Synthesis and Characterization of Ruthenium bis-Bipyridine Mono- and Disulfinato Complexes

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Supplementary Information

Figure S1. The effect on the predicted TD-DFT electronic spectrum (CH_3CN) of species **1** of excluding the solvent correction (red trace) compared with its inclusion (blue). Inset shows expansion of lower energy region. Note that the lack of a high energy transition near 50,000 cm^{-1} in the red spectrum is due to the calculation not extending to that energy region

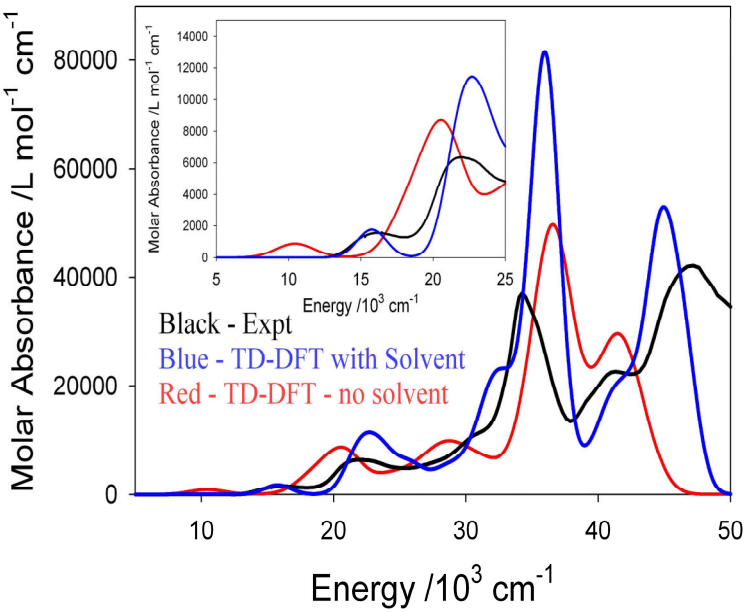
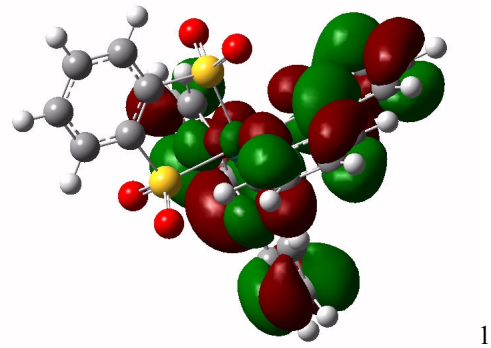


Figure S2 Frontier MOs of Species **2** (DFT/B3LYP, TZVP and DGDZV –PCM, acetonitrile see text)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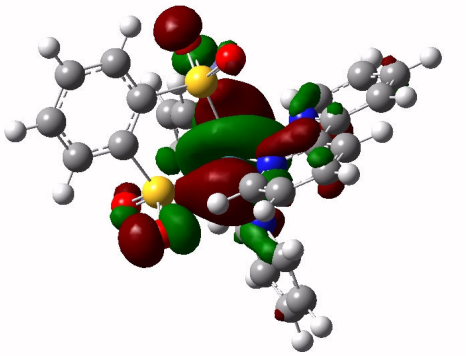
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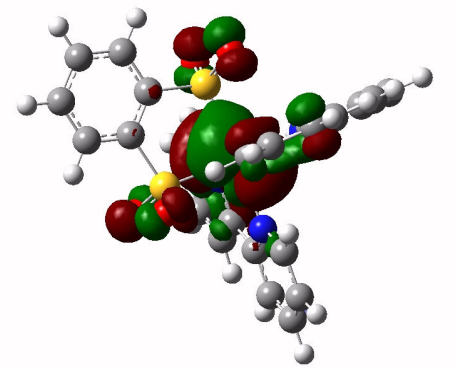
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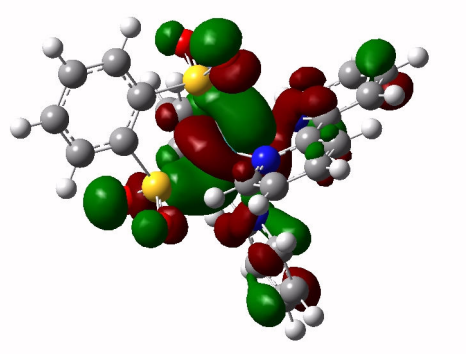
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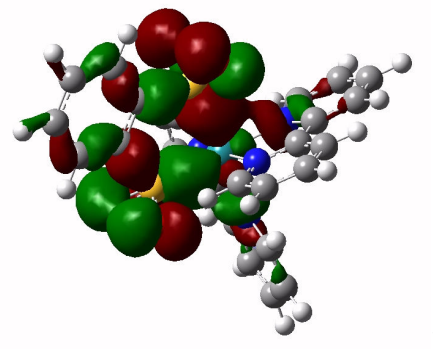
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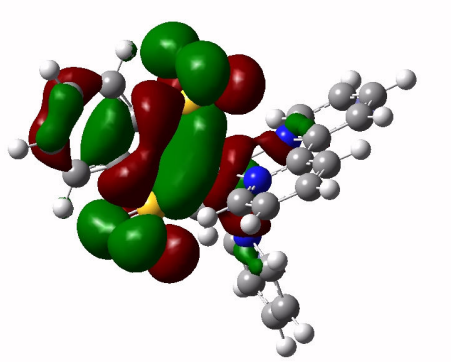
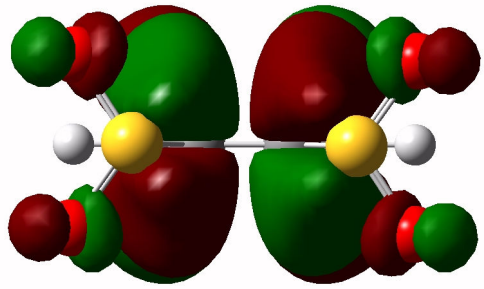

152

Figure S3 Frontier MOs of (SO_2.SO_2) ligand (DFT/B3LYP, TZVP and DGDZV –PCM, acetonitrile see text)



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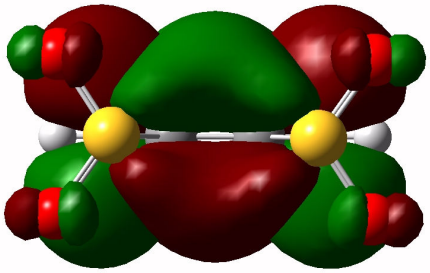

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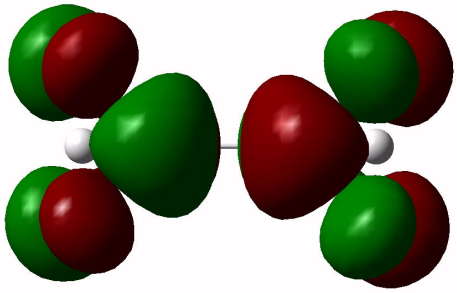

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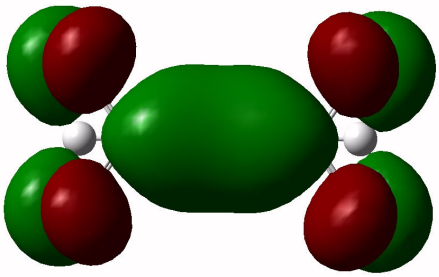

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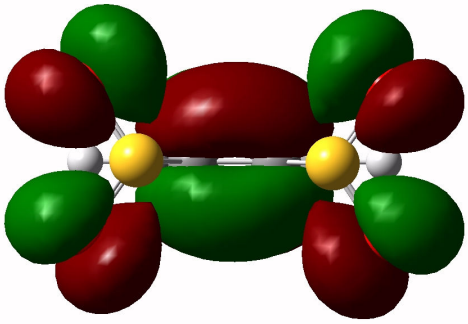

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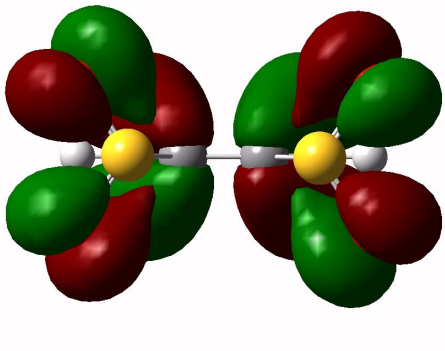

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Table S1. Molecular Orbital Percent Contributions- Species **1** - DFT- B3LYP/TZVP and DGDZVP(Ru)-PCM (CH3CN) -see main text. (AOMIX, Mulliken) E(SCF)= -6612.0876 a.u.

Fragment 1 is Ruthenium, s,p and d
Fragment 2 is S.SO_2 ligand
Fragment 3 is bipyridine

MO#	E(eV)	MO Compositions (%)			
	Fragment:	1	2	3	
159	10	0.02	4.2	2.4	93.5
158	9	-0.11	57.8	12.3	29.9
157	8	-0.18	13.9	79.6	6.5
156	7	-0.31	45	42.7	12.2
155	6	-0.57	2.3	96.8	0.9
154	5	-1.14	1	0.4	98.5
153	4	-1.21	1.9	0.3	97.8
152	3	-1.32	2.2	0.3	97.5
151	2	-1.56	0.7	0.5	98.8
150	1	-2.25	4.9	0.6	94.5
149L	0	-2.3	2.4	0.5	97.1
occupied – unoccupied orbital gap 2.630 eV					
148H	0	-4.93	30.2	65.5	4.2
147	-1	-5.79	72.2	13.3	14.5
146	-2	-5.92	78.6	9.1	12.3
145	-3	-6.16	52.6	38.6	8.7
144	-4	-6.43	14	78.8	7.3
143	-5	-6.72	0.7	97.7	1.7
142	-6	-6.98	16.1	71.9	12
141	-7	-7.11	0.5	1.7	97.8
140	-8	-7.15	2	8.6	89.4
139	-9	-7.27	4.3	80.5	15.1
138	-10	-7.8	3.5	90	6.5
137	-11	-7.92	3	93	4
136	-12	-7.99	1.8	95.7	2.5
135	-13	-8.48	0.3	5.1	94.6
134	-14	-8.54	1.2	1	97.8
133	-15	-8.6	1.1	6.4	92.5
132	-16	-8.66	3	3.5	93.5
131	-17	-8.7	1.4	2.4	96.1
130	-18	-8.81	3	18.7	78.3
129	-19	-8.89	5.5	8.2	86.4
128	-20	-9.14	5.9	44	50.1
127	-21	-9.37	6	13.5	80.5
126	-22	-9.51	12.9	19.5	67.6
125	-23	-9.72	11.8	2.2	85.9
124	-24	-9.8	0.4	98.9	0.7
123	-25	-10.28	0.7	90.2	9.2
122	-26	-10.43	0.9	6.3	92.8
121	-27	-10.5	0.3	5.1	94.6

120	-28	-10.69	0.2	5.6	94.3
119	-29	-10.7	1	34.6	64.4
118	-30	-10.78	3.4	49.5	47.1

Table S2. Molecular Orbital Percent Contributions- Species 2 - DFT- B3LYP/TZVP and DGDZVP(Ru)-PCM (CH3CN) -see main text. (AOMIX, Mulliken) E(SCF)=-6762.546 a.u.

Fragment 1is Ruthenium, s,p and d
Fragment 2 is $SO_2.SO_2$ ligand
Fragment 3 is bipyridine

MO#	E(eV)	MO Compositions (%)			
		Fragment: 1	2	3	
166	9	-0.5	57.5	27.7	14.8
165	8	-0.51	62.8	9.2	28
164	7	-0.86	1.7	95.3	3
163	6	-0.87	-0.6	100.1	0.4
162	5	-1.25	0.6	2.5	96.9
161	4	-1.31	1.6	0.4	98
160	3	-1.42	1.9	0.1	98
159	2	-1.64	0.4	1.1	98.4
158	1	-2.38	4.1	0.3	95.5
157L	0	-2.41	1.9	0.3	97.8
--- occupied - unoccupied orbital gap --- 3.780 eV					
156H	0	-6.19	81	10.2	8.7
155	-1	-6.28	79.2	10.3	10.5
154	-2	-6.37	67.2	16.1	16.7
153	-3	-6.6	13.8	77.7	8.5
152	-4	-6.91	20.7	72.7	6.6
151	-5	-6.97	-0.1	98.7	1.4
150	-6	-7.06	0.2	99.3	0.5
149	-7	-7.19	0.2	1.7	98.2
148	-8	-7.25	0.9	1.8	97.4
147	-9	-7.49	3.4	88.1	8.5
146	-10	-7.67	5.8	84.9	9.3
145	-11	-8.1	1.2	91.7	7.1
144	-12	-8.23	-0.2	94.8	5.4
143	-13	-8.28	4.6	90.8	4.6
142	-14	-8.32	1.3	91.4	7.3
141	-15	-8.61	0.6	3.5	95.8
140	-16	-8.64	1.1	2.3	96.6
139	-17	-8.7	2.2	4.8	93
138	-18	-8.79	6.1	7.6	86.3
137	-19	-8.83	0.3	4.7	95
136	-20	-8.97	5	2.2	92.8
135	-21	-9.05	9.2	2.8	88
134	-22	-9.45	5.6	6.8	87.6
133	-23	-9.55	10.3	6.4	83.3

132	-24	-9.83	11.6	4	84.3
131	-25	-10.07	0.4	96.7	3
130	-26	-10.38	0.3	98.8	0.9
129	-27	-10.53	0.4	38.5	61.1
128	-28	-10.56	0.6	2.7	96.7
127	-29	-10.59	0.4	63.2	36.3
126	-30	-10.78	0	0.6	99.4

Table S3. TD-DFT Predicted Electronic Spectrum. Species **1**
TD-DFT- B3LYP/TZVP and DGDZVP(Ru)-PCM (CH3CN) -see main text. (SWizard Output from Gaussian TD-DFT File)

#	(nm	1000 cm-1	eV)	(f)	(Assignment; MO# -> MO#)
1	636.7	15.7	1.95	0.0151	148->149(+77%) 148->150(18%)
2	625.8	16.0	1.98	0.0044	148->150(+78%) 148->149(+19%)
3	465.8	21.5	2.66	0.0147	147->150(+54%) 147->149(+38%)
4	461.3	21.7	2.69	0.0273	147->149(+33%) 146->149(+26%) 147->150(19%) 146->150(13%)
5	452.1	22.1	2.74	0.0025	148->151(+87%) 146->149(8%)
6	448.1	22.3	2.77	0.0560	146->149(+60%) 147->149(19%) 147->150(+9%) 148->151(+6%)
7	425.5	23.5	2.91	0.0360	146->150(+31%) 148->153(+22%) 148->152(+16%) 148->157(+7%)
8	421.5	23.7	2.94	0.0284	146->150(+34%) 148->152(32%) 147->150(7%)
9	414.6	24.1	2.99	0.0102	148->152(+48%) 148->153(18%) 148->157(8%) 148->158(+6%)
10	399.9	25.0	3.10	0.0055	148->153(+41%) 145->149(17%) 148->154(16%) 148->157(7%)
11	394.0	25.4	3.15	0.0125	148->154(+68%) 145->150(+7%)
12	385.0	26.0	3.22	0.0083	145->149(+48%) 145->150(+35%)148->154(6%)
13	384.6	26.0	3.22	0.0339	145->150(+47%) 145->149(26%) 148->153(10%)
14	362.3	27.6	3.42	0.0031	148->158(+26%) 147->157(+14%) 148->157(+12%) 148->159(+8%) 147->156(+8%) 148->156(+6%)
15	355.9	28.1	3.48	0.0094	144->150(+38%) 147->151(38%) 144->149(+18%)
16	355.2	28.2	3.49	0.0192	147->151(+51%) 144->150(+22%) 144->149(+18%)
17	350.7	28.5	3.54	0.0010	144->149(+58%) 144->150(35%)
18	345.1	29.0	3.59	0.0034	146->151(+22%) 148->155(22%) 146->158(+20%) 146->159(+7%) 147->158(+5%)
19	344.5	29.0	3.60	0.0117	148->155(+56%) 146->151(+37%)
20	343.2	29.1	3.61	0.0025	146->151(+32%) 148->155(14%) 146->158(11%) 147->157(7%)
21	340.6	29.4	3.64	0.0070	147->157(+22%) 146->158(13%) 147->156(+13%) 147->153(+5%)
22	333.5	30.0	3.72	0.0180	147->152(+83%)
23	325.8	30.7	3.81	0.0202	147->153(+55%) 146->152(20%) 147->154(12%)
24	321.4	31.1	3.86	0.0156	147->154(+49%) 146->152(35%)
25	319.5	31.3	3.88	0.0059	146->153(+79%)
26	316.8	31.6	3.91	0.0671	146->152(+26%) 147->154(+24%) 147->153(+15%) 145->151(6%)
27	312.5	32.0	3.97	0.0069	146->154(+63%) 145->151(24%)

28	310.9	32.2	3.99	0.0436	145->151(+65%) 146->154(+16%)
29	308.0	32.5	4.03	0.0083	143->149(+51%) 143->150(+27%) 142->149(+13%)
30	306.8	32.6	4.04	0.0283	143->150(+39%) 142->149(20%) 142->150(+9%) 146->157(6%)
31	304.2	32.9	4.08	0.0179	146->157(+19%) 146->156(+12%) 143->150(+8%) 147->158(7%) 145->152(+6%) 146->153(6%) 148->156(6%)
32	302.8	33.0	4.09	0.0829	148->156(+40%) 148->157(23%) 143->150(+10%) 143->149(10%)
33	301.3	33.2	4.12	0.0016	142->149(+52%) 143->149(27%)
34	298.8	33.5	4.15	0.0021	142->150(+51%) 147->158(12%) 143->150(6%) 145->152(+6%)
35	296.2	33.8	4.19	0.0144	145->152(+42%) 142->150(16%) 145->153(+7%)
36	293.6	34.1	4.22	0.0025	145->152(+32%) 147->158(+27%) 147->159(+8%) 142->150(+5%) 146->158(5%)
37	290.3	34.4	4.27	0.0073	144->151(+53%) 145->153(+34%)
38	289.0	34.6	4.29	0.0113	144->151(+31%) 148->159(+26%) 145->153(15%) 148->158(12%)
39	287.5	34.8	4.31	0.0429	141->149(+42%) 145->154(+23%) 145->153(+13%)
40	287.1	34.8	4.32	0.0277	148->159(+36%) 145->153(+15%) 141->149(13%) 148->158(10%) 144->151(6%)
41	285.2	35.1	4.35	0.0589	140->149(+51%) 145->154(27%) 141->150(6%)
42	283.6	35.3	4.37	0.0220	141->150(+55%) 140->150(15%) 145->154(14%) 141->149(+6%)
43	280.1	35.7	4.43	0.1561	140->150(+66%)
44	279.4	35.8	4.44	0.0195	148->160(+91%)
45	277.9	36.0	4.46	0.0768	147->155(+80%)
46	277.0	36.1	4.48	0.4102	145->154(+18%) 140->149(+17%) 141->150(+11%) 147->155(11%) 141->149(7%) 145->153(6%) 144->152(5%)
47	275.1	36.3	4.51	0.0235	144->152(+79%) 144->153(+6%)
48	273.5	36.6	4.53	0.1353	139->150(+56%) 139->149(+24%)
49	271.1	36.9	4.57	0.0035	144->153(+77%) 144->154(+11%) 144->152(6%)
50	269.7	37.1	4.60	0.0008	139->149(+46%) 146->155(+31%) 139->150(17%)
51	269.2	37.1	4.61	0.0031	146->155(+57%) 139->149(23%) 139->150(+10%)
52	266.6	37.5	4.65	0.0029	145->157(+41%) 145->156(+23%) 148->157(6%)
53	265.1	37.7	4.68	0.0002	144->154(+85%) 144->153(10%)
54	258.9	38.6	4.79	0.0189	143->151(+81%) 142->151(+7%)
55	257.7	38.8	4.81	0.0016	147->156(+55%) 147->157(30%) 145->155(10%)
56	256.4	39.0	4.84	0.0160	145->155(+66%) 144->155(+9%) 147->156(+7%)
57	253.6	39.4	4.89	0.0015	142->151(+47%) 145->158(+23%) 145->159(+7%)

58	253.1	39.5	4.90	0.0036	142->151(+34%) 145->158(29%) 145->159(9%) 144->155(+6%)
59	251.4	39.8	4.93	0.0055	144->155(+77%) 145->155(6%)
60	249.8	40.0	4.96	0.0067	146->156(+44%) 146->157(27%) 141->151(+12%)
61	249.4	40.1	4.97	0.0061	141->151(+32%) 147->159(14%) 146->156(13%) 146->157(+7%) 138->149(+6%) 140->151(6%)
62	247.8	40.4	5.00	0.0051	143->152(+67%) 143->153(+11%) 142->152(+5%)
63	246.7	40.5	5.03	0.0332	140->151(+41%) 138->149(12%) 141->151(+8%) 138->150(+7%)
64	245.9	40.7	5.04	0.0197	138->149(+48%) 147->159(+17%) 143->152(6%) 147->158(6%)
65	244.7	40.9	5.07	0.0140	138->149(+23%) 141->151(12%) 147->159(12%) 147->160(+8%) 143->153(7%) 140->151(+6%)
66	243.9	41.0	5.08	0.0083	138->150(+66%) 147->159(8%) 141->151(6%)
67	243.2	41.1	5.10	0.0241	137->150(+38%) 143->153(16%) 137->149(+14%) 140->151(8%) 147->159(+6%)
68	242.8	41.2	5.11	0.0115	148->161(+81%) 148->162(5%)
69	242.6	41.2	5.11	0.0144	142->152(+41%) 143->153(19%) 137->150(12%) 138->150(+8%)
70	242.3	41.3	5.12	0.0004	142->152(+34%) 143->153(+17%) 143->152(11%) 137->150(+10%) 142->153(+8%)
71	240.6	41.6	5.15	0.0059	146->159(+38%) 146->158(15%) 141->151(7%) 147->160(6%) 143->153(6%)
72	239.8	41.7	5.17	0.0198	147->160(+40%) 146->159(+18%) 140->151(9%) 146->158(7%)
73	239.4	41.8	5.18	0.0052	143->154(+45%) 142->153(18%) 147->160(+13%) 137->149(+7%)
74	238.5	41.9	5.20	0.0018	137->149(+54%) 137->150(17%) 142->153(+15%)
75	238.1	42.0	5.21	0.0034	142->153(+30%) 143->154(+15%) 143->153(11%) 145->156(+6%) 137->149(6%) 144->156(+5%)
76	236.7	42.2	5.24	0.0079	141->152(+38%) 146->160(+16%) 140->151(+7%) 141->154(+5%)
77	236.1	42.3	5.25	0.0091	145->156(+21%) 142->153(10%) 145->157(10%) 142->154(+9%) 144->156(+9%) 140->153(6%) 140->154(+5%)
78	235.6	42.4	5.26	0.0249	141->153(+15%) 143->154(+9%) 141->152(+9%) 141->154(8%) 142->154(6%) 144->156(6%)
79	235.0	42.5	5.28	0.0172	142->154(+29%) 141->152(+9%) 147->160(+9%) 145->156(6%) 136->150(+5%)
80	234.8	42.6	5.28	0.0099	142->154(+25%) 140->152(+10%) 141->153(+9%) 141->152(8%) 147->160(7%) 141->154(+6%)
81	234.6	42.6	5.29	0.0125	136->150(+20%) 144->157(14%) 144->158(+14%) 136->149(+11%) 140->152(+8%) 145->157(5%) 144->156(5%)

82	234.1	42.7	5.30	0.0203	136->150(+20%) 144->158(14%) 136->149(+10%) 146->160(+9%) 144->157(+7%) 144->156(+7%)
83	234.0	42.7	5.30	0.0125	139->151(+33%) 140->152(20%) 136->150(+15%) 136->149(+7%)
84	233.5	42.8	5.31	0.0082	146->160(+35%) 140->152(25%) 139->151(16%)
85	231.8	43.1	5.35	0.0152	139->151(+25%) 146->160(+20%) 136->149(18%) 141->153(11%) 140->153(7%)
86	231.3	43.2	5.36	0.0040	136->149(+43%) 136->150(32%)
87	230.7	43.3	5.37	0.0007	144->157(+43%) 144->156(38%)
88	227.6	43.9	5.45	0.0162	133->149(+27%) 132->149(+23%) 131->149(14%) 135->149(6%) 140->153(+5%)
89	227.2	44.0	5.46	0.0006	141->154(+32%) 140->153(30%) 141->153(+12%) 140->154(11%)
90	226.3	44.2	5.48	0.0063	140->154(+44%) 141->154(+17%) 141->153(14%)
91	225.3	44.4	5.50	0.0937	133->150(+16%) 132->150(+12%) 148->162(+11%) 131->150(11%) 145->159(+7%) 144->158(7%)
92	224.8	44.5	5.52	0.0199	148->162(+48%) 133->150(6%) 132->150(5%) 131->150(+5%)
93	224.2	44.6	5.53	0.1697	148->162(+20%) 145->159(19%) 144->158(+8%) 145->158(+8%) 140->154(+5%)
94	223.9	44.7	5.54	0.0170	139->152(+74%) 139->153(+8%)
95	222.8	44.9	5.57	0.1374	145->159(+40%) 144->158(+13%) 145->158(10%)
96	221.5	45.1	5.60	0.0027	142->155(+74%) 143->155(+10%)
97	220.9	45.3	5.61	0.0139	139->153(+62%) 139->154(+20%)
98	219.3	45.6	5.65	0.0257	145->160(+45%) 134->149(+23%)
99	218.3	45.8	5.68	0.0320	145->160(+34%) 134->149(32%) 134->150(7%) 135->150(6%)
100	217.2	46.0	5.71	0.0178	135->149(+43%) 132->149(+10%) 145->160(+9%)
101	216.9	46.1	5.72	0.0126	134->150(+36%) 134->149(14%) 139->154(13%) 135->149(8%)
102	216.8	46.1	5.72	0.0122	135->150(+34%) 139->154(+21%) 139->153(12%) 134->149(9%)
103	216.4	46.2	5.73	0.0045	139->154(+31%) 134->150(+26%) 135->150(17%)
104	215.0	46.5	5.77	0.1350	143->155(+40%) 143->156(+8%) 139->155(+8%)
105	214.9	46.5	5.77	0.0399	143->156(+30%) 142->156(+11%) 142->158(+9%) 143->155(9%) 138->151(5%)
106	214.0	46.7	5.79	0.0060	133->149(+35%) 132->149(12%) 138->151(10%) 131->149(+6%)
107	213.3	46.9	5.81	0.0196	138->151(+41%) 133->149(+10%)
108	213.1	46.9	5.82	0.0051	144->159(+39%) 138->151(+12%) 144->158(10%) 132->150(+9%) 133->150(6%)
109	212.5	47.1	5.84	0.0047	132->150(+32%) 133->150(26%) 138->151(10%) 144->159(9%)
110	211.9	47.2	5.85	0.0011	143->157(+65%) 142->156(8%)

Table S4. TD-DFT Predicted Electronic Spectrum. Species **2**
TD-DFT- B3LYP/TZVP and DGDZVP(Ru)-PCM (CH_3CN) -see main text. (SWizard Output from Gaussian TD-DFT File)

#	(nm	1000 cm-1	eV)	(f)	(Assignment; MO# -> MO#)
1	423.6	23.6	2.93	0.0001	156->158(+89%) 156->157(+6%)
2	421.2	23.7	2.94	0.0014	156->157(+92%) 156->158(5%)
3	406.1	24.6	3.05	0.0104	155->158(+90%)
4	404.4	24.7	3.07	0.0031	155->157(+87%) 154->158(8%)
5	388.5	25.7	3.19	0.1054	154->157(+90%) 155->158(+5%)
6	375.8	26.6	3.30	0.0557	154->158(+82%) 155->157(+6%)
7	353.4	28.3	3.51	0.0013	156->165(+58%) 155->166(+15%) 154->165(+11%)
8	349.2	28.6	3.55	0.0013	155->165(+64%) 156->166(+24%)
9	348.9	28.7	3.55	0.0012	153->157(+97%)
10	346.7	28.8	3.58	0.0013	153->158(+97%)
11	327.0	30.6	3.79	0.0028	156->159(+76%) 154->166(10%)
12	325.0	30.8	3.82	0.0037	154->166(+36%) 156->166(24%) 156->159(+20%) 155->165(+5%)
13	320.4	31.2	3.87	0.0014	152->157(+89%)
14	318.4	31.4	3.89	0.0005	155->159(+56%) 152->158(37%)
15	318.0	31.4	3.90	0.0028	152->158(+52%) 155->159(+39%)
16	310.5	32.2	3.99	0.0000	156->160(+83%) 155->166(+6%)
17	310.0	32.3	4.00	0.0140	154->159(+85%)
18	306.8	32.6	4.04	0.0042	151->157(+84%)
19	304.9	32.8	4.07	0.0009	151->158(+57%) 155->160(12%) 154->166(+6%) 151->157(5%) 150->157(5%)
20	304.1	32.9	4.08	0.0017	155->160(+37%) 151->158(+25%) 154->166(12%) 156->166(6%)
21	303.1	33.0	4.09	0.0126	156->161(+61%) 155->166(10%) 154->160(9%)
22	299.6	33.4	4.14	0.0198	155->160(+28%) 155->161(+28%) 156->166(+7%) 155->166(+6%) 154->166(+5%)
23	298.9	33.5	4.15	0.0029	155->166(+30%) 156->165(12%) 155->161(9%) 156->161(+7%) 154->165(+6%)
24	297.9	33.6	4.16	0.0203	156->162(+71%) 155->161(+11%)
25	296.4	33.7	4.18	0.0008	150->157(+85%) 151->158(+7%)
26	295.8	33.8	4.19	0.0117	155->162(+22%) 149->157(+21%) 154->161(20%) 154->160(+8%) 155->166(7%) 148->158(6%)
27	294.9	33.9	4.20	0.0250	155->161(+26%) 156->162(14%) 155->160(10%) 156->166(9%) 154->166(8%) 149->158(7%) 155->165(+6%) 154->162(6%)
28	294.3	34.0	4.21	0.0002	150->158(+89%)
29	289.6	34.5	4.28	0.0053	154->160(+34%) 154->161(+27%) 154->165(12%) 155->162(+7%)
30	288.5	34.7	4.30	0.0037	149->157(+42%) 149->158(+17%) 148->158(+14%) 148->157(+9%)
31	287.6	34.8	4.31	0.0204	149->158(+25%) 155->162(+22%) 148->157(+12%) 154->161(+9%) 156->161(8%) 154->165(+7%)
32	287.2	34.8	4.32	0.0420	155->162(+24%) 148->157(20%) 154->160(15%) 148->158(+10%) 154->165(6%) 154->162(+6%)149->158(5%)
33	287.0	34.8	4.32	0.1002	154->162(+25%) 149->158(+14%) 148->158(12%) 154->161(10%) 155->161(+8%) 154->165(7%)

34 286.4 34.9 4.33 0.0457 154->162(15%) 148->157(+15%)
154->165(14%) 154->160(12%)
148->158(9%) 155->162(+8%) 155->166(+5%)
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36 278.7 35.9 4.45 0.2374 148->158(+37%) 154->161(24%)
154->160(+8%) 149->157(8%)
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Reference 44.
Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

CIF File species **2**

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C6 C 0.7275(6) 0.4782(4) 0.0526(4) 0.0242(11) Uani 1 1 d . . .
C7 C 0.7605(6) 0.5233(5) -0.0385(4) 0.0317(13) Uani 1 1 d . . .
H7A H 0.7291 0.5913 -0.0525 0.038 Uiso 1 1 calc R . .
C8 C 0.8407(6) 0.4676(5) -0.1103(4) 0.0333(13) Uani 1 1 d . . .
H8A H 0.8650 0.5000 -0.1697 0.040 Uiso 1 1 calc R . .
C9 C 0.8811(6) 0.3680(5) -0.0919(4) 0.0312(13) Uani 1 1 d . . .
H9A H 0.9339 0.3289 -0.1375 0.037 Uiso 1 1 calc R . .
C10 C 0.8411(6) 0.3253(5) -0.0018(4) 0.0246(11) Uani 1 1 d . . .
H10A H 0.8670 0.2551 0.0111 0.030 Uiso 1 1 calc R . .
C11 C 0.7498(6) 0.0779(4) 0.1301(4) 0.0246(11) Uani 1 1 d . . .
H11A H 0.6448 0.0566 0.1033 0.030 Uiso 1 1 calc R . .
C12 C 0.8320(6) -0.0058(5) 0.1078(4) 0.0288(12) Uani 1 1 d . . .
H12A H 0.7829 -0.0812 0.0676 0.035 Uiso 1 1 calc R . .
C13 C 0.9803(7) 0.0206(5) 0.1433(5) 0.0399(15) Uani 1 1 d . . .
H13A H 1.0397 -0.0340 0.1292 0.048 Uiso 1 1 calc R . .
C14 C 1.0400(6) 0.1288(5) 0.2000(5) 0.0373(14) Uani 1 1 d . . .
H14A H 1.1450 0.1516 0.2262 0.045 Uiso 1 1 calc R . .
C15 C 0.9528(6) 0.2088(4) 0.2217(4) 0.0246(11) Uani 1 1 d . . .
C16 C 1.0098(6) 0.3273(4) 0.2837(4) 0.0236(11) Uani 1 1 d . . .
C17 C 1.1524(6) 0.3631(5) 0.3340(4) 0.0273(12) Uani 1 1 d . . .
H17A H 1.2218 0.3148 0.3289 0.033 Uiso 1 1 calc R . .
C18 C 1.1928(6) 0.4740(5) 0.3937(4) 0.0298(13) Uani 1 1 d . . .
H18A H 1.2931 0.5026 0.4327 0.036 Uiso 1 1 calc R . .
C19 C 1.0947(6) 0.5459(5) 0.3998(4) 0.0268(12) Uani 1 1 d . . .
H19A H 1.1264 0.6227 0.4414 0.032 Uiso 1 1 calc R . .
C20 C 0.9564(6) 0.5057(4) 0.3468(4) 0.0235(11) Uani 1 1 d . . .
H20A H 0.8867 0.5539 0.3498 0.028 Uiso 1 1 calc R . .
C21 C 0.4945(5) 0.1336(4) 0.3158(4) 0.0210(10) Uani 1 1 d . . .
C22 C 0.4363(5) 0.1099(4) 0.2098(4) 0.0213(11) Uani 1 1 d . . .
C23 C 0.3436(6) 0.0043(4) 0.1688(4) 0.0258(11) Uani 1 1 d . . .
H23A H 0.3033 -0.0173 0.0931 0.031 Uiso 1 1 calc R . .
C24 C 0.3056(6) -0.0740(5) 0.2358(4) 0.0306(12) Uani 1 1 d . . .
H24A H 0.2406 -0.1473 0.2040 0.037 Uiso 1 1 calc R . .
C25 C 0.3585(6) -0.0482(5) 0.3425(4) 0.0310(13) Uani 1 1 d . . .
H25A H 0.3300 -0.0998 0.3881 0.037 Uiso 1 1 calc R . .
C26 C 0.4539(6) 0.0546(5) 0.3820(4) 0.0280(12) Uani 1 1 d . . .
H26A H 0.4960 0.0752 0.4574 0.034 Uiso 1 1 calc R . .

O5 O 0.9596(10) -0.2175(7) 0.2672(8) 0.139(4) Uani 1 1 d . . .
N5 N 0.8721(7) -0.1364(5) 0.4100(6) 0.0613(18) Uani 1 1 d . . .
C27 C 0.9453(14) -0.1900(8) 0.3365(14) 0.129(6) Uani 1 1 d . . .
H27 H 1.0244 -0.2093 0.3825 0.155 Uiso 1 1 calc R . .
C28 C 0.7626(10) -0.0784(7) 0.3755(6) 0.069(2) Uani 1 1 d . . .
H28C H 0.7564 -0.0766 0.2985 0.103 Uiso 1 1 calc R . .
H28D H 0.7881 0.0012 0.4178 0.103 Uiso 1 1 calc R . .
H28A H 0.6661 -0.1189 0.3857 0.103 Uiso 1 1 calc R . .
C29 C 0.8867(11) -0.1420(9) 0.5215(9) 0.101(4) Uani 1 1 d . . .
H29C H 0.8227 -0.0964 0.5538 0.151 Uiso 1 1 calc R . .
H29D H 0.9909 -0.1105 0.5593 0.151 Uiso 1 1 calc R . .
H29A H 0.8565 -0.2229 0.5283 0.151 Uiso 1 1 calc R . .

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S1 0.0165(6) 0.0236(7) 0.0210(6) 0.0053(5) -0.0008(5) 0.0018(5)
S2 0.0234(7) 0.0212(6) 0.0179(6) 0.0011(5) 0.0007(5) -0.0018(5)
O1 0.027(2) 0.031(2) 0.0203(17) -0.0011(15) -0.0082(15) -0.0007(16)
O2 0.021(2) 0.032(2) 0.037(2) 0.0094(17) 0.0000(16) 0.0060(16)
O3 0.038(2) 0.025(2) 0.0246(19) -0.0027(15) 0.0079(17) -0.0001(17)
O4 0.031(2) 0.029(2) 0.0233(18) 0.0078(15) -0.0098(16) -0.0026(17)
N1 0.019(2) 0.020(2) 0.026(2) 0.0031(18) -0.0016(18) 0.0003(18)
N2 0.0100(19) 0.017(2) 0.0140(18) 0.0048(15) -0.0063(15) -0.0069(16)
N3 0.017(2) 0.021(2) 0.0170(19) 0.0038(16) -0.0013(16) 0.0020(17)
N4 0.014(2) 0.022(2) 0.0126(18) 0.0059(16) -0.0001(15) -0.0016(17)
C1 0.027(3) 0.030(3) 0.032(3) 0.004(2) 0.009(2) 0.006(2)
C2 0.030(3) 0.031(3) 0.048(4) -0.001(3) 0.006(3) 0.010(3)
C3 0.032(3) 0.023(3) 0.060(4) 0.009(3) 0.005(3) 0.010(3)
C4 0.027(3) 0.026(3) 0.042(3) 0.014(2) -0.002(3) 0.003(2)
C5 0.017(3) 0.026(3) 0.030(3) 0.005(2) -0.002(2) -0.002(2)
C6 0.023(3) 0.023(3) 0.021(2) 0.005(2) -0.005(2) -0.002(2)
C7 0.026(3) 0.035(3) 0.030(3) 0.015(2) -0.006(2) -0.001(2)
C8 0.029(3) 0.039(3) 0.024(3) 0.012(2) -0.003(2) -0.010(3)
C9 0.030(3) 0.034(3) 0.022(3) 0.001(2) 0.004(2) -0.005(2)
C10 0.023(3) 0.026(3) 0.021(2) 0.002(2) 0.004(2) 0.000(2)
C11 0.022(3) 0.024(3) 0.022(2) 0.002(2) -0.002(2) 0.000(2)
C12 0.023(3) 0.025(3) 0.034(3) -0.002(2) 0.000(2) 0.008(2)
C13 0.028(3) 0.033(3) 0.049(4) -0.008(3) -0.003(3) 0.010(3)
C14 0.022(3) 0.039(3) 0.042(3) -0.004(3) -0.007(2) 0.007(3)
C15 0.015(3) 0.028(3) 0.024(3) 0.002(2) -0.004(2) -0.001(2)
C16 0.025(3) 0.024(3) 0.017(2) 0.004(2) -0.002(2) 0.000(2)
C17 0.017(3) 0.033(3) 0.028(3) 0.007(2) -0.001(2) -0.002(2)
C18 0.023(3) 0.035(3) 0.021(2) 0.002(2) -0.001(2) -0.012(2)
C19 0.027(3) 0.022(3) 0.023(3) -0.002(2) 0.000(2) -0.005(2)
C20 0.022(3) 0.020(3) 0.021(2) -0.002(2) -0.003(2) -0.003(2)
C21 0.013(2) 0.024(3) 0.022(2) 0.000(2) 0.0013(19) 0.001(2)
C22 0.016(3) 0.022(3) 0.024(2) 0.005(2) 0.001(2) 0.001(2)
C23 0.017(3) 0.026(3) 0.029(3) 0.002(2) -0.001(2) 0.000(2)
C24 0.020(3) 0.027(3) 0.039(3) 0.002(2) -0.001(2) -0.001(2)

C25 0.028(3) 0.027(3) 0.032(3) 0.008(2) 0.001(2) -0.004(2)
C26 0.025(3) 0.028(3) 0.027(3) 0.009(2) 0.002(2) -0.001(2)
O5 0.112(7) 0.108(6) 0.170(8) -0.064(6) 0.093(6) -0.025(5)
N5 0.066(5) 0.049(4) 0.086(5) 0.024(3) 0.038(4) 0.024(3)
C27 0.115(10) 0.042(6) 0.244(18) 0.003(8) 0.125(12) -0.005(6)
C28 0.078(6) 0.081(6) 0.049(4) 0.016(4) 0.009(4) 0.022(5)
C29 0.084(7) 0.119(9) 0.143(10) 0.098(8) 0.039(7) 0.055(7)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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S1 C22 1.841(5) . ?
S2 O4 1.423(4) . ?
S2 O3 1.523(4) . ?
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N4 C16 1.368(6) . ?
C1 C2 1.383(8) . ?
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C7 C8 1.441(8) . ?
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C9 C10 1.413(7) . ?
C11 C12 1.397(7) . ?
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C14 C15 1.396(7) . ?
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C25 C26 1.339(7) . ?
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O4 S2 C21 100.1(2) . . ?
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O4 S2 Ru1 110.96(17) . . ?
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C21 S2 Ru1 106.57(17) . . ?
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C5 N1 Ru1 114.0(3) . . ?
C1 N1 Ru1 126.9(3) . . ?
C6 N2 C10 118.9(4) . . ?
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C6 N2 Ru1 113.6(3) . . ?
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C15 N3 C11 114.9(4) . . ?
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C11 N3 Ru1 128.1(3) . . ?
C20 N4 C16 121.6(4) . . ?
C20 N4 Ru1 124.8(3) . . ?
C16 N4 Ru1 113.5(3) . . ?
C2 C1 N1 122.8(5) . . ?
C1 C2 C3 117.1(5) . . ?
C2 C3 C4 120.5(5) . . ?
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N2 C10 C9 124.3(5) . . ?
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