Supporting Information (SI)

Polymorphism, Mesomorphism and Anti-Oxidant Character of Homoleptic *Bis*[(*E*)-2-(1-((*o*-ethylphenyl)imino)ethyl)phenolato-κ^2-*N*,*O*]Ni/Cu(II) Complexes

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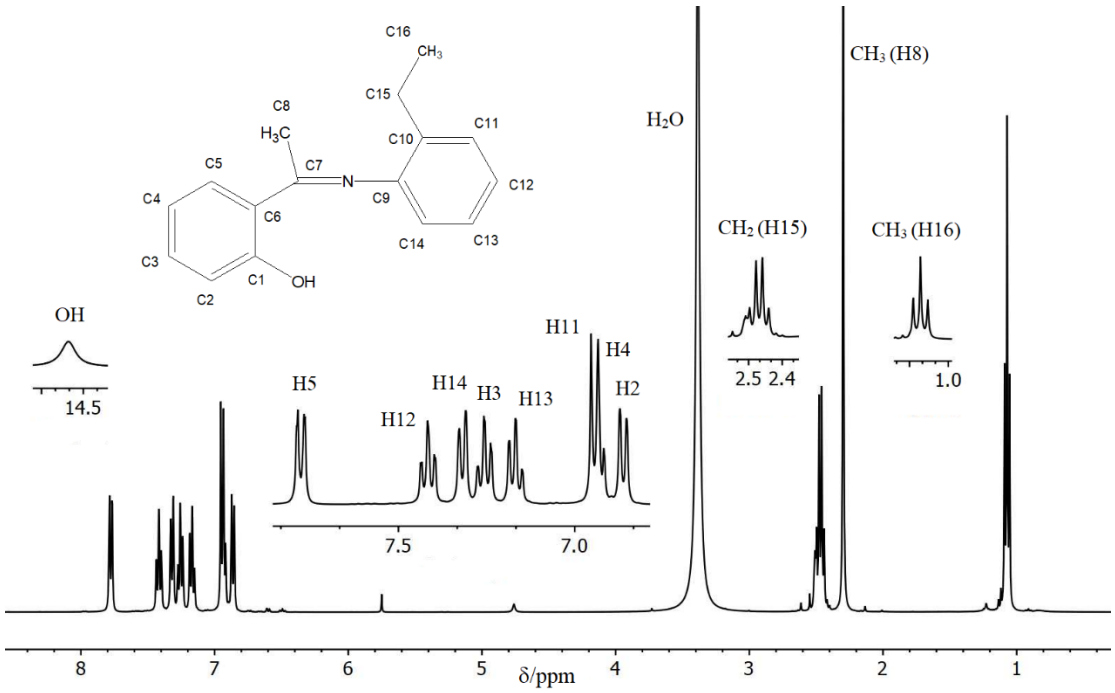


Figure S1a. ^{1}H NMR (400Hz) spectrum of H**L** in DMSO-d_6 solvent at 20 °C.

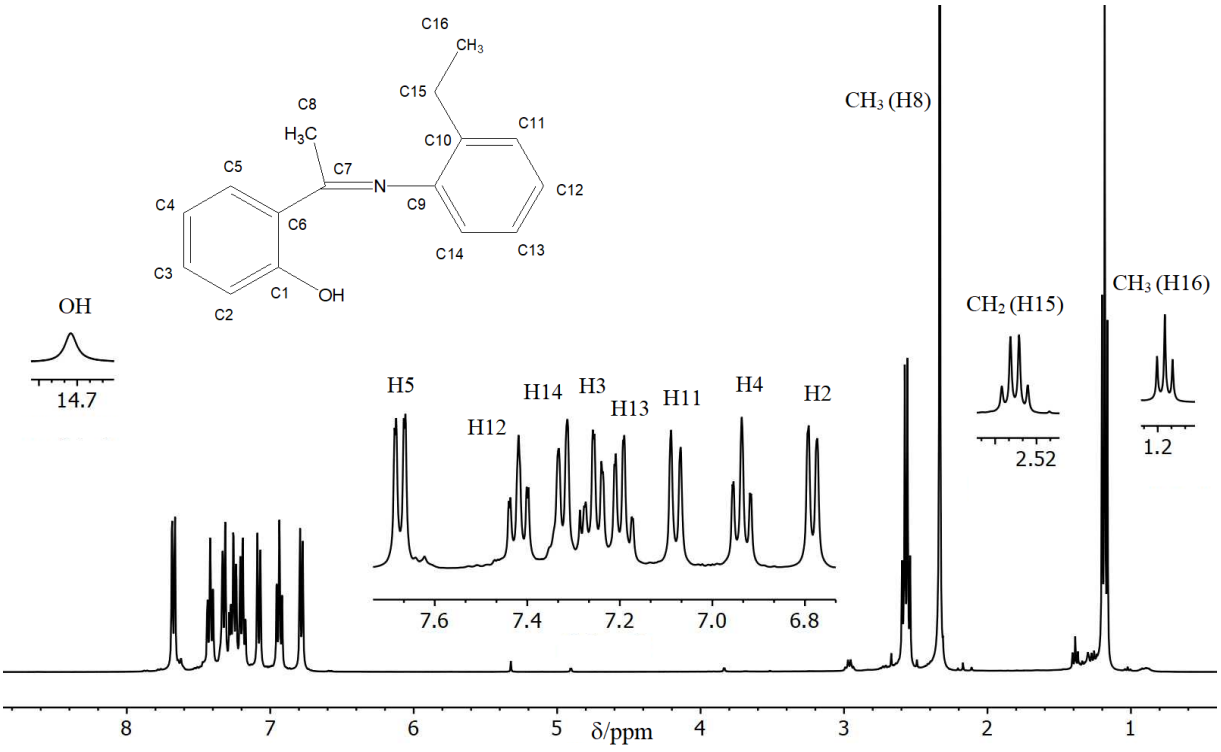


Figure S1b. ^{1}H NMR spectrum for H**L** in $CDCl_3$ at 20 °C.

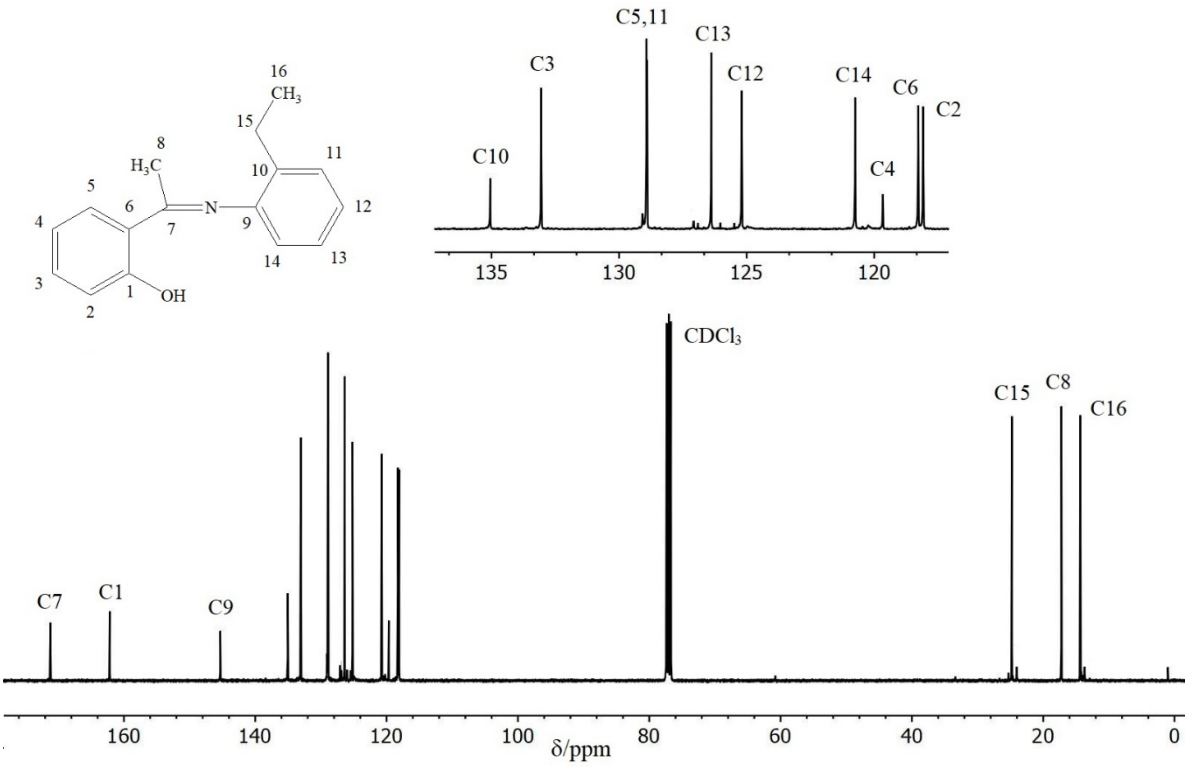
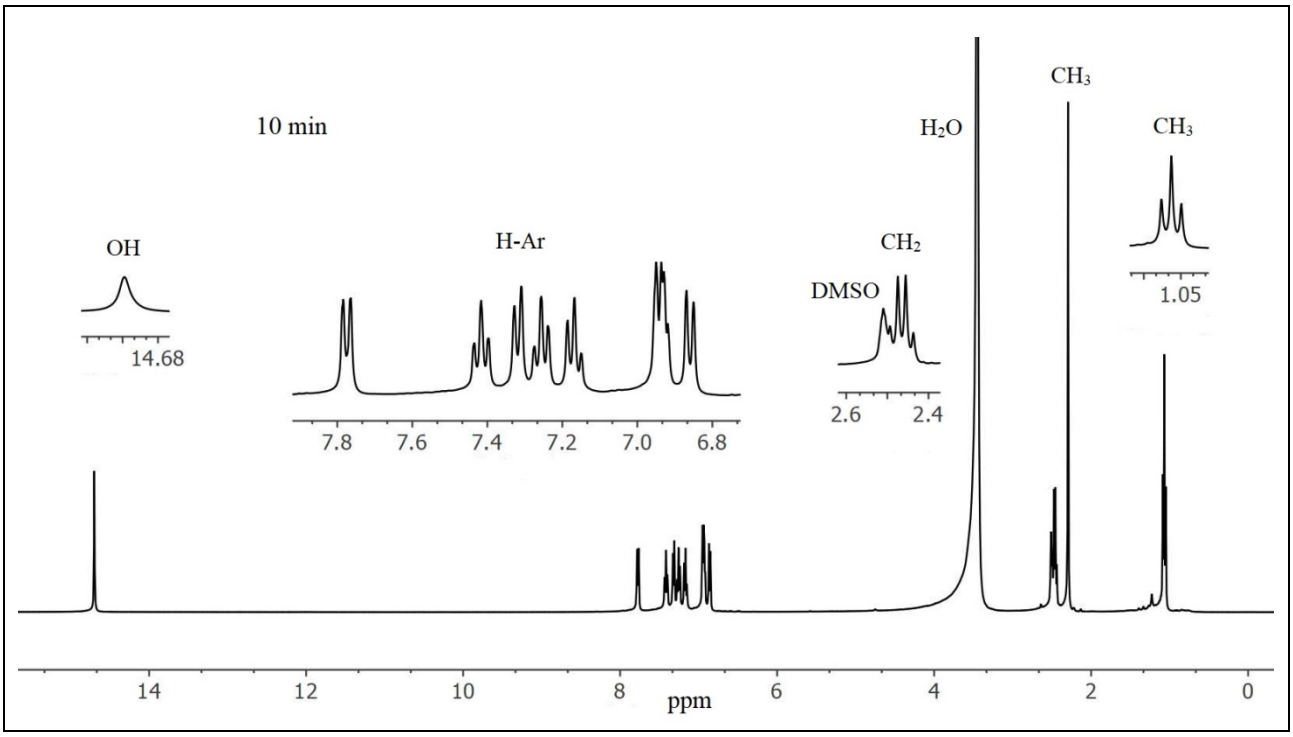


Figure S2. ^{13}C NMR spectrum for H**L** in $CDCl_3$ at 20 °C.



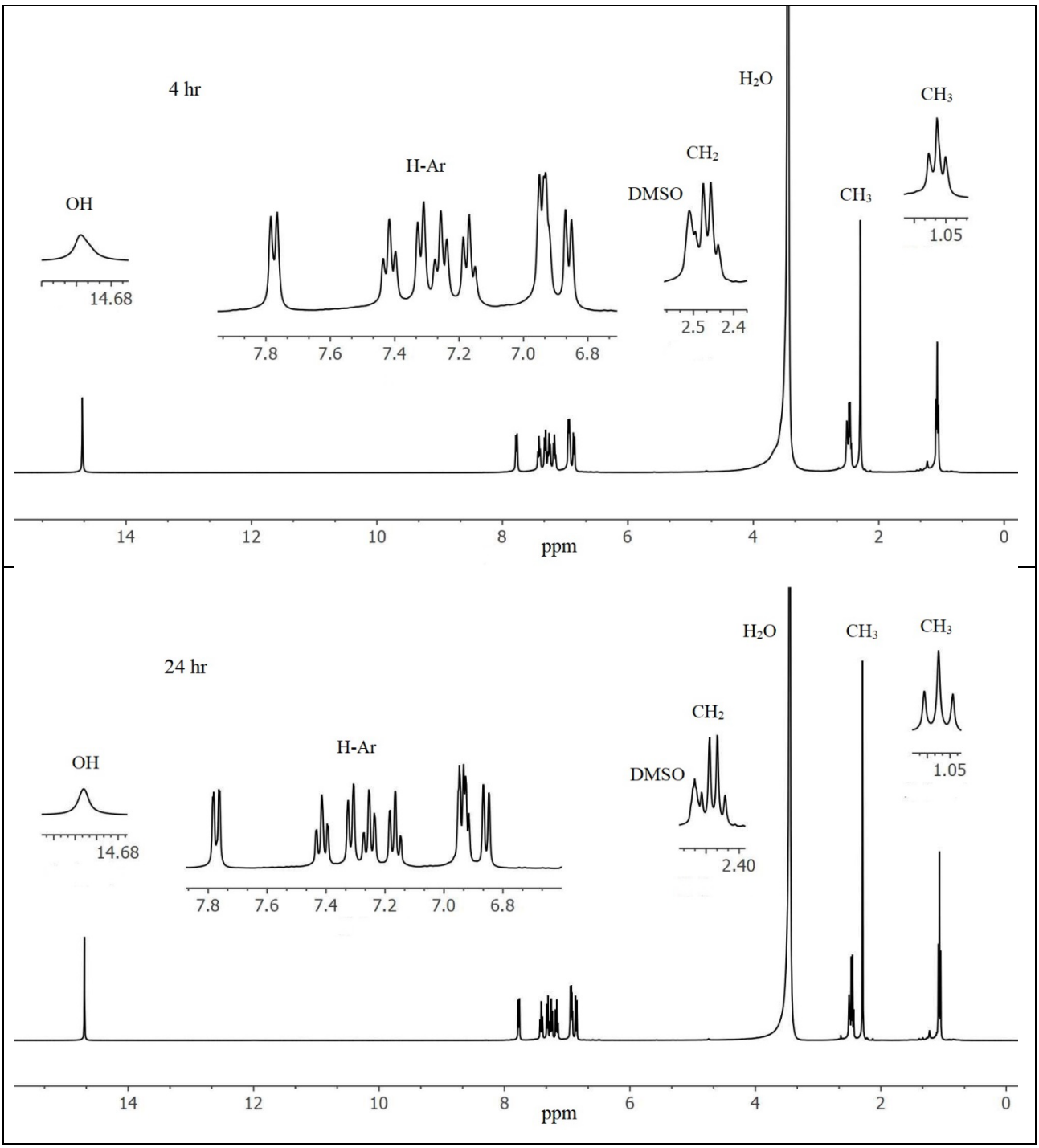
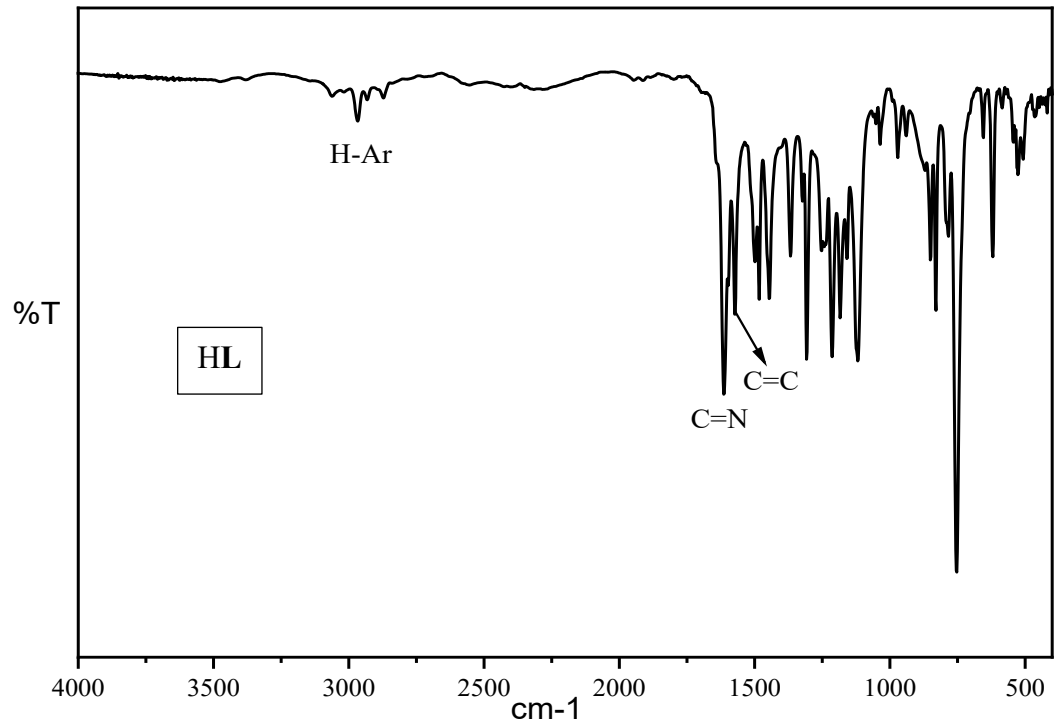


Figure S3. ^{1}H NMR spectra for H**L** at different time intervals in DMSO-d_6 at 20 °C.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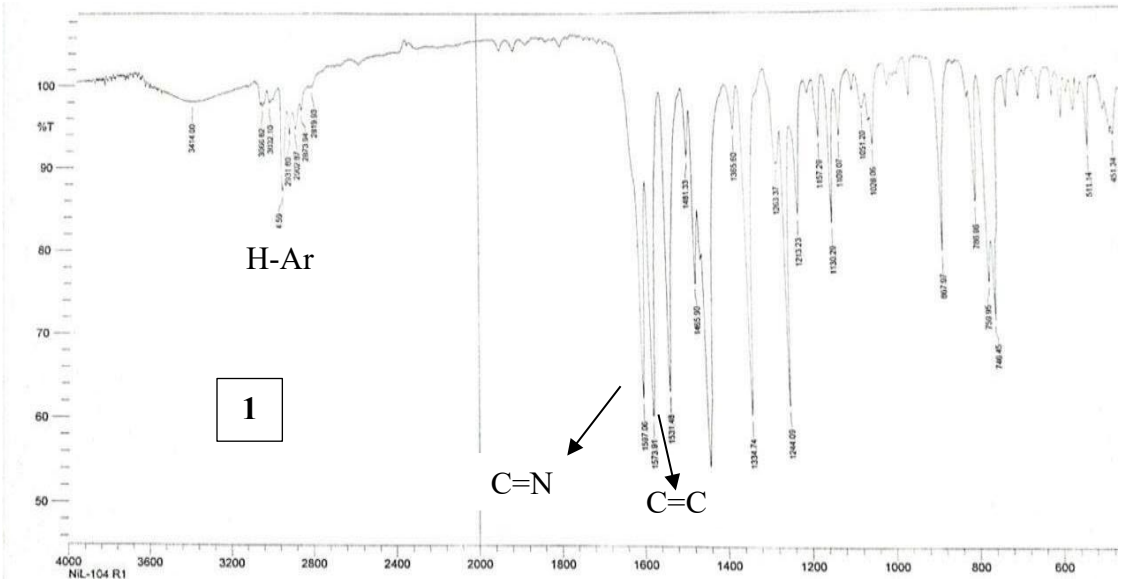
C=N
4000
3500
3000
2500
2000
1500
1000
500
cm-1


H-Ar
1
C=N
C=C
100
%T
90
80
70
60
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3200
2800
2400
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1800
1600
1400
1200
1000
800
600
NiL-104 R1

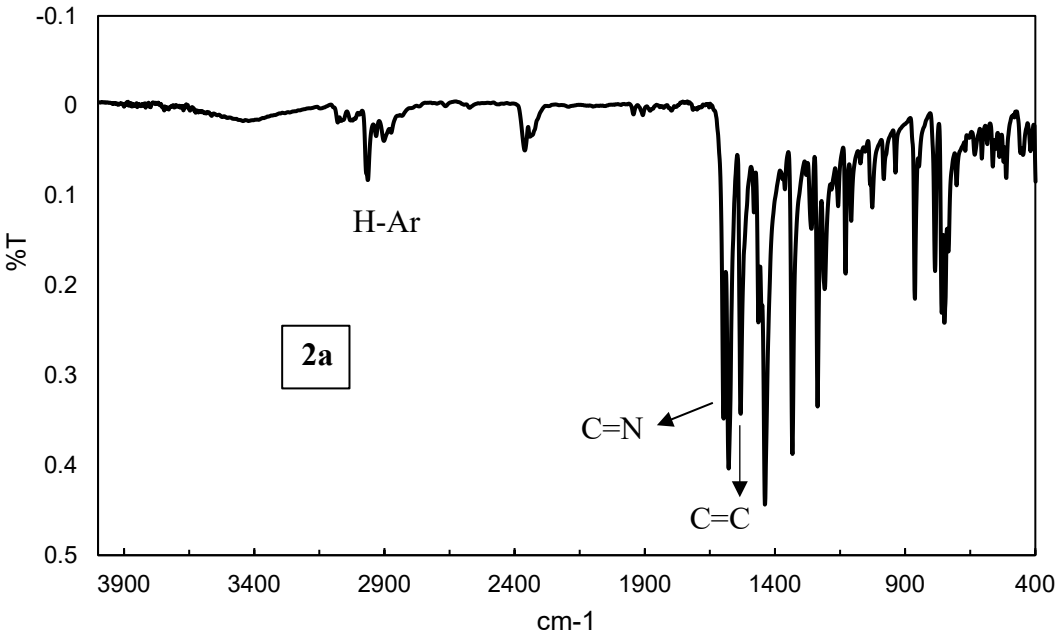
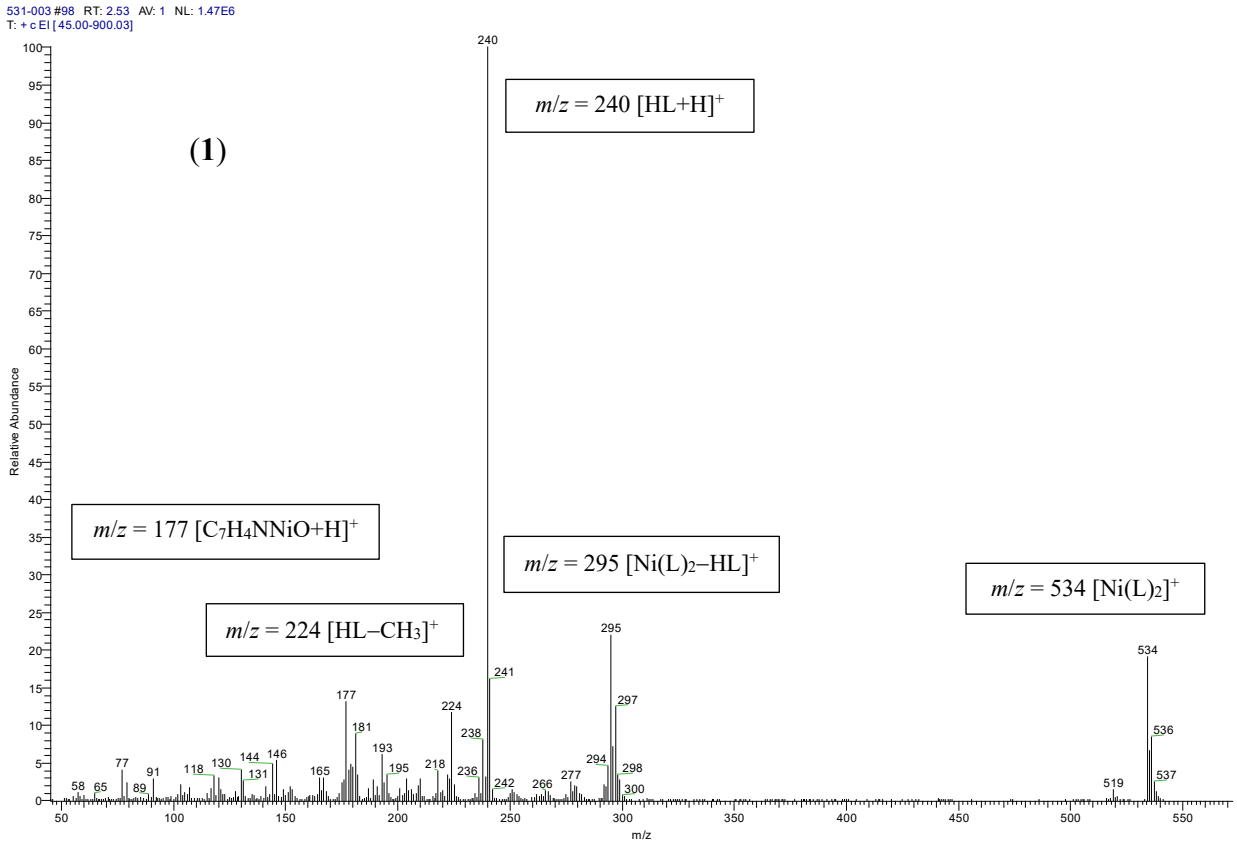


Figure S4. IR (KBr) spectra for H**L**, **1** and **2a** at ambient temperature.



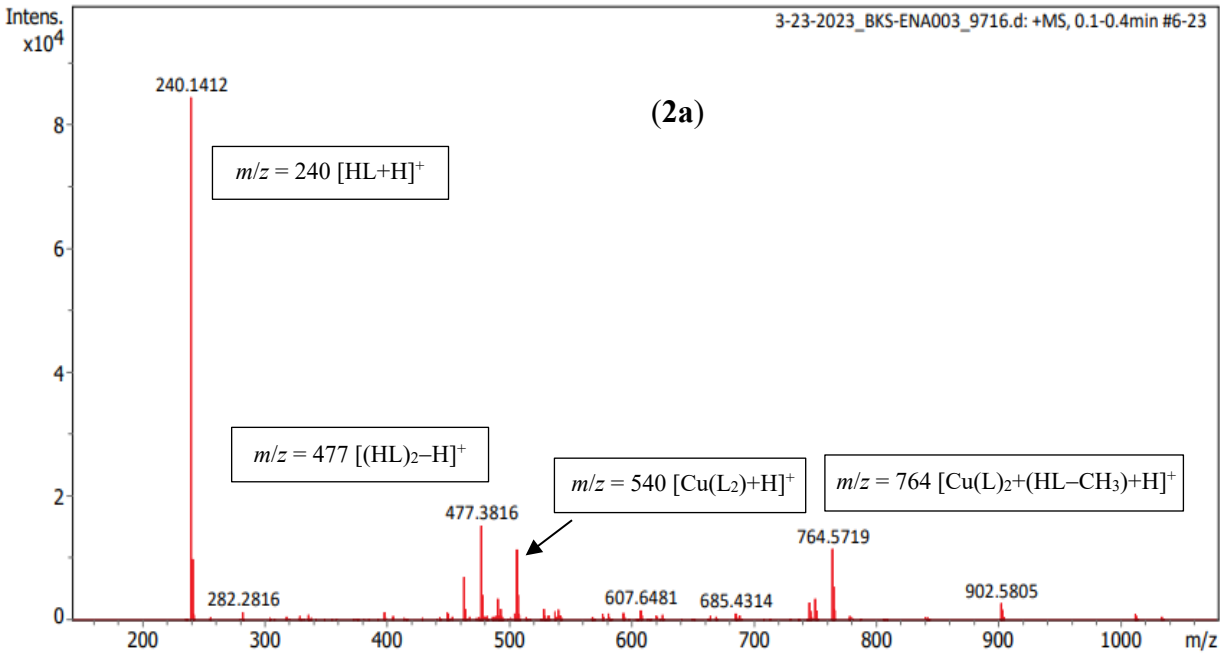


Figure S5. EI-mass spectrum for **1** and ESI-mass spectrum for **2a**.

Decomplexation of the complexes with NaCN and isolation of the ligand (HL)

H**L** (obtained from **1**): ^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm = 1.18 (t, J_{HH} = 7.6 Hz, 3H, CH_3), 2.33 (s, 3H, H_8), 2.54-2.63 (m, 2H, CH_2), 6.78 (dd, J_{HH} = 7.6, 1.6 Hz,1H, H_2), 6.93 (t, J_{HH} = 8.4, 1.6 Hz, 1H, H_4), 7.07 (dd, J_{HH} = 8.0, 1.6 Hz, 1H, H_{11}), 7.19 (dt, J_{HH} = 7.6, 1.6 Hz, 1H, H_{13}), 7.25 (dt, J_{HH} = 7.2, 1.6 Hz, 1H, H_3), 7.32 (dd, J_{HH} = 7.6, 1.6 Hz,1H, H_{14}), 7.41 (dt, J_{HH} = 8.8, 1.6 Hz , 1H, H_{12}) and 7.67 (dd, J_{HH} = 8.0, 1.6 Hz, 1H, H_5) and 14.83 (br, OH) (see Figure S6a for detailed peak assignments with hydrogen atoms numbering).

H**L** (obtained from **2a**): ^{1}H NMR (400 MHz, DMSO-d_6): δ/ppm = 1.07 (t, J_{HH} = 7.6 Hz, 3H, CH_3), 2.30 (s, 3H, H_8), 2.47 (q, J_{HH} = 7.6 Hz, 2H, CH_2), 6.87 (dd, J_{HH} = 7.6, 1.6 Hz, 1H, H_2), 6.93 (t, J_{HH} = 8.0, 1H, H_4), 6.94 (d, J_{HH} = 8.0, 1H, H_{11}), 7.17 (dt, J_{HH} = 7.6, 1.6 Hz, 1H, H_{13}), 7.26 (dt, J_{HH} = 7.6, 1.6 Hz, 1H, H_3), 7.32 (dd, J_{HH} = 7.6, 1.6 Hz, 1H, H_{14}), 7.42 (dt, J_{HH} = 8.0, 1.6 Hz, 1H, H_{12}) and 7.78 (dd, J_{HH} = 8.4, 1.6 Hz, 1H, H_5) and 14.67 (br, 1H, OH) (see Figure S6b for detailed peak assignments with hydrogen atoms numbering).

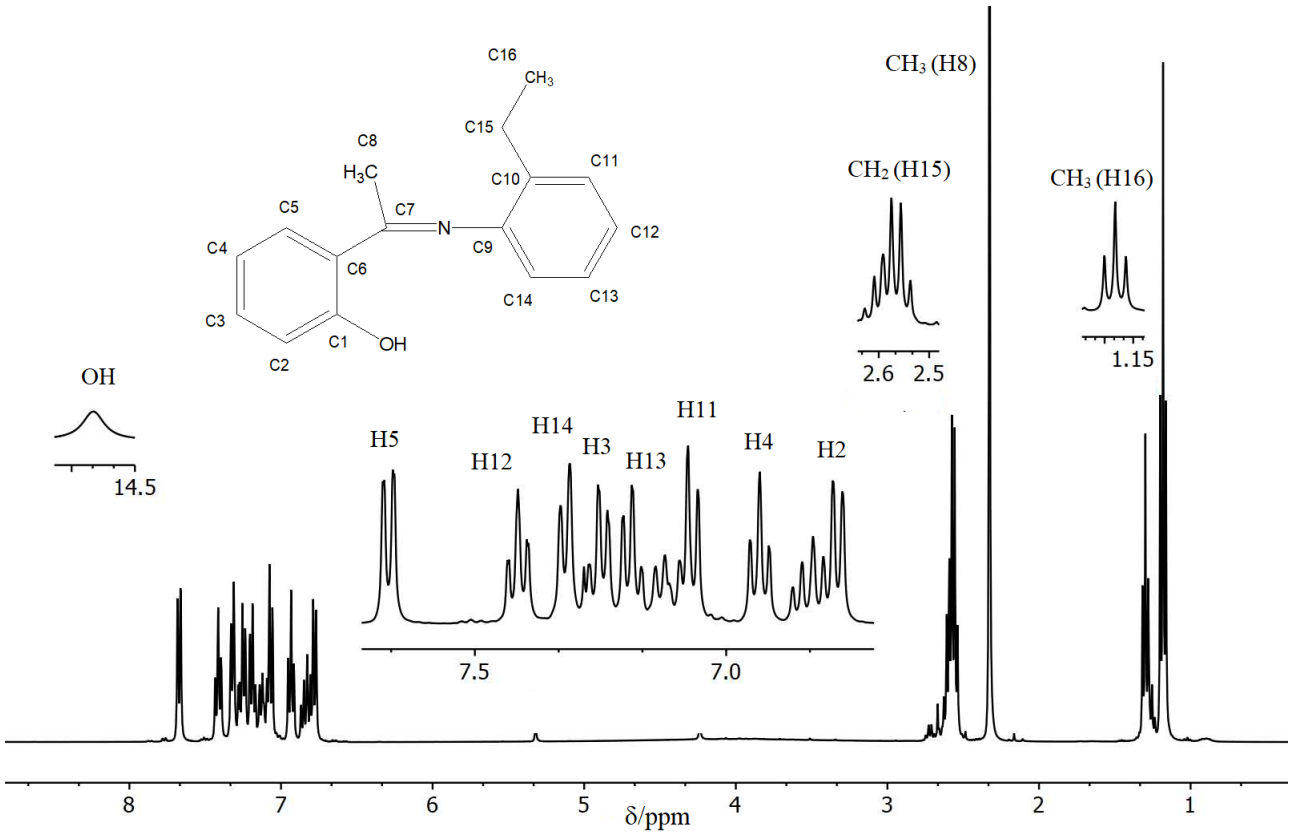


Figure S6a. ^{1}H NMR spectrum for **HL** in $CDCl_3$ at 20 °C (isolated via decomplexation of **1** with NaCN).

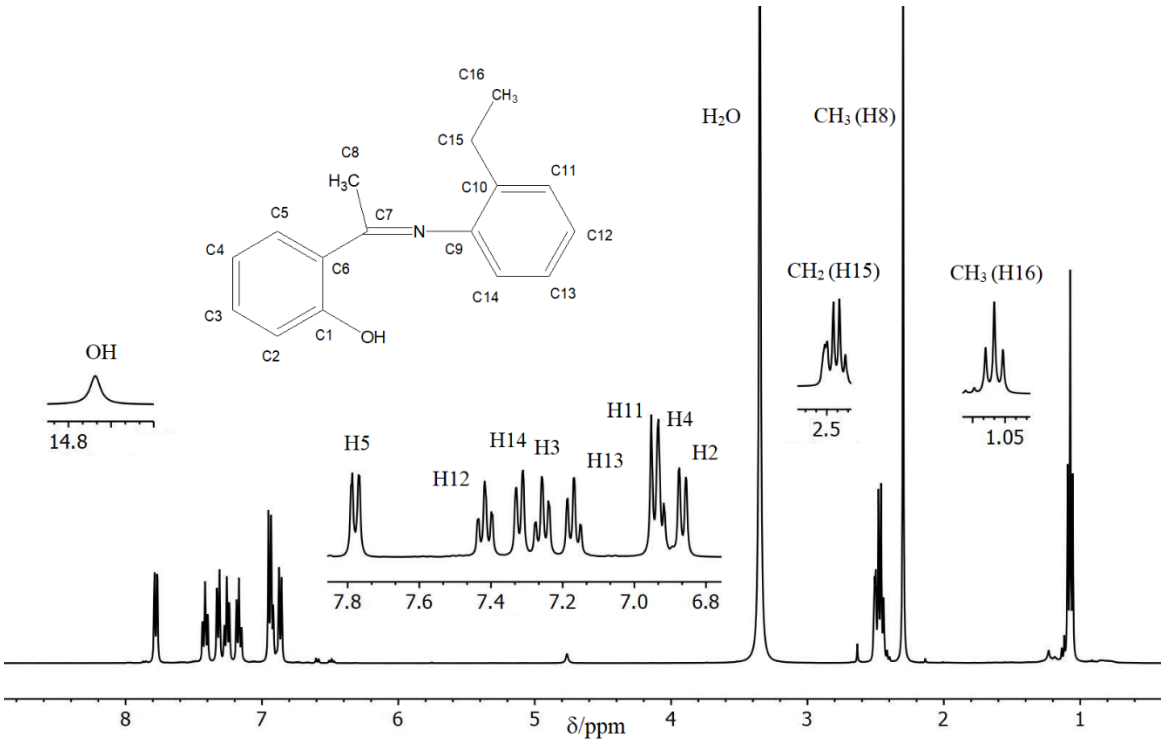


Figure S6b. ^{1}H NMR spectrum for **HL** in DMSO-d_6 at 20 °C (isolated via decomplexation of **2a** with NaCN).

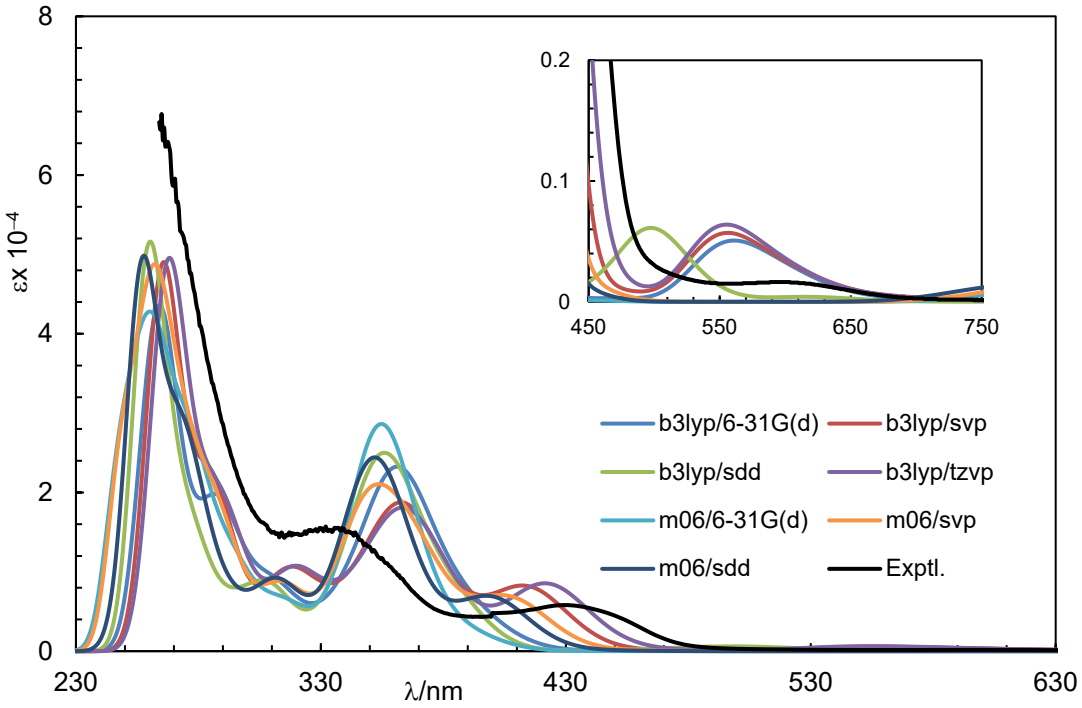


Figure S7a. Calculated UV/Vis spectra for **1** (HS, S = 1, m = 3) using PCM $CHCl_3$. Experimental spectrum for **1** (ca. 0.033 mM) in $CHCl_3$. Spectra in the visible range are shown in the inset. The Gaussian band shape with exponential half-width of σ = 0.16 eV.

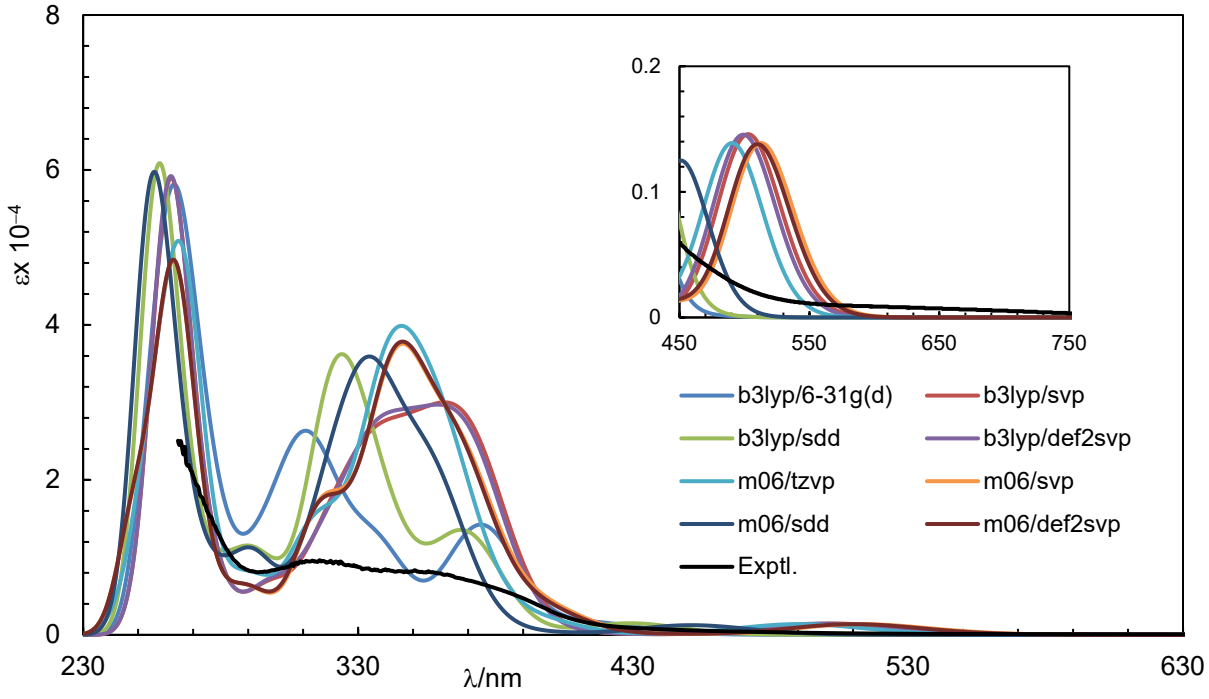
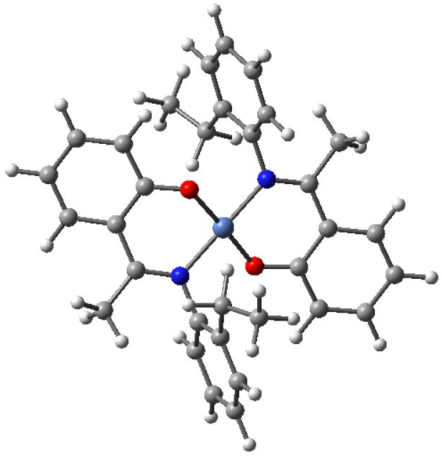
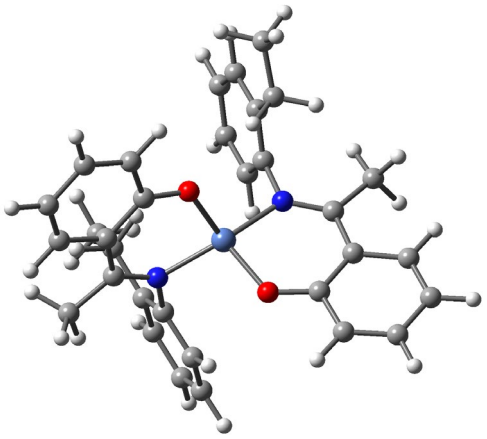
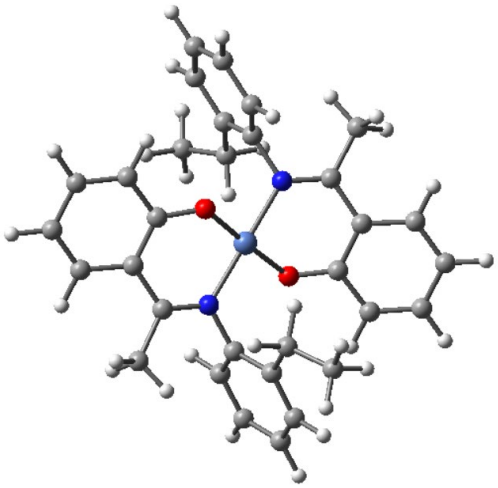
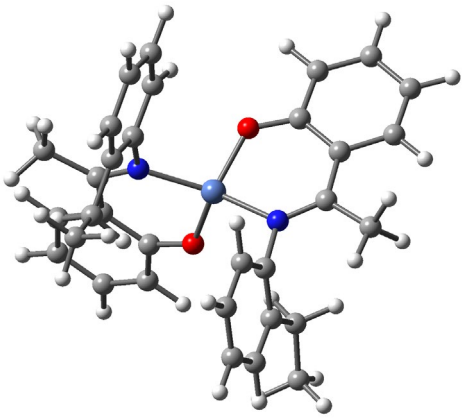


Figure S7b. Calculated UV-vis. spectra for **2a** using different combinations of the functionals and the basis sets with PCM in $CHCl_3$. Experimental spectrum (ca. 0.10 mM) in $CHCl_3$. Spectra in

visible range are shown in the inset. Gaussian band shape with exponential half-width of σ = 0.16 eV.

 Ni(II) complex (**1**), LS (S = 0, m = 1) (Molecule A) (–3006.401475 a.u.)	 Ni(II) complex (**1**), HS (S = 1, m = 3), (Molecule A) (–3006.407113 a.u., stable by + 3.54 kcal/mol)
 Ni(II) complex (**1**), LS (S = 0, m = 1) (Molecule B) (–3006.401481 a.u.)	 Ni(II) complex (**1**), HS (S = 1, m = 3) (Molecule B) (–3006.407113 a.u., stable by + 3.53 kcal/mol)

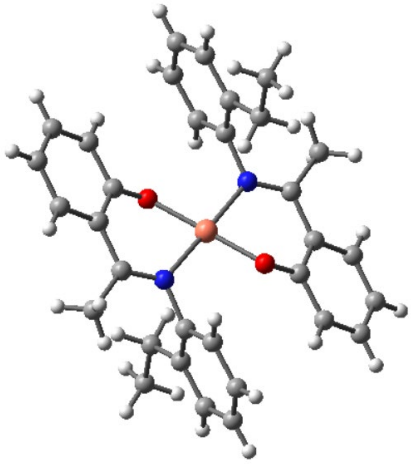
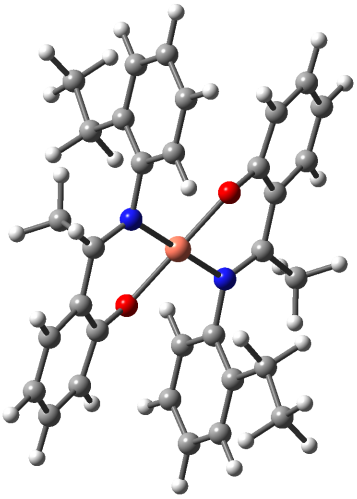
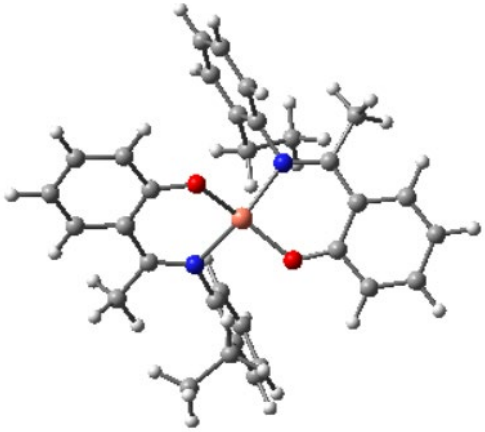
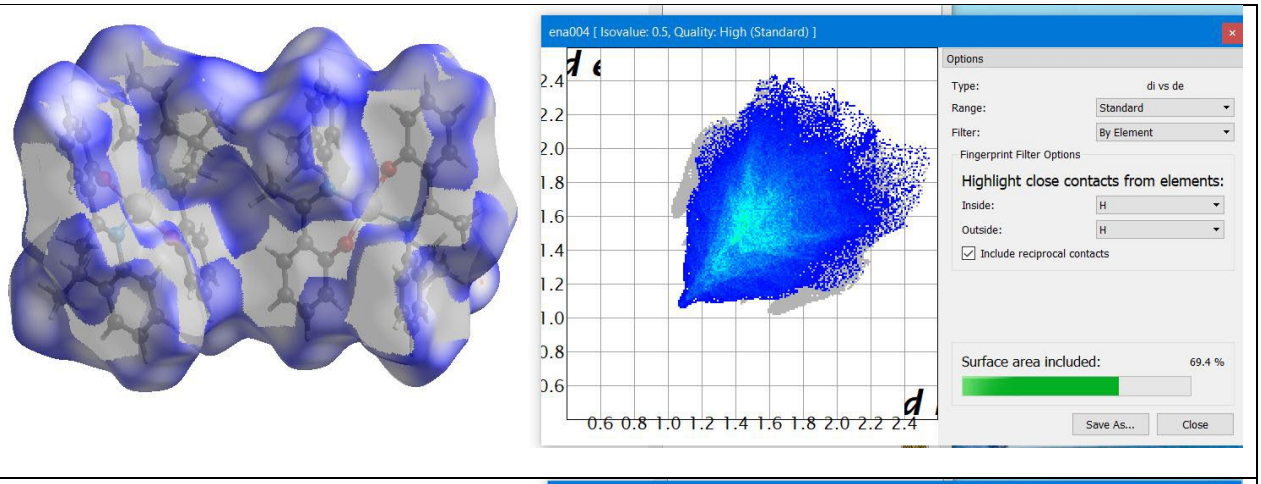
 Cu(II) complex (**2a**) (Molecule A) (–3138.532999 a.u.)	 Cu(II) complex (**2a**) (Molecule B) (–3138.532969 a.u.)
 Cu(II) complex (**2b**) (–3138.534580 a.u.), +0.99 kcal/mol (A) and	

Figure S8. Optimized structures for compounds **1** (HS and LS), **2a** and **2b**, calculated at B3LYP/6-31G(d).

Compound **1**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Fingerprint Filter Options
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Inside: H
Outside: H
Include reciprocal contacts
Surface area included: 69.4 %
Save As...
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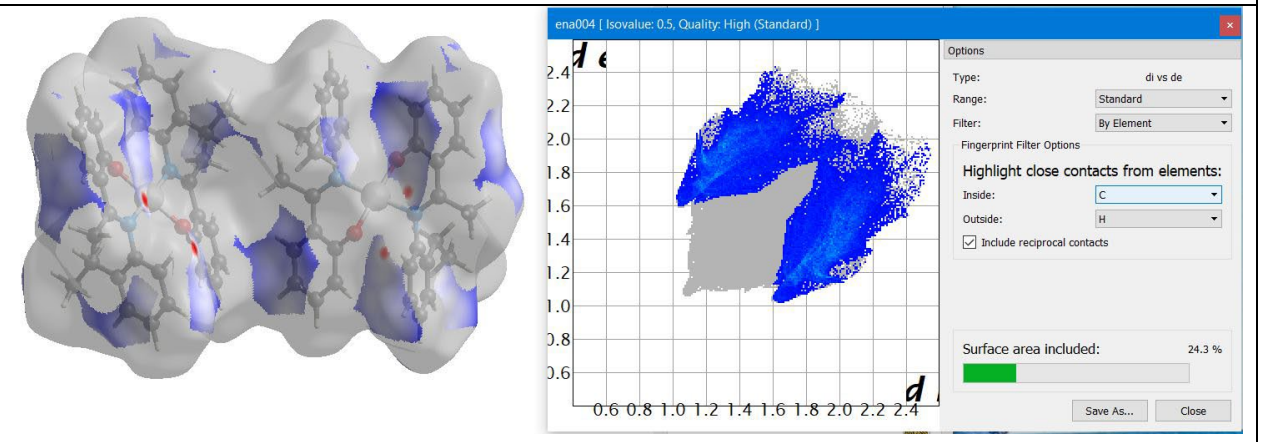
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Fingerprint Filter Options
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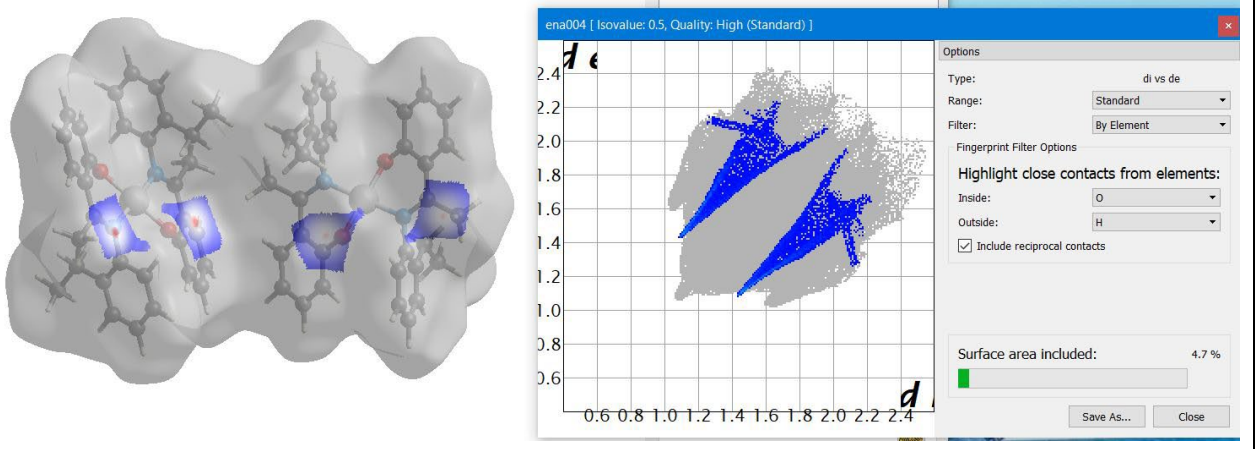
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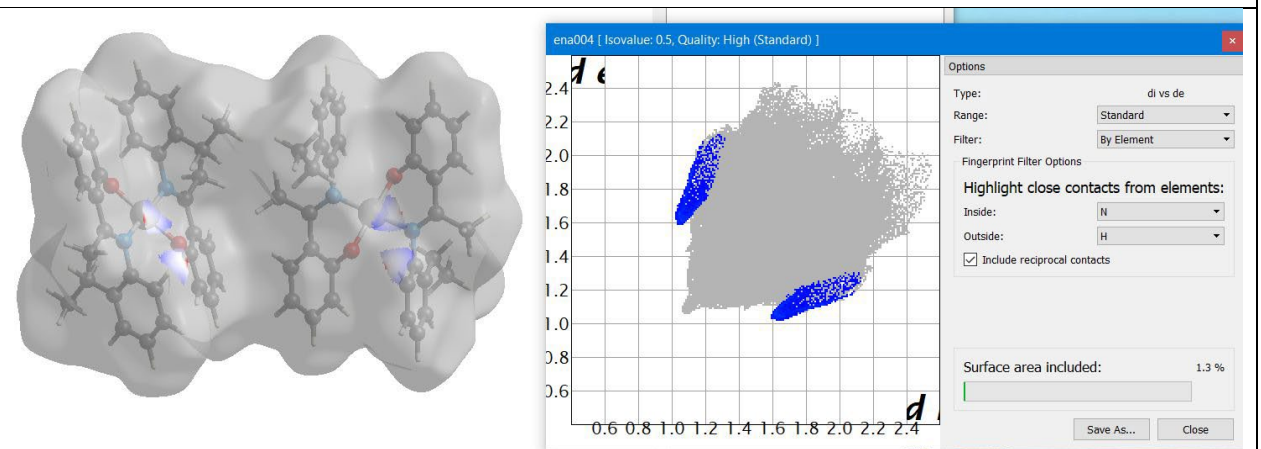
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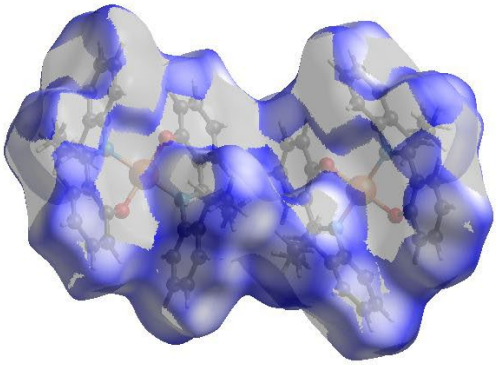
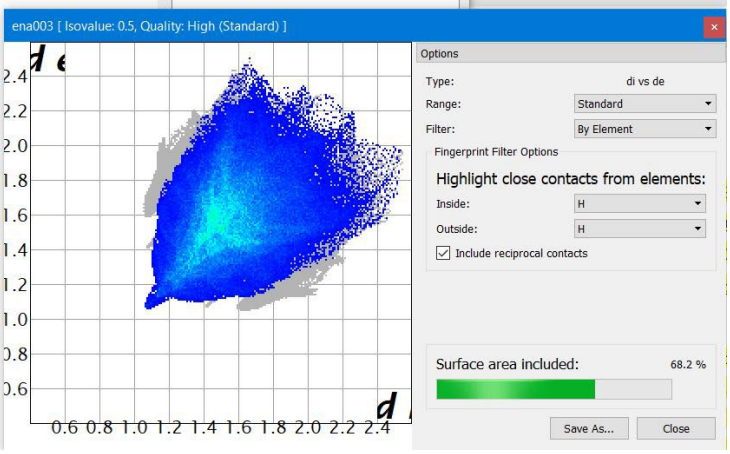
Compound **2a**

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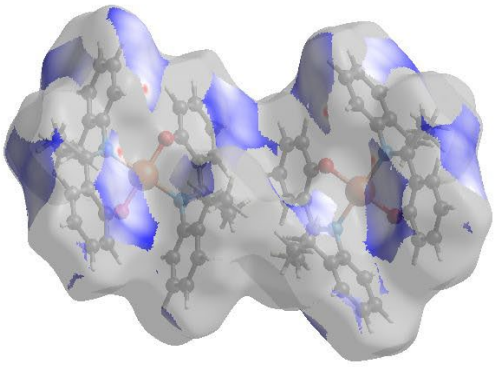

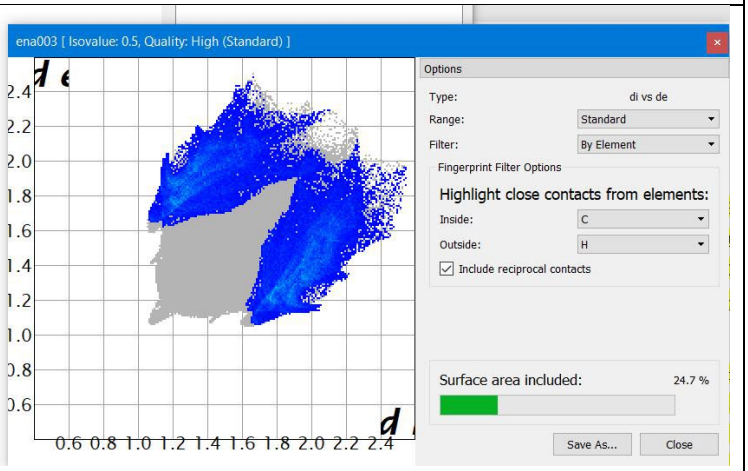
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Options
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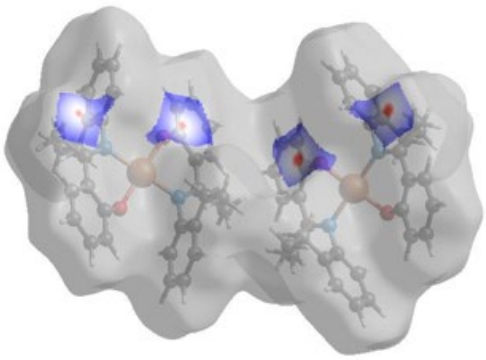
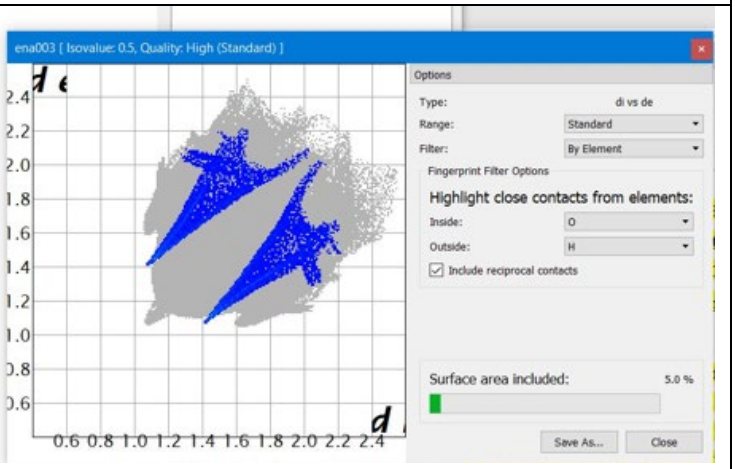
Fingerprint Filter Options
Highlight close contacts from elements:
Inside: C
Outside: H
Include reciprocal contacts
Surface area included: 24.7 %
Save As...
Close
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4

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Range: Standard
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Fingerprint Filter Options
Highlight close contacts from elements:
Inside: O
Outside: H
Include reciprocal contacts
Surface area included: 5.0 %
Save As...
Close
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4

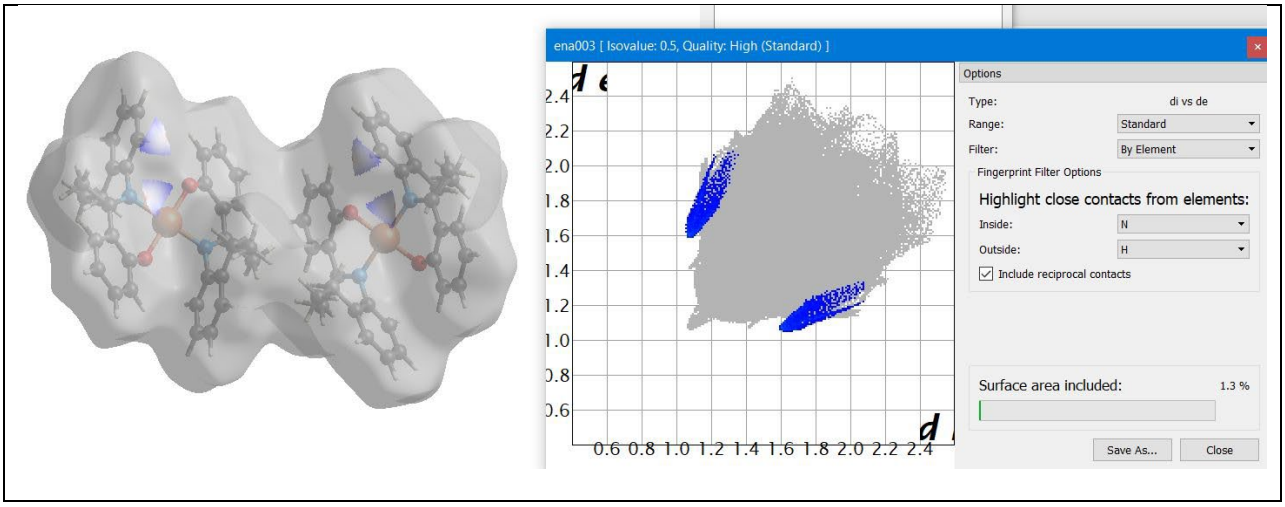
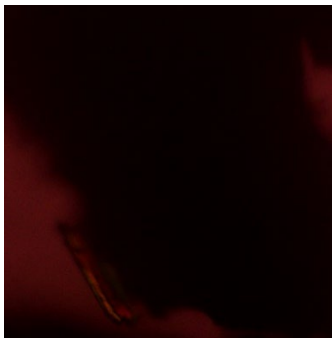
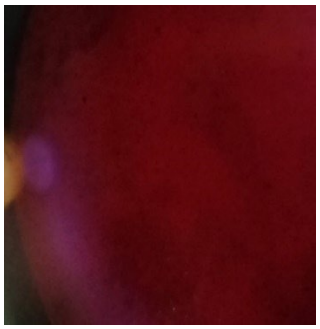
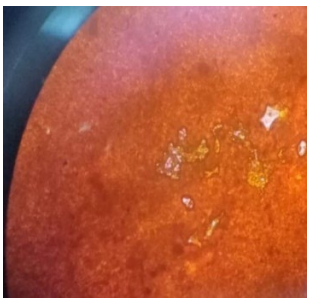
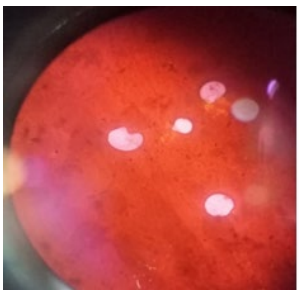
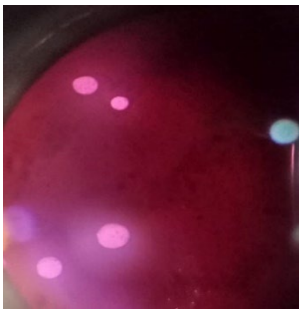


Figure S9. Hirshfeld surface mapped with d-norm property (right side) and 2D fingerprint plots (left side) showing breakdown of all possible contributions from close contacts. The di/de are the distances from the surface to the nearest atoms interior/exterior to the surface.

First heating cycle	
 (a) Crystalline-solid phase (Cr) at 30-185 °C.	 (b) Crystalline-solid melted or isotropic-liquid phase (I or m. p.) at 190-193 °C.

Second heating cycle	
 (c) Cold crystals (CCr) phase at 70-140 °C.	 (d) Cold crystals melted at 145-160 °C.

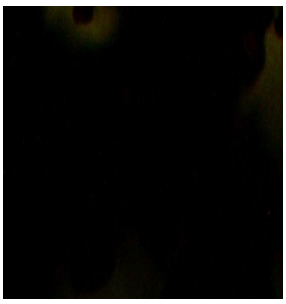
(e) Liquid crystals (LC) phase at 165-180 °C.



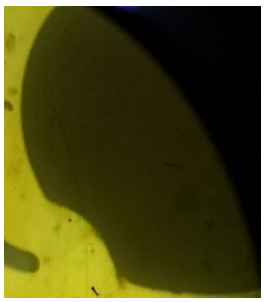
(f) Liquid crystals melted or isotropic-liquid (I or m. p) phase at 183-187 °C.

Figure S10. Optical texture observations under polarizing light microscopic (PLM) through second heating cycle for **2b**.

First heating cycle



(a) Crystalline-solid phase (Cr) at 30-185 °C.

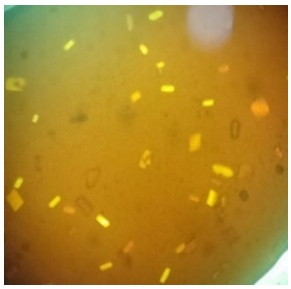


(b) Crystalline-solid melted or isotropic-liquid phase (I or m. p.) at 188-190 °C.

Second heating cycle

(c) Cold crystals (CCr) phase at 70-150 °C.

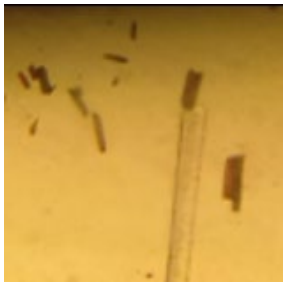
(d) Cold crystals melted at 155-165°C.



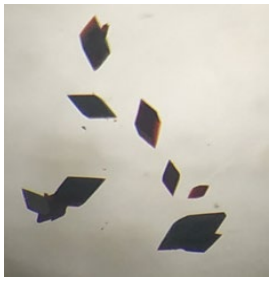
(e) Liquid crystals (LC) phase at 170-185°C.

(f) Liquid crystals melted or isotropic-liquid (I or m. p) phase at 188-190°C.

Figure S11. Optical texture observations through polarizing light microscope (PLM) during second heating cycle for bulk microcrystals **2**.



(**2a**)



(**2b**)

Figure S12. Crystals pictures of polymorphs **2a** and **2b**.

Table S1. Analysis of X-H...Cg(π-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) in **1**.

==========

- 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
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-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	Transformed J-Plane P, Q, R, S	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C(2) -H(2)	[1] ->	Cg(4)	[2556.01]	2.97	0.5186 0.3373-0.7857 -6.6006	2.90	13.19	125	3.599(4)	48
C(11) -H(11)	[1] ->	Cg(3)	[2656.01]	2.85	0.4343-0.6387 0.6352 7.7801	-2.84	3.19	141	3.632(4)	47
C(18) -H(18)	[2] ->	Cg(8)	[2665.02]	2.96	-0.5216 0.4547-0.7219 2.5330	-2.89	12.18	126	3.605(4)	49
C(27) -H(27)	[2] ->	Cg(7)	[2765.02]	2.79	0.4416 0.1609-0.8827 6.7484	-2.79	3.03	141	3.579(4)	48
			Min or Max	2.790		-2.893	3.0	141.00	3.579	49.00

[2556] = -X,-Y,1-Z
[2656] = 1-X,-Y,1-Z
[2665] = 1-X,1-Y,-Z
[2765] = 2-X,1-Y,-Z
Cg3 = centroid of ring C1-C2-C3-C4-C5-C6
Cg7 = centroid of ring C17-C18-C19-C20-C21-C22

Table S2. Analysis of potential hydrogen bonds with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg in **2a**.

==========

Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)

==========

Nr	Typ	Res	Donor --- H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A	A..H..A*	A'..H..A"	Sum(XY,YZ)	Sum(XZ)

---

1 1 C(8) --H(8A) ..O(1) [1655.01] 0.98 2.59 3.532(3) 161

Table S3. Analysis of X-H...Cg(π-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) in **2a**.

- 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
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-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	Transformed J-Plane P, Q, R, S	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C(11) -H(11)	[1]	-> Cg(3)	[2765.01]	2.76	0.4477 0.1704-0.8778 6.9010	-2.76	3.34	141	3.554(2)	50
C(27) -H(27)	[2]	-> Cg(7)	[2656.02]	2.83	0.4426-0.6342 0.6340 7.9756	-2.82	2.15	141	3.612(3)	49
			Min or Max	2.760		-2.824	2.2	141.00	3.554	50.00

[2765] = 2-X,1-Y,-Z
[2656] = 1-X,-Y,1-Z

Cg3 = centroid of ring C1-C2-C3-C4-C5-C6
Cg7 = centroid of ring C17-C18-C19-C20-C21-C22

Table S4. Excited states, excitation energy (eV), wavelength (nm) and oscillator strength (*f*) for **1** (HS, S = 1, m = 3) at B3LYP/SVP with PCM in chloroform.

Excitation energies and oscillator strengths:

Excited State 1: 3.003-A 0.7996 eV 1550.61 nm f=0.0007 <S**2>=2.005

123B ->141B 0.13290

128B ->141B -0.24555

130B ->141B 0.50357

130B ->143B 0.15931

131B ->141B -0.17589

134B ->141B -0.19980

135B ->141B -0.36717

135B ->143B -0.11790

136B ->141B 0.40407

136B ->143B 0.11953

140B ->141B 0.37727

140B ->143B 0.12117

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3005.81460262

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.005-A 0.9819 eV 1262.72 nm f=0.0001 <S**2>=2.007

129B ->141B -0.27636

132B ->141B 0.33705

132B ->143B 0.10940

135B ->141B 0.27091

136B ->141B 0.33322

136B ->143B 0.11394

138B ->141B 0.63690

138B ->143B 0.20164

Excited State 3: 3.005-A 1.1634 eV 1065.71 nm f=0.0004 <S**2>=2.008

122B ->141B -0.10477

128B ->141B 0.30713

128B ->143B 0.10460

129B ->142B -0.10946

129B ->144B 0.15704

130B ->141B 0.28527

131B ->141B 0.29273

132B ->141B -0.13977

132B ->142B 0.13572

132B ->144B -0.18846

133B ->141B -0.10676

134B ->141B 0.20001

135B ->142B 0.11006

135B ->144B -0.15183

136B ->142B 0.13000

136B ->144B -0.17527

137B ->141B 0.34004

137B ->143B 0.10710

138B ->142B 0.25482

138B ->144B -0.33166

138B ->148B -0.14933

140B ->141B -0.13861

Excited State 4: 3.006-A 1.8002 eV 688.74 nm f=0.0003 <S**2>=2.009

128B ->142B -0.13541

128B ->144B 0.19602

130B ->142B -0.37079

130B ->144B 0.48636

130B ->148B 0.21976

131B ->142B -0.15528

131B ->144B 0.19278

132B ->144B -0.12565

134B ->144B 0.10231

135B ->144B -0.11271

136B ->142B -0.11521

136B ->144B 0.13990

137B ->142B -0.28240

137B ->144B 0.35447

137B ->148B 0.14834

Excited State 5: 3.010-A 2.0571 eV 602.72 nm f=0.0020 <S**2>=2.015

128B ->141B 0.18540

129B ->142B 0.10550

129B ->144B -0.16182

130B ->141B 0.36727

130B ->143B 0.10715

131B ->141B 0.22651

132B ->141B -0.11181

132B ->142B -0.14713

132B ->144B 0.19749

134B ->141B 0.13544

135B ->142B -0.13188

135B ->144B 0.17207

136B ->142B -0.13782

136B ->144B 0.18188

137B ->141B 0.34155

137B ->143B 0.10691

138B ->142B -0.31881

138B ->144B 0.38360

138B ->148B 0.15457

Excited State 6: 3.057-A 2.2506 eV 550.89 nm f=0.0051 <S**2>=2.086

141A ->144A -0.10318

128B ->142B -0.18160

128B ->144B 0.24789

128B ->148B 0.11507

130B ->142B 0.13879

130B ->144B -0.18863

131B ->142B -0.18688

131B ->144B 0.22062

131B ->148B 0.10114

134B ->142B -0.16514

134B ->144B 0.19714

135B ->142B -0.18392

135B ->144B 0.22039

136B ->142B 0.22604

136B ->144B -0.27774

136B ->148B -0.11312

138B ->141B 0.13315

140B ->142B 0.38739

140B ->144B -0.32669

140B ->148B -0.11955

Excited State 7: 4.001-A 2.6178 eV 473.62 nm f=0.0007 <S**2>=3.752

140A ->143A 0.20473

141A ->143A 0.45671

141A ->144A -0.13209

142A ->144A 0.49242

139B ->142B 0.42835

139B ->144B 0.10558

140B ->141B -0.24013

140B ->142B 0.15888

140B ->143B 0.39928

Excited State 8: 3.975-A 2.6378 eV 470.02 nm f=0.0001 <S**2>=3.700

140A ->144A 0.21133

141A ->143A -0.15536

141A ->144A 0.37369

142A ->143A 0.49882

142A ->144A 0.20340

139B ->141B 0.24244

139B ->143B -0.35004

140B ->141B -0.10153

140B ->142B -0.36702

140B ->143B 0.15076

140B ->144B -0.23747

Excited State 9: 3.134-A 2.9586 eV 419.06 nm f=0.0117 <S**2>=2.205

139B ->141B 0.89334

139B ->143B 0.24582

140B ->142B 0.13080

Excited State 10: 3.147-A 2.9955 eV 413.90 nm f=0.0647 <S**2>=2.226

128B ->141B 0.11383

130B ->141B -0.10663

134B ->141B 0.12742

135B ->141B 0.20195

136B ->141B -0.17493

136B ->143B -0.14126

139B ->142B 0.14426

140B ->141B 0.81405

140B ->143B 0.21516

Excited State 11: 3.325-A 3.0964 eV 400.41 nm f=0.0019 <S**2>=2.514

139A ->143A -0.20754

139A ->144A 0.14757

140A ->143A -0.34536

140A ->144A 0.31586

141A ->143A 0.43533

141A ->144A -0.43233

142A ->143A 0.38076

142A ->144A -0.34680

140B ->142B -0.14023

Excited State 12: 3.309-A 3.1184 eV 397.59 nm f=0.0027 <S**2>=2.487

139A ->143A 0.13085

139A ->144A 0.19102

140A ->143A -0.36480

140A ->144A -0.37421

141A ->143A 0.51450

141A ->144A 0.56439

140B ->142B 0.10597

140B ->143B -0.14358

Excited State 13: 3.589-A 3.2489 eV 381.62 nm f=0.0180 <S**2>=2.970

135A ->143A -0.13631

135A ->144A 0.15510

136A ->143A 0.12620

138A ->143A -0.19330

138A ->144A 0.12342

139A ->144A 0.12034

141A ->143A -0.18330

141A ->144A 0.17011

142A ->144A -0.18944

133B ->142B -0.10448

135B ->142B -0.11921

135B ->144B -0.12098

136B ->143B 0.11708

137B ->142B 0.18614

137B ->143B 0.13688

138B ->142B -0.13633

138B ->144B -0.14272

139B ->142B 0.61556

139B ->144B -0.20415

140B ->142B 0.10801

140B ->150B -0.10608

Excited State 14: 3.564-A 3.2698 eV 379.17 nm f=0.0200 <S**2>=2.926

135A ->143A -0.12005

136A ->144A -0.14367

137A ->143A 0.15427

137A ->144A 0.14416

138A ->144A 0.10934

139A ->143A -0.14490

141A ->143A -0.14362

142A ->143A 0.38702

142A ->144A 0.11952

130B ->142B -0.10670

132B ->143B 0.12529

134B ->143B -0.10072

135B ->144B -0.13360

136B ->143B -0.15181

136B ->144B 0.17204

137B ->142B 0.12122

139B ->142B -0.25993

139B ->144B 0.11725

140B ->142B 0.59594

Excited State 15: 3.830-A 3.3488 eV 370.23 nm f=0.0240 <S**2>=3.418

135A ->143A 0.13650

136A ->143A 0.12085

136A ->144A 0.19708

137A ->143A -0.21509

137A ->144A -0.24126

138A ->144A -0.13577

140A ->144A 0.11670

141A ->144A 0.11688

142A ->143A 0.19950

142A ->144A -0.13755

142A ->149A -0.10574

142A ->150A -0.10556

132B ->143B -0.16173

136B ->141B -0.16521

136B ->142B -0.19949

136B ->143B 0.25334

137B ->142B -0.12255

138B ->143B 0.14596

139B ->141B -0.13787

139B ->142B -0.19172

139B ->143B -0.17725

140B ->142B 0.39552

140B ->143B 0.24074

140B ->149B -0.11836

Excited State 16: 3.594-A 3.3769 eV 367.15 nm f=0.0446 <S**2>=2.980

135A ->143A 0.15906

135A ->144A -0.16147

136A ->143A -0.12689

138A ->143A 0.21002

138A ->144A -0.13705

139A ->144A -0.11316

141A ->143A -0.16108

142A ->143A 0.27186

134B ->142B 0.13082

135B ->141B -0.10111

135B ->142B 0.16831

137B ->142B -0.14633

137B ->143B -0.10207

138B ->142B 0.20230

139B ->142B 0.42542

139B ->144B -0.24304

140B ->141B -0.12511

140B ->142B 0.17094

140B ->143B -0.33052

Excited State 17: 3.536-A 3.4389 eV 360.54 nm f=0.0859 <S**2>=2.876

137A ->144A 0.11457

141A ->144A 0.14606

142A ->143A -0.10623

142A ->144A -0.56985

140B ->141B -0.22336

140B ->143B 0.64737

Excited State 18: 3.254-A 3.5290 eV 351.32 nm f=0.0194 <S**2>=2.397

140A ->144A -0.22741

141A ->143A -0.14058

142A ->143A 0.37698

142A ->144A 0.14413

131B ->142B -0.10044

139B ->141B -0.17999

139B ->143B 0.72539

140B ->142B -0.16403

140B ->143B 0.17673

Excited State 19: 3.668-A 3.5583 eV 348.44 nm f=0.0032 <S**2>=3.113

134A ->147A -0.10123

136A ->146A -0.11591

138A ->146A -0.10316

139A ->147A -0.10974

139A ->148A 0.15284

140A ->143A 0.38144

140A ->144A -0.36749

140A ->146A -0.10805

140A ->147A -0.12108

141A ->143A 0.14317

141A ->144A -0.16024

142A ->143A 0.30283

142A ->144A -0.21726

134B ->146B -0.14160

135B ->142B -0.12698

135B ->146B 0.12213

137B ->141B -0.12635

137B ->147B -0.14075

138B ->142B 0.21008

138B ->148B 0.11566

140B ->142B -0.13679

Excited State 20: 3.776-A 3.5889 eV 345.47 nm f=0.0239 <S**2>=3.315

134A ->145A 0.13828

135A ->145A 0.16727

138A ->146A 0.10131

138A ->148A 0.12437

139A ->144A -0.12246

139A ->146A -0.17173

139A ->148A -0.13263

140A ->143A 0.37603

140A ->144A 0.22747

140A ->145A 0.10439

140A ->146A 0.11501

140A ->148A 0.12678

141A ->143A 0.27298

141A ->144A 0.22640

131B ->141B -0.11465

133B ->145B 0.20535

136B ->141B -0.12602

136B ->147B -0.11265

137B ->141B 0.12053

137B ->144B 0.11489

137B ->147B 0.14102

137B ->148B -0.13105

138B ->141B 0.16017

138B ->147B 0.10381

139B ->143B 0.21670

140B ->143B -0.14840

140B ->144B -0.14123

Excited State 21: 3.581-A 3.6071 eV 343.72 nm f=0.0065 <S**2>=2.956

135A ->145A -0.12221

138A ->148A -0.13473

139A ->146A 0.17809

140A ->143A 0.50886

140A ->144A 0.25513

140A ->148A -0.15259

141A ->143A 0.18370

141A ->144A 0.24800

142A ->144A -0.22696

132B ->141B 0.10197

133B ->145B -0.13744

136B ->141B 0.12604

137B ->144B -0.10544

137B ->148B 0.14422

138B ->141B -0.14139

138B ->147B -0.12264

139B ->144B 0.16342

140B ->143B -0.18030

140B ->144B 0.13055

Excited State 22: 3.823-A 3.6282 eV 341.73 nm f=0.0099 <S**2>=3.403

136A ->146A -0.10274

138A ->146A -0.11417

139A ->148A 0.16576

140A ->143A -0.21090

140A ->144A 0.50507

140A ->146A -0.12695

141A ->144A 0.22413

142A ->143A -0.21306

142A ->144A 0.13517

131B ->141B 0.10377

133B ->145B -0.11743

134B ->146B -0.11828

135B ->146B 0.10308

136B ->142B -0.10841

136B ->144B 0.11183

137B ->141B -0.10810

137B ->147B -0.14586

138B ->142B 0.19553

138B ->148B 0.10492

139B ->143B 0.32673

140B ->144B -0.15021

Excited State 23: 3.621-A 3.7318 eV 332.23 nm f=0.0123 <S**2>=3.028

139A ->144A 0.10260

141A ->143A -0.13962

135B ->141B -0.10229

136B ->144B -0.10156

137B ->142B -0.13692

138B ->142B -0.51645

138B ->144B -0.17772

139B ->142B 0.17454

139B ->144B 0.53391

140B ->144B 0.17603

Excited State 24: 3.218-A 3.7705 eV 328.82 nm f=0.0064 <S**2>=2.339

140A ->144A 0.18026

141A ->144A 0.11448

129B ->141B -0.12109

134B ->142B -0.11706

135B ->142B -0.21073

135B ->144B 0.10692

136B ->142B 0.18660

137B ->142B -0.13107

138B ->141B -0.21536

138B ->142B 0.16318

138B ->143B 0.14838

139B ->144B -0.14516

140B ->144B 0.72588

Excited State 25: 3.593-A 3.8251 eV 324.14 nm f=0.0143 <S**2>=2.978

139A ->143A 0.13880

139A ->144A 0.10613

140A ->144A 0.13102

142A ->150A 0.10611

131B ->142B 0.18768

132B ->143B 0.12560

136B ->141B 0.11677

138B ->141B -0.36270

138B ->142B 0.22550

138B ->143B 0.46380

138B ->144B 0.11468

139B ->142B 0.14218

139B ->143B 0.15453

139B ->144B 0.40608

139B ->150B -0.10393

140B ->144B -0.26006

140B ->149B 0.11211

Excited State 26: 3.503-A 3.8473 eV 322.27 nm f=0.0258 <S**2>=2.818

139A ->143A -0.12877

140A ->143A -0.14284

131B ->141B -0.11386

132B ->143B -0.10146

134B ->141B -0.10588

137B ->141B 0.15188

138B ->141B 0.26172

138B ->142B 0.41940

138B ->143B -0.30354

138B ->144B 0.27097

139B ->142B 0.13765

139B ->143B -0.13908

139B ->144B 0.48799

140B ->143B -0.12681

140B ->144B 0.12598

Excited State 27: 3.267-A 3.8784 eV 319.68 nm f=0.0103 <S**2>=2.418

129B ->141B 0.26762

131B ->144B 0.12988

132B ->141B -0.20896

135B ->141B -0.24426

136B ->141B -0.34301

137B ->144B -0.10715

138B ->141B 0.34287

138B ->143B 0.58402

140B ->144B 0.13192

Excited State 28: 3.188-A 3.9427 eV 314.46 nm f=0.0286 <S**2>=2.291

128B ->141B 0.16985

130B ->141B -0.18141

131B ->141B -0.50152

131B ->143B -0.13018

132B ->141B 0.12442

134B ->141B -0.21892

137B ->141B 0.60031

137B ->143B 0.10641

138B ->144B -0.15607

Excited State 29: 3.362-A 3.9728 eV 312.09 nm f=0.0073 <S**2>=2.576

139A ->143A 0.78540

139A ->144A -0.33022

140A ->143A -0.12099

140A ->144A 0.17966

138B ->141B 0.13614

138B ->142B -0.11359

138B ->143B -0.11336

140B ->144B 0.13408

Excited State 30: 3.343-A 3.9836 eV 311.23 nm f=0.0206 <S**2>=2.544

139A ->143A 0.36443

139A ->144A 0.81133

140A ->143A 0.18257

140A ->144A 0.13576

138B ->143B -0.12501

139B ->144B -0.12694

Excited State 31: 4.025-A 4.0680 eV 304.78 nm f=0.0009 <S**2>=3.800

137A ->143A -0.10999

137A ->144A -0.13523

140A ->149A 0.19219

140A ->150A 0.12945

141A ->149A 0.17301

142A ->149A 0.35140

142A ->150A 0.31957

132B ->143B -0.11126

136B ->142B -0.18848

136B ->143B 0.28259

138B ->143B -0.20446

139B ->149B -0.25239

139B ->150B -0.24289

140B ->149B 0.32820

140B ->150B 0.20835

Excited State 32: 3.971-A 4.0794 eV 303.93 nm f=0.0065 <S**2>=3.692

138A ->143A	-0.11245
139A ->143A	0.14023
139A ->144A	-0.17376
140A ->149A	-0.10372
140A ->150A	0.16559
141A ->149A	-0.24245
141A ->150A	0.32502
142A ->149A	0.23126
142A ->150A	-0.19217
135B ->142B	-0.10874
136B ->143B	0.12035
137B ->142B	0.34197
137B ->143B	0.15482
137B ->144B	0.11918
138B ->142B	0.10937
139B ->149B	-0.23938
139B ->150B	0.22232
140B ->149B	-0.19685
140B ->150B	0.29425

Excited State 33: 3.676-A 4.1756 eV 296.93 nm f=0.0100 <S**2>=3.128

134A ->144A	0.10221
135A ->143A	0.10604
129B ->141B	-0.11041
131B ->144B	0.10577
134B ->144B	0.13923
135B ->142B	0.20870
135B ->143B	0.15968
135B ->144B	0.12741
136B ->142B	-0.20357

137B ->142B 0.67865

137B ->143B -0.16022

137B ->144B 0.18515

Excited State 34: 3.688-A 4.1902 eV 295.89 nm f=0.0060 <S**2>=3.150

128B ->141B 0.12891

131B ->141B -0.11872

132B ->142B 0.14941

132B ->143B -0.15036

134B ->143B 0.16901

135B ->142B 0.31525

135B ->143B 0.11427

136B ->141B 0.15099

136B ->142B 0.19543

136B ->143B -0.26714

137B ->141B -0.21387

137B ->143B 0.62423

138B ->144B 0.11162

Excited State 35: 3.507-A 4.2399 eV 292.42 nm f=0.0420 <S**2>=2.825

129B ->142B -0.21648

132B ->142B 0.14007

133B ->141B 0.15261

134B ->143B -0.10092

135B ->142B 0.34392

136B ->141B -0.11031

136B ->142B 0.52372

136B ->143B 0.21734

137B ->141B 0.12270

137B ->143B -0.24005

138B ->144B 0.35733

Excited State 36: 3.462-A 4.2790 eV 289.75 nm f=0.0071 <S**2>=2.746

134A ->147A	0.10586
139A ->146A	-0.11346
139A ->147A	0.11779
140A ->146A	-0.10938
140A ->147A	0.18679
141A ->147A	-0.11077
129B ->141B	-0.27833
131B ->141B	-0.12690
132B ->141B	0.14429
132B ->142B	0.11184
133B ->141B	0.11974
134B ->141B	0.40601
134B ->142B	0.36216
134B ->147B	0.10121
135B ->141B	-0.37249
136B ->141B	-0.15282
137B ->144B	0.11777

Excited State 37: 3.434-A 4.2984 eV 288.45 nm f=0.0137 <S**2>=2.697

139A ->147A	-0.10303
139A ->148A	-0.10340
140A ->145A	-0.16710
140A ->146A	0.11843
141A ->145A	0.16512
129B ->141B	-0.23754
131B ->142B	0.22614
132B ->142B	-0.15073
133B ->141B	0.59331
134B ->144B	0.11819
135B ->142B	0.14467
136B ->141B	-0.19366

136B ->142B -0.19194

136B ->144B -0.11076

137B ->143B 0.16604

137B ->144B 0.10933

Excited State 38: 3.455-A 4.3191 eV 287.06 nm f=0.0106 <S**2>=2.734

138A ->144A -0.14084

139A ->145A 0.17284

140A ->145A -0.18004

141A ->145A 0.17347

129B ->141B 0.28281

130B ->141B -0.11918

130B ->143B -0.14340

131B ->141B 0.28178

131B ->142B -0.18651

131B ->143B 0.13969

132B ->141B 0.34214

133B ->141B 0.10952

133B ->142B -0.14114

133B ->144B 0.11508

134B ->143B 0.12331

135B ->141B -0.22359

135B ->142B -0.12943

136B ->141B 0.15344

136B ->142B -0.10285

137B ->141B 0.15226

137B ->142B 0.13745

137B ->143B -0.16212

137B ->145B 0.11970

Excited State 39: 3.094-A 4.3370 eV 285.87 nm f=0.0138 <S**2>=2.143

129B ->141B -0.12622

130B ->141B 0.21672

130B ->143B 0.10838

131B ->141B 0.20899

132B ->141B 0.56987

132B ->143B 0.12238

133B ->141B -0.28776

134B ->141B -0.33209

134B ->143B -0.10697

136B ->141B -0.42689

137B ->143B 0.10450

138B ->141B -0.12421

Excited State 40: 3.421-A 4.3635 eV 284.14 nm f=0.0791 <S**2>=2.675

135A ->143A -0.11307

138A ->143A -0.20175

138A ->144A 0.23900

130B ->141B -0.26009

130B ->143B -0.16745

130B ->144B -0.13292

131B ->141B 0.20816

131B ->142B 0.28885

133B ->141B -0.20546

135B ->141B -0.29050

135B ->142B 0.32186

136B ->141B 0.24363

136B ->142B -0.15593

136B ->143B -0.11259

136B ->144B -0.20590

137B ->141B 0.13472

137B ->142B -0.16996

137B ->143B -0.17172

138B ->144B 0.11152

Excited State 41: 3.637-A 4.3782 eV 283.19 nm f=0.0058 <S**2>=3.057

137A ->144A -0.11281

138A ->145A 0.11574

139A ->145A -0.18471

140A ->145A 0.14873

141A ->145A -0.18761

129B ->141B -0.21261

129B ->143B -0.14890

130B ->143B -0.15005

131B ->143B 0.17785

131B ->144B -0.11612

133B ->141B 0.20143

133B ->142B 0.13190

133B ->145B -0.10236

134B ->142B -0.19779

134B ->143B 0.21854

135B ->141B -0.24120

135B ->142B -0.17074

135B ->143B 0.34276

135B ->144B -0.13694

136B ->142B 0.11775

136B ->143B -0.23654

136B ->145B 0.10306

137B ->145B -0.12741

138B ->145B -0.10180

Excited State 42: 3.421-A 4.3943 eV 282.15 nm f=0.0267 <S**2>=2.675

133A ->144A 0.13781

134A ->143A -0.11540

138A ->143A -0.27798

142A ->149A 0.10906

130B ->141B 0.40038

130B ->143B -0.13614

131B ->141B -0.31330

132B ->142B 0.11967

133B ->141B -0.12149

133B ->142B -0.12989

135B ->141B 0.21760

136B ->141B -0.13027

136B ->143B -0.28955

137B ->141B -0.13725

137B ->143B -0.36313

138B ->143B 0.10128

Excited State 43: 3.372-A 4.3999 eV 281.79 nm f=0.0035 <S**2>=2.593

138A ->144A 0.23713

139A ->147A 0.11303

140A ->145A 0.17168

141A ->145A -0.18012

128B ->141B -0.11904

129B ->141B 0.42877

129B ->143B 0.10033

130B ->141B 0.13330

132B ->141B 0.20211

132B ->142B 0.11413

133B ->141B 0.37824

134B ->142B 0.11495

135B ->141B 0.32701

135B ->146B 0.12543

136B ->142B -0.13341

136B ->143B -0.10318

137B ->145B -0.13707

138B ->146B -0.11771

Excited State 44: 3.493-A 4.4206 eV 280.47 nm f=0.0105 <S**2>=2.800

136A ->143A -0.17332

136A ->147A 0.11702

137A ->144A 0.17063

138A ->143A -0.18364

140A ->148A -0.11330

129B ->141B 0.12341

131B ->141B -0.18764

132B ->141B 0.20463

132B ->142B -0.16632

132B ->143B 0.10480

133B ->142B 0.14139

134B ->141B 0.50695

134B ->142B -0.38064

134B ->146B -0.10338

135B ->141B -0.18673

135B ->142B 0.14008

136B ->143B 0.16537

137B ->144B -0.11683

Excited State 45: 3.440-A 4.4385 eV 279.34 nm f=0.0059 <S**2>=2.708

133A ->143A 0.12468

133A ->144A -0.18113

134A ->143A 0.27901

134A ->144A -0.12486

136A ->143A 0.22316

136A ->144A -0.12514

137A ->144A -0.15327

138A ->143A 0.47495

138A ->144A -0.17156

129B ->141B 0.12334

130B ->141B 0.11338

130B ->142B -0.11961

131B ->141B -0.16519

131B ->142B 0.13458

132B ->141B 0.20577

133B ->142B -0.10467

134B ->141B 0.30564

135B ->143B -0.10532

136B ->142B -0.14951

136B ->143B -0.17641

136B ->144B -0.11847

Excited State 46: 3.514-A 4.4743 eV 277.11 nm f=0.0061 <S**2>=2.837

133A ->143A -0.21117

133A ->144A -0.15372

134A ->143A 0.11905

134A ->144A 0.24879

135A ->144A -0.11873

136A ->144A 0.16137

137A ->143A -0.23784

137A ->144A -0.16194

138A ->143A 0.34447

138A ->144A 0.56357

139A ->145A 0.10013

140A ->145A -0.11966

141A ->145A 0.15267

131B ->142B -0.10028

133B ->141B -0.16349

134B ->142B -0.13455

Excited State 47: 3.518-A 4.4776 eV 276.90 nm f=0.0029 <S**2>=2.844

136A ->144A -0.11917

137A ->143A 0.10898

128B ->141B 0.17751

129B ->141B 0.25383

130B ->143B 0.11613

131B ->141B -0.16344

131B ->142B 0.10951

131B ->143B 0.21527

132B ->143B 0.20732

133B ->143B -0.18065

133B ->145B -0.10879

134B ->142B 0.13354

134B ->143B 0.16849

135B ->143B 0.42217

136B ->143B 0.39177

136B ->144B -0.14572

137B ->141B -0.15451

137B ->143B -0.12310

137B ->144B 0.14922

138B ->143B -0.12398

Excited State 48: 3.642-A 4.4985 eV 275.61 nm f=0.0140 <S**2>=3.066

134A ->143A -0.17249

138A ->143A -0.20587

138A ->144A 0.14063

139A ->147A -0.15884

140A ->146A 0.14880

140A ->147A -0.21326

141A ->146A -0.17124

141A ->147A 0.20107

142A ->146A -0.10352

142A ->147A 0.16010

129B ->141B 0.15495

130B ->142B 0.11543

130B ->144B 0.10694

131B ->143B -0.12668

132B ->141B 0.16057

132B ->143B -0.14804

133B ->142B 0.11626

134B ->141B 0.18699

134B ->142B 0.26643

135B ->142B -0.16700

135B ->143B -0.20443

135B ->146B -0.11911

136B ->143B -0.10508

137B ->146B -0.14175

138B ->146B 0.12378

140B ->146B 0.11105

Excited State 49: 3.699-A 4.5284 eV 273.79 nm f=0.0068 <S**2>=3.172

134A ->144A -0.19071

134A ->145A -0.10123

135A ->145A -0.15096

138A ->144A -0.14505

138A ->145A 0.10915

139A ->146A -0.10449

139A ->148A -0.11073

140A ->146A 0.16450

140A ->147A 0.19229

140A ->148A 0.11122

141A ->146A -0.23997

141A ->147A -0.22479

141A ->148A -0.15847

142A ->147A -0.14383

131B ->143B -0.10344

133B ->141B -0.17544

133B ->142B 0.30885

133B ->143B -0.15793

133B ->145B -0.23779

134B ->142B -0.13755

134B ->143B -0.11421

134B ->146B -0.11267

135B ->142B -0.14141

135B ->143B -0.12213

135B ->146B 0.13551

136B ->142B -0.15691

137B ->147B 0.13575

140B ->147B -0.12934

Excited State 50: 3.520-A 4.5670 eV 271.48 nm f=0.0100 <S**2>=2.847

134A ->143A 0.13153

136A ->143A -0.14889

136A ->144A 0.12955

136A ->146A -0.11571

136A ->147A 0.15117

137A ->143A -0.10245

137A ->144A 0.16141

139A ->146A 0.11827

140A ->148A -0.18599

141A ->148A 0.22496

142A ->148A 0.10542

129B ->142B -0.10189

129B ->144B 0.12830

131B ->143B 0.15900

132B ->142B 0.13343

132B ->144B -0.12133

132B ->146B -0.11672

134B ->142B 0.30472

134B ->143B 0.15639

134B ->145B 0.10052

134B ->146B -0.20807

135B ->142B -0.29479

135B ->144B -0.10173

136B ->144B -0.10239

137B ->144B -0.11944

138B ->144B 0.20647

140B ->145B -0.11283

140B ->146B 0.17459

Excited State 51: 3.403-A 4.5808 eV 270.66 nm f=0.0266 <S**2>=2.645

134A ->143A 0.11042

135A ->144A 0.16295

135A ->145A 0.10029

136A ->143A 0.17235

141A ->145A 0.14643

142A ->145A 0.10888

128B ->141B -0.16320

130B ->143B -0.14964

131B ->143B -0.14933

132B ->142B 0.19707

133B ->142B 0.60759

133B ->143B -0.14069

133B ->144B -0.12711

133B ->145B 0.12264

134B ->142B 0.17943

135B ->143B 0.27582

136B ->144B 0.10124

137B ->145B 0.11714

Excited State 52: 3.350-A 4.5944 eV 269.86 nm f=0.0077 <S**2>=2.556

140A ->146A	-0.13696
141A ->146A	0.25409
142A ->146A	0.11613
128B ->141B	0.29949
129B ->142B	-0.10503
129B ->144B	0.13467
130B ->143B	0.14932
132B ->141B	0.12671
132B ->143B	-0.13771
133B ->141B	0.23107
133B ->142B	0.34760
133B ->143B	-0.10479
134B ->141B	-0.11089
134B ->142B	-0.25653
134B ->146B	0.11515
135B ->141B	-0.10947
135B ->143B	-0.22652
135B ->144B	-0.12227
136B ->142B	-0.16163
137B ->141B	-0.11567
138B ->144B	0.22019
140B ->146B	-0.10797

Excited State 53: 3.518-A 4.6244 eV 268.11 nm f=0.0338 <S**2>=2.845

136A ->143A	-0.35164
136A ->144A	0.19031
137A ->143A	-0.24140
137A ->144A	0.25655
128B ->141B	0.12436
130B ->142B	-0.10104
130B ->143B	-0.20530

131B ->143B -0.29969

132B ->142B 0.43247

132B ->143B 0.11533

133B ->142B -0.18847

134B ->143B -0.21704

135B ->142B -0.12265

135B ->143B 0.14338

135B ->144B 0.15300

Excited State 54: 3.472-A 4.6372 eV 267.37 nm f=0.0277 <S**2>=2.763

136A ->143A -0.12785

141A ->145A 0.26622

141A ->146A 0.22633

141A ->147A 0.10007

141A ->148A -0.10158

142A ->145A 0.40091

142A ->146A 0.22951

128B ->141B -0.36466

129B ->142B -0.13359

130B ->142B -0.15587

133B ->141B -0.21155

133B ->142B -0.10669

134B ->141B 0.15678

134B ->142B -0.15732

135B ->143B 0.12979

136B ->143B -0.10811

136B ->144B -0.10692

137B ->141B 0.12838

137B ->143B 0.15175

138B ->144B 0.10255

140B ->145B 0.16850

Excited State 55: 3.533-A 4.6458 eV 266.88 nm f=0.0139 <S**2>=2.870

134A ->143A	-0.22513
134A ->144A	0.14688
135A ->144A	-0.13185
136A ->143A	0.17865
136A ->144A	-0.19022
137A ->143A	0.41243
137A ->144A	-0.13882
138A ->144A	0.14392
141A ->145A	0.10683
141A ->147A	0.13190
142A ->145A	-0.17812
129B ->141B	-0.11781
129B ->142B	-0.16729
131B ->142B	-0.27453
131B ->143B	-0.15514
132B ->142B	0.28172
133B ->142B	-0.13697
134B ->142B	-0.17058
136B ->142B	-0.25529
137B ->143B	0.10658
138B ->144B	0.15144

Excited State 56: 3.577-A 4.6489 eV 266.70 nm f=0.0658 <S**2>=2.949

134A ->144A	0.11620
135A ->143A	0.13652
137A ->143A	0.22708
137A ->144A	0.15480
138A ->143A	0.11661
141A ->146A	-0.15327
141A ->147A	-0.10064
141A ->148A	0.11195

142A ->145A 0.61855

142A ->146A 0.10312

129B ->142B 0.13802

130B ->142B 0.15979

131B ->142B 0.14744

132B ->142B 0.26249

132B ->143B -0.12079

136B ->143B 0.12888

136B ->144B 0.12253

140B ->145B 0.17651

Excited State 57: 3.550-A 4.6651 eV 265.77 nm f=0.0123 <S**2>=2.901

130A ->144A 0.15694

133A ->143A 0.17322

134A ->144A -0.11686

137A ->144A 0.18189

138A ->143A 0.12060

138A ->144A 0.12022

141A ->146A 0.21299

129B ->142B -0.24147

129B ->143B 0.11963

129B ->144B 0.13032

130B ->142B 0.36265

130B ->143B -0.22241

130B ->144B 0.12002

131B ->142B 0.13575

131B ->143B -0.10418

131B ->144B 0.12264

132B ->142B -0.28541

135B ->143B 0.23007

135B ->144B -0.19198

137B ->143B 0.15284

137B ->144B 0.14411

138B ->144B 0.14247

Excited State 58: 3.451-A 4.6791 eV 264.97 nm f=0.1507 <S**2>=2.728

134A ->144A -0.15335

135A ->143A -0.19030

137A ->143A -0.12750

137A ->144A -0.21297

138A ->143A -0.14316

141A ->145A -0.12130

141A ->147A -0.16460

141A ->148A 0.20968

142A ->145A 0.36972

142A ->146A 0.12720

128B ->141B 0.28060

129B ->142B -0.10202

130B ->143B -0.14874

131B ->142B -0.29691

131B ->143B -0.19076

132B ->142B -0.24114

132B ->143B 0.11488

133B ->141B 0.10692

134B ->141B -0.11587

134B ->142B 0.14737

134B ->143B -0.18084

137B ->141B -0.17872

Excited State 59: 3.529-A 4.6864 eV 264.56 nm f=0.0362 <S**2>=2.864

133A ->144A -0.10808

134A ->143A 0.18461

134A ->144A 0.30261

135A ->143A 0.32446

135A ->144A 0.26746

136A ->144A 0.14005

137A ->143A 0.13873

138A ->143A -0.11016

138A ->144A -0.11878

141A ->145A 0.25070

141A ->146A -0.19612

141A ->148A -0.17006

142A ->146A -0.14581

142A ->147A -0.17717

128B ->141B 0.15984

130B ->142B -0.24289

132B ->142B -0.21525

134B ->143B -0.11474

136B ->142B 0.10307

140B ->145B 0.25981

140B ->147B -0.10305

Excited State 60: 3.636-A 4.6982 eV 263.90 nm f=0.0098 <S**2>=3.055

133A ->143A 0.10765

134A ->144A -0.22612

135A ->143A -0.23926

137A ->143A -0.12918

141A ->145A 0.32726

141A ->146A 0.24724

141A ->147A 0.36580

142A ->146A -0.23626

142A ->147A -0.28615

142A ->148A 0.17177

128B ->141B 0.10522

129B ->142B 0.15094

129B ->144B -0.10193

134B ->142B 0.10883

135B ->143B -0.11551

138B ->144B -0.12406

140B ->145B 0.31263

140B ->146B 0.10191

140B ->147B -0.14515

Excited State 61: 3.495-A 4.7032 eV 263.62 nm f=0.0517 <S**2>=2.804

134A ->143A -0.29766

135A ->144A -0.24067

137A ->144A -0.27789

141A ->145A -0.16771

141A ->146A 0.12998

141A ->147A 0.20234

142A ->146A 0.18160

142A ->147A -0.13815

142A ->148A 0.14069

130B ->142B -0.20000

130B ->144B 0.14017

131B ->142B 0.39423

131B ->143B -0.14842

134B ->143B -0.16460

135B ->142B -0.21287

135B ->143B 0.14007

136B ->142B 0.17103

137B ->144B -0.15413

140B ->145B -0.14380

140B ->147B -0.11755

Excited State 62: 3.509-A 4.7161 eV 262.90 nm f=0.0013 <S**2>=2.829

141A ->145A 0.29341

141A ->146A -0.28935

141A ->148A 0.20824

142A ->145A -0.35396

142A ->146A 0.74897

142A ->148A 0.15730

140B ->145B 0.10625

Excited State 63: 3.660-A 4.7243 eV 262.44 nm f=0.0052 <S**2>=3.098

133A ->144A 0.12404

134A ->143A -0.23433

135A ->144A -0.16621

141A ->145A 0.16107

141A ->146A -0.19640

141A ->147A -0.25004

141A ->148A 0.24361

142A ->145A -0.14042

142A ->146A -0.22020

142A ->147A 0.21702

142A ->148A -0.27155

131B ->142B 0.15937

135B ->143B 0.10492

140B ->145B 0.54084

Excited State 64: 3.617-A 4.7448 eV 261.30 nm f=0.0093 <S**2>=3.021

135A ->143A 0.12700

137A ->143A 0.16695

141A ->145A 0.19661

141A ->146A 0.51158

141A ->147A -0.47147

142A ->145A -0.16852

142A ->147A 0.16105

129B ->142B 0.13497

132B ->143B -0.12437

133B ->143B -0.17590

140B ->146B 0.33104

Excited State 65: 3.474-A 4.7506 eV 260.99 nm f=0.0026 <S**2>=2.767

130A ->143A 0.12389

133A ->143A 0.17304

133A ->144A 0.21877

134A ->143A -0.19131

134A ->144A -0.10721

136A ->144A 0.19021

137A ->143A 0.25903

138A ->143A 0.15951

138A ->144A 0.23286

129B ->142B -0.14043

130B ->142B -0.35801

130B ->143B -0.14820

131B ->143B 0.10935

132B ->142B -0.13761

132B ->144B 0.11377

133B ->142B 0.14236

133B ->143B 0.40958

134B ->143B 0.18516

135B ->143B -0.11792

135B ->144B 0.11725

137B ->142B 0.10191

140B ->145B -0.13061

Excited State 66: 3.490-A 4.7551 eV 260.74 nm f=0.0024 <S**2>=2.794

133A ->143A -0.13764

136A ->143A 0.14940

136A ->144A -0.23547

137A ->143A -0.26008

138A ->144A -0.10968

141A ->145A 0.22604

141A ->146A 0.13773

141A ->147A -0.15058

142A ->147A 0.13031

128B ->141B 0.11534

129B ->142B 0.13723

131B ->142B 0.17749

132B ->143B 0.29232

132B ->144B -0.12327

133B ->142B 0.11931

133B ->143B 0.61624

Excited State 67: 3.692-A 4.7621 eV 260.36 nm f=0.0024 <S**2>=3.157

133A ->143A -0.16386

133A ->144A 0.25573

134A ->143A -0.17751

136A ->143A 0.45771

137A ->143A -0.24271

137A ->144A 0.44638

138A ->143A 0.14070

141A ->147A 0.18614

142A ->147A 0.33319

130B ->142B -0.14156

132B ->142B -0.12873

133B ->143B -0.22104

140B ->147B -0.14484

Excited State 68: 3.697-A 4.7707 eV 259.89 nm f=0.0091 <S**2>=3.166

133A ->143A 0.11223

133A ->144A -0.12401

134A ->143A 0.11942

136A ->143A -0.18275

136A ->144A 0.22658

137A ->143A 0.20509

137A ->144A -0.14453

141A ->147A 0.17893

142A ->147A 0.61913

142A ->148A -0.16976

140B ->146B -0.11938

140B ->147B -0.43289

Excited State 69: 3.394-A 4.7753 eV 259.64 nm f=0.0125 <S**2>=2.630

136A ->143A 0.13045

139A ->145A 0.12700

140A ->145A -0.18087

141A ->145A -0.37872

141A ->147A -0.11652

141A ->148A -0.41864

142A ->146A 0.14242

142A ->148A 0.25076

133B ->143B 0.12468

139B ->145B -0.19060

139B ->146B -0.11157

140B ->145B 0.42857

140B ->146B 0.35723

Excited State 70: 3.583-A 4.7857 eV 259.07 nm f=0.0017 <S**2>=2.959

136A ->143A -0.10235

142A ->146A -0.18222

142A ->147A 0.24868

142A ->148A 0.74091

140B ->145B 0.11520

140B ->146B -0.43498

140B ->147B 0.24756

Excited State 71: 3.410-A 4.7934 eV 258.66 nm f=0.0019 <S**2>=2.657

134A ->144A -0.11063

136A ->143A 0.34445

136A ->144A 0.38811

137A ->144A 0.26854

141A ->145A -0.14837

141A ->146A 0.10157

141A ->148A 0.33396

142A ->147A -0.14431

129B ->142B 0.23142

130B ->143B 0.11777

133B ->143B 0.21561

134B ->143B -0.23356

135B ->143B 0.12345

136B ->144B -0.11316

139B ->145B -0.13197

140B ->145B 0.17020

140B ->146B -0.16541

Excited State 72: 3.597-A 4.7965 eV 258.49 nm f=0.0147 <S**2>=2.985

134A ->143A -0.11324

134A ->144A -0.10220

135A ->143A -0.16950

136A ->143A 0.15063

136A ->144A 0.33084

137A ->143A 0.17197

141A ->145A 0.13850

141A ->148A -0.47128

142A ->146A 0.14866

142A ->147A 0.11989

142A ->148A -0.18298

129B ->142B 0.13408

134B ->143B -0.11149

135B ->144B -0.10171

137B ->144B -0.11196

139B ->145B 0.15953

140B ->147B 0.47556

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 72 LETran= 1306.

Table S5. Excited states, excitation energy (eV), wavelength (nm) and oscillator strength (*f*) for **2a** at M06/SVP with PCM in chloroform.

Excitation energies and oscillator strengths:

Excited State 1: 2.009-A 1.5173 eV 817.15 nm f=0.0000 <S**2>=0.759

112B ->142B 0.12759

116B ->142B 0.10784

117B ->142B -0.23154

125B ->142B 0.16781

130B ->142B -0.27447

131B ->142B -0.13809

132B ->142B 0.32851

141B ->142B 0.78037

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3136.71488957

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.004-A 2.1080 eV 588.17 nm f=0.0000 <S**2>=0.754

107B ->142B -0.11590

109B ->142B 0.23127

112B ->142B 0.26191

117B ->142B 0.16676

121B ->142B 0.29534

124B ->142B -0.13027

125B ->142B 0.27399

130B ->142B 0.25484

131B ->142B 0.40084

132B ->142B 0.57595

141B ->142B -0.23438

Excited State 3: 2.003-A 2.3924 eV 518.23 nm f=0.0000 <S**2>=0.753

106B ->142B -0.12267

113B ->142B 0.20583

116B ->142B 0.12665

122B ->142B -0.15754

125B ->142B -0.55724

129B ->142B 0.70109

132B ->142B 0.12360

135B ->142B -0.10925

136B ->142B -0.11732

Excited State 4: 2.056-A 2.4174 eV 512.88 nm f=0.0137 <S**2>=0.807

140B ->142B 0.98019

Excited State 5: 2.010-A 2.4958 eV 496.76 nm f=0.0000 <S**2>=0.760

107B ->142B -0.10081

113B ->142B -0.35916

114B ->142B -0.17860

116B ->142B -0.16329

117B ->142B -0.17022

121B ->142B -0.14811

124B ->142B -0.45883

125B ->142B -0.28358

130B ->142B -0.25735

131B ->142B 0.47869

135B ->142B 0.30352

138B ->142B -0.14026

Excited State 6: 3.415-A 2.7245 eV 455.08 nm f=0.0010 <S**2>=2.665

140A ->144A 0.42582

141A ->143A -0.20162

142A ->143A 0.52297

140B ->144B -0.41487

141B ->143B 0.53428

Excited State 7: 3.421-A 2.7268 eV 454.69 nm f=0.0000 <S**2>=2.676

140A ->143A 0.42981

141A ->144A -0.19581

142A ->144A 0.49339

140B ->143B -0.44164

141B ->144B 0.52993

Excited State 8: 2.135-A 3.0375 eV 408.18 nm f=0.0000 <S**2>=0.889

102B ->142B 0.15764

116B ->142B -0.15375

117B ->142B 0.44480

124B ->142B 0.12438

130B ->142B 0.43594

131B ->142B 0.25003

132B ->142B -0.18656

138B ->142B -0.19163

141B ->142B 0.54174

Excited State 9: 2.477-A 3.1109 eV 398.54 nm f=0.0313 <S**2>=1.284

139A ->144A -0.11026

139A ->148A -0.15027

141A ->143A -0.35620

141A ->147A -0.11096

142A ->143A -0.12266

136B ->146B 0.12516

137B ->145B -0.10031

138B ->147B -0.14860

139B ->142B 0.78077

139B ->148B 0.13990

Excited State 10: 2.336-A 3.1828 eV 389.54 nm f=0.0011 <S**2>=1.114

133A ->144A -0.12941

139A ->144A 0.11881

141A ->143A 0.61084

142A ->143A 0.57029

139B ->142B 0.37508

140B ->144B 0.13355

141B ->143B -0.24967

Excited State 11: 2.585-A 3.1954 eV 388.01 nm f=0.0000 <S**2>=1.421

133A ->143A -0.13597

139A ->143A 0.18444

141A ->144A 0.65901

142A ->144A 0.54767

139B ->143B -0.11234

139B ->147B -0.10081

141B ->144B -0.16908

Excited State 12: 3.329-A 3.3129 eV 374.24 nm f=0.0091 <S**2>=2.520

135A ->144A 0.35081

136A ->143A -0.36619

137A ->144A 0.15630

138A ->143A -0.18496

140A ->144A -0.10887

140A ->149A -0.17269

141A ->143A 0.15977

142A ->150A 0.18146

133B ->142B -0.19909

133B ->144B -0.11611

134B ->142B 0.17877

134B ->144B -0.30967

135B ->143B 0.36860

137B ->144B -0.15673

138B ->143B -0.16332

140B ->149B 0.19016

141B ->150B 0.20176

Excited State 13: 3.254-A 3.3140 eV 374.12 nm f=0.0000 <S**2>=2.396

135A ->143A -0.31962

136A ->144A 0.32703

137A ->143A -0.14462

138A ->144A 0.18457

140A ->150A -0.18060

141A ->144A -0.20278

142A ->144A -0.22858

142A ->149A 0.18114

134B ->143B 0.29795

135B ->142B 0.11694

135B ->144B -0.32719

137B ->143B 0.15050

138B ->142B 0.19162

138B ->144B 0.17182

139B ->143B -0.11325

140B ->143B -0.14757

140B ->150B 0.17918

141B ->149B 0.17013

Excited State 14: 2.196-A 3.3708 eV 367.82 nm f=0.1941 <S**2>=0.956

140A ->144A 0.16519

141A ->143A -0.26956

142A ->143A 0.23373

133B ->142B 0.66612

134B ->142B -0.24315

134B ->144B -0.11823

135B ->143B 0.12577

137B ->142B -0.14607

139B ->142B -0.21326

140B ->144B 0.15268

141B ->143B -0.36010

Excited State 15: 2.984-A 3.3861 eV 366.16 nm f=0.0000 <S**2>=1.976

134A ->145A -0.12036

135A ->143A 0.16847

136A ->144A -0.16725

137A ->146A -0.16189

138A ->148A 0.14830

139A ->146A 0.11087

139A ->147A 0.24205

141A ->144A -0.12825

141A ->145A 0.14941

141A ->148A 0.19154

142A ->144A -0.12416

117B ->142B 0.13463

130B ->142B 0.10914

134B ->143B -0.14779

135B ->144B 0.17528

136B ->142B -0.14700

136B ->145B -0.18380

137B ->146B 0.15674

138B ->142B 0.49333

138B ->148B 0.20636

139B ->146B -0.12130

139B ->147B -0.22775

141B ->142B 0.14584

Excited State 16: 2.028-A 3.4631 eV 358.01 nm f=0.0000 <S**2>=0.778

140A ->143A -0.35734

141A ->144A 0.50856

142A ->144A -0.36474

140B ->143B -0.27502

141B ->144B 0.60064

Excited State 17: 2.878-A 3.5499 eV 349.26 nm f=0.0906 <S**2>=1.820

134A ->143A 0.10212

134A ->146A 0.13225

134A ->147A 0.10372

137A ->145A 0.17905

138A ->146A 0.12696

138A ->147A -0.15106

139A ->145A -0.12140

139A ->148A -0.24110

140A ->144A -0.18009

141A ->143A 0.30745

141A ->146A -0.15082

141A ->147A -0.21334

133B ->142B 0.30636

134B ->142B -0.15881

136B ->146B 0.21694

137B ->142B -0.13994

137B ->145B -0.18711

138B ->143B -0.11879

138B ->147B -0.21970

139B ->142B -0.26112

139B ->144B 0.12901

139B ->148B 0.25146

141B ->143B 0.28655

Excited State 18: 2.373-A 3.6153 eV 342.94 nm f=0.2530 <S**2>=1.158

137A ->145A -0.11389

139A ->148A 0.15095

141A ->143A 0.29257

141A ->147A 0.11733

142A ->143A -0.32880

133B ->142B 0.29794

134B ->142B -0.39269

136B ->146B -0.12712

137B ->142B -0.15085

137B ->145B 0.11139

138B ->147B 0.12959

139B ->142B 0.32769

139B ->148B -0.14652

141B ->143B 0.43119

Excited State 19: 2.536-A 3.6677 eV 338.04 nm f=0.0000 <S**2>=1.358

134A ->145A 0.11084

137A ->146A 0.15782

138A ->145A 0.10363

138A ->148A -0.10190

139A ->147A -0.14963

141A ->145A -0.11485

141A ->148A -0.10532

136B ->142B 0.18242

136B ->145B 0.16560

137B ->146B -0.15377

138B ->142B 0.77281

138B ->148B -0.15803

139B ->143B 0.15625

139B ->147B 0.15440

140B ->143B 0.11409

Excited State 20: 2.159-A 3.7758 eV 328.36 nm f=0.0187 <S**2>=0.916

133B ->142B 0.30402

137B ->142B 0.89612

140B ->144B 0.18112

141B ->143B 0.15582

Excited State 21: 3.094-A 3.7888 eV 327.24 nm f=0.0000 <S**2>=2.143

140A ->143A -0.13688

141A ->144A -0.14632

142A ->144A 0.20025

136B ->142B -0.27014

140B ->143B 0.73595

141B ->144B 0.51142

Excited State 22: 3.270-A 3.8046 eV 325.88 nm f=0.0088 <S**2>=2.424

140A ->144A -0.27900

141A ->143A -0.23978

142A ->143A 0.27243

134B ->142B 0.13511

137B ->142B -0.21481

140B ->144B 0.70167

141B ->143B 0.43211

Excited State 23: 2.193-A 3.8392 eV 322.95 nm f=0.0000 <S**2>=0.952

139A ->147A 0.11252

140A ->143A 0.22502

142A ->144A -0.13186

135B ->142B -0.20912

136B ->142B 0.80918

138B ->148B 0.10174

139B ->143B -0.11029

140B ->143B 0.28479

141B ->144B 0.17324

Excited State 24: 2.538-A 3.8459 eV 322.38 nm f=0.0000 <S**2>=1.360

140A ->143A 0.75527

141A ->144A 0.33883

142A ->144A -0.38644

136B ->142B -0.30752

140B ->143B 0.18972

Excited State 25: 2.249-A 3.8482 eV 322.18 nm f=0.0022 <S**2>=1.015

140A ->144A 0.59136

141A ->143A 0.23494

142A ->143A -0.33811

133B ->142B 0.22695

134B ->142B 0.56154

137B ->142B -0.14909

140B ->144B 0.23625

Excited State 26: 2.145-A 3.9058 eV 317.44 nm f=0.0000 <S**2>=0.900

140A ->150A 0.11019

113B ->142B 0.17939

124B ->142B 0.15312

129B ->142B 0.13703

131B ->142B -0.10542

135B ->142B 0.87075

136B ->142B 0.20046

Excited State 27: 2.126-A 3.9158 eV 316.62 nm f=0.1502 <S**2>=0.880

140A ->144A -0.52603

133B ->142B 0.37602

134B ->142B 0.58198

140B ->144B -0.39153

Excited State 28: 3.412-A 4.0842 eV 303.57 nm f=0.0008 <S**2>=2.661

135A ->144A -0.14602

136A ->143A 0.18110

138A ->143A 0.10385

139A ->144A 0.17554

140A ->149A -0.33696

140A ->151A 0.13345

141A ->150A -0.16042

142A ->150A 0.37285

134B ->142B 0.13819

134B ->144B 0.15221

135B ->143B -0.18026

138B ->143B 0.14824

139B ->144B -0.21800

140B ->149B 0.34504

140B ->151B -0.12958

141B ->150B 0.40385

Excited State 29: 3.382-A 4.0919 eV 303.00 nm f=0.0000 <S**2>=2.609

135A ->143A 0.14827

136A ->144A -0.18085

139A ->143A -0.16969

140A ->150A -0.36220

141A ->149A -0.15001

142A ->149A 0.33535

142A ->151A -0.12847

134B ->143B -0.15685

135B ->142B 0.17801

135B ->144B 0.18405

137B ->143B -0.10243

138B ->144B -0.12198

139B ->143B 0.19691

140B ->150B 0.37652

141B ->149B 0.37486

141B ->151B -0.13643

141B ->153B 0.10388

Excited State 30: 2.989-A 4.2040 eV 294.92 nm f=0.0000 <S**2>=1.984

135A ->143A -0.11447

137A ->146A -0.12909

138A ->145A -0.10662

134B ->143B 0.17711

135B ->144B -0.13050

136B ->144B 0.14381

136B ->145B -0.12459

137B ->146B 0.11073

138B ->144B -0.27929

139B ->143B 0.80139

Excited State 31: 3.053-A 4.2215 eV 293.70 nm f=0.0314 <S**2>=2.080

135A ->144A -0.10908

137A ->145A -0.11647

139A ->144A -0.10691

141A ->146A 0.10460

134B ->144B 0.19916

135B ->143B -0.17581

136B ->143B 0.13283

136B ->146B -0.12552

137B ->145B 0.10633

138B ->143B -0.32583

139B ->144B 0.76427

141B ->150B 0.11557

Excited State 32: 2.649-A 4.3083 eV 287.78 nm f=0.0000 <S**2>=1.504

134A ->144A -0.18482

135A ->143A 0.10124

139A ->143A 0.88366

136B ->145B 0.10753

137B ->146B -0.10045

139B ->143B 0.17518

Excited State 33: 2.703-A 4.3229 eV 286.81 nm f=0.0235 <S**2>=1.576

134A ->143A -0.14430

138A ->143A 0.14780

139A ->144A 0.76178

139A ->145A -0.18850

141A ->146A -0.23972

142A ->146A -0.10215

136B ->143B 0.10768

138B ->143B -0.12581

138B ->146B -0.12133

139B ->144B 0.21688

139B ->145B 0.18104

Excited State 34: 3.288-A 4.3470 eV 285.22 nm f=0.0000 <S**2>=2.453

134A ->145A -0.14858

137A ->143A -0.13582

137A ->147A -0.14919

138A ->144A -0.13725

138A ->148A -0.17481

139A ->146A 0.35941

139A ->147A -0.13236

141A ->145A 0.45780

141A ->148A -0.12427

142A ->145A 0.16399

136B ->142B 0.16800

136B ->144B -0.12544

136B ->148B -0.14635

137B ->143B 0.15328

137B ->147B 0.16906

138B ->144B -0.12757

138B ->145B 0.28669

138B ->148B -0.11858

139B ->146B -0.33962

139B ->147B 0.14714

141B ->145B -0.21754

Excited State 35: 3.217-A 4.3698 eV 283.73 nm f=0.0147 <S**2>=2.338

134A ->143A -0.16515

134A ->146A -0.10852

135A ->144A 0.10390

137A ->144A -0.11289

137A ->148A -0.16789

138A ->146A 0.15856

138A ->147A -0.17427

139A ->144A 0.43809

139A ->145A 0.30797

139A ->148A -0.10470

141A ->146A 0.36340

142A ->146A 0.11177

136B ->143B -0.15102

136B ->147B -0.15732

137B ->144B 0.12495

137B ->148B 0.16710

138B ->146B 0.25591

138B ->147B -0.14167

139B ->145B -0.31051

141B ->146B -0.17221

Excited State 36: 3.359-A 4.4986 eV 275.60 nm f=0.0047 <S**2>=2.570

134A ->147A -0.13037

136A ->146A -0.12763

137A ->145A 0.28570

138A ->143A 0.16534

138A ->146A 0.27887

139A ->144A -0.18677

139A ->148A 0.23618

141A ->147A 0.34815

142A ->147A 0.13600

134B ->145B 0.12047

136B ->143B 0.11617

136B ->146B 0.28565

136B ->147B -0.14996

137B ->145B -0.30773

138B ->143B 0.20001

138B ->146B 0.14926

138B ->147B 0.14599

139B ->144B 0.18301

139B ->148B -0.22958

141B ->147B -0.15570

Excited State 37: 3.277-A 4.5174 eV 274.46 nm f=0.0000 <S**2>=2.435

134A ->148A 0.12984

136A ->145A 0.11111

137A ->146A -0.26305

137A ->147A 0.10315

138A ->145A -0.25729

139A ->143A 0.20189

139A ->147A -0.22776

141A ->148A -0.31088

142A ->148A -0.11603

132B ->144B -0.12801

133B ->143B 0.39062

134B ->143B -0.21065

136B ->145B -0.26609

136B ->148B 0.11341

137B ->146B 0.26872

137B ->147B -0.10309

138B ->145B -0.14017

138B ->148B -0.15599

139B ->146B 0.10342

139B ->147B 0.21952

141B ->148B 0.15208

Excited State 38: 2.987-A 4.5244 eV 274.04 nm f=0.0000 <S**2>=1.980

135A ->143A -0.13348

137A ->146A 0.13325

138A ->145A 0.13174

139A ->147A 0.11818

141A ->148A 0.15969

132B ->142B 0.19448

132B ->144B -0.24550

133B ->143B 0.64330

134B ->143B -0.25084

136B ->145B 0.13237

137B ->143B -0.20749

137B ->146B -0.13222

138B ->144B 0.13925

139B ->143B 0.19055

139B ->147B -0.10725

Excited State 39: 2.914-A 4.5667 eV 271.49 nm f=0.0192 <S**2>=1.873

133A ->144A -0.10533

132B ->143B -0.31486

133B ->144B 0.71543

134B ->144B -0.26651

137B ->144B -0.17862

138B ->143B 0.33615

139B ->144B 0.27297

Excited State 40: 2.649-A 4.6124 eV 268.81 nm f=0.0912 <S**2>=1.505

135A ->144A 0.16188

136A ->143A -0.12445

138A ->143A -0.20676

141A ->147A -0.13362

133B ->144B -0.29880

134B ->144B 0.22054

138B ->143B 0.75763

139B ->144B 0.29641

Excited State 41: 2.412-A 4.6221 eV 268.24 nm f=0.0000 <S**2>=1.204

135A ->143A 0.16449

136A ->144A -0.18220

137A ->143A 0.13075

138A ->144A -0.10156

109B ->142B 0.14734

112B ->142B 0.16749

121B ->142B 0.13883

125B ->142B 0.15689

129B ->142B 0.15029

131B ->142B 0.12290

132B ->142B -0.37735

133B ->143B 0.14656

135B ->144B -0.10126

138B ->144B 0.62471

139B ->143B 0.28385

Excited State 42: 3.130-A 4.6453 eV 266.90 nm f=0.0100 <S**2>=2.199

135A ->144A -0.16348

136A ->143A -0.12891

137A ->144A 0.37960

137A ->148A 0.12323

138A ->143A 0.69414

139A ->145A 0.13482

139A ->148A -0.11983

141A ->146A 0.21301

141A ->147A -0.22300

133B ->144B -0.10054

135B ->143B 0.13027

136B ->143B 0.14160

137B ->144B -0.17379

Excited State 43: 2.911-A 4.6494 eV 266.67 nm f=0.0000 <S**2>=1.869

135A ->143A -0.11074

136A ->144A -0.15182

137A ->143A 0.43797

138A ->144A 0.34213

139A ->146A 0.10385

141A ->145A 0.17346

142A ->145A 0.10204

109B ->142B 0.10404

112B ->142B 0.11851

125B ->142B 0.10674

129B ->142B 0.10613

132B ->142B -0.26531

133B ->143B 0.19027

135B ->144B -0.13021

136B ->144B 0.25447

137B ->143B -0.19307

138B ->144B -0.38322

139B ->143B -0.22125

Excited State 44: 3.004-A 4.6576 eV 266.20 nm f=0.0000 <S**2>=2.006

135A ->143A -0.13073

137A ->143A 0.33066

138A ->144A 0.36778

139A ->147A -0.12322

141A ->145A 0.16669

141A ->148A -0.21721

142A ->148A -0.10423

109B ->142B -0.11997

112B ->142B -0.13512

121B ->142B -0.10906

125B ->142B -0.11389

129B ->142B -0.11664

132B ->142B 0.29764

133B ->143B -0.26712

135B ->144B 0.17638

137B ->143B -0.18568

138B ->144B 0.43561

Excited State 45: 2.948-A 4.6983 eV 263.89 nm f=0.1273 <S**2>=1.923

133A ->144A -0.23351

134A ->143A 0.21238

135A ->144A 0.12975

136A ->143A -0.26201

137A ->144A 0.23040

138A ->143A -0.23142

139A ->144A 0.17257

142A ->150A 0.13619

133B ->144B 0.13999

134B ->144B 0.28332

135B ->143B -0.26885

136B ->143B 0.47234

137B ->144B -0.16597

139B ->144B -0.19519

139B ->145B -0.10983

141B ->146B -0.14459

Excited State 46: 2.396-A 4.7059 eV 263.46 nm f=0.0000 <S**2>=1.186

133A ->143A 0.15186

134A ->144A -0.11416

137A ->143A 0.21727

138A ->144A 0.41633

139A ->143A -0.10586

134B ->143B -0.26187

136B ->144B -0.48488

137B ->143B 0.52149

138B ->144B -0.12188

138B ->145B -0.10722

139B ->146B 0.13406

141B ->145B 0.16881

Excited State 47: 2.406-A 4.7181 eV 262.78 nm f=0.0000 <S**2>=1.197

133A ->143A -0.34111

134A ->144A 0.26344

135A ->143A 0.14711

136A ->144A -0.23217

137A ->143A 0.36510

138A ->144A -0.27568

139A ->143A 0.15575

141A ->144A -0.12736

142A ->145A -0.13011

142A ->149A -0.12292

125B ->142B -0.10593

131B ->142B -0.10546

132B ->142B 0.24140

134B ->143B 0.19282

135B ->144B -0.25102

137B ->143B 0.34540

141B ->145B 0.11369

Excited State 48: 2.164-A 4.7198 eV 262.69 nm f=0.1760 <S**2>=0.921

135A ->144A 0.12063

136A ->143A -0.32693

137A ->144A 0.39267

138A ->143A 0.13640

133B ->144B 0.11753

135B ->143B -0.30444

136B ->143B -0.45075

137B ->144B 0.51034

139B ->145B 0.12592

141B ->147B -0.10162

Excited State 49: 2.575-A 4.7960 eV 258.51 nm f=0.0955 <S**2>=1.408

130A ->144A -0.15378

131A ->143A 0.18110

133A ->144A -0.33429

134A ->143A 0.41188

135A ->144A -0.24899

136A ->143A 0.13937

139A ->144A 0.17741

142A ->152A -0.11530

128B ->144B 0.15097

130B ->143B -0.15592

131B ->143B 0.12644

132B ->143B 0.10515

133B ->144B -0.26248

135B ->143B 0.31221

135B ->152B -0.10579

136B ->143B -0.17386

137B ->144B 0.15626

141B ->150B 0.11907

141B ->152B -0.10661

Excited State 50: 2.672-A 4.7974 eV 258.44 nm f=0.0000 <S**2>=1.535

130A ->143A -0.16738

131A ->144A 0.20015

133A ->143A -0.29709

134A ->144A 0.31413

135A ->143A -0.26187

136A ->144A 0.15416

139A ->143A 0.12332

140A ->152A -0.13485

142A ->145A 0.16421

142A ->148A 0.14434

142A ->153A 0.11646

128B ->143B 0.16658

130B ->144B -0.15758

131B ->144B 0.11632

132B ->142B -0.16039

133B ->143B -0.23591

134B ->143B -0.17847

135B ->144B 0.28139

135B ->153B 0.10306

136B ->144B -0.11802

137B ->143B 0.12336

138B ->144B 0.11725

140B ->150B -0.10066

141B ->149B -0.16612

Excited State 51: 3.189-A 4.8321 eV 256.58 nm f=0.0220 <S**2>=2.292

130A ->144A -0.17960

131A ->143A 0.20307

132A ->143A -0.11377

133A ->144A 0.32938

134A ->143A -0.28135

135A ->144A 0.10803

135A ->153A 0.10668

136A ->143A -0.15290

136A ->152A 0.10704

137A ->144A -0.24328

138A ->143A 0.18018

140A ->149A -0.10137

140A ->153A 0.15033

141A ->146A -0.10461

142A ->146A -0.14237

142A ->152A -0.22920

128B ->142B -0.11905

128B ->144B 0.16795

130B ->143B -0.17185

131B ->143B 0.13851

135B ->152B -0.11625

137B ->144B 0.17026

140B ->153B -0.16235

141B ->146B -0.12624

141B ->152B -0.24849

Excited State 52: 3.108-A 4.8329 eV 256.54 nm f=0.0002 <S**2>=2.165

130A ->143A 0.17361

131A ->144A -0.18956

133A ->143A -0.29482

134A ->144A 0.21928

135A ->143A -0.16999

135A ->152A 0.10300

136A ->144A 0.21418

137A ->143A 0.14017

138A ->144A -0.24840

140A ->152A 0.15145

142A ->145A 0.30675

142A ->148A -0.11071

142A ->153A -0.14824

128B ->143B -0.17274

130B ->144B 0.16269

131B ->144B -0.14521

135B ->153B -0.10278

137B ->143B -0.19057

138B ->144B -0.10707

140B ->152B -0.18514

141B ->145B 0.14189

141B ->148B -0.12569

141B ->153B -0.17532

Excited State 53: 2.893-A 4.8706 eV 254.55 nm f=0.0000 <S**2>=1.843

133A ->143A 0.17959

134A ->144A -0.10509

135A ->143A 0.12076

140A ->150A 0.10225

141A ->145A 0.13357

141A ->149A 0.11176

142A ->145A 0.67448

142A ->148A 0.17456

132B ->142B 0.11263

136B ->144B 0.10521

141B ->145B 0.47862

141B ->148B 0.13308

Excited State 54: 2.092-A 4.9172 eV 252.14 nm f=0.0000 <S**2>=0.844

137A ->143A -0.15293

139A ->146A 0.13314

141A ->145A 0.33955

142A ->145A -0.48953

142A ->148A -0.17312

137B ->143B -0.13294

141B ->145B 0.68594

Excited State 55: 2.944-A 4.9295 eV 251.52 nm f=0.0000 <S**2>=1.917

133A ->143A -0.41670

134A ->144A 0.10601

135A ->143A 0.27799

136A ->144A -0.26088

137A ->143A -0.48166

138A ->144A 0.48842

140A ->152A 0.12912

142A ->145A 0.16308

142A ->148A -0.16010

142A ->153A -0.10015

140B ->152B -0.12708

141B ->148B -0.16636

141B ->153B -0.10279

Excited State 56: 3.119-A 4.9335 eV 251.31 nm f=0.0222 <S**2>=2.181

135A ->144A 0.14902

136A ->143A -0.16367

137A ->144A -0.39609

138A ->143A 0.12833

141A ->146A 0.12207

142A ->146A 0.55434

142A ->147A 0.15655

142A ->152A 0.10995

136B ->143B 0.20812

137B ->144B 0.15052

141B ->146B 0.47058

141B ->152B 0.10569

Excited State 57: 2.819-A 4.9392 eV 251.02 nm f=0.0169 <S**2>=1.737

133A ->144A 0.35540

134A ->143A -0.13802

135A ->144A -0.23549

136A ->143A 0.19122

137A ->144A 0.50221

138A ->143A -0.32961

141A ->147A 0.10396

142A ->146A 0.32590

142A ->147A 0.36926

141B ->146B 0.16358

141B ->147B 0.19544

Excited State 58: 2.629-A 4.9589 eV 250.02 nm f=0.0000 <S**2>=1.478

133A ->143A 0.11738

138A ->144A -0.12563

142A ->148A -0.18129

134B ->143B -0.24377

135B ->144B 0.18619

136B ->144B 0.68604

137B ->143B 0.49439

140B ->152B -0.11003

141B ->148B -0.15350

Excited State 59: 2.598-A 4.9590 eV 250.02 nm f=0.0015 <S**2>=1.437

137A ->144A 0.13217

142A ->146A -0.14836

142A ->147A -0.13922

134B ->144B -0.29264

135B ->143B 0.16013

136B ->143B 0.58050

137B ->144B 0.64220

Excited State 60: 2.555-A 4.9792 eV 249.00 nm f=0.0436 <S**2>=1.383

133A ->144A -0.21578

134A ->143A 0.12726

138A ->143A 0.23998

138A ->146A -0.11042

138A ->147A -0.11668

139A ->145A -0.13063

141A ->146A -0.24920

141A ->147A 0.12882

142A ->146A 0.17484

142A ->147A 0.52227

140B ->145B -0.12287

141B ->146B -0.51886

141B ->147B 0.25497

Excited State 61: 3.176-A 4.9933 eV 248.30 nm f=0.0000 <S**2>=2.272

130A ->143A 0.15731

131A ->144A -0.19435

133A ->143A -0.24622

134A ->144A 0.11900

135A ->143A 0.12090

138A ->144A 0.18817

140A ->152A -0.13875

142A ->145A -0.15578

142A ->148A 0.50310

128B ->143B -0.14865

130B ->144B 0.13862

131B ->144B -0.14396

134B ->143B -0.18962

136B ->144B 0.28791

137B ->143B 0.13449

140B ->152B 0.13800

141B ->148B 0.33775

141B ->153B 0.10143

Excited State 62: 2.520-A 5.0044 eV 247.75 nm f=0.0571 <S**2>=1.338

133A ->144A -0.10569

140A ->145A 0.13818

141A ->146A 0.14987

141A ->147A 0.15422

142A ->146A -0.54322

142A ->147A 0.21697

135B ->143B -0.10964

141B ->146B 0.40916

141B ->147B 0.55163

Excited State 63: 3.282-A 5.0263 eV 246.67 nm f=0.0028 <S**2>=2.442

130A ->144A -0.15683

131A ->143A 0.21115

134A ->143A -0.17209

137A ->144A 0.14804

137A ->148A -0.12503

138A ->147A -0.12175

140A ->148A -0.16532

140A ->153A -0.22289

141A ->146A -0.16280

141A ->147A 0.10962

141A ->152A -0.11630

142A ->146A -0.10062

142A ->147A -0.12358

142A ->152A 0.32106

128B ->144B 0.15291

130B ->143B -0.13294

131B ->143B 0.18481

134B ->144B 0.17043

135B ->143B 0.11858

140B ->148B 0.19958

140B ->153B 0.23194

141B ->147B 0.11596

141B ->152B 0.38047

Excited State 64: 2.198-A 5.0498 eV 245.52 nm f=0.0036 <S**2>=0.958

139A ->148A 0.10640

140A ->145A -0.12542

140A ->148A 0.10827

141A ->147A 0.19996

142A ->146A 0.27092

142A ->147A -0.57202

137B ->148B -0.10905

140B ->145B -0.12270

141B ->146B -0.12251

141B ->147B 0.60705

Excited State 65: 3.067-A 5.0631 eV 244.88 nm f=0.0000 <S**2>=2.102

133A ->143A 0.10127

134A ->144A 0.17194

135A ->147A -0.10862

136A ->144A -0.20103

136A ->148A -0.10109

137A ->143A -0.31796

137A ->146A 0.15858

137A ->147A 0.27367

138A ->145A 0.14703

138A ->148A 0.25517

140A ->152A -0.13552

141A ->145A 0.34248

141A ->148A -0.15354

142A ->148A -0.14669

142A ->153A 0.11771

134B ->143B -0.10133

136B ->145B 0.12830

137B ->147B -0.11677

138B ->145B -0.14672

138B ->148B 0.11731

139B ->146B 0.18908

139B ->147B -0.12740

140B ->152B 0.15898

141B ->145B -0.25689

141B ->151B -0.10292

141B ->153B 0.12056

Excited State 66: 2.532-A 5.0735 eV 244.38 nm f=0.0000 <S**2>=1.352

133A ->143A 0.13522

134A ->144A 0.13849

135A ->143A -0.12955

136A ->144A -0.17412

140A ->146A 0.12909

141A ->145A 0.25257

142A ->145A -0.11043

142A ->148A 0.61968

138B ->145B -0.11168

138B ->148B -0.11453

139B ->146B 0.13799

140B ->152B -0.13894

141B ->148B -0.46215

141B ->153B -0.10908

Excited State 67: 2.885-A 5.0759 eV 244.26 nm f=0.0003 <S**2>=1.831

133A ->144A -0.42517

134A ->143A -0.35675

135A ->144A 0.39293

136A ->143A 0.47539

137A ->144A 0.23396

137A ->148A -0.10597

138A ->143A 0.15869

141A ->146A -0.13834

142A ->146A 0.12632

142A ->147A -0.13331

141B ->146B 0.14432

141B ->152B -0.12667

Excited State 68: 2.664-A 5.0868 eV 243.74 nm f=0.0000 <S**2>=1.525

133A ->143A -0.26510

134A ->144A -0.35602

135A ->143A 0.37528

136A ->144A 0.49803

137A ->143A 0.10752

140A ->152A -0.10483

141A ->145A 0.11203

141A ->148A -0.30986

141B ->148B -0.38177

Excited State 69: 2.632-A 5.1066 eV 242.79 nm f=0.0000 <S**2>=1.482

133A ->143A -0.14597

134A ->144A -0.18855

134A ->145A 0.10658

135A ->143A 0.14674

136A ->144A 0.17020

139A ->146A -0.11813

140A ->146A 0.13014

140A ->152A 0.13156

141A ->145A 0.35840

141A ->148A 0.27391

141A ->149A 0.15940

142A ->149A 0.11932

134B ->143B 0.26549

135B ->144B 0.26290

137B ->143B 0.10591

139B ->146B 0.12519

140B ->146B -0.15894

140B ->147B 0.10023

141B ->145B -0.15851

141B ->148B 0.44337

141B ->149B 0.11292

Excited State 70: 3.007-A 5.1167 eV 242.31 nm f=0.0047 <S**2>=2.011

134A ->143A 0.21225

135A ->144A -0.17282

136A ->143A -0.22176

136A ->147A 0.11297

137A ->145A -0.15267

137A ->148A -0.25516

138A ->143A 0.11036

138A ->146A -0.14434

138A ->147A -0.25532

141A ->146A -0.22134

141A ->147A 0.30721

142A ->147A -0.20216

132B ->143B 0.10669

134B ->144B -0.26510

135B ->143B -0.25709

136B ->146B -0.11127

137B ->144B -0.13074

137B ->148B 0.13649

138B ->147B -0.12936

139B ->145B -0.11133

140B ->145B 0.29915

141B ->146B 0.11247

141B ->147B -0.17849

Excited State 71: 3.027-A 5.1354 eV 241.43 nm f=0.0000 <S**2>=2.040

141A ->145A -0.19262

141A ->148A -0.21860

141A ->149A -0.11502

132B ->144B -0.18197

133B ->143B 0.20299

134B ->143B 0.50437

135B ->144B 0.57095

137B ->143B 0.20356

139B ->146B -0.11987

Excited State 72: 3.103-A 5.1374 eV 241.34 nm f=0.0084 <S**2>=2.157

135A ->144A -0.10033

136A ->143A -0.16471

141A ->146A -0.14196

128B ->144B -0.10874

132B ->143B -0.24505

133B ->144B 0.19011

134B ->144B 0.55770

135B ->143B 0.52518

137B ->144B 0.17438

139B ->145B -0.12264

140B ->145B 0.19647

141B ->146B 0.10943

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 72 LETran= 1306.