Supporting Information

Schiff base ligands derived from 1,2-*bis*(2'-nitro-/amino-phenoxy)-3-R-benzene and 2-hydroxy-1-naphthaldehyde and their Cu/Zn(II) complexes: Synthesis, characterization, X-ray structures and computational studies†

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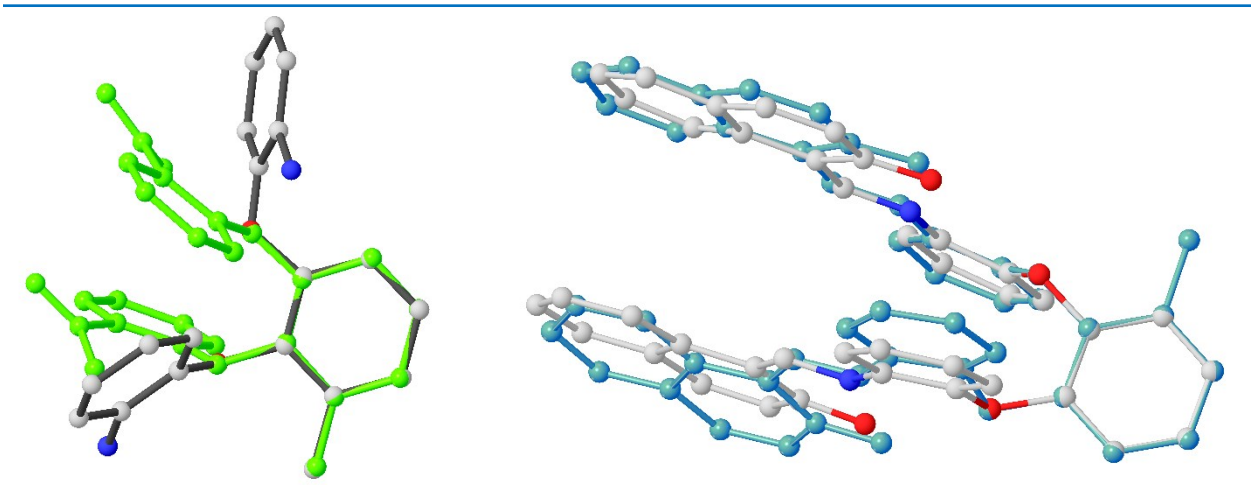


Fig. S1 (a) Left: a view of the structural overlap of compounds **2** (in green) and **5** (in black); (b) Right: a view of the structural overlap of compounds $\mathbf{H_2L^1}$ (grey green) and $\mathbf{H_2L^2}$ (in blue).

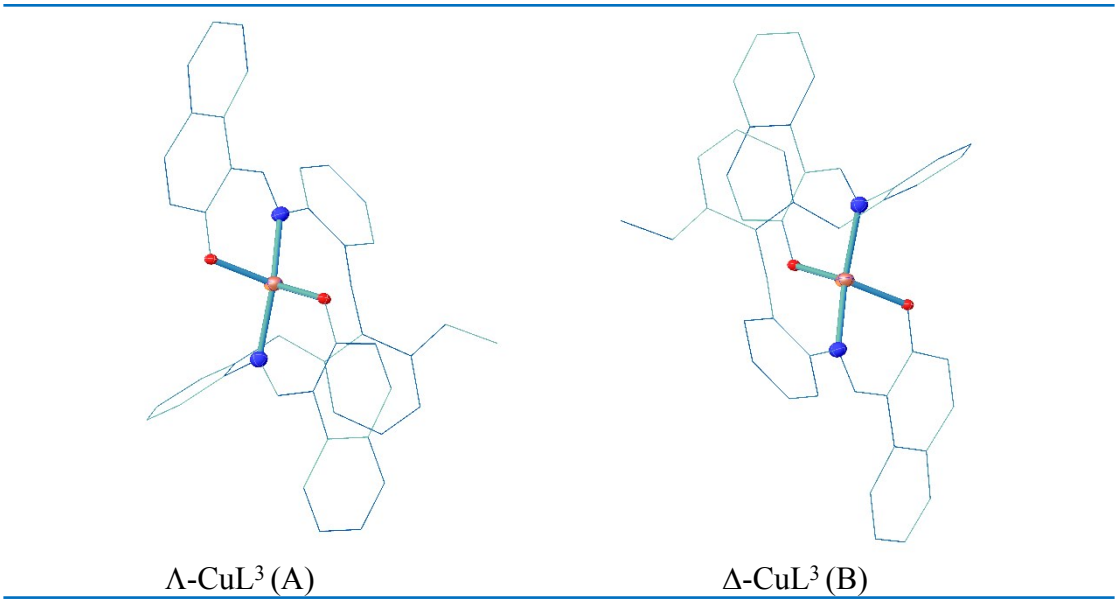


Fig. S2 View of opposite configured Λ-Cu (A) and Δ-Cu (B) in **CuL^3**.

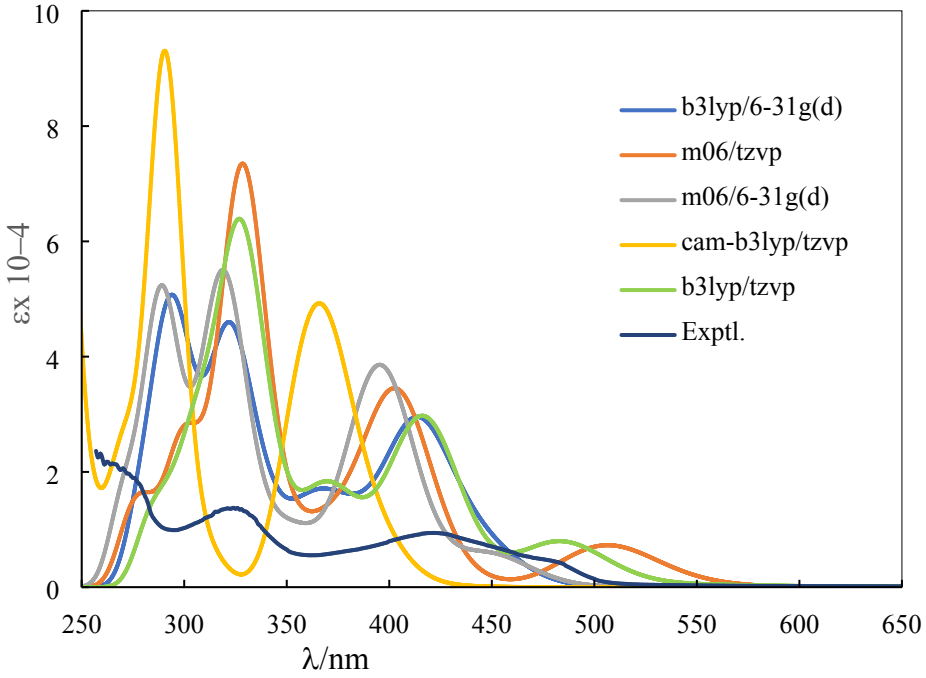


Fig. S3 Computed UV-Vis. spectra for CuL^3 at different combinations of the functionals and basis sets using PCM in chloroform (Gaussian band shape with exponential half-width, σ = 0.16 eV). Experimental spectrum for CuL^3 (0.12 mM) in chloroform at 25 ^{o}C.

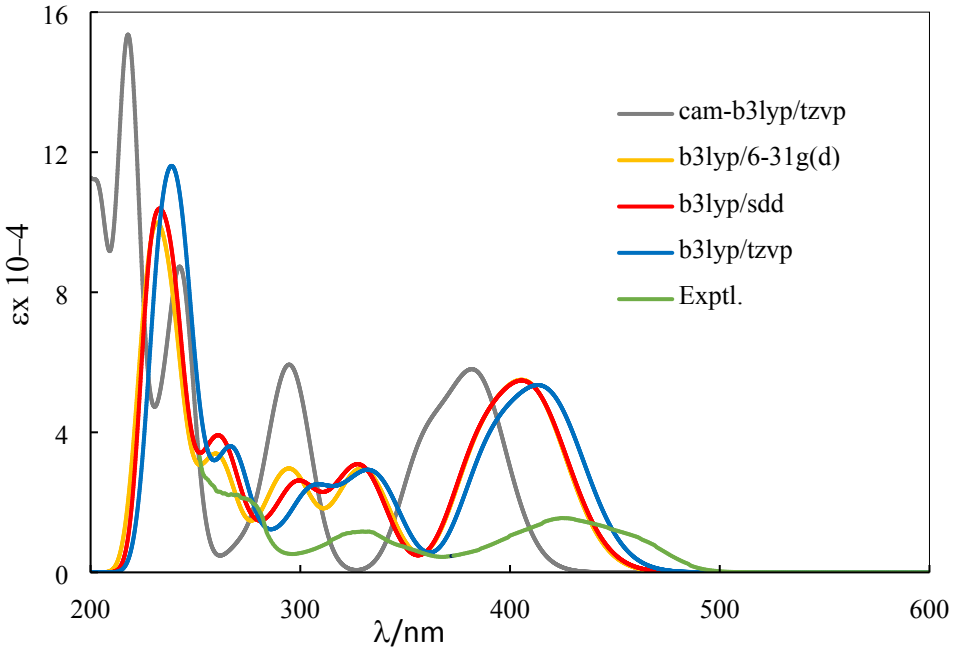
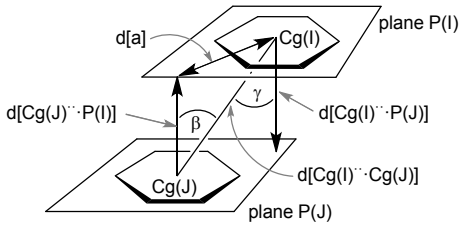


Fig. S4 Computed UV-Vis. spectra for ZnL^3 at different combinations of the functionals and basis sets using PCM in chloroform (Gaussian band shape with exponential half-width, σ = 0.16 eV). Experimental spectrum for ZnL^3 (0.11 mM) in chloroform at 25 °C.

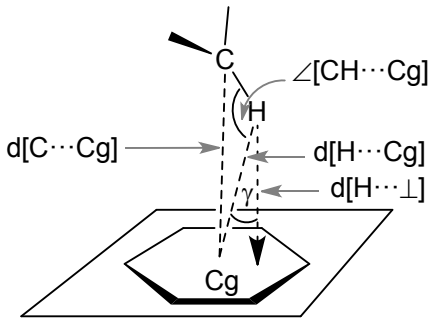
Crystal packing analyses:

Significant π-stacking involves rather short centroid-centroid contacts (<3.8 Å), near parallel ring planes (alpha < 10° to ~0° or even exactly 0° by symmetry), small slip angles (β, γ <25°) and vertical displacements (slippage <1.5 Å) which translate into a sizable overlap of the aryl-plane areas (Scheme S1).[1]



Scheme S1 Graphical presentation of the parameters used for the description of π–π stacking.[2]

Significant intermolecular C-H···π contacts start below around 2.7 Å for the (C-)H···ring centroid distances with H-perp also starting at below 2.6-2.7 Å and C-H··Cg > 145° (Scheme S2).[3]



Scheme S2 Graphical presentation of the parameters used for the description of CH-π interactions.

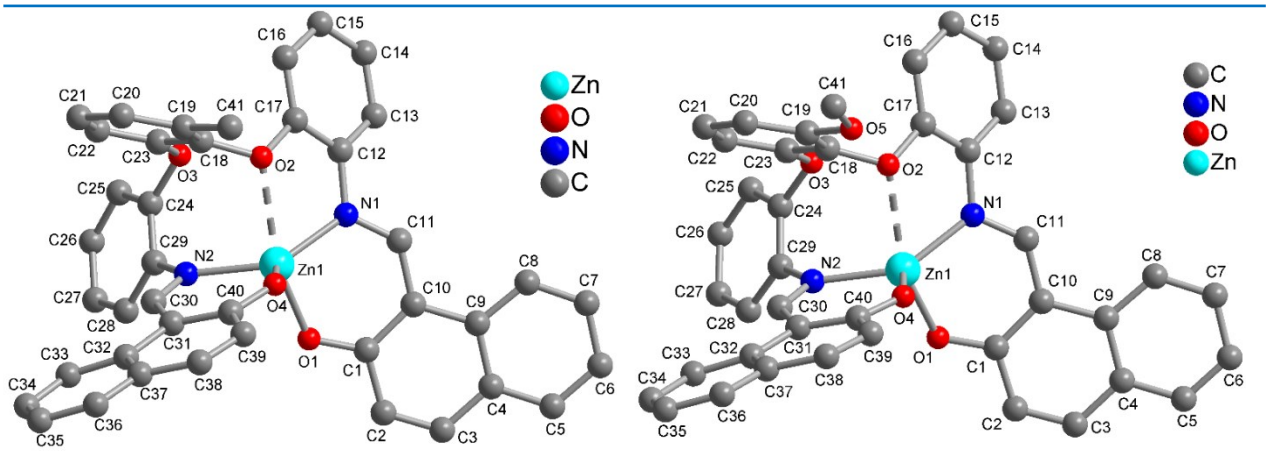


Fig. S5 X-ray molecular structures of **ZnL²** (left) and **ZnL³** (right) with atoms numbering. Grey dashed lines indicate weak bond between etheric oxygen and zinc atoms. Hydrogen atoms are omitted for clarity.

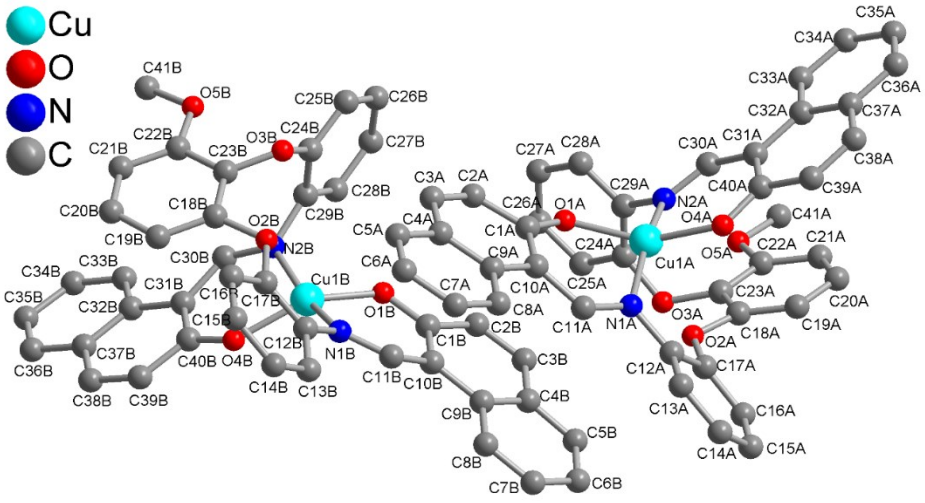


Fig. S6 (a) X-ray molecular structure of **CuL³** (A: right and B: left) with atoms numbering. Grey dashed lines indicate weak bond between etheric oxygen and copper atoms. There are two symmetry independent molecules in the asymmetric unit which happen to have the identical Λ-configuration at-metal (Λ-Cu) (note

that the asymmetric unit could have also been chosen with both Δ-Cu or one Λ and one Δ molecule as A and B). Hydrogen atoms are omitted for clarity.

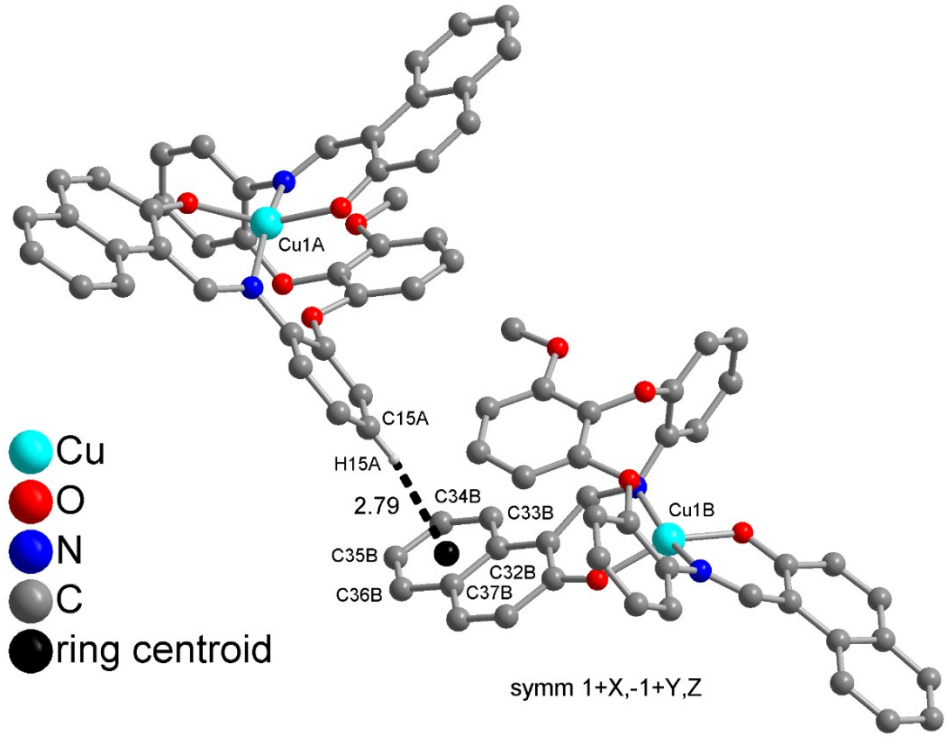


Fig. S7 Shortest intermolecular C-H···π interaction in the packing of **CuL^3**, indicated as dashed black line with the (C-)H-centroid contact [in Å] given. Further details of this C-H···π interaction are listed in Table S3.

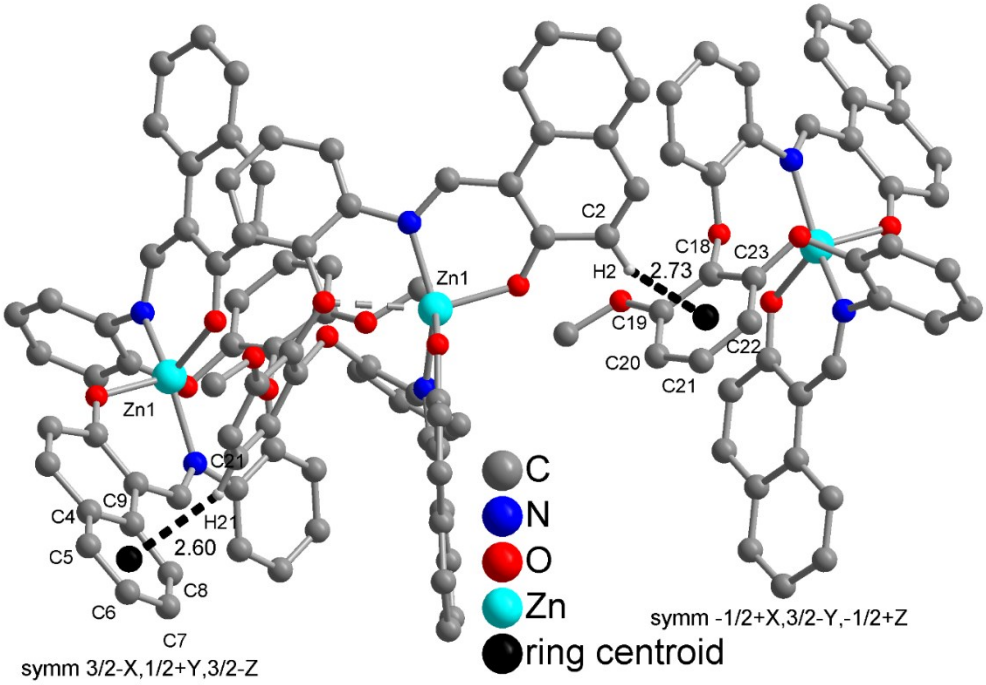


Fig. S8 Two shortest intermolecular C-H···π interactions in the packing of **ZnL^3**, indicated as dashed black lines with the (C-)H-centroid contacts [in Å] given. Both C-H···π interactions involve the methoxyaryl ring, MeC_6H_3- either as donor or as acceptor. Further details of these C-H···π interactions are listed in Table S4.

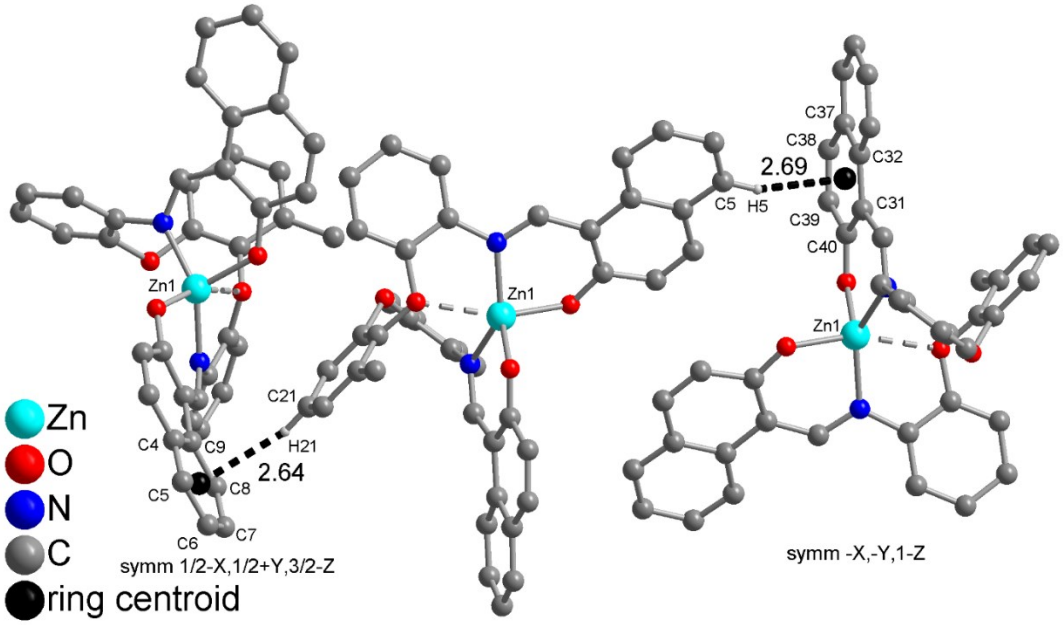


Fig. S9 Two shortest intermolecular C-H···π interactions in the packing of **ZnL^2**, indicated as dashed black lines with the (C-)H-centroid contacts [in Å] given. In addition, there is also a C-H···π interaction which involves the methylaryl ring, MeC_6H_3- as acceptor as in **ZnL^3**. Further details of these C-H···π interactions are listed in Table S5.

Table S1. Packing analysis of **CuL^3** for possible intermolecular π–π interactions (see Scheme S1 for explanation).

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Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.000 Deg. and Beta < 60.0 Deg.

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- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg4	[1] ->	Cg14	[1555.02]	3.8294(18)	4.44(14)	26.0	26.1	3.4377(12)	3.4416(13)	1.679
Cg9	[1] ->	Cg19	[1545.02]	3.6725(17)	4.87(14)	17.2	19.4	3.4639(12)	3.5079(13)	1.087
Cg14	[2] ->	Cg4	[1555.01]	3.8294(18)	4.44(14)	26.1	26.0	3.4416(13)	3.4377(12)	1.687
Cg19	[2] ->	Cg9	[1565.01]	3.6724(17)	4.87(14)	19.4	17.2	3.5078(13)	3.4638(12)	1.220

[1555] = X,Y,Z
[1545] = X,-1+Y,Z
[1554] = X,Y,-1+Z
[1565] = X,1+Y,Z

Cg(I) refers to the Ring Centre-of-Gravity in
Cg4 = Ring C1A-C2A-C3A-C4A-C9A-C10A
Cg9 = Ring C31A-C32A-C37A-C38A-C39A-C40A
Cg14 = Ring C1B-C2B-C3B-C4B-C9B-C10B
Cg19 = Ring C31B-C32B-C37B-C38B-C39B-C40B

Table S2. Packing analysis of **ZnL^3** for possible intramolecular $\pi-\pi$ interactions (see Scheme S1 for explanation).

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.000 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg3	[1] ->	Cg7	[1555.01]	3.9550(9)	36.57(7)	20.1	36.0	3.1979(5)	3.7151(7)	
Cg7	[1] ->	Cg3	[1555.01]	3.9549(9)	36.57(7)	36.0	20.1	3.7151(7)	3.1978(5)	

[1555] = X,Y,Z

Cg(I) refers to the Ring Centre-of-Gravity in
Cg3 = Zn1-O4-N2-C30-C31-C40
Cg7 = C18-C19-C20-C21-C22-C23

Table S3 Analysis of *inter*molecular C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) in **CuL^3** (see Scheme S2 for explanation).

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- C-H..Cg = C-H-Cg angle (degrees)
- C..Cg = Distance of X to Cg (Angstrom)
- C-H, Pi = Angle of the X-H bond with the Pi-plane (i.e.' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Res(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	C..Cg	X-H,Pi
C13A -H13A	[1] ->	Cg5	[2765.01]	2.89	-2.81	13.44	121	3.479(3)	20
C15A -H15A	[1] ->	Cg20	[1645.02]	2.79	-2.78	4.55	152	3.654(3)	57
C41A -H41B	[1] ->	Cg15	[2766.02]	2.93	2.82	15.99	132	3.665(4)	33

[2765] = 2-X,1-Y,-Z
[1645] = 1+X,-1+Y,Z
[2766] = 2-X,1-Y,1-Z

Cg(I) refers to the Ring Centre-of-Gravity in
Cg5 = Ring C4A-C5A-C6A-C7A-C8A-C9A
Cg15 = Ring C4B-C5B-C6B-C7B-C8B-C9B
Cg20 = Ring C32B-C33B-C34B-C35B-C36B-C37B

Table S4. Analysis of *inter*molecular C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) in **ZnL^3** (see Scheme S2 for explanation).

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal

- C-H..Cg = C-H-Cg angle (degrees)
- C..Cg = Distance of X to Cg (Angstrom)
- C-H, Pi = Angle of the X-H bond with the Pi-plane (i.e.' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Res(I)	Cg(J) [ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	C..Cg	X-H,Pi
C2 -H2	[1] ->	Cg7 [4464.01]	2.73	2.61	16.76	149	3.5750(18)	74
C5 -H5	[1] ->	Cg9 [3666.01]	2.97	-2.70	24.52	145	3.7852(19)	79
C21 -H21	[1] ->	Cg5 [2656.01]	2.60	-2.57	8.47	153	3.4727(19)	68
C21 -H21	[1] ->	Cg11 [2656.01]	2.89	2.55	28.07	130	3.5754(19)	67

[4464] = -1/2+X,3/2-Y,-1/2+Z
[3666] = 1-X,1-Y,1-Z
[2656] = 3/2-X,1/2+Y,3/2-Z

Cg(I) refers to the Ring Centre-of-Gravity in
Cg5 = Ring C4-C5-C6-C7-C8-C9
Cg7 = Ring C18-C19-C20-C21-C22-C23
Cg9 = Ring C31-C32-C37-C38-C39-C40
Cg11 = Ring C1-C2-C3-C4-C5-C6-C7-C8-C9-C10

Table S5 Analysis of *inter*molecular C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) in **ZnL^2** (see Scheme S2 for explanation).

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- C-H..Cg = C-H-Cg angle (degrees)
- C..Cg = Distance of X to Cg (Angstrom)
- C-H, Pi = Angle of the X-H bond with the Pi-plane (i.e.' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Res(I)	Cg(J) [ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	C..Cg	X-H,Pi
C2 -H2	[1] ->	Cg7 [4454.01]	2.75	2.65	15.04	145	3.571(2)	69
C5 -H5	[1] ->	Cg9 [3556.01]	2.69	-2.63	11.65	155	3.573(3)	73
C21 -H21	[1] ->	Cg5 [2556.01]	2.64	2.61	9.45	162	3.557(3)	69
C35 -H35	[1] ->	Cg8 [4455.01]	2.77	-2.69	13.39	164	3.691(3)	61

[4454] = -1/2+X,1/2-Y,-1/2+Z
[3556] = -X,-Y,1-Z
[2556] = 1/2-X,1/2+Y,3/2-Z
[4455] = -1/2+X,1/2-Y,1/2+Z

Cg5 = centroid of ring C4-C5-C6-C7-C8-C9
Cg7 = centroid of ring C18-C19-C20-C21-C22-C23
Cg8 = centroid of ring C24-C25-C26-C27-C28-C29
Cg9 = centroid of ring C31-C32-C37-C38-C39-C40

Table S6 List of excited states with excitation energy (eV), Wavelength (nm) and Osilator Strenth (*f*) for **CuL^3** at m06/6-31g(d)//b3lyp/6-31g(d) with PCM using chloroform as solvent.

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Excitation energies and oscillator strengths:

 Excited State   1:  2.005-A      1.1956 eV 1036.98 nm  f=0.0003
<S**2>=0.755
    157B ->179B       -0.23999
    158B ->179B       -0.37816
    164B ->179B        0.30920
    168B ->179B       -0.15832
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    169B ->179B        0.41956
    171B ->179B        0.12663
    173B ->179B       -0.14132
    178B ->179B        0.56322
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3703.69931592
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:  2.003-A      1.5360 eV  807.16 nm  f=0.0005
<S**2>=0.753
    147B ->179B        0.21467
    152B ->179B        0.15225
    153B ->179B        0.11566
    154B ->179B        0.18062
    157B ->179B        0.10773
    158B ->179B       -0.11812
    159B ->179B       -0.15513
    160B ->179B       -0.25491
    161B ->179B       -0.20256
    162B ->179B       -0.11455
    163B ->179B       -0.21545
    165B ->179B       -0.25310
    166B ->179B        0.47434
    167B ->179B        0.43627
    170B ->179B        0.10816
    174B ->179B       -0.13098
    177B ->179B       -0.18726

 Excited State   3:  2.002-A      1.6994 eV  729.58 nm  f=0.0002
<S**2>=0.752
    149B ->179B        0.10118
    152B ->179B        0.12993
    160B ->179B       -0.51243
    161B ->179B        0.26563
    162B ->179B        0.19465
    163B ->179B        0.62778
    163B ->181B        0.10664
    164B ->179B        0.13201
    174B ->179B        0.15470

 Excited State   4:  2.002-A      1.7645 eV  702.68 nm  f=0.0006
<S**2>=0.752
    139B ->179B       -0.10567
    149B ->179B        0.21355
    152B ->179B       -0.16626
    153B ->179B        0.13232
    156B ->179B        0.19277
    161B ->179B       -0.27171
    162B ->179B        0.47131
    163B ->179B       -0.15390
    164B ->179B        0.57753
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    166B ->179B        0.13256
    167B ->179B       -0.10015
    169B ->179B       -0.17290
    173B ->179B       -0.16454

 Excited State   5:  3.441-A      2.3178 eV  534.92 nm  f=0.0003
<S**2>=2.710
    177A ->180A       -0.11509
    178A ->180A        0.28604
    179A ->180A        0.60307
    177B ->180B       -0.31787
    178B ->179B       -0.15914
    178B ->180B       -0.57436

 Excited State   6:  3.425-A      2.3904 eV  518.67 nm  f=0.0001
<S**2>=2.683
    178A ->181A        0.54377
    179A ->181A       -0.39692
    177B ->179B        0.16094
    177B ->181B       -0.45904
    178B ->179B       -0.11591
    178B ->181B        0.45808

 Excited State   7:  2.205-A      2.7275 eV  454.58 nm  f=0.0089
<S**2>=0.966
    174A ->180A        0.11874
    158B ->179B        0.11115
    165B ->179B       -0.12863
    169B ->179B       -0.17461
    171B ->179B       -0.11402
    174B ->180B       -0.12403
    177B ->179B        0.71892
    177B ->180B       -0.11444
    178B ->179B        0.45350
    178B ->180B       -0.14734

 Excited State   8:  2.430-A      2.7540 eV  450.20 nm  f=0.0403
<S**2>=1.227
    173A ->181A       -0.22264
    173A ->183A        0.10840
    175A ->181A       -0.11003
    157B ->179B        0.11108
    158B ->179B        0.20984
    164B ->179B       -0.10437
    168B ->179B        0.10631
    169B ->179B       -0.22829
    171B ->179B       -0.11783
    172B ->179B        0.13823
    173B ->181B        0.24298
    177B ->179B       -0.47601
    178B ->179B        0.55959
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 Excited State   9:  3.384-A      2.8183 eV  439.92 nm  f=0.0017
<S**2>=2.612
    174A ->180A        0.51719
    174A ->182A       -0.25211
    176A ->180A       -0.13771
    179A ->182A        0.11680
    173B ->180B        0.15600
    174B ->180B       -0.47383
    174B ->182B        0.23659
    175B ->180B        0.10930
    176B ->180B        0.16220
    177B ->179B       -0.15238
    178B ->179B       -0.18613
    178B ->182B       -0.10933

 Excited State  10:  3.222-A      2.8525 eV  434.65 nm  f=0.0087
<S**2>=2.346
    173A ->181A        0.45322
    173A ->183A       -0.20848
    175A ->181A        0.23290
    178A ->183A        0.11210
    179A ->181A       -0.13347
    172B ->181B        0.12332
    173B ->179B        0.15716
    173B ->181B       -0.44855
    173B ->183B        0.19296
    174B ->181B       -0.14494
    177B ->179B       -0.30792
    177B ->183B       -0.10404
    178B ->179B        0.20970
    178B ->181B        0.13335

 Excited State  11:  2.239-A      3.0902 eV  401.21 nm  f=0.2248
<S**2>=1.003
    177A ->180A        0.15113
    178A ->180A        0.35593
    179A ->180A        0.54512
    179A ->182A        0.11134
    176B ->179B       -0.11595
    177B ->180B        0.16714
    178B ->180B        0.59986
    178B ->181B       -0.12037

 Excited State  12:  2.831-A      3.1555 eV  392.91 nm  f=0.0508
<S**2>=1.754
    171A ->180A        0.14983
    172A ->180A        0.15011
    173A ->180A        0.10765
    175A ->180A       -0.15323
    177A ->180A        0.39189
    178A ->180A        0.29034
    178A ->181A        0.11063
```

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    178A ->182A        0.12128
    179A ->180A       -0.37650
    179A ->182A        0.17492
    170B ->180B       -0.12177
    171B ->180B        0.11493
    176B ->179B       -0.23688
    176B ->180B       -0.12570
    177B ->182B       -0.11009
    178B ->180B       -0.29714
    178B ->182B       -0.19733

 Excited State  13:  2.534-A      3.1719 eV  390.88 nm  f=0.0695
<S**2>=1.355
    168A ->181A        0.10589
    175A ->181A       -0.19914
    177A ->180A       -0.10650
    177A ->181A        0.35302
    178A ->180A       -0.11717
    178A ->181A        0.63349
    178A ->183A        0.11466
    177B ->181B        0.19223
    178B ->181B       -0.44146

 Excited State  14:  2.165-A      3.2364 eV  383.09 nm  f=0.0709
<S**2>=0.922
    175A ->181A       -0.14967
    177A ->181A        0.29453
    179A ->181A        0.70732
    178B ->180B        0.13514
    178B ->181B        0.53124

 Excited State  15:  2.531-A      3.2726 eV  378.86 nm  f=0.0150
<S**2>=1.352
    168A ->180A       -0.10110
    170A ->180A        0.14028
    173A ->180A        0.12784
    175A ->180A       -0.19586
    176A ->180A       -0.12444
    177A ->180A        0.15507
    178A ->180A        0.55676
    178A ->181A        0.10291
    179A ->180A       -0.18734
    179A ->182A       -0.13393
    175B ->179B        0.13533
    176B ->179B        0.58276
    178B ->182B        0.12765

 Excited State  16:  2.789-A      3.2983 eV  375.91 nm  f=0.0038
<S**2>=1.694
    170A ->180A       -0.10524
    176A ->180A        0.11455
    178A ->180A       -0.29024
```

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    178A ->181A        0.12201
    179A ->180A        0.11255
    179A ->181A        0.14336
    179A ->182A        0.18431
    176B ->179B        0.63018
    176B ->180B       -0.17494
    176B ->184B        0.11228
    178B ->182B       -0.17253

 Excited State  17:  3.234-A      3.3910 eV  365.63 nm  f=0.0031
<S**2>=2.365
    172A ->181A       -0.10231
    172A ->185A        0.10170
    172A ->190A        0.14730
    173A ->181A       -0.11908
    175A ->181A       -0.14057
    178A ->181A       -0.24383
    178A ->183A        0.22646
    179A ->181A       -0.27412
    179A ->183A       -0.17757
    172B ->181B        0.12699
    172B ->190B       -0.14439
    173B ->181B        0.17824
    175B ->179B        0.15415
    176B ->179B        0.33329
    177B ->181B        0.17965
    177B ->183B       -0.19191
    178B ->181B        0.16626
    178B ->183B        0.20210

 Excited State  18:  3.428-A      3.4138 eV  363.18 nm  f=0.0007
<S**2>=2.688
    174A ->180A       -0.10401
    175A ->184A        0.10418
    175A ->185A       -0.20313
    175A ->186A        0.15204
    175A ->190A        0.10464
    176A ->184A        0.13373
    176A ->185A        0.12213
    176A ->191A        0.20780
    177A ->184A        0.12940
    177A ->185A       -0.15690
    177A ->186A        0.10576
    177A ->190A        0.13518
    178A ->181A        0.10173
    179A ->181A        0.10919
    179A ->182A        0.14285
    172B ->185B        0.12003
    174B ->180B        0.10079
    175B ->179B        0.13967
    175B ->185B       -0.20319
    175B ->186B        0.10125
```

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    175B ->189B       -0.13251
    175B ->191B       -0.18499
    176B ->181B        0.11574
    176B ->184B       -0.19452
    176B ->185B        0.21487
    176B ->186B       -0.13074
    176B ->190B       -0.14105
    177B ->182B       -0.10262
    178B ->182B       -0.13859

 Excited State  19:  3.309-A      3.4801 eV  356.27 nm  f=0.0086
<S**2>=2.488
    173A ->181A        0.13538
    173A ->183A        0.10087
    177A ->181A        0.11548
    177A ->183A        0.11300
    178A ->183A       -0.26921
    179A ->181A       -0.20100
    179A ->182A        0.12708
    179A ->183A        0.17952
    173B ->179B        0.14222
    173B ->181B       -0.12745
    177B ->181B        0.46837
    177B ->183B        0.29587
    178B ->180B        0.12149
    178B ->181B        0.28513
    178B ->182B       -0.13517
    178B ->183B       -0.19242

 Excited State  20:  3.048-A      3.4846 eV  355.81 nm  f=0.0270
<S**2>=2.073
    172A ->185A       -0.10124
    172A ->190A       -0.11249
    175A ->181A       -0.15168
    178A ->181A        0.14417
    179A ->181A       -0.14199
    179A ->182A       -0.10234
    172B ->190B        0.10847
    175B ->179B       -0.13251
    176B ->181B        0.17021
    177B ->180B        0.41452
    177B ->181B        0.50002
    178B ->180B       -0.11792
    178B ->181B        0.33101
    178B ->182B        0.10295

 Excited State  21:  3.238-A      3.4911 eV  355.14 nm  f=0.0243
<S**2>=2.372
    177A ->180A        0.13951
    178A ->180A       -0.12208
    178A ->183A       -0.13562
    179A ->180A        0.17893
```

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    179A ->182A       -0.10252
    179A ->183A        0.11059
    173B ->179B        0.11258
    175B ->179B        0.14143
    177B ->179B        0.11691
    177B ->180B        0.61336
    177B ->181B       -0.19560
    177B ->182B        0.12774
    177B ->183B        0.12948
    178B ->180B       -0.25853
    178B ->183B       -0.13170

 Excited State  22:  3.096-A      3.5360 eV  350.63 nm  f=0.0183
<S**2>=2.146
    169A ->184A       -0.14735
    171A ->182A       -0.11784
    174A ->180A       -0.18015
    176A ->191A       -0.10336
    177A ->182A       -0.11449
    177A ->185A        0.11221
    178A ->180A        0.17787
    179A ->182A        0.20288
    179A ->188A       -0.10295
    179A ->189A        0.13366
    168B ->184B        0.13963
    170B ->182B        0.12205
    171B ->182B       -0.11143
    174B ->180B        0.14954
    175B ->179B        0.16138
    176B ->179B       -0.12340
    176B ->185B       -0.13184
    177B ->180B        0.45030
    177B ->181B       -0.10731
    177B ->182B       -0.12851
    178B ->180B       -0.15575
    178B ->182B       -0.22065
    178B ->189B       -0.13154

 Excited State  23:  2.207-A      3.5591 eV  348.36 nm  f=0.0038
<S**2>=0.968
    177A ->180A        0.12073
    172B ->179B        0.13089
    175B ->179B        0.86729
    176B ->179B       -0.14721
    177B ->180B       -0.13843
    177B ->181B        0.15567

 Excited State  24:  2.427-A      3.6280 eV  341.74 nm  f=0.0156
<S**2>=1.222
    173A ->181A        0.18755
    175A ->180A        0.12100
    175A ->181A       -0.26755
```

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    176A ->181A       -0.15571
    177A ->180A       -0.26250
    177A ->181A        0.49741
    178A ->180A        0.18021
    178A ->181A       -0.25814
    179A ->181A       -0.29404
    172B ->179B       -0.16161
    173B ->179B       -0.22018
    175B ->179B        0.22479
    177B ->181B       -0.25888

 Excited State  25:  2.631-A      3.6341 eV  341.17 nm  f=0.0039
<S**2>=1.480
    169A ->184A       -0.10551
    170A ->180A        0.12786
    173A ->180A        0.11503
    175A ->180A       -0.23907
    175A ->181A       -0.12812
    177A ->180A        0.57130
    177A ->181A        0.27826
    178A ->180A       -0.35984
    178A ->181A       -0.13363
    179A ->180A        0.21594
    179A ->181A       -0.14299
    168B ->184B        0.10720
    174B ->179B       -0.14700
    177B ->180B       -0.18288

 Excited State  26:  2.234-A      3.7082 eV  334.35 nm  f=0.0276
<S**2>=0.998
    175A ->181A       -0.16932
    177A ->181A        0.14119
    178A ->181A       -0.11064
    161B ->179B       -0.11008
    172B ->179B        0.23161
    173B ->179B        0.48105
    174B ->179B        0.67341
    177B ->181B       -0.11113

 Excited State  27:  2.212-A      3.7447 eV  331.09 nm  f=0.0250
<S**2>=0.974
    175A ->180A        0.14087
    175A ->181A       -0.10208
    176A ->180A        0.13339
    178A ->180A        0.11425
    158B ->179B       -0.11083
    162B ->179B        0.10797
    164B ->179B        0.13842
    169B ->179B        0.12189
    172B ->179B        0.23592
    173B ->179B        0.59723
    174B ->179B       -0.58190
```

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    175B ->179B       -0.10662

 Excited State  28:  3.196-A      3.8100 eV  325.42 nm  f=0.0348
<S**2>=2.303
    169A ->184A        0.14330
    173A ->180A        0.11217
    174A ->180A       -0.32913
    175A ->180A       -0.20698
    176A ->180A       -0.20454
    176A ->184A       -0.10253
    178A ->180A       -0.12737
    168B ->184B       -0.13219
    174B ->179B       -0.21372
    175B ->180B        0.24278
    176B ->180B        0.61531

 Excited State  29:  2.401-A      3.8330 eV  323.47 nm  f=0.0747
<S**2>=1.191
    174A ->180A        0.20318
    175A ->180A       -0.12654
    175A ->181A        0.17164
    176A ->180A       -0.15627
    177A ->180A       -0.10619
    177A ->181A        0.16426
    172B ->179B        0.69896
    173B ->179B       -0.32088
    174B ->180B        0.22254
    175B ->179B       -0.10419
    175B ->181B        0.11650
    176B ->180B       -0.13140
    176B ->181B       -0.18572

 Excited State  30:  2.390-A      3.8550 eV  321.62 nm  f=0.2099
<S**2>=1.177
    173A ->180A        0.11635
    174A ->180A        0.29954
    175A ->180A       -0.32601
    175A ->181A       -0.26308
    176A ->180A       -0.37411
    177A ->180A       -0.21001
    177A ->181A       -0.17728
    172B ->179B       -0.24122
    173B ->179B        0.11357
    173B ->180B       -0.16367
    173B ->181B       -0.11279
    174B ->179B       -0.11438
    174B ->180B        0.39026
    175B ->180B       -0.13261
    176B ->180B       -0.23517
    176B ->181B        0.16410
```

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 Excited State  31:  2.801-A      3.8715 eV  320.25 nm  f=0.0007
<S**2>=1.711
    173A ->181A        0.13724
    171B ->179B       -0.12919
    172B ->179B        0.29695
    173B ->179B       -0.18974
    175B ->181B       -0.21079
    176B ->181B        0.79760

 Excited State  32:  2.457-A      3.8772 eV  319.77 nm  f=0.0030
<S**2>=1.259
    173A ->181A       -0.23605
    175A ->180A       -0.12606
    175A ->181A        0.64976
    176A ->180A       -0.11321
    177A ->181A        0.44889
    172B ->179B       -0.26398
    172B ->181B       -0.10925
    173B ->179B        0.14754
    173B ->181B        0.11504
    176B ->181B        0.24383

 Excited State  33:  2.579-A      3.9430 eV  314.44 nm  f=0.1577
<S**2>=1.412
    173A ->181A        0.46069
    174A ->180A       -0.14876
    175A ->180A       -0.12140
    175A ->181A        0.14754
    176A ->180A       -0.13349
    177A ->180A       -0.10165
    178A ->187A        0.11587
    171B ->179B        0.18308
    173B ->181B        0.40307
    174B ->181B        0.12504
    175B ->181B       -0.15326
    176B ->180B       -0.25762
    177B ->187B       -0.22560
    177B ->188B        0.13444
    178B ->186B        0.12065
    178B ->187B        0.20845

 Excited State  34:  3.415-A      3.9503 eV  313.86 nm  f=0.0061
<S**2>=2.666
    166A ->180A        0.10002
    169A ->180A        0.12653
    171A ->180A        0.11981
    173A ->181A        0.12052
    174A ->188A        0.11113
    175A ->180A       -0.11759
    177A ->186A       -0.10845
    177A ->188A       -0.14253
    178A ->186A        0.10813
```

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    178A ->188A        0.12428
    179A ->182A        0.14239
    179A ->186A        0.18476
    179A ->188A        0.34324
    179A ->189A        0.10272
    169B ->180B       -0.15722
    170B ->180B       -0.12727
    176B ->188B        0.10793
    177B ->186B       -0.17858
    177B ->187B       -0.11032
    177B ->188B       -0.15444
    178B ->182B       -0.16166
    178B ->186B       -0.20939
    178B ->188B       -0.33435

 Excited State  35:  2.995-A      3.9621 eV  312.93 nm  f=0.0461
<S**2>=1.993
    168A ->181A       -0.13240
    173A ->181A       -0.17055
    174A ->180A        0.22473
    175A ->180A        0.15430
    175A ->181A        0.13097
    175A ->187A        0.12946
    176A ->180A        0.11001
    176A ->181A        0.25283
    177A ->180A        0.13247
    177A ->181A        0.16825
    178A ->187A        0.28479
    178A ->188A       -0.10852
    179A ->187A       -0.21747
    167B ->181B        0.10529
    172B ->181B        0.10594
    173B ->180B       -0.10890
    173B ->181B       -0.21790
    174B ->180B        0.23184
    176B ->180B        0.23038
    176B ->181B       -0.12117
    177B ->183B       -0.10626
    177B ->187B       -0.25594
    178B ->183B        0.11810
    178B ->187B        0.21234

 Excited State  36:  2.167-A      3.9710 eV  312.22 nm  f=0.0359
<S**2>=0.924
    173A ->180A       -0.10910
    173A ->181A        0.34259
    174A ->180A        0.40137
    175A ->180A        0.18741
    176A ->180A        0.13239
    176A ->181A       -0.14628
    177A ->180A        0.18065
    178A ->187A       -0.14353
```

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    172B ->179B       -0.11041
    173B ->181B        0.41921
    174B ->180B        0.40553
    176B ->180B        0.29639

 Excited State  37:  3.139-A      3.9887 eV  310.84 nm  f=0.0026
<S**2>=2.214
    174A ->181A        0.12744
    175A ->181A       -0.15598
    176A ->181A        0.85436
    177A ->181A        0.12339
    178A ->187A       -0.12712
    179A ->187A        0.10834
    173B ->181B        0.10646
    175B ->181B       -0.19873
    177B ->187B        0.10700
    178B ->187B       -0.10858

 Excited State  38:  2.469-A      4.0214 eV  308.31 nm  f=0.0046
<S**2>=1.274
    176A ->181A        0.24787
    174B ->181B        0.18255
    175B ->180B        0.17729
    175B ->181B        0.86300
    176B ->181B        0.22521

 Excited State  39:  3.310-A      4.0395 eV  306.93 nm  f=0.0018
<S**2>=2.489
    170A ->180A       -0.11364
    171A ->180A        0.13596
    171A ->184A        0.10529
    176A ->184A        0.16009
    177A ->184A        0.12784
    177A ->185A        0.10791
    178A ->184A        0.17821
    179A ->184A        0.29726
    179A ->185A        0.14629
    179A ->188A       -0.12243
    179A ->189A       -0.10370
    168B ->179B       -0.10902
    168B ->180B       -0.11619
    170B ->179B       -0.14744
    170B ->180B       -0.12445
    171B ->179B        0.25976
    171B ->180B        0.13722
    174B ->180B        0.10559
    175B ->184B       -0.13111
    176B ->184B       -0.14942
    176B ->185B       -0.13502
    177B ->184B       -0.10828
    178B ->182B        0.11101
    178B ->184B       -0.27312
```

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    178B ->185B       -0.13756
    178B ->188B        0.12833

 Excited State  40:  3.014-A      4.0722 eV  304.47 nm  f=0.0102
<S**2>=2.021
    172A ->180A       -0.10078
    172A ->181A       -0.24977
    173A ->181A       -0.13785
    175A ->180A        0.21186
    176A ->180A       -0.25341
    177A ->180A        0.19703
    169B ->179B       -0.10171
    170B ->179B        0.23169
    171B ->179B        0.47900
    172B ->180B        0.14967
    172B ->181B        0.31352
    175B ->180B        0.24151
    176B ->180B       -0.11754
    176B ->181B        0.17974

 Excited State  41:  3.264-A      4.0772 eV  304.09 nm  f=0.0032
<S**2>=2.413
    172A ->180A        0.11634
    172A ->181A       -0.15044
    173A ->180A        0.11047
    175A ->180A       -0.27507
    176A ->180A        0.41073
    177A ->180A       -0.21565
    169B ->180B        0.14372
    170B ->179B        0.21889
    171B ->179B        0.28703
    172B ->180B       -0.11097
    172B ->181B        0.21481
    175B ->180B       -0.40392
    175B ->181B        0.13491
    176B ->180B        0.26421

 Excited State  42:  2.124-A      4.1186 eV  301.04 nm  f=0.0045
<S**2>=0.878
    172A ->180A        0.13832
    175A ->180A       -0.32014
    176A ->180A        0.50352
    177A ->180A       -0.18417
    169B ->179B       -0.10066
    169B ->180B       -0.16476
    172B ->180B        0.24291
    173B ->180B        0.15276
    174B ->180B        0.13247
    175B ->180B        0.54068
    175B ->181B       -0.15296
    176B ->180B       -0.21252
```

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 Excited State  43:  2.665-A      4.1420 eV  299.33 nm  f=0.0379
<S**2>=1.525
    172A ->181A        0.13866
    174A ->180A        0.10560
    157B ->179B        0.10746
    158B ->179B        0.14687
    164B ->179B       -0.11271
    166B ->179B        0.11560
    169B ->179B        0.22763
    169B ->181B       -0.10401
    170B ->179B       -0.28822
    170B ->180B        0.11102
    171B ->179B        0.53006
    171B ->180B       -0.10711
    172B ->181B       -0.28280
    173B ->181B       -0.10882
    174B ->181B       -0.12591
    175B ->180B        0.15112
    178B ->183B        0.11355

 Excited State  44:  3.354-A      4.1621 eV  297.88 nm  f=0.0155
<S**2>=2.562
    166A ->180A        0.13963
    169A ->180A        0.13707
    170A ->180A       -0.17593
    171A ->180A        0.13875
    174A ->182A       -0.26166
    174A ->189A       -0.11891
    179A ->182A       -0.23427
    179A ->184A       -0.11275
    179A ->189A        0.11931
    165B ->180B        0.14778
    169B ->180B       -0.22181
    170B ->180B       -0.19353
    174B ->180B        0.10472
    174B ->182B        0.25030
    174B ->189B        0.10252
    175B ->180B       -0.12868
    178B ->182B        0.31238
    178B ->184B        0.10582
    178B ->189B       -0.11727

 Excited State  45:  2.701-A      4.1971 eV  295.40 nm  f=0.0231
<S**2>=1.574
    172A ->185A       -0.14975
    172A ->190A       -0.10769
    173A ->181A       -0.15949
    177A ->185A        0.10174
    158B ->179B        0.11101
    166B ->179B        0.17032
    167B ->179B       -0.12811
    168B ->179B       -0.15939
```

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    169B ->179B        0.38290
    169B ->181B       -0.20621
    170B ->179B       -0.24907
    170B ->181B       -0.15692
    171B ->179B       -0.13478
    171B ->181B       -0.20828
    172B ->181B        0.38152
    172B ->185B        0.12052

 Excited State  46:  3.029-A      4.2081 eV  294.63 nm  f=0.0023
<S**2>=2.044
    172A ->180A       -0.13089
    175A ->180A       -0.10752
    166B ->180B       -0.15895
    168B ->180B        0.14702
    169B ->180B       -0.31473
    170B ->179B       -0.26294
    171B ->180B       -0.19018
    172B ->180B        0.36503
    173B ->180B        0.46012
    175B ->180B       -0.38314

 Excited State  47:  2.775-A      4.2301 eV  293.10 nm  f=0.0076
<S**2>=1.675
    170A ->181A        0.13608
    172A ->181A        0.18322
    173A ->183A        0.10064
    178A ->183A        0.10662
    179A ->182A       -0.10721
    179A ->184A        0.10499
    165B ->179B        0.11806
    168B ->179B       -0.17754
    169B ->180B       -0.13064
    169B ->181B       -0.27932
    170B ->179B        0.48103
    171B ->179B       -0.12578
    172B ->180B        0.10358
    172B ->181B        0.12098
    173B ->180B        0.14111
    173B ->183B       -0.10859
    174B ->181B       -0.15267
    178B ->182B       -0.23720
    178B ->184B       -0.10202

 Excited State  48:  2.177-A      4.2439 eV  292.15 nm  f=0.1163
<S**2>=0.935
    172A ->181A        0.15507
    178A ->182A        0.23397
    179A ->182A        0.57978
    169B ->181B       -0.16333
    172B ->181B        0.16664
    174B ->180B       -0.10704
```

```
    175B ->180B       -0.11003
    177B ->182B        0.19817
    178B ->182B        0.52089

 Excited State  49:  2.491-A      4.2654 eV  290.67 nm  f=0.0744
<S**2>=1.301
    172A ->180A        0.26632
    172A ->181A        0.28317
    173A ->180A        0.35649
    175A ->180A        0.24180
    179A ->182A       -0.18499
    158B ->179B       -0.11908
    166B ->179B       -0.12990
    167B ->179B        0.10851
    168B ->179B        0.20189
    169B ->179B       -0.17992
    169B ->181B       -0.17188
    170B ->179B       -0.23144
    171B ->181B       -0.11486
    172B ->181B        0.31115
    173B ->180B        0.10791
    174B ->181B       -0.11328
    178B ->183B        0.12722

 Excited State  50:  2.337-A      4.2747 eV  290.04 nm  f=0.0509
<S**2>=1.115
    168A ->180A       -0.10518
    170A ->180A        0.10323
    172A ->180A        0.32564
    172A ->181A       -0.20301
    173A ->180A        0.50114
    175A ->180A        0.36131
    179A ->182A        0.11953
    166B ->179B        0.10687
    167B ->179B       -0.10251
    169B ->179B        0.19860
    170B ->179B        0.11969
    172B ->181B       -0.20873
    173B ->180B        0.24561
    177B ->183B        0.10217
    178B ->183B       -0.15528

 Excited State  51:  3.298-A      4.3047 eV  288.02 nm  f=0.0044
<S**2>=2.469
    167A ->181A        0.11031
    172A ->181A        0.35985
    173A ->180A       -0.17455
    173A ->183A       -0.17339
    176A ->184A        0.14696
    176A ->185A       -0.21054
    176A ->186A        0.12698
    176A ->190A        0.10023
```

```
    178A ->183A       -0.14345
    168B ->179B        0.11138
    170B ->179B        0.20527
    170B ->184B        0.10663
    173B ->180B        0.13124
    173B ->183B        0.15383
    175B ->184B       -0.11718
    175B ->185B        0.23147
    175B ->186B       -0.11829
    176B ->184B       -0.11726
    176B ->191B       -0.13750

 Excited State  52:  3.150-A      4.3092 eV  287.72 nm  f=0.0244
<S**2>=2.230
    172A ->181A        0.38411
    173A ->180A        0.26681
    174A ->181A       -0.12524
    175A ->180A        0.16999
    176A ->184A       -0.16560
    176A ->191A       -0.12985
    178A ->183A       -0.17613
    179A ->183A        0.16585
    168B ->179B       -0.19174
    169B ->181B        0.12109
    170B ->179B        0.10091
    170B ->181B       -0.13732
    171B ->179B        0.15623
    173B ->180B       -0.22248
    174B ->181B        0.28163
    175B ->184B        0.17755
    175B ->191B        0.12340
    176B ->180B       -0.10645
    178B ->184B       -0.12588

 Excited State  53:  2.975-A      4.3258 eV  286.62 nm  f=0.0419
<S**2>=1.963
    176A ->185A        0.13478
    177A ->184A       -0.12709
    178A ->183A       -0.11884
    179A ->183A        0.10171
    169B ->179B        0.10107
    169B ->180B        0.12682
    169B ->181B        0.14708
    170B ->179B        0.22093
    173B ->180B        0.30433
    173B ->181B       -0.17658
    173B ->183B       -0.10945
    174B ->180B        0.19370
    174B ->181B        0.35633
    175B ->184B       -0.12098
    175B ->185B       -0.11894
    175B ->191B       -0.12008
```

```
    176B ->184B        0.11794
    176B ->185B       -0.11839
    177B ->183B       -0.16272
    178B ->183B        0.25866

 Excited State  54:  3.276-A      4.3274 eV  286.51 nm  f=0.0218
<S**2>=2.433
    167A ->181A       -0.11285
    172A ->181A       -0.19919
    173A ->180A        0.11447
    173A ->183A        0.14644
    175A ->191A        0.10849
    176A ->185A       -0.26012
    176A ->186A        0.14989
    176A ->190A        0.10798
    177A ->191A        0.11321
    167B ->181B       -0.10425
    171B ->179B       -0.10391
    171B ->181B        0.11604
    172B ->181B        0.12801
    173B ->183B       -0.18243
    174B ->181B        0.23803
    175B ->181B       -0.11259
    175B ->185B        0.27073
    175B ->186B       -0.12377
    175B ->189B        0.11648
    176B ->184B       -0.11271
    176B ->191B       -0.13868
    177B ->183B       -0.12879
    178B ->183B        0.25452

 Excited State  55:  2.803-A      4.3424 eV  285.52 nm  f=0.0700
<S**2>=1.714
    167A ->181A        0.10810
    170A ->181A        0.12838
    173A ->183A       -0.14871
    174A ->181A        0.47200
    178A ->183A       -0.27423
    178A ->184A        0.14354
    178A ->186A       -0.10947
    179A ->183A        0.26621
    169B ->179B        0.10748
    169B ->180B       -0.11192
    170B ->179B       -0.20167
    171B ->179B       -0.14895
    171B ->181B        0.17065
    177B ->183B       -0.13881
    178B ->183B        0.16061

 Excited State  56:  2.998-A      4.3563 eV  284.61 nm  f=0.0125
<S**2>=1.997
    171A ->181A       -0.11854
```

```
    172A ->180A       -0.10527
    172A ->181A       -0.17417
    174A ->181A        0.67437
    169B ->179B       -0.10279
    169B ->180B        0.19234
    170B ->179B        0.10380
    171B ->181B       -0.15703
    172B ->181B       -0.18015
    173B ->180B        0.19780
    174B ->181B       -0.16368

 Excited State  57:  2.799-A      4.3579 eV  284.50 nm  f=0.0077
<S**2>=1.708
    171A ->181A        0.10365
    172A ->180A       -0.14250
    174A ->181A       -0.31578
    176A ->184A       -0.10511
    176A ->191A       -0.10137
    178A ->183A       -0.12983
    166B ->180B        0.11164
    168B ->180B       -0.14885
    169B ->180B        0.35937
    170B ->179B       -0.18560
    171B ->180B        0.17615
    172B ->180B       -0.17871
    173B ->180B        0.50974
    174B ->180B        0.14239
    174B ->181B       -0.16931
    175B ->184B        0.12122
    175B ->191B        0.10075
    178B ->183B        0.10289

 Excited State  58:  2.231-A      4.3679 eV  283.85 nm  f=0.0532
<S**2>=0.994
    172A ->181A        0.23245
    174A ->181A        0.25645
    178A ->183A        0.30862
    179A ->183A       -0.27677
    169B ->180B        0.12540
    170B ->179B       -0.12997
    171B ->181B        0.12395
    172B ->181B        0.24125
    173B ->180B        0.11925
    173B ->181B       -0.18648
    174B ->180B        0.11260
    174B ->181B        0.46325
    177B ->183B        0.24291
    178B ->183B       -0.34094

 Excited State  59:  3.091-A      4.4125 eV  280.98 nm  f=0.0035
<S**2>=2.138
    169A ->184A       -0.14226
```

```
    171A ->180A        0.12176
    172A ->180A        0.28367
    172A ->181A       -0.10298
    173A ->180A       -0.17169
    175A ->184A        0.12814
    176A ->180A       -0.23421
    176A ->184A       -0.17482
    176A ->191A       -0.22865
    168B ->179B        0.36692
    168B ->184B        0.14235
    169B ->179B        0.16312
    175B ->180B        0.20510
    175B ->184B        0.19495
    175B ->190B        0.10649
    175B ->191B        0.21121
    176B ->184B       -0.14301
    178B ->189B        0.10322

 Excited State  60:  2.807-A      4.4235 eV  280.29 nm  f=0.0096
<S**2>=1.719
    172A ->180A       -0.22830
    172A ->181A        0.27034
    173A ->180A        0.18052
    174A ->181A        0.11163
    165B ->181B        0.11380
    168B ->179B        0.27013
    168B ->181B       -0.14735
    169B ->179B        0.15439
    169B ->181B        0.41826
    170B ->181B        0.10678
    171B ->181B        0.25305
    172B ->181B        0.16836
    173B ->181B        0.12397
    174B ->181B       -0.38955
    178B ->184B       -0.14501

 Excited State  61:  3.021-A      4.4292 eV  279.92 nm  f=0.0010
<S**2>=2.032
    171A ->180A        0.10957
    172A ->180A        0.43870
    172A ->181A        0.15271
    173A ->180A       -0.26400
    174A ->182A        0.18048
    176A ->180A       -0.10078
    168B ->179B       -0.32768
    169B ->179B       -0.14048
    169B ->181B        0.23880
    171B ->180B        0.10770
    171B ->181B        0.10191
    172B ->181B        0.12154
    174B ->181B       -0.20768
    174B ->182B       -0.16277
```

```
    178B ->184B        0.20027
    178B ->185B        0.14061

 Excited State  62:  2.928-A      4.4424 eV  279.09 nm  f=0.0013
<S**2>=1.894
    168A ->180A       -0.15074
    169A ->180A       -0.10095
    169A ->184A        0.11302
    170A ->180A        0.14132
    172A ->180A        0.41987
    173A ->180A       -0.37663
    174A ->182A       -0.15628
    179A ->184A        0.13860
    169B ->180B        0.24267
    170B ->180B        0.22967
    171B ->180B       -0.13606
    172B ->180B        0.32551
    174B ->182B        0.16999
    175B ->180B       -0.12860
    178B ->184B       -0.18023

 Excited State  63:  2.880-A      4.4710 eV  277.30 nm  f=0.0193
<S**2>=1.824
    169A ->180A       -0.22957
    170A ->180A        0.10872
    171A ->180A       -0.13766
    172A ->180A       -0.15154
    174A ->182A       -0.18023
    176A ->182A        0.14653
    177A ->182A        0.13965
    177A ->184A        0.11715
    179A ->184A        0.16781
    179A ->189A       -0.16882
    168B ->179B       -0.32680
    168B ->184B        0.10634
    169B ->179B       -0.14195
    172B ->180B        0.13255
    174B ->182B        0.13230
    178B ->183B        0.11637
    178B ->184B        0.45915
    178B ->188B       -0.10236
    178B ->189B        0.11589

 Excited State  64:  2.956-A      4.5094 eV  274.95 nm  f=0.0007
<S**2>=1.935
    169A ->180A        0.14487
    170A ->180A       -0.19182
    171A ->180A        0.24839
    179A ->184A       -0.24961
    165B ->180B       -0.10314
    168B ->179B       -0.12327
    168B ->180B       -0.11362
```

```
    169B ->180B        0.35562
    171B ->180B        0.19234
    172B ->180B        0.63067
    172B ->181B       -0.13522

 Excited State  65:  2.588-A      4.5291 eV  273.75 nm  f=0.0432
<S**2>=1.424
    168A ->181A        0.11226
    170A ->181A        0.12428
    171A ->181A        0.10805
    178A ->183A        0.11134
    178A ->186A        0.10180
    179A ->183A        0.14443
    179A ->184A        0.39717
    168B ->179B        0.40950
    168B ->180B       -0.16870
    169B ->179B        0.13612
    170B ->180B       -0.12257
    170B ->181B        0.12315
    171B ->180B        0.23757
    172B ->180B        0.15324
    176B ->184B        0.12432
    178B ->184B        0.34088

 Excited State  66:  3.195-A      4.5385 eV  273.18 nm  f=0.0090
<S**2>=2.302
    168A ->181A        0.19743
    170A ->181A        0.26425
    171A ->181A        0.28296
    172A ->186A       -0.14723
    173A ->183A       -0.14925
    177A ->186A        0.13458
    178A ->184A       -0.16830
    178A ->186A        0.16868
    168B ->179B       -0.23514
    168B ->180B        0.12402
    169B ->179B       -0.14144
    169B ->181B       -0.11522
    170B ->180B        0.11381
    170B ->181B        0.20784
    171B ->180B       -0.12039
    171B ->181B        0.28738
    172B ->180B       -0.17243
    172B ->186B        0.12620
    173B ->183B        0.12025
    178B ->184B       -0.14133
    178B ->188B       -0.10664

 Excited State  67:  3.099-A      4.5812 eV  270.64 nm  f=0.0104
<S**2>=2.152
    170A ->181A       -0.14230
    170A ->190A        0.10867
```

```
    171A ->180A        0.21395
    171A ->181A       -0.20071
    171A ->185A        0.14005
    172A ->181A        0.19759
    172A ->186A       -0.11299
    177A ->183A        0.12081
    178A ->183A        0.10642
    178A ->184A        0.25215
    178A ->185A       -0.21557
    178A ->190A       -0.15180
    179A ->184A       -0.14539
    179A ->185A        0.10397
    170B ->180B        0.19021
    170B ->190B        0.10596
    171B ->180B       -0.22455
    171B ->185B        0.14572
    172B ->180B       -0.16954
    172B ->181B       -0.20972
    172B ->186B        0.10577
    177B ->184B       -0.10686
    178B ->183B        0.10913
    178B ->184B        0.11303
    178B ->185B       -0.19337

 Excited State  68:  2.205-A      4.5988 eV  269.60 nm  f=0.0652
<S**2>=0.965
    168A ->180A       -0.20145
    169A ->180A       -0.10534
    170A ->180A        0.30301
    171A ->180A       -0.35038
    173A ->180A       -0.11224
    178A ->184A        0.10156
    178A ->185A       -0.11833
    179A ->184A       -0.35406
    169B ->180B       -0.14813
    170B ->180B       -0.30029
    171B ->180B        0.41235
    172B ->180B        0.10204
    172B ->181B       -0.12303
    178B ->184B       -0.27163

 Excited State  69:  2.244-A      4.6285 eV  267.87 nm  f=0.0194
<S**2>=1.009
    170A ->181A        0.30154
    171A ->181A        0.52858
    179A ->183A       -0.15316
    169B ->181B        0.23595
    170B ->181B       -0.35555
    171B ->181B       -0.41296
    177B ->184B       -0.11369
    178B ->185B       -0.19984
```

```
 Excited State  70:  2.860-A      4.6539 eV  266.41 nm  f=0.0027
<S**2>=1.794
    168A ->180A       -0.10714
    168A ->181A        0.49608
    169A ->181A        0.26581
    170A ->181A        0.14004
    171A ->180A        0.13523
    171A ->181A       -0.37650
    172A ->181A       -0.14901
    173A ->181A       -0.11090
    174A ->181A       -0.18226
    177A ->181A       -0.12305
    178A ->183A        0.15709
    179A ->183A        0.17549
    168B ->181B       -0.11788
    169B ->181B        0.18598
    171B ->181B       -0.15062
    178B ->183B       -0.14349

 Excited State  71:  2.908-A      4.6700 eV  265.49 nm  f=0.0059
<S**2>=1.865
    168A ->180A       -0.35152
    168A ->181A       -0.28457
    169A ->180A       -0.18615
    169A ->181A       -0.12092
    170A ->180A        0.21969
    171A ->180A        0.50653
    171A ->181A        0.14155
    172A ->180A       -0.23198
    173A ->180A       -0.11468
    178A ->184A       -0.15844
    179A ->183A        0.14514
    174B ->182B       -0.12883

 Excited State  72:  3.378-A      4.6730 eV  265.32 nm  f=0.0009
<S**2>=2.603
    163A ->180A        0.13187
    164A ->180A        0.14418
    165A ->180A        0.21220
    166A ->180A       -0.12832
    170A ->180A        0.16514
    174A ->180A       -0.11089
    174A ->182A       -0.25859
    174A ->186A        0.16122
    174A ->188A        0.28865
    177A ->182A        0.10080
    178A ->182A        0.34860
    179A ->182A       -0.17230
    179A ->188A       -0.11581
    162B ->180B        0.17173
    163B ->180B       -0.11607
    164B ->180B       -0.17614
```

```
    170B ->180B        0.11656
    174B ->182B        0.21282
    174B ->186B       -0.16565
    174B ->188B       -0.24778
    177B ->182B       -0.11176
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   72
LETran=    1306.
```

Table S7 List of excited states with excitation energy (eV), Wavelength (nm) and Osilator Strenth (*f*) for **ZnL^3** at b3lyp/tzvp//b3lyp/6-31g(d) with PCM using chloroform as solvent.

```
Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.9374 eV  422.09 nm  f=0.3753
<S**2>=0.000
     179 -> 180        0.68938
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3844.93701909
 Copying the excited state density for this state as the 1-particle
RhoCI density.

 Excited State   2:      Singlet-A      3.0218 eV  410.30 nm  f=0.0276
<S**2>=0.000
     178 -> 180        0.17440
     179 -> 181        0.67849

 Excited State   3:      Singlet-A      3.0523 eV  406.21 nm  f=0.1103
<S**2>=0.000
     178 -> 180        0.67443
     179 -> 180        0.11644
     179 -> 181       -0.16346

 Excited State   4:      Singlet-A      3.1798 eV  389.91 nm  f=0.2850
<S**2>=0.000
     178 -> 181        0.69697

 Excited State   5:      Singlet-A      3.6456 eV  340.09 nm  f=0.1821
<S**2>=0.000
     176 -> 180        0.15846
     177 -> 180        0.65618

 Excited State   6:      Singlet-A      3.7630 eV  329.48 nm  f=0.0230
<S**2>=0.000
     172 -> 180        0.10177
     176 -> 180        0.37391
     176 -> 181        0.51332
     177 -> 180       -0.12699
     177 -> 181       -0.15048
```

```
 Excited State   7:      Singlet-A      3.7863 eV  327.46 nm  f=0.0763
<S**2>=0.000
     169 -> 180        0.22424
     170 -> 180       -0.17496
     172 -> 180       -0.20781
     173 -> 180        0.29979
     175 -> 180       -0.23239
     175 -> 181       -0.14981
     176 -> 180       -0.23504
     176 -> 181        0.33384
     177 -> 180        0.12717

 Excited State   8:      Singlet-A      3.8222 eV  324.38 nm  f=0.0695
<S**2>=0.000
     175 -> 180        0.15154
     175 -> 181        0.58652
     176 -> 180       -0.13446
     177 -> 181       -0.27310

 Excited State   9:      Singlet-A      3.8597 eV  321.23 nm  f=0.0017
<S**2>=0.000
     169 -> 180        0.16125
     170 -> 180       -0.13717
     172 -> 180       -0.12827
     173 -> 180        0.30653
     174 -> 180       -0.27351
     176 -> 180        0.42538
     176 -> 181       -0.20001

 Excited State  10:      Singlet-A      3.8684 eV  320.50 nm  f=0.0041
<S**2>=0.000
     168 -> 181        0.11811
     172 -> 181        0.16809
     173 -> 180        0.12948
     173 -> 181        0.13457
     174 -> 180        0.11373
     174 -> 181        0.28555
     175 -> 181        0.20438
     176 -> 180        0.12770
     177 -> 181        0.49695

 Excited State  11:      Singlet-A      3.9062 eV  317.40 nm  f=0.0022
<S**2>=0.000
     174 -> 180        0.50136
     175 -> 180       -0.36071
     176 -> 180        0.22906
     176 -> 181       -0.12561
     177 -> 181       -0.13944

 Excited State  12:      Singlet-A      3.9490 eV  313.97 nm  f=0.0032
<S**2>=0.000
```

```
     173 -> 180        0.15920
     174 -> 180        0.32468
     175 -> 180        0.49900
     175 -> 181       -0.22668
     177 -> 181       -0.14235

 Excited State  13:      Singlet-A      3.9559 eV  313.41 nm  f=0.0043
<S**2>=0.000
     168 -> 181       -0.14832
     169 -> 181       -0.10558
     172 -> 180       -0.12966
     172 -> 181       -0.26088
     173 -> 181       -0.28392
     174 -> 180        0.13279
     174 -> 181       -0.30340
     175 -> 180        0.16189
     176 -> 181        0.19889
     177 -> 181        0.30360

 Excited State  14:      Singlet-A      4.0004 eV  309.93 nm  f=0.1281
<S**2>=0.000
     179 -> 182        0.66914

 Excited State  15:      Singlet-A      4.0767 eV  304.13 nm  f=0.0021
<S**2>=0.000
     168 -> 181       -0.17903
     172 -> 180       -0.13914
     172 -> 181       -0.42806
     174 -> 181        0.45691

 Excited State  16:      Singlet-A      4.1154 eV  301.27 nm  f=0.0471
<S**2>=0.000
     169 -> 180        0.12012
     170 -> 180       -0.11875
     172 -> 180       -0.26973
     173 -> 180       -0.32282
     178 -> 183        0.47824
     179 -> 183       -0.16666

 Excited State  17:      Singlet-A      4.1224 eV  300.76 nm  f=0.0714
<S**2>=0.000
     169 -> 180       -0.15357
     170 -> 180        0.14024
     172 -> 180        0.26514
     172 -> 181       -0.15948
     173 -> 180        0.34354
     178 -> 183        0.41983
     179 -> 183       -0.15466

 Excited State  18:      Singlet-A      4.2056 eV  294.81 nm  f=0.0005
<S**2>=0.000
     172 -> 181       -0.19677
```

```
     173 -> 181        0.56976
     174 -> 181       -0.29509

 Excited State  19:      Singlet-A      4.2431 eV  292.20 nm  f=0.0028
<S**2>=0.000
     178 -> 182       -0.28932
     178 -> 184       -0.34138
     179 -> 184        0.51568

 Excited State  20:      Singlet-A      4.2521 eV  291.58 nm  f=0.0028
<S**2>=0.000
     178 -> 183        0.21619
     179 -> 183        0.65483

 Excited State  21:      Singlet-A      4.2861 eV  289.27 nm  f=0.0119
<S**2>=0.000
     169 -> 180        0.13765
     171 -> 180        0.19154
     172 -> 180        0.16254
     178 -> 182        0.32726
     178 -> 184        0.35675
     179 -> 184        0.38328

 Excited State  22:      Singlet-A      4.2945 eV  288.70 nm  f=0.0346
<S**2>=0.000
     169 -> 180        0.30770
     170 -> 180       -0.16168
     171 -> 180        0.29499
     172 -> 180        0.35648
     178 -> 182       -0.18868
     179 -> 184       -0.25940

 Excited State  23:      Singlet-A      4.3606 eV  284.33 nm  f=0.0032
<S**2>=0.000
     178 -> 182        0.50488
     178 -> 184       -0.44352

 Excited State  24:      Singlet-A      4.3683 eV  283.83 nm  f=0.0105
<S**2>=0.000
     169 -> 180       -0.21157
     170 -> 180        0.22452
     171 -> 180        0.50139
     172 -> 180       -0.22581
     172 -> 181        0.11467
     179 -> 185       -0.10920
     179 -> 186        0.16265

 Excited State  25:      Singlet-A      4.3988 eV  281.86 nm  f=0.0196
<S**2>=0.000
     168 -> 181        0.42301
     169 -> 181        0.30722
     170 -> 181        0.13183
```

```
     171 -> 181       -0.16526
     172 -> 181       -0.29327
     173 -> 181       -0.13541
     178 -> 184        0.14852

 Excited State  26:      Singlet-A      4.5129 eV  274.73 nm  f=0.0121
<S**2>=0.000
     168 -> 181       -0.17171
     169 -> 180        0.12487
     169 -> 181       -0.14276
     170 -> 180        0.24485
     170 -> 181        0.57856
     178 -> 184        0.10319

 Excited State  27:      Singlet-A      4.5516 eV  272.39 nm  f=0.0249
<S**2>=0.000
     168 -> 180        0.12832
     169 -> 180        0.36008
     170 -> 180        0.41853
     170 -> 181       -0.28155
     171 -> 180       -0.16372
     179 -> 185       -0.10937
     179 -> 186        0.18047

 Excited State  28:      Singlet-A      4.5714 eV  271.22 nm  f=0.0388
<S**2>=0.000
     168 -> 180        0.15642
     168 -> 181        0.31417
     169 -> 181       -0.31235
     170 -> 180        0.10005
     171 -> 181        0.46446

 Excited State  29:      Singlet-A      4.5835 eV  270.50 nm  f=0.0360
<S**2>=0.000
     169 -> 180        0.13914
     170 -> 180        0.19119
     170 -> 181       -0.10655
     171 -> 180        0.21159
     179 -> 185        0.45451
     179 -> 186       -0.37385

 Excited State  30:      Singlet-A      4.6040 eV  269.29 nm  f=0.1156
<S**2>=0.000
     177 -> 182       -0.24104
     178 -> 185       -0.20635
     179 -> 185        0.33578
     179 -> 186        0.33441
     179 -> 187       -0.17969
     179 -> 189        0.25703

 Excited State  31:      Singlet-A      4.6382 eV  267.31 nm  f=0.0075
<S**2>=0.000
```

```
     168 -> 180       -0.13279
     168 -> 181       -0.11486
     169 -> 181        0.39470
     171 -> 181        0.45589
     177 -> 182        0.10715
     178 -> 185       -0.15933
     179 -> 189       -0.14101

 Excited State  32:      Singlet-A      4.6454 eV  266.89 nm  f=0.0139
<S**2>=0.000
     168 -> 181       -0.12469
     169 -> 181        0.18031
     171 -> 180        0.10627
     177 -> 182       -0.25466
     178 -> 185        0.25007
     178 -> 186        0.15550
     179 -> 185       -0.22190
     179 -> 186       -0.24495
     179 -> 187       -0.17430
     179 -> 189        0.29297
     179 -> 190       -0.10427

 Excited State  33:      Singlet-A      4.6710 eV  265.44 nm  f=0.0128
<S**2>=0.000
     178 -> 185        0.49812
     178 -> 186        0.22643
     179 -> 185        0.25872
     179 -> 186        0.26851

 Excited State  34:      Singlet-A      4.6814 eV  264.85 nm  f=0.0069
<S**2>=0.000
     169 -> 181        0.11760
     177 -> 182       -0.12343
     178 -> 186       -0.10001
     178 -> 187       -0.22729
     179 -> 187        0.56021
     179 -> 189        0.20645

 Excited State  35:      Singlet-A      4.7085 eV  263.32 nm  f=0.0236
<S**2>=0.000
     168 -> 180        0.59825
     168 -> 181       -0.17382
     170 -> 180       -0.10023
     177 -> 182        0.10917
     178 -> 188       -0.11121
     179 -> 189       -0.13254

 Excited State  36:      Singlet-A      4.7235 eV  262.48 nm  f=0.0769
<S**2>=0.000
     168 -> 180        0.16407
     175 -> 183       -0.27582
     176 -> 183        0.18824
```

```
     178 -> 186        0.10140
     178 -> 187        0.35026
     178 -> 188        0.31788
     179 -> 187        0.23014
     179 -> 188       -0.14683

 Excited State  37:      Singlet-A      4.7434 eV  261.38 nm  f=0.0288
<S**2>=0.000
     175 -> 183        0.16888
     176 -> 183       -0.13023
     178 -> 186        0.22473
     178 -> 187        0.43916
     178 -> 188       -0.35953
     179 -> 187        0.15217

 Excited State  38:      Singlet-A      4.8031 eV  258.13 nm  f=0.0039
<S**2>=0.000
     178 -> 185       -0.25875
     178 -> 186        0.53669
     178 -> 187       -0.23991
     178 -> 189       -0.17687
     178 -> 190       -0.14214
     179 -> 190        0.12945

 Excited State  39:      Singlet-A      4.8341 eV  256.48 nm  f=0.0010
<S**2>=0.000
     178 -> 188        0.13995
     179 -> 188        0.59930
     179 -> 190        0.27345

 Excited State  40:      Singlet-A      4.8471 eV  255.79 nm  f=0.0226
<S**2>=0.000
     176 -> 182        0.10621
     176 -> 184        0.19897
     177 -> 184       -0.11020
     178 -> 185        0.10421
     178 -> 186       -0.10844
     179 -> 188       -0.29368
     179 -> 189        0.23474
     179 -> 190        0.42936

 Excited State  41:      Singlet-A      4.8804 eV  254.04 nm  f=0.0696
<S**2>=0.000
     175 -> 184        0.18209
     176 -> 182        0.16610
     176 -> 184        0.36749
     177 -> 184       -0.14050
     178 -> 186        0.15804
     178 -> 189        0.19640
     178 -> 190        0.23397
     179 -> 189       -0.10736
     179 -> 190       -0.18605
```

```
 Excited State  42:      Singlet-A      4.9009 eV  252.98 nm  f=0.0280
<S**2>=0.000
     176 -> 184       -0.16075
     178 -> 189        0.34624
     178 -> 190        0.42261
     179 -> 190        0.29425

 Excited State  43:      Singlet-A      4.9945 eV  248.24 nm  f=0.0914
<S**2>=0.000
     175 -> 183        0.10654
     176 -> 183        0.26968
     177 -> 182       -0.17372
     177 -> 183       -0.13682
     178 -> 189        0.40818
     178 -> 190       -0.32948
     179 -> 189       -0.18083
     179 -> 190        0.10069
     179 -> 191       -0.10953

 Excited State  44:      Singlet-A      5.0072 eV  247.61 nm  f=0.0015
<S**2>=0.000
     175 -> 183        0.27282
     176 -> 183        0.46935
     177 -> 183       -0.28985
     178 -> 189       -0.17507
     178 -> 190        0.24264

 Excited State  45:      Singlet-A      5.0300 eV  246.49 nm  f=0.1811
<S**2>=0.000
     166 -> 180        0.23971
     173 -> 182       -0.12007
     174 -> 182        0.16265
     177 -> 182        0.23950
     178 -> 189        0.24632
     178 -> 190       -0.15647
     179 -> 189        0.13502
     179 -> 191        0.45348

 Excited State  46:      Singlet-A      5.0630 eV  244.88 nm  f=0.0647
<S**2>=0.000
     166 -> 180        0.22242
     167 -> 181       -0.12437
     174 -> 182       -0.23460
     174 -> 184       -0.21987
     176 -> 184       -0.13731
     177 -> 182       -0.27662
     177 -> 184       -0.21143
     179 -> 189       -0.10581
     179 -> 190        0.10145
     179 -> 191        0.28338
```

```
 Excited State  47:      Singlet-A      5.0946 eV  243.36 nm  f=0.0675
<S**2>=0.000
     167 -> 181        0.18137
     175 -> 184       -0.17788
     176 -> 182        0.50996
     176 -> 185        0.10940
     177 -> 182       -0.10491
     177 -> 183        0.21120
     177 -> 184        0.12938

 Excited State  48:      Singlet-A      5.0998 eV  243.11 nm  f=0.0038
<S**2>=0.000
     174 -> 183        0.15802
     175 -> 183        0.11949
     176 -> 182       -0.22619
     176 -> 183        0.24376
     177 -> 183        0.53844
     177 -> 184       -0.17464

 Excited State  49:      Singlet-A      5.1206 eV  242.13 nm  f=0.1887
<S**2>=0.000
     167 -> 181       -0.33287
     174 -> 184        0.13118
     176 -> 183        0.10705
     177 -> 183        0.16560
     177 -> 184        0.43238
     178 -> 188       -0.15590

 Excited State  50:      Singlet-A      5.1253 eV  241.91 nm  f=0.1424
<S**2>=0.000
     166 -> 180        0.14783
     167 -> 181        0.13106
     173 -> 182        0.22249
     174 -> 182       -0.11122
     174 -> 184        0.21101
     175 -> 182       -0.20135
     176 -> 182       -0.22878
     176 -> 184        0.23991
     177 -> 182       -0.10847
     177 -> 184        0.21103
     179 -> 189       -0.13126
     179 -> 190        0.13055
     179 -> 191        0.13783

 Excited State  51:      Singlet-A      5.1479 eV  240.84 nm  f=0.0604
<S**2>=0.000
     166 -> 180        0.10259
     167 -> 181        0.24801
     174 -> 182       -0.11584
     175 -> 182        0.50151
     175 -> 184        0.22008
     176 -> 182       -0.14387
```

```
     176 -> 184       -0.11080
     177 -> 184        0.12978
     178 -> 188        0.10476

 Excited State  52:      Singlet-A      5.1878 eV  238.99 nm  f=0.1607
<S**2>=0.000
     166 -> 180        0.38197
     167 -> 180       -0.17812
     174 -> 182       -0.22889
     175 -> 182       -0.12764
     177 -> 182        0.12862
     179 -> 189        0.14727
     179 -> 191       -0.30101

 Excited State  53:      Singlet-A      5.1977 eV  238.54 nm  f=0.0127
<S**2>=0.000
     167 -> 181       -0.21284
     172 -> 184        0.14256
     173 -> 183        0.11829
     173 -> 184        0.12582
     174 -> 183        0.21362
     174 -> 184        0.12358
     175 -> 182        0.31678
     175 -> 184       -0.23668
     176 -> 184        0.12858
     177 -> 184       -0.12864

 Excited State  54:      Singlet-A      5.2205 eV  237.50 nm  f=0.0718
<S**2>=0.000
     166 -> 180        0.11108
     173 -> 182        0.19436
     173 -> 184        0.16660
     174 -> 182        0.32310
     174 -> 184        0.28713
     175 -> 184        0.17212
     176 -> 184       -0.28132
     177 -> 182       -0.11515
     177 -> 184       -0.18652

 Excited State  55:      Singlet-A      5.2353 eV  236.83 nm  f=0.0088
<S**2>=0.000
     173 -> 183        0.24411
     174 -> 183        0.49739
     175 -> 182       -0.10922
     175 -> 184        0.31618
     176 -> 184       -0.10897
     177 -> 183       -0.11326

 Excited State  56:      Singlet-A      5.2599 eV  235.72 nm  f=0.0423
<S**2>=0.000
     166 -> 180       -0.16645
     167 -> 181       -0.14161
```

```
     172 -> 182        0.12748
     173 -> 182       -0.17700
     173 -> 184        0.11235
     174 -> 182       -0.29926
     174 -> 183       -0.10197
     174 -> 184        0.13478
     175 -> 182       -0.13049
     175 -> 184        0.32840
     176 -> 187       -0.15012
     179 -> 191        0.13083

 Excited State  57:      Singlet-A      5.2780 eV  234.91 nm  f=0.1695
<S**2>=0.000
     166 -> 180        0.13175
     167 -> 180        0.26379
     167 -> 181        0.11546
     172 -> 183        0.12145
     173 -> 182       -0.20134
     174 -> 184        0.12391
     175 -> 183       -0.23319
     176 -> 183        0.10128
     178 -> 188       -0.19127
     178 -> 191        0.39427

 Excited State  58:      Singlet-A      5.2947 eV  234.17 nm  f=0.0184
<S**2>=0.000
     167 -> 181       -0.12480
     172 -> 183       -0.13231
     172 -> 184        0.12989
     174 -> 182        0.11249
     174 -> 184       -0.26040
     175 -> 183        0.10617
     175 -> 184        0.14651
     176 -> 184        0.10214
     176 -> 185        0.15995
     177 -> 186       -0.12088
     178 -> 191        0.41915

 Excited State  59:      Singlet-A      5.3048 eV  233.72 nm  f=0.0254
<S**2>=0.000
     167 -> 180        0.37179
     169 -> 182        0.10657
     173 -> 182        0.31293
     174 -> 183       -0.10853
     174 -> 184       -0.13293
     175 -> 182        0.10050
     175 -> 183       -0.12958
     177 -> 182        0.11470
     178 -> 188       -0.11616
     178 -> 191       -0.17362
```

```
 Excited State  60:      Singlet-A      5.3125 eV  233.38 nm  f=0.2551
<S**2>=0.000
     167 -> 180        0.28481
     167 -> 181       -0.19108
     173 -> 182        0.16319
     174 -> 182       -0.15982
     174 -> 184        0.11966
     175 -> 183        0.19213
     175 -> 184       -0.13804
     176 -> 185       -0.15307
     176 -> 187        0.10209
     178 -> 188        0.14804
     178 -> 191        0.27034

 Excited State  61:      Singlet-A      5.3322 eV  232.52 nm  f=0.0224
<S**2>=0.000
     166 -> 180        0.26151
     167 -> 180        0.34902
     167 -> 181       -0.18154
     172 -> 183       -0.12042
     173 -> 182       -0.21724
     174 -> 182        0.12126
     175 -> 183        0.11287
     177 -> 182       -0.12306
     178 -> 188        0.10202
     178 -> 191       -0.20630

 Excited State  62:      Singlet-A      5.3722 eV  230.79 nm  f=0.0140
<S**2>=0.000
     172 -> 182       -0.17621
     172 -> 183       -0.11240
     173 -> 186        0.10047
     174 -> 186        0.10752
     175 -> 185        0.14488
     175 -> 186       -0.15219
     176 -> 185        0.34926
     176 -> 186       -0.34000
     177 -> 185       -0.15907
     177 -> 186        0.22967

 Excited State  63:      Singlet-A      5.3802 eV  230.44 nm  f=0.0496
<S**2>=0.000
     172 -> 182        0.24290
     172 -> 183       -0.17941
     172 -> 184        0.23280
     173 -> 184        0.26620
     174 -> 184       -0.13383
     174 -> 185        0.12153
     175 -> 183       -0.12429
     175 -> 187        0.11858
     176 -> 184       -0.10316
     176 -> 187        0.18479
```

```
     177 -> 184        0.11760
     177 -> 185        0.13999
     177 -> 187       -0.16375

 Excited State  64:      Singlet-A      5.3889 eV  230.07 nm  f=0.0568
<S**2>=0.000
     168 -> 183        0.12934
     172 -> 182        0.10985
     172 -> 183        0.46069
     173 -> 183        0.22449
     173 -> 184        0.14519
     174 -> 183       -0.19667
     175 -> 183        0.17134
     176 -> 186       -0.11877
     178 -> 188        0.10608

 Excited State  65:      Singlet-A      5.4098 eV  229.18 nm  f=0.0124
<S**2>=0.000
     171 -> 184        0.12142
     172 -> 184       -0.21138
     173 -> 183       -0.24468
     173 -> 184        0.34249
     174 -> 183        0.16034
     174 -> 184       -0.19292
     174 -> 185       -0.10779
     174 -> 187       -0.11174
     176 -> 184        0.11103
     176 -> 185       -0.14637
     176 -> 186       -0.13105
     176 -> 187       -0.16666

 Excited State  66:      Singlet-A      5.4177 eV  228.85 nm  f=0.0965
<S**2>=0.000
     171 -> 182        0.17609
     172 -> 183       -0.14762
     173 -> 183        0.21221
     173 -> 186       -0.11247
     174 -> 182        0.19929
     174 -> 184       -0.10540
     176 -> 185       -0.11130
     176 -> 186        0.13466
     177 -> 185       -0.28127
     177 -> 186        0.30112
     177 -> 187       -0.14214
     177 -> 189        0.10223

 Excited State  67:      Singlet-A      5.4261 eV  228.50 nm  f=0.0091
<S**2>=0.000
     172 -> 182       -0.18742
     172 -> 183       -0.21602
     173 -> 183        0.45590
     173 -> 184        0.16117
```

```
     174 -> 183       -0.17586
     177 -> 185        0.19730
     177 -> 186       -0.11023

 Excited State  68:      Singlet-A      5.4401 eV  227.91 nm  f=0.0191
<S**2>=0.000
     169 -> 182       -0.17990
     170 -> 182        0.14976
     171 -> 182       -0.10411
     172 -> 182        0.31709
     172 -> 183       -0.10942
     172 -> 184       -0.18696
     173 -> 182        0.22275
     174 -> 185       -0.10225
     176 -> 186       -0.20970
     177 -> 185       -0.11858
     177 -> 187        0.16125
     177 -> 189       -0.18914

 Excited State  69:      Singlet-A      5.4770 eV  226.37 nm  f=0.0162
<S**2>=0.000
     170 -> 182       -0.10160
     172 -> 184        0.35566
     173 -> 184       -0.14115
     173 -> 185       -0.11274
     174 -> 185       -0.19994
     174 -> 187        0.12796
     176 -> 185       -0.28345
     176 -> 186       -0.25815

 Excited State  70:      Singlet-A      5.4889 eV  225.88 nm  f=0.0020
<S**2>=0.000
     166 -> 181        0.67100
     167 -> 181       -0.11829

 Excited State  71:      Singlet-A      5.4959 eV  225.59 nm  f=0.0218
<S**2>=0.000
     172 -> 182        0.11196
     173 -> 184       -0.14069
     176 -> 187       -0.14366
     177 -> 185        0.42152
     177 -> 186        0.37233
     177 -> 187        0.14490

 Excited State  72:      Singlet-A      5.5309 eV  224.17 nm  f=0.0383
<S**2>=0.000
     164 -> 180        0.10152
     165 -> 180        0.21413
     172 -> 182       -0.17518
     173 -> 184        0.14309
     174 -> 184       -0.10345
     174 -> 186        0.18289
```

```
     176 -> 186        0.16711
     177 -> 185       -0.10496
     177 -> 186        0.18625
     177 -> 187        0.32173
     177 -> 189       -0.25257
 SavETr:  write IOETrn=   770 NScale= 10 NData=  16 NLR=1 NState=   72
LETran=    1306.
```

References

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