# Electronic Supplementary Information for

## Liquid crystalline radicals: Discotic behavior of unsymmetric derivatives of 1,3,5-triphenyl-6-oxoverdazyl

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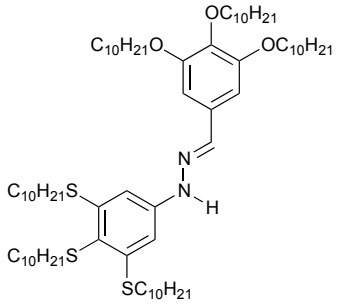
**Table of Content**:

## 1. Additional synthetic details

Reagents and solvents were obtained commercially. Reactions were carried out under Ar, and subsequent manipulations were conducted in air. $^1$H NMR spectra were obtained at 400 MHz ($^1$H) in $CDCl_3$ and referenced to the solvent unless stated otherwise.

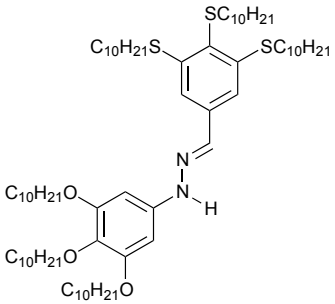
**Hydrazones 4[10]. General Procedure.** To a solution of crude 3,4,5-tri(decyloxyphenyl)hydrazine[1] or 3,4,5-tri(decylsulfanyl)phenylhydrazine[1] (**2[10]**, 1.3 mmol) and 3,4,5-tri(decyloxy)benzaldehyde[2,3] or 3,4,5-tri(decylsulfanyl)benzaldehyde[4] (**3[10]**, 1.0 mmol) in EtOH (4 mL) 1 drop of AcOH was added. The mixture was refluxed for 1 h under Ar, cooled to rt, solvent was evaporated, and traces of AcOH removed on vacuum to give 90~% yield of crude hydrazone **4[10]** (~70% pure), which was used for the next step without additional purification.

**3,4,5-Tri(decyloxy)benzaldehyde 3,4,5-tri(decylsulfanyl)phenylhydrazone 4[10] (X=S,Y=O).**




$^1$H NMR (400 MHz, $CDCl_3$) δ 0.85-0.91 (m, 18H), 1.20-1.42 (m, 72H), 1.43-1.52 (m, 12H), 1.55-1.62 (m, 2H), 1.75 (quin, $J$ = 7.2 Hz, 6H), 1.80 (quin, $J$ = 7.0 Hz, 4H), 2.79 (t, $J$ = 6.6 Hz, 2H), 2.89 (t, $J$ = 6.6 Hz, 4H), 3.98 (t, $J$ = 6.1 Hz, 2H), 4.01 (t, $J$ = 6.4 Hz, 4H), 6.65 (s, 2H), 6.84 (s, 2H), 7.57 (s, 1H), 7.58 (s, 1H).

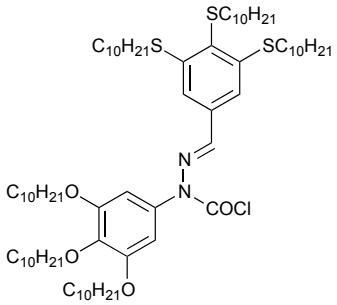
**3,4,5-Tri(decylsulfanyl)benzaldehyde 3,4,5-tri(decyloxy)phenylhydrazone 4[10] (X=O,Y=S).**




$^1$H NMR (400 MHz, $CDCl_3$) (major signals) d 0.84-0.92 (m, 18H), 1.20-1.41 (m, 72H), 1.43-1.52 (m, 12H), 1.55-1.64 (m, 2H), 1.68-1.86 (m, 10H), 2.85 (t, *J* = 7.4 Hz, 2H), 2.92 (t, *J* = 7.5 Hz, 4H), 3.89 (t, *J* = 6.5 Hz, 2H), 3.98 (t, *J* = 6.4 Hz, 4H), 6.33 (s, 2H), 7.15 (s, 2H), 7.56 (s, 2H).

**Carbamoyl chlorides 5[10]. General Procedure.** To a solution of crude hydrazone **4[10]** (1.0 mmol) in dry $CH_2Cl_2$ (10 mL) pyridine (1.2 mmol) followed by triphosgene (297 mg, 1.0 mmol) were added under Ar. The mixture was stirred at ambient temperature for 4 hrs, 1% HCl was added, organic products were extracted ($CH_2Cl_2$), extracts dried ($Na_2SO_4$), and solvent evaporated. The crude product was purified on a short silica gel column (hexane / $CH_2Cl_2$, 4:1) to give chloride **5[10]** as yellowish viscous oil in yields ~50%.

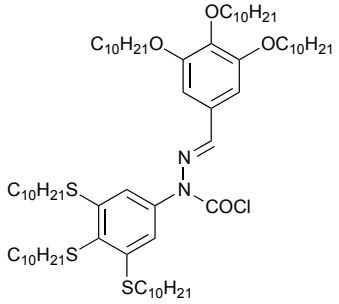
**3,4,5-Tri(decylsulfanyl)benzaldehyde-chloroformyl-3,4,5-tri(decyloxy)phenylhydrazone 5[10](X=O,Y=S).**




$^1$H NMR (400 MHz, $CDCl_3$) δ 0.84-0.91 (m, 18H), 1.20-1.38 (m, 72H), 1.42-1.52 (m, 12H), 1.53-1.62 (m, 2H), 1.73 (quin, *J* = 7.5 Hz, 6H), 1.80 (quin, *J* = 7.1 Hz, 4H), 2.84 (t,

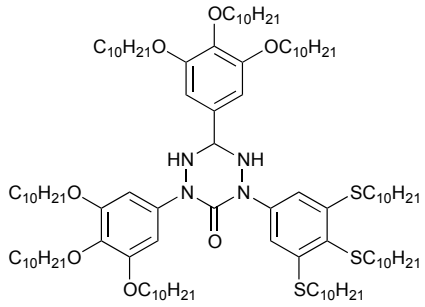
*J* = 7.4 Hz, 2H), 2.89 (t, *J* = 7.3 Hz, 4H), 3.93 (t, *J* = 6.5 Hz, 4H), 4.03 (t, *J* = 6.5 Hz, 2H), 6.40 (s, 2H), 7.15 (s, 2H), 7.24 (s, 1H). Molecular ions in MS were not observed.

**3,4,5-Tri(decyloxy)benzaldehyde-chloroformyl-3,4,5-tri(decylsulfanyl)phenylhydrazone 5[10] (X=S,Y=O).**




$^1$H NMR (400 MHz, $CDCl_3$) δ 0.84-0.91 (m, 18H), 1.20-1.38 (m, 72H), 1.39-1.50 (m, 12H), 1.62 -1.76 (m, 8H), 1.80 (quin, *J* = 7.4 Hz, 4H), 2.81 (t, *J* = 7.4 Hz, 4H), 2.91 (t, *J* = 7.4 Hz, 2H), 3.98 (t, *J* = 6.5 Hz, 6H), 6.67 (s, 2H), 6.87 (s, 2H), 7.28 (s, 1H). HRMS calcd for $C_{74}H_{132}ClN_2O_4S_3$ m/z 1243.9032; found m/z 1243.9018.

**2,6-Di(3,4,5-tridecyloxyphenyl)-4-(3,4,5-tridecylsulfanylphenyl)-1,2,4,5-tetrazine-3-one 6[10]d.**




$^1$H NMR (400 MHz, $CDCl_3$) δ 0.84-0.94 (m, 27H), 1.20-1.51 (m, 126H), 1.52-1.64 (m, 8H), 1.65-1.83 (m, 10H), 2.61 (t, *J* = 7.1 Hz, 4H), 2.81 (t, *J* = 7.5 Hz, 2H), 3.91 (t, *J* = 6.6 Hz, 4H), 3.93 (t, *J* = 6.5 Hz, 8H), 4.71 (d, *J* = 8.5 Hz, 2H), 5.46 (t, *J* = 8.5 Hz, 1H), 6.81 (s, 4H), 6.99 (s, 2H). The molecular ion in MS was not observed.

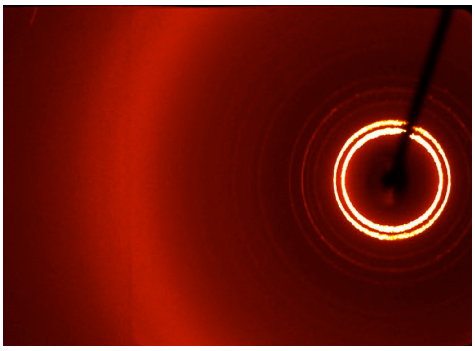
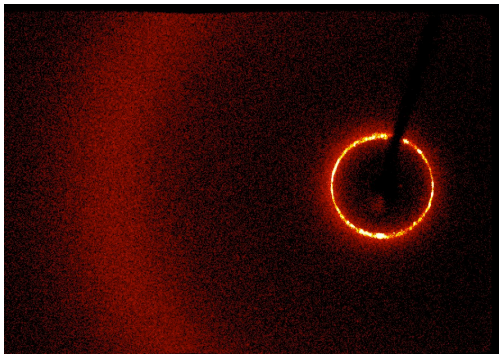
**2. Powder XRD measurements**

X-ray diffraction experiments were performed with Bruker D8 GADDS (Cu Kα

radiation, Göbel mirror, point collimator, Vantec 2000 area detector) equipped with a modified Linkam heating stage and with Bruker NanoStar small angle diffractometer (Cu $K_\alpha$ radiation, cross-coupled Göbel mirrors, 3 pinhole collimator, Vantec 2000 area detector). Samples were prepared in a form of a thin film or a droplet on heated surface. The X-ray beam was incident nearly parallel to sample surface, and resulting XRD patterns were recorded as a function of temperature.

Experimental pattern was at first indexed using indexing procedure implemented in Topas I software (Bruker), in this step a space group was found as well rough estimation of unit cell parameter. Next, the whole pattern was fitted using Topas software, assuming previously determined lattice symmetry and taking unit cell dimensions and background parameters as fitted variables (so called 'hkl phase'). In this procedure the intensity of each simulated peak is an independent variable with no physical meaning.

Results are shown in Fig. S1 and S2 and Tables S1- S5.

a)  b) 

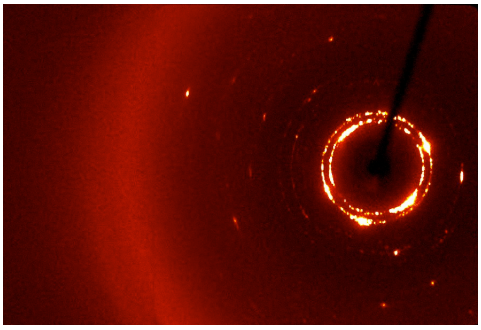
c) 

**Fig. S1**. 2D patterns for **1[10]d**: a) $Col_{h(3D)}$ phase at 70 °C, sample heated from the crystalline phase; b) $Col_h$ phase at 78 °C, sample cooled from the isotropic phase; c) $Col_{h(3D)}$ phase at 70 °C, sample cooled from the $Col_h$ phase.

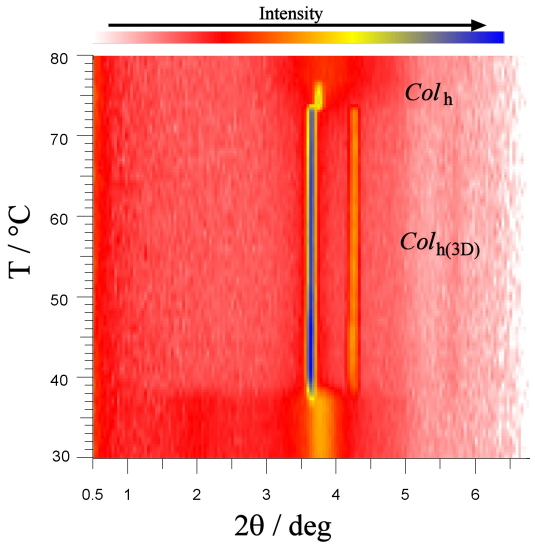



**Fig. S2**. Temperature dependence of the position of low angle reflections for **1d[10]** recorded on cooling.

**Table S1.** Selected X-ray diffraction data for **1[10]c**.

| Temp /ºC | Phase | Miller indices *hk* | $d_{meas}$ /Å obs | $d_{calcd}$ /Å calcd | Cell parameter /Å |
|---|---|---|---|---|---|
| 75 | $Col_h$ | 10 | 23.55 | 23.55 | $a$ = 27.19 |
| | | 11 | 13.58 | 13.59 | |
| | | 20 | 11.78 | 11.77 | |

**Table S2.** Selected X-ray diffraction data for **1[10]d** at 78 ºC.

| Temp /ºC | Phase | Miller indices *hk* | $d_{meas}$ /Å obs | $d_{calcd}$ /Å calcd | Cell parameter /Å |
|---|---|---|---|---|---|
| 78 | $Col_h$ | 10 | 23.44 | 23.43 | $a$ = 27.05 |
| | | 11 | 13.52 | 13.53 | |

**Table S3.** X-ray diffraction data for **1[10]d** at 70 ºC.

| Temp /ºC | Phase | Miller indices *hkl* | $d_{meas}$ /Å obs | $D_{calcd}$ /Å calcd | Cell parameters /Å |
|---|---|---|---|---|---|
| 70 | $Col_{h(3D)}$ | 100 | 24.15 | 24.14 | $a$ = 27.9 |
| | | 101 | 20.64 | 20.63 | $c$ = 39.7 |
| | | 102 | 15.36 | 15.36 | |
| | | 110 | 13.98 | 13.97 | |
| | | 111 | 13.19 | 13.18 | |
| | | 201 | 11.57 | 11.57 | |
| | | 210 | 9.15 | 9.14 | |
| | | 211 | 8.92 | 8.92 | |
| | | 212 | 8.32 | 8.32 | |
| | | 300 | 8.06 | 8.06 | |
| | | 213 | 7.49 | 7.52 | |
| | | 302 | 7.49 | 7.47 | |
| | | 220 | 6.98 | 6.98 | |
| | | 214 | 6.72 | 6.73 | |
| | | 310 | 6.72 | 6.71 | |
| | | 400 | 6.05 | 6.05 | |
| | | 314 | 5.57 | 5.56 | |

**Table S4.** X-ray diffraction data for **1[10]e**.

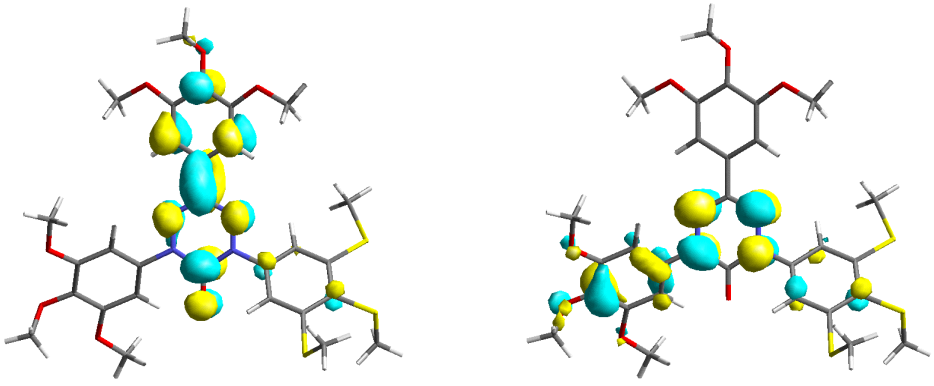
| Temp /ºC | Phase | Miller indices *hkl* | $d_{meas}$ /Å obs | $d_{calcd}$ /Å calcd | Cell parameters /Å |
|---|---|---|---|---|---|
| 65 | $Col_{h(3D)}$ | 100 | 24.01 | 24.01 | $a$ = 27.72 |
| | | 101 | 20.34 | 20.34 | $c$ = 38.26 |
| | | 102 | 14.95 | 14.96 | |
| | | 110 | 13.88 | 13.86 | |
| | | 111 | 13.05 | 13.03 | |
| | | 201 | 11.47 | 11.45 | |
| | | 210 | 9.08 | 9.08 | |
| | | 211 | 8.85 | 8.83 | |
| | | 212 | 8.21 | 8.20 | |
| | | 300 | 8.02 | 8.00 | |
| | | 213 | 7.40 | 7.39 | |
| | | 220 | 6.96 | 6.93 | |
| | | 310 | 6.68 | 6.66 | |
| | | 400 | 6.02 | 6.00 | |

**Table S5.** X-ray diffraction data for **1[10]f**.

| Temp /ºC | Phase | Miller indices *hkl* | $d_{meas}$ /Å obs | $d_{calcd}$ /Å calcd | Cell parameters /Å |
|---|---|---|---|---|---|
| 90 | $Col_{h(3D)}$ | 100 | 24.47 | 24.47 | $a$ = 27.72 |
| | | 101 | 21.75 | 21.75 | $c$ = 38.26 |
| | | 102 | 17.03 | 17.04 | |
| | | 110 | 14.14 | 14.12 | |
| | | 111 | 13.55 | 13.54 | |
| | | 201 | 11.86 | 11.85 | |
| | | 202 | 10.86 | 10.87 | |
| | | 210 | 9.26 | 9.25 | |
| | | 211 | 9.09 | 9.08 | |
| | | 212 | 8.62 | 8.62 | |
| | | 300 | 8.17 | 8.15 | |
| | | 213 | 7.99 | 7.98 | |
| | | 302 | 7.72 | 7.71 | |
| | | 303 | 7.26 | 7.25 | |
| | | 220 | 7.06 | 7.06 | |
| | | 310 | 6.79 | 6.79 | |
| | | 223 | 6.46 | 6.45 | |
| | | 400 | 6.14 | 6.12 | |
| | | 320 | 5.63 | 5.61 | |

## 3. α-FMO contours

Contours of α-FMOs are shown in Fig. S3.



α-LUMO, E = -1.24 eV  α-HOMO, E = -5.20 eV

**Fig. S3**. Contours and energies α-FMOs involved in low energy excitations in **1[1]c**.

## 4. Partial data for TD-DFT calculation (B3LYP/6-31G(d,p)) for 1[1]

### 1[1]a

```
Excited State   1:  2.062-A      2.0457 eV  606.07 nm  f=0.0010
<S**2>=0.812
    192B ->194B       -0.37502
    193B ->194B        0.91979
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -5002.80596109
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:  2.063-A      2.0755 eV  597.38 nm  f=0.0003
<S**2>=0.814
    191B ->194B        0.99310

 Excited State   3:  2.042-A      2.1024 eV  589.73 nm  f=0.0157
<S**2>=0.792
    192B ->194B        0.92314
    193B ->194B        0.37741

 Excited State   4:  2.040-A      2.1163 eV  585.84 nm  f=0.0524
<S**2>=0.790
    194A ->195A       -0.16144
    184B ->194B       -0.28351
    190B ->194B        0.92868

 Excited State   5:  2.113-A      2.3260 eV  533.03 nm  f=0.0139
<S**2>=0.866
    183B ->194B        0.19690
    188B ->194B        0.96046

 Excited State   6:  2.086-A      2.3418 eV  529.44 nm  f=0.0272
<S**2>=0.838
    194A ->195A       -0.13465
    189B ->194B        0.97350
```

### 1[1]b

```
Excited State   1:  2.028-A      2.0192 eV  614.01 nm  f=0.0731
<S**2>=0.778
    158A ->159A       -0.12199
    158A ->160A       -0.10337
    150B ->158B        0.11329
    157B ->158B        0.96577
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2095.97900447
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:  2.075-A      2.4130 eV  513.82 nm  f=0.0480
<S**2>=0.827
    158A ->159A       -0.21386
    151B ->158B       -0.15964
    154B ->158B       -0.10715
    155B ->158B        0.11502
    156B ->158B        0.92556
```

```
 Excited State   3:  2.121-A      2.4543 eV  505.17 nm  f=0.0432
<S**2>=0.874
    158A ->161A       -0.10493
    152B ->158B        0.14003
    155B ->158B        0.95141
    156B ->158B       -0.12615

 Excited State   4:  2.061-A      2.4845 eV  499.03 nm  f=0.0016
<S**2>=0.812
    154B ->158B        0.98271
    156B ->158B        0.11600

 Excited State   5:  2.063-A      2.5311 eV  489.84 nm  f=0.0076
<S**2>=0.814
    152B ->158B        0.83172
    153B ->158B        0.51881
    155B ->158B       -0.15783

 Excited State   6:  2.048-A      2.5765 eV  481.21 nm  f=0.0001
<S**2>=0.799
    152B ->158B       -0.52395
    153B ->158B        0.84328

 Excited State   7:  2.049-A      2.7375 eV  452.91 nm  f=0.0069
<S**2>=0.800
    144B ->158B       -0.13496
    147B ->158B       -0.31954
    149B ->158B        0.12092
    150B ->158B       -0.23389
    151B ->158B        0.85417
    154B ->158B       -0.10152
    156B ->158B        0.15774
```

**1[1]c**

```
Excited State   1:  2.026-A      1.9656 eV  630.78 nm  f=0.0597
<S**2>=0.776
    170A ->171A       -0.100045
    162B ->170B        0.12621
    169B ->170B        0.96559
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3064.92111189
 Copying the excited state density for this state as the 1-
particle RhoCI density.

 Excited State   2:  2.078-A      2.3174 eV  535.01 nm  f=0.0529
<S**2>=0.830
    170A ->171A        0.13680
    161B ->170B        0.10648
    166B ->170B        0.10625
    167B ->170B       -0.65912
    168B ->170B        0.69312
```

```
 Excited State   3:  2.091-A      2.3508 eV  527.42 nm  f=0.0103
<S**2>=0.843
    165B ->170B       -0.30728
    167B ->170B        0.64834
    168B ->170B        0.67073

 Excited State   4:  2.065-A      2.4031 eV  515.94 nm  f=0.0092
<S**2>=0.816
    164B ->170B       -0.10479
    165B ->170B        0.93130
    167B ->170B        0.28536
    168B ->170B        0.15511

 Excited State   5:  2.050-A      2.4585 eV  504.31 nm  f=0.0102
<S**2>=0.801
    164B ->170B        0.81843
    165B ->170B        0.10050
    166B ->170B       -0.54151

 Excited State   6:  2.086-A      2.4948 eV  496.98 nm  f=0.0026
<S**2>=0.838
    162B ->170B       -0.10932
    164B ->170B        0.55103
    166B ->170B        0.79953

 Excited State   7:  2.045-A      2.6883 eV  461.19 nm  f=0.0032
<S**2>=0.796
    158B ->170B       -0.16749
    159B ->170B        0.36856
    161B ->170B        0.76239
    162B ->170B        0.33580
    163B ->170B       -0.22405
    166B ->170B        0.12215
    167B ->170B        0.11657
```

**1d[1]**

```
Excited State   1:  2.051-A      2.0722 eV  598.31 nm  f=0.1094
<S**2>=0.802
    170A ->171A       -0.13870
    162B ->170B        0.15620
    169B ->170B        0.95268
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3064.91744100
 Copying the excited state density for this state as the 1-
particle RhoCI density.
```

```
 Excited State   2:  2.077-A      2.3594 eV  525.48 nm  f=0.0252
<S**2>=0.829
    170A ->171A       -0.11459
    165B ->170B       -0.33336
    166B ->170B        0.59988
    168B ->170B        0.68593

 Excited State   3:  2.062-A      2.3895 eV  518.86 nm  f=0.0196
<S**2>=0.813
    170A ->171A       -0.12203
    165B ->170B        0.76209
    166B ->170B       -0.26231
    168B ->170B        0.55569

 Excited State   4:  2.076-A      2.4364 eV  508.89 nm  f=0.0136
<S**2>=0.827
    170A ->171A        0.19281
    164B ->170B        0.35388
    165B ->170B        0.47831
    166B ->170B        0.63992
    167B ->170B       -0.15284
    168B ->170B       -0.34637

 Excited State   5:  2.070-A      2.4689 eV  502.17 nm  f=0.0122
<S**2>=0.821
    164B ->170B        0.92325
    165B ->170B       -0.21577
    166B ->170B       -0.26740

 Excited State   6:  2.043-A      2.5320 eV  489.67 nm  f=0.0042
<S**2>=0.794
    164A ->171A       -0.10052
    170A ->171A       -0.45989
    162B ->170B        0.24131
    166B ->170B        0.22386
    167B ->170B        0.76931
    168B ->170B       -0.17918
```

**1e[1]**

```
Excited State   1:  2.055-A      2.0470 eV  605.69 nm  f=0.0963
<S**2>=0.805
    182A ->183A       -0.11942
    173B ->182B        0.19487
    177B ->182B        0.17639
    180B ->182B       -0.15938
```

```
    181B ->182B        0.92122
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -4033.85816745
 Copying the excited state density for this state as the 1-
particle RhoCI density.

 Excited State   2:  2.077-A      2.2127 eV  560.33 nm  f=0.0130
<S**2>=0.829
    177B ->182B       -0.17248
    179B ->182B       -0.21704
    180B ->182B        0.91712
    181B ->182B        0.21408

 Excited State   3:  2.052-A      2.3153 eV  535.51 nm  f=0.0148
<S**2>=0.803
    176B ->182B       -0.32462
    177B ->182B        0.56653
    178B ->182B        0.29515
    179B ->182B        0.60515
    180B ->182B        0.28610

 Excited State   4:  2.058-A      2.3328 eV  531.49 nm  f=0.0028
<S**2>=0.809
    176B ->182B        0.87178
    178B ->182B        0.11872
    179B ->182B        0.45662

 Excited State   5:  2.083-A      2.3621 eV  524.89 nm  f=0.0176
<S**2>=0.835
    173B ->182B       -0.11925
    176B ->182B        0.32863
    177B ->182B        0.67897
    178B ->182B        0.19478
    179B ->182B       -0.57600
    181B ->182B       -0.11738

 Excited State   6:  2.045-A      2.4245 eV  511.38 nm  f=0.0061
<S**2>=0.795
    182A ->183A       -0.17279
    173B ->182B        0.17363
    177B ->182B       -0.29491
    178B ->182B        0.89509
    179B ->182B       -0.13599

 Excited State   7:  2.030-A      2.6129 eV  474.50 nm  f=0.0037
<S**2>=0.781
```

```
    176A ->183A       -0.14223
    182A ->183A        0.66800
    169B ->182B        0.10135
    170B ->182B       -0.15862
    171B ->182B        0.14837
    172B ->182B        0.18732
    173B ->182B       -0.47388
    174B ->182B        0.10463
    175B ->182B        0.15035
    177B ->182B       -0.19943
    178B ->182B        0.18923
    180B ->182B       -0.16608
    181B ->182B        0.18493
```

**1f[1]**

```
Excited State   1:  2.019-A      1.9102 eV  649.07 nm  f=0.0325
<S**2>=0.769
    182A ->184A        0.10392
    173B ->182B        0.13331
    181B ->182B        0.96748
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -4033.86347112
 Copying the excited state density for this state as the 1-
particle RhoCI density.

 Excited State   2:  2.087-A      2.1927 eV  565.44 nm  f=0.0074
<S**2>=0.839
    180B ->182B        0.98430

 Excited State   3:  2.088-A      2.2688 eV  546.49 nm  f=0.0150
<S**2>=0.840
    177B ->182B        0.16754
    179B ->182B        0.96771

 Excited State   4:  2.040-A      2.3272 eV  532.76 nm  f=0.0111
<S**2>=0.791
    176B ->182B        0.94343
    177B ->182B       -0.22535
    178B ->182B        0.23171

 Excited State   5:  2.075-A      2.3915 eV  518.44 nm  f=0.0121
<S**2>=0.827
    173B ->182B       -0.10209
    177B ->182B        0.63171
    178B ->182B        0.73518
```

```
    179B ->182B       -0.16225

 Excited State   6:  2.075-A      2.3963 eV  517.39 nm  f=0.0039
<S**2>=0.826
    170B ->182B       -0.11477
    171B ->182B        0.10840
    176B ->182B        0.31818
    177B ->182B        0.68620
    178B ->182B       -0.60514

 Excited State   7:  2.049-A      2.6249 eV  472.33 nm  f=0.0046
<S**2>=0.799
    170B ->182B        0.57246
    171B ->182B       -0.51760
    173B ->182B        0.48849
    174B ->182B        0.21853
    175B ->182B       -0.14318
    177B ->182B        0.16370
```

## 5. Archive data for B3LYP/6-31G(d,p) geometry optimizations

**1[1]a**

```
1\1\GINC-OCTOPUS\SP\UTD-B3LYP-FC\6-31G(d,p)\C29H33N4O1S9(2)\PIOTR\25-J
 an-2011\0\\#P UB3LYP/6-31G(d,p) TD(NStates=20) SCF=tight Geom(NoAngle,
  noDistance, check) #P guess=check\\1,3,5-(3,4,5-MeSphenyl)-6-oxoverda
 zyl, C1 at the DFT geom\\0,2\O,0,0.0282047059,-0.115285422,-0.09465078
 99\C,0,0.0341840566,-0.0158818497,1.1184053093\N,0,1.2097727394,0.0339
 011276,1.8840053605\N,0,1.2340553281,0.1850049261,3.2418620169\C,0,0.0
 48203188,0.2620406031,3.84516135\N,0,-1.143869026,0.2099718223,3.25153
 81388\N,0,-1.1338265255,0.0584091974,1.8935521975\C,0,-2.4298307769,0.
 1060734125,1.2734936909\C,0,-2.7271343253,-0.7013505819,0.1760860063\C
 ,0,-4.0075412247,-0.6488514385,-0.3856674812\C,0,-4.9923138599,0.19663
 30979,0.169240541\C,0,-4.6696778266,1.0070263069,1.279757275\C,0,-3.38
 55819849,0.9572960119,1.8299860019\C,0,0.0556756319,0.3989309154,5.327
 44636\C,0,-1.1534535099,0.4743015972,6.025603415\C,0,-1.1542485945,0.6
 055537273,7.4180091668\C,0,0.0697690933,0.6598762735,8.1198555002\C,0,
 1.2866297692,0.5802930479,7.4080520535\C,0,1.2717575348,0.4492071069,6
 .0157040126\C,0,2.501389754,0.0545208574,1.2533969821\C,0,3.4792162582
 ,0.8855578587,1.8019937329\C,0,4.7595346629,0.9085084079,1.2413020042\
 C,0,5.0561092081,0.0916381292,0.1282705941\C,0,4.0494072474,-0.7330613
 711,-0.418504681\C,0,2.7728041052,-0.7588496906,0.1536758186\S,0,-6.62
 71232111,0.2791084541,-0.5617215003\S,0,6.6862605348,0.140041174,-0.61
 6033722\H,0,-3.1062504279,1.5593719515,2.6814660276\S,0,-5.9491868546,
 2.0722232786,1.9255112552\C,0,-5.1408147936,2.8423316662,3.3693073\H,0
 ,-5.9055064081,3.4834902871,3.8128002351\H,0,-4.8322103338,2.098626375
 7,4.1080419798\H,0,-4.2897339292,3.4627763604,3.0794249038\C,0,-7.4891
 455773,-1.0407079487,0.3822540247\H,0,-7.5136681529,-0.7975797553,1.44
 56970601\H,0,-8.510036824,-1.0742661012,-0.0049805729\H,0,-7.008246138
 8,-2.0060160205,0.2163973514\S,0,-4.4649706139,-1.6364660507,-1.800664
 5879\H,0,-1.9640660583,-1.3427671169,-0.23190469\H,0,2.1876515405,0.38
 1412344,5.4471690179\C,0,-2.9382690651,-2.576204754,-2.1471581968\H,0,
 -2.1037004468,-1.9153001577,-2.3916871807\H,0,-2.6683405766,-3.2393203
```

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9242997\H,0,5.0215800534,0.3042804772,7.6353902463\H,0,3.9305359804,-0
.6281766788,6.5867818037\H,0,4.1268229066,1.1369261066,6.3483957757\S,
0,0.0792919426,0.8788192227,9.8998544905\C,0,0.0636384143,-0.870203847
5,10.4616920193\H,0,0.0686461157,-0.8387241185,11.5535863105\H,0,-0.84
14781448,-1.3737119037,10.1185292538\H,0,0.9551868454,-1.3922614894,10
.1108238073\S,0,-2.6600067656,0.7018927474,8.3748782276\H,0,-2.0751590
978,0.4255118041,5.4645627751\H,0,1.9932053974,-1.38416112,-0.24801468
83\C,0,-3.9529310866,0.4153033619,7.1186648149\H,0,-3.9908360325,1.221
1065019,6.3815372498\H,0,-3.8292624298,-0.5477204422,6.6183531074\H,0,
-4.8921384593,0.4070108377,7.6758104419\S,0,4.4745492048,-1.7298931141
,-1.8371082576\C,0,2.925744853,-2.6374273299,-2.1711405915\H,0,2.64874
77024,-3.2948979875,-1.3435722751\H,0,2.1032150372,-1.9591687025,-2.40
88467854\H,0,3.1429793178,-3.2497408205,-3.048929553\C,0,7.5282979477,
-1.1973609942,0.3212018714\H,0,7.0260678353,-2.1524606859,0.1595133211
\H,0,8.5450784576,-1.2522040072,-0.0743274305\H,0,7.5665482906,-0.9547
109069,1.3843494595\S,0,6.0662234341,1.9467359545,1.8764617715\H,0,3.2
194669676,1.4932908733,2.6556526095\C,0,5.2858610184,2.7335650972,3.32
66366595\H,0,6.0673163762,3.3587287796,3.763699623\H,0,4.4455071774,3.
3715369396,3.0435830274\H,0,4.9679407495,1.9964770963,4.0680467273\\Ve
rsion=EM64L-G09RevA.02\State=2-A\HF=-5002.8811391\S2=0.773538\S2-1=0.\
S2A=0.750252\RMSD=8.579e-09\PG=C01 [X(C29H33N4O1S9)]\\

**1[1]b**

1\1\GINC-OCTOPUS\FOpt\UB3LYP\6-31G(d,p)\C29H33N4O10(2)\PIOTR\16-Nov-20
11\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck freq=n
oraman\\1,3,5-(3,4,5-MeOphenyl)-6-oxoverdazyl, C1\\0,2\O,-0.0621290594
,-0.5197023953,0.0730087124\C,-0.024801063,-0.2280759499,1.2564537525\
N,1.1666267504,-0.1400466245,1.9913766149\N,1.2256409684,0.2086402802,
3.3129166548\C,0.0568983977,0.4234807479,3.9155208874\N,-1.1480708619,
0.3515544799,3.3509420331\N,-1.1699541074,0.0515776475,2.016747988\C,-
2.4874435072,-0.0712729003,1.4543303311\C,-2.7474635592,0.3202968131,0
.1388263337\C,-4.0529924142,0.2125388405,-0.3508282226\C,-5.0927302628
,-0.2635614568,0.4669578281\C,-4.8034803184,-0.6544762729,1.7863624197
\C,-3.5021076976,-0.55328083,2.2861700673\C,0.1012886246,0.7796759617,
5.357363623\C,-1.0468675288,1.2791738755,5.9835667064\C,-1.0038580246,
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108702\C,2.447951363,-0.3065343764,1.3604719719\C,3.5040245383,0.48220
01352,1.8260099935\C,4.7746348522,0.3210187438,1.2662880949\C,4.986448
412,-0.6110257577,0.2349136431\C,3.9096319767,-1.3980230882,-0.2092187
257\C,2.6370426581,-1.2558304547,0.3528503832\O,-6.384303573,-0.302071
2307,0.0134842806\O,6.2155742801,-0.6984720803,-0.3625153785\H,-3.2594
615007,-0.833193218,3.3003759832\O,-5.8628106999,-1.1275027158,2.50101
97412\C,-5.6395421623,-1.516552129,3.8467072505\H,-6.6078784584,-1.844
5231107,4.2271903197\H,-4.9237144585,-2.3456033809,3.9180058309\H,-5.2
768127177,-0.6787718051,4.4557839884\C,-6.7019301346,-1.4362707585,-0.
7964157809\H,-6.5635863573,-2.3701473221,-0.2379779904\H,-7.754333513,
-1.3326383048,-1.0685300009\H,-6.0920370419,-1.4566537354,-1.706182194
1\O,-4.4205053524,0.5536451934,-1.6187002579\H,-1.9463442974,0.6799289
666,-0.4853841489\H,2.1587815696,0.2177042726,5.5686411309\C,-3.419650
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282\H,-2.6181848301,0.3184399905,-2.65378394\H,-3.9246051254,1.2448131
679,-3.4433461442\O,2.4302930289,0.8205012331,8.2293951419\C,3.6245649
091,0.3288502347,7.6418910241\H,4.3680223183,0.3180423512,8.4401982064
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407909544,8.0878224526\O,4.2085312688,-2.2866131383,-1.1993899532\C,3.
1514755489,-3.0663240869,-1.7409975456\H,2.7164054755,-3.7376666895,-0
.9897309058\H,2.3584512048,-2.4348712146,-2.1590511675\H,3.5990716253,
-3.6616294075,-2.5379586516\C,7.0270886939,-1.7840536956,0.090877702\H
,6.5505615925,-2.7487091902,-0.1156653992\H,7.9648933466,-1.7176513659
,-0.4645100841\H,7.2364758588,-1.6980937703,1.1642033257\O,5.874223005
,1.0284194143,1.6493332333\H,3.320145299,1.1883349643,2.6216216972\C,5
.7137808375,2.0236798417,2.6477541952\H,6.6993194643,2.4709148746,2.78
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685872,3.6002269771\\Version=EM64L-G09RevA.02\State=2-A\HF=-2096.05321
03\S2=0.772626\S2-1=0.\S2A=0.750245\RMSD=3.626e-09\RMSF=1.600e-06\Dipo
le=0.1055986,-1.1993507,0.2654743\Quadrupole=-2.3578312,2.2960605,0.06
17708,1.4339123,3.98176,-2.9366495\PG=C01 [X(C29H33N4O10)]\\@

**1[1]c**

1\1\GINC-OCTOPUS\FOpt\UB3LYP\6-31G(d,p)\C29H33N4O7S3(2)\PIOTR\20-Aug-2
013\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck\\1-(3
,4,5-MeOphenyl)-3-(3,4,5-MeOphenyl)-5-(3,4,5-MeSphenyl)-6-oxoverdazyl\
\0,2\O,0.0869327903,-0.4800583921,0.1030521906\C,0.109680264,-0.258109
8435,1.3002635168\N,1.292617213,-0.2463984304,2.0553246609\N,1.3513040
236,0.0518044637,3.389888133\C,0.1819020704,0.2695042002,3.9895518379\
N,-1.0185383142,0.2510086391,3.4080052172\N,-1.0362577376,0.0139294847
,2.062652975\C,-2.3507336534,-0.0470862808,1.4821096116\C,-2.583877089
3,0.4044183196,0.1808267318\C,-3.8860388161,0.3528530128,-0.3267464336
\C,-4.9480379348,-0.1268038432,0.4600659061\C,-4.6852095746,-0.5782694
501,1.7658638647\C,-3.3875455621,-0.5339546987,2.283254669\C,0.2168575
013,0.5636243794,5.4447962462\C,-0.9256722284,1.0695006377,6.076692663
7\C,-0.889066301,1.3537413047,7.4441294401\C,0.2853689032,1.1324836297
,8.1868789089\C,1.4218830159,0.6099784822,7.5423430321\C,1.3909786182,
0.3341711692,6.1720649765\C,2.5695114224,-0.4313539734,1.4286763754\C,
3.6493579719,0.3027148504,1.9224989739\C,4.9238282374,0.1405834325,1.3
718779116\C,5.1233946584,-0.7770661184,0.3128598091\C,4.0251740986,-1.
5300940509,-0.1542475613\C,2.7515177191,-1.3531316136,0.3954440871\O,-
6.2343520203,-0.1115406476,-0.0074159275\H,-3.1653738294,-0.8626164394
,3.2873643976\O,-5.7651586005,-1.0493920861,2.449560268\C,-5.566355298
3,-1.5085441437,3.7770287901\H,-6.5474432421,-1.8255233747,4.133239469
1\H,-4.8755489673,-2.3606794175,3.8140247541\H,-5.1854136691,-0.711666
0972,4.4284441685\C,-6.5710633728,-1.1950243476,-0.8778348868\H,-6.465
4098962,-2.1588090685,-0.365079459\H,-7.6164602285,-1.0486822751,-1.15
68664456\H,-5.949465479,-1.1862812275,-1.7795427159\O,-4.229307401,0.7
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.2536513255,-0.0679604771,5.6599301268\C,-3.203359981,1.2508741832,-2.
4327153003\H,-2.7410359784,2.1563271261,-2.0206202524\H,-2.4253555811,
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548328\H,-0.0995241333,0.9375365258,11.4123736201\H,-1.3237897296,0.44
08570444,10.2124691129\H,0.229398842,-0.4457701532,10.3345594242\O,-1.
9403582424,1.8546512608,8.1558845932\H,-1.8168324436,1.2397799216,5.48
93338006\H,1.9231195353,-1.9318467232,0.0162509632\C,-3.1381806697,2.1

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5820740075,1.2592006282,7.0046311192\H,-3.8251189427,2.5611200241,8.20
02430076\H,3.4682285555,0.9892360929,2.7359792876\S,6.3329523246,1.079
8729086,1.9446999759\S,6.7748908292,-0.9751999249,-0.3625787401\S,4.14
73713378,-2.6951304876,-1.5214969532\C,5.5968126412,2.1785408243,3.204
7991276\H,4.8343067963,2.8357387085,2.7802796312\H,5.1839121743,1.6182
85176,4.0471078035\H,6.4272494594,2.7899629185,3.5643086355\C,6.651959
456,0.055011804,-1.8756421204\H,5.9041953447,-0.3582405972,-2.55400315
64\H,6.4151798349,1.0881114495,-1.6159739651\H,7.6355356562,0.01787424
74,-2.3496889346\C,5.0546467214,-4.0895304065,-0.7510444298\H,6.061059
7915,-3.7832228558,-0.4636797926\H,4.5068246961,-4.4768436565,0.110056
6321\H,5.1147819183,-4.8665885398,-1.5168347278\\Version=EM64L-G09RevC
.01\State=2-A\HF=-3064.9933458\S2=0.772959\S2-1=0.\S2A=0.750248\RMSD=5
.875e-09\RMSF=1.887e-06\Dipole=-0.3057323,-0.3859247,0.3450768\Quadrup
ole=-3.9192783,2.4127344,1.5065439,6.5083461,-4.8723851,-9.2870465

**1[1]d**

1\1\GINC-OCTOPUS\FOpt\UB3LYP\6-31G(d,p)\C29H33N4O7S3(2)\PIOTR\18-Aug-2
013\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck\\1-(3
,4,5-MeOphenyl)-3-(3,4,5-MeSphenyl)-5-(3,4,5-MeOphenyl)-6-oxoverdazyl\
\0,2\O,-0.0948893496,-0.494777948,0.1446276066\C,-0.0613065851,-0.1758
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442\N,-1.1941383411,0.4809235444,3.3864331229\N,-1.2092919839,0.145948
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379\C,-5.1177867578,-0.1146386781,0.4681410645\C,-4.8517580175,-0.4990
477659,1.794467785\C,-3.5545330597,-0.4168846307,2.3089469264\C,0.0467
909334,0.9330684534,5.3919214787\C,-1.1090054432,1.4066471299,6.019426
3949\C,-1.0898455081,1.7828346131,7.3668173281\C,0.1118326413,1.679053
2758,8.1085973648\C,1.2715065019,1.1863420909,7.4714894053\C,1.2344140
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,-1.4812652885,-0.0707075818\C,2.5836577577,-1.2861167935,0.4683165323
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2.4193797606,8.202308283\S,0.0991439125,2.1302575349,9.8469852265\S,2.

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064218\H,-4.6647420814,2.9248779542,7.3224114343\H,-3.4493407813,3.161
6474886,6.0482851232\H,-4.0149027967,1.5137046451,6.4632413192\C,0.824
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56,9.1526015644\C,2.6318073319,-0.3933771308,9.3725524995\H,1.86143175
95,-0.2011186913,10.1202658947\H,2.381156943,-1.2724207341,8.775847953
2\H,3.5899676878,-0.5587263266,9.8709669016\\Version=EM64L-G09RevC.01\
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-09\RMSF=2.956e-06\Dipole=-0.1674502,-0.5739845,-0.0790236\Quadrupole=
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(C29H33N4O7S3)]

**1[1]e**

1\1\GINC-OCTOPUS\FOpt\UB3LYP\6-31G(d,p)\C29H33N4O4S6(2)\PIOTR\18-Aug-2
013\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck\\1-(3
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86\N,-1.0386887345,0.4255402934,3.4492133148\N,-1.050818404,0.15085560
28,2.1118274982\C,-2.3618443369,0.0934573876,1.5223980527\C,-2.5809133
973,0.5245959117,0.2120231857\C,-3.880449969,0.477470791,-0.3035578702
\C,-4.9527670837,0.0260856744,0.4859500449\C,-4.7035265779,-0.40726695
05,1.8005706825\C,-3.4086257647,-0.3691264288,2.3251556136\C,0.1895379
071,0.770666902,5.4847018145\C,-0.9653022117,1.2362894029,6.1199282571
\C,-0.9529316411,1.5600155803,7.4810421292\C,0.2411700381,1.4127966785
,8.2277749558\C,1.4004972546,0.9314808871,7.581656857\C,1.3694790141,0
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6612611792,0.272616286,2.0465093157\C,4.9369527682,0.0477267043,1.5208
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.4630053693\C,-6.5949505994,-1.0730175493,-0.8009229279\H,-6.525715360
8,-2.0067197784,-0.2299037504\H,-7.6316651666,-0.9116896142,-1.1028953
752\H,-5.9627159716,-1.1378213144,-1.6932090717\O,-4.2107310258,0.8582
45178,-1.5688554523\H,-1.7560205769,0.8675543912,-0.3899348285\H,2.262
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73334\H,-2.7008493306,2.2275724958,-2.0320068584\H,-2.4042046273,0.551
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8623302639,1.3453515901,5.5270730041\H,1.8635323191,-1.8653322494,0.09
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7,4.2465847221\H,6.5462121971,2.5319910842,3.8283522619\C,6.7021174367
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072,-3.903225126,-0.3377858342\H,4.3307422023,-4.5352296983,0.20865788
65\H,4.9430529865,-4.9344807848,-1.4144213508\S,-2.399092793,2.1816806
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31,0.7724912564,8.413963128\C,-3.6207713693,2.3317524276,6.9793442596\
H,-4.5126916428,2.7480486137,7.4525007794\H,-3.2843040013,3.0159943979
,6.1971674523\H,-3.8745963801,1.3611697822,6.5463053791\C,0.9514372758

,3.4751299214,9.9823348685\H,0.9453057197,3.8087971349,11.0225676586\H
,1.9786601657,3.4405025063,9.6165473735\H,0.3451256062,4.1555127786,9.
3821312943\C,2.7334863411,-0.7334870844,9.4277540725\H,1.9589490624,-0
.5648486532,10.1768768858\H,2.4807081882,-1.5857154407,8.7942545889\H,
3.6865061751,-0.9264989773,9.9259784522\\Version=EM64L-G09RevC.01\Stat
e=2-A\HF=-4033.9333935\S2=0.772905\S2-1=0.\S2A=0.750255\RMSD=3.039e-09
\RMSF=2.746e-06\Dipole=-0.4347406,0.0720259,-0.0435535\Quadrupole=-8.0
10213,8.8706763,-0.8604633,8.1241289,0.3454511,-2.0617092\PG=C01 [X(C2
9H33N4O4S6)]\\

**1[1]f**

1\1\GINC-OCTOPUS\FOpt\UB3LYP\6-31G(d,p)\C29H33N4O4S6(2)\PIOTR\19-Aug-2
013\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck\\1-(3
,4,5-MeSphenyl)-3-(3,4,5-MeOphenyl)-5-(3,4,5-MeSphenyl)-6-oxoverdazyl\
\0,2\O,0.0673654934,-0.3638337654,-0.0256197189\C,0.0748876462,-0.1662
118346,1.1761099746\N,1.244405981,-0.179788957,1.9497896316\N,1.284153
4958,0.0880143682,3.2897010379\C,0.1068072763,0.3010050621,3.879805459
6\N,-1.0836186732,0.305879066,3.2790097851\N,-1.0797420142,0.100269980
7,1.9273203926\C,-2.3832055393,0.063368103,1.3264265249\C,-2.595957201
3,0.5274913446,0.0279676133\C,-3.8808049475,0.487791145,-0.5264145196\
C,-4.9697423109,0.0000340843,0.2343882187\C,-4.7384328838,-0.434207990
4,1.5573115736\C,-3.449513622,-0.4094890598,2.0948404652\C,0.123973872
4,0.5548185299,5.3422854172\C,-1.0381221331,1.0028411647,5.9820359807\
C,-1.0188671456,1.2436039549,7.3581860186\C,0.159070661,1.0396221845,8
.1008754161\C,1.3157495431,0.5753056484,7.447700035\C,1.3012400276,0.3
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,0.7361970327,11.3162992606\H,-1.4361840445,0.2303965736,10.0924328335
\H,0.146638858,-0.6039091657,10.2035618474\O,-2.0901484467,1.683542854
3,8.0788152672\H,-1.9322996544,1.1606543556,5.3960830603\H,1.891490619
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2\H,-3.1790571676,2.7146895628,6.624058707\H,-3.6965523432,1.028180744
9,6.9108137948\H,-4.0113741586,2.2819601965,8.1412292182\H,3.416743831
9,1.0498282708,2.6574811425\S,6.2913966307,1.1287787595,1.8981258567\S
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,-1.5958179475\C,5.5442692396,2.2332445706,3.1465505454\H,4.7914362473
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,-1.0379113361\H,-5.9428969906,-1.9913087785,-1.7515524471\H,-6.693184
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4O4S6)]\\.

**7**

1\1\GINC-OCTOPUS\FOpt\UB3LYP\6-31G(2d,p)\C20H15N4O1(2)\PIOTR\24-Sep-20
13\0\\#P UB3LYP/6-31G(2d,p) FOpt freq(noraman, ReadIso) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Diphenyl Ph oxoverdazyl, C2 symm\\0,
2\O,-0.0000001195,0.0000000097,0.\C,-0.0000001237,0.0000000026,1.21229
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,-0.0000000135,3.945118\N,-1.1861712621,0.0277789801,3.3439289921\N,-1
.1689042527,-0.0000000039,1.9818749919\C,-2.460316,0.080132,1.363616\C
,-2.750996,-0.609957,0.183738\C,-4.030179,-0.523959,-0.358266\C,-5.018
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6,0.1744949473,6.1386050103\C,2.4603157516,-0.0801319966,1.3636160161\
C,3.4471297472,-0.841553004,1.9955600139\C,4.720681751,-0.9168199975,1
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7.2363581,-0.6478339,-1.7822696,0.,0.\PG=C02 [C2(H1C1C1C1C1O1),X(C16H1
4N4)]\\@

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1 A. Jankowiak, P. Kaszynski *Beils. J. Org. Chem.* 2012, **8**, 275.

2 A. Nowak-Król, D. Gryko, D. T. Gryko *Chem. Asian J.* 2010, **5**, 904.

3 A. Jankowiak, D. Pociecha, H. Monobe, J. Szczytko, P. Kaszyński *Chem. Commun.* 2012, **48**, 7064

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