375244 -2.147210
6 0.000000 7.593873 -1.495791
1 0.000000 8.608387 0.418665
1 0.000000 6.334580 -3.233095
1 0.000000 8.514672 -2.070267
8 0.000000 1.499106 -1.818081
8 0.000000 -1.499106 -1.818081
1 0.000000 -3.841166 -3.178108
1 0.000000 3.841166 -3.178108

S3.11 Molecule 11

Ground-state

SCF[PCM-M06/6-31G(d)]= -1761,36232633 au.

6 0.071490 -2.407303 0.445268
6 0.063829 -3.430381 -0.479600
6 -0.123739 -3.139391 -1.871985
6 -0.226248 -1.774599 -2.294202

6 -0.039184 -0.728971 -1.314939
6 0.000000 -1.073798 0.029848
1 -0.197229 -5.199500 -2.513614
6 -0.287005 -4.166848 -2.828539
6 -0.615052 -1.521147 -3.630022
6 -0.790788 -2.544444 -4.534448
6 -0.595749 -3.879903 -4.138278
1 -0.831930 -0.504553 -3.932101
1 -1.099461 -2.318394 -5.549861
1 -0.725290 -4.684900 -4.854269
6 0.192733 -4.645416 0.316526
6 0.254007 -4.194299 1.668661
6 0.272378 -6.001631 0.074840
6 0.377049 -5.015024 2.751394
6 0.400155 -6.899852 1.162400
1 0.249070 -6.411657 -0.928856
6 0.481487 -8.305776 0.945464
6 0.450554 -6.408773 2.506274
6 0.603536 -9.175572 1.995321
1 0.443242 -8.674289 -0.076246
6 0.577750 -7.341103 3.573890
6 0.651927 -8.686115 3.327264
1 0.663719 -10.243958 1.814277
1 0.614663 -6.961607 4.591380
1 0.748584 -9.385542 4.151616
8 0.177073 -2.824297 1.734181
1 0.419300 -4.619060 3.760551
6 0.039184 0.728971 -1.314939
6 0.226248 1.774599 -2.294202
6 0.000000 1.073798 0.029848
6 0.123739 3.139391 -1.871985
6 0.615052 1.521147 -3.630022
6 -0.071490 2.407303 0.445268
6 -0.063829 3.430381 -0.479600
6 0.287005 4.166848 -2.828539
6 0.790788 2.544444 -4.534448
1 0.831930 0.504553 -3.932101
8 -0.177073 2.824297 1.734181
6 -0.192733 4.645416 0.316526
1 0.197229 5.199500 -2.513614
6 0.595749 3.879903 -4.138278
1 1.099461 2.318394 -5.549861
6 -0.254007 4.194299 1.668661
6 -0.272378 6.001631 0.074840
1 0.725290 4.684900 -4.854269
6 -0.377049 5.015024 2.751394
6 -0.400155 6.899852 1.162400
1 -0.249070 6.411657 -0.928856
6 -0.450554 6.408773 2.506274
1 -0.419300 4.619060 3.760551
6 -0.481487 8.305776 0.945464
6 -0.577750 7.341103 3.573890
6 -0.603536 9.175572 1.995321
1 -0.443242 8.674289 -0.076246

6 -0.651927 8.686115 3.327264
1 -0.614663 6.961607 4.591380
1 -0.663719 10.243958 1.814277
1 -0.748584 9.385542 4.151616
8 0.000000 0.000000 0.858214

Excited-state

SCF[PCM-M06/6-31G(d)]= -1761,83706826 au.

6 0.049749 2.390034 0.526549
6 0.106867 3.426315 -0.442539
6 0.319605 3.101345 -1.825674
6 0.372607 1.724998 -2.221928
6 0.100695 0.695404 -1.223914
6 0.082813 1.078663 0.154296
1 0.526489 5.137094 -2.506077
6 0.567318 4.093756 -2.793410
6 0.784943 1.421281 -3.526264
6 1.042554 2.419700 -4.457357
6 0.906721 3.761337 -4.094553
1 0.941890 0.385919 -3.804294
1 1.359592 2.151674 -5.459620
1 1.098118 4.546263 -4.818857
6 0.000000 4.638754 0.304889
6 -0.093084 4.237820 1.680248
6 -0.044606 6.002901 0.019332
6 -0.205918 5.096705 2.727193
6 -0.161434 6.935366 1.071570
1 -0.006786 6.377504 -0.997254
6 -0.206545 8.336203 0.809231
6 -0.239690 6.491931 2.434954
6 -0.318559 9.244568 1.829947
1 -0.148534 8.669661 -0.223482
6 -0.354907 7.456904 3.463236
6 -0.393178 8.801295 3.172723
1 -0.350583 10.307381 1.612247
1 -0.413448 7.114105 4.492765
1 -0.481598 9.527422 3.974575
8 -0.057201 2.869867 1.797440
1 -0.271673 4.738432 3.748923
6 -0.100695 -0.695404 -1.223914
6 -0.372607 -1.724998 -2.221928
6 -0.082813 -1.078663 0.154296
6 -0.319605 -3.101345 -1.825674
6 -0.784943 -1.421281 -3.526264
6 -0.049749 -2.390034 0.526549
6 -0.106867 -3.426315 -0.442539
6 -0.567318 -4.093756 -2.793410
6 -1.042554 -2.419700 -4.457357
1 -0.941890 -0.385919 -3.804294
8 0.057201 -2.869867 1.797440

6 0.000000 -4.638754 0.304889
1 -0.526489 -5.137094 -2.506077
6 -0.906721 -3.761337 -4.094553
1 -1.359592 -2.151674 -5.459620
6 0.093084 -4.237820 1.680248
6 0.044606 -6.002901 0.019332
1 -1.098118 -4.546263 -4.818857
6 0.205918 -5.096705 2.727193
6 0.161434 -6.935366 1.071570
1 0.006786 -6.377504 -0.997254
6 0.239690 -6.491931 2.434954
1 0.271673 -4.738432 3.748923
6 0.206545 -8.336203 0.809231
6 0.354907 -7.456904 3.463236
6 0.318559 -9.244568 1.829947
1 0.148534 -8.669661 -0.223482
6 0.393178 -8.801295 3.172723
1 0.413448 -7.114105 4.492765
1 0.350583 -10.307381 1.612247
1 0.481598 -9.527422 3.974575
8 0.000000 0.000000 0.987595

S3.12 Molecule 12

Ground-state

SCF[PCM-M06/6-31G(d)]= -2450,13611992 au.

6 0.000000 2.650446 0.475010
6 0.000000 3.181008 -0.810633
6 0.000000 4.600563 -0.844506
6 0.000000 5.122593 0.417364
16 0.000000 3.907221 1.668508
1 0.000000 5.205054 -1.746831
1 0.000000 6.169144 0.702997
6 0.000000 1.233595 0.477008
6 0.000000 0.708065 -0.810969
16 0.000000 0.000000 1.715167
6 0.000000 -0.708065 -0.810969
6 0.000000 -1.233595 0.477008
6 0.000000 -2.650446 0.475010
6 0.000000 -3.181008 -0.810633
16 0.000000 -3.907221 1.668508
6 0.000000 -4.600563 -0.844506
6 0.000000 -5.122593 0.417364
1 0.000000 -5.205054 -1.746831
1 0.000000 -6.169144 0.702997
16 0.000000 1.940728 -2.049580

16 0.000000 -1.940728 -2.049580

Excited-state

SCF[PCM-M06/6-31G(d)]= -2450,1268605 au.

6 0.000000 2.616285 0.482349
6 0.000000 3.170350 -0.827517
6 0.000000 4.567620 -0.845653
6 0.000000 5.095886 0.432820
16 0.000000 3.882353 1.690497
1 0.000000 5.183551 -1.740571
1 0.000000 6.144157 0.712873
6 0.000000 1.237706 0.490605
6 0.000000 0.685937 -0.837754
16 0.000000 0.000000 1.748867
6 0.000000 -0.685937 -0.837754
6 0.000000 -1.237706 0.490605
6 0.000000 -2.616285 0.482349
6 0.000000 -3.170350 -0.827517
16 0.000000 -3.882353 1.690497
6 0.000000 -4.567620 -0.845653
6 0.000000 -5.095886 0.432820
1 0.000000 -5.183551 -1.740571
1 0.000000 -6.144157 0.712873
16 0.000000 1.932144 -2.086268
16 0.000000 -1.932144 -2.086268

S3.13 Molecule 13

Ground-state

SCF[PCM-M06/6-31G(d)]= -1501,49618454 au.

6 0.000000 3.181818 -0.324965
6 0.000000 2.660372 0.937104
6 0.000000 1.239685 0.904693
6 0.000000 0.709436 -0.380203
6 0.000000 -1.239685 0.904693
6 0.000000 -0.709436 -0.380203
6 0.000000 -2.660372 0.937104
6 0.000000 -3.181818 -0.324965
1 0.000000 -4.228203 -0.611471
16 0.000000 -1.965147 -1.575005
16 0.000000 1.965147 -1.575005
1 0.000000 4.228203 -0.611471

1 0.000000 -3.265603 1.839021
1 0.000000 3.265603 1.839021
16 0.000000 0.000000 2.144095

Excited-state

SCF[PCM-M06/6-31G(d)]= -1501,48522572 au.

6 0.000000 3.162234 -0.346837
6 0.000000 2.630753 0.950081
6 0.000000 1.248138 0.941697
6 0.000000 0.683086 -0.385611
6 0.000000 -1.248138 0.941697
6 0.000000 -0.683086 -0.385611
6 0.000000 -2.630753 0.950081
6 0.000000 -3.162234 -0.346837
1 0.000000 -4.212216 -0.621750
16 0.000000 -1.951195 -1.612659
16 0.000000 1.951195 -1.612659
1 0.000000 4.212216 -0.621750
1 0.000000 -3.257612 1.837295
1 0.000000 3.257612 1.837295
16 0.000000 0.000000 2.203879

S3.14 Molecule 14

Ground-state

SCF[PCM-M06/6-31G(d)]= -1855,40453376 au.

6 1.321153 0.065345 0.000000
6 0.847289 1.380284 0.000000
6 -0.542357 1.435057 0.000000
6 -1.152527 0.169362 0.000000
6 -3.002250 1.579206 0.000000
6 -2.556140 0.254316 0.000000
6 -4.412732 1.699381 0.000000
6 -5.005988 0.466500 0.000000
1 -6.069436 0.250228 0.000000
16 -3.885113 -0.860198 0.000000
16 0.000000 -1.112067 0.000000
1 -4.963784 2.634503 0.000000
1 1.503313 2.247286 0.000000
16 -1.703119 2.748391 0.000000
6 2.697955 -0.287595 0.000000
6 3.281309 -1.547250 0.000000

6 3.612234 0.822044 0.000000
7 4.346703 1.721826 0.000000
6 4.696596 -1.696471 0.000000
7 5.853782 -1.826488 0.000000
6 2.534305 -2.755284 0.000000
7 1.946448 -3.760967 0.000000

Excited-state

SCF[PCM-M06/6-31G(d)]= -1855,40154313 au.

6 1.328537 -0.071116 0.000000
6 0.877545 -1.398593 0.000000
6 -0.514070 -1.469947 0.000000
6 -1.152143 -0.203492 0.000000
6 -2.971712 -1.658190 0.000000
6 -2.537551 -0.314115 0.000000
6 -4.362168 -1.794804 0.000000
6 -4.982230 -0.554302 0.000000
1 -6.051379 -0.365638 0.000000
16 -3.895319 0.785915 0.000000
16 0.000000 1.100088 0.000000
1 -4.908240 -2.732810 0.000000
1 1.549141 -2.252312 0.000000
16 -1.639001 -2.804839 0.000000
6 2.710810 0.318100 0.000000
6 3.221898 1.642426 0.000000
6 3.646840 -0.743067 0.000000
7 4.399821 -1.636416 0.000000
6 4.619755 1.859543 0.000000
7 5.775123 2.034787 0.000000
6 2.436450 2.814315 0.000000
7 1.829032 3.814714 0.000000