Group 16 substitution effects on the electronic and optical properties of 1-dimensional conjugated heterocycle oligomers: A relativistic self-interaction corrected real-space TDDFT study

Supporting Information

Joëlle Mérgola-Greef[*][1] and Bruce F. Milne[†][1]

[1]Marine Biodiscovery Centre, Department of Chemistry, University of Aberdeen, Meston Building, Meston Walk, AB24 3UE, Old Aberdeen, UK.

_____

[*]j.mergola-greef.21@abdn.ac.uk
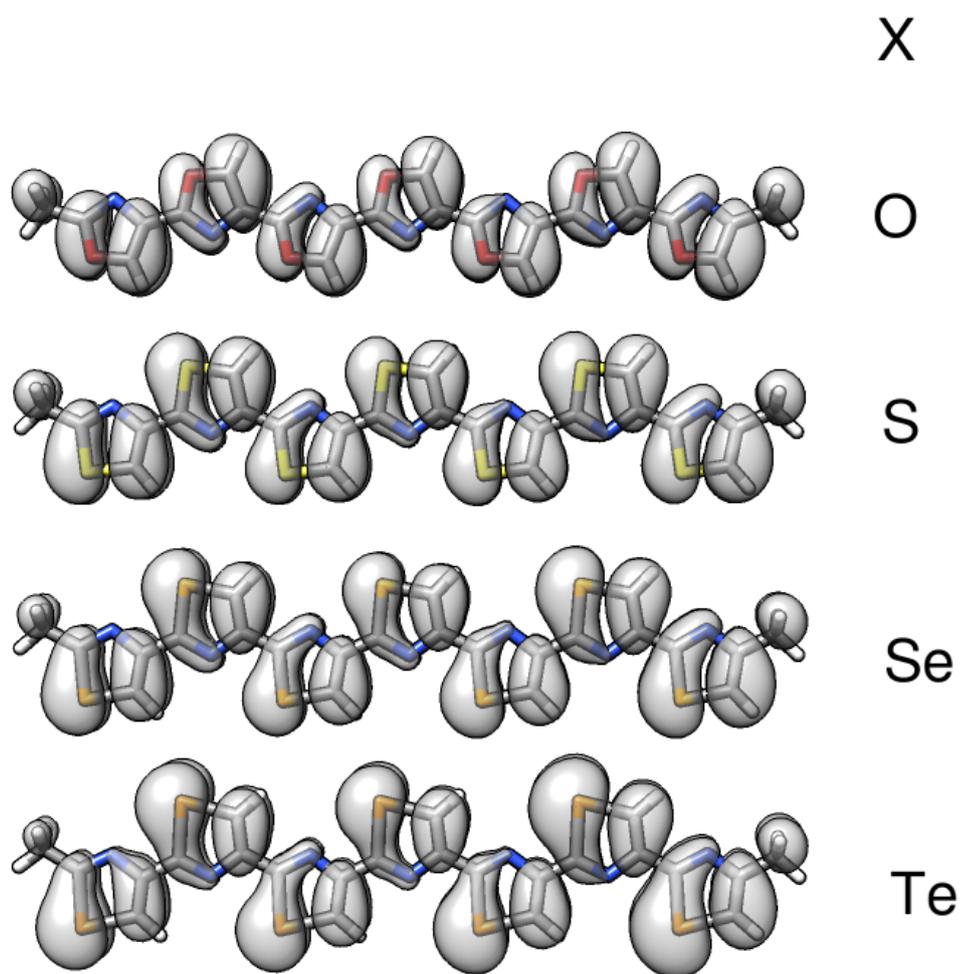[†]bruce.milne@abdn.ac.uk

X

O

S

Se

Te

Figure S1: Hole density distribution for the monocationic azole chain species. Surface cutoff = 0.0001 e$^-$.
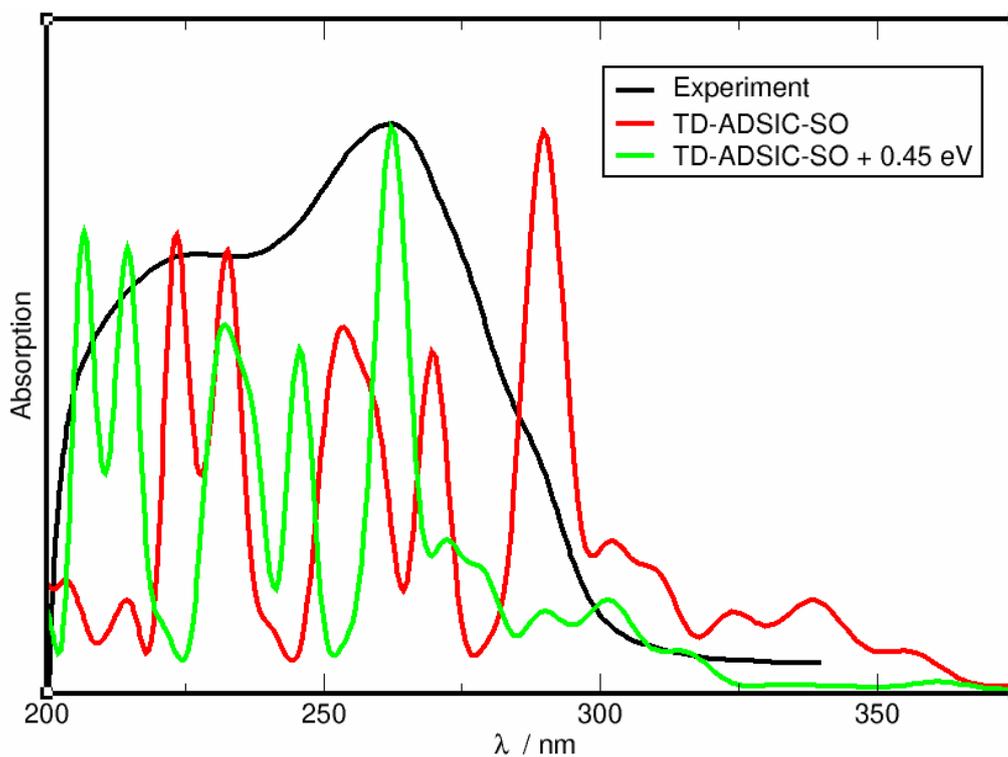
Figure S2: Comparison of telomestatin absorption spectra. The experimental UV-Vis spectrum is shown in black whilst the TD-ADSIC-SO calculated spectrum is shown in red and the shifted spectrum in green. Both calculated spectra are normalised to the largest peak in the experimental spectrum. Applying a shift of +0.45 eV aligns the largest peak in the calculated spectrum with the experimental λ-max at $\sim$260 nm. Unfortunately, the experimental spectrum cuts off before the position of the highest energy peak in the calculated spectrum, however a small rise in intensity just before the cut-off suggests the presence of the peaks in the region predicted by the calculations.
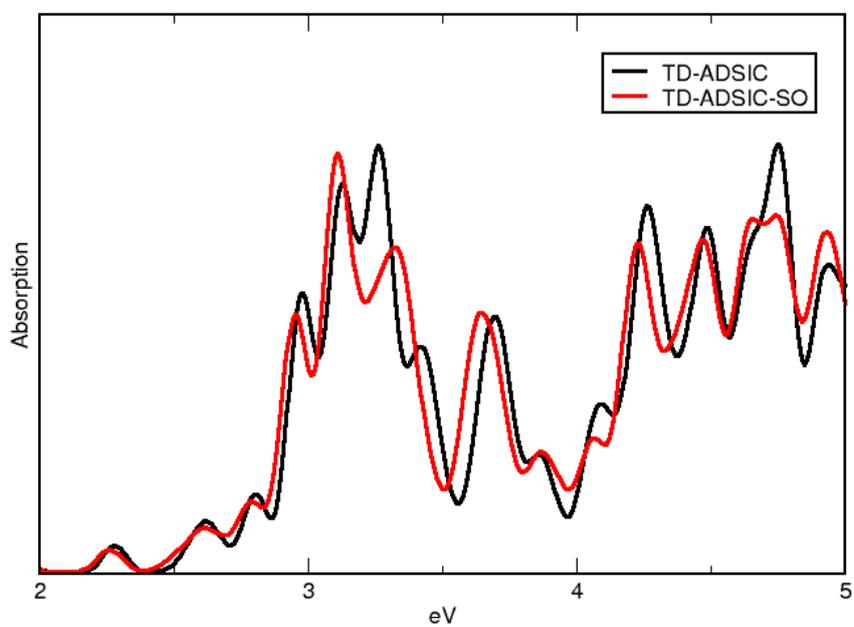
Figure S3: Detail of TD-ADSIC absorption spectrum for neutral 7-tellurazole compound with and without inclusion of spin-orbit coupling.
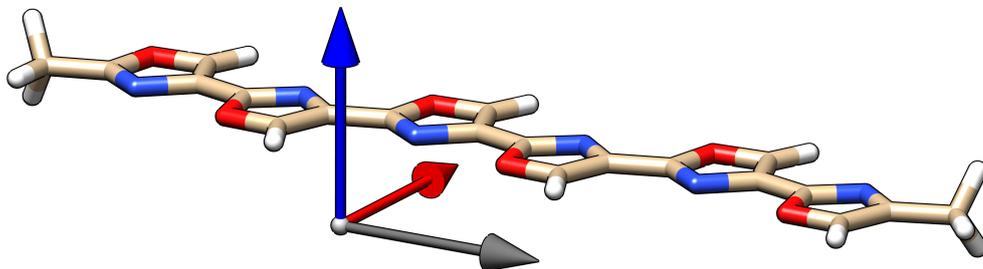
Figure S4: Geometry of 6-oxazole chain showing axes of polarisation for application of impulse ('kick') prior to time-propagation. Axis colours: black = longitudinal, red = transverse (in plane), blue = transverse (through plane).

r²SCAN-D4/Def2-TZVP geometry: x = O

50
N -10.497943 0.636825 -0.000000
C -9.441791 -0.261433 -0.000000
C -9.931205 -1.530463 -0.000000
O -11.289090 -1.444072 -0.000000
C -11.558039 -0.102240 -0.000000
C -8.063425 0.143879 -0.000001
N -7.009895 -0.616647 -0.000001
C -5.949740 0.268647 -0.000001
C -6.427754 1.545228 -0.000001
O -7.783569 1.478176 -0.000001
C -4.573779 -0.145689 -0.000001
O -4.300560 -1.481082 -0.000001
C -2.944571 -1.554197 -0.000001
C -2.460717 -0.279802 -0.000001
N -3.517069 0.609996 -0.000001
C -1.083455 0.130797 -0.000001
N -0.027894 -0.626557 -0.000001
C 1.029823 0.261838 -0.000001
C 0.547440 1.536833 -0.000001
O -0.808609 1.465624 -0.000001
C 2.407666 -0.147372 -0.000001
N 3.460539 0.613651 -0.000001
C 4.521868 -0.270597 -0.000001
C 4.043705 -1.547206 -0.000001
O 2.686652 -1.480911 -0.000001
C 5.897920 0.145707 -0.000001
C -12.977964 0.309997 -0.000000
H 4.496126 -2.522899 -0.000001
H 0.996601 2.514075 -0.000001
H -2.496900 -2.532139 -0.000001
H -5.975556 2.521098 -0.000001
H -9.490347 -2.511482 -0.000000
H -13.625743 -0.564693 0.000000
H -13.195106 0.917294 -0.880741
H -13.195106 0.917293 0.880741
O 6.168329 1.480300 -0.000000
C 7.525965 1.553704 -0.000000
C 8.012647 0.280204 -0.000000

N 6.955057 -0.609471 -0.000001
H 7.972126 2.532139 -0.000000
C 9.392654 -0.126301 -0.000000
O 9.675633 -1.451750 -0.000001
C 11.043902 -1.499975 -0.000001
C 11.520031 -0.228895 -0.000000
N 10.443355 0.641427 -0.000000
H 11.489659 -2.479694 -0.000001
C 12.921624 0.258124 -0.000000
H 13.625743 -0.574568 -0.000000
H 13.113636 0.876870 0.880108
H 13.113636 0.876870 -0.880109

r²SCAN-D4/Def2-TZVP geometry: x = S

50

N -10.566748 0.507526 0.000000
C -9.485751 -0.335748 0.000000
C -9.780308 -1.676955 0.000000
S -11.471232 -1.882221 0.000000
C -11.686099 -0.154299 0.000000
C -8.151818 0.222768 0.000000
N -7.044514 -0.469942 0.000001
C -5.955027 0.354365 0.000001
C -6.232795 1.701797 0.000001
S -7.917582 1.948655 0.000001
C -4.627542 -0.219440 0.000001
S -4.408280 -1.947340 0.000001
C -2.720774 -1.715653 0.000001
C -2.431586 -0.370852 0.000001
N -3.514049 0.462740 0.000001
C -1.100905 0.195206 0.000001
N 0.010177 -0.490901 0.000001
C 1.094953 0.339673 0.000001
C 0.809651 1.685436 0.000001
S -0.876690 1.922443 0.000001
C 2.426090 -0.225168 0.000001
N 3.533608 0.466479 0.000001
C 4.623273 -0.357500 0.000001
C 4.345082 -1.704788 0.000001
S 2.659381 -1.950727 0.000001
C 5.949850 0.218130 0.000000
C -13.038401 0.468448 -0.000000
H 5.052543 -2.518693 0.000001
H 1.512951 2.502931 0.000001
H -2.020617 -2.535875 0.000001
H -5.525170 2.515589 0.000001
H -9.088626 -2.504049 0.000000
H -13.826030 -0.284606 -0.000000
H -13.159185 1.101910 -0.881608
H -13.159185 1.101910 0.881608
S 6.165301 1.945856 0.000000
C 7.853236 1.716013 0.000000

```
C 8.146172 0.371531 0.000000
N 7.063894 -0.462690 0.000000
H 8.553562 2.535875 0.000000
C 9.481711 -0.184450 0.000000
S 9.729578 -1.902950 0.000001
C 11.418452 -1.626569 0.000000
C 11.688685 -0.282088 0.000000
N 10.583217 0.521286 0.000000
H 12.121227 -2.445774 0.000000
C 13.043640 0.339584 -0.000000
H 13.826030 -0.419258 -0.000000
H 13.171190 0.975378 0.879733
H 13.171190 0.975377 -0.879733
```

r²SCAN-D4/Def2-TZVP geometry: x = Se

50

N -10.585775 0.456841 -0.000000
C -9.497105 -0.382996 -0.000000
C -9.737051 -1.730987 -0.000000
Se -11.555276 -2.045822 -0.000000
C -11.722468 -0.154440 -0.000000
C -8.179572 0.214285 -0.000000
N -7.053176 -0.428565 -0.000000
C -5.959577 0.397480 -0.000000
C -6.187031 1.750618 -0.000000
Se -7.999760 2.100182 -0.000000
C -4.646549 -0.210147 -0.000001
Se -4.477552 -2.097465 -0.000001
C -2.662029 -1.759137 -0.000001
C -2.427064 -0.407567 -0.000001
N -3.516046 0.424770 -0.000001
C -1.111924 0.195246 -0.000001
N 0.017455 -0.441612 -0.000001
C 1.107435 0.389482 -0.000001
C 0.874135 1.741411 -0.000001
Se -0.940614 2.082443 -0.000001
C 2.423366 -0.211612 -0.000001
N 3.549926 0.429959 -0.000001
C 4.644108 -0.395463 -0.000001
C 4.416884 -1.748434 -0.000001
Se 2.603107 -2.097736 -0.000001
C 5.956832 0.213170 -0.000001
C -13.046816 0.525199 -0.000000
H 5.170443 -2.520278 -0.000001
H 1.624149 2.516684 -0.000001
H -1.913674 -2.536031 -0.000001
H -5.433749 2.522755 -0.000000
H -8.997960 -2.516429 -0.000001
H -13.869068 -0.189285 -0.000000
H -13.137735 1.164205 -0.881681
H -13.137735 1.164205 0.881681
Se 6.124678 2.100526 -0.000001
C 7.940587 1.761062 -0.000001

C 8.177233 0.409400 -0.000000
N 7.086829 -0.421578 -0.000001
H 8.690733 2.536031 -0.000000
C 9.496747 -0.186058 -0.000000
Se 9.689517 -2.066806 -0.000000
C 11.506376 -1.686714 0.000000
C 11.726794 -0.338037 0.000000
N 10.618209 0.468423 -0.000000
H 12.253625 -2.465903 0.000000
C 13.071684 0.310847 0.000000
H 13.869068 -0.432217 0.000000
H 13.186325 0.949321 0.879813
H 13.186325 0.949321 -0.879812

r²SCAN-D4/Def2-TZVP geometry: x = Te

50

N -10.602947 0.395305 -0.000000
C -9.505027 -0.437178 -0.000000
C -9.678380 -1.794752 -0.000000
Te -11.660777 -2.260577 -0.000000
C -11.764404 -0.156740 -0.000000
C -8.210555 0.214343 -0.000000
N -7.060394 -0.374782 -0.000001
C -5.961186 0.450965 -0.000001
C -6.126407 1.812809 -0.000001
Te -8.107395 2.305063 -0.000001
C -4.669275 -0.206270 -0.000001
Te -4.575132 -2.298345 -0.000001
C -2.590985 -1.815679 -0.000001
C -2.420219 -0.454921 -0.000001
N -3.516123 0.375783 -0.000001
C -1.126866 0.199114 -0.000001
N 0.026047 -0.383235 -0.000001
C 1.121778 0.447791 -0.000001
C 0.950880 1.808584 -0.000001
Te -1.033238 2.291394 -0.000001
C 2.416413 -0.203773 -0.000001
N 3.566917 0.382886 -0.000001
C 4.666536 -0.442802 -0.000001
C 4.501376 -1.804303 -0.000001
Te 2.518958 -2.295734 -0.000001
C 5.958926 0.214123 -0.000001
C -13.040724 0.613042 0.000000
H 5.322049 -2.506375 -0.000001
H 1.768218 2.514493 -0.000001
H -1.774169 -2.522192 -0.000001
H -5.306181 2.515385 -0.000001
H -8.870932 -2.511596 -0.000000
H -13.913307 -0.038712 0.000000
H -13.085565 1.257437 -0.881955
H -13.085565 1.257437 0.881955
Te 6.055344 2.307140 -0.000000
C 8.039083 1.820172 -0.000000

C 8.209043 0.458855 -0.000000
N 7.110663 -0.368661 -0.000001
H 8.859671 2.522192 -0.000000
C 9.507238 -0.188177 -0.000000
Te 9.626558 -2.278237 -0.000001
C 11.609082 -1.750889 -0.000000
C 11.765091 -0.393760 0.000000
N 10.652214 0.411714 0.000000
H 12.423690 -2.461159 0.000000
C 13.094402 0.294529 0.000001
H 13.913307 -0.424663 0.000001
H 13.189420 0.936705 0.879716
H 13.189420 0.936705 -0.879715

r²SCAN-D4/Def2-TZVP geometry: Telomestatin

56

S -4.144991 4.474603 -0.699226
O -5.379616 0.002862 0.472739
O -3.355168 -3.819537 -0.033265
O 0.183109 5.950949 -0.296770
O 0.762218 -5.358061 -0.221710
O 4.296951 4.572488 0.025956
O 4.824444 -3.559834 -0.117794
O 6.310454 0.637311 0.053924
N -2.823107 2.634365 0.644976
N -3.168919 -0.138267 0.227497
N -1.554702 -2.500279 -0.007269
N -0.245351 3.850141 0.336634
N 1.170503 -3.170148 -0.068021
N 2.543504 3.215873 0.283398
N 3.529799 -1.752427 0.044260
N 4.103943 0.920506 0.203280
C -4.177236 2.130188 0.569206
C -4.940456 2.843498 -0.577127
C -4.167487 0.645137 0.409977
C -2.698525 3.770762 0.092113
C -3.723735 -1.412344 0.171300
C -5.079299 -1.329131 0.316689
C -2.841970 -2.542915 0.033147
C -1.433423 4.487095 0.039632
C -1.156043 -3.821231 -0.100724
C -6.201728 -2.283883 0.349168
C -2.253147 -4.635893 -0.118928
C -1.165897 5.767405 -0.345904
C 0.260706 -4.081757 -0.132270
C 0.670075 4.733548 0.111699
C -2.486257 -6.088056 -0.205245
C 2.094487 4.510609 0.147056
C 2.369941 -3.850529 -0.113684
C 3.559687 -3.037217 -0.056038
C 3.829944 3.296971 0.196024
C 2.122170 -5.186392 -0.208186
C 4.711724 2.155334 0.182384

C 4.849677 -1.357689 0.047986
C 3.165734 5.341191 -0.005880
C 5.067870 0.066916 0.119836
C 5.643160 -2.462067 -0.049587
C 6.062037 1.984626 0.094236
H -4.675039 2.362785 1.524771
H -4.810626 2.315588 -1.524771
H -6.002782 2.954872 -0.364714
H -6.918875 -2.074498 -0.450272
H -5.827217 -3.297914 0.223632
H -6.740926 -2.223057 1.299187
H -1.757743 6.610326 -0.660531
H -3.070663 -6.340723 -1.095240
H -1.532345 -6.610326 -0.255927
H -3.038732 -6.451346 0.666514
H 2.721652 -6.077757 -0.270252
H 3.303331 6.399839 -0.140965
H 6.702272 -2.648981 -0.084155
H 6.918875 2.634001 0.049039