Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Electronic Supplementary Information (ESI)

Synthesis, Photochromic Properties and Thermal Bleaching Kinetics of Pyrazolone Phenylsemicarbazones Containing a Thiophene Ring

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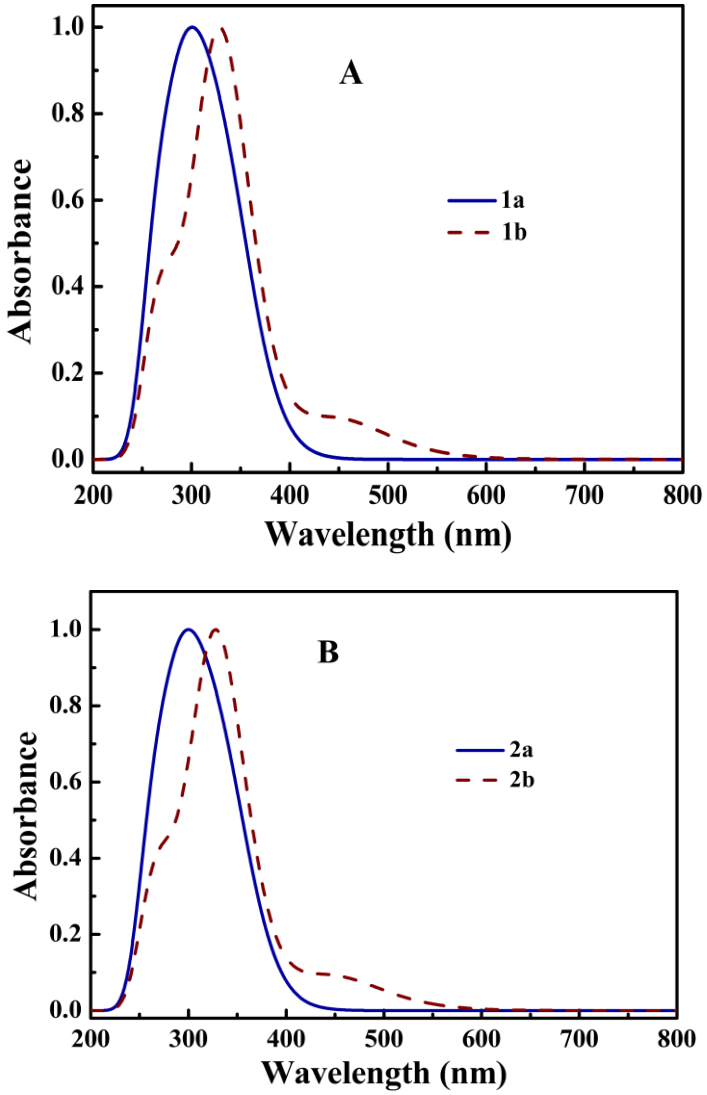

Figure S1. Absorption spectra of **1**(A) and **2**(B) by TDDFT calculations at the b3lyp/6-31+g(d) level.

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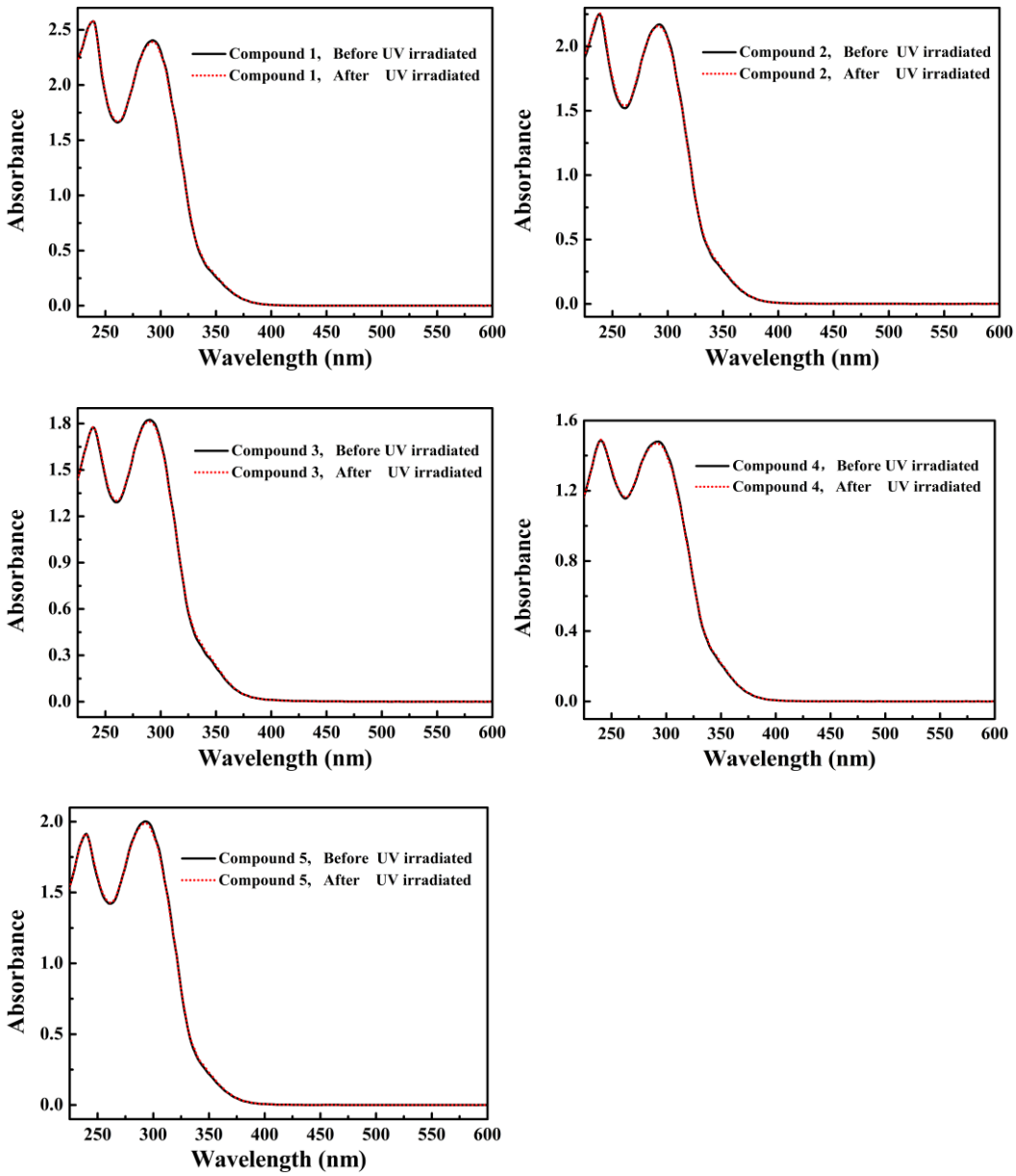

Figure S2. Absorption spectra of **1, 2, 3, 4** and **5** before and after UV irradiated in ethanol(3.0×10^{-5} M).

The absorption spectra of **1**, **2**, **3**, **4** and **5** in ethanol are shown in Figure S2. Unfortunately, no absorption spectral changes were observed upon photoirradiation at any wavelength in ethanol. This result indicates that the five compounds have no photochromic properties in solution because the probability of intermolecular reaction has been reduced in the solution due to the dilution of concentrations.

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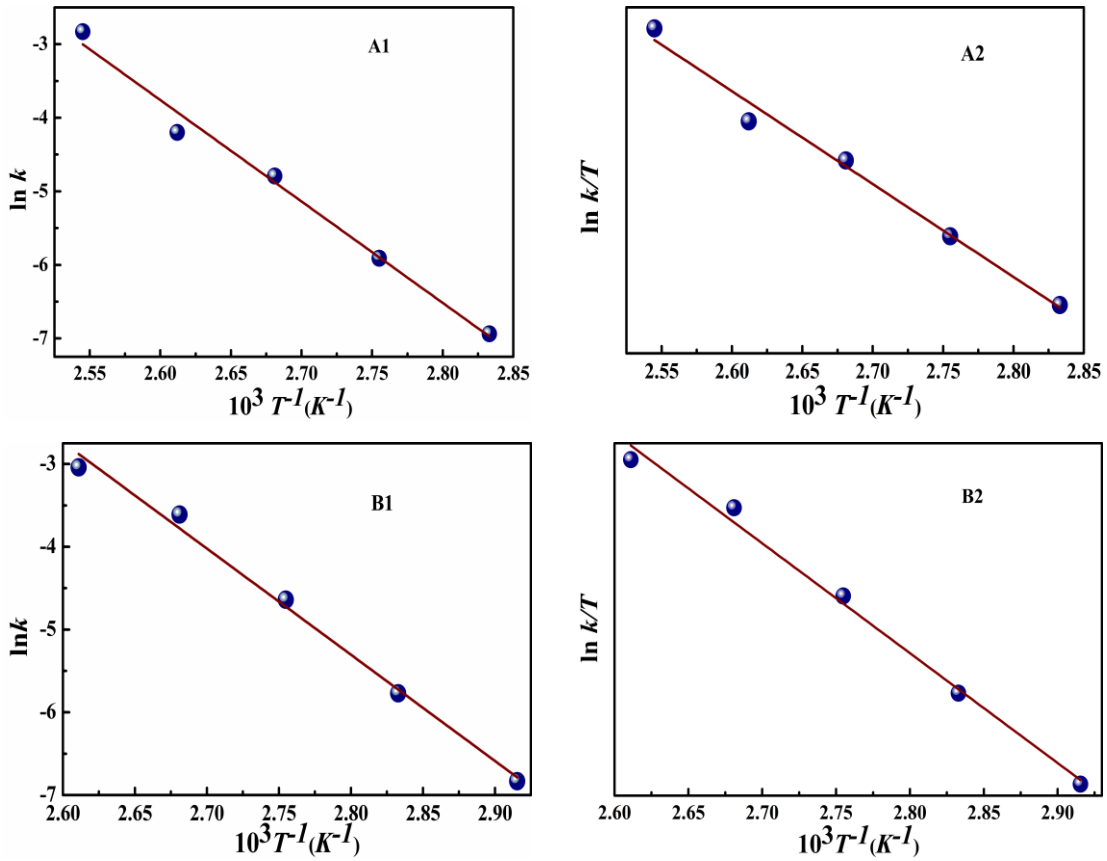

Figure S3. Arrhenius plots of the thermal bleaching rate constant of **1b**→**1a**(A1) and **2b**→**2a**(B1); (A2) and (B2) Eyring plots for the thermal bleaching reaction in the ranging of 353~393K for **1b** and 343~383K for **2b**.

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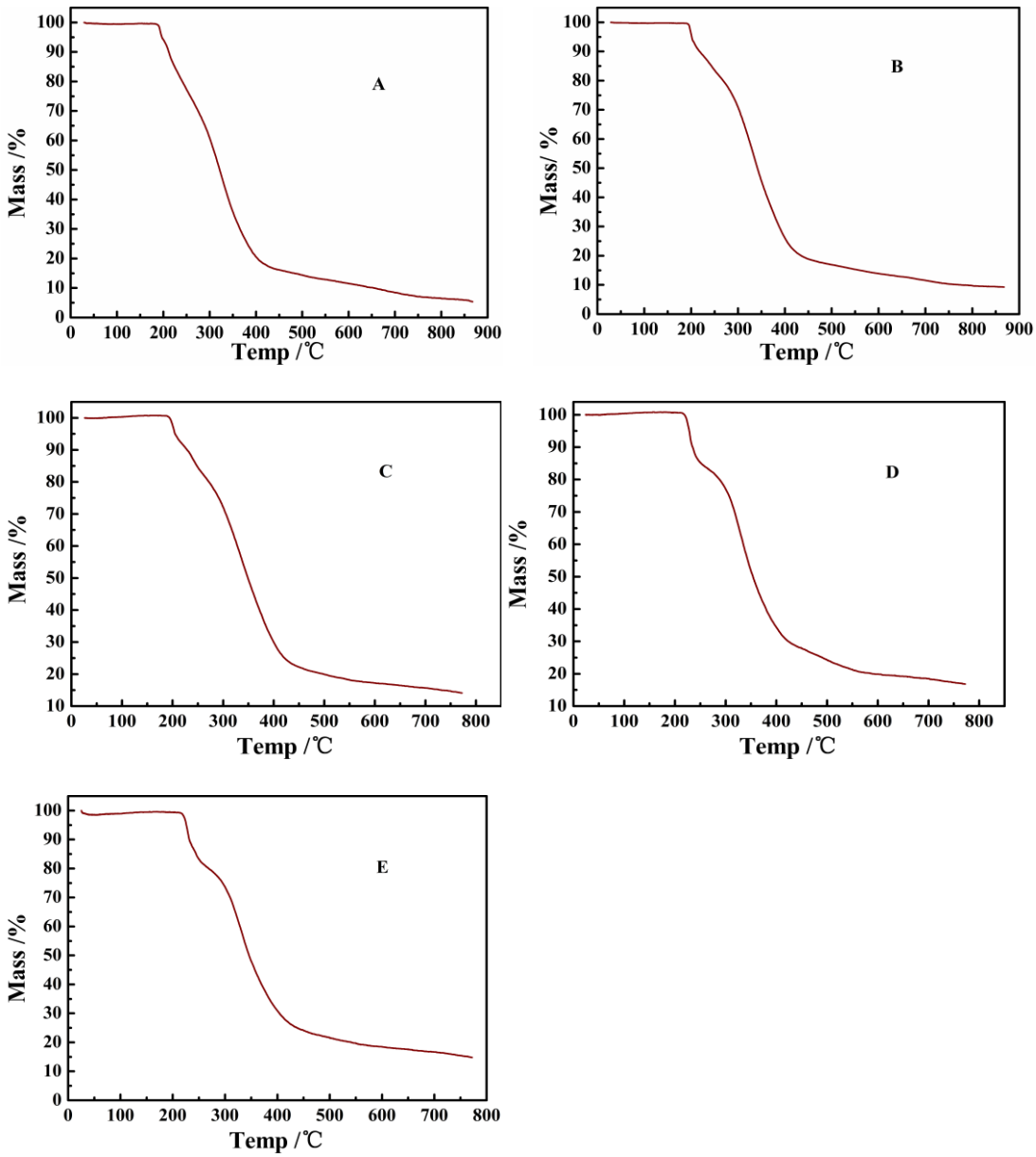

Figure S4. TGA curves of **1**(A), **2**(B), **3**(C), **4**(D) and **5**(E) powder in N_2 atmosphere.

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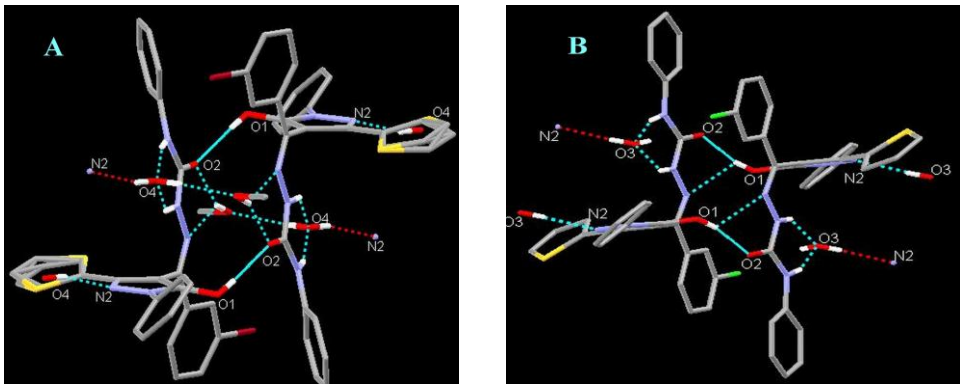

Figure S5. Hydrogen bond connection diagram of **1a**(A) and **2a**(B); the other H atoms are omitted for clarity.

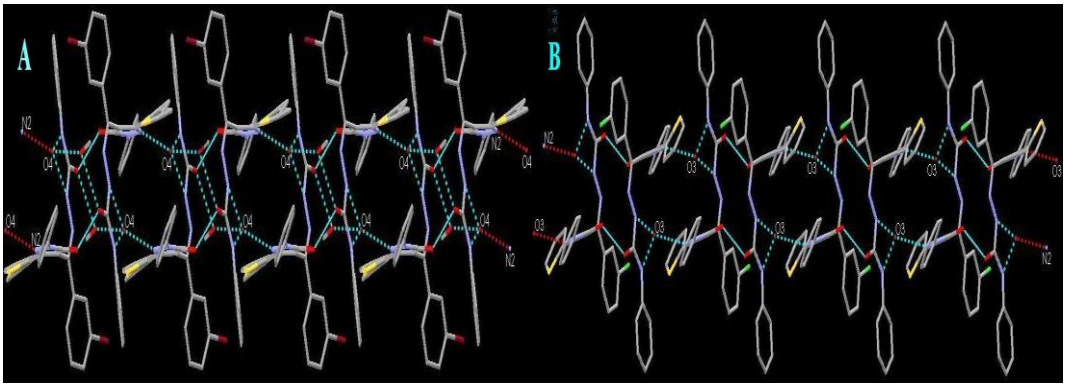

Figure S6. One-dimensional hydrogen-bonded chains in the crystal structure of **1a**(A) and **2a**(B), all the H atoms are omitted for clarity.

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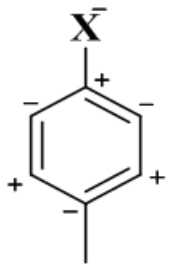

Scheme S1. The electron density distribution

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Table S1. Crystal data for **1a** and **2a.**

Compound	**1a**	**2a**
Empirical formula	C28H26 Br1 N5 O4 S1	C27 H20 Cl1 N5 O2 S1
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Monoclinic
space group	P-1	P2(1) /n
Unit cell dimensions	a = 11.497 (2)Å b =11.542 (2) Å c = 12.417 (3)Å α = 113.90 (3)^o β = 106.80 (3)^o γ= 99.11(3)^o	a = 12.380 (3) Å b = 11.605 (2) Å c = 19.026 (4) Å α= 90^o β= 104.66(3)^o γ= 90^o
Volume	1368.9(5) Å^3	2644.6(9)Å^3
Calculated density	1.476 mg/m^3	0.334 Mg/m^3
Goodness-of-fit on F^2	1.080	1.057
Final *R* indices [I>2sigma(I)]	R1 = 0.0404, *w*R2 = 0.0983	R1 = 0.0670, *w*R2 = 0.1671
R indices (all data)	R1 = 0.0705, *w*R2 = 0.1405	R1 = 0.1096, *w*R2 = 0.1884

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Table S2. Selected bond lengths (Å) of **1a** and **2a.**

1a		**2a**	
Br-C(17)	1.894(3)	S-C(13)	1.673(5)
O(1)-C(9)	1.331(4)	S-C(10)	1.690(4)
O(1)-H(1O)	0.80(3)	Cl-C(17)	1.744(4)
O(2)-C(21)	1.233(4)	O(1)-C(9)	1.328(4)
O(3)-C(28)	1.379(6)	O(1)-H(1A)	0.79(4)
N(1)-C(9)	1.356(4)	N(1)-C(9)	1.354(4)
N(1)-N(2)	1.372(4)	N(1)-N(2)	1.378(3)
N(1)-C(6)	1.428(4)	N(1)-C(6)	1.433(4)
N(2)-C(7)	1.333(4)	O(2)-C(21)	1.229(3)
N(3)-C(14)	1.293(4)	N(2)-C(7)	1.332(4)
N(3)-N(4)	1.368(4)	C(2)-C(3)	1.354(7)
N(4)-C(21)	1.357(4)	N(3)-C(14)	1.291(4)
N(5)-C(21)	1.356(4)	N(3)-N(4)	1.363(3)
N(5)-C(22)	1.407(5)	N(4)-C(21)	1.370(4)
C(7)-C(8)	1.416(4)	N(5)-C(21)	1.352(4)
C(7)-C(10)	1.467(4)	N(5)-C(22)	1.409(4)
C(8)-C(9)	1.370(5)	C(7)-C(8)	1.410(4)
C(8)-C(14)	1.489(4)	C(7)-C(10)	1.463(4)
C(10)-C(11)	1.3802(12)	C(8)-C(9)	1.370(4)
C(10)-C(11')	1.3802(11)	C(8)-C(14)	1.483(4)
C(10)-S'	1.6506(13)	C(10)-C(11)	1.464(5)
C(10)-S	1.6519(11)	C(11)-C(12)	1.429(6)
S-C(13)	1.6500(13)	C(12)-C(13)	1.323(7)
C(11)-C(12)	1.4500(12)	C(14)-C(15)	1.489(4)
C(12)-C(13)	1.3800(11)	C(15)-C(20)	1.382(4)
S'-C(13')	1.6500(12)	C(15)-C(16)	1.393(4)
C(11')-C(12')	1.4501(13)	C(16)-C(17)	1.377(4)
C(12')-C(13')	1.3801(11)	C(17)-C(18)	1.359(5)
C(14)-C(15)	1.483(4)	C(18)-C(19)	1.381(6)
C(15)-C(20)	1.373(5)	C(19)-C(20)	1.383(5)
C(15)-C(16)	1.407(4)		
C(16)-C(17)	1.383(5)		
C(17)-C(18)	1.381(5)		
C(18)-C(19)	1.371(5)		
C(19)-C(20)	1.395(5)		

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Table S3. Selected torsion angles of (°) for **1a** and **2a**.

1a		**2a**	
N(2)-N(1)-C(6)-C(5)	129.2(4)	N(2)-N(1)-C(6)-C(5)	-141.3(3)
C(21)-N(5)-C(22)-C(27)	-25.1(6)	C(21)-N(5)-C(22)-C(27)	10.9(6)
C(21)-N(5)-C(22)-C(23)	159.3(4)	C(21)-N(5)-C(22)-C(23)	-171.3(3)

Table S4. Hydrogen bonds for **1a** and **2a** (Å and °).

1a				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4N)...O(4)#1	0.83(2)	2.21(3)	2.881(4)	138(3)
N(5)-H(5N)...O(4)#1	0.84(2)	2.03(3)	2.844(4)	163(3)
O(1)-H(1O)...O(2)#1	0.80(3)	1.84(3)	2.615(3)	162(4)
O(4)-H(4AO)...O(3)	0.84(3)	1.95(3)	2.763(5)	163(5)
O(3)-H(3O)...O(2)	0.83(3)	2.01(4)	2.769(4)	152(6)
O(3)-H(3O)...N(3)	0.83(3)	2.64(5)	3.310(4)	139(5)
O(4)-H(4BO)...N(2)#2	0.84(3)	2.07(3)	2.886(4)	166(5)
Symmetry codes: #1 -x+1, -y+1, -z+1 ; #2 x+1, y, z				
2a				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4A)...O(3)	0.88	2.30	3.058(4)	146.4
N(5)-H(5A)...O(3)	0.88	2.03	2.864(4)	161.8
O(1)-H(1A)...O(2)#1	0.79(4)	1.80(4)	2.582(4)	168(4)
O(3)-H(3)...N(2)#2	0.81(5)	2.04(5)	2.846(4)	175(4)
Symmetry codes: #1 -x+1, -y, -z ; #2 -x+1, -y+1, -z				

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Results of Time-Dependent DFT Calculations:
b3lyp/6-31+g(d) (states=20) in the gas phase

1a

Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	3.6010 eV	344.31 nm	f=0.0622
141 ->143	0.60149			
142 ->143	0.36393			

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

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

Excited State 2:	Singlet-A	3.6547 eV	339.24 nm	f=0.3456
141 ->143	-0.35889			
142 ->143	0.59003			
142 ->144	0.10885			
Excited State 3:	Singlet-A	3.8889 eV	318.81 nm	f=0.0964
140 ->144	-0.11405			
142 ->144	0.68325			
Excited State 4:	Singlet-A	4.0708 eV	304.57 nm	f=0.1613
139 ->143	0.11684			
140 ->143	-0.46000			
141 ->144	0.49453			
Excited State 5:	Singlet-A	4.1582 eV	298.16 nm	f=0.3882
140 ->143	0.46506			
141 ->144	0.48643			
Excited State 6:	Singlet-A	4.2942 eV	288.72 nm	f=0.0084
137 ->143	0.14972			
139 ->143	0.55846			
140 ->145	0.18088			
142 ->145	-0.30948			
Excited State 7:	Singlet-A	4.3814 eV	282.98 nm	f=0.0047
137 ->143	-0.15823			
140 ->144	0.65895			
142 ->144	0.12551			
Excited State 8:	Singlet-A	4.5019 eV	275.41 nm	f=0.2501
135 ->143	-0.21780			
136 ->143	-0.12188			
137 ->143	0.51082			
138 ->143	0.12264			
139 ->143	-0.19223			
140 ->143	-0.20575			
140 ->144	0.20284			
142 ->145	-0.11372			
Excited State 9:	Singlet-A	4.6219 eV	268.25 nm	f=0.0062

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137 ->143	-0.12566			
138 ->143	0.65278			
142 ->149	0.16179			
142 ->151	0.10456			
Excited State 10:	Singlet-A	4.6469 eV	266.81 nm	f=0.0517
137 ->143	0.11617			
139 ->143	0.18659			
141 ->145	0.18386			
142 ->145	0.48467			
142 ->146	0.37363			
Excited State 11:	Singlet-A	4.6982 eV	263.90 nm	f=0.0576
137 ->143	-0.23627			
139 ->143	-0.16130			
141 ->145	-0.10029			
142 ->145	-0.28915			
142 ->146	0.51101			
142 ->148	0.11169			
Excited State 12:	Singlet-A	4.6985 eV	263.88 nm	f=0.0236
141 ->145	0.59972			
141 ->146	0.22413			
142 ->145	-0.15573			
Excited State 13:	Singlet-A	4.7532 eV	260.85 nm	f=0.0115
134 ->144	-0.18575			
134 ->146	0.11553			
136 ->143	0.15454			
141 ->145	0.23833			
141 ->146	-0.32930			
141 ->147	0.43804			
142 ->147	0.15849			
Excited State 14:	Singlet-A	4.7585 eV	260.55 nm	f=0.0317
134 ->144	-0.14590			
136 ->143	-0.14348			
136 ->144	-0.10273			
141 ->145	-0.15765			
141 ->146	0.46780			
141 ->147	0.38500			
142 ->147	0.10220			
Excited State 15:	Singlet-A	4.7660 eV	260.14 nm	f=0.0472
135 ->143	0.56393			
136 ->143	-0.28455			
137 ->143	0.15704			
Excited State 16:	Singlet-A	4.7826 eV	259.24 nm	f=0.0078
133 ->143	0.17469			
135 ->143	0.24700			

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136 ->143 0.54982
137 ->143 0.18030
141 ->146 0.20471
Excited State 17: Singlet-A 4.8216 eV 257.15 nm f=0.0109 <S**2>=0.000
141 ->147 -0.13026
142 ->146 -0.16386
142 ->147 0.27348
142 ->148 0.51905
142 ->150 0.21938
142 ->152 0.13821
Excited State 18: Singlet-A 4.8519 eV 255.54 nm f=0.0153
137 ->144 -0.35196
139 ->144 0.56432
141 ->146 0.11541
Excited State 19: Singlet-A 4.8631 eV 254.95 nm f=0.0032
133 ->143 0.65133
136 ->143 -0.20344
Excited State 20: Singlet-A 4.9412 eV 250.92 nm f=0.0036
138 ->143 -0.12061
138 ->144 -0.10595
138 ->151 -0.10585
140 ->147 -0.11049
141 ->147 -0.15105
141 ->148 -0.10144
142 ->147 0.47843
142 ->148 -0.25776
142 ->149 0.24380
142 ->150 -0.13211
142 ->151 0.10997

1b

Excitation energies and oscillator strengths:
Excited State 1: Singlet-A 3.6058 eV 343.85 nm f=0.0769
132 ->134 0.58470
133 ->134 0.39015
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited State 2: Singlet-A 3.6551 eV 339.21 nm f=0.3296
132 ->134 -0.38551
133 ->134 0.57229
133 ->135 -0.11296
Excited State 3: Singlet-A 3.8868 eV 318.99 nm f=0.0994
131 ->135 -0.11262
133 ->135 0.68262
Excited State 4: Singlet-A 4.0756 eV 304.21 nm f=0.1538

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129 ->134	-0.14429			
131 ->134	0.46597			
132 ->135	0.48895			
Excited State 5:	Singlet-A	4.1646 eV	297.71 nm	f=0.3981
129 ->134	0.13326			
131 ->134	-0.45965			
132 ->135	0.49208			
Excited State 6:	Singlet-A	4.3617 eV	284.26 nm	f=0.0181
128 ->134	-0.33154			
129 ->134	0.41568			
131 ->135	-0.13411			
131 ->136	-0.18433			
133 ->136	0.32764			
133 ->137	-0.11475			
Excited State 7:	Singlet-A	4.3849 eV	282.75 nm	f=0.0018
128 ->134	-0.15987			
131 ->135	0.64687			
133 ->135	0.11934			
133 ->136	0.12937			
Excited State 8:	Singlet-A	4.5086 eV	274.99 nm	f=0.2407
126 ->134	0.23670			
127 ->134	0.10615			
128 ->134	0.32516			
129 ->134	0.40114			
130 ->134	-0.16453			
131 ->134	0.20135			
131 ->135	0.19838			
133 ->136	-0.15063			
Excited State 9:	Singlet-A	4.6231 eV	268.18 nm	f=0.0055
129 ->134	0.17709			
130 ->134	0.63776			
133 ->140	-0.16841			
133 ->141	0.10696			
Excited State 10:	Singlet-A	4.6565 eV	266.26 nm	f=0.0629
131 ->137	-0.11475			
132 ->136	0.13760			
133 ->136	0.36876			
133 ->137	0.52463			
Excited State 11:	Singlet-A	4.7144 eV	262.99 nm	f=0.0249
126 ->135	-0.10235			
132 ->136	0.55624			
132 ->137	0.27735			
132 ->138	-0.10570			
133 ->137	-0.19969			

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Excited State 12:	Singlet-A	4.7424 eV	261.44 nm	f=0.0567
126 ->134	-0.24774			
128 ->134	0.41614			
132 ->137	-0.22669			
133 ->136	0.35352			
133 ->137	-0.21220			
Excited State 13:	Singlet-A	4.7553 eV	260.73 nm	f=0.0118
125 ->135	-0.22567			
125 ->137	0.13400			
132 ->137	0.10805			
132 ->138	0.57269			
133 ->138	0.18610			
Excited State 14:	Singlet-A	4.7678 eV	260.05 nm	f=0.0512
124 ->134	0.13571			
126 ->134	-0.32759			
127 ->134	0.40245			
132 ->136	-0.22944			
132 ->137	0.32091			
133 ->136	-0.10667			
Excited State 15:	Singlet-A	4.7765 eV	259.57 nm	f=0.0055
126 ->134	0.35265			
129 ->134	-0.16247			
132 ->136	-0.27787			
132 ->137	0.31755			
133 ->136	0.19638			
133 ->137	-0.14943			
133 ->138	-0.10725			
133 ->139	-0.24132			
Excited State 16:	Singlet-A	4.7865 eV	259.03 nm	f=0.0085
124 ->134	0.17845			
126 ->134	0.24299			
127 ->134	0.49289			
128 ->134	-0.11687			
129 ->134	-0.15785			
132 ->136	0.11341			
132 ->137	-0.30114			
Excited State 17:	Singlet-A	4.8179 eV	257.34 nm	f=0.0194
126 ->134	0.16966			
132 ->138	-0.13013			
133 ->136	0.10105			
133 ->137	-0.23121			
133 ->138	0.26336			
133 ->139	0.49820			
133 ->142	0.15211			

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Excited State 18:	Singlet-A	4.8617 eV	255.02 nm	f=0.0054
124 ->134	0.64605			
127 ->134	-0.22465			
Excited State 19:	Singlet-A	4.8681 eV	254.69 nm	f=0.0216
128 ->135	0.12071			
129 ->135	0.63658			
130 ->135	-0.16381			
Excited State 20:	Singlet-A	4.9341 eV	251.28 nm	f=0.0019
131 ->138	-0.12412			
132 ->138	-0.16629			
133 ->138	0.54165			
133 ->139	-0.30838			
133 ->140	0.13396			

2a

Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	2.7628 eV	448.76 nm	f=0.0691
132 ->134	0.13069			
133 ->134	0.69104			

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

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

Excited State 2:	Singlet-A	3.2895 eV	376.91 nm	f=0.0061
132 ->134	0.68565			
133 ->134	-0.13818			
Excited State 3:	Singlet-A	3.6179 eV	342.69 nm	f=0.2300
131 ->134	0.70065			
Excited State 4:	Singlet-A	3.7231 eV	333.01 nm	f=0.0902
130 ->134	0.66886			
133 ->135	-0.19549			
Excited State 5:	Singlet-A	3.7940 eV	326.79 nm	f=0.3958
130 ->134	0.20031			
133 ->135	0.66561			
Excited State 6:	Singlet-A	3.9903 eV	310.71 nm	f=0.0010
129 ->134	0.70496			
Excited State 7:	Singlet-A	4.0307 eV	307.60 nm	f=0.1334
128 ->134	0.68017			
Excited State 8:	Singlet-A	4.1953 eV	295.53 nm	f=0.0033
124 ->134	-0.10742			
126 ->134	-0.13157			
127 ->134	0.65785			
Excited State 9:	Singlet-A	4.3013 eV	288.25 nm	f=0.0318
132 ->135	-0.20013			
132 ->136	0.12624			
133 ->136	0.63479			
133 ->137	0.13611			

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Excited State 10:	Singlet-A	4.3087 eV	287.75 nm	f=0.0279
132 ->135	0.64270			
133 ->136	0.19815			
Excited State 11:	Singlet-A	4.4009 eV	281.72 nm	f=0.0178
122 ->134	-0.13172			
124 ->134	0.21158			
125 ->134	-0.23996			
126 ->134	0.51977			
127 ->134	0.19494			
133 ->136	0.10798			
133 ->137	-0.15122			
Excited State 12:	Singlet-A	4.4251 eV	280.19 nm	f=0.0049
126 ->134	0.11468			
133 ->136	-0.11748			
133 ->137	0.66868			
Excited State 13:	Singlet-A	4.4745 eV	277.09 nm	f=0.0096
124 ->134	0.11619			
125 ->134	0.10972			
130 ->135	0.39938			
131 ->135	0.25774			
132 ->139	-0.18141			
133 ->139	-0.37673			
133 ->140	0.14706			
Excited State 14:	Singlet-A	4.5178 eV	274.43 nm	f=0.0415
124 ->134	0.22451			
125 ->134	0.58933			
126 ->134	0.17599			
130 ->135	-0.11493			
131 ->137	0.10849			
133 ->139	0.10254			
Excited State 15:	Singlet-A	4.5469 eV	272.68 nm	f=0.0262
122 ->134	-0.18955			
123 ->134	0.16178			
124 ->134	0.46650			
125 ->134	-0.14750			
126 ->134	-0.33209			
131 ->135	0.13626			
131 ->137	-0.14075			
Excited State 16:	Singlet-A	4.5796 eV	270.73 nm	f=0.0520
124 ->134	-0.11886			
130 ->135	-0.12728			
131 ->135	0.62173			
133 ->138	-0.15196			
133 ->139	0.12350			

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Excited State 17:	Singlet-A	4.6487 eV	266.70 nm	f=0.0199
122 ->134	0.15270			
123 ->134	0.10296			
131 ->135	0.10306			
132 ->138	0.13631			
133 ->138	0.61955			
133 ->139	0.13005			
Excited State 18:	Singlet-A	4.7214 eV	262.60 nm	f=0.0137
123 ->134	0.59514			
124 ->134	-0.16661			
133 ->138	-0.14675			
133 ->140	-0.18650			
Excited State 19:	Singlet-A	4.7426 eV	261.43 nm	f=0.0167
122 ->134	-0.14052			
123 ->134	0.19295			
124 ->134	-0.10670			
132 ->140	0.11513			
133 ->139	0.26339			
133 ->140	0.55184			
Excited State 20:	Singlet-A	4.7860 eV	259.06 nm	f=0.0985
128 ->135	0.12235			
129 ->135	-0.27446			
129 ->143	-0.10420			
130 ->135	0.32839			
132 ->136	0.14671			
133 ->139	0.31283			
133 ->140	-0.10476			
133 ->142	0.32823			

2b

Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	2.7557 eV	449.92 nm	f=0.0711
141 ->143	0.12803			
142 ->143	0.69150			

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

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

Excited State 2:	Singlet-A	3.2803 eV	377.96 nm	f=0.0062
141 ->143	0.68577			
142 ->143	-0.13562			
Excited State 3:	Singlet-A	3.6000 eV	344.40 nm	f=0.2026
140 ->143	0.69320			
Excited State 4:	Singlet-A	3.6513 eV	339.56 nm	f=0.0718
139 ->143	0.69048			
Excited State 5:	Singlet-A	3.7848 eV	327.58 nm	f=0.4402
142 ->144	0.68876			

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Excited State 6:	Singlet-A	3.9811 eV	311.43 nm	f=0.0011
138 ->143	0.70610			
Excited State 7:	Singlet-A	4.0197 eV	308.44 nm	f=0.1344
137 ->143	0.68014			
Excited State 8:	Singlet-A	4.1841 eV	296.32 nm	f=0.0032
133 ->143	-0.10197			
135 ->143	-0.13083			
136 ->143	0.65969			
Excited State 9:	Singlet-A	4.3014 eV	288.24 nm	f=0.0479
141 ->144	0.54163			
142 ->145	0.39213			
142 ->146	-0.10666			
Excited State 10:	Singlet-A	4.3050 eV	288.00 nm	f=0.0094
141 ->144	-0.39616			
141 ->145	0.10705			
142 ->145	0.53338			
Excited State 11:	Singlet-A	4.3917 eV	282.31 nm	f=0.0190
130 ->143	0.12840			
133 ->143	0.21425			
134 ->143	-0.23369			
135 ->143	0.53132			
136 ->143	0.19316			
142 ->146	-0.10057			
Excited State 12:	Singlet-A	4.4249 eV	280.20 nm	f=0.0084
139 ->144	-0.23951			
140 ->144	0.14096			
142 ->146	0.56506			
142 ->147	-0.19148			
142 ->148	0.12020			
Excited State 13:	Singlet-A	4.4266 eV	280.09 nm	f=0.0004
139 ->144	0.35506			
140 ->144	-0.22655			
141 ->147	0.13382			
142 ->145	0.13221			
142 ->146	0.37226			
142 ->147	0.28098			
142 ->148	-0.17061			
Excited State 14:	Singlet-A	4.5019 eV	275.41 nm	f=0.0417
131 ->143	0.10264			
133 ->143	0.25284			
134 ->143	0.59320			
135 ->143	0.14798			
Excited State 15:	Singlet-A	4.5350 eV	273.39 nm	f=0.0233
130 ->143	0.17969			

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131 ->143	0.17096			
133 ->143	0.46084			
134 ->143	-0.18126			
135 ->143	-0.33925			
140 ->144	-0.13138			
140 ->146	0.13735			
Excited State 16:	Singlet-A	4.5707 eV	271.26 nm	f=0.0585
133 ->143	0.11861			
139 ->144	0.17614			
140 ->144	0.61858			
142 ->147	0.17789			
Excited State 17:	Singlet-A	4.6488 eV	266.70 nm	f=0.0222
130 ->143	-0.15195			
132 ->143	0.12534			
141 ->148	0.12462			
142 ->147	0.36720			
142 ->148	0.51003			
Excited State 18:	Singlet-A	4.7072 eV	263.40 nm	f=0.0149
131 ->143	0.22685			
132 ->143	0.55151			
139 ->144	0.16023			
142 ->147	-0.22132			
142 ->149	-0.11743			
Excited State 19:	Singlet-A	4.7312 eV	262.06 nm	f=0.0929
130 ->143	0.10119			
139 ->144	0.33412			
142 ->147	-0.28496			
142 ->148	0.34655			
142 ->149	0.34413			
Excited State 20:	Singlet-A	4.7455 eV	261.27 nm	f=0.0247
130 ->143	0.11326			
132 ->143	0.23238			
139 ->144	-0.24127			
142 ->147	0.13660			
142 ->148	-0.14051			
142 ->149	0.51232			