Electronic Supplementary Information (ESI)

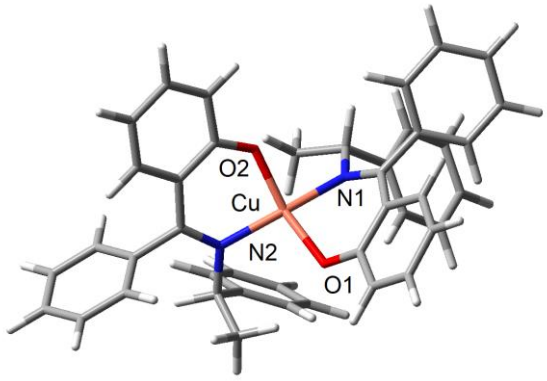
Pseudotetrahedral copper(II)-complexes with enantiopure (*R*- or *S*)-2-(((aryl)ethylimino)ethyl)phenolate Schiff base ligands

Mohammed Enamullah,[a,*] Mohammad Anwar Hossain,[a] Mohammad Khairul Islam,[a] Dennis Woschko,[b] Christoph Janiak[b,*]

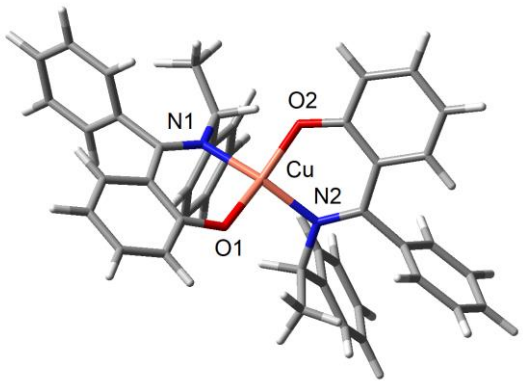
[a] Department of Chemistry, Jahangirnagar University, Dhaka-1342, Bangladesh. E-mail: enamullah@juniv.edu

[b] Institut für Anorganische Chemie und Strukturchemie, Universität Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf, Germany. E-mail: janiak@hhu.de

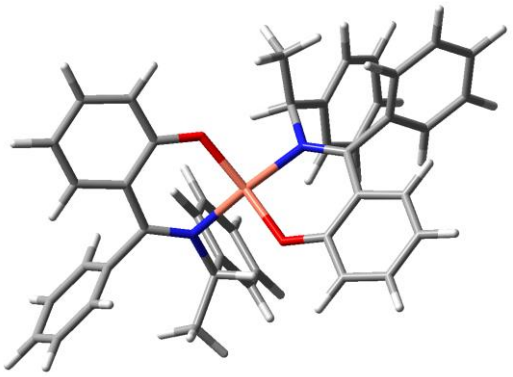
Emails: enamullah@juniv.edu, anwar3842@gmail.com, khairul_chemist@outlook.com, dennis.woschko@hhu.de, janiak@hhu.de



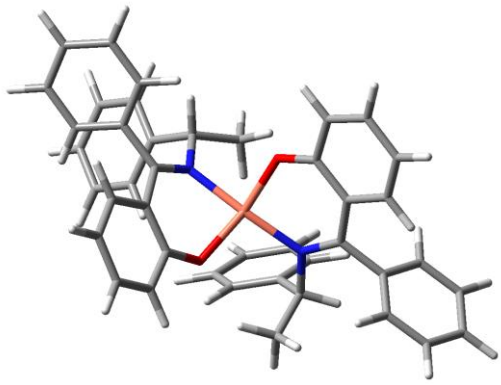
Λ-Cu-*R*-L[1] (-3521.885971 a.u., stable by +7.58 kcal/mol)



Δ-Cu-*R*-L[1] (- 3521.873888 a.u.)

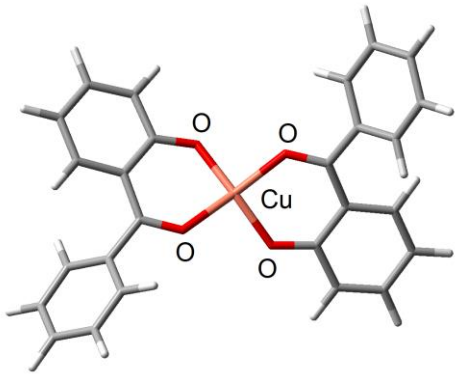


Λ-Cu-*S*-L[1] (-3521.873874 a.u.)

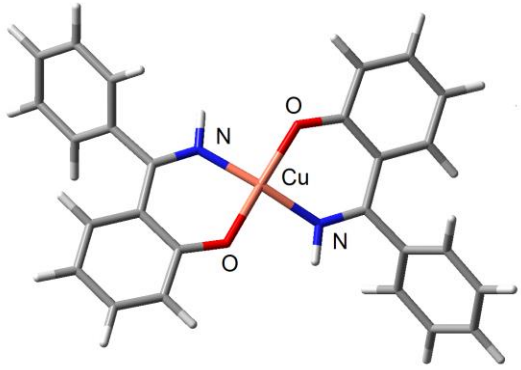


Δ-Cu-*S*-L[1] (-3521.885968 a.u., stable by +7.59 kcal/mol)

Fig. S1 DFT optimized structures for diastereomeric pairs Λ-Cu-*R*-L[1]/Δ-Cu-*R*-L[1] and Λ-Cu-*S*-L[1]/ Δ-Cu-*S*-L[1], calculated at b3lyp/6-31g(d), respectively.



CuL'$_2$ (-2942.583295 a.u., stable by +24,950.41 kcal/mol)



CuL"$_2$ (-2902.822321 a.u.)

Fig. S2 DFT optimized structures for CuL'$_2$ and CuL"$_2$ at b3lyp/6-31g(d), respectively.

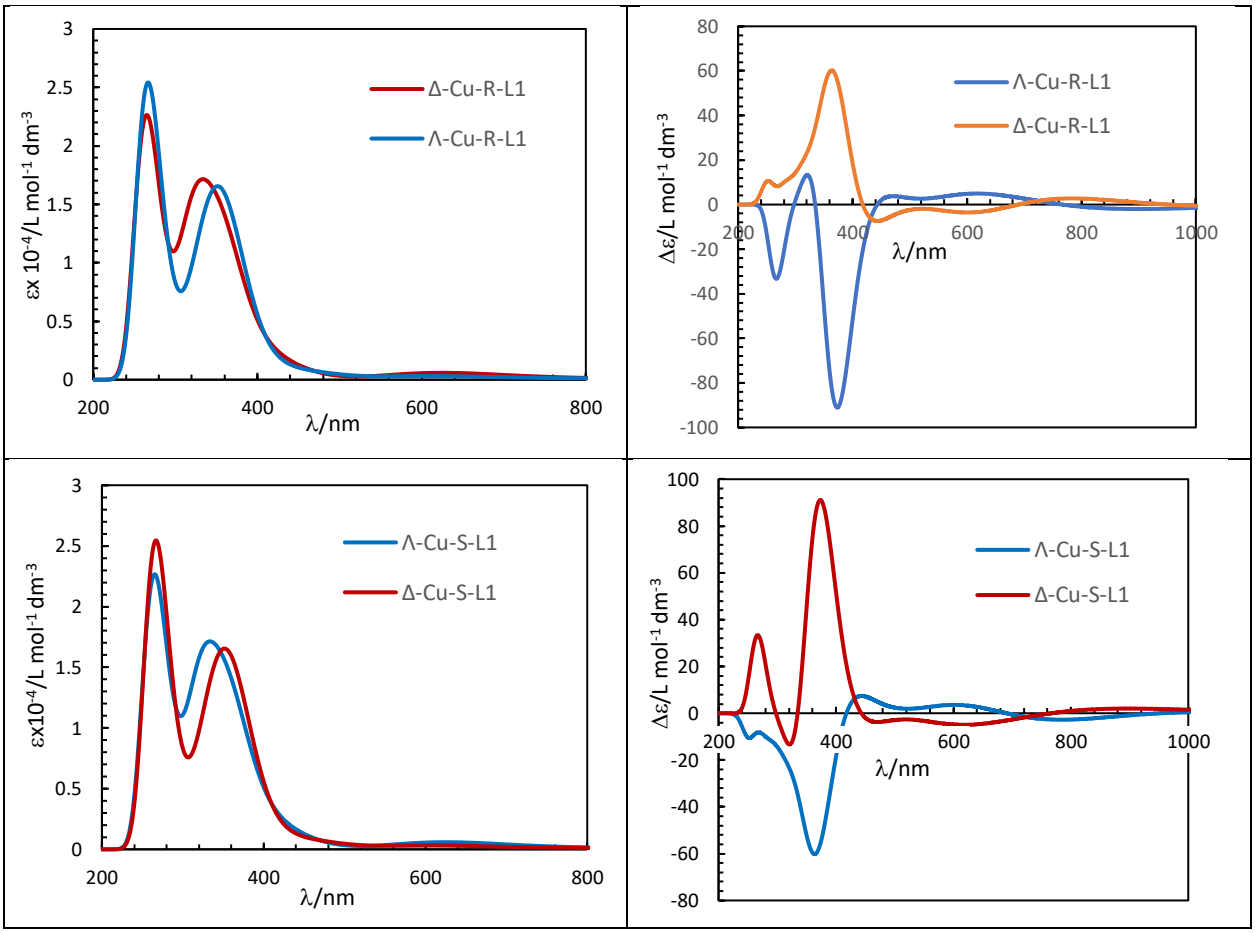


Fig. S3 Calculated UV-Vis. and ECD spectra for diastereomeric pairs Λ-Cu-*R*-L[1]/Δ-Cu-*R*-L[1] and Λ-Cu-*S*-L[1]/Δ-Cu-*S*-L[1] at m06/sdd//b3lyp/6-31g(d), (Gaussian band shape with exponential half-width σ = 0.33 eV).

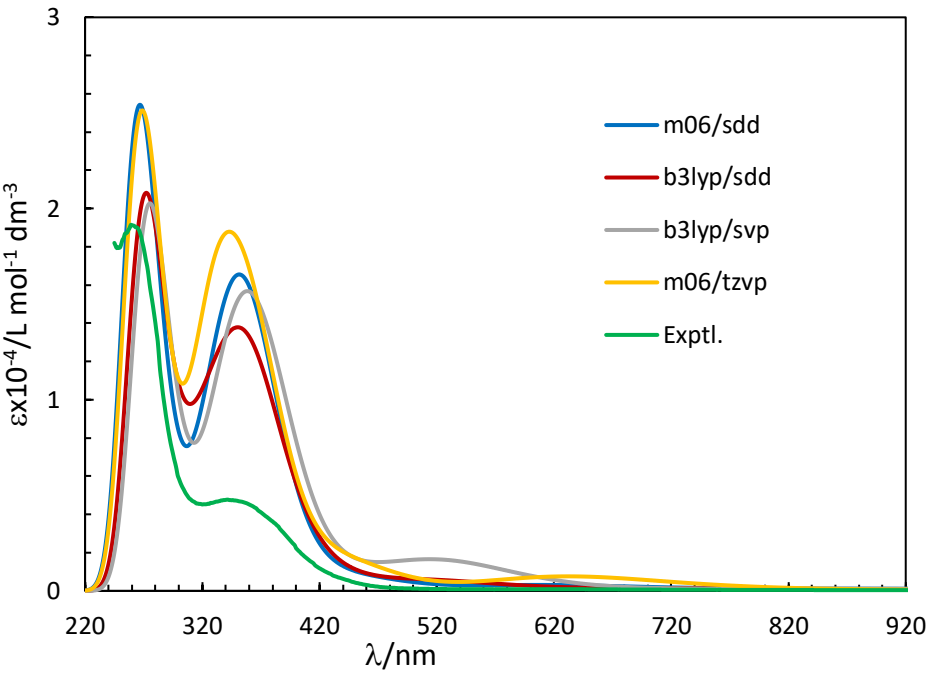


Fig. S4. Computed UV-Vis. spectra for Λ-Cu-*R*-L[1] with different combinations of the functionals and basis sets using PCM in chloroform (Gaussian band shape with exponential half-width, σ = 0.33 eV). Experimental spectrum for Cu-*R*-L[1] (0.10 mM) in chloroform at 25 °C.

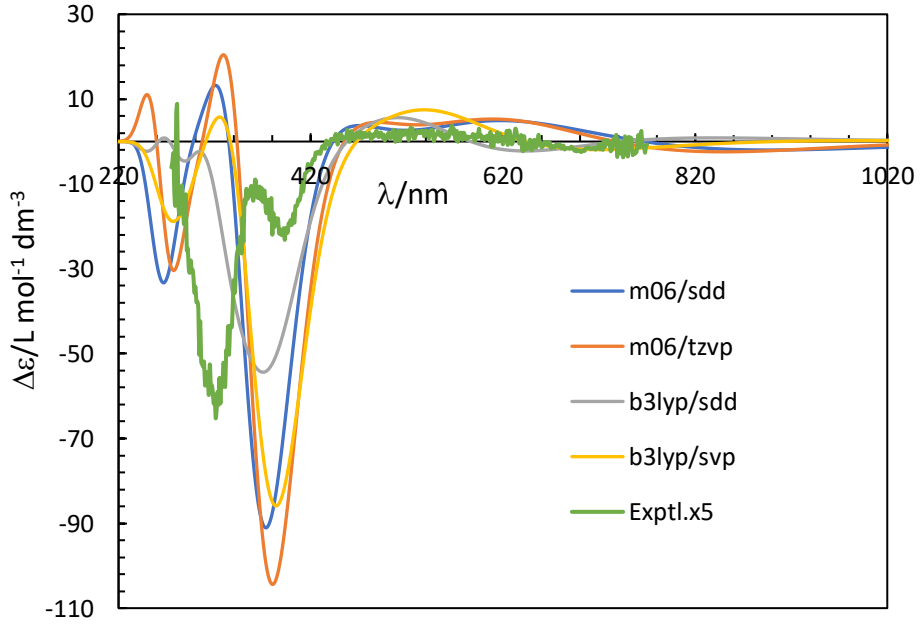


Fig. S5a. Computed ECD spectra for Λ-Cu-*R*-L[1] with different combinations of the functionals and the basis sets using PCM in chloroform (Gaussian band shape with exponential half-width σ = 0.33 eV). Experimental spectrum for Cu-*R*-L[1] (1.21 mM) in chloroform at 25 °C (Δεx5).

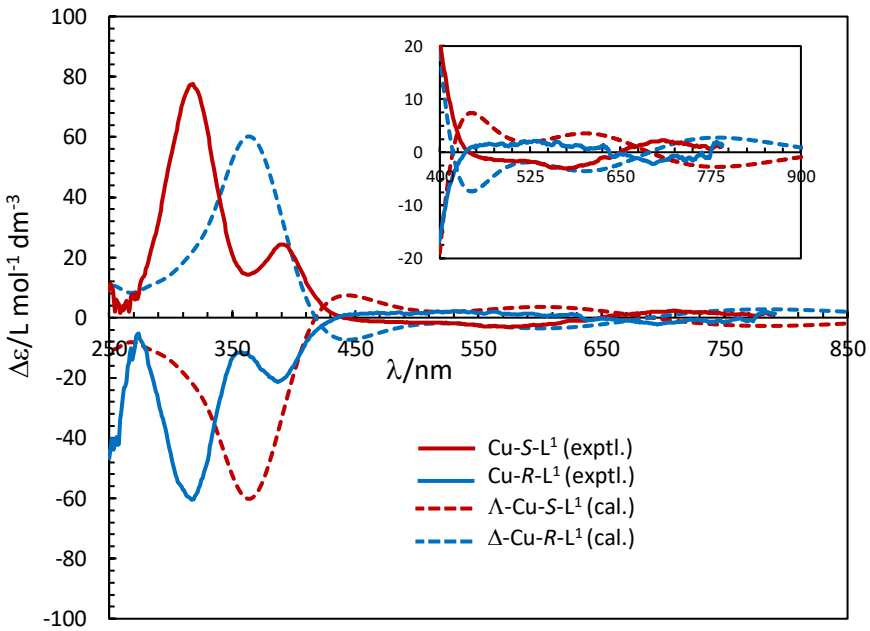
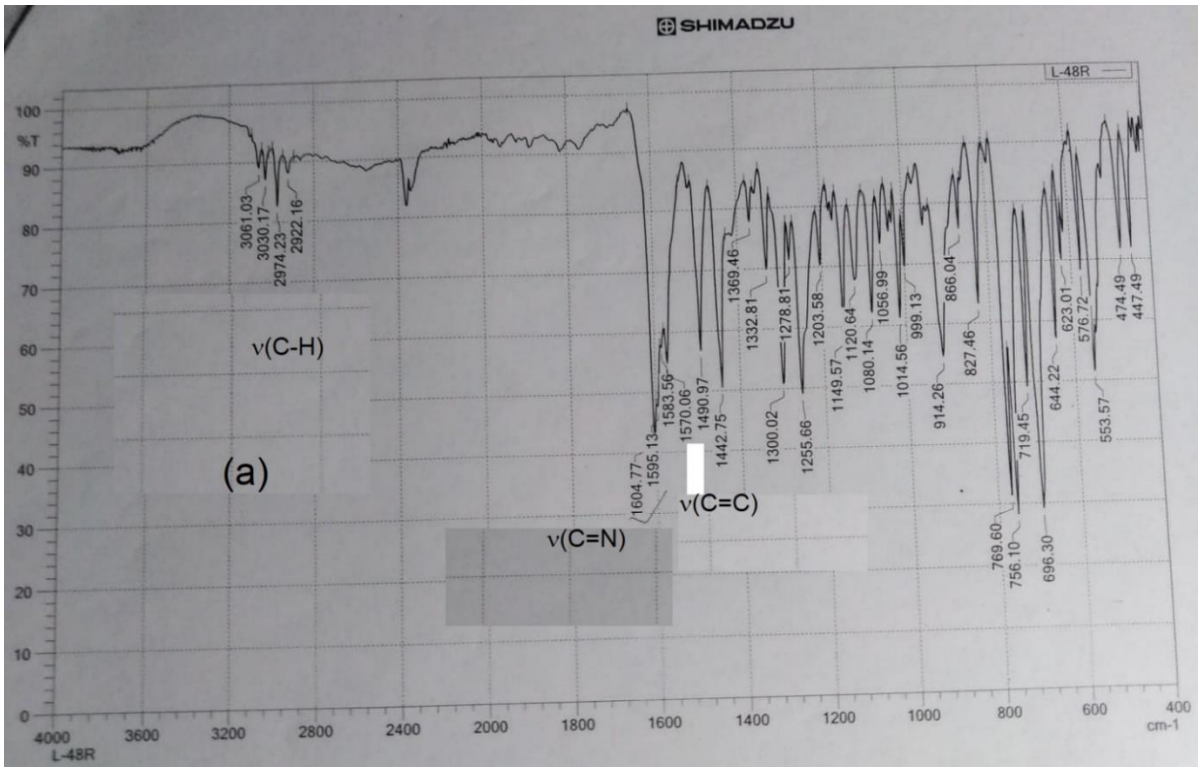
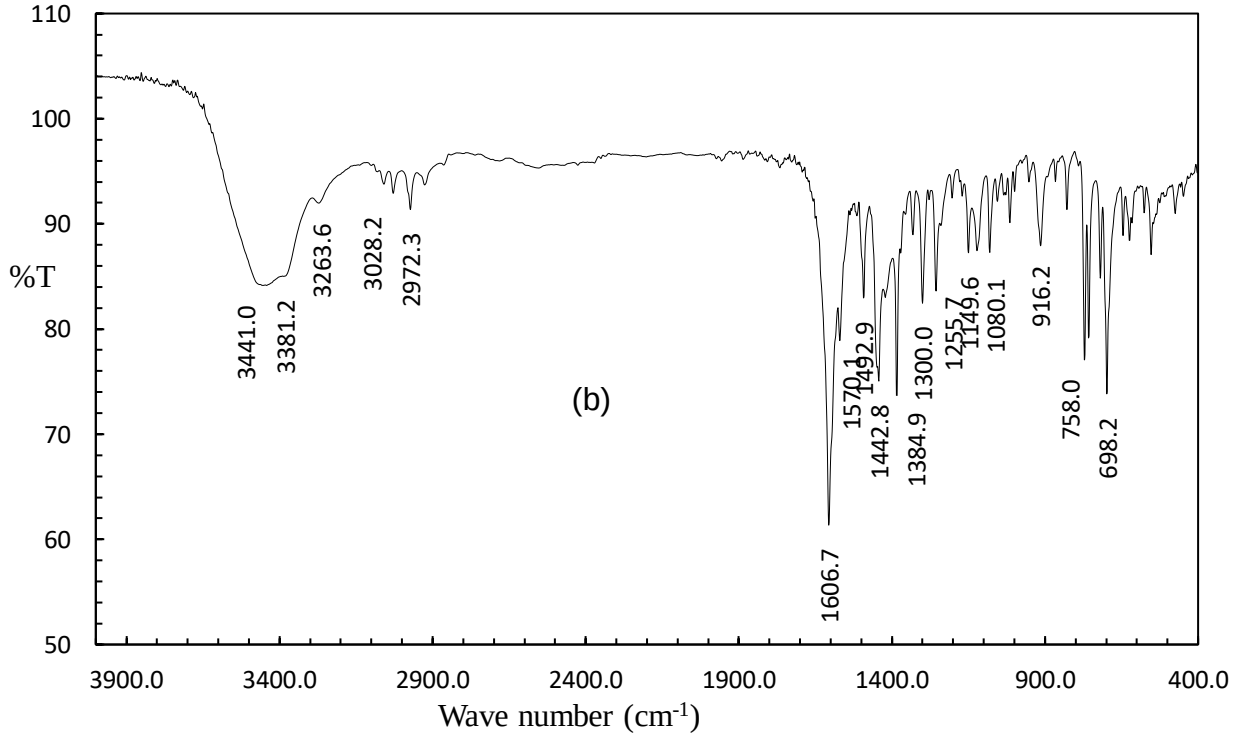


Fig. S5b. Experimental ECD spectra for Cu-*R*-L^1/Cu-*S*-L^1 (1.21/1.33 mM) in chloroform at 25 °C (values of Δε are increased by 5 times) as in Fig. 8. Calculated spectra for Δ-Cu-*R*-L^1/Λ-Cu-*S*-L^1 at the m06/sdd//b3lyp/6-31g(d) level with PCM in chloroform (Gaussian band shape with exponential half-width σ = 0.33 eV). The calculated spectra for the most likely correct diastereomeric pairs Λ-Cu-*R*-L^1/Δ-Cu-*S*-L^1 were also given in Fig. 8 in the main text.


SHIMADZU
L-48R
%T
100
90
80
70
60
50
40
30
20
10
0
3061.03
3030.17
2974.23
2922.16
ν(C-H)
(a)
1604.77
1595.13
1583.56
1570.06
1490.97
1442.75
1369.46
1332.81
1300.02
1278.81
1255.66
1203.58
1149.57
1120.64
1080.14
1056.99
1014.56
999.13
914.26
866.04
827.46
769.60
756.10
719.45
696.30
644.22
623.01
576.72
553.57
474.49
447.49
ν(C=C)
ν(C=N)
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
400
cm-1
L-48R


%T
110
100
90
80
70
60
50
3441.0
3381.2
3263.6
3028.2
2972.3
(b)
1606.7
1570.1
1492.9
1442.8
1384.9
1300.0
1255.7
1149.6
1080.1
916.2
758.0
698.2
3900.0
3400.0
2900.0
2400.0
1900.0
1400.0
900.0
400.0
Wave number (cm-1)

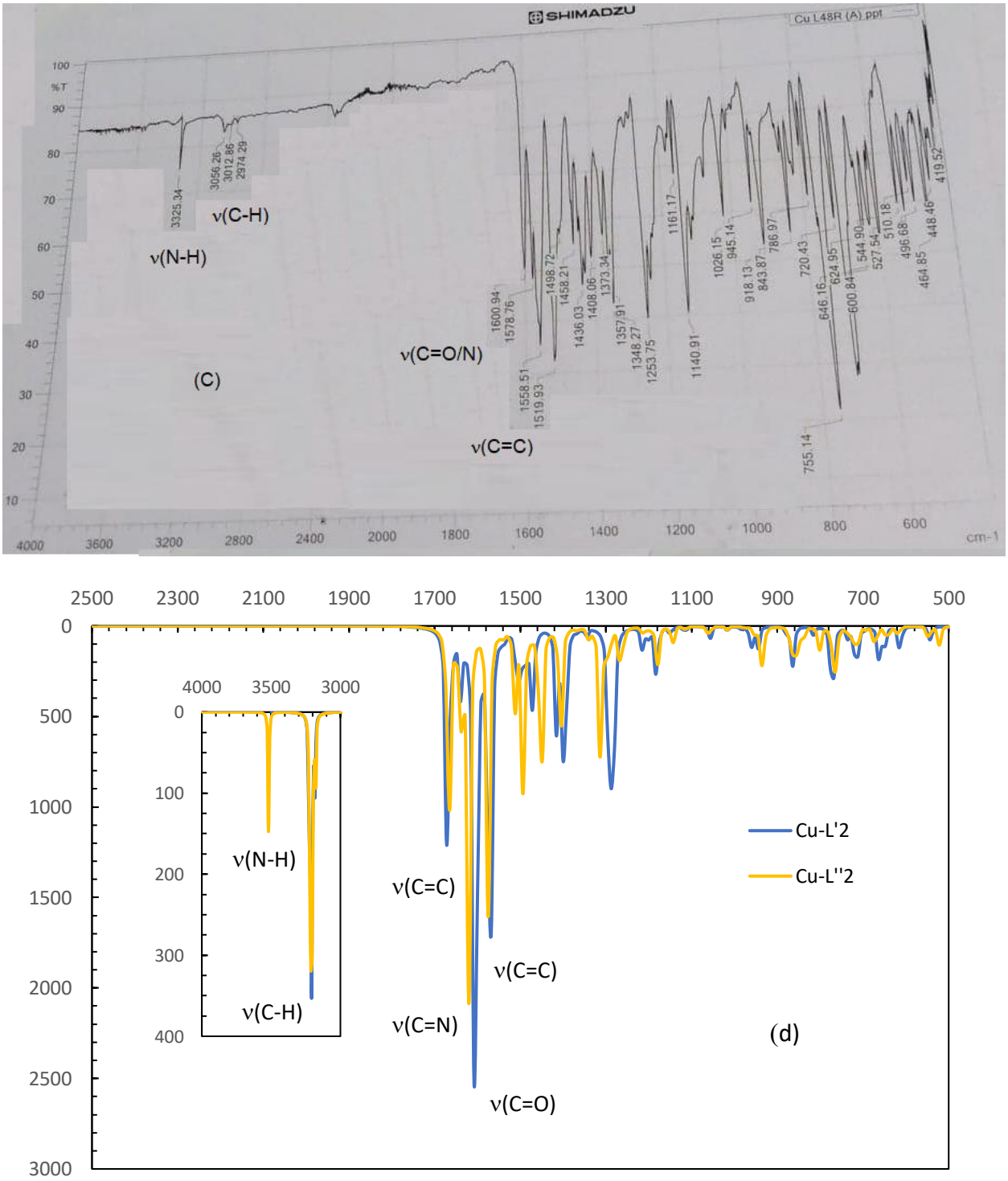


Fig. S6. IR spectra (KBr, cm^{-1}) for (a) *R*-HL^1, (b) Cu-*R*-L^1, (c) admixture of CuL'_2 and CuL''_2 and (d) calculated spectra for CuL'_2 and CuL''_2 at b3lyp/6-31g(d).

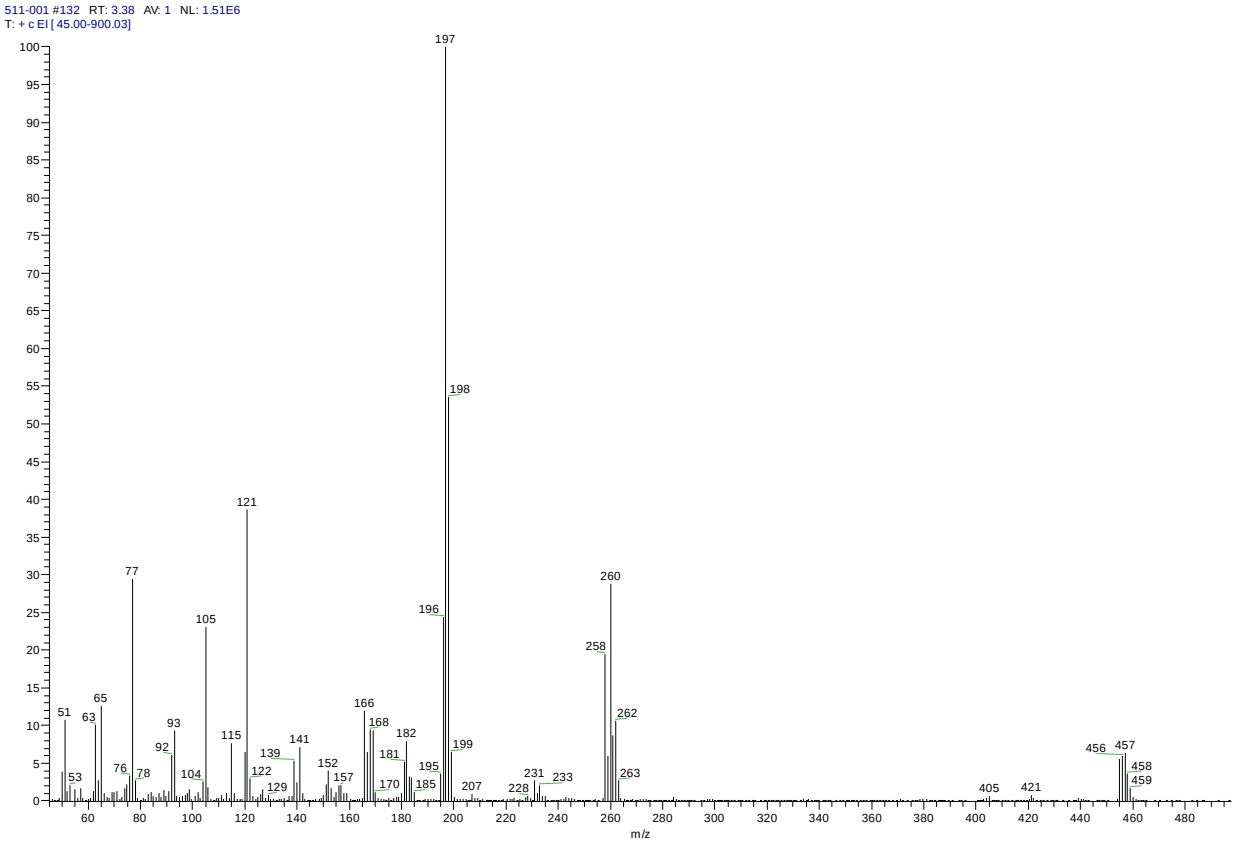


Fig. S7. EI-MS spectrum for dark green block shaped crystals of admixture of CuL'_2 and CuL''_2, obtained from crystallization of Cu-*R*-L^1.

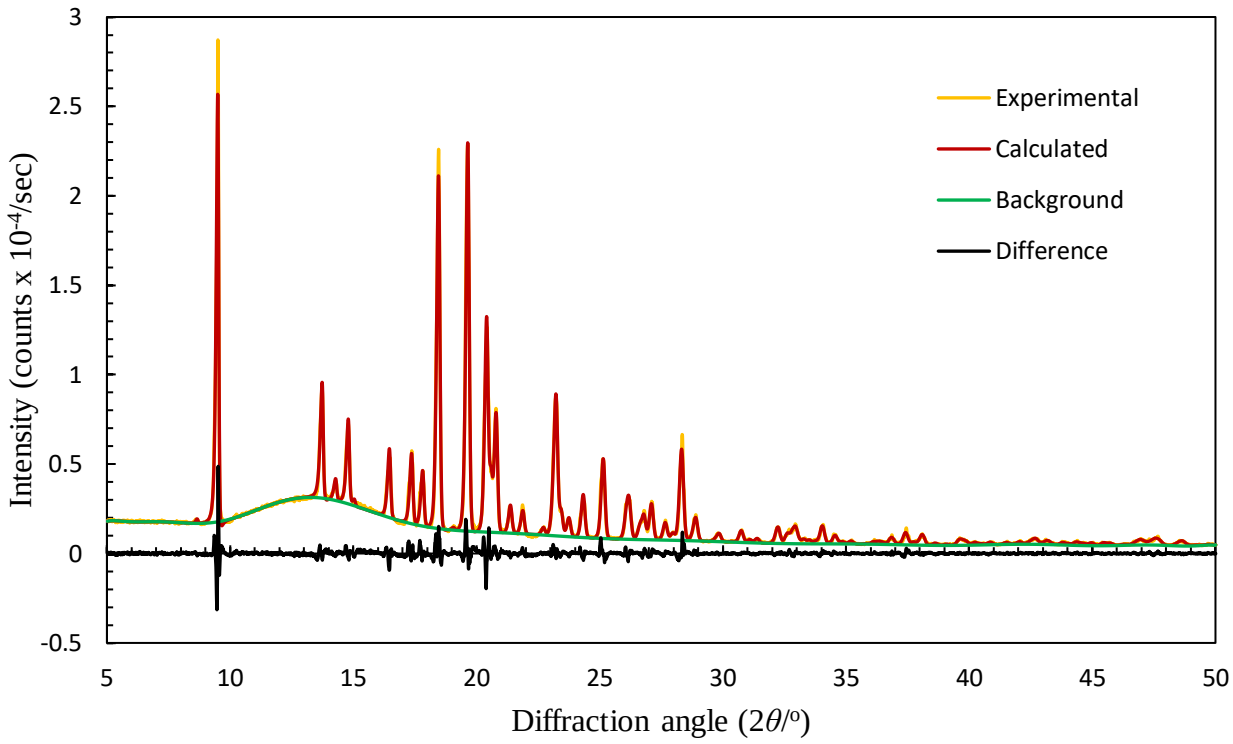


Fig. S8. Experimental and calculated Rietveld refinement plots for *R*-HL[1].

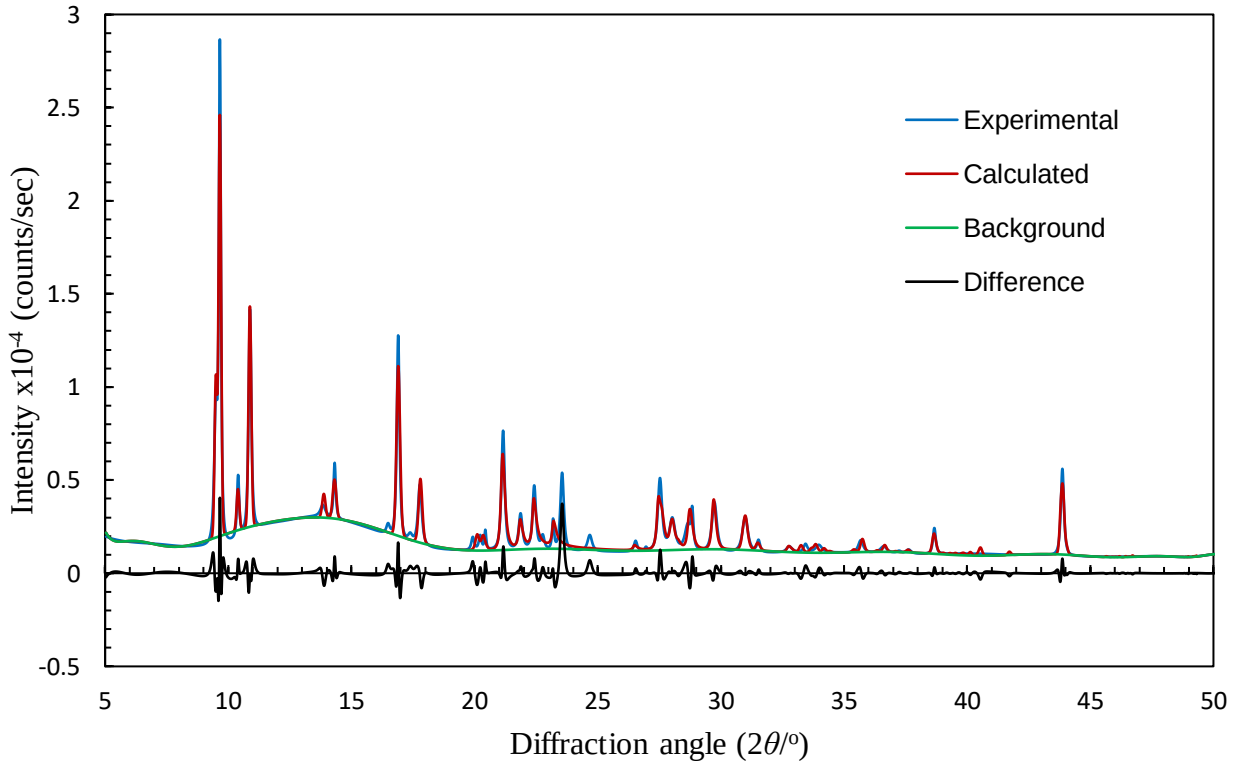


Fig. S9. Experimental and calculated Rietveld refinement plots for Cu-*R*-L[1] (calculated for Δ-Cu-*R*-L[1]).

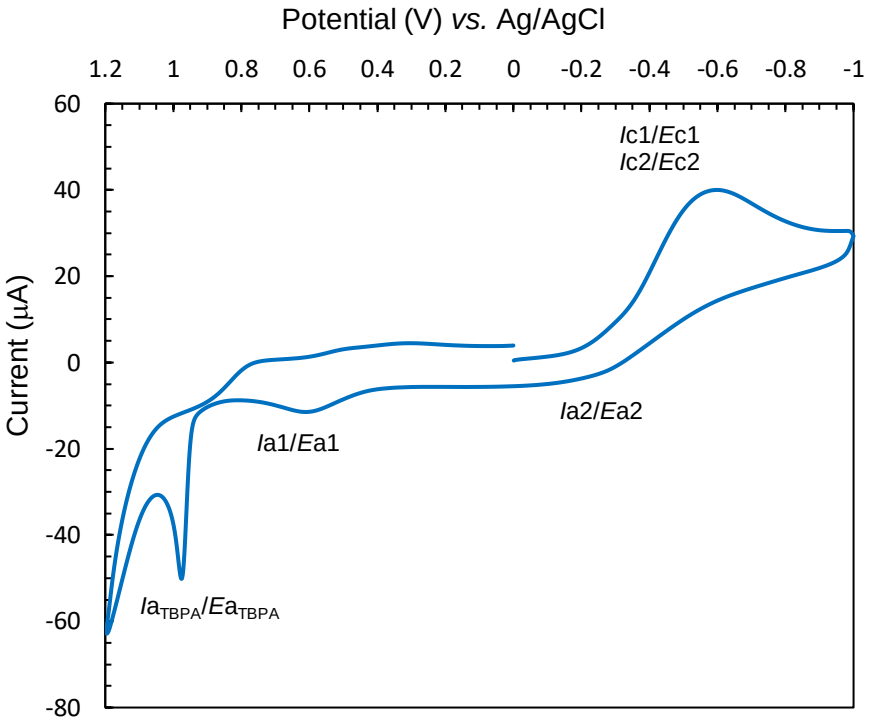


Fig. S10. Cyclic voltammogram for Cu-*R*-L[1] (0.5 mM); TBAP (0.1 M) at scan rate of 0.10 [Vs^{-1}] in acetonitrile at 25 °C.

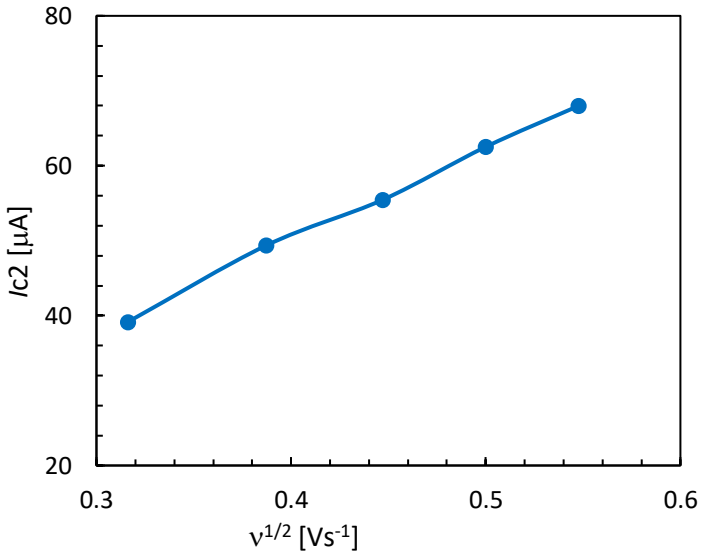


Fig. S11. Plot of *I*c2 *vs.* $\nu^{1/2}$ [Vs^{-1}] for Cu-*R*-L[1] (0.5 mM); TBAP (0.1 M) in acetonitrile at 25 °C.

Table S1. Excited states, excitation energy (eV), wavelength (nm) and oscillator strength (*f*) for Λ-Cu-*R*-L^1 at m06/sdd//b3lyp/631g(d) with PCM in chloroform.

Excited State 1: 2.015-A 1.3140 eV 943.57 nm f=0.0013 <S**2>=0.765
137B ->169B -0.14805
141B ->169B 0.14860
142B ->169B -0.19253
151B ->169B -0.16036
153B ->169B -0.40091
153B ->171B 0.10737
154B ->169B -0.13784
155B ->169B -0.17804
165B ->169B -0.11816
166B ->169B 0.12754
168B ->169B 0.72305
168B ->171B -0.11507
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2077.87388905
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.008-A 1.3994 eV 885.98 nm f=0.0008 <S**2>=0.758
132B ->169B -0.13119
135B ->169B -0.10999
140B ->169B -0.14715
141B ->169B -0.24085
144B ->169B 0.10057
148B ->169B 0.18126
149B ->169B -0.22597
151B ->169B 0.18057
152B ->169B -0.25626
154B ->169B -0.20931
155B ->169B 0.48548
155B ->171B -0.13145
163B ->169B -0.11325
164B ->169B 0.11772
165B ->169B -0.12839
167B ->169B 0.47452
168B ->169B 0.11770

Excited State 3: 2.003-A 1.8186 eV 681.76 nm f=0.0011 <S**2>=0.753
145B ->169B 0.12819

147B ->169B 0.22368
149B ->169B -0.31360
150B ->169B -0.15806
151B ->169B 0.56230
151B ->171B -0.15491
152B ->169B 0.41893
152B ->171B -0.11566
153B ->169B -0.22105
155B ->169B -0.16127
162B ->169B 0.12263
163B ->169B -0.16679

Excited State 4: 2.008-A 2.0400 eV 607.77 nm f=0.0053 <S**2>=0.758
132B ->169B 0.11052
136B ->169B 0.11882
143B ->169B 0.18665
144B ->169B 0.24975
145B ->169B -0.17761
146B ->169B 0.44913
146B ->171B -0.12777
147B ->169B 0.26745
149B ->169B 0.17158
150B ->169B 0.24128
152B ->169B -0.21566
154B ->169B 0.33727
155B ->169B -0.10979
164B ->169B 0.10441
165B ->169B -0.16164
166B ->169B 0.33557
167B ->169B 0.10395
168B ->169B -0.10213

Excited State 5: 2.708-A 2.5194 eV 492.12 nm f=0.0009 <S**2>=1.584
168A ->170A -0.12314
168A ->171A 0.16285
169A ->170A 0.26470
169A ->171A -0.11779
141B ->169B 0.15125
149B ->169B 0.11456
151B ->169B -0.16117
155B ->169B -0.25410
167B ->169B 0.67505

167B ->171B 0.15878
168B ->169B -0.18624
168B ->170B -0.27966
168B ->171B -0.19798

Excited State 6: 2.949-A 2.6567 eV 466.68 nm f=0.0055 <S**2>=1.924
168A ->170A 0.32728
169A ->171A 0.37440
142B ->169B 0.14955
153B ->169B 0.17911
154B ->169B 0.16155
161B ->169B -0.14964
165B ->169B 0.14287
166B ->169B -0.11725
167B ->169B 0.31644
167B ->170B -0.34380
168B ->169B 0.38715
168B ->170B -0.13325
168B ->171B 0.33468

Excited State 7: 3.109-A 2.7417 eV 452.21 nm f=0.0026 <S**2>=2.166
168A ->171A -0.33680
169A ->170A -0.44479
169A ->171A -0.14993
155B ->169B -0.12180
167B ->169B 0.40000
167B ->170B 0.18727
167B ->171B -0.30849
168B ->169B 0.12828
168B ->170B 0.46875

Excited State 8: 2.543-A 2.8776 eV 430.85 nm f=0.0085 <S**2>=1.367
168A ->170A -0.25463
169A ->170A 0.22720
169A ->171A -0.29167
137B ->169B 0.11426
141B ->169B -0.13272
142B ->169B 0.20483
150B ->169B 0.11171
151B ->169B 0.16426
153B ->169B 0.24939
154B ->169B 0.14849

155B ->169B 0.12925
161B ->169B -0.16669
165B ->169B 0.16610
166B ->169B -0.20114
167B ->170B 0.22444
167B ->171B 0.11616
168B ->169B 0.45614
168B ->171B -0.28349

Excited State 9: 3.284-A 3.1773 eV 390.22 nm f=0.0030 <S**2>=2.446
164A ->170A -0.27419
164A ->171A 0.21859
165A ->170A -0.17342
165A ->171A 0.13713
166A ->170A -0.21106
166A ->171A 0.16764
167A ->170A -0.13512
168A ->170A -0.11679
168A ->182A -0.12366
169A ->170A 0.10387
169A ->171A -0.10343
169A ->182A 0.13966
163B ->169B 0.19585
163B ->170B 0.16559
163B ->171B 0.20630
164B ->169B -0.14721
166B ->169B 0.36292
166B ->170B 0.21879
166B ->171B 0.25698
167B ->171B 0.11269
167B ->182B -0.13068
168B ->182B 0.14720

Excited State 10: 3.453-A 3.2865 eV 377.26 nm f=0.0003 <S**2>=2.730
163A ->170A -0.17550
163A ->171A -0.20045
164A ->170A -0.16628
164A ->171A -0.19362
165A ->170A 0.25121
165A ->171A 0.28651
168A ->181A -0.20622
169A ->181A -0.19468

161B ->170B -0.18636
161B ->171B 0.12074
164B ->169B -0.11356
164B ->170B 0.40593
164B ->171B -0.25689
164B ->181B -0.12372
167B ->181B 0.20321
168B ->181B 0.20301

Excited State 11: 2.059-A 3.3515 eV 369.94 nm f=0.0339 <S**2>=0.810
167A ->170A 0.23614
167A ->171A -0.10988
168A ->171A 0.19531
169A ->170A 0.62342
167B ->171B -0.14934
168B ->170B 0.63462
168B ->171B 0.18463

Excited State 12: 2.443-A 3.3908 eV 365.65 nm f=0.0512 <S**2>=1.243
167A ->170A 0.52652
167A ->171A -0.23112
169A ->171A 0.16965
146B ->169B 0.12457
152B ->169B -0.17139
153B ->169B -0.16294
161B ->169B -0.16545
163B ->169B 0.17596
163B ->171B 0.12030
165B ->169B 0.21941
166B ->169B -0.31813
168B ->169B -0.13836
168B ->171B -0.26004

Excited State 13: 2.156-A 3.4139 eV 363.17 nm f=0.1245 <S**2>=0.912
167A ->170A 0.49979
167A ->171A -0.22662
168A ->170A -0.30685
168A ->171A -0.11126
169A ->170A -0.12151
169A ->171A -0.38927
153B ->169B 0.11667
163B ->169B -0.11663

165B ->169B -0.14357
166B ->169B 0.10753
167B ->170B -0.24622
168B ->170B -0.26036
168B ->171B 0.35859

Excited State 14: 3.415-A 3.4872 eV 355.54 nm f=0.0044 <S**2>=2.665
157A ->176A -0.30931
159A ->173A 0.10516
159A ->174A 0.21855
159A ->180A 0.10663
160A ->170A -0.12300
160A ->173A -0.11482
160A ->174A -0.23387
160A ->180A -0.11502
164A ->174A -0.13091
164A ->176A 0.17270
157B ->176B 0.31047
158B ->176B -0.10413
159B ->169B 0.16555
159B ->170B 0.10904
159B ->171B 0.12558
159B ->173B 0.12429
159B ->174B 0.31443
159B ->175B 0.16607
159B ->180B 0.15687
163B ->169B 0.10920
163B ->176B -0.16187
165B ->176B 0.13752

Excited State 15: 3.457-A 3.5303 eV 351.20 nm f=0.0005 <S**2>=2.738
156A ->173A -0.11881
156A ->174A 0.18753
156A ->175A -0.33834
158A ->173A -0.36830
158A ->175A 0.19516
162A ->173A -0.14705
163A ->173A -0.14782
156B ->173B 0.11035
156B ->174B -0.21174
156B ->175B 0.32844
157B ->173B 0.11150

158B ->173B 0.38017
158B ->175B -0.17530
160B ->173B -0.12815
161B ->173B -0.14818

Excited State 16: 3.173-A 3.5406 eV 350.18 nm f=0.0010 <S**2>=2.267
161A ->178A 0.16616
161A ->179A 0.14027
162A ->178A -0.23275
162A ->179A 0.10748
163A ->177A -0.19391
165A ->177A -0.17779
166A ->174A -0.10311
166A ->180A 0.15587
167A ->170A 0.24133
167A ->171A 0.36074
168A ->171A -0.12433
169A ->171A 0.14838
160B ->177B -0.11088
160B ->178B 0.11410
160B ->179B 0.16769
161B ->177B -0.10649
161B ->178B -0.15374
162B ->177B -0.12230
162B ->178B 0.21416
162B ->179B -0.10480
163B ->177B -0.14422
164B ->177B -0.14099
165B ->177B -0.10022
165B ->180B -0.12047
166B ->169B 0.11607
166B ->180B -0.10409

Excited State 17: 2.827-A 3.5471 eV 349.53 nm f=0.0024 <S**2>=1.749
159A ->170A -0.11453
161A ->178A -0.11018
162A ->178A 0.16662
163A ->177A 0.13476
165A ->177A 0.12161
166A ->180A -0.10188
167A ->170A 0.33644
167A ->171A 0.52416

168A ->170A -0.18615
168A ->171A -0.21296
169A ->171A 0.27001
160B ->179B -0.11039
161B ->178B 0.10344
162B ->178B -0.14850
163B ->177B 0.10224
164B ->169B -0.12658
166B ->169B 0.11013
167B ->170B 0.11451

Excited State 18: 3.448-A 3.5633 eV 347.95 nm f=0.0006 <S**2>=2.723
157A ->180A -0.10371
161A ->177A 0.20668
161A ->178A -0.10188
161A ->179A 0.17116
162A ->178A 0.20201
162A ->179A 0.12381
163A ->179A -0.21663
165A ->179A -0.12081
166A ->174A -0.17998
166A ->180A 0.31554
157B ->180B 0.10491
160B ->177B 0.24121
161B ->178B 0.10011
161B ->179B -0.17249
162B ->178B -0.19147
162B ->179B -0.20032
163B ->179B -0.15465
165B ->174B 0.13975
165B ->180B -0.27911
166B ->174B 0.11660
166B ->180B -0.18980

Excited State 19: 2.216-A 3.6161 eV 342.87 nm f=0.0610 <S**2>=0.978
164A ->170A 0.11010
167A ->170A 0.23153
167A ->171A -0.41795
168A ->170A 0.22169
168A ->171A 0.11403
169A ->171A 0.19259
146B ->169B -0.10670

164B ->169B -0.26039
166B ->169B 0.48224
167B ->170B 0.33806
168B ->171B -0.17513

Excited State 20: 3.108-A 3.6733 eV 337.53 nm f=0.0034 <S**2>=2.165
168A ->170A -0.18159
168A ->171A 0.12129
169A ->171A 0.20832
163B ->169B -0.11419
164B ->169B 0.12103
166B ->169B -0.18260
167B ->170B 0.67430
167B ->171B 0.13453
168B ->171B 0.55374

Excited State 21: 2.739-A 3.6890 eV 336.09 nm f=0.0243 <S**2>=1.626
168A ->170A 0.40040
168A ->171A -0.33942
169A ->170A 0.30405
169A ->171A -0.38035
153B ->169B -0.11722
163B ->169B 0.30780
165B ->169B 0.14246
167B ->170B 0.22044
167B ->171B -0.32171
168B ->170B -0.26294
168B ->171B 0.26218

Excited State 22: 2.440-A 3.7221 eV 333.10 nm f=0.0765 <S**2>=1.238
168A ->170A -0.41022
168A ->171A 0.22535
169A ->170A -0.16047
153B ->169B -0.18085
161B ->169B -0.14443
162B ->169B -0.12893
163B ->169B 0.56962
165B ->169B 0.26302
166B ->169B 0.17834
167B ->170B -0.17557
167B ->182B 0.10632
168B ->171B 0.18756

168B ->182B -0.11251

Excited State 23: 2.893-A 3.7381 eV 331.67 nm f=0.0041 <S**2>=1.843
167A ->170A 0.18120
167A ->171A 0.25477
168A ->170A 0.40594
168A ->171A 0.15478
169A ->170A -0.21628
169A ->171A -0.38274
167B ->171B 0.60111
168B ->170B 0.27012
168B ->171B 0.13153

Excited State 24: 2.109-A 3.7844 eV 327.61 nm f=0.0103 <S**2>=0.862
168A ->171A -0.31473
169A ->170A 0.12351
169A ->171A 0.11153
146B ->169B -0.10895
163B ->169B 0.16245
164B ->169B 0.76016
166B ->169B 0.21992
167B ->171B 0.27600

Excited State 25: 2.155-A 3.8076 eV 325.63 nm f=0.0079 <S**2>=0.911
167A ->170A 0.17249
167A ->171A 0.25392
168A ->170A 0.14675
168A ->171A 0.60453
169A ->170A -0.20133
169A ->171A -0.15045
164B ->169B 0.39750
167B ->171B -0.46591

Excited State 26: 2.178-A 3.8693 eV 320.43 nm f=0.0031 <S**2>=0.936
161B ->169B 0.11435
163B ->169B -0.40619
165B ->169B 0.80981
166B ->169B 0.30593

Excited State 27: 3.055-A 3.9755 eV 311.87 nm f=0.0017 <S**2>=2.083
164A ->170A 0.12896
166A ->170A 0.14975

166A ->171A -0.10058
168A ->176A -0.11408
168A ->182A -0.23653
169A ->176A 0.14659
169A ->182A 0.27716
152B ->169B 0.11664
161B ->169B 0.38395
162B ->169B -0.20668
163B ->169B 0.22831
166B ->170B -0.20235
166B ->171B -0.21769
167B ->176B 0.12723
167B ->182B -0.26062
168B ->176B -0.16311
168B ->182B 0.29844

Excited State 28: 2.993-A 3.9892 eV 310.80 nm f=0.0048 <S**2>=1.989
164A ->170A -0.10587
165A ->171A 0.12153
167A ->171A -0.10622
168A ->175A -0.11404
168A ->181A 0.24139
169A ->175A -0.13101
169A ->181A 0.23479
169A ->182A -0.12807
160B ->169B 0.11281
161B ->169B 0.47293
162B ->169B -0.22034
164B ->170B 0.15208
164B ->171B -0.11198
165B ->170B -0.13142
166B ->169B -0.10675
166B ->170B 0.21933
166B ->171B 0.10918
167B ->175B 0.10975
167B ->181B -0.24206
168B ->175B 0.13784
168B ->181B -0.24636
168B ->182B -0.11864

Excited State 29: 2.927-A 4.0157 eV 308.75 nm f=0.0018 <S**2>=1.892
164A ->171A 0.12006

165A ->170A -0.15501
165A ->171A -0.11096
168A ->175A 0.11309
168A ->181A -0.21983
169A ->175A 0.12189
169A ->181A -0.22936
154B ->169B 0.10283
161B ->169B 0.48735
162B ->169B -0.33172
164B ->170B -0.18579
166B ->169B -0.12409
166B ->171B 0.12429
167B ->175B -0.11478
167B ->181B 0.22377
168B ->174B 0.10591
168B ->175B -0.12650
168B ->181B 0.24557

Excited State 30: 2.109-A 4.0507 eV 306.08 nm f=0.0019 <S**2>=0.862
160B ->169B 0.45958
161B ->169B 0.23327
162B ->169B 0.75646
163B ->169B 0.31125
166B ->169B -0.12677

Excited State 31: 2.758-A 4.1799 eV 296.62 nm f=0.0184 <S**2>=1.652
164A ->170A 0.15988
165A ->171A -0.10471
169A ->182A 0.10452
153B ->169B -0.13862
155B ->169B 0.21043
159B ->169B 0.34365
160B ->170B 0.10937
161B ->170B 0.21755
161B ->171B 0.12237
163B ->170B -0.27255
163B ->171B -0.11767
165B ->170B -0.33650
165B ->171B -0.13617
166B ->170B 0.44551
166B ->171B 0.18275
168B ->182B 0.12177

Excited State 32: 2.138-A 4.2364 eV 292.67 nm f=0.0011 <S**2>=0.893
160B ->169B 0.83569
161B ->169B -0.35040
162B ->169B -0.37126

Excited State 33: 2.488-A 4.2656 eV 290.66 nm f=0.0152 <S**2>=1.297
157A ->176A 0.13879
157B ->176B -0.12411
159B ->169B 0.81315
159B ->170B 0.14081
163B ->170B 0.17477
165B ->170B 0.21672
166B ->170B -0.26268

Excited State 34: 2.773-A 4.2982 eV 288.45 nm f=0.0001 <S**2>=1.672
168B ->172B 0.97992

Excited State 35: 2.853-A 4.3436 eV 285.44 nm f=0.0383 <S**2>=1.784
164A ->171A -0.10141
165A ->170A 0.13016
152B ->170B 0.11411
155B ->170B 0.18659
159B ->169B -0.14096
160B ->171B 0.10274
161B ->171B 0.21129
163B ->170B 0.16284
163B ->171B -0.28872
165B ->170B 0.18885
165B ->171B -0.41601
166B ->170B -0.20656
166B ->171B 0.57430

Excited State 36: 2.880-A 4.3749 eV 283.40 nm f=0.0000 <S**2>=1.823
169A ->172A 0.98187

Excited State 37: 2.738-A 4.3849 eV 282.75 nm f=0.0128 <S**2>=1.624
157A ->174A -0.11526
160A ->176A -0.11940
164A ->170A 0.12217
166A ->170A -0.19460
166A ->171A 0.13391

155B ->169B 0.11137
157B ->169B 0.68223
157B ->170B 0.12377
157B ->171B 0.11065
157B ->174B 0.12573
158B ->169B -0.32622
159B ->176B 0.11991
163B ->171B -0.13193
165B ->170B 0.15014

Excited State 38: 3.261-A 4.4102 eV 281.13 nm f=0.0006 <S**2>=2.408
166A ->170A -0.16392
168A ->174A 0.15684
169A ->173A -0.16668
169A ->174A -0.25026
169A ->176A 0.12572
155B ->169B -0.21522
157B ->169B -0.11385
158B ->169B 0.10029
159B ->169B -0.10108
167B ->174B -0.23341
167B ->175B -0.10669
167B ->176B 0.12127
168B ->173B 0.22437
168B ->174B 0.39980
168B ->175B 0.22025
168B ->176B -0.19249

Excited State 39: 2.411-A 4.4294 eV 279.91 nm f=0.0163 <S**2>=1.203
163A ->170A 0.10311
141B ->169B 0.14205
149B ->169B 0.10135
151B ->169B -0.13753
152B ->169B 0.15126
153B ->169B -0.17555
154B ->169B 0.28060
155B ->169B 0.47493
157B ->169B -0.30352
158B ->169B -0.31594
159B ->169B -0.15961
161B ->170B -0.11401
164B ->169B 0.11038

164B ->170B 0.11190
166B ->170B -0.17806
168B ->173B 0.11883
168B ->174B 0.14181

Excited State 40: 3.003-A 4.4705 eV 277.34 nm f=0.0043 <S**2>=2.005
164A ->170A -0.21995
164A ->171A 0.15772
166A ->170A 0.54580
166A ->171A -0.32740
166A ->179A 0.13448
157B ->169B 0.36102
165B ->171B -0.11796
167B ->174B -0.13301
168B ->173B 0.17238
168B ->174B 0.22532
168B ->175B 0.11761

Excited State 41: 2.500-A 4.4744 eV 277.10 nm f=0.0223 <S**2>=1.312
156A ->175A 0.12831
160A ->170A 0.12366
164A ->170A 0.13428
152B ->169B 0.14443
155B ->169B 0.19599
156B ->169B 0.22823
156B ->175B -0.11792
157B ->169B 0.13954
158B ->169B 0.68787
158B ->170B -0.10389
163B ->170B 0.10369

Excited State 42: 3.115-A 4.4922 eV 276.00 nm f=0.0010 <S**2>=2.175
168A ->173A -0.11875
169A ->173A -0.13356
169A ->174A 0.11243
167B ->172B -0.53493
167B ->173B 0.35795
168B ->173B 0.61345
168B ->174B -0.24646

Excited State 43: 2.706-A 4.5107 eV 274.86 nm f=0.0456 <S**2>=1.581
157A ->170A 0.12619

157A ->176A 0.10092
160A ->170A -0.25370
160A ->171A 0.14359
161A ->170A -0.10691
164A ->170A -0.20304
164A ->171A 0.15989
165A ->170A -0.22155
166A ->170A -0.11354
167A ->171A -0.10723
169A ->176A 0.10318
154B ->169B 0.27198
157B ->169B 0.18001
158B ->169B 0.32850
159B ->169B -0.12185
159B ->176B -0.10088
163B ->171B -0.11234
164B ->170B 0.14229
166B ->170B -0.17217
166B ->171B -0.15951
167B ->172B -0.19129
168B ->173B -0.12455

Excited State 44: 2.781-A 4.5212 eV 274.23 nm f=0.0028 <S**2>=1.683
168A ->172A 0.14806
168A ->173A -0.11941
169A ->174A 0.14731
167B ->172B 0.79261
167B ->173B 0.20261
168B ->173B 0.36158
168B ->174B -0.17527

Excited State 45: 2.338-A 4.5589 eV 271.96 nm f=0.0083 <S**2>=1.117
168A ->172A -0.26315
168A ->174A -0.25973
168A ->175A -0.11013
169A ->173A 0.60703
169A ->174A 0.31454
169A ->176A -0.11141
167B ->174B -0.10933
167B ->175B -0.10449
168B ->173B 0.27286
168B ->174B 0.32799

Excited State 46: 2.987-A 4.5640 eV 271.66 nm f=0.0188 <S**2>=1.980

159A ->170A	0.11637
161A ->170A	0.14795
161A ->177A	-0.10319
161A ->178A	0.14700
162A ->170A	0.16759
162A ->171A	0.11576
162A ->177A	0.16427
162A ->178A	-0.10607
163A ->170A	0.36469
163A ->171A	0.24169
163A ->178A	0.12616
165A ->170A	0.13095
165A ->171A	0.11044
165A ->178A	0.10728
167A ->171A	0.14875
168A ->174A	0.10414
169A ->173A	-0.14847
156B ->169B	-0.20800
160B ->178B	0.19062
161B ->177B	0.10817
162B ->177B	-0.15733
162B ->178B	0.13717
164B ->170B	0.21357
168B ->175B	-0.19114

Excited State 47: 2.752-A 4.5655 eV 271.57 nm f=0.0014 <S**2>=1.643

168A ->172A	0.78308
168A ->173A	-0.20681
169A ->174A	0.32992
169A ->175A	0.10642
167B ->172B	-0.10341
167B ->173B	-0.11655
168B ->173B	-0.10076
168B ->174B	0.27547
168B ->175B	0.11231

Excited State 48: 2.873-A 4.5788 eV 270.78 nm f=0.0096 <S**2>=1.814

156A ->173A	-0.12619
157A ->176A	0.12389
158A ->175A	-0.12292

160A ->170A -0.17237
166A ->170A 0.10029
168A ->172A -0.11265
156B ->169B 0.45638
156B ->173B 0.14357
157B ->176B -0.13494
158B ->175B 0.10510
159B ->169B -0.11148
165B ->170B 0.21609
165B ->171B 0.19880
166B ->170B 0.18340
168B ->176B -0.10415

Excited State 49: 3.198-A 4.5808 eV 270.66 nm f=0.0008 <S**2>=2.307
161A ->177A -0.10322
161A ->179A 0.11131
162A ->170A 0.17796
162A ->171A 0.14002
162A ->178A 0.20867
163A ->177A -0.16668
165A ->177A -0.16219
165A ->178A 0.13166
166A ->170A -0.10227
169A ->174A -0.17693
156B ->169B 0.29664
156B ->173B 0.10673
157B ->169B -0.10279
158B ->169B -0.12259
160B ->177B -0.16063
160B ->179B 0.13779
161B ->170B 0.14234
161B ->178B 0.14315
162B ->170B -0.17756
162B ->177B -0.12557
162B ->178B -0.17637
163B ->177B -0.11797
164B ->177B -0.12680
164B ->178B 0.12214
165B ->170B -0.12775
165B ->177B -0.12531
168B ->177B -0.11008

Excited State 50: 3.142-A 4.5868 eV 270.31 nm f=0.0051 <S**2>=2.219

159A ->170A	-0.19874
160A ->171A	-0.10030
161A ->177A	-0.10334
161A ->178A	0.11509
161A ->179A	-0.13966
162A ->170A	-0.13609
162A ->178A	-0.14294
162A ->179A	-0.13046
163A ->177A	0.12571
164A ->170A	-0.18223
165A ->177A	0.12198
166A ->170A	-0.10397
166A ->180A	0.13990
156B ->169B	0.34361
156B ->173B	0.11003
160B ->170B	0.10569
160B ->178B	0.11523
160B ->179B	-0.13514
161B ->170B	0.12537
161B ->177B	0.13795
162B ->178B	0.15773
162B ->179B	0.15377
163B ->177B	0.12126
164B ->177B	0.10411
165B ->171B	-0.17549
165B ->174B	0.11043
165B ->180B	-0.11534
166B ->170B	-0.11857

Excited State 51: 2.562-A 4.5893 eV 270.16 nm f=0.0097 <S**2>=1.390

160A ->170A	0.14584
163A ->170A	0.11939
164A ->170A	0.13486
166A ->171A	0.13630
168A ->172A	-0.30440
168A ->173A	-0.24588
169A ->173A	-0.32154
169A ->174A	0.34805
155B ->169B	-0.14245
156B ->169B	0.18751
164B ->170B	0.11601

165B ->170B -0.19801
165B ->171B -0.12364
168B ->173B -0.13318
168B ->174B 0.22508

Excited State 52: 3.036-A 4.5973 eV 269.69 nm f=0.0117 <S**2>=2.054
159A ->170A 0.18815
161A ->179A -0.12069
162A ->177A -0.16082
163A ->170A 0.19764
164A ->171A 0.13989
166A ->170A 0.22204
166A ->174A -0.10085
166A ->179A -0.17059
166A ->180A 0.12172
167A ->171A 0.11474
168A ->172A 0.20265
168A ->173A 0.14410
169A ->173A 0.23041
169A ->174A -0.10681
169A ->175A -0.10160
155B ->169B -0.11590
156B ->169B 0.18095
160B ->178B -0.10799
162B ->177B 0.17060
165B ->171B 0.12740
165B ->179B 0.15775
166B ->179B 0.10871

Excited State 53: 3.007-A 4.6023 eV 269.40 nm f=0.0007 <S**2>=2.010
160A ->170A 0.11490
161A ->170A 0.18832
161A ->177A 0.17184
162A ->178A -0.10918
162A ->179A 0.10693
163A ->170A 0.10707
163A ->179A -0.11550
164A ->170A 0.12124
165A ->178A -0.10450
166A ->170A -0.11792
166A ->171A 0.13146
166A ->179A 0.12828

168A ->172A 0.30566
168A ->173A 0.25363
169A ->173A 0.26184
169A ->174A -0.25814
156B ->169B 0.14031
160B ->177B 0.19105
162B ->179B -0.13889
165B ->170B -0.18693
165B ->171B -0.15850
165B ->179B -0.13439

Excited State 54: 3.051-A 4.6144 eV 268.69 nm f=0.0068 <S**2>=2.077
157A ->176A -0.19988
159A ->170A -0.20822
159A ->174A -0.14084
160A ->170A 0.13008
160A ->171A -0.13581
160A ->174A 0.14410
161A ->179A 0.13064
163A ->179A -0.10112
164A ->170A -0.12638
164A ->176A 0.14078
165A ->170A -0.13050
166A ->170A 0.10513
166A ->174A 0.11265
166A ->180A -0.14773
155B ->169B -0.13988
157B ->176B 0.22109
159B ->169B 0.21052
159B ->171B -0.10385
159B ->174B -0.19381
162B ->177B -0.10357
162B ->179B -0.12082
163B ->170B -0.12035
163B ->171B -0.15594
163B ->176B -0.14740
165B ->170B 0.18534
165B ->171B 0.16702
165B ->176B 0.11270
165B ->180B 0.14016

Excited State 55: 3.208-A 4.6246 eV 268.10 nm f=0.0119 <S**2>=2.322

156A ->174A -0.11751
156A ->175A 0.36168
158A ->170A 0.12100
158A ->171A 0.12376
158A ->173A -0.25589
158A ->174A 0.15598
162A ->173A -0.12734
163A ->173A -0.10345
163A ->175A 0.11791
165A ->170A 0.10685
169A ->175A 0.17991
156B ->174B 0.17507
156B ->175B -0.35995
158B ->169B -0.23910
158B ->173B 0.26580
158B ->174B -0.12612
161B ->173B -0.11128
164B ->170B -0.15840
168B ->175B 0.11398

Excited State 56: 2.528-A 4.6288 eV 267.86 nm f=0.0326 <S**2>=1.348
159A ->170A 0.13611
160A ->170A 0.15293
161A ->170A 0.11953
163A ->170A 0.15963
165A ->170A 0.17380
165A ->171A 0.18599
166A ->171A 0.11222
166A ->179A -0.12002
168A ->172A -0.10297
168A ->175A 0.11092
169A ->175A 0.22598
157B ->169B 0.17474
159B ->176B -0.11237
163B ->170B -0.13852
164B ->170B -0.18123
164B ->171B 0.10897
165B ->170B -0.13292
167B ->174B -0.14232
167B ->175B 0.18716
168B ->174B -0.13852
168B ->175B 0.49145

Excited State 57: 3.053-A 4.6386 eV 267.29 nm f=0.0031 <S**2>=2.081

157A ->174A	-0.10304
159A ->171A	0.12762
160A ->171A	0.13093
160A ->176A	-0.11771
161A ->171A	0.11255
163A ->171A	0.15040
164A ->179A	-0.10801
166A ->170A	0.14476
166A ->177A	0.15213
166A ->179A	0.22910
154B ->169B	0.10440
157B ->169B	-0.13528
158B ->169B	0.12302
159B ->176B	0.15288
162B ->180B	-0.10467
165B ->170B	0.19861
165B ->171B	0.23919
165B ->177B	-0.12250
165B ->179B	-0.18828
166B ->170B	0.13221
166B ->179B	-0.13020
168B ->174B	-0.14394
168B ->175B	0.21581

Excited State 58: 2.830-A 4.6719 eV 265.38 nm f=0.0140 <S**2>=1.752

157A ->170A	-0.15163
157A ->171A	0.10863
157A ->174A	-0.12239
159A ->176A	0.11101
160A ->174A	-0.10826
160A ->176A	-0.11089
164A ->170A	-0.18203
164A ->171A	0.14173
165A ->170A	-0.14533
169A ->176A	0.13419
157B ->169B	-0.29903
157B ->174B	0.11092
159B ->174B	0.11657
159B ->176B	0.14363
163B ->170B	-0.24870

163B ->171B -0.19224
164B ->170B 0.11589
167B ->176B -0.11946
168B ->174B 0.12454
168B ->175B 0.15459
168B ->176B 0.31082

Excited State 59: 2.972-A 4.6843 eV 264.68 nm f=0.0106 <S**2>=1.958
156A ->171A -0.10412
156A ->173A 0.27504
156A ->174A -0.12156
158A ->175A 0.29845
165A ->170A 0.11914
165A ->171A 0.10020
156B ->169B 0.53864
156B ->173B -0.26996
158B ->169B -0.10405
158B ->174B 0.14123
158B ->175B -0.30422
168B ->175B -0.14084

Excited State 60: 2.586-A 4.6955 eV 264.05 nm f=0.0562 <S**2>=1.422
159A ->170A 0.12156
159A ->171A -0.26320
160A ->170A 0.10818
160A ->171A -0.19890
161A ->171A -0.21357
162A ->171A -0.16308
163A ->170A 0.14986
163A ->171A -0.29265
164A ->170A 0.13536
165A ->170A -0.22097
165A ->171A -0.28655
166A ->171A -0.13279
167A ->170A -0.14691
154B ->169B 0.19158
155B ->169B -0.10230
156B ->169B 0.11249
164B ->170B 0.23925
167B ->175B 0.13068
168B ->174B -0.16240
168B ->175B 0.34363

168B ->181B 0.10155

Excited State 61: 2.604-A 4.7052 eV 263.50 nm f=0.0852 <S**2>=1.445
159A ->170A -0.16237
159A ->171A 0.19832
160A ->170A -0.11031
160A ->171A 0.13346
161A ->170A -0.10870
161A ->171A 0.12735
163A ->170A -0.14660
163A ->171A 0.26684
164A ->170A 0.15643
164A ->171A 0.15153
165A ->170A -0.24898
165A ->171A -0.10069
169A ->176A -0.17113
154B ->169B -0.13594
156B ->169B 0.12070
163B ->170B 0.18612
164B ->170B 0.23880
164B ->171B -0.13204
165B ->170B -0.14368
167B ->175B 0.11536
167B ->176B 0.10583
167B ->181B 0.10370
168B ->174B -0.20682
168B ->175B 0.31553
168B ->176B -0.25651
168B ->181B 0.11413

Excited State 62: 3.088-A 4.7404 eV 261.55 nm f=0.0135 <S**2>=2.134
157A ->174A -0.12501
159A ->171A -0.12417
160A ->176A -0.12730
163A ->170A 0.13066
164A ->170A -0.10226
168A ->175A 0.15918
169A ->175A 0.42965
169A ->176A -0.12145
154B ->169B 0.12165
157B ->174B 0.11499
159B ->176B 0.17140

165B ->170B -0.17072
165B ->171B -0.13205
166B ->170B -0.16737
167B ->176B 0.14433
168B ->174B -0.11454
168B ->175B -0.20273
168B ->176B -0.38887

Excited State 63: 3.208-A 4.7437 eV 261.37 nm f=0.0309 <S**2>=2.323
151A ->171A -0.11068
152A ->170A 0.11518
153A ->171A 0.10653
162A ->177A -0.13483
163A ->171A 0.15537
168A ->175A 0.14257
169A ->173A -0.12292
169A ->174A -0.13306
169A ->175A 0.33994
151B ->170B 0.16202
154B ->169B -0.11127
159B ->176B -0.13237
162B ->177B 0.12338
163B ->171B -0.11979
164B ->170B 0.29938
164B ->181B 0.10748
165B ->170B 0.20214
168B ->176B 0.11562

Excited State 64: 3.214-A 4.7649 eV 260.20 nm f=0.0156 <S**2>=2.333
152A ->171A -0.12668
153A ->170A -0.11092
159A ->171A 0.11367
160A ->170A 0.10576
163A ->170A -0.11900
165A ->170A -0.13178
166A ->170A -0.10236
168A ->175A 0.14273
168A ->181A 0.12681
169A ->174A -0.25839
169A ->175A 0.30524
169A ->176A -0.17274
169A ->181A 0.13368

151B ->171B 0.10109
159B ->176B -0.11460
163B ->170B -0.23486
165B ->170B 0.10385
165B ->171B 0.12890
167B ->181B -0.13241
168B ->175B -0.14812
168B ->176B -0.25782
168B ->181B -0.15150

Excited State 65: 2.717-A 4.7690 eV 259.98 nm f=0.0500 <S**2>=1.595
162A ->170A -0.12610
163A ->170A -0.16612
164A ->170A 0.22366
166A ->170A 0.18374
168A ->175A 0.16391
168A ->181A 0.11404
169A ->175A 0.39980
169A ->176A 0.18219
169A ->181A 0.12444
163B ->170B 0.26014
163B ->171B 0.13952
164B ->171B -0.12164
165B ->170B -0.14845
167B ->176B -0.12972
168B ->174B 0.10991
168B ->176B 0.46432

Excited State 66: 3.070-A 4.8041 eV 258.08 nm f=0.0037 <S**2>=2.106
159A ->170A -0.11762
159A ->171A -0.13859
160A ->170A -0.15566
166A ->171A -0.10731
168A ->176A 0.11760
169A ->174A -0.19240
169A ->176A -0.31215
154B ->169B 0.10138
155B ->170B -0.12913
166B ->170B -0.10378
167B ->173B 0.41258
168B ->173B -0.22309
168B ->174B 0.20483

168B ->175B 0.12171
168B ->176B 0.11501
168B ->177B -0.35578
168B ->178B -0.26234
168B ->179B 0.11756

Excited State 67: 2.954-A 4.8189 eV 257.29 nm f=0.0082 <S**2>=1.932
159A ->170A 0.10829
163A ->171A -0.11006
164A ->170A -0.10234
168A ->176A -0.11637
169A ->173A 0.13768
169A ->176A 0.33626
154B ->169B -0.13153
158B ->170B -0.16108
158B ->171B 0.12464
160B ->170B 0.16702
161B ->170B 0.32827
162B ->170B -0.14465
163B ->170B 0.24727
163B ->171B -0.13703
166B ->170B 0.11448
166B ->171B -0.17094
167B ->173B 0.15605
168B ->173B -0.17411
168B ->176B -0.21231
168B ->177B -0.28574
168B ->178B -0.16020
168B ->182B -0.11894

Excited State 68: 2.708-A 4.8385 eV 256.25 nm f=0.0125 <S**2>=1.583
158A ->170A 0.17758
158A ->171A 0.16532
159A ->170A -0.31406
160A ->171A -0.16682
161A ->170A -0.11301
162A ->170A 0.13637
162A ->171A 0.18049
163A ->171A 0.14777
166A ->171A -0.19393
168A ->176A -0.15943
169A ->174A 0.11738

169A ->175A 0.14371
169A ->176A 0.51292
169A ->182A -0.12766
160B ->170B -0.11596
161B ->170B -0.25459
163B ->171B 0.11272
168B ->176B -0.12508

Excited State 69: 3.137-A 4.8491 eV 255.68 nm f=0.0031 <S**2>=2.210
158A ->170A -0.17642
158A ->171A -0.17736
159A ->170A 0.13078
162A ->170A -0.12485
163A ->171A -0.10333
166A ->170A 0.10511
166A ->171A 0.17201
169A ->174A 0.13300
169A ->176A 0.23350
169A ->177A -0.11220
151B ->170B 0.10245
158B ->170B 0.16467
158B ->171B -0.10922
158B ->173B 0.10123
163B ->170B -0.22783
163B ->171B 0.13107
166B ->170B -0.19624
166B ->171B 0.17247
167B ->173B 0.37999
168B ->173B -0.10302
168B ->175B 0.10388
168B ->176B -0.12581
168B ->177B -0.19275

Excited State 70: 3.022-A 4.8672 eV 254.73 nm f=0.0045 <S**2>=2.034
159A ->170A 0.10757
162A ->170A 0.12988
164A ->171A -0.10880
165A ->170A -0.13750
166A ->170A -0.16642
166A ->171A -0.18251
168A ->173A 0.17940
169A ->173A -0.15347

169A ->177A -0.12560
155B ->170B 0.19542
163B ->171B -0.11353
166B ->170B 0.14727
166B ->171B -0.15731
167B ->173B 0.23783
167B ->174B 0.50354
167B ->175B 0.25482
168B ->174B 0.28066
168B ->175B 0.11667

Excited State 71: 2.741-A 4.8709 eV 254.54 nm f=0.0059 <S**2>=1.629
157A ->170A -0.12849
158A ->171A -0.10821
159A ->170A -0.23002
159A ->171A 0.14664
160A ->170A 0.19115
160A ->171A -0.13710
161A ->170A -0.12104
162A ->170A -0.23697
164A ->171A 0.12621
165A ->170A 0.26319
166A ->170A 0.19107
166A ->171A 0.14881
168A ->173A -0.15173
169A ->174A -0.12838
169A ->177A 0.10795
154B ->169B 0.21921
155B ->170B -0.13004
167B ->174B 0.43276
167B ->175B 0.22840
168B ->174B 0.13117
168B ->176B -0.15341

Excited State 72: 2.588-A 4.8746 eV 254.35 nm f=0.0173 <S**2>=1.424
157A ->170A 0.11250
159A ->170A 0.11112
160A ->170A -0.12167
161A ->170A -0.18343
161A ->171A 0.13950
162A ->170A -0.18692
163A ->170A 0.36421

163A ->171A -0.13900
164A ->170A -0.18615
165A ->170A 0.11719
165A ->171A -0.27944
166A ->170A -0.11791
167A ->172A -0.23970
168A ->173A -0.21332
168A ->174A 0.11868
169A ->173A 0.14872
169A ->177A 0.15800
169A ->178A 0.10142
154B ->169B -0.23262
163B ->170B -0.10009
164B ->170B 0.12336
166B ->171B 0.10152
167B ->174B 0.10303
168B ->177B 0.14705
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 72 LETran= 1306.