Supporting Information

Ancillary Ligand Control of Electronic Structure in *o*-Benzoquinonediimine-Ruthenium Complex Redox Series: Structures, Electron Paramagnetic Resonance (EPR), and Ultraviolet-Visible-Near-Infrared (UV-vis-NIR) Spectroelectrochemistry

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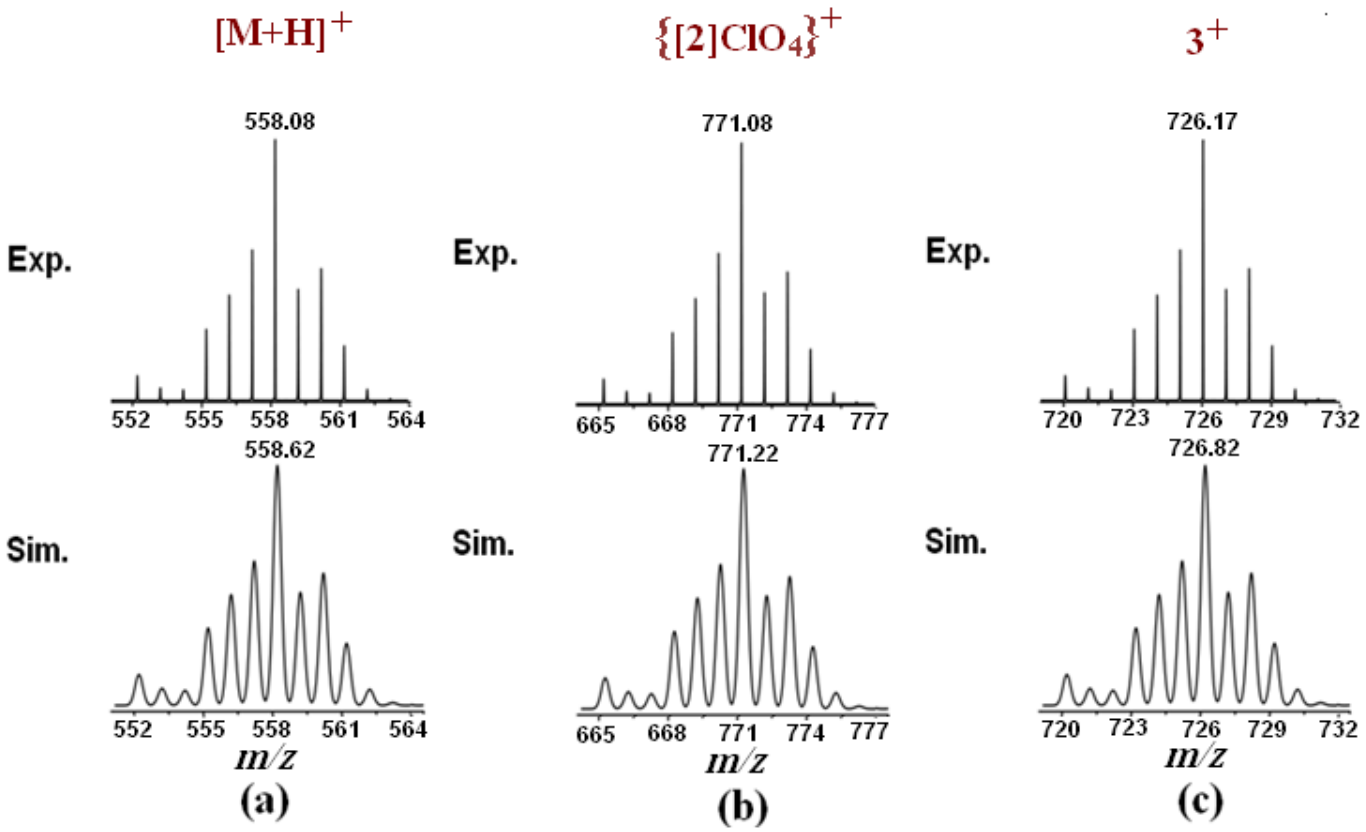


Figure S1. ESI-MS of (a) **1**, (b) [**2**]$(ClO_4)_2$ and (c) [**3**]PF_6 in CH_3CN.

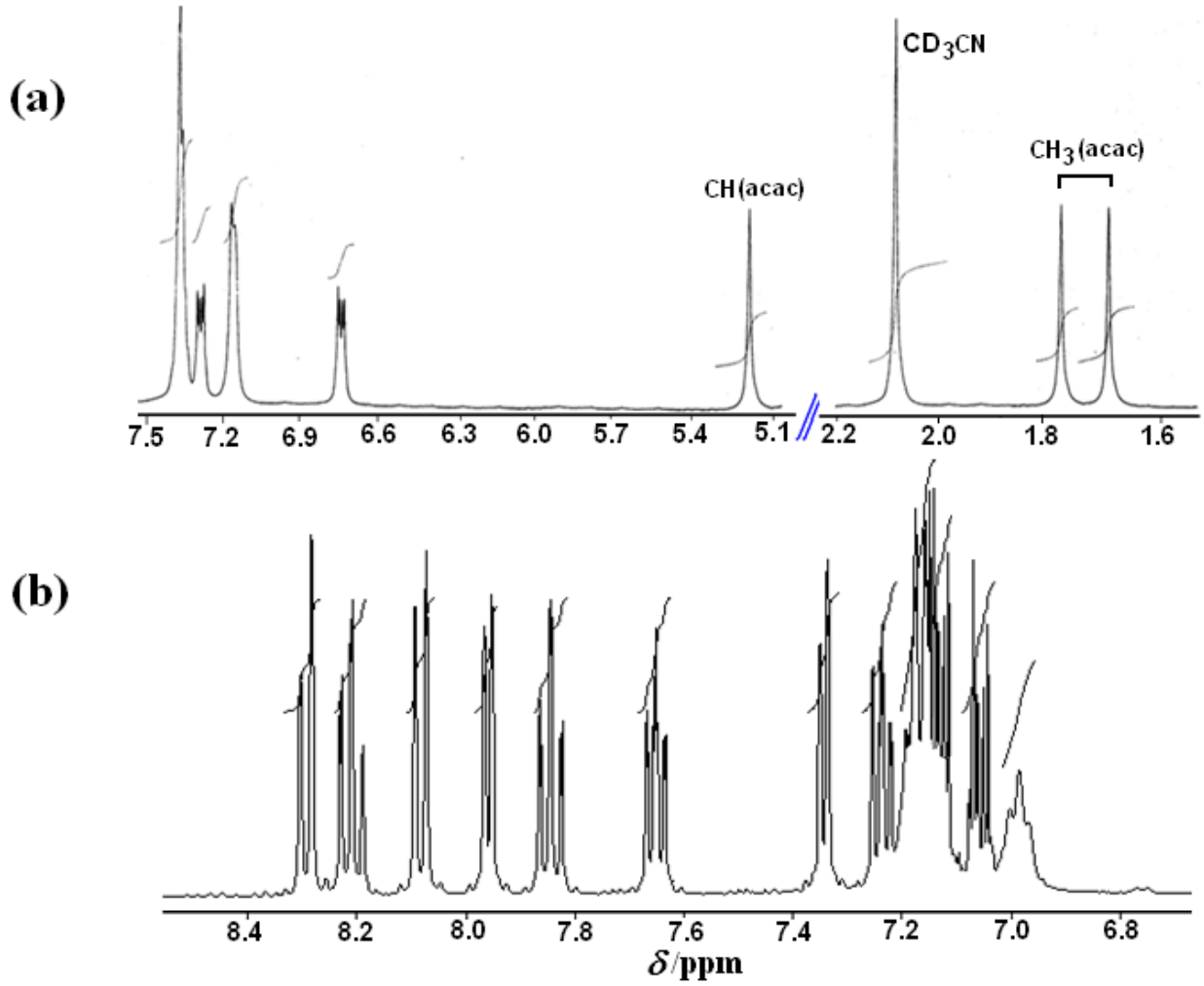


Figure S2. ^{1}H-NMR spectra of (a) **1** and (b) [**2**]$(ClO_4)_2$ in CD_3CN.

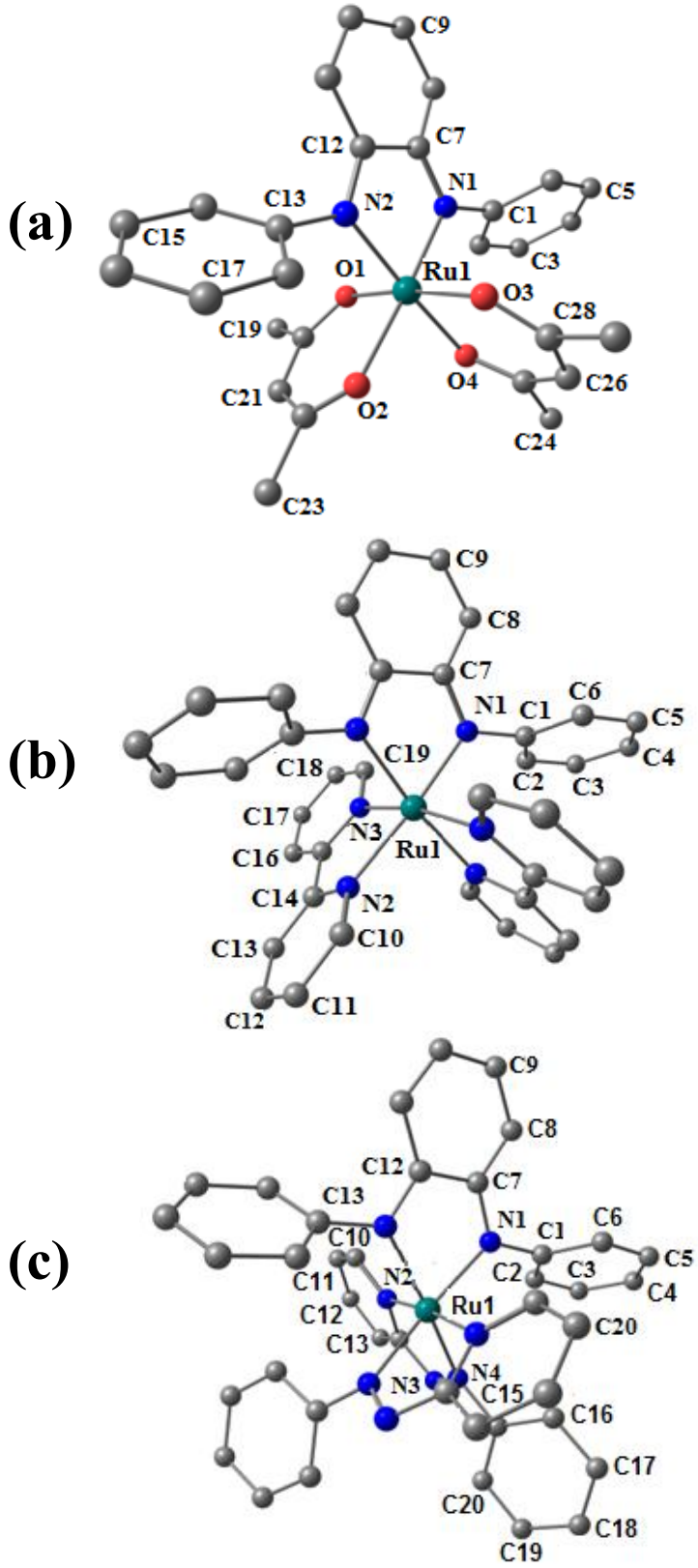


Figure S3. DFT optimized geometry of **1**, $\mathbf{2}^{2+}$ and $\mathbf{3}^{+}$.

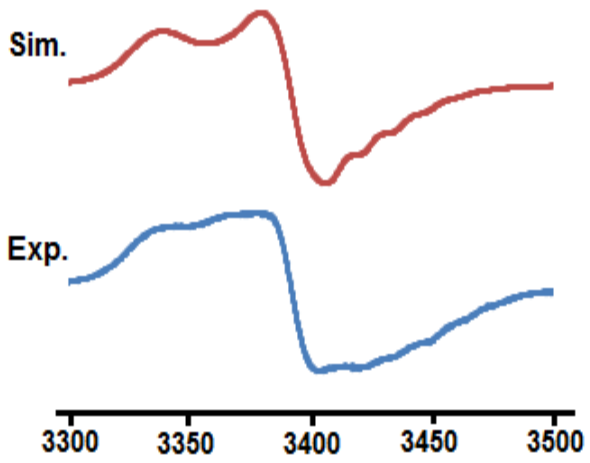


Figure S4. EPR spectra of electrogenerated $\mathbf{2}^{+}$ (blue: experimental and red: simulated) at 120 K in CH_2Cl_2/0.1 M $NBu_4^{+}PF_6^{-}$.

Table S1. Experimental and DFT Calculated Selected Bond Lengths (Å) for 1^n

bond	exp.	calc.		
	1	$\mathbf{1}^+$ (S=1/2)	**1** (S=0)	$\mathbf{1}^-$ (S=1/2)
Ru1-N1	1.963(2)	2.044	2.020	2.056
Ru1-N2	1.9821(19)	2.044	2.020	2.057
Ru1-O1	2.036(16)	2.028	2.067	2.086
Ru1-O2	2.0652(19)	2.055	2.097	2.123
Ru1-O3	2.0152(15)	2.028	2.068	2.086
Ru1-O4	2.0643(17)	2.055	2.098	2.123
N1-C7	1.346(3)	1.328	1.341	1.367
N2-C12	1.336(3)	1.328	1.341	1.368
C7-C8	1.409(4)	1.437	1.431	1.416
C8-C9	1.367(4)	1.363	1.370	1.389
C9-C10	1.412(4)	1.438	1.427	1.404
C10-C11	1.349(4)	1.363	1.370	1.389
C11-C12	1.427(4)	1.437	1.431	1.416
C7-C12	1.450(4)	1.469	1.455	1.445

Table S2. Experimental and DFT Calculated Selected Bond Angles (deg) for 1^n

bond angles (deg)	exp.	calc.		
	1	$\mathbf{1}^+$ (S=1/2)	**1** (S=0)	$\mathbf{1}^-$ (S=1/2)
N1-Ru1-N2	80.09(8)	78.91	78.98	78.90
N1-Ru1-O1	90.49(8)	89.79	90.34	89.99
N1-Ru1-O2	175.96(7)	175.98	176.51	176.91
N1-Ru1-O3	93.08(8)	92.57	94.73	93.20
N1-Ru1-O4	95.10(8)	97.03	97.39	97.83
N2-Ru1-O1	95.34(8)	92.47	94.47	92.95
N2-Ru1-O2	95.87(8)	97.19	97.52	98.01
N2-Ru1-O3	86.89(8)	89.84	90.63	90.14
N2-Ru1-O4	174.48(8)	175.85	176.37	176.73
O1-Ru1-O2	89.82(7)	89.40	89.93	90.38
O1-Ru1-O3	176.08(7)	176.96	173.40	175.92
O1-Ru1-O4	87.37(7)	88.35	85.30	86.74
O2-Ru1-O3	86.74(7)	88.36	85.25	86.56
O2-Ru1-O4	88.94(7)	86.86	86.09	85.24
O3-Ru1-O4	90.68(7)	89.47	89.86	90.31

Table S3. Experimental and DFT Calculated Selected Bond Lengths (Å) for 2^n

bond	exp.	calc.				
	$\mathbf{2}^{2+}$	$\mathbf{2}^{3+}$ (S=1/2)	$\mathbf{2}^{2+}$ (S=0)	$\mathbf{2}^{+}$ (S=1/2)	**2** (S=1)	**2** (S=0)
Ru1-N1	2.020(2)	2.083	2.096	2.114	2.116	2.116
Ru1-N2	2.0881(19)	2.144	2.137	2.131	2.112	2.116
Ru1-N3	2.073 (2)	2.134	2.122	2.108	2.098	2.117
N1-C7	1.318(3)	1.352	1.328	1.361	1.361	1.397
C7-C8	1.419(4)	1.427	1.440	1.424	1.423	1.410
C8-C9	1.350(4)	1.377	1.362	1.379	1.381	1.392
C7-C7#1	1.468(4)	1.461	1.474	1.450	1.450	1.426
C9-C9#1	1.411(7)	1.423	1.440	1.415	1.412	1.401

Symmetry transformations used to generate equivalent atoms: #1= -x+1,y,-z+1/2

Table S4. Experimental and DFT Calculated Selected Bond Angles (deg) for 2^n

bond angles (deg)	exp.	calc.				
	$\mathbf{2}^{2+}$	$\mathbf{2}^{3+}$ (S=1/2)	$\mathbf{2}^{2+}$ (S=0)	$\mathbf{2}^{+}$ (S=1/2)	**2** (S=1)	**2** (S=0)
N1-Ru1-N2	173.91(7)	172.93	172.67	171.39	172.86	174.34
N1-Ru1-N3	97.71(9)	96.23	98.10	96.21	96.58	97.74
N1-Ru1-N1#1	78.16(12)	79.17	77.51	77.93	77.49	79.09
N1-Ru1-N2#1	97.74(8)	99.86	99.63	99.26	99.27	96.19
N1-Ru1-N3#1	92.58(9)	91.37	90.48	89.73	91.47	87.32
N2-Ru1-N3	77.85(9)	77.00	77.12	77.16	77.91	77.15
N2-Ru1-N1#1	97.74(8)	98.31	96.72	96.24	97.83	98.25
N2-Ru1-N2#1	86.68(10)	82.93	86.44	87.22	85.85	87.15
N2-Ru1-N3#1	92.44(8)	95.57	94.88	97.24	94.46	97.84
N3-Ru1-N1#1	92.58(9)	87.60	89.35	88.75	90.31	89.15
N3-Ru1-N2#1	92.44(8)	95.06	95.38	98.07	95.24	99.82
N3-Ru1-N3#1	166.75(12)	170.14	169.47	173.01	170.23	174.73

Symmetry transformations used to generate equivalent atoms: #1= -x+1,y,-z+1/2

Table S5. Experimental and DFT Calculated Selected Bond Lengths (Å) for 3^n

bond	exp.	calc.			
	$\mathbf{3}^{+}$	$\mathbf{3}^{2+}$ (S=0)	$\mathbf{3}^{+}$ (S=1/2)	$\mathbf{3}$ (S=1)	$\mathbf{3}^{-}$ (S=3/2)
Ru1-N1	2.065(3)	2.094	2.105	2.131	2.111
Ru1-N2	2.050(3)	2.109	2.094	2.087	2.102
Ru1-N4	2.030(3)	2.137	2.115	2.086	2.146
N1-C7	1.351(4)	1.326	1.357	1.357	1.363
C7-C8	1.422(5)	1.442	1.425	1.425	1.422
C8-C9	1.369(5)	1.361	1.377	1.379	1.384
C7-C7#1	1.445(7)	1.476	1.451	1.451	1.449
C9-C9#1	1.406(8)	1.442	1.417	1.414	1.408
N3-N4	1.283(4)	1.273	1.279	1.313	1.341

Symmetry transformations used to generate equivalent atoms: #1= -x,-y+1/2,z

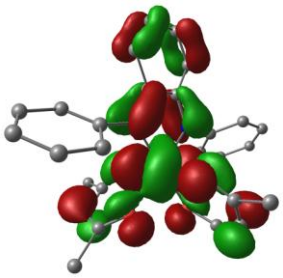
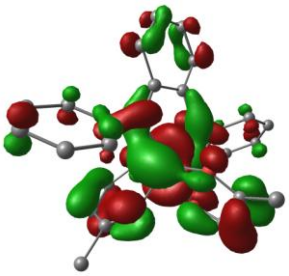
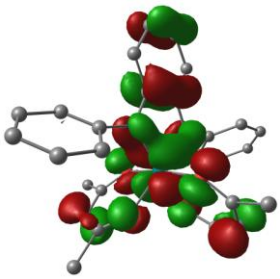
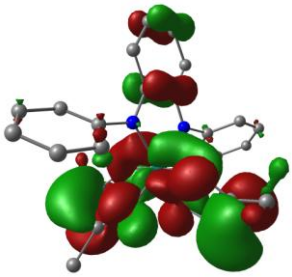
Table S6. Experimental and DFT Calculated Selected Bond Angles (deg) for 3^n

bond angles (deg)	exp.	calc.			
	$\mathbf{3}^{+}$	$\mathbf{3}^{2+}$ (S=0)	$\mathbf{3}^{+}$ (S=1/2)	$\mathbf{3}$ (S=1)	$\mathbf{3}^{-}$ (S=3/2)
N1-Ru1-N2	97.90(11)	90.762	89.71	90.46	90.16
N1-Ru1-N4	173.19(11)	101.221	100.47	99.36	100.23
N2-Ru1-N4	75.69(12)	74.954	100.72	75.76	75.29
N1-Ru1-N1#1	77.96(16)	77.313	77.71	76.87	77.56
N1-Ru1-N2#1	91.35(11)	96.331	94.78	95.59	95.12
N1-Ru1-N4#1	99.65(11)	171.198	169.53	170.65	170.22
N2-Ru1-N1#1	91.35(11)	96.331	94.78	95.59	95.12
N2-Ru1-N2#1	168.10(16)	170.923	174.22	172.26	173.22
N2-Ru1-N4#1	95.31(11)	98.033	98.12	98.45	99.53
N4-Ru1-N1#1	99.65(11)	171.198	169.53	170.65	170.22
N4-Ru1-N2#1	95.31(11)	98.033	100.72	98.45	99.53
N4-Ru1-N4#1	83.43(15)	81.540	83.13	85.59	83.50

Symmetry transformations used to generate equivalent atoms: #1= -x,-y+1/2,z

Table S7. Composition and Energies of Selected Molecular Orbitals of 1 (*S*=0)

MO	energy(eV)	composition		
		Ru	Q	acac
HOMO-10	-7.099	0.05	0.46	0.50
HOMO-9	-6.811	0.05	0.81	0.14
HOMO-8	-6.777	0.04	0.77	0.19
HOMO-7	-6.455	0.03	0.51	0.46
HOMO-6	-6.393	0.05	0.81	0.14
HOMO-5	-6.200	0.17	0.52	0.31
HOMO-4	-6.009	0.27	0.37	0.37
HOMO-3	-5.914	0.19	0.14	0.67
HOMO-2	-5.081	0.40	0.28	0.32
HOMO-1	-5.034	0.53	0.18	0.30
HOMO	-4.577	0.61	0.19	0.20
LUMO	-2.472	0.32	0.60	0.08
LUMO+1	-0.695	0.03	0.89	0.08
LUMO+2	-0.412	0.05	0.62	0.33
LUMO+3	-0.312	0.04	0.11	0.85
LUMO+4	-0.288	0.04	0.35	0.60
LUMO+5	0.119	0.02	0.96	0.02
LUMO+6	0.219	0.11	0.82	0.07
LUMO+7	0.683	0.10	0.86	0.04
LUMO+8	0.873	0.33	0.38	0.29
LUMO+9	1.028	0.15	0.72	0.13
LUMO+10	1.359	0.71	0.07	0.22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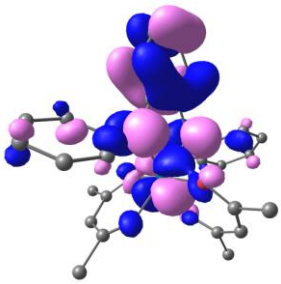
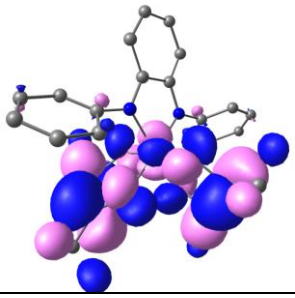
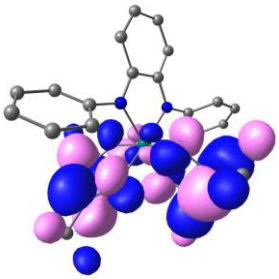
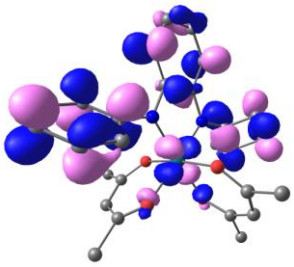
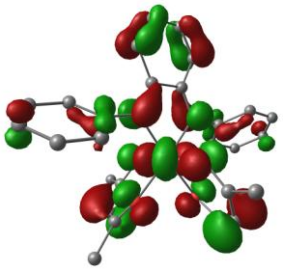
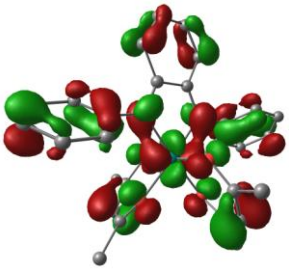
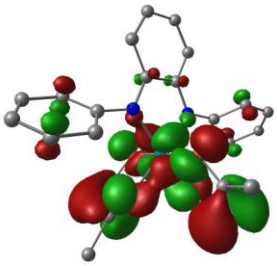
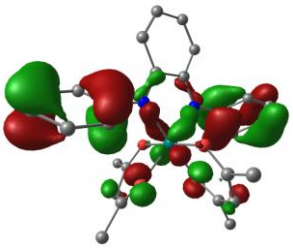
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S8. Composition and Energies of Selected Molecular Orbitals of 1^+ (*S*=1/2)

MO	energy (eV)	composition		
		Ru	Q	acac
		α-spin		
HOMO-10	-10.516	0.27	0.18	0.55
HOMO-9	-10.319	0.10	0.14	0.75
HOMO-8	-10.134	0.59	0.19	0.22
HOMO-7	-9.851	0.42	0.14	0.44
HOMO-6	-9.838	0.19	0.68	0.13
HOMO-5	-9.677	0.01	0.91	0.08
HOMO-4	-9.601	0.03	0.93	0.03
HOMO-3	-9.551	0.05	0.82	0.12
HOMO-2	-9.010	0.12	0.09	0.79
HOMO-1	-8.966	0.14	0.84	0.02
SOMO	-8.947	0.16	0.05	0.79
LUMO	-6.568	0.15	0.81	0.04
LUMO+1	-4.293	0.54	0.11	0.36
LUMO+2	-4.000	0.41	0.43	0.16
LUMO+3	-3.942	0.04	0.05	0.90
LUMO+4	-3.912	0.01	0.03	0.96
LUMO+5	-3.259	0.09	0.88	0.03
LUMO+6	-3.128	0.02	0.96	0.01
LUMO+7	-2.866	0.03	0.94	0.02
LUMO+8	-2.798	0.03	0.94	0.02
LUMO+9	-2.495	0.03	0.96	0.01
LUMO+10	-2.334	0.12	0.84	0.04
		β-spin		
HOMO-10	-10.588	0.08	0.09	0.83

HOMO-9	-10.248	0.06	0.13	0.81
HOMO-8	-10.055	0.18	0.72	0.09
HOMO-7	-9.882	0.54	0.25	0.20
HOMO-6	-9.675	0.02	0.91	0.07
HOMO-5	-9.633	0.18	0.57	0.25
HOMO-4	-9.613	0.12	0.85	0.03
HOMO-3	-9.452	0.31	0.39	0.29
HOMO-2	-9.314	0.12	0.50	0.38
HOMO-1	-8.831	0.22	0.41	0.37
HOMO	-8.824	0.16	0.13	0.71
LUMO	-6.727	0.68	0.12	0.19
LUMO+1	-6.456	0.23	0.72	0.05
LUMO+2	-4.000	0.49	0.12	0.39
LUMO+3	-3.898	0.10	0.06	0.84
LUMO+4	-3.890	0.01	0.02	0.96
LUMO+5	-3.752	0.33	0.54	0.12
LUMO+6	-3.203	0.15	0.80	0.05
LUMO+7	-3.111	0.04	0.94	0.02
LUMO+8	-2.866	0.04	0.94	0.02
LUMO+9	-2.797	0.04	0.94	0.02
LUMO+10	-2.485	0.04	0.95	0.02

α-spin			
			
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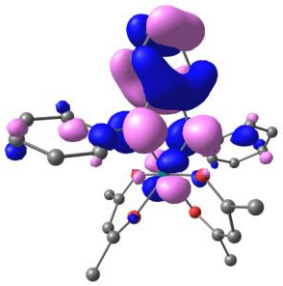
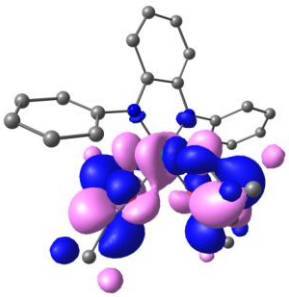
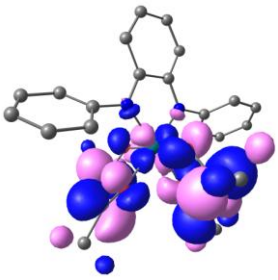
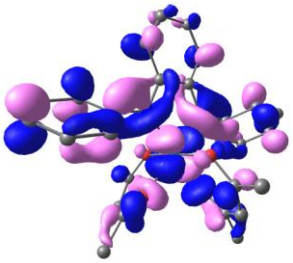
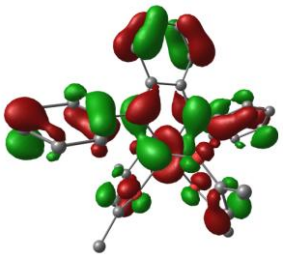
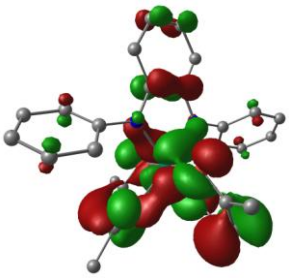
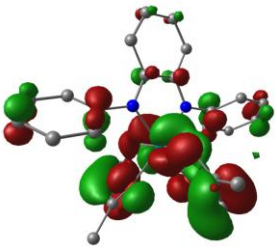
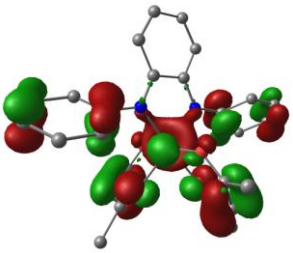
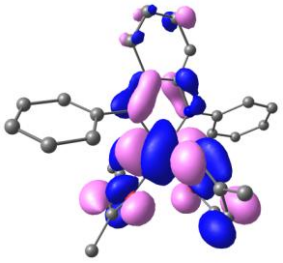
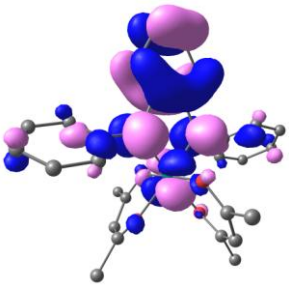
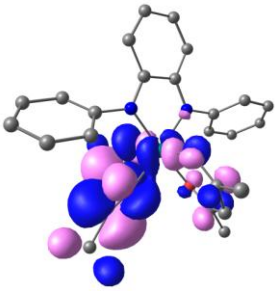
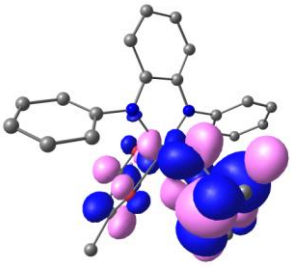
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S9. Composition and Energies of Selected Molecular Orbitals of 1^- (*S*=1/2)

MO	energy (eV)	composition		
		Ru	Q	acac
		α-spin		
HOMO-10	-3.782	0.00	0.97	0.03
HOMO-9	-3.722	0.04	0.32	0.64
HOMO-8	-3.351	0.06	0.79	0.15
HOMO-7	-3.226	0.03	0.73	0.24
HOMO-6	-3.031	0.17	0.12	0.70
HOMO-5	-2.854	0.14	0.07	0.79
HOMO-4	-2.551	0.18	0.69	0.13
HOMO-3	-2.002	0.52	0.19	0.29
HOMO-2	-1.562	0.69	0.14	0.17
HOMO-1	-1.088	0.67	0.19	0.15
SOMO	-0.242	0.22	0.73	0.05
LUMO	2.409	0.02	0.03	0.95
LUMO+1	2.438	0.06	0.07	0.87
LUMO+2	2.892	0.10	0.85	0.05
LUMO+3	3.027	0.05	0.91	0.04
LUMO+4	3.088	0.05	0.91	0.03
LUMO+5	3.106	0.07	0.87	0.06
LUMO+6	3.885	0.56	0.12	0.32
LUMO+7	3.986	0.57	0.12	0.31
LUMO+8	4.140	0.55	0.08	0.37
LUMO+9	4.166	0.16	0.71	0.12
LUMO+10	4.228	0.53	0.23	0.24
		β-spin		
HOMO-10	-3.776	0.01	0.83	0.16

HOMO-9	-3.762	0.00	0.97	0.03
HOMO-8	-3.683	0.04	0.25	0.72
HOMO-7	-3.286	0.05	0.80	0.15
HOMO-6	-3.183	0.03	0.74	0.24
HOMO-5	-2.994	0.15	0.10	0.75
HOMO-4	-2.768	0.04	0.05	0.90
HOMO-3	-2.268	0.25	0.62	0.13
HOMO-2	-1.383	0.70	0.13	0.17
HOMO-1	-1.193	0.48	0.37	0.15
HOMO	-0.840	0.62	0.26	0.12
LUMO	1.468	0.29	0.58	0.12
LUMO+1	2.452	0.06	0.08	0.86
LUMO+2	2.469	0.06	0.04	0.90
LUMO+3	2.937	0.10	0.86	0.04
LUMO+4	3.048	0.05	0.92	0.03
LUMO+5	3.139	0.07	0.89	0.05
LUMO+6	3.141	0.06	0.90	0.04
LUMO+7	3.897	0.57	0.09	0.33
LUMO+8	4.023	0.62	0.09	0.29
LUMO+9	4.245	0.53	0.22	0.25
LUMO+10	4.245	0.47	0.13	0.40

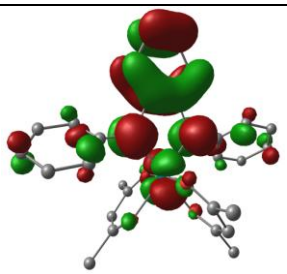
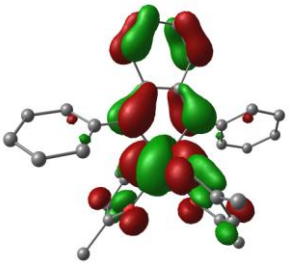
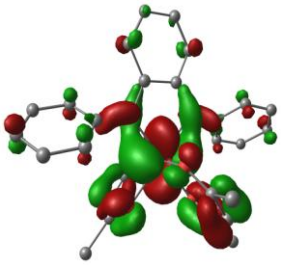
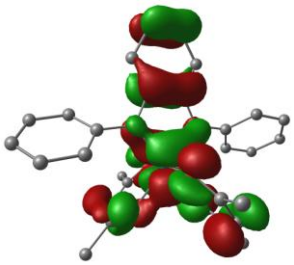
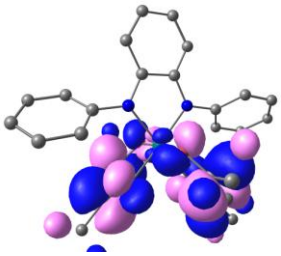
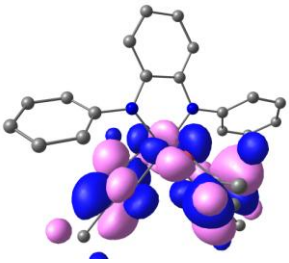
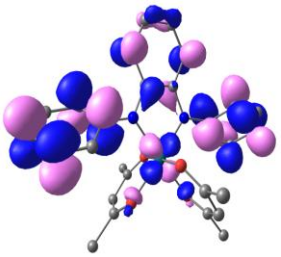
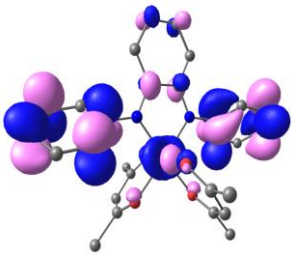
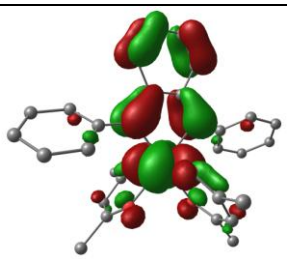
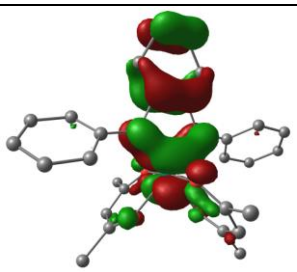
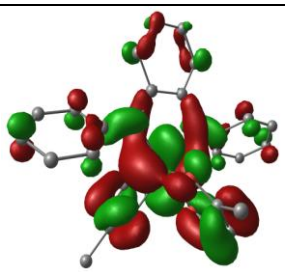
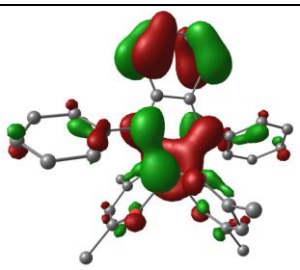
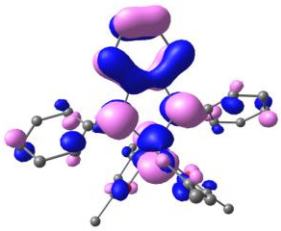
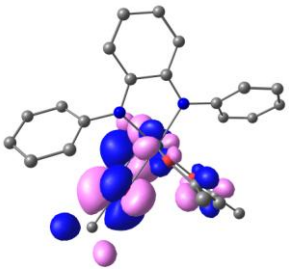
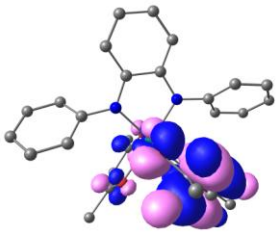
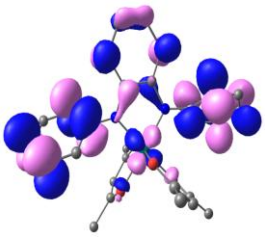
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S10. Composition and Energies of Selected Molecular Orbitals of 2^{2+} (*S*=0)

MO	energy(eV)	composition		
		Ru	Q	bpy
HOMO-10	-13.694	0.01	0.08	0.91
HOMO-9	-13.651	0.02	0.02	0.96
HOMO-8	-12.464	0.01	0.01	0.97
HOMO-7	-12.386	0.24	0.66	0.10
HOMO-6	-12.130	0.16	0.77	0.07
HOMO-5	-11.819	0.25	0.68	0.08
HOMO-4	-11.761	0.05	0.91	0.04
HOMO-3	-11.669	0.13	0.81	0.06
HOMO-2	-11.591	0.60	0.27	0.13
HOMO-1	-11.309	0.68	0.20	0.12
HOMO	-10.902	0.45	0.48	0.07
LUMO	-8.369	0.17	0.74	0.09
LUMO+1	-7.539	0.05	0.03	0.93
LUMO+2	-7.457	0.08	0.02	0.89
LUMO+3	-6.714	0.04	0.03	0.93
LUMO+4	-6.536	0.03	0.03	0.93
LUMO+5	-6.357	0.03	0.01	0.96
LUMO+6	-6.339	0.03	0.02	0.96
LUMO+7	-5.449	0.19	0.70	0.12
LUMO+8	-5.268	0.35	0.30	0.35
LUMO+9	-5.169	0.09	0.52	0.39
LUMO+10	-5.072	0.09	0.65	0.26

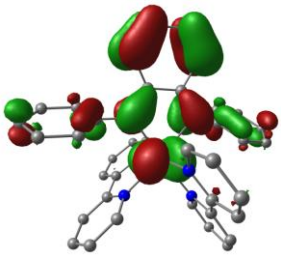
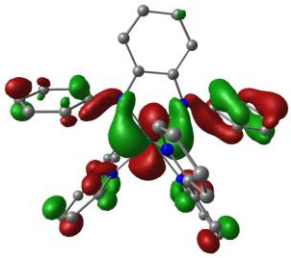
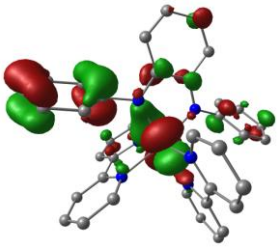
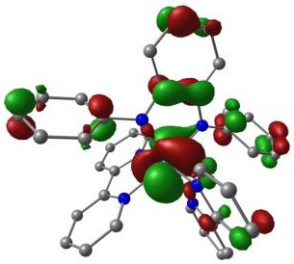
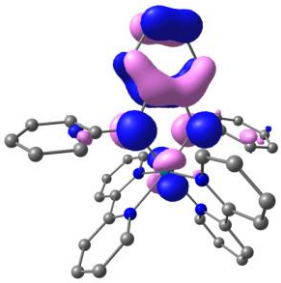
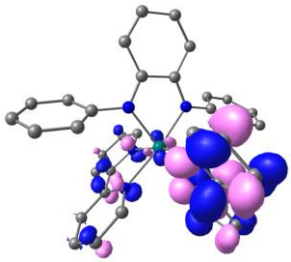
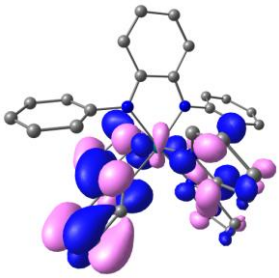
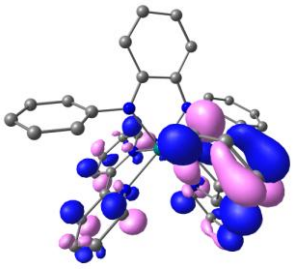
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S11. Composition and Energies of Selected Molecular Orbitals of 2^{3+} (*S*=1/2)

MO	energy (eV)	composition		
		Ru	Q	bpy
		α-spin		
HOMO-10	-16.266	0.01	0.02	0.97
HOMO-9	-15.992	0.01	0.10	0.40
HOMO-8	-15.540	0.51	0.14	0.20
HOMO-7	-15.378	0.66	0.08	0.28
HOMO-6	-15.122	0.64	0.76	0.11
HOMO-5	-15.047	0.13	0.06	0.91
HOMO-4	-14.996	0.04	0.05	0.92
HOMO-3	-14.653	0.01	0.96	0.03
HOMO-2	-14.604	0.06	0.91	0.02
HOMO-1	-14.576	0.01	0.96	0.03
SOMO	-14.254	0.04	0.92	0.04
LUMO	-12.004	0.11	0.86	0.04
LUMO+1	-10.346	0.05	0.02	0.94
LUMO+2	-10.285	0.05	0.01	0.94
LUMO+3	-9.643	0.47	0.09	0.44
LUMO+4	-9.502	0.45	0.32	0.23
LUMO+5	-9.411	0.03	0.06	0.92
LUMO+6	-9.268	0.02	0.04	0.94
LUMO+7	-9.064	0.04	0.03	0.93
LUMO+8	-9.058	0.01	0.01	0.98
LUMO+9	-8.567	0.02	0.95	0.03
LUMO+10	-8.349	0.03	0.91	0.05
		β-spin		
HOMO-10	-16.516	0.01	0.08	0.92

HOMO-9	-16.264	0.00	0.02	0.97
HOMO-8	-15.301	0.64	0.16	0.19
HOMO-7	-15.188	0.54	0.24	0.23
HOMO-6	-15.133	0.18	0.49	0.34
HOMO-5	-15.029	0.15	0.16	0.69
HOMO-4	-14.993	0.09	0.04	0.87
HOMO-3	-14.638	0.01	0.96	0.03
HOMO-2	-14.572	0.02	0.95	0.03
HOMO-1	-14.525	0.09	0.88	0.03
HOMO	-14.311	0.23	0.70	0.07
LUMO	-12.870	0.62	0.31	0.08
LUMO+1	-11.818	0.13	0.82	0.04
LUMO+2	-10.325	0.04	0.02	0.94
LUMO+3	-10.268	0.06	0.01	0.93
LUMO+4	-9.426	0.46	0.09	0.46
LUMO+5	-9.399	0.03	0.06	0.91
LUMO+6	-9.254	0.37	0.30	0.33
LUMO+7	-9.235	0.14	0.11	0.76
LUMO+8	-9.055	0.01	0.01	0.98
LUMO+9	-9.049	0.07	0.04	0.89
LUMO+10	-8.480	0.03	0.94	0.04

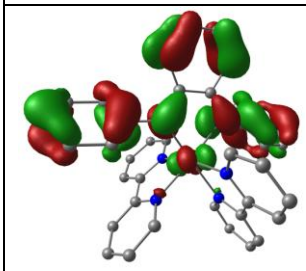
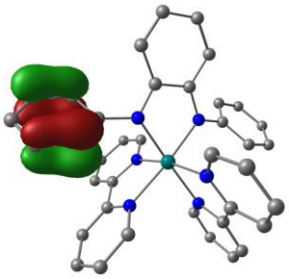
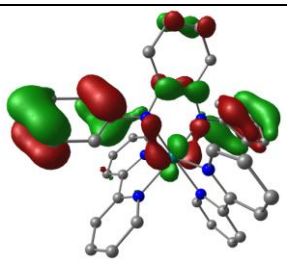
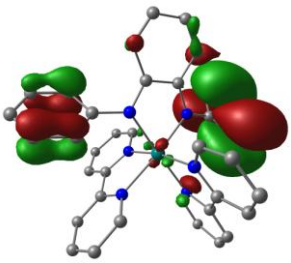
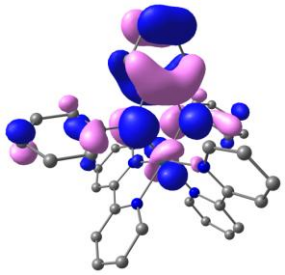
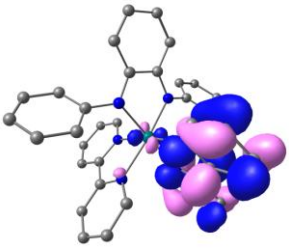
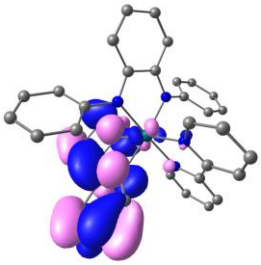
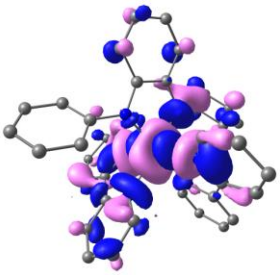
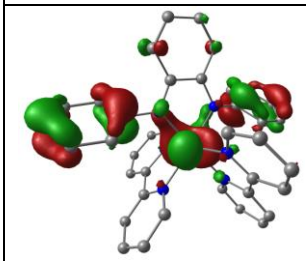
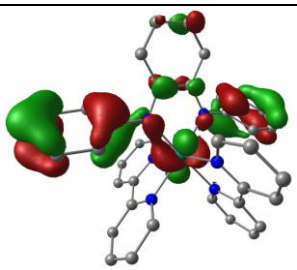
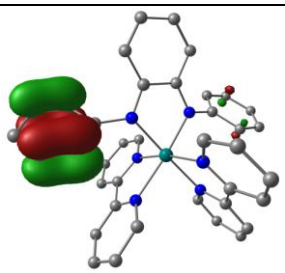
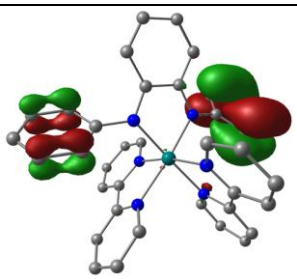
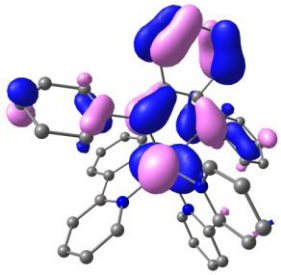
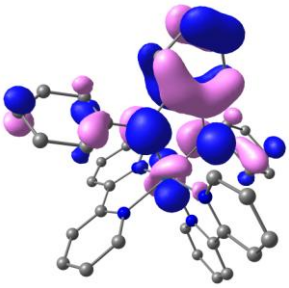
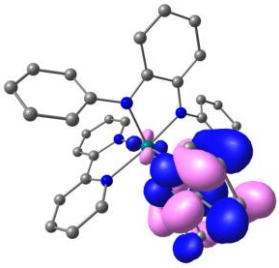
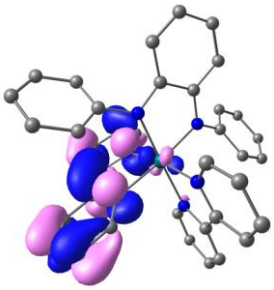
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S12. Composition and Energies of Selected Molecular Orbitals of 2^+ (*S*=1/2)

MO	energy (eV)	composition		
		Ru	Q	bpy
		α-spin		
HOMO-10	-9.648	0.01	0.01	0.98
HOMO-9	-9.611	0.00	0.01	0.99
HOMO-8	-8.919	0.02	0.94	0.03
HOMO-7	-8.882	0.01	0.97	0.02
HOMO-6	-8.675	0.13	0.83	0.04
HOMO-5	-8.645	0.06	0.89	0.05
HOMO-4	-8.333	0.52	0.37	0.10
HOMO-3	-8.284	0.70	0.19	0.11
HOMO-2	-7.971	0.75	0.13	0.12
HOMO-1	-7.456	0.42	0.52	0.06
SOMO	-6.044	0.14	0.80	0.06
LUMO	-4.779	0.04	0.02	0.94
LUMO+1	-4.668	0.08	0.01	0.90
LUMO+2	-3.940	0.04	0.04	0.92
LUMO+3	-3.728	0.06	0.03	0.92
LUMO+4	-3.647	0.03	0.03	0.94
LUMO+5	-3.609	0.01	0.01	0.98
LUMO+6	-2.511	0.26	0.54	0.21
LUMO+7	-2.408	0.30	0.21	0.48
LUMO+8	-2.367	0.07	0.10	0.83
LUMO+9	-2.294	0.04	0.14	0.82
LUMO+10	-2.199	0.08	0.79	0.13
		β-spin		
HOMO-10	-9.985	0.09	0.82	0.09

HOMO-9	-9.645	0.01	0.01	0.98
HOMO-8	-9.609	0.00	0.01	0.99
HOMO-7	-8.888	0.02	0.95	0.03
HOMO-6	-8.856	0.01	0.97	0.03
HOMO-5	-8.622	0.14	0.82	0.04
HOMO-4	-8.575	0.05	0.91	0.05
HOMO-3	-8.243	0.61	0.27	0.12
HOMO-2	-7.944	0.77	0.11	0.12
HOMO-1	-7.902	0.71	0.18	0.11
HOMO	-7.111	0.28	0.67	0.05
LUMO	-4.789	0.02	0.04	0.94
LUMO+1	-4.657	0.09	0.01	0.90
LUMO+2	-4.328	0.13	0.78	0.09
LUMO+3	-3.934	0.04	0.04	0.92
LUMO+4	-3.726	0.06	0.03	0.92
LUMO+5	-3.643	0.03	0.03	0.94
LUMO+6	-3.603	0.01	0.01	0.98
LUMO+7	-2.471	0.24	0.53	0.23
LUMO+8	-2.380	0.17	0.14	0.69
LUMO+9	-2.352	0.18	0.16	0.65
LUMO+10	-2.282	0.08	0.14	0.77

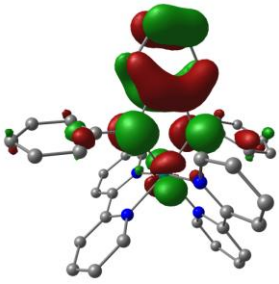
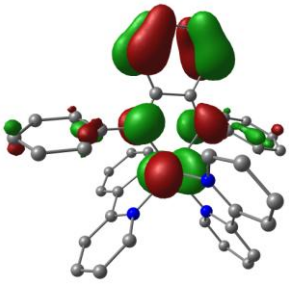
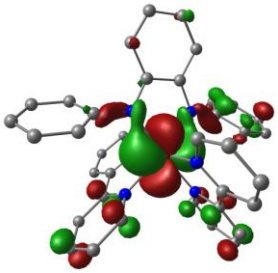
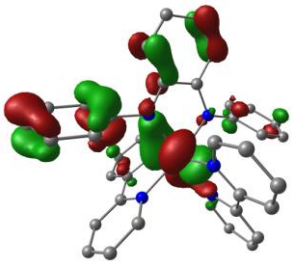
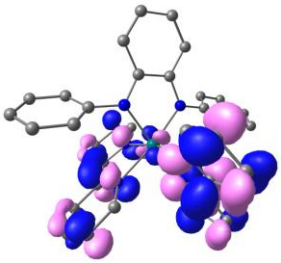
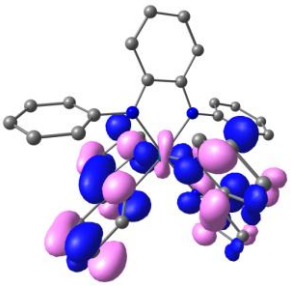
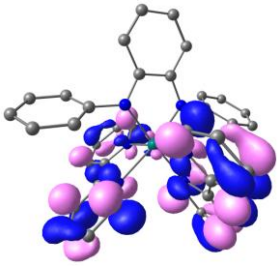
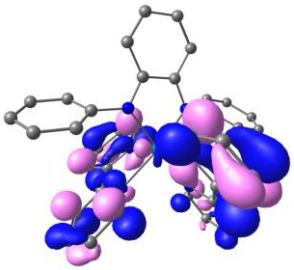
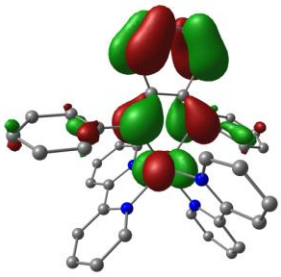
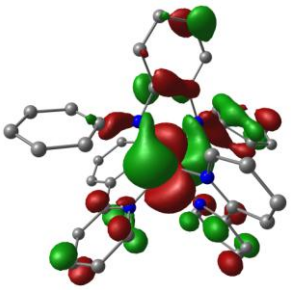
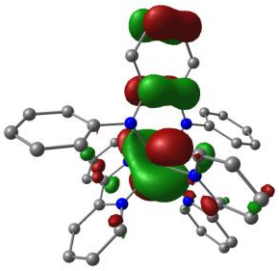
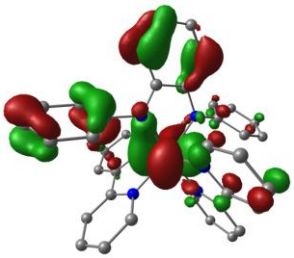
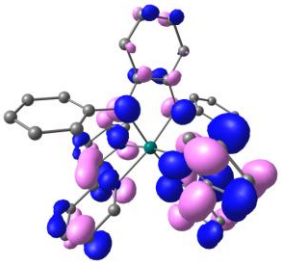
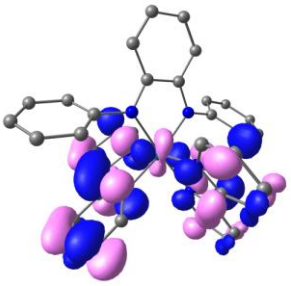
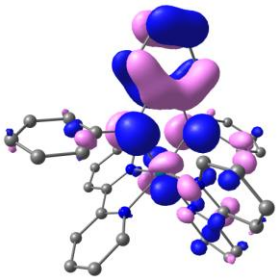
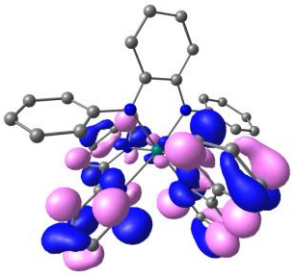
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S13. Composition and Energies of Selected Molecular Orbitals of 2 (*S*=0)

MO	energy(eV)	composition		
		Ru	Q	bpy
HOMO-10	-6.794	0.00	0.04	0.96
HOMO-9	-6.733	0.00	0.02	0.98
HOMO-8	-6.172	0.01	0.97	0.02
HOMO07	-6.136	0.00	0.97	0.03
HOMO-6	-5.773	0.12	0.83	0.04
HOMO-5	-5.672	0.05	0.90	0.06
HOMO-4	-5.249	0.62	0.24	0.13
HOMO-3	-5.115	0.71	0.16	0.12
HOMO-2	-4.969	0.77	0.11	0.12
HOMO-1	-4.111	0.27	0.68	0.05
HOMO	-2.663	0.07	0.66	0.26
LUMO	-1.888	0.09	0.14	0.77
LUMO+1	-1.805	0.10	0.04	0.87
LUMO+2	-1.097	0.04	0.04	0.92
LUMO+3	-0.867	0.08	0.02	0.90
LUMO+4	-0.796	0.03	0.02	0.96
LUMO+5	-0.742	0.02	0.02	0.96
LUMO+6	0.327	0.23	0.56	0.22
LUMO+7	0.472	0.05	0.17	0.78
LUMO+8	0.514	0.21	0.27	0.52
LUMO+9	0.561	0.04	0.60	0.36
LUMO+10	0.588	0.12	0.49	0.39

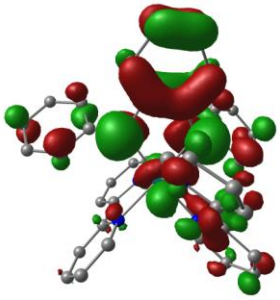
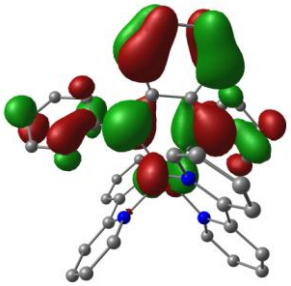
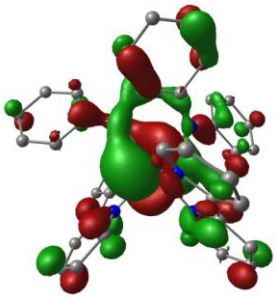
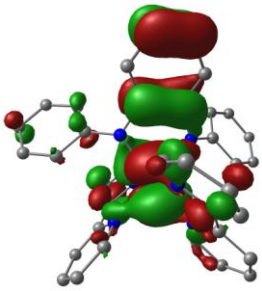
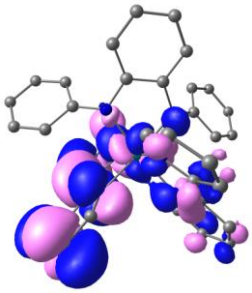
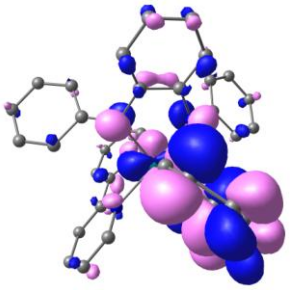
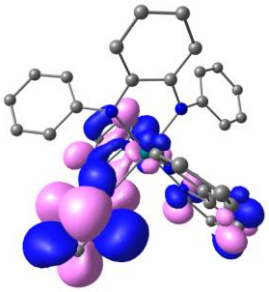
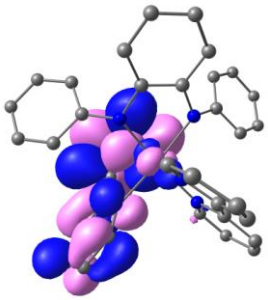
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S14. Composition and Energies of Selected Molecular Orbitals of 2 (*S*=1)

MO	energy (eV)	composition		
		Ru	Q	bpy
		α-spin		
HOMO-10	-6.464	0.01	0.65	0.34
HOMO-9	-6.451	0.01	0.45	0.55
HOMO-8	-6.437	0.01	0.70	0.29
HOMO-7	-6.167	0.05	0.90	0.05
HOMO-6	-6.143	0.04	0.90	0.06
HOMO-5	-5.591	0.35	0.57	0.09
HOMO-4	-5.498	0.65	0.24	0.11
HOMO-3	-5.004	0.78	0.08	0.14
HOMO-2	-4.633	0.61	0.30	0.08
SOMO 2	-3.654	0.18	0.77	0.05
SOMO 1	-2.445	0.04	0.02	0.95
LUMO	-1.771	0.09	0.02	0.89
LUMO+1	-0.764	0.05	0.05	0.90
LUMO+2	-0.569	0.06	0.04	0.90
LUMO+3	-0.494	0.03	0.02	0.96
LUMO+4	-0.453	0.03	0.02	0.95
LUMO+5	0.103	0.17	0.70	0.13
LUMO+6	0.203	0.05	0.90	0.05
LUMO+7	0.301	0.07	0.82	0.11
LUMO+8	0.350	0.14	0.74	0.12
LUMO+9	0.730	0.01	0.09	0.90
LUMO+10	0.768	0.06	0.12	0.82
		β-spin		
HOMO-10	-7.261	0.02	0.73	0.25

HOMO-9	-6.430	0.00	0.95	0.04
HOMO-8	-6.418	0.00	0.96	0.03
HOMO-7	-6.326	0.01	0.02	0.96
HOMO-6	-6.261	0.01	0.05	0.94
HOMO-5	-6.095	0.05	0.87	0.07
HOMO-4	-6.059	0.03	0.89	0.07
HOMO-3	-5.366	0.48	0.40	0.12
HOMO-2	-4.925	0.79	0.08	0.13
HOMO-1	-4.915	0.69	0.19	0.11
HOMO	-1.954	0.44	0.50	0.06
LUMO	-1.329	0.16	0.75	0.09
LUMO+1	-1.233	0.06	0.03	0.91
LUMO+2	-0.709	0.07	0.02	0.90
LUMO+3	-0.512	0.06	0.05	0.89
LUMO+4	-0.380	0.07	0.04	0.89
LUMO+5	-0.323	0.03	0.03	0.95
LUMO+6	0.152	0.02	0.03	0.96
LUMO+7	0.256	0.17	0.71	0.12
LUMO+8	0.333	0.04	0.91	0.05
LUMO+9	0.397	0.06	0.84	0.10
LUMO+10	0.989	0.15	0.73	0.12

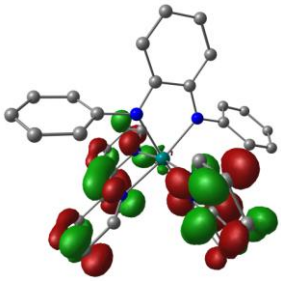
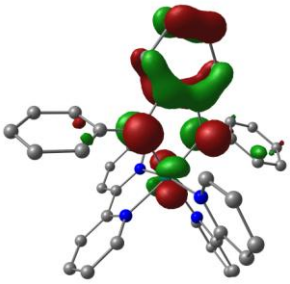
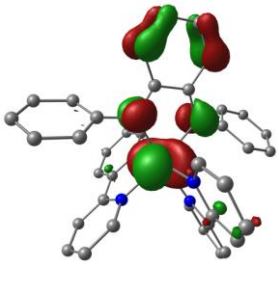
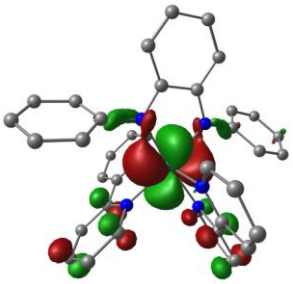
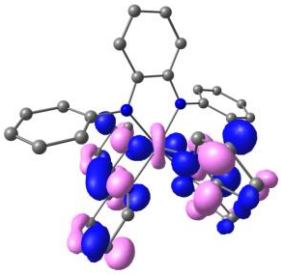
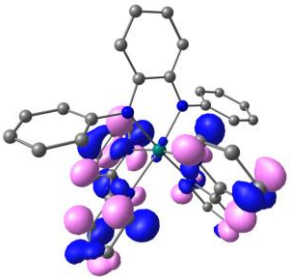
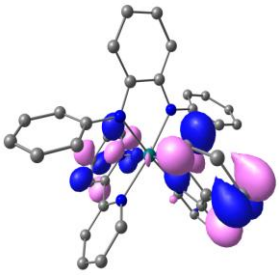
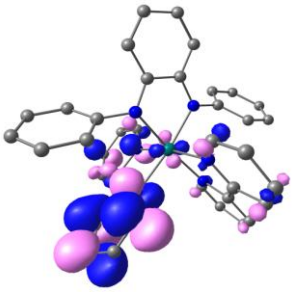
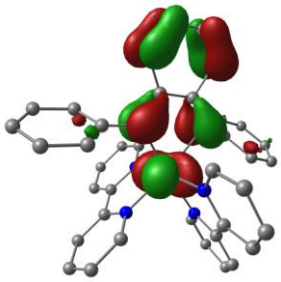
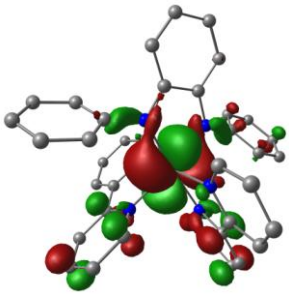
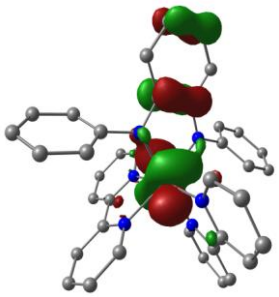
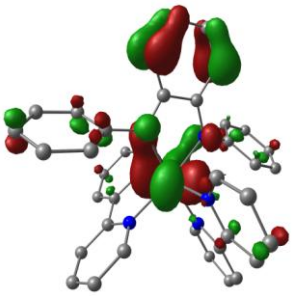
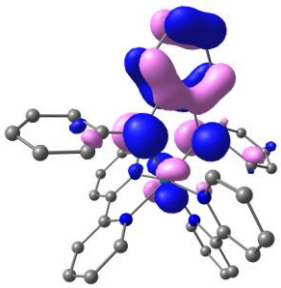
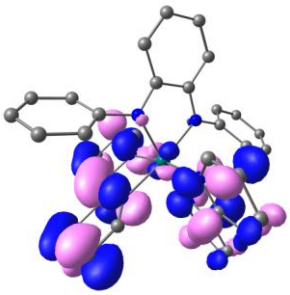
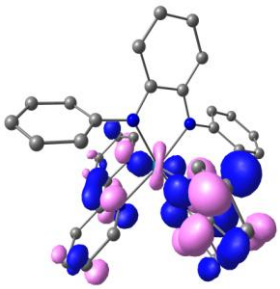
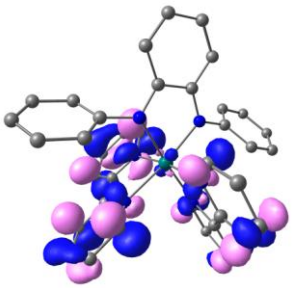
α-spin			
			
SOMO	SOMO 1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S15. Composition and Energies of Selected Molecular Orbitals of 3^+ (*S*=1/2)

MO	energy (eV)	composition		
		Ru	Q	pap
		α-spin		
HOMO-10	-9.456	0.13	0.07	0.80
HOMO-9	-9.366	0.01	0.03	0.96
HOMO-8	-9.212	0.46	0.26	0.27
HOMO-7	-9.166	0.09	0.80	0.12
HOMO-6	-9.143	0.06	0.90	0.04
HOMO-5	-9.018	0.60	0.28	0.12
HOMO-4	-8.957	0.25	0.60	0.15
HOMO-3	-8.803	0.11	0.74	0.15
HOMO-2	-8.699	0.47	0.38	0.15
HOMO-1	-7.994	0.32	0.61	0.07
SOMO	-6.679	0.10	0.71	0.19
LUMO	-5.710	0.10	0.11	0.79
LUMO+1	-5.437	0.22	0.03	0.76
LUMO+2	-3.929	0.03	0.02	0.95
LUMO+3	-3.861	0.05	0.02	0.93
LUMO+4	-2.970	0.22	0.30	0.48
LUMO+5	-2.915	0.03	0.02	0.95
LUMO+6	-2.795	0.03	0.01	0.95
LUMO+7	-2.748	0.08	0.16	0.76
LUMO+8	-2.637	0.04	0.07	0.90
LUMO+9	-2.580	0.27	0.20	0.53
LUMO+10	-2.433	0.03	0.71	0.26
		β-spin		
HOMO-10	-9.529	0.00	0.01	0.99
HOMO-9	-9.445	0.13	0.08	0.78

HOMO-8	-9.355	0.01	0.03	0.96
HOMO-7	-9.210	0.48	0.21	0.31
HOMO-6	-9.142	0.05	0.87	0.08
HOMO-5	-9.122	0.01	0.96	0.03
HOMO-4	-8.901	0.41	0.48	0.11
HOMO-3	-8.888	0.31	0.53	0.16
HOMO-2	-8.680	0.51	0.35	0.14
HOMO-1	-8.675	0.38	0.47	0.15
HOMO	-7.632	0.21	0.73	0.05
LUMO	-5.641	0.04	0.05	0.92
LUMO+1	-5.352	0.20	0.03	0.77
LUMO+2	-5.003	0.13	0.79	0.08
LUMO+3	-3.906	0.03	0.02	0.95
LUMO+4	-3.837	0.05	0.02	0.93
LUMO+5	-2.951	0.21	0.29	0.50
LUMO+6	-2.891	0.03	0.02	0.95
LUMO+7	-2.792	0.05	0.01	0.96
LUMO+8	-2.720	0.21	0.14	0.78
LUMO+9	-2.615	0.03	0.11	0.84
LUMO+10	-2.557	0.03	0.21	0.52

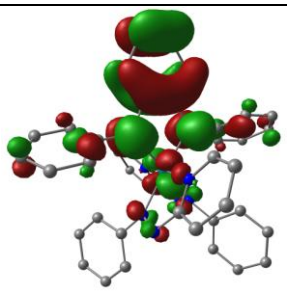
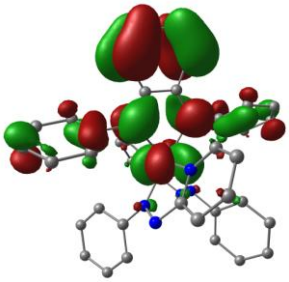
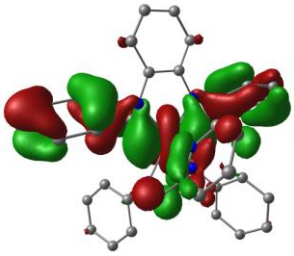
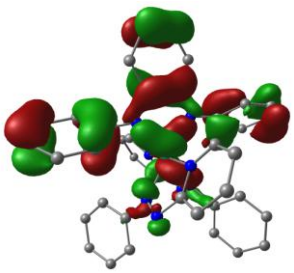
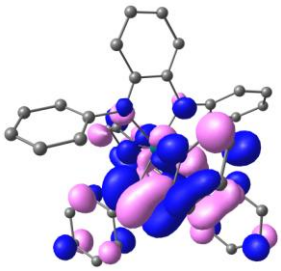
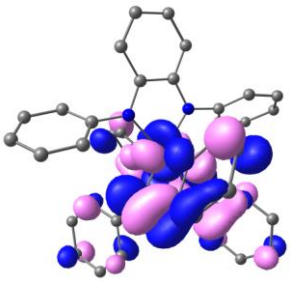
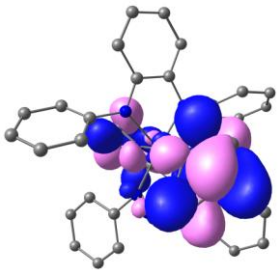
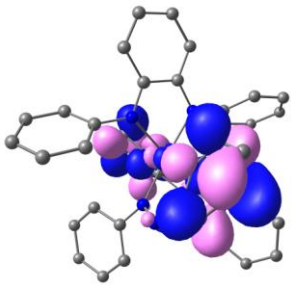
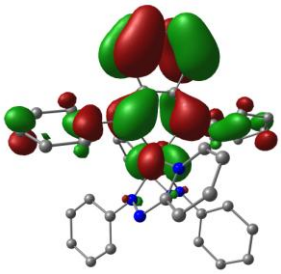
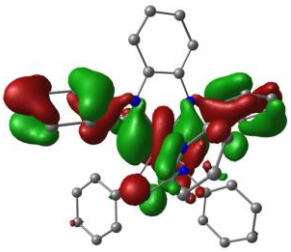
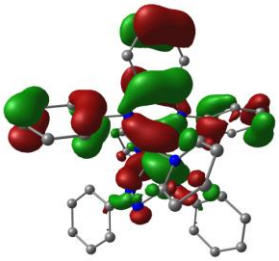
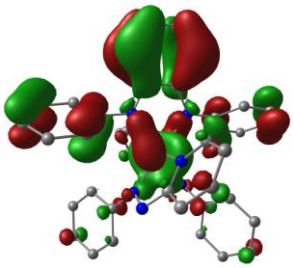
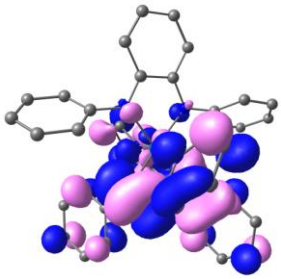
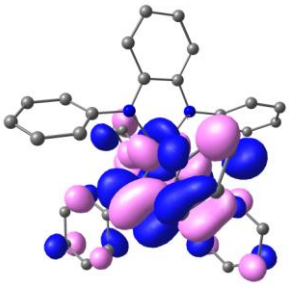
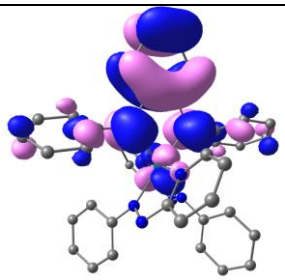
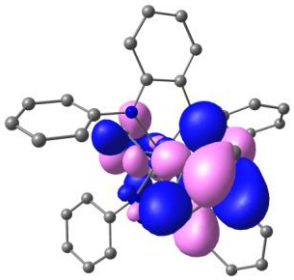
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S16. Composition and Energies of Selected Molecular Orbitals of 3^{2+} (*S*=0)

MO	energy(eV)	composition		
		Ru	Q	pap
HOMO-10	-12.182	0.60	0.15	0.25
HOMO-9	-12.063	0.64	0.23	0.13
HOMO-8	-11.954	0.05	0.45	0.50
HOMO-7	-11.952	0.10	0.78	0.12
HOMO-6	-11.926	0.08	0.33	0.59
HOMO-5	-11.890	0.01	0.22	0.77
HOMO-4	-11.855	0.17	0.37	0.46
HOMO-3	-11.837	0.02	0.43	0.56
HOMO-2	-11.729	0.05	0.35	0.60
HOMO-1	-11.561	0.43	0.20	0.36
HOMO	-11.075	0.27	0.65	0.08
LUMO	-8.964	0.13	0.80	0.08
LUMO+1	-8.394	0.07	0.04	0.89
LUMO+2	-8.307	0.14	0.02	0.84
LUMO+3	-6.576	0.02	0.02	0.96
LUMO+4	-6.520	0.04	0.02	0.94
LUMO+5	-6.186	0.38	0.40	0.22
LUMO+6	-5.931	0.44	0.15	0.40
LUMO+7	-5.545	0.06	0.79	0.14
LUMO+8	-5.472	0.02	0.14	0.84
LUMO+9	-5.447	0.06	0.18	0.76
LUMO+10	-5.383	0.07	0.71	0.22

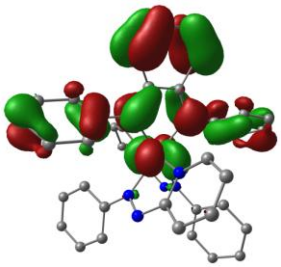
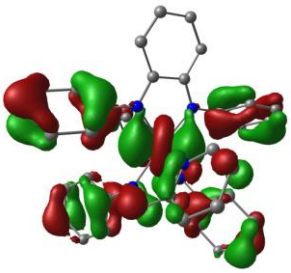
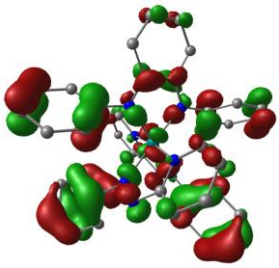
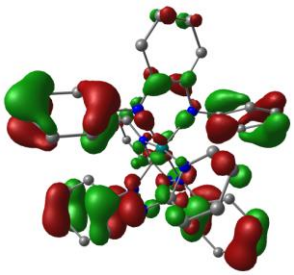
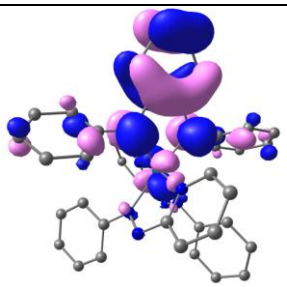
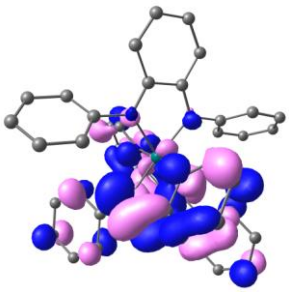
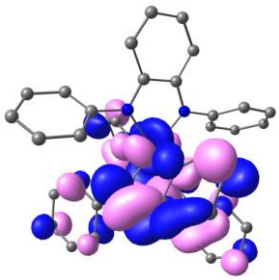
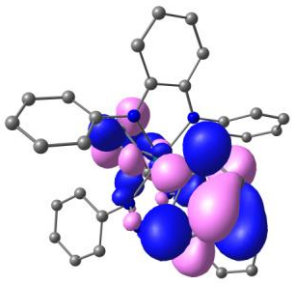
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S17. Composition and Energies of Selected Molecular Orbitals of 3 (*S*=1)

MO	energy (eV)	composition		
		Ru	Q	pap
		α-spin		
HOMO-10	-6.594	0.01	0.09	0.90
HOMO-9	-6.528	0.08	0.69	0.23
HOMO-8	-6.361	0.05	0.24	0.71
HOMO-7	-6.335	0.03	0.28	0.69
HOMO-6	-6.256	0.21	0.38	0.41
HOMO-5	-6.039	0.35	0.48	0.17
HOMO-4	-5.928	0.56	0.25	0.20
HOMO-3	-5.524	0.63	0.16	0.21
HOMO-2	-5.065	0.54	0.34	0.12
SOMO 2	-4.021	0.14	0.78	0.08
SOMO 1	-3.502	0.07	0.04	0.89
LUMO	-2.528	0.23	0.03	0.75
LUMO+1	-0.865	0.03	0.02	0.94
LUMO+2	-0.786	0.06	0.02	0.92
LUMO+3	-0.276	0.23	0.60	0.17
LUMO+4	-0.011	0.17	0.60	0.22
LUMO+5	0.054	0.07	0.77	0.16
LUMO+6	0.084	0.04	0.67	0.29
LUMO+7	0.096	0.01	0.07	0.92
LUMO+8	0.163	0.02	0.21	0.77
LUMO+9	0.205	0.01	0.31	0.67
LUMO+10	0.270	0.02	0.04	0.94
		β-spin		
HOMO-10	-6.641	0.00	0.95	0.05
HOMO-9	-6.558	0.04	0.19	0.77

HOMO-8	-6.544	0.01	0.07	0.92
HOMO-7	-6.484	0.13	0.66	0.21
HOMO-6	-6.237	0.09	0.21	0.70
HOMO-5	-6.210	0.04	0.44	0.52
HOMO-4	-6.111	0.07	0.28	0.65
HOMO-3	-5.971	0.55	0.25	0.20
HOMO-2	-5.500	0.67	0.18	0.15
HOMO-1	-5.469	0.64	0.17	0.19
HOMO	-4.762	0.35	0.58	0.07
LUMO	-2.343	0.10	0.73	0.17
LUMO+1	-2.047	0.10	0.10	0.79
LUMO+2	-1.983	0.13	0.02	0.85
LUMO+3	-0.762	0.03	0.03	0.94
LUMO+4	-0.703	0.05	0.02	0.93
LUMO+5	-0.208	0.22	0.61	0.17
LUMO+6	0.036	0.18	0.81	0.20
LUMO+7	0.107	0.07	0.65	0.12
LUMO+8	0.111	0.05	0.19	0.30
LUMO+9	0.166	0.00	0.16	0.80
LUMO+10	0.292	0.03	0.19	0.81

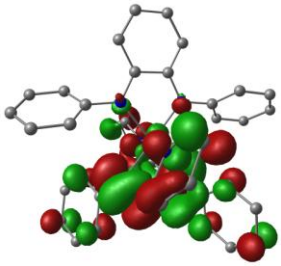
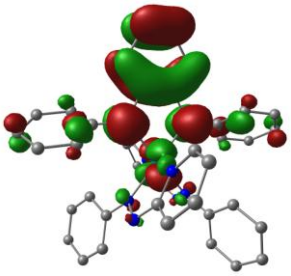
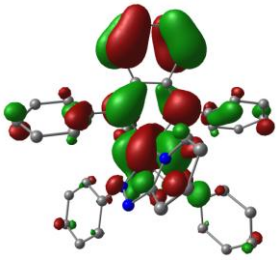
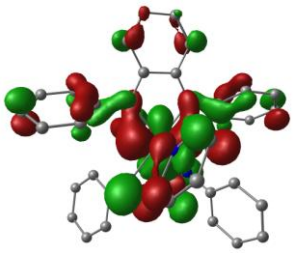
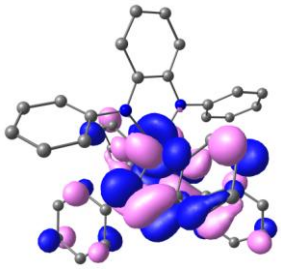
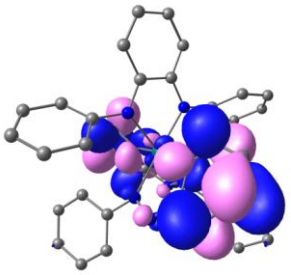
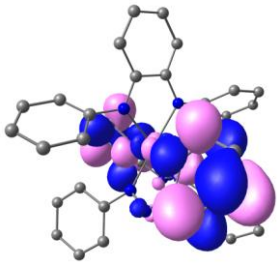
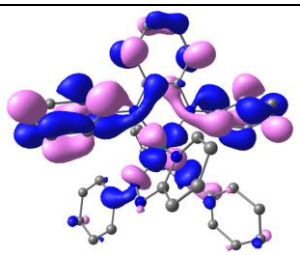
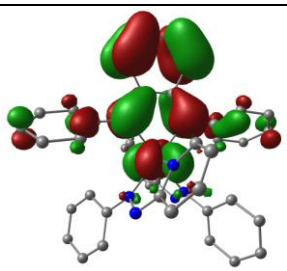
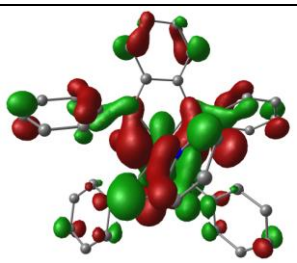
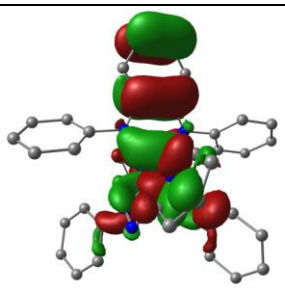
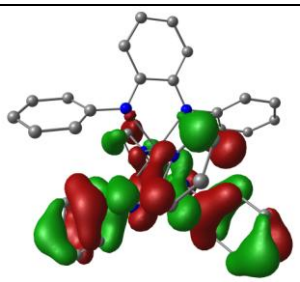
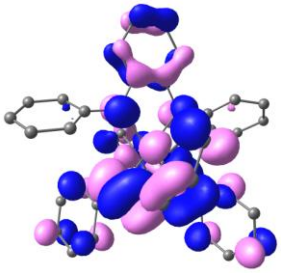
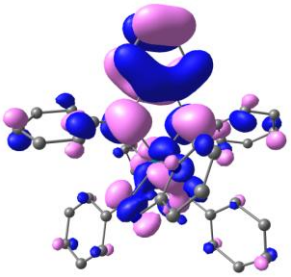
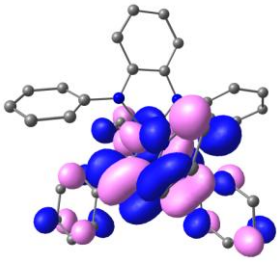
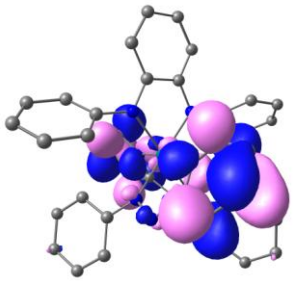
α-spin			
			
SOMO 1	SOMO 2	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S18. Composition and Energies of Selected Molecular Orbitals of 3^- (*S*=3/2)

MO	energy (eV)	composition		
		Ru	Q	pap
		α-spin		
HOMO-10	-3.673	0.13	0.07	0.80
HOMO-9	-3.462	0.07	0.06	0.87
HOMO-8	-3.432	0.09	0.37	0.54
HOMO-7	-3.266	0.01	0.04	0.95
HOMO-6	-3.264	0.28	0.51	0.21
HOMO-5	-2.967	0.66	0.19	0.15
HOMO-4	-2.640	0.45	0.32	0.24
HOMO-3	-2.072	0.72	0.15	0.13
SOMO 3	-1.194	0.17	0.77	0.77
SOMO 2	-0.894	0.06	0.03	0.91
SOMO 1	-0.535	0.21	0.02	0.77
LUMO	2.173	0.05	0.05	0.91
LUMO+1	2.277	0.06	0.05	0.90
LUMO+2	2.421	0.11	0.83	0.06
LUMO+3	2.582	0.06	0.88	0.05
LUMO+4	2.639	0.06	0.84	0.11
LUMO+5	2.657	0.04	0.90	0.07
LUMO+6	2.944	0.04	0.01	0.95
LUMO+7	3.049	0.01	0.02	0.96
LUMO+8	3.085	0.06	0.15	0.79
LUMO+9	3.119	0.03	0.03	0.95
LUMO+10	3.451	0.12	0.75	0.13
		β-spin		
HOMO-10	-3.876	0.03	0.67	0.30

HOMO-9	-3.750	0.01	0.23	0.76
HOMO-8	-3.730	0.01	0.08	0.91
HOMO-7	-3.467	0.08	0.09	0.83
HOMO-6	-3.259	0.05	0.38	0.57
HOMO-5	-3.204	0.13	0.05	0.82
HOMO-4	-2.906	0.01	0.01	0.98
HOMO-3	-2.803	0.27	0.60	0.13
HOMO-2	-2.175	0.65	0.23	0.12
HOMO-1	-2.029	0.63	0.10	0.27
HOMO	-1.726	0.57	0.30	0.13
LUMO	0.499	0.20	0.71	0.09
LUMO+1	0.960	0.08	0.04	0.88
LUMO+2	1.385	0.19	0.03	0.78
LUMO+3	2.308	0.05	0.06	0.88
LUMO+4	2.397	0.06	0.09	0.85
LUMO+5	2.496	0.09	0.85	0.05
LUMO+6	2.630	0.06	0.86	0.08
LUMO+7	2.705	0.04	0.89	0.08
LUMO+8	2.713	0.05	0.84	0.11
LUMO+9	3.048	0.04	0.02	0.95
LUMO+10	3.130	0.02	0.02	0.96

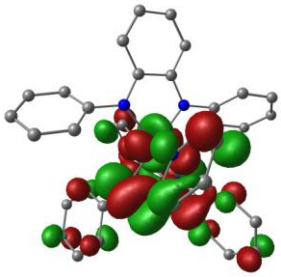
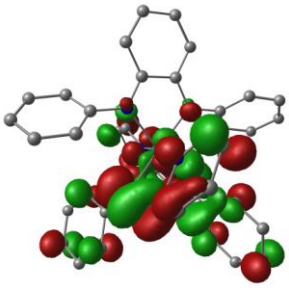
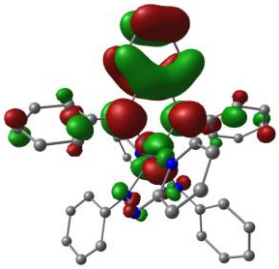
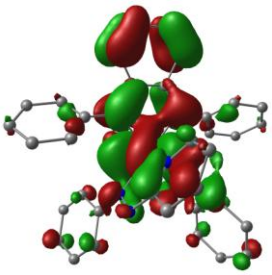
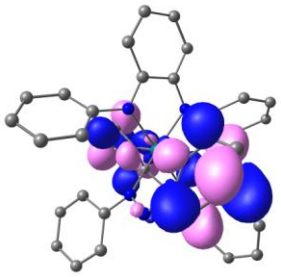
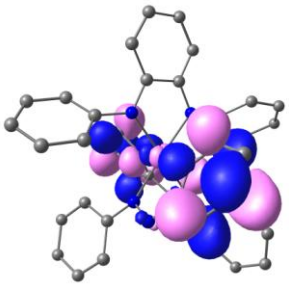
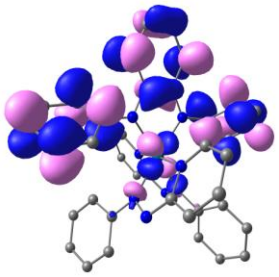
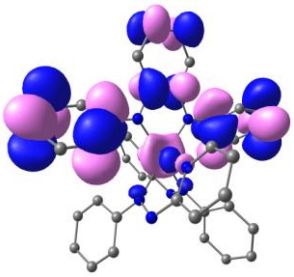
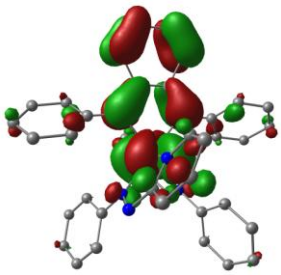
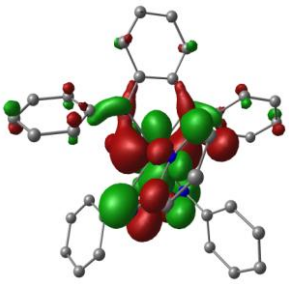
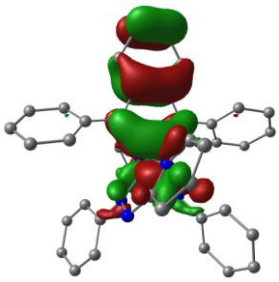
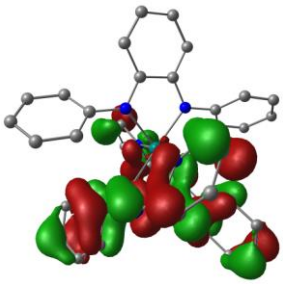
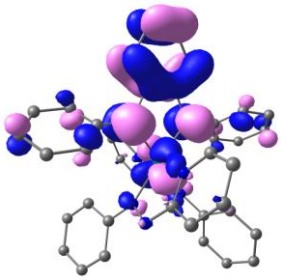
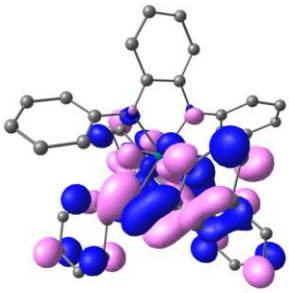
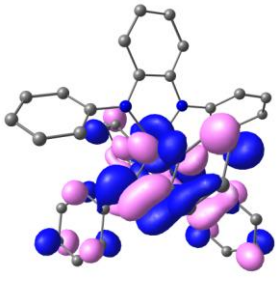
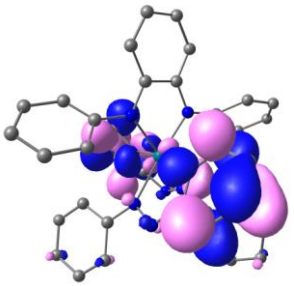
α-spin			
			
SOMO 1	SOMO 2	SOMO 3	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S19. Energies of DFT Optimized 2^n (n = 0) and 3^n (n = 2+, 0, 1–)

complex	*E* (Hartrees)				$\Delta E_{(HE-LE)}$[a]
	S = 0	*S* = 1/2	*S* = 1	*S* = 3/2	
2	-1888.5547728		-1888.5520952		0.0026776 Hartrees 587.6652693cm^{-1} 7.030039336 kJ/mol
3^{2+}	-2074.9561984		-2074.929554		0.0266444 Hartrees 5847.769832 cm^{-1} 69.95487753 kJ/mol
3	-2075.4036244		-2075.4150574		0.011433 Hartrees 2509.25344 cm^{-1} 30.0173438 kJ/mol
3^{-}		-2075.4709879		-2075.4780221	0.0070342 Hartrees 1543.828442 cm^{-1} 18.46829351 kJ/mol

[a]HE = Spin state in higher in energy and LE = Spin state in lower in energy.

Table S20. DFT Optimized Coordinates of 1 (*S*=0)

sym	x	y	z
Ru	4.084292000	10.165076000	0.004532000
O	5.716039000	11.433835000	0.054937000
O	4.227796000	10.067360000	-2.085740000
O	2.573725000	8.768228000	-0.205539000
O	5.502883000	8.619583000	0.030658000
N	3.863736000	10.349623000	2.004207000
N	2.722993000	11.654725000	0.106928000
C	4.566000000	9.538861000	2.938492000
C	3.878938000	8.709232000	3.837683000
H	2.793127000	8.698932000	3.830760000
C	4.592000000	7.890026000	4.713441000
H	4.052946000	7.244087000	5.401467000
C	5.988454000	7.894864000	4.703289000
C	6.670606000	8.717425000	3.802112000
C	5.968251000	9.530141000	2.913168000
H	6.541248000	7.258427000	5.388919000
H	7.757404000	8.724803000	3.787434000
H	6.479287000	10.161564000	2.195149000
C	3.016561000	11.304582000	2.415448000
C	2.753381000	11.684995000	3.769933000
H	3.299106000	11.199727000	4.570446000
C	1.822849000	12.654214000	4.040507000
H	1.626722000	12.939971000	5.070196000
C	1.099187000	13.293348000	2.988829000
H	0.342885000	14.032640000	3.237480000
C	1.348878000	12.992368000	1.675139000
H	0.799785000	13.481020000	0.879082000
C	2.344572000	12.020026000	1.340977000
C	2.178657000	12.285354000	-1.045949000
C	2.342823000	13.661468000	-1.266194000
H	2.880876000	14.258071000	-0.535647000
C	1.836600000	14.246727000	-2.427093000
H	1.974643000	15.311767000	-2.593888000
C	1.162003000	13.469684000	-3.371211000
H	0.765655000	13.928514000	-4.272927000
C	1.006169000	12.097737000	-3.153182000

H	0.483998000	11.486565000	-3.884787000
C	1.519853000	11.499860000	-2.003176000
H	1.423440000	10.434767000	-1.825049000
C	7.523113000	12.761466000	-0.639357000
H	7.185867000	13.590656000	-0.007390000
H	8.008552000	13.163902000	-1.531965000
H	8.260552000	12.193599000	-0.059875000
C	6.347355000	11.864335000	-0.973756000
C	6.063584000	11.583001000	-2.316270000
H	6.700257000	12.050161000	-3.058442000
C	5.054023000	10.720423000	-2.795005000
C	4.903462000	10.524072000	-4.291235000
H	4.925108000	9.453672000	-4.523509000
H	5.682984000	11.033597000	-4.863410000
H	3.924465000	10.905095000	-4.604825000
C	6.444593000	6.466337000	0.087992000
H	7.178235000	6.746701000	-0.675798000
H	6.186136000	5.410899000	-0.029757000
H	6.921038000	6.610247000	1.064879000
C	5.237280000	7.378679000	-0.010884000
C	3.953709000	6.804826000	-0.134149000
H	3.902766000	5.723032000	-0.173115000
C	2.741678000	7.498546000	-0.241887000
C	1.456688000	6.716233000	-0.431686000
H	0.741087000	6.987577000	0.352660000
H	1.618633000	5.635626000	-0.411891000
H	1.002467000	6.990119000	-1.391151000

Table S21. DFT Optimized Coordinates of 1^+ (*S*=1/2)

sym	x	y	z
Ru	4.047829000	10.209099000	0.048680000
O	5.564228000	11.555823000	0.044678000
O	4.159806000	10.109233000	-2.001052000
O	2.585365000	8.805918000	-0.021017000
O	5.456013000	8.712308000	0.085918000
N	3.865333000	10.431739000	2.072799000
N	2.627696000	11.675773000	0.156474000
C	4.585702000	9.633066000	3.008283000
C	3.898474000	8.828442000	3.931406000
H	2.812697000	8.820647000	3.937154000
C	4.618790000	8.019423000	4.809091000
H	4.086489000	7.389091000	5.515169000
C	6.015517000	8.017519000	4.778655000
C	6.694020000	8.817530000	3.854527000
C	5.986478000	9.614112000	2.956382000
H	6.572921000	7.391624000	5.468988000
H	7.779781000	8.820322000	3.830835000
H	6.498650000	10.233988000	2.229993000
C	2.998953000	11.357548000	2.468254000
C	2.754000000	11.760230000	3.826591000
H	3.336808000	11.315019000	4.623029000
C	1.803215000	12.702373000	4.088423000
H	1.620834000	13.013117000	5.112571000
C	1.023786000	13.293946000	3.034473000
H	0.244316000	14.003574000	3.294355000
C	1.249833000	12.986959000	1.724897000
H	0.662540000	13.435949000	0.933966000
C	2.277633000	12.040693000	1.384832000
C	2.066114000	12.297151000	-0.996976000
C	2.199639000	13.680982000	-1.194588000
H	2.728288000	14.282374000	-0.461167000
C	1.681101000	14.264344000	-2.349825000
H	1.794297000	15.332847000	-2.506942000
C	1.022613000	13.479453000	-3.299610000
H	0.613454000	13.938737000	-4.194393000
C	0.896959000	12.101560000	-3.099519000

H	0.383096000	11.489612000	-3.834991000
C	1.430360000	11.501666000	-1.960571000
H	1.346565000	10.433927000	-1.795581000
C	7.589042000	12.582732000	-0.574625000
H	7.239678000	13.567469000	-0.244431000
H	8.271076000	12.709573000	-1.417591000
H	8.135157000	12.136687000	0.264322000
C	6.404635000	11.715936000	-0.924329000
C	6.270191000	11.199357000	-2.216420000
H	7.044046000	11.453585000	-2.930076000
C	5.157373000	10.484778000	-2.706111000
C	5.059615000	10.154914000	-4.175467000
H	4.876535000	9.082278000	-4.300284000
H	5.959824000	10.435910000	-4.725600000
H	4.199892000	10.682052000	-4.605334000
C	6.486983000	6.627225000	-0.272994000
H	7.250610000	7.091030000	-0.906420000
H	6.278176000	5.618577000	-0.634989000
H	6.901725000	6.563328000	0.739873000
C	5.252784000	7.495340000	-0.247060000
C	3.990673000	6.934372000	-0.531876000
H	3.968721000	5.886135000	-0.802985000
C	2.758088000	7.576132000	-0.379772000
C	1.474476000	6.813472000	-0.596696000
H	0.866032000	6.850430000	0.313789000
H	1.653426000	5.770662000	-0.865773000
H	0.893049000	7.293307000	-1.392336000

Table S22. DFT Optimized Coordinates of 1^- (*S*=1/2)

sym	x	y	z
Ru	4.093470000	10.150580000	-0.011576000
O	5.691429000	11.491920000	0.018801000
O	4.226595000	10.017925000	-2.126984000
O	2.570019000	8.731256000	-0.144040000
O	5.548929000	8.604249000	0.000148000
N	3.884227000	10.354192000	2.024270000
N	2.692047000	11.652730000	0.094055000
C	4.554176000	9.536811000	2.948359000
C	3.868615000	8.764599000	3.908846000
H	2.784999000	8.822485000	3.949758000
C	4.562638000	7.926753000	4.781381000
H	4.008573000	7.335289000	5.508311000
C	5.955578000	7.832718000	4.719620000
C	6.644458000	8.589907000	3.766332000
C	5.958331000	9.429668000	2.890790000
H	6.495070000	7.178075000	5.400634000
H	7.729880000	8.530196000	3.706749000
H	6.482766000	10.015390000	2.144082000
C	2.995848000	11.313061000	2.427243000
C	2.724734000	11.692496000	3.764812000
H	3.271616000	11.210545000	4.568434000
C	1.776676000	12.664854000	4.059537000
H	1.586906000	12.933396000	5.097103000
C	1.065407000	13.293632000	3.024267000
H	0.301895000	14.034338000	3.254601000
C	1.335877000	12.976200000	1.698589000
H	0.783572000	13.464735000	0.902673000
C	2.325409000	12.020993000	1.359591000
C	2.186773000	12.309827000	-1.038648000
C	2.284377000	13.706686000	-1.207418000
H	2.747389000	14.297036000	-0.422356000
C	1.812436000	14.322595000	-2.366175000
H	1.906897000	15.401799000	-2.474101000
C	1.233848000	13.565681000	-3.388577000
H	0.866347000	14.047804000	-4.291834000
C	1.139171000	12.178619000	-3.234317000

H	0.689202000	11.574627000	-4.020447000
C	1.608677000	11.555359000	-2.079487000
H	1.545825000	10.480193000	-1.954249000
C	7.463409000	12.843668000	-0.719540000
H	7.086297000	13.713971000	-0.169731000
H	7.973584000	13.186499000	-1.624831000
H	8.190260000	12.343022000	-0.068685000
C	6.312041000	11.893355000	-1.017174000
C	6.048975000	11.557934000	-2.357721000
H	6.679454000	12.023669000	-3.107985000
C	5.052159000	10.675117000	-2.827528000
C	4.913670000	10.474578000	-4.330338000
H	4.894767000	9.402467000	-4.556824000
H	5.719671000	10.949815000	-4.898152000
H	3.954977000	10.894789000	-4.658143000
C	6.477988000	6.444564000	0.063038000
H	7.226056000	6.741320000	-0.680954000
H	6.219255000	5.391489000	-0.085028000
H	6.937185000	6.560944000	1.052341000
C	5.271946000	7.368763000	-0.030654000
C	3.987737000	6.789954000	-0.126940000
H	3.942744000	5.706265000	-0.156968000
C	2.759938000	7.473790000	-0.188058000
C	1.481358000	6.658693000	-0.323072000
H	0.810303000	6.890486000	0.512308000
H	1.667491000	5.580580000	-0.343673000
H	0.960049000	6.948044000	-1.243459000

Table S23. DFT Optimized Coordinates of 2^{2+} (*S*=0)

sym	x	y	z
Ru	0.219981547	2.577527662	3.396460873
N	-0.710807751	0.945641083	4.326154744
N	1.009922360	0.963129417	2.363631747
N	-1.179557435	2.866183014	1.827079715
N	1.137836640	4.103909983	2.214706108
N	-0.525881918	4.162268132	4.624418690
N	1.645831480	2.676911695	4.958389638
C	-1.788269818	1.034642663	5.263479510
C	-1.604949431	1.696992468	6.485088671
H	-0.628844916	2.094523764	6.736868878
C	-2.660582942	1.792983846	7.390311497
H	-2.503411848	2.282702173	8.346723226
C	-3.912356196	1.254388183	7.078546403
H	-4.732936687	1.337753301	7.784160714
C	-4.099561178	0.598066946	5.860223846
H	-5.066098465	0.169391685	5.613312916
C	-3.042202634	0.476377145	4.958762570
H	-3.184783628	-0.057559939	4.023322681
C	-0.293933531	-0.250253891	3.924026263
C	-0.691677634	-1.518212242	4.481276281
H	-1.359177228	-1.535622036	5.333536217
C	-0.193733518	-2.673992733	3.958349732
H	-0.474393291	-3.627218947	4.395580809
C	0.728707674	-2.663553108	2.851778370
H	1.110584224	-3.609415329	2.480199774
C	1.150861560	-1.495734380	2.290896890
H	1.868203920	-1.492096260	1.479597332
C	0.665921339	-0.240591624	2.805156558
C	1.783049067	1.076801876	1.161763749
C	1.233834828	0.666770658	-0.062727049
H	0.231551663	0.249240253	-0.090117471
C	1.976761267	0.802356770	-1.236299037
H	1.547357626	0.483503902	-2.181341398
C	3.268362682	1.332089708	-1.194862395
H	3.848859636	1.424334293	-2.107478261
C	3.814713246	1.734794002	0.026963666

H	4.824649142	2.131971547	0.066592945
C	3.073345562	1.620192567	1.202752973
H	3.501323906	1.923801811	2.152671374
C	-2.348665059	2.209192357	1.701902916
H	-2.580195017	1.502500779	2.487734036
C	-3.225103220	2.423514799	0.643719929
H	-4.155011805	1.867608495	0.592992866
C	-2.878318070	3.356946043	-0.332396136
H	-3.533601766	3.551662183	-1.175378840
C	-1.673263970	4.042302739	-0.207113536
H	-1.391566807	4.772757492	-0.955323502
C	-0.834044417	3.785089062	0.882214967
C	0.449935606	4.479367094	1.102599468
C	0.947788611	5.468294167	0.247761212
H	0.395471011	5.760956279	-0.636789787
C	2.161432813	6.085525875	0.536249565
H	2.553878784	6.855160843	-0.120631862
C	2.856484682	5.697673983	1.680203156
H	3.805273825	6.149524360	1.948589066
C	2.310038019	4.704609088	2.486229701
H	2.822351607	4.368344167	3.379088264
C	-1.669774030	4.837119432	4.418770690
H	-2.288390479	4.488388968	3.600781701
C	-2.056322522	5.921497808	5.200799232
H	-2.991587603	6.429977083	4.993428644
C	-1.218754578	6.330234686	6.236923063
H	-1.479748025	7.177381526	6.863128188
C	-0.037637749	5.627729398	6.463429764
H	0.620120778	5.928987360	7.269782118
C	0.287230330	4.538072266	5.649511392
C	1.483924774	3.694643600	5.852112564
C	2.389893909	3.873032267	6.903121129
H	2.257309544	4.683637762	7.609286683
C	3.462478105	2.996985533	7.051466710
H	4.167310514	3.128774381	7.866166412
C	3.605586990	1.947839021	6.144395680
H	4.417735265	1.233592158	6.225782823
C	2.677112815	1.823943165	5.115999964
H	2.748759540	1.023807992	4.389525836

Table S24. DFT Optimized Coordinates of 2^{3+} (*S*=1/2)

sym	x	y	z
Ru	0.280756000	2.552503000	3.420395000
N	-0.719846000	0.966742000	4.329198000
N	1.017817000	0.965472000	2.346485000
N	-1.131070000	2.846160000	1.846845000
N	1.159385000	4.137802000	2.273476000
N	-0.436748000	4.179069000	4.624982000
N	1.699168000	2.624261000	4.990913000
C	-1.830375000	1.045871000	5.200060000
C	-1.773075000	1.858150000	6.351432000
H	-0.853457000	2.372164000	6.597523000
C	-2.861147000	1.915466000	7.213255000
H	-2.795872000	2.500780000	8.125074000
C	-4.038181000	1.211535000	6.918998000
H	-4.890358000	1.275264000	7.588523000
C	-4.113314000	0.423279000	5.763782000
H	-5.026818000	-0.113753000	5.528429000
C	-3.015884000	0.320981000	4.917563000
H	-3.079122000	-0.289547000	4.021662000
C	-0.295391000	-0.250201000	3.919307000
C	-0.659322000	-1.495077000	4.516304000
H	-1.302862000	-1.505721000	5.386920000
C	-0.139779000	-2.672585000	4.024395000
H	-0.399237000	-3.613380000	4.500292000
C	0.775520000	-2.673457000	2.934384000
H	1.194481000	-3.615312000	2.593358000
C	1.180061000	-1.494655000	2.345966000
H	1.928218000	-1.503048000	1.563020000
C	0.660513000	-0.251673000	2.813693000
C	1.716590000	1.052217000	1.118679000
C	1.215979000	0.402325000	-0.034316000
H	0.277126000	-0.140616000	0.015738000
C	1.902523000	0.506691000	-1.238983000
H	1.505542000	0.026254000	-2.127778000
C	3.105458000	1.220932000	-1.303584000
H	3.650613000	1.280663000	-2.240517000
C	3.611064000	1.853345000	-0.158324000

H	4.558774000	2.380667000	-0.205159000
C	2.912701000	1.793650000	1.041737000
H	3.317986000	2.253402000	1.935729000
C	-2.276726000	2.151673000	1.691877000
H	-2.490462000	1.406591000	2.446601000
C	-3.157956000	2.378691000	0.641097000
H	-4.069764000	1.796033000	0.565308000
C	-2.840004000	3.361488000	-0.296634000
H	-3.500232000	3.567063000	-1.133519000
C	-1.657768000	4.082182000	-0.141786000
H	-1.400694000	4.848361000	-0.862689000
C	-0.812364000	3.814782000	0.939511000
C	0.444816000	4.545998000	1.189958000
C	0.892293000	5.606012000	0.394823000
H	0.320208000	5.930936000	-0.465652000
C	2.080823000	6.258605000	0.714794000
H	2.433436000	7.083876000	0.104053000
C	2.801257000	5.835813000	1.831134000
H	3.730550000	6.314105000	2.121759000
C	2.305004000	4.774229000	2.581038000
H	2.839390000	4.412184000	3.450822000
C	-1.541232000	4.906426000	4.382323000
H	-2.163627000	4.578424000	3.558582000
C	-1.887010000	6.021771000	5.141070000
H	-2.790995000	6.574027000	4.907587000
C	-1.049913000	6.403395000	6.187961000
H	-1.280391000	7.272035000	6.796910000
C	0.093669000	5.648482000	6.447164000
H	0.750671000	5.934276000	7.259767000
C	0.382079000	4.532893000	5.655825000
C	1.546902000	3.650454000	5.880534000
C	2.443131000	3.804252000	6.942664000
H	2.320916000	4.614217000	7.651508000
C	3.497510000	2.905777000	7.100039000
H	4.194956000	3.021745000	7.923878000
C	3.636052000	1.858050000	6.189177000
H	4.438785000	1.133562000	6.275282000
C	2.716339000	1.751873000	5.151976000
H	2.788569000	0.954761000	4.421812000

Table S25. DFT Optimized Coordinates of 2^+ (*S*=1/2)

sym	x	y	z
Ru	0.227402000	2.626684000	3.404957000
N	-0.731011000	0.985776000	4.332611000
N	1.063811000	0.995129000	2.383251000
N	-1.159995000	2.841840000	1.831822000
N	1.115768000	4.139124000	2.193641000
N	-0.491386000	4.194681000	4.654418000
N	1.639766000	2.665657000	4.954918000
C	-1.805199000	1.071946000	5.255770000
C	-1.637655000	1.728370000	6.486127000
H	-0.657884000	2.112139000	6.747295000
C	-2.701614000	1.854676000	7.379077000
H	-2.544972000	2.355760000	8.330761000
C	-3.956621000	1.328114000	7.065698000
H	-4.783317000	1.426214000	7.762957000
C	-4.132706000	0.659811000	5.852156000
H	-5.099645000	0.232698000	5.600250000
C	-3.070321000	0.528679000	4.958184000
H	-3.209763000	-0.019139000	4.030165000
C	-0.297100000	-0.232778000	3.909230000
C	-0.695299000	-1.485094000	4.458394000
H	-1.386489000	-1.498342000	5.292951000
C	-0.196048000	-2.667620000	3.954295000
H	-0.505160000	-3.611471000	4.393879000
C	0.730367000	-2.661390000	2.883757000
H	1.122111000	-3.600403000	2.503745000
C	1.156106000	-1.470816000	2.333900000
H	1.883270000	-1.467929000	1.529771000
C	0.666525000	-0.227456000	2.825284000
C	1.808534000	1.108315000	1.179718000
C	1.263590000	0.692830000	-0.048479000
H	0.273818000	0.245521000	-0.062179000
C	1.985347000	0.846444000	-1.232264000
H	1.549646000	0.516869000	-2.171737000
C	3.260796000	1.416583000	-1.213853000
H	3.823193000	1.530848000	-2.135906000
C	3.809861000	1.829707000	0.001995000

H	4.806650000	2.262001000	0.029805000
C	3.091202000	1.678278000	1.188339000
H	3.524294000	1.988920000	2.134508000
C	-2.300294000	2.135943000	1.711345000
H	-2.504757000	1.442649000	2.515939000
C	-3.167079000	2.282875000	0.633969000
H	-4.072921000	1.687904000	0.588469000
C	-2.842529000	3.195380000	-0.369473000
H	-3.491735000	3.335686000	-1.227906000
C	-1.664447000	3.926208000	-0.253050000
H	-1.392405000	4.636329000	-1.024447000
C	-0.833414000	3.735260000	0.856169000
C	0.429862000	4.468198000	1.065336000
C	0.913103000	5.443600000	0.185720000
H	0.361015000	5.694697000	-0.711948000
C	2.109373000	6.095392000	0.464988000
H	2.491594000	6.852911000	-0.211821000
C	2.803106000	5.755515000	1.625813000
H	3.740985000	6.233762000	1.887242000
C	2.272566000	4.773894000	2.454687000
H	2.784884000	4.469049000	3.359531000
C	-1.617099000	4.903203000	4.456548000
H	-2.230896000	4.590417000	3.619812000
C	-1.989991000	5.971217000	5.265027000
H	-2.911544000	6.505853000	5.061449000
C	-1.159215000	6.328517000	6.326852000
H	-1.412097000	7.159931000	6.977124000
C	0.002281000	5.594428000	6.545285000
H	0.657142000	5.852816000	7.368934000
C	0.315506000	4.523039000	5.701260000
C	1.493474000	3.652367000	5.885666000
C	2.393842000	3.774818000	6.949988000
H	2.270611000	4.562404000	7.683994000
C	3.444172000	2.870298000	7.075345000
H	4.144444000	2.955619000	7.900163000
C	3.568377000	1.849806000	6.132481000
H	4.359991000	1.111094000	6.197396000
C	2.647646000	1.781546000	5.092560000
H	2.693211000	1.007856000	4.336345000

Table S26. DFT Optimized Coordinates of 2 (*S*=0)

sym	x	y	z
Ru	0.421578000	2.759836000	3.496690000
N	-0.602076000	1.186484000	4.475589000
N	1.174946000	1.073401000	2.443886000
N	-0.969862000	3.075507000	1.932353000
N	1.345395000	4.275182000	2.343743000
N	-0.173855000	4.270501000	4.814261000
N	1.861442000	2.620120000	4.987481000
C	-1.936048000	1.144620000	4.887063000
C	-2.490982000	2.159282000	5.702527000
H	-1.843422000	2.941593000	6.075121000
C	-3.834483000	2.146752000	6.071433000
H	-4.213562000	2.943343000	6.708754000
C	-4.688245000	1.122093000	5.654781000
H	-5.733963000	1.113818000	5.949658000
C	-4.160048000	0.101161000	4.859136000
H	-4.800604000	-0.710817000	4.520359000
C	-2.820198000	0.108509000	4.479913000
H	-2.433976000	-0.695511000	3.861020000
C	0.077897000	-0.020196000	4.286393000
C	-0.061000000	-1.143015000	5.128064000
H	-0.742585000	-1.079680000	5.971468000
C	0.651166000	-2.315795000	4.892638000
H	0.529219000	-3.164789000	5.560861000
C	1.531500000	-2.390416000	3.805329000
H	2.097688000	-3.299800000	3.618151000
C	1.698948000	-1.289260000	2.970212000
H	2.390913000	-1.339525000	2.133975000
C	0.988440000	-0.089781000	3.190621000
C	1.377024000	0.974174000	1.064454000
C	0.721955000	0.003690000	0.265620000
H	0.054837000	-0.704720000	0.747118000
C	0.918554000	-0.053399000	-1.110715000
H	0.393168000	-0.809382000	-1.690956000
C	1.769170000	0.852967000	-1.753862000
H	1.920075000	0.804270000	-2.828974000
C	2.428841000	1.812478000	-0.983322000

H	3.111317000	2.515274000	-1.457575000
C	2.241782000	1.871390000	0.397400000
H	2.790387000	2.596960000	0.987749000
C	-2.100472000	2.369265000	1.748179000
H	-2.333067000	1.645518000	2.518508000
C	-2.931918000	2.553267000	0.648456000
H	-3.833991000	1.957785000	0.556703000
C	-2.578319000	3.498600000	-0.314597000
H	-3.196628000	3.660908000	-1.192363000
C	-1.408064000	4.226545000	-0.136481000
H	-1.100918000	4.949907000	-0.882618000
C	-0.615862000	4.002890000	0.996859000
C	0.639975000	4.719954000	1.264764000
C	1.106465000	5.790782000	0.489233000
H	0.524018000	6.147605000	-0.352357000
C	2.316067000	6.397009000	0.800828000
H	2.686277000	7.224684000	0.203660000
C	3.042180000	5.920490000	1.897452000
H	3.995414000	6.355865000	2.178935000
C	2.518958000	4.869659000	2.637540000
H	3.041427000	4.468689000	3.498440000
C	-1.157748000	5.171920000	4.609639000
H	-1.657137000	5.104054000	3.649862000
C	-1.548217000	6.098797000	5.561770000
H	-2.357273000	6.788145000	5.343644000
C	-0.896856000	6.102890000	6.805250000
H	-1.187342000	6.801159000	7.584137000
C	0.130415000	5.197097000	7.021431000
H	0.653367000	5.189210000	7.971259000
C	0.497633000	4.290831000	6.012926000
C	1.626491000	3.370182000	6.109229000
C	2.490409000	3.288050000	7.216308000
H	2.292817000	3.878403000	8.103950000
C	3.596690000	2.455101000	7.169389000
H	4.264408000	2.383355000	8.022882000
C	3.838551000	1.712701000	6.004982000
H	4.686059000	1.040371000	5.926185000
C	2.949382000	1.823894000	4.945455000
H	3.062111000	1.258751000	4.028144000

Table S27. DFT Optimized Coordinates of 2 (*S*=1)

sym	x	y	z
Ru	0.230727000	2.553985000	3.388286000
N	-0.743278000	0.915356000	4.307861000
N	1.069193000	0.905475000	2.386718000
N	-1.151224000	2.812016000	1.830697000
N	1.136674000	4.079097000	2.241130000
N	-0.532473000	4.118674000	4.584541000
N	1.640714000	2.651190000	4.930720000
C	-1.805483000	1.024681000	5.235505000
C	-1.619978000	1.718123000	6.443819000
H	-0.639656000	2.123249000	6.667518000
C	-2.671714000	1.874037000	7.345682000
H	-2.501318000	2.411065000	8.275551000
C	-3.933385000	1.343726000	7.065693000
H	-4.751782000	1.468631000	7.769486000
C	-4.129331000	0.647921000	5.870622000
H	-5.104814000	0.227812000	5.637421000
C	-3.079788000	0.487163000	4.966546000
H	-3.238333000	-0.065850000	4.045019000
C	-0.330904000	-0.310235000	3.883263000
C	-0.752220000	-1.559245000	4.419356000
H	-1.450635000	-1.565439000	5.248458000
C	-0.270803000	-2.750751000	3.911268000
H	-0.602973000	-3.691447000	4.342704000
C	0.662128000	-2.753366000	2.850737000
H	1.040430000	-3.695904000	2.463636000
C	1.113989000	-1.562737000	2.315232000
H	1.848839000	-1.565710000	1.517593000
C	0.644656000	-0.314076000	2.810187000
C	1.849541000	1.011997000	1.209598000
C	1.325437000	0.640447000	-0.041783000
H	0.316878000	0.240524000	-0.089837000
C	2.083919000	0.790105000	-1.202362000
H	1.659102000	0.500706000	-2.160516000
C	3.378411000	1.312244000	-1.139245000
H	3.968148000	1.428691000	-2.044491000
C	3.906559000	1.682672000	0.099255000

H	4.914400000	2.085710000	0.162761000
C	3.151238000	1.535063000	1.262844000
H	3.564426000	1.816738000	2.226241000
C	-2.250073000	2.062329000	1.616888000
H	-2.382414000	1.236530000	2.304930000
C	-3.166592000	2.324140000	0.610318000
H	-4.038829000	1.689936000	0.494198000
C	-2.937146000	3.426518000	-0.233734000
H	-3.636942000	3.673806000	-1.026671000
C	-1.799379000	4.188717000	-0.045155000
H	-1.600753000	5.033009000	-0.695659000
C	-0.889229000	3.868264000	0.984784000
C	0.364444000	4.559927000	1.208845000
C	0.830051000	5.632759000	0.416328000
H	0.218982000	6.008259000	-0.396681000
C	2.064330000	6.200039000	0.668419000
H	2.422614000	7.024890000	0.059298000
C	2.847572000	5.689341000	1.718565000
H	3.822267000	6.101631000	1.955976000
C	2.340143000	4.636118000	2.465227000
H	2.902225000	4.212270000	3.289197000
C	-1.710049000	4.747274000	4.426386000
H	-2.352819000	4.341687000	3.652798000
C	-2.097161000	5.846028000	5.179535000
H	-3.057567000	6.316374000	4.999438000
C	-1.209217000	6.327236000	6.160974000
H	-1.469328000	7.190253000	6.767334000
C	-0.003970000	5.681425000	6.352735000
H	0.682633000	6.031190000	7.115914000
C	0.334857000	4.556189000	5.565153000
C	1.522478000	3.754507000	5.756174000
C	2.504098000	3.995524000	6.745509000
H	2.428882000	4.876338000	7.373771000
C	3.548883000	3.109352000	6.922521000
H	4.300408000	3.295421000	7.684394000
C	3.616182000	1.956678000	6.113697000
H	4.405442000	1.222479000	6.233189000
C	2.644412000	1.776634000	5.141830000
H	2.651883000	0.916251000	4.481864000

Table S28. DFT Optimized Coordinates of 3^+ (*S*=1/2)

sym	x	y	z
Ru	0.000031000	3.463224000	16.399750000
N	0.889463000	4.440081000	18.039568000
N	1.443481000	1.949589000	16.294234000
N	0.145687000	1.260884000	14.444130000
N	-0.629011000	2.208393000	14.817031000
C	1.930197000	5.403263000	17.928710000
C	1.693756000	6.628008000	17.284134000
H	0.696617000	6.852240000	16.922482000
C	2.719261000	7.560381000	17.131466000
H	2.513217000	8.505158000	16.636249000
C	4.000182000	7.290954000	17.618819000
H	4.796865000	8.018805000	17.498534000
C	4.243670000	6.081464000	18.272427000
H	5.232425000	5.863562000	18.666717000
C	3.220399000	5.146050000	18.429124000
H	3.415117000	4.218288000	18.959328000
C	0.486014000	4.002248000	19.259722000
C	0.914689000	4.537610000	20.508823000
H	1.600687000	5.376147000	20.515369000
C	0.451911000	4.009320000	21.693868000
H	0.782820000	4.434096000	22.636912000
C	2.475812000	1.722492000	17.126054000
H	2.578782000	2.418367000	17.948064000
C	3.359404000	0.661597000	16.948277000
H	4.172654000	0.522871000	17.652539000
C	3.178906000	-0.209130000	15.868635000
H	3.856369000	-1.041451000	15.707517000
C	2.105834000	0.004736000	15.012475000
H	1.896727000	-0.639407000	14.166180000
C	1.249918000	1.084889000	15.260311000
C	-1.745293000	2.405451000	13.950702000
C	-2.977455000	2.771551000	14.508676000
H	-3.073054000	2.862074000	15.583679000
C	-4.080417000	2.945044000	13.675056000
H	-5.043405000	3.201576000	14.106246000
C	-3.951872000	2.782919000	12.292998000

H	-4.811574000	2.932339000	11.646509000
C	-2.717127000	2.424804000	11.741062000
H	-2.616134000	2.300794000	10.667010000
C	-1.613795000	2.222781000	12.564139000
H	-0.650770000	1.941061000	12.154064000
N	-0.889394000	2.486369000	18.039582000
C	-1.930265000	1.523335000	17.928754000
C	-1.694024000	0.298535000	17.284206000
H	-0.696922000	0.074129000	16.922563000
C	-2.719675000	-0.633683000	17.131575000
H	-2.513781000	-1.578508000	16.636387000
C	-4.000551000	-0.364041000	17.618928000
H	-4.797349000	-1.091769000	17.498667000
C	-4.243846000	0.845509000	18.272496000
H	-5.232567000	1.063582000	18.666777000
C	-3.220427000	1.780766000	18.429163000
H	-3.415000000	2.708584000	18.959322000
C	-0.485875000	2.924163000	19.259731000
C	-0.914498000	2.388784000	20.508843000
H	-1.600495000	1.550246000	20.515407000
C	-0.451668000	2.917053000	21.693878000
H	-0.782535000	2.492259000	22.636929000
N	-1.443426000	4.976845000	16.294239000
N	-0.145589000	5.665626000	14.444193000
N	0.629090000	4.718091000	14.817057000
C	-2.475795000	5.203884000	17.126028000
H	-2.578792000	4.507962000	17.947996000
C	-3.359395000	6.264774000	16.948264000
H	-4.172677000	6.403454000	17.652498000
C	-3.178865000	7.135554000	15.868671000
H	-3.856334000	7.967874000	15.707564000
C	-2.105759000	6.921741000	15.012539000
H	-1.896633000	7.565920000	14.166276000
C	-1.249838000	5.841590000	15.260359000
C	1.745378000	4.521049000	13.950731000
C	2.977519000	4.154872000	14.508701000
H	3.073099000	4.064283000	15.583700000
C	4.080488000	3.981393000	13.675086000
H	5.043461000	3.724801000	14.106275000
C	3.951968000	4.143606000	12.293037000

H	4.811674000	3.994195000	11.646551000
C	2.717243000	4.501795000	11.741104000
H	2.616270000	4.625872000	10.667057000
C	1.613906000	4.703805000	12.564176000
H	0.650896000	4.985579000	12.154103000

Table S29. DFT Optimized Coordinates of 3^{2+} (*S*=0)

sym	x	y	z
Ru	-0.000006000	3.463266000	16.430967000
N	0.879533000	4.431580000	18.066315000
N	1.441923000	1.932281000	16.264037000
N	0.121427000	1.339977000	14.388491000
N	-0.673664000	2.240606000	14.812016000
C	1.921725000	5.405408000	17.950989000
C	1.683421000	6.605660000	17.266582000
H	0.695585000	6.813987000	16.872832000
C	2.703844000	7.545887000	17.137329000
H	2.506128000	8.483304000	16.626615000
C	3.973488000	7.289427000	17.663362000
H	4.767052000	8.021550000	17.552258000
C	4.215786000	6.090515000	18.337841000
H	5.198169000	5.885520000	18.752343000
C	3.194792000	5.152987000	18.492209000
H	3.383694000	4.228186000	19.029676000
C	0.491606000	4.014136000	19.264253000
C	0.909276000	4.569352000	20.528321000
H	1.571007000	5.425944000	20.537222000
C	0.443076000	4.032179000	21.689494000
H	0.742292000	4.462095000	22.640404000
C	2.485424000	1.660821000	17.066279000
H	2.605506000	2.304184000	17.928787000
C	3.376653000	0.619254000	16.811045000
H	4.200940000	0.443593000	17.493876000
C	3.190630000	-0.178287000	15.679630000
H	3.872466000	-0.992281000	15.455762000
C	2.104654000	0.083893000	14.848950000
H	1.892544000	-0.505966000	13.964535000
C	1.245697000	1.137467000	15.176165000
C	-1.819983000	2.432394000	13.988688000
C	-3.036276000	2.790879000	14.590157000
H	-3.097276000	2.887859000	15.666850000
C	-4.172109000	2.938879000	13.798557000
H	-5.122744000	3.184633000	14.261590000
C	-4.093115000	2.761658000	12.413669000

H	-4.978941000	2.890838000	11.799326000
C	-2.875069000	2.414084000	11.816891000
H	-2.814787000	2.279898000	10.741421000
C	-1.739021000	2.235421000	12.597559000
H	-0.790309000	1.962235000	12.150378000
N	-0.879537000	2.494966000	18.066329000
C	-1.921727000	1.521136000	17.951018000
C	-1.683430000	0.320884000	17.266608000
H	-0.695600000	0.112560000	16.872844000
C	-2.703852000	-0.619346000	17.137370000
H	-2.506141000	-1.556762000	16.626654000
C	-3.973490000	-0.362888000	17.663421000
H	-4.767053000	-1.095014000	17.552329000
C	-4.215781000	0.836023000	18.337903000
H	-5.198159000	1.041016000	18.752419000
C	-3.194787000	1.773553000	18.492256000
H	-3.383684000	2.698353000	19.029727000
C	-0.491600000	2.912418000	19.264261000
C	-0.909258000	2.357209000	20.528335000
H	-1.570988000	1.500616000	20.537247000
C	-0.443048000	2.894389000	21.689501000
H	-0.742255000	2.464478000	22.640416000
N	-1.441939000	4.994246000	16.264026000
N	-0.121445000	5.586541000	14.388475000
N	0.673649000	4.685918000	14.812007000
C	-2.485443000	5.265706000	17.066264000
H	-2.605523000	4.622347000	17.928775000
C	-3.376678000	6.307266000	16.811020000
H	-4.200967000	6.482927000	17.493848000
C	-3.190657000	7.104799000	15.679599000
H	-3.872498000	7.918788000	15.455724000
C	-2.104679000	6.842618000	14.848923000
H	-1.892571000	7.432472000	13.964504000
C	-1.245717000	5.789052000	15.176147000
C	1.819983000	4.494148000	13.988695000
C	3.036277000	4.135697000	14.590184000
H	3.097266000	4.038733000	15.666879000
C	4.172124000	3.987714000	13.798600000
H	5.122759000	3.741987000	14.261649000
C	4.093144000	4.164919000	12.413710000

H	4.978981000	4.035754000	11.799380000
C	2.875099000	4.512461000	11.816913000
H	2.814827000	4.646636000	10.741441000
C	1.739036000	4.691106000	12.597563000
H	0.790324000	4.964267000	12.150367000

Table S30. DFT Optimized Coordinates of 3 (*S*=1)

sym	x	y	z
Ru	0.000006000	3.463274000	16.345740000
N	0.901448000	4.434366000	18.015219000
N	1.420681000	1.939850000	16.204934000
N	0.107849000	1.323662000	14.347644000
N	-0.711756000	2.237769000	14.815061000
C	1.942169000	5.391212000	17.919008000
C	1.731914000	6.596306000	17.228892000
H	0.752780000	6.798720000	16.810677000
C	2.763991000	7.522501000	17.085627000
H	2.577804000	8.448309000	16.547586000
C	4.026902000	7.268904000	17.625660000
H	4.829907000	7.991169000	17.508326000
C	4.246330000	6.075876000	18.317480000
H	5.223983000	5.863187000	18.742904000
C	3.217051000	5.146445000	18.465242000
H	3.393572000	4.223238000	19.009663000
C	0.485763000	4.002730000	19.233192000
C	0.898729000	4.544770000	20.484921000
H	1.575455000	5.391138000	20.491194000
C	0.442990000	4.014338000	21.674212000
H	0.769504000	4.447034000	22.616068000
C	2.442684000	1.652917000	17.035502000
H	2.517131000	2.282149000	17.914632000
C	3.352603000	0.638425000	16.783037000
H	4.161186000	0.453692000	17.482056000
C	3.207601000	-0.126305000	15.609964000
H	3.915269000	-0.916630000	15.376998000
C	2.142708000	0.128248000	14.768350000
H	1.962967000	-0.446064000	13.866610000
C	1.229499000	1.155070000	15.097125000
C	-1.900516000	2.359024000	14.053378000
C	-3.086734000	2.776297000	14.677112000
H	-3.092311000	2.953289000	15.744011000
C	-4.257780000	2.908212000	13.933360000
H	-5.171950000	3.219419000	14.431807000
C	-4.263403000	2.635529000	12.563888000

H	-5.176945000	2.746937000	11.986197000
C	-3.083577000	2.212423000	11.942320000
H	-3.076712000	1.998574000	10.876571000
C	-1.911096000	2.065474000	12.675747000
H	-0.992807000	1.737947000	12.203723000
N	-0.901443000	2.492188000	18.015218000
C	-1.942173000	1.535351000	17.919004000
C	-1.731924000	0.330252000	17.228895000
H	-0.752789000	0.127826000	16.810689000
C	-2.764009000	-0.595933000	17.085627000
H	-2.577826000	-1.521746000	16.547592000
C	-4.026922000	-0.342322000	17.625647000
H	-4.829933000	-1.064579000	17.508311000
C	-4.246343000	0.850713000	18.317459000
H	-5.223998000	1.063414000	18.742873000
C	-3.217057000	1.780133000	18.465225000
H	-3.393574000	2.703346000	19.009639000
C	-0.485763000	2.923828000	19.233192000
C	-0.898735000	2.381793000	20.484922000
H	-1.575460000	1.535425000	20.491195000
C	-0.443001000	2.912230000	21.674213000
H	-0.769519000	2.479538000	22.616068000
N	-1.420668000	4.986698000	16.204926000
N	-0.107822000	5.602889000	14.347646000
N	0.711777000	4.688775000	14.815062000
C	-2.442676000	5.273631000	17.035488000
H	-2.517130000	4.644397000	17.914616000
C	-3.352591000	6.288126000	16.783019000
H	-4.161179000	6.472858000	17.482033000
C	-3.207580000	7.052858000	15.609950000
H	-3.915245000	7.843185000	15.376980000
C	-2.142681000	6.798307000	14.768342000
H	-1.962933000	7.372620000	13.866605000
C	-1.229475000	5.771483000	15.097122000
C	1.900526000	4.567499000	14.053367000
C	3.086736000	4.150179000	14.677082000
H	3.092318000	3.973167000	15.743978000
C	4.257771000	4.018240000	13.933317000
H	5.171937000	3.706997000	14.431750000
C	4.263390000	4.290945000	12.563849000

H	5.176923000	4.179517000	11.986148000
C	3.083570000	4.714095000	11.942299000
H	3.076702000	4.927959000	10.876553000
C	1.911101000	4.861067000	12.675739000
H	0.992817000	5.188629000	12.203729000

Table S31. DFT Optimized Coordinates of 3⁻ (*S*=3/2)

sym	x	y	z
Ru	0.000000000	3.463273000	16.419271000
N	0.897160000	4.434733000	18.065024000
N	1.439581000	1.936493000	16.295016000
N	0.186377000	1.263836000	14.407987000
N	-0.677361000	2.204469000	14.817709000
C	1.947898000	5.370928000	17.959872000
C	1.784021000	6.533899000	17.185212000
H	0.831295000	6.710552000	16.702012000
C	2.829711000	7.442124000	17.031606000
H	2.674882000	8.330007000	16.423010000
C	4.066606000	7.218956000	17.641871000
H	4.881482000	7.927241000	17.513485000
C	4.244118000	6.066974000	18.411397000
H	5.203058000	5.869446000	18.886379000
C	3.201288000	5.155353000	18.570593000
H	3.350114000	4.262214000	19.170203000
C	0.483998000	4.002813000	19.290449000
C	0.886611000	4.548088000	20.540881000
H	1.555506000	5.401376000	20.546966000
C	0.436201000	4.016455000	21.737188000
H	0.760585000	4.456772000	22.677577000
C	2.457444000	1.686715000	17.139672000
H	2.523892000	2.355073000	17.990947000
C	3.376896000	0.667356000	16.948392000
H	4.180831000	0.519766000	17.662041000
C	3.235629000	-0.153419000	15.806762000
H	3.945291000	-0.955215000	15.615000000
C	2.185765000	0.063670000	14.944553000
H	2.021829000	-0.547001000	14.063160000
C	1.254345000	1.110144000	15.204298000
C	-1.780485000	2.335365000	13.963923000
C	-2.981162000	2.891264000	14.448735000
H	-3.037105000	3.195156000	15.485278000
C	-4.090887000	3.020253000	13.618119000
H	-5.006459000	3.447410000	14.021610000
C	-4.039987000	2.603168000	12.284641000

H	-4.907651000	2.710955000	11.637728000
C	-2.853904000	2.043362000	11.796875000
H	-2.794492000	1.715852000	10.760282000
C	-1.739878000	1.903453000	12.617675000
H	-0.820521000	1.469621000	12.244772000
N	-0.897161000	2.491822000	18.065029000
C	-1.947897000	1.555625000	17.959880000
C	-1.784017000	0.392650000	17.185225000
H	-0.831290000	0.215997000	16.702027000
C	-2.829704000	-0.515579000	17.031623000
H	-2.674873000	-1.403464000	16.423032000
C	-4.066600000	-0.292410000	17.641887000
H	-4.881474000	-1.000699000	17.513503000
C	-4.244116000	0.859575000	18.411407000
H	-5.203056000	1.057103000	18.886388000
C	-3.201288000	1.771199000	18.570599000
H	-3.350116000	2.664340000	19.170205000
C	-0.484001000	2.923749000	19.290452000
C	-0.886617000	2.378481000	20.540886000
H	-1.555511000	1.525194000	20.546975000
C	-0.436208000	2.910121000	21.737190000
H	-0.760594000	2.469810000	22.677582000
N	-1.439582000	4.990053000	16.295007000
N	-0.186376000	5.662700000	14.407975000
N	0.677361000	4.722069000	14.817703000
C	-2.457445000	5.239835000	17.139661000
H	-2.523893000	4.571482000	17.990939000
C	-3.376897000	6.259193000	16.948375000
H	-4.180833000	6.406787000	17.662022000
C	-3.235630000	7.079962000	15.806740000
H	-3.945291000	7.881756000	15.614973000
C	-2.185765000	6.862869000	14.944533000
H	-2.021829000	7.473534000	14.063137000
C	-1.254345000	5.816396000	15.204285000
C	1.780486000	4.591168000	13.963918000
C	2.981160000	4.035267000	14.448732000
H	3.037102000	3.731378000	15.485277000
C	4.090885000	3.906271000	13.618117000
H	5.006456000	3.479113000	14.021611000
C	4.039987000	4.323350000	12.284638000

H	4.907650000	4.215557000	11.637726000
C	2.853906000	4.883157000	11.796869000
H	2.794495000	5.210663000	10.760274000
C	1.739880000	5.023073000	12.617668000
H	0.820525000	5.456906000	12.244763000

Table S32. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 1(*S*=0)

```
 Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    0.2834 eV 4374.60 nm
f=0.0044  <S**2>=0.000
     120 ->129         0.21692
     121 ->129        -0.22633
     123 ->129        -0.11299
     128 ->129         0.69251
     128 <-129        -0.28565
 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 symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    0.3300 eV 3757.23 nm
f=0.0016  <S**2>=0.000
     122 ->129         0.36065
     125 ->129        -0.16383
     127 ->129         0.62540
     127 <-129        -0.21317

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    0.9347 eV 1326.39 nm
f=0.0028  <S**2>=0.000
     123 ->129        -0.20720
     126 ->129         0.65385
     128 ->129        -0.10877

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    0.9429 eV 1314.90 nm
f=0.0257  <S**2>=0.000
     122 ->129        -0.15033
     124 ->129        -0.27561
     125 ->129         0.57581
     127 ->129         0.24862

 Excited state symmetry could not be determined.
 Excited State   5:      Singlet-?Sym    1.0071 eV 1231.08 nm
f=0.0184  <S**2>=0.000
     120 ->129        -0.14469
     121 ->129         0.15815
     122 ->129         0.20349
     123 ->129         0.29594
     124 ->129         0.44202
     125 ->129         0.26454
     126 ->129         0.17053
```

```
     128 ->129         0.13804

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    1.0128 eV 1224.22 nm
f=0.0132  <S**2>=0.000
     120 ->129        -0.18554
     121 ->129         0.20621
     122 ->129        -0.15009
     123 ->129         0.39644
     124 ->129        -0.33163
     125 ->129        -0.23240
     126 ->129         0.18326
     128 ->129         0.17759

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    1.2185 eV 1017.53 nm
f=0.0487  <S**2>=0.000
     122 ->129         0.53012
     124 ->129        -0.34219
     127 ->129        -0.30513
     127 <-129         0.10570

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    1.4207 eV  872.70 nm
f=0.0655  <S**2>=0.000
     120 ->129         0.28090
     121 ->129        -0.41314
     123 ->129         0.43671
     127 ->130         0.15597
     128 ->129        -0.17013

 Excited state symmetry could not be determined.
 Excited State   9:      Singlet-?Sym    1.6547 eV  749.28 nm
f=0.0196  <S**2>=0.000
     119 ->129         0.57128
     128 ->130        -0.39763

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    1.6913 eV  733.06 nm
f=0.0787  <S**2>=0.000
     119 ->129         0.38914
     128 ->130         0.56004

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    1.7023 eV  728.35 nm
f=0.0104  <S**2>=0.000
     120 ->129         0.49502
     121 ->129         0.28570
     122 ->130        -0.11539
     127 ->130        -0.35388
```

```
 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    1.9226 eV  644.88 nm
f=0.0475  <S**2>=0.000
     118 ->129        -0.18816
     120 ->129         0.19643
     121 ->129         0.26745
     122 ->130        -0.17104
     127 ->130         0.56276

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    2.0569 eV  602.79 nm
f=0.0016  <S**2>=0.000
     118 ->129         0.63778
     122 ->130        -0.14469
     125 ->130         0.18385
     127 ->130         0.12757

 Excited state symmetry could not be determined.
 Excited State  14:      Singlet-?Sym    2.1394 eV  579.53 nm
f=0.0159  <S**2>=0.000
     123 ->130         0.13849
     126 ->130         0.68929

 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    2.2105 eV  560.88 nm
f=0.0003  <S**2>=0.000
     118 ->129        -0.14083
     124 ->130        -0.19066
     125 ->130         0.65058

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    2.2643 eV  547.55 nm
f=0.0842  <S**2>=0.000
     121 ->130         0.20150
     123 ->130         0.64501
     126 ->130        -0.14060

 Excited state symmetry could not be determined.
 Excited State  17:      Singlet-?Sym    2.2925 eV  540.82 nm
f=0.0109  <S**2>=0.000
     124 ->130         0.66609
     125 ->130         0.17368

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    2.5862 eV  479.40 nm
f=0.0028  <S**2>=0.000
     120 ->130        -0.21018
     121 ->130         0.62152
     123 ->130        -0.22396
```

```
 Excited state symmetry could not be determined.
 Excited State  19:      Singlet-?Sym    2.6568 eV  466.67 nm
f=0.0047  <S**2>=0.000
     115 ->129         0.16287
     117 ->129         0.67227

 Excited state symmetry could not be determined.
 Excited State  20:      Singlet-?Sym    2.7720 eV  447.27 nm
f=0.1177  <S**2>=0.000
     114 ->129         0.21334
     116 ->129         0.48900
     121 ->129         0.11365
     122 ->130         0.41769

 Excited state symmetry could not be determined.
 Excited State  21:      Singlet-?Sym    2.8247 eV  438.93 nm
f=0.0051  <S**2>=0.000
     120 ->130         0.65295
     121 ->130         0.23030

 Excited state symmetry could not be determined.
 Excited State  22:      Singlet-?Sym    2.9360 eV  422.29 nm
f=0.0962  <S**2>=0.000
     116 ->129         0.42826
     119 ->130        -0.27122
     120 ->129        -0.10859
     121 ->129        -0.14496
     122 ->130        -0.41235

 Excited state symmetry could not be determined.
 Excited State  23:      Singlet-?Sym    3.1741 eV  390.61 nm
f=0.1049  <S**2>=0.000
     116 ->129         0.12777
     119 ->130         0.63100
     121 ->129        -0.10777
     122 ->130        -0.20170

 Excited state symmetry could not be determined.
 Excited State  24:      Singlet-?Sym    3.2684 eV  379.34 nm
f=0.0327  <S**2>=0.000
     115 ->129         0.63783
     117 ->129        -0.15437
     122 ->131        -0.12665
     127 ->131        -0.18076

 Excited state symmetry could not be determined.
 Excited State  25:      Singlet-?Sym    3.2998 eV  375.74 nm
f=0.0005  <S**2>=0.000
     114 ->129         0.61915
```

```
     116 ->129        -0.20466
     122 ->130        -0.10769
     128 ->131         0.18556

 Excited state symmetry could not be determined.
 Excited State  26:      Singlet-?Sym    3.3341 eV  371.87 nm
f=0.0117  <S**2>=0.000
     115 ->129         0.22098
     122 ->131         0.33719
     125 ->131        -0.14718
     127 ->131         0.51110

 Excited state symmetry could not be determined.
 Excited State  27:      Singlet-?Sym    3.4837 eV  355.90 nm
f=0.0047  <S**2>=0.000
     112 ->129        -0.12013
     114 ->129         0.13078
     118 ->130         0.48839
     121 ->131         0.13877
     123 ->131         0.15936
     128 ->131        -0.38665

 Excited state symmetry could not be determined.
 Excited State  28:      Singlet-?Sym    3.4844 eV  355.83 nm
f=0.0049  <S**2>=0.000
     112 ->129         0.11650
     114 ->129        -0.12910
     118 ->130         0.49303
     121 ->131        -0.13747
     123 ->131        -0.15820
     128 ->131         0.38512

 Excited state symmetry could not be determined.
 Excited State  29:      Singlet-?Sym    3.5289 eV  351.34 nm
f=0.0035  <S**2>=0.000
     111 ->129        -0.11125
     112 ->129         0.65588
     114 ->129         0.10327
     128 ->131        -0.13511

 Excited state symmetry could not be determined.
 Excited State  30:      Singlet-?Sym    3.5849 eV  345.86 nm
f=0.0046  <S**2>=0.000
     109 ->129        -0.14560
     113 ->129         0.67168

 Excited state symmetry could not be determined.
 Excited State  31:      Singlet-?Sym    3.6537 eV  339.33 nm
f=0.0522  <S**2>=0.000
     120 ->132         0.16656
```

```
     120 ->133         0.24361
     121 ->132        -0.11417
     121 ->133        -0.16721
     123 ->133        -0.11030
     128 ->132         0.29265
     128 ->133         0.42686
     128 ->134        -0.15348

 Excited state symmetry could not be determined.
 Excited State  32:      Singlet-?Sym    3.7764 eV  328.32 nm
f=0.0026  <S**2>=0.000
     111 ->129         0.63952
     112 ->129         0.11974
     123 ->131         0.11196
     127 ->133         0.12578

 Excited state symmetry could not be determined.
 Excited State  33:      Singlet-?Sym    3.8191 eV  324.64 nm
f=0.0092  <S**2>=0.000
     108 ->129        -0.21406
     109 ->129         0.38527
     110 ->129         0.51833

 Excited state symmetry could not be determined.
 Excited State  34:      Singlet-?Sym    3.8271 eV  323.96 nm
f=0.0183  <S**2>=0.000
     111 ->129        -0.22115
     121 ->131         0.22803
     122 ->132         0.11111
     122 ->133         0.16259
     123 ->131         0.30356
     126 ->131         0.15155
     127 ->132         0.18509
     127 ->133         0.26657
     128 ->131         0.28475

 Excited state symmetry could not be determined.
 Excited State  35:      Singlet-?Sym    3.8785 eV  319.67 nm
f=0.0154  <S**2>=0.000
     109 ->129         0.54031
     110 ->129        -0.40845
     113 ->129         0.12424

 Excited state symmetry could not be determined.
 Excited State  36:      Singlet-?Sym    3.9962 eV  310.26 nm
f=0.0028  <S**2>=0.000
     106 ->129        -0.14014
     108 ->129         0.41037
     110 ->129         0.14467
     122 ->131         0.35911
```

```
     124 ->131        -0.10021
     125 ->131        -0.17862
     127 ->131        -0.32041

 Excited state symmetry could not be determined.
 Excited State  37:      Singlet-?Sym    3.9972 eV  310.18 nm
f=0.0022  <S**2>=0.000
     108 ->129         0.46717
     109 ->129         0.10948
     110 ->129         0.17945
     122 ->131        -0.30213
     125 ->131         0.15472
     127 ->131         0.26455

 Excited state symmetry could not be determined.
 Excited State  38:      Singlet-?Sym    4.0436 eV  306.62 nm
f=0.0000  <S**2>=0.000
     104 ->129         0.14807
     105 ->129         0.28566
     107 ->129         0.50382
     117 ->130         0.20209
     128 ->132         0.15655
     128 ->133        -0.11188

 Excited state symmetry could not be determined.
 Excited State  39:      Singlet-?Sym    4.0628 eV  305.17 nm
f=0.0026  <S**2>=0.000
     107 ->129         0.10350
     121 ->131        -0.21108
     123 ->131        -0.32316
     126 ->131        -0.16784
     127 ->132         0.27820
     127 ->133         0.39826
     127 ->134        -0.10079
     128 ->131        -0.13052

 Excited state symmetry could not be determined.
 Excited State  40:      Singlet-?Sym    4.1046 eV  302.06 nm
f=0.0032  <S**2>=0.000
     106 ->129         0.63802
     108 ->129         0.18554
     116 ->130         0.12326

 Excited state symmetry could not be determined.
 Excited State  41:      Singlet-?Sym    4.1474 eV  298.94 nm
f=0.0076  <S**2>=0.000
     104 ->129         0.17100
     105 ->129         0.52066
     107 ->129        -0.37631
     117 ->130        -0.10655
```

```
 Excited state symmetry could not be determined.
 Excited State  42:      Singlet-?Sym    4.1834 eV  296.37 nm
f=0.0113  <S**2>=0.000
     104 ->129        -0.12268
     107 ->129        -0.15596
     115 ->130         0.13973
     117 ->130         0.55849
     120 ->131         0.10446
     128 ->132        -0.23280
     128 ->133         0.16325

 Excited state symmetry could not be determined.
 Excited State  43:      Singlet-?Sym    4.2276 eV  293.28 nm
f=0.0305  <S**2>=0.000
     114 ->130         0.10402
     116 ->130         0.62826
     128 ->134         0.17608

 Excited state symmetry could not be determined.
 Excited State  44:      Singlet-?Sym    4.2572 eV  291.23 nm
f=0.0101  <S**2>=0.000
     104 ->129         0.41054
     105 ->129        -0.30080
     107 ->129        -0.18491
     117 ->130         0.21391
     128 ->132         0.29068
     128 ->133        -0.19310

 Excited state symmetry could not be determined.
 Excited State  45:      Singlet-?Sym    4.2764 eV  289.93 nm
f=0.0043  <S**2>=0.000
     104 ->129        -0.35286
     116 ->130        -0.10806
     127 ->132         0.10277
     127 ->134         0.15831
     128 ->132         0.34845
     128 ->134         0.37821

 Excited state symmetry could not be determined.
 Excited State  46:      Singlet-?Sym    4.2795 eV  289.72 nm
f=0.0066  <S**2>=0.000
     104 ->129         0.27494
     116 ->130        -0.12008
     127 ->132         0.12181
     127 ->134        -0.14100
     128 ->132        -0.15040
     128 ->133         0.27316
     128 ->134         0.47652
```

```
 Excited state symmetry could not be determined.
 Excited State  47:      Singlet-?Sym    4.3262 eV  286.59 nm
f=0.0014  <S**2>=0.000
     117 ->130        -0.17466
     120 ->131         0.27518
     121 ->131        -0.23313
     126 ->131         0.52455
     128 ->131        -0.13588
     128 ->132        -0.10151

 Excited state symmetry could not be determined.
 Excited State  48:      Singlet-?Sym    4.3422 eV  285.53 nm
f=0.0063  <S**2>=0.000
     103 ->129         0.50653
     125 ->131         0.12833
     127 ->132         0.30624
     127 ->133        -0.21622

 Excited state symmetry could not be determined.
 Excited State  49:      Singlet-?Sym    4.3862 eV  282.67 nm
f=0.0216  <S**2>=0.000
     106 ->129         0.10554
     116 ->130        -0.14271
     122 ->131         0.24023
     123 ->133         0.10837
     125 ->131         0.56516
     127 ->132        -0.10745

 Excited state symmetry could not be determined.
 Excited State  50:      Singlet-?Sym    4.4019 eV  281.66 nm
f=0.0086  <S**2>=0.000
     103 ->129         0.47043
     121 ->133        -0.11067
     123 ->133        -0.11009
     127 ->132        -0.30885
     127 ->133         0.20805
     128 ->134         0.14545

 Excited state symmetry could not be determined.
 Excited State  51:      Singlet-?Sym    4.4139 eV  280.90 nm
f=0.0007  <S**2>=0.000
     102 ->129         0.54434
     122 ->134        -0.10393
     127 ->133        -0.11371
     127 ->134        -0.36559

 Excited state symmetry could not be determined.
 Excited State  52:      Singlet-?Sym    4.4536 eV  278.39 nm
f=0.0047  <S**2>=0.000
     124 ->131         0.63376
```

```
     125 ->131        -0.17482
     127 ->132        -0.10491

 Excited state symmetry could not be determined.
 Excited State  53:      Singlet-?Sym    4.4695 eV  277.40 nm
f=0.1189  <S**2>=0.000
     114 ->130         0.20442
     120 ->132        -0.10766
     120 ->133        -0.16289
     121 ->132         0.15040
     121 ->133         0.22306
     122 ->131        -0.15255
     123 ->132         0.13235
     123 ->133         0.18529
     124 ->131        -0.22639
     125 ->131        -0.14609
     127 ->132        -0.16788
     127 ->133         0.10681
     128 ->132         0.17576
     128 ->133         0.25596

 Excited state symmetry could not be determined.
 Excited State  54:      Singlet-?Sym    4.4774 eV  276.91 nm
f=0.0007  <S**2>=0.000
     101 ->129         0.10106
     102 ->129         0.39606
     104 ->129         0.14514
     115 ->130        -0.10157
     123 ->131        -0.11132
     126 ->131         0.10088
     127 ->134         0.45040

 Excited state symmetry could not be determined.
 Excited State  55:      Singlet-?Sym    4.4983 eV  275.63 nm
f=0.0140  <S**2>=0.000
     101 ->129         0.40812
     105 ->129         0.10428
     115 ->130        -0.25045
     120 ->131        -0.21284
     122 ->132        -0.11521
     122 ->133        -0.16342
     123 ->131        -0.12244
     125 ->133         0.12626
     126 ->131         0.20600
     127 ->134        -0.15534

 Excited state symmetry could not be determined.
 Excited State  56:      Singlet-?Sym    4.5224 eV  274.15 nm
f=0.0040  <S**2>=0.000
     101 ->129         0.17868
```

```
     102 ->129         0.12655
     115 ->130        -0.15980
     120 ->131         0.31828
     121 ->131        -0.20543
     122 ->132        -0.11704
     122 ->133        -0.17177
     122 ->134         0.10822
     123 ->131         0.32281
     125 ->133         0.11015
     126 ->131        -0.25724
     127 ->133         0.10235

 Excited state symmetry could not be determined.
 Excited State  57:      Singlet-?Sym    4.5448 eV  272.80 nm
f=0.0590  <S**2>=0.000
     113 ->130         0.11113
     115 ->130         0.54794
     117 ->130        -0.12757
     122 ->132        -0.12062
     122 ->133        -0.17504
     125 ->132         0.11442
     125 ->133         0.16482
     127 ->133         0.10778

 Excited state symmetry could not be determined.
 Excited State  58:      Singlet-?Sym    4.5553 eV  272.18 nm
f=0.0013  <S**2>=0.000
     114 ->130         0.38412
     120 ->132         0.15925
     120 ->133         0.23036
     123 ->132         0.12819
     123 ->133         0.18684
     126 ->132         0.21151
     126 ->133         0.30479
     128 ->132        -0.10240
     128 ->133        -0.14973

 Excited state symmetry could not be determined.
 Excited State  59:      Singlet-?Sym    4.5909 eV  270.06 nm
f=0.0009  <S**2>=0.000
     101 ->129         0.48949
     113 ->130         0.11143
     115 ->130         0.16432
     120 ->131         0.15914
     122 ->132         0.18983
     122 ->133         0.27529
     125 ->133        -0.10376
     127 ->133        -0.11612

 Excited state symmetry could not be determined.
```

```
 Excited State  60:      Singlet-?Sym    4.6086 eV  269.03 nm
f=0.1407  <S**2>=0.000
     112 ->130         0.12494
     114 ->130         0.52225
     120 ->133        -0.11501
     123 ->132        -0.13475
     123 ->133        -0.19190
     126 ->132        -0.15330
     126 ->133        -0.20907

 Excited state symmetry could not be determined.
 Excited State  61:      Singlet-?Sym    4.6596 eV  266.08 nm
f=0.0169  <S**2>=0.000
     105 ->130        -0.11938
     111 ->130        -0.17943
     112 ->130         0.62274

 Excited state symmetry could not be determined.
 Excited State  62:      Singlet-?Sym    4.7540 eV  260.80 nm
f=0.0063  <S**2>=0.000
      98 ->129         0.27120
     100 ->129         0.32495
     125 ->132         0.26389
     125 ->133        -0.14923
     125 ->134         0.11238
     126 ->132         0.36592
     126 ->134         0.18414

 Excited state symmetry could not be determined.
 Excited State  63:      Singlet-?Sym    4.7574 eV  260.61 nm
f=0.0026  <S**2>=0.000
      98 ->129         0.30535
     100 ->129         0.38855
     124 ->134         0.10690
     125 ->134        -0.16002
     126 ->132        -0.31768
     126 ->133         0.27248

 Excited state symmetry could not be determined.
 Excited State  64:      Singlet-?Sym    4.7627 eV  260.32 nm
f=0.0101  <S**2>=0.000
      98 ->129        -0.11270
     100 ->129        -0.15732
     125 ->132         0.41299
     125 ->133        -0.30124
     125 ->134        -0.14606
     126 ->132        -0.19175
     126 ->133         0.21800
     126 ->134         0.20932
```

```
 Excited state symmetry could not be determined.
 Excited State  65:      Singlet-?Sym    4.7876 eV  258.97 nm
f=0.0004  <S**2>=0.000
      99 ->129         0.59302
     125 ->132         0.11444
     125 ->133         0.21363
     125 ->134         0.13097

 Excited state symmetry could not be determined.
 Excited State  66:      Singlet-?Sym    4.7930 eV  258.68 nm
f=0.0031  <S**2>=0.000
      99 ->129        -0.17738
     123 ->134         0.11960
     124 ->132        -0.34048
     125 ->133         0.26039
     125 ->134        -0.10377
     126 ->133         0.10315
     126 ->134         0.41077

 Excited state symmetry could not be determined.
 Excited State  67:      Singlet-?Sym    4.7942 eV  258.62 nm
f=0.0081  <S**2>=0.000
      98 ->129        -0.10525
      99 ->129         0.19568
     122 ->133        -0.18411
     123 ->132         0.14327
     124 ->133         0.33329
     125 ->132        -0.26534
     125 ->133        -0.23268
     125 ->134         0.15002
     126 ->134         0.26866

 Excited state symmetry could not be determined.
 Excited State  68:      Singlet-?Sym    4.8023 eV  258.18 nm
f=0.0007  <S**2>=0.000
      98 ->129         0.46550
     100 ->129        -0.44124
     125 ->134         0.10039
     126 ->133         0.15243

 Excited state symmetry could not be determined.
 Excited State  69:      Singlet-?Sym    4.8029 eV  258.14 nm
f=0.0003  <S**2>=0.000
      99 ->129        -0.23840
     119 ->134         0.10861
     122 ->134        -0.10277
     123 ->132        -0.13256
     123 ->133         0.11748
     124 ->134         0.13084
     125 ->134         0.52834
```

```
     126 ->132        -0.11946
     127 ->134         0.11680

 Excited state symmetry could not be determined.
 Excited State  70:      Singlet-?Sym    4.8269 eV  256.86 nm
f=0.0049  <S**2>=0.000
      98 ->129        -0.19066
     120 ->132        -0.13776
     120 ->133        -0.19926
     123 ->132        -0.21056
     123 ->133        -0.29994
     126 ->132         0.22389
     126 ->133         0.34723
     126 ->134        -0.19113

 Excited state symmetry could not be determined.
 Excited State  71:      Singlet-?Sym    4.8306 eV  256.67 nm
f=0.0378  <S**2>=0.000
     121 ->131        -0.10805
     122 ->133         0.11011
     123 ->132        -0.22775
     123 ->133         0.14831
     124 ->132         0.25731
     124 ->133         0.39340
     124 ->134        -0.31497

 Excited state symmetry could not be determined.
 Excited State  72:      Singlet-?Sym    4.8523 eV  255.52 nm
f=0.0052  <S**2>=0.000
     113 ->130         0.62034
     120 ->131        -0.10484
     121 ->131        -0.11621

 Excited state symmetry could not be determined.
 Excited State  73:      Singlet-?Sym    4.8729 eV  254.44 nm
f=0.0106  <S**2>=0.000
     121 ->134         0.15489
     122 ->132         0.23728
     122 ->133        -0.11796
     123 ->134         0.44797
     124 ->132         0.33154
     124 ->133        -0.17318

 Excited state symmetry could not be determined.
 Excited State  74:      Singlet-?Sym    4.8786 eV  254.14 nm
f=0.0574  <S**2>=0.000
     118 ->131         0.10533
     120 ->131         0.31435
     121 ->131         0.36638
     122 ->134         0.11442
```

```
     123 ->131        -0.24683
     124 ->133         0.20906
     125 ->132         0.13423
     125 ->133         0.20056

 Excited state symmetry could not be determined.
 Excited State  75:      Singlet-?Sym    4.9131 eV  252.36 nm
f=0.0125  <S**2>=0.000
     113 ->130        -0.16834
     120 ->131        -0.17745
     121 ->131        -0.19494
     122 ->132         0.12993
     122 ->133         0.18445
     122 ->134         0.30072
     123 ->132         0.25629
     123 ->133        -0.19777
     124 ->133         0.13248
     124 ->134         0.22186
     125 ->133         0.13618

 Excited state symmetry could not be determined.
 Excited State  76:      Singlet-?Sym    4.9659 eV  249.67 nm
f=0.0166  <S**2>=0.000
      97 ->129         0.51024
     119 ->131         0.10573
     122 ->132        -0.28995
     122 ->133         0.20922
     124 ->132         0.14242

 Excited state symmetry could not be determined.
 Excited State  77:      Singlet-?Sym    4.9789 eV  249.02 nm
f=0.0079  <S**2>=0.000
      97 ->129        -0.30545
     121 ->134        -0.10314
     122 ->132        -0.14758
     122 ->133         0.10189
     123 ->134        -0.26072
     124 ->132         0.32876
     124 ->133        -0.21723
     125 ->132        -0.14978
     126 ->134         0.27924

 Excited state symmetry could not be determined.
 Excited State  78:      Singlet-?Sym    4.9855 eV  248.69 nm
f=0.0013  <S**2>=0.000
     123 ->132        -0.23259
     123 ->133         0.14888
     124 ->133         0.10010
     124 ->134         0.50499
     125 ->134        -0.18740
```

```
     126 ->132         0.23067
     126 ->133        -0.16956

 Excited state symmetry could not be determined.
 Excited State  79:      Singlet-?Sym    4.9893 eV  248.50 nm
f=0.0100  <S**2>=0.000
      97 ->129         0.32501
     119 ->131        -0.22295
     119 ->132         0.12521
     122 ->132         0.28334
     122 ->133        -0.19633
     123 ->133        -0.12572
     123 ->134        -0.28569
     124 ->132         0.11659
     124 ->133        -0.10291
     126 ->134         0.17219

 Excited state symmetry could not be determined.
 Excited State  80:      Singlet-?Sym    5.0133 eV  247.31 nm
f=0.0051  <S**2>=0.000
     111 ->130         0.65431
     112 ->130         0.19854
```

Table S33. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 1^+(*S*=1/2)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  2.014-?Sym    0.7558 eV 1640.37 nm  f=0.0013
<S**2>=0.764
    120B ->129B       -0.19531
    121B ->129B        0.35950
    123B ->129B        0.41216
    125B ->129B        0.35379
    128B ->129B        0.71717
 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 symmetry could not be determined.
 Excited State   2:  2.153-?Sym    0.8545 eV 1450.95 nm  f=0.0001
<S**2>=0.909
    128A ->130A       -0.16311
    124B ->129B       -0.13228
    126B ->129B        0.49769
    127B ->129B        0.79543
    128B ->130B       -0.20114

 Excited state symmetry could not be determined.
 Excited State   3:  3.196-?Sym    0.9858 eV 1257.71 nm  f=0.0006
<S**2>=2.303
    121A ->130A       -0.10619
    122A ->130A        0.14019
    128A ->130A       -0.37868
    129A ->130A        0.60618
    120B ->130B        0.14921
    126B ->129B       -0.14208
    127B ->129B       -0.21636
    128B ->130B       -0.60459
    129A <-130A        0.12442
    128B <-130B       -0.14094

 Excited state symmetry could not be determined.
 Excited State   4:  3.421-?Sym    1.5137 eV  819.07 nm  f=0.0055
<S**2>=2.676
    124A ->130A       -0.40534
    126A ->130A       -0.10976
    127A ->130A       -0.41562
    124B ->130B       -0.15333
    126B ->130B        0.37673
    127B ->130B        0.69417
```

```
 Excited state symmetry could not be determined.
 Excited State   5:  2.638-?Sym    1.6755 eV  739.97 nm  f=0.0150
<S**2>=1.490
    128A ->130A        0.42039
    129A ->130A        0.69772
    121B ->130B        0.15022
    123B ->130B        0.17967
    125B ->130B        0.14609
    127B ->129B        0.10568
    128B ->130B        0.47565

 Excited state symmetry could not be determined.
 Excited State   6:  2.229-?Sym    1.8083 eV  685.63 nm  f=0.0310
<S**2>=0.992
    128A ->130A        0.71289
    121B ->130B       -0.21330
    123B ->130B       -0.28097
    125B ->130B       -0.31050
    128B ->130B       -0.49194

 Excited state symmetry could not be determined.
 Excited State   7:  2.048-?Sym    1.9149 eV  647.45 nm  f=0.0375
<S**2>=0.798
    124B ->129B       -0.12914
    126B ->129B        0.81719
    127B ->129B       -0.53794

 Excited state symmetry could not be determined.
 Excited State   8:  2.040-?Sym    1.9445 eV  637.61 nm  f=0.0041
<S**2>=0.790
    124A ->130A        0.12548
    127A ->130A        0.21001
    121B ->129B       -0.27647
    123B ->129B       -0.33756
    125B ->129B       -0.55071
    127B ->130B        0.11971
    128B ->129B        0.63889

 Excited state symmetry could not be determined.
 Excited State   9:  2.039-?Sym    2.0927 eV  592.45 nm  f=0.0696
<S**2>=0.789
    126A ->130A       -0.14594
    127A ->130A       -0.17100
    120B ->129B        0.31934
    121B ->129B       -0.41394
    123B ->129B       -0.39563
    125B ->129B        0.63369
    127B ->130B       -0.16739
    128B ->129B        0.22278
```

```
 Excited state symmetry could not be determined.
 Excited State  10:  3.010-?Sym    2.1287 eV  582.45 nm  f=0.0737
<S**2>=2.015
    121A ->130A        0.49122
    125A ->130A       -0.21116
    128A ->130A       -0.30463
    129A ->130A        0.32217
    121B ->130B       -0.27832
    123B ->130B       -0.42561
    125B ->130B       -0.40829
    128B ->130B        0.23869

 Excited state symmetry could not be determined.
 Excited State  11:  2.560-?Sym    2.2021 eV  563.04 nm  f=0.0069
<S**2>=1.388
    127A ->130A       -0.27140
    124B ->130B       -0.16320
    125B ->129B       -0.19649
    126B ->130B        0.66755
    127B ->130B       -0.62712

 Excited state symmetry could not be determined.
 Excited State  12:  3.427-?Sym    2.2989 eV  539.32 nm  f=0.0000
<S**2>=2.687
    124A ->130A       -0.38044
    126A ->130A        0.63119
    127A ->130A        0.23461
    123B ->130B       -0.10353
    124B ->130B       -0.57491
    126B ->130B       -0.11266

 Excited state symmetry could not be determined.
 Excited State  13:  3.250-?Sym    2.3263 eV  532.97 nm  f=0.0181
<S**2>=2.390
    121A ->130A        0.12628
    122A ->130A       -0.31211
    125A ->130A       -0.37600
    120B ->130B       -0.19810
    121B ->130B       -0.13222
    123B ->130B       -0.27364
    124B ->129B        0.27412
    125B ->130B        0.69317
    128B ->130B       -0.12324

 Excited state symmetry could not be determined.
 Excited State  14:  3.014-?Sym    2.3288 eV  532.39 nm  f=0.0221
<S**2>=2.021
    124A ->130A       -0.23073
    126A ->130A       -0.21990
    127A ->130A        0.77222
```

```
    124B ->130B        0.14899
    125B ->129B        0.19389
    126B ->130B        0.45574

 Excited state symmetry could not be determined.
 Excited State  15:  2.175-?Sym    2.4034 eV  515.87 nm  f=0.0002
<S**2>=0.932
    125A ->130A        0.14926
    119B ->129B       -0.22134
    123B ->129B        0.15393
    124B ->129B        0.88803
    125B ->130B       -0.19454
    126B ->129B        0.17153

 Excited state symmetry could not be determined.
 Excited State  16:  2.511-?Sym    2.5106 eV  493.84 nm  f=0.0784
<S**2>=1.326
    121A ->130A        0.39531
    122A ->130A        0.67378
    125A ->130A        0.33717
    126A ->130A       -0.10223
    128A ->130A        0.15093
    129A ->130A       -0.11181
    120B ->130B        0.13561
    123B ->130B       -0.13043
    125B ->130B        0.39788

 Excited state symmetry could not be determined.
 Excited State  17:  2.187-?Sym    2.5210 eV  491.80 nm  f=0.0042
<S**2>=0.946
    124A ->130A        0.28255
    126A ->130A        0.67069
    120B ->129B       -0.15046
    123B ->129B       -0.20203
    124B ->130B        0.42894
    125B ->129B        0.18501
    126B ->130B        0.32557
    127B ->130B        0.13172

 Excited state symmetry could not be determined.
 Excited State  18:  2.275-?Sym    2.5381 eV  488.48 nm  f=0.0261
<S**2>=1.044
    121A ->130A       -0.42964
    122A ->130A       -0.22466
    125A ->130A        0.50989
    128A ->130A       -0.12446
    120B ->130B        0.24639
    121B ->130B       -0.30995
    123B ->130B       -0.49363
    125B ->130B        0.12204
```

```
    128B ->130B        0.20679

 Excited state symmetry could not be determined.
 Excited State  19:  2.964-?Sym    2.6263 eV  472.08 nm  f=0.0019
<S**2>=1.946
    123A ->130A        0.62660
    124A ->130A        0.11558
    125A ->130A       -0.12136
    120B ->129B       -0.17045
    121B ->129B        0.35637
    122B ->130B       -0.41784
    123B ->129B       -0.41549

 Excited state symmetry could not be determined.
 Excited State  20:  3.267-?Sym    2.6305 eV  471.34 nm  f=0.0007
<S**2>=2.418
    121A ->130A        0.39082
    122A ->130A       -0.39048
    123A ->130A        0.15879
    125A ->130A        0.50497
    120B ->130B       -0.26673
    121B ->130B       -0.29913
    122B ->129B        0.26964
    122B ->130B       -0.10482
    123B ->129B       -0.10836
    123B ->130B        0.33719

 Excited state symmetry could not be determined.
 Excited State  21:  2.615-?Sym    2.6460 eV  468.57 nm  f=0.0134
<S**2>=1.459
    123A ->130A        0.53176
    124A ->130A       -0.15244
    126A ->130A        0.16715
    120B ->129B        0.26908
    121B ->129B       -0.38664
    122B ->130B       -0.26132
    123B ->129B        0.46821
    124B ->130B        0.34997

 Excited state symmetry could not be determined.
 Excited State  22:  2.163-?Sym    2.6730 eV  463.84 nm  f=0.0015
<S**2>=0.920
    121A ->130A       -0.16904
    122A ->130A        0.14123
    125A ->130A       -0.19705
    119B ->129B       -0.21645
    120B ->130B        0.17971
    122B ->129B        0.88826
    124B ->129B       -0.12885
```

```
 Excited state symmetry could not be determined.
 Excited State  23:  2.065-?Sym    2.7122 eV  457.13 nm  f=0.0313
<S**2>=0.816
    123A ->130A        0.42907
    124A ->130A        0.40632
    120B ->129B       -0.24193
    121B ->129B       -0.31708
    122B ->130B        0.51203
    123B ->129B        0.15423
    124B ->130B       -0.37374
    125B ->129B        0.10717
    126B ->130B        0.13602
    127B ->130B        0.10567

 Excited state symmetry could not be determined.
 Excited State  24:  2.526-?Sym    2.7233 eV  455.28 nm  f=0.0005
<S**2>=1.346
    125A ->130A        0.28695
    120B ->130B       -0.36477
    121B ->130B        0.70736
    122B ->129B        0.20986
    123B ->130B       -0.44227

 Excited state symmetry could not be determined.
 Excited State  25:  2.125-?Sym    2.7606 eV  449.12 nm  f=0.0293
<S**2>=0.879
    123A ->130A        0.30808
    124A ->130A       -0.33471
    120B ->129B        0.29078
    121B ->129B        0.35568
    122B ->130B        0.67482
    123B ->129B       -0.18471
    124B ->130B        0.22040

 Excited state symmetry could not be determined.
 Excited State  26:  2.073-?Sym    2.8221 eV  439.33 nm  f=0.0004
<S**2>=0.824
    121A ->130A       -0.10901
    122A ->130A        0.10180
    119B ->129B        0.90166
    120B ->130B       -0.17011
    122B ->129B        0.24377
    124B ->129B        0.17573

 Excited state symmetry could not be determined.
 Excited State  27:  2.376-?Sym    2.8893 eV  429.12 nm  f=0.0031
<S**2>=1.161
    119A ->130A       -0.13766
    121A ->130A        0.39433
    122A ->130A       -0.37955
```

```
    119B ->129B        0.22215
    120B ->130B        0.69740
    121B ->130B        0.31990

 Excited state symmetry could not be determined.
 Excited State  28:  2.082-?Sym    2.9434 eV  421.23 nm  f=0.1302
<S**2>=0.833
    124A ->130A        0.42539
    129A ->131A        0.13828
    118B ->129B        0.18261
    119B ->130B        0.11919
    120B ->129B        0.67441
    121B ->129B        0.31258
    123B ->129B        0.10358
    124B ->130B       -0.20315
    126B ->130B        0.19181
    127B ->130B        0.17565

 Excited state symmetry could not be determined.
 Excited State  29:  2.983-?Sym    3.0967 eV  400.38 nm  f=0.0025
<S**2>=1.975
    119A ->134A        0.10079
    124A ->132A        0.13282
    126A ->132A        0.10059
    127A ->132A       -0.24917
    128A ->131A        0.44378
    129A ->131A        0.48044
    118B ->129B        0.22951
    120B ->129B       -0.21753
    125B ->131B       -0.20183
    125B ->132B       -0.10270
    126B ->131B       -0.12773
    126B ->132B        0.18603
    127B ->131B        0.16840
    127B ->132B       -0.22999
    128B ->131B       -0.24817
    128B ->132B       -0.13651

 Excited state symmetry could not be determined.
 Excited State  30:  3.237-?Sym    3.1328 eV  395.76 nm  f=0.0012
<S**2>=2.369
    121A ->133A       -0.10389
    124A ->134A       -0.11523
    127A ->131A       -0.35705
    128A ->132A        0.41090
    129A ->132A        0.41702
    125B ->131B        0.12820
    125B ->132B       -0.21894
    126B ->131B        0.16414
    126B ->132B        0.12430
```

```
    126B ->134B        0.12297
    127B ->131B       -0.33405
    127B ->132B       -0.22229
    128B ->131B        0.13891
    128B ->132B       -0.26064

 Excited state symmetry could not be determined.
 Excited State  31:  2.192-?Sym    3.1581 eV  392.59 nm  f=0.0016
<S**2>=0.951
    121A ->134A       -0.11131
    122A ->134A       -0.12226
    129A ->131A       -0.26919
    129A ->134A       -0.26432
    118B ->129B        0.81101
    120B ->129B       -0.17432
    127B ->132B        0.13780
    128B ->134B        0.11121

 Excited state symmetry could not be determined.
 Excited State  32:  3.215-?Sym    3.1779 eV  390.15 nm  f=0.0004
<S**2>=2.334
    120A ->130A       -0.21777
    121A ->131A        0.24618
    121A ->134A        0.29436
    122A ->131A        0.16753
    122A ->134A        0.20791
    128A ->131A       -0.13497
    128A ->134A       -0.21701
    129A ->131A        0.26225
    129A ->134A        0.18948
    118B ->129B        0.33456
    119B ->130B        0.28229
    121B ->134B       -0.16616
    123B ->131B        0.10910
    123B ->134B       -0.19493
    125B ->134B       -0.16438
    128B ->131B        0.19075
    128B ->132B        0.10693
    128B ->134B       -0.30550

 Excited state symmetry could not be determined.
 Excited State  33:  3.387-?Sym    3.2266 eV  384.25 nm  f=0.0000
<S**2>=2.619
    120A ->130A       -0.53580
    127A ->134A       -0.10182
    129A ->131A       -0.11079
    118B ->129B       -0.18212
    119B ->130B        0.68242
    127B ->134B        0.13283
```

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 Excited state symmetry could not be determined.
 Excited State  34:  3.364-?Sym    3.2279 eV  384.11 nm  f=0.0001
<S**2>=2.580
    119A ->130A       -0.17327
    120A ->130A        0.16477
    124A ->131A       -0.27959
    124A ->134A       -0.29610
    126A ->131A       -0.14361
    126A ->134A       -0.13738
    127A ->131A       -0.16863
    127A ->134A       -0.32101
    128A ->132A       -0.10896
    129A ->132A       -0.17138
    119B ->130B       -0.20413
    126B ->131B       -0.23170
    126B ->132B       -0.13195
    126B ->134B        0.26760
    126B ->136B        0.10043
    127B ->131B       -0.16311
    127B ->134B        0.41845
    127B ->136B        0.15156

 Excited state symmetry could not be determined.
 Excited State  35:  3.049-?Sym    3.2476 eV  381.77 nm  f=0.0005
<S**2>=2.074
    116A ->130A       -0.13524
    118A ->130A        0.10288
    119A ->130A        0.63173
    121A ->132A        0.10857
    121A ->133A        0.21898
    121A ->135A       -0.10531
    122A ->133A        0.12778
    127A ->131A       -0.10768
    128A ->133A       -0.26602
    118B ->130B        0.10557
    120B ->130B        0.21278
    121B ->133B       -0.12427
    123B ->133B       -0.12841
    123B ->135B       -0.11654
    128B ->133B       -0.28848

 Excited state symmetry could not be determined.
 Excited State  36:  3.161-?Sym    3.2729 eV  378.82 nm  f=0.0004
<S**2>=2.248
    116A ->130A       -0.13110
    119A ->130A        0.57649
    121A ->132A       -0.13017
    121A ->133A       -0.24542
    122A ->133A       -0.13813
    127A ->131A        0.10017
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    128A ->133A        0.26969
    129A ->132A       -0.18382
    120B ->130B        0.10175
    121B ->133B        0.17039
    123B ->133B        0.19209
    125B ->133B        0.14607
    127B ->131B        0.11489
    128B ->133B        0.28293
    128B ->135B        0.19344

 Excited state symmetry could not be determined.
 Excited State  37:  2.501-?Sym    3.3367 eV  371.58 nm  f=0.0111
<S**2>=1.314
    119A ->131A        0.13508
    119A ->134A        0.11280
    120A ->130A        0.49439
    127A ->132A        0.21517
    128A ->134A        0.24657
    129A ->131A        0.13681
    129A ->134A        0.38922
    118B ->129B        0.13221
    119B ->130B        0.40326
    126B ->132B       -0.11743
    127B ->131B       -0.12566
    127B ->132B        0.20060
    128B ->134B        0.17786

 Excited state symmetry could not be determined.
 Excited State  38:  2.352-?Sym    3.3540 eV  369.66 nm  f=0.0199
<S**2>=1.133
    119A ->131A       -0.11917
    119A ->134A       -0.10757
    120A ->130A        0.58285
    124A ->133A       -0.11913
    127A ->132A       -0.22300
    128A ->134A       -0.23426
    129A ->131A       -0.11760
    129A ->134A       -0.37498
    119B ->130B        0.45011
    127B ->132B       -0.13448
    128B ->134B       -0.11207

 Excited state symmetry could not be determined.
 Excited State  39:  2.188-?Sym    3.5011 eV  354.13 nm  f=0.0019
<S**2>=0.947
    118A ->133A        0.12425
    119A ->132A        0.11826
    119A ->133A        0.19210
    124A ->134A        0.11515
    127A ->131A        0.20471
```

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    128A ->133A        0.27035
    128A ->135A       -0.10336
    129A ->132A        0.25881
    129A ->133A        0.66090
    129A ->135A       -0.17158
    126B ->131B       -0.15657
    126B ->134B        0.13315
    127B ->134B        0.22019

 Excited state symmetry could not be determined.
 Excited State  40:  3.392-?Sym    3.5077 eV  353.47 nm  f=0.0003
<S**2>=2.626
    124A ->132A       -0.18437
    124A ->133A       -0.29545
    124A ->135A        0.12149
    126A ->132A       -0.11905
    126A ->133A       -0.19426
    127A ->132A       -0.12268
    127A ->133A       -0.35043
    127A ->135A        0.10553
    129A ->134A        0.17563
    126B ->132B       -0.16934
    126B ->133B        0.31722
    126B ->135B        0.16071
    127B ->132B       -0.13760
    127B ->133B        0.46832
    127B ->135B        0.22651
    127B ->140B        0.13373

 Excited state symmetry could not be determined.
 Excited State  41:  3.127-?Sym    3.5988 eV  344.51 nm  f=0.0023
<S**2>=2.195
    116A ->130A       -0.13128
    118A ->130A       -0.34378
    119A ->130A       -0.14966
    116B ->130B        0.16342
    118B ->130B        0.85184

 Excited state symmetry could not be determined.
 Excited State  42:  2.065-?Sym    3.6576 eV  338.98 nm  f=0.0103
<S**2>=0.816
    118A ->130A        0.12112
    121A ->132A       -0.11674
    121A ->133A       -0.21766
    122A ->133A       -0.12558
    124A ->131A       -0.19455
    124A ->134A       -0.22588
    126A ->131A       -0.10365
    126A ->134A       -0.10336
    127A ->131A       -0.25464
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    127A ->134A       -0.25668
    128A ->132A        0.22518
    128A ->133A        0.31097
    121B ->133B       -0.11669
    123B ->133B       -0.14199
    125B ->133B       -0.15115
    126B ->131B        0.11342
    126B ->134B       -0.15608
    127B ->131B        0.24841
    127B ->132B        0.14582
    127B ->134B       -0.23373
    128B ->131B       -0.12214
    128B ->132B        0.19201
    128B ->133B       -0.24558
    128B ->135B       -0.12590

 Excited state symmetry could not be determined.
 Excited State  43:  2.273-?Sym    3.7313 eV  332.28 nm  f=0.0067
<S**2>=1.041
    118A ->130A       -0.59104
    119A ->130A        0.20108
    115B ->129B        0.11035
    117B ->129B        0.63942
    118B ->130B       -0.26033

 Excited state symmetry could not be determined.
 Excited State  44:  2.283-?Sym    3.7462 eV  330.96 nm  f=0.0031
<S**2>=1.054
    118A ->130A        0.62138
    119A ->130A       -0.13468
    129A ->132A        0.11321
    129A ->133A        0.10062
    115B ->129B        0.12087
    117B ->129B        0.66115
    118B ->130B        0.17069

 Excited state symmetry could not be determined.
 Excited State  45:  3.318-?Sym    3.7702 eV  328.85 nm  f=0.0019
<S**2>=2.502
    122A ->133A       -0.17872
    123A ->137A        0.24258
    125A ->138A        0.21759
    126A ->134A       -0.17392
    126A ->136A       -0.16620
    126A ->139A       -0.13770
    128A ->133A       -0.26011
    128A ->140A        0.10688
    129A ->133A        0.17416
    117B ->129B       -0.12811
    118B ->130B       -0.11731
```

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    120B ->133B       -0.15473
    121B ->135B        0.14570
    121B ->138B       -0.11426
    122B ->137B       -0.24793
    123B ->133B        0.11563
    123B ->138B        0.18768
    124B ->134B        0.17739
    124B ->136B       -0.12964
    124B ->139B        0.12830
    125B ->133B        0.26739
    127B ->131B        0.12841
    128B ->135B        0.12907
    128B ->140B        0.16094

 Excited state symmetry could not be determined.
 Excited State  46:  3.456-?Sym    3.7792 eV  328.07 nm  f=0.0000
<S**2>=2.736
    122A ->137A        0.17077
    123A ->135A       -0.14425
    123A ->138A       -0.23372
    124A ->133A        0.16465
    125A ->136A       -0.13408
    125A ->137A       -0.20349
    125A ->139A       -0.11651
    126A ->133A       -0.20862
    126A ->138A        0.10357
    126A ->140A        0.17512
    128A ->134A       -0.15132
    128A ->136A       -0.15488
    128A ->137A        0.11635
    129A ->136A        0.16637
    121B ->137B        0.19066
    122B ->135B       -0.15362
    122B ->138B        0.22916
    123B ->137B       -0.18264
    124B ->133B        0.25980
    124B ->140B       -0.14902
    125B ->134B        0.18284
    125B ->136B       -0.11014
    125B ->139B        0.10019
    128B ->134B       -0.13371
    128B ->136B        0.18016
    128B ->137B        0.12888
    128B ->139B       -0.10453

 Excited state symmetry could not be determined.
 Excited State  47:  3.434-?Sym    3.7986 eV  326.39 nm  f=0.0012
<S**2>=2.698
    109A ->130A        0.14064
    112A ->130A        0.11965
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    115A ->130A       -0.50687
    117A ->130A        0.33491
    120A ->130A        0.13063
    128A ->139A        0.10722
    129A ->136A        0.11766
    129A ->139A       -0.13284
    109B ->130B       -0.11672
    115B ->130B        0.52228
    117B ->130B       -0.22018
    128B ->136B        0.13800
    128B ->139B        0.14390

 Excited state symmetry could not be determined.
 Excited State  48:  3.334-?Sym    3.8042 eV  325.91 nm  f=0.0000
<S**2>=2.528
    107A ->130A        0.11028
    111A ->130A       -0.12989
    114A ->130A        0.19211
    116A ->130A        0.45508
    119A ->130A        0.28057
    128A ->135A        0.14732
    129A ->135A       -0.18462
    105B ->130B       -0.11153
    111B ->130B        0.11575
    114B ->130B       -0.27985
    116B ->130B       -0.36311
    118B ->130B        0.31794
    128B ->133B        0.17544
    128B ->135B       -0.13827

 Excited state symmetry could not be determined.
 Excited State  49:  2.147-?Sym    3.8409 eV  322.80 nm  f=0.0016
<S**2>=0.902
    121A ->131A       -0.13970
    121A ->134A       -0.20318
    122A ->131A       -0.10667
    122A ->134A       -0.16922
    127A ->133A       -0.10485
    128A ->131A        0.42937
    128A ->134A        0.27738
    114B ->129B       -0.11867
    116B ->129B        0.32861
    123B ->131B        0.10354
    125B ->131B        0.12554
    125B ->134B       -0.10091
    127B ->132B        0.15784
    128B ->131B        0.43967
    128B ->132B        0.25062
    128B ->134B       -0.21302
```

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 Excited state symmetry could not be determined.
 Excited State  50:  2.324-?Sym    3.8537 eV  321.73 nm  f=0.0094
<S**2>=1.100
    118A ->130A       -0.24071
    121A ->132A        0.12259
    121A ->133A        0.20541
    121A ->135A       -0.10707
    122A ->132A        0.11511
    122A ->133A        0.21944
    124A ->131A       -0.14916
    124A ->134A       -0.18339
    127A ->131A       -0.16101
    127A ->134A       -0.22126
    128A ->132A       -0.13235
    128A ->133A       -0.14910
    129A ->132A        0.30586
    129A ->133A        0.22012
    116B ->130B        0.10719
    118B ->130B       -0.13175
    121B ->133B        0.13514
    123B ->133B        0.11656
    126B ->134B       -0.10648
    127B ->131B        0.28352
    127B ->132B        0.12826
    127B ->134B       -0.13415
    128B ->133B        0.31015
    128B ->135B        0.11272

 Excited state symmetry could not be determined.
 Excited State  51:  2.111-?Sym    3.9352 eV  315.06 nm  f=0.0001
<S**2>=0.864
    124A ->132A        0.10670
    124A ->133A        0.11050
    127A ->132A        0.10649
    127A ->133A        0.15454
    128A ->131A       -0.12331
    113B ->129B       -0.11660
    114B ->129B       -0.27186
    116B ->129B        0.79229
    127B ->131B        0.12089
    127B ->132B       -0.19541
    127B ->133B        0.10249
    128B ->131B       -0.11025

 Excited state symmetry could not be determined.
 Excited State  52:  2.858-?Sym    3.9980 eV  310.12 nm  f=0.0157
<S**2>=1.791
    122A ->133A       -0.10583
    127A ->131A        0.16303
    129A ->132A        0.48704
```

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    129A ->133A       -0.32785
    123B ->132B        0.10703
    125B ->132B        0.10585
    127B ->131B       -0.11082
    128B ->131B       -0.36305
    128B ->132B        0.55838
    128B ->133B        0.12590

 Excited state symmetry could not be determined.
 Excited State  53:  2.671-?Sym    4.0238 eV  308.13 nm  f=0.0009
<S**2>=1.534
    117A ->130A        0.10123
    124A ->133A       -0.19655
    127A ->133A       -0.25513
    128A ->131A       -0.18912
    128A ->134A       -0.14832
    129A ->131A        0.41054
    129A ->134A       -0.18886
    116B ->129B        0.21924
    126B ->131B       -0.11097
    126B ->132B        0.18819
    127B ->131B       -0.30866
    127B ->132B        0.52771
    128B ->131B       -0.17617
    128B ->132B       -0.16086

 Excited state symmetry could not be determined.
 Excited State  54:  3.015-?Sym    4.0363 eV  307.17 nm  f=0.0013
<S**2>=2.022
    121A ->134A       -0.15723
    122A ->134A       -0.12491
    127A ->132A        0.13153
    128A ->131A       -0.36615
    129A ->131A        0.46111
    129A ->134A       -0.33154
    121B ->134B        0.10355
    123B ->134B        0.13359
    125B ->134B        0.14417
    127B ->131B        0.17001
    127B ->132B       -0.24700
    128B ->131B        0.37092
    128B ->132B        0.21913
    128B ->134B        0.26506

 Excited state symmetry could not be determined.
 Excited State  55:  2.981-?Sym    4.0626 eV  305.18 nm  f=0.0090
<S**2>=1.971
    127A ->131A        0.40302
    129A ->132A        0.35917
    129A ->133A       -0.27352
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    126B ->134B        0.17780
    127B ->131B        0.38191
    127B ->132B        0.26307
    127B ->134B        0.26677
    128B ->131B        0.19199
    128B ->132B       -0.32778
    128B ->133B       -0.15293

 Excited state symmetry could not be determined.
 Excited State  56:  2.487-?Sym    4.1392 eV  299.54 nm  f=0.0052
<S**2>=1.296
    121A ->133A        0.12779
    124A ->131A        0.10538
    127A ->132A       -0.12238
    128A ->132A        0.48889
    128A ->133A       -0.18193
    129A ->132A       -0.32148
    129A ->133A        0.11865
    126B ->131B        0.26874
    126B ->132B        0.21251
    126B ->134B        0.18872
    127B ->131B        0.27120
    127B ->132B        0.17265
    127B ->134B        0.30546
    128B ->131B       -0.12860
    128B ->132B        0.29756

 Excited state symmetry could not be determined.
 Excited State  57:  2.634-?Sym    4.1400 eV  299.48 nm  f=0.0003
<S**2>=1.485
    124A ->132A        0.20869
    124A ->133A        0.12700
    126A ->132A        0.12795
    127A ->132A        0.51115
    127A ->133A        0.18095
    128A ->131A        0.32355
    128A ->134A       -0.15453
    129A ->134A       -0.18877
    116B ->129B       -0.15328
    117B ->130B       -0.20411
    126B ->132B        0.12480
    126B ->133B        0.21575
    127B ->132B        0.12718
    127B ->133B        0.41374
    127B ->135B        0.16280

 Excited state symmetry could not be determined.
 Excited State  58:  2.630-?Sym    4.1594 eV  298.08 nm  f=0.0001
<S**2>=1.479
    127A ->132A       -0.35775
```

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    129A ->131A       -0.25032
    129A ->134A        0.21942
    117B ->130B       -0.13032
    121B ->134B        0.11548
    123B ->134B        0.13967
    125B ->131B       -0.10764
    125B ->134B        0.13091
    126B ->131B       -0.30063
    126B ->132B        0.39408
    127B ->131B       -0.14166
    127B ->132B        0.14610
    127B ->133B        0.11062
    128B ->131B        0.35807
    128B ->132B        0.18645
    128B ->134B        0.28815

 Excited state symmetry could not be determined.
 Excited State  59:  2.845-?Sym    4.2234 eV  293.57 nm  f=0.0102
<S**2>=1.773
    121A ->133A        0.12202
    124A ->131A       -0.21431
    126A ->131A       -0.13487
    127A ->131A        0.32191
    128A ->132A        0.61014
    128A ->133A       -0.20347
    126B ->131B       -0.34938
    126B ->132B       -0.22814
    126B ->134B       -0.10916
    127B ->131B       -0.16161
    127B ->132B       -0.10555
    127B ->134B       -0.27869

 Excited state symmetry could not be determined.
 Excited State  60:  3.337-?Sym    4.2695 eV  290.40 nm  f=0.0006
<S**2>=2.534
    115A ->130A       -0.26348
    117A ->130A       -0.42447
    115B ->130B        0.24557
    117B ->130B        0.75165
    127B ->132B        0.10141
    127B ->133B        0.12234

 Excited state symmetry could not be determined.
 Excited State  61:  2.420-?Sym    4.3185 eV  287.10 nm  f=0.0000
<S**2>=1.214
    117A ->130A       -0.16611
    121A ->131A        0.10084
    121A ->134A        0.19729
    122A ->131A        0.14032
    122A ->134A        0.11747
```

```
    124A ->132A       -0.21329
    126A ->132A       -0.18300
    127A ->133A       -0.14941
    128A ->131A        0.45301
    128A ->134A       -0.43989
    116B ->129B        0.11700
    117B ->130B       -0.17744
    126B ->131B        0.11886
    126B ->132B       -0.20753
    127B ->133B       -0.24536
    128B ->131B        0.11128
    128B ->134B        0.29746

 Excited state symmetry could not be determined.
 Excited State  62:  2.994-?Sym    4.3622 eV  284.22 nm  f=0.0142
<S**2>=1.991
    116A ->130A        0.16628
    121A ->133A       -0.11845
    124A ->134A       -0.22818
    125A ->138A       -0.12611
    126A ->131A        0.10930
    127A ->131A        0.34444
    127A ->134A       -0.24712
    128A ->133A       -0.14188
    128A ->135A       -0.12440
    129A ->133A        0.13305
    129A ->135A        0.20408
    116B ->130B       -0.31981
    120B ->135B       -0.10379
    123B ->138B       -0.10720
    126B ->131B        0.28247
    126B ->132B        0.16624
    126B ->134B       -0.15672
    127B ->131B       -0.20441
    127B ->132B       -0.12243
    128B ->133B       -0.19880
    128B ->135B        0.18064

 Excited state symmetry could not be determined.
 Excited State  63:  3.032-?Sym    4.3797 eV  283.09 nm  f=0.0173
<S**2>=2.048
    116A ->130A       -0.24724
    121A ->132A        0.11164
    121A ->133A        0.15132
    122A ->135A       -0.10776
    123A ->137A        0.11302
    124A ->131A        0.10144
    124A ->134A       -0.19748
    125A ->138A        0.14064
    126A ->131A        0.11211
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    126A ->134A       -0.12871
    127A ->131A        0.30144
    127A ->134A       -0.25299
    128A ->133A        0.21148
    128A ->135A        0.12062
    129A ->132A       -0.12569
    129A ->135A       -0.21380
    116B ->130B        0.15944
    122B ->137B       -0.11391
    123B ->138B        0.12223
    126B ->131B        0.29179
    126B ->132B        0.17219
    126B ->134B       -0.14552
    127B ->131B       -0.18226
    127B ->132B       -0.10980
    128B ->133B        0.21081
    128B ->135B       -0.16513

 Excited state symmetry could not be determined.
 Excited State  64:  2.372-?Sym    4.4171 eV  280.69 nm  f=0.0002
<S**2>=1.157
    115A ->130A        0.12115
    117A ->130A        0.40134
    124A ->132A        0.11130
    124A ->133A       -0.20506
    126A ->132A        0.14938
    126A ->133A       -0.10942
    127A ->132A        0.33819
    127A ->133A       -0.25761
    128A ->134A       -0.12561
    129A ->131A       -0.10022
    129A ->134A        0.12950
    117B ->130B        0.30161
    121B ->131B       -0.15547
    123B ->131B       -0.16550
    125B ->131B       -0.23134
    125B ->132B       -0.14183
    126B ->131B       -0.12511
    126B ->132B        0.19990
    126B ->133B       -0.12397
    127B ->131B        0.12456
    127B ->132B       -0.20552
    127B ->133B       -0.13671
    128B ->131B        0.18859
    128B ->132B        0.12086

 Excited state symmetry could not be determined.
 Excited State  65:  2.532-?Sym    4.4257 eV  280.14 nm  f=0.0107
<S**2>=1.353
    115A ->130A        0.19712
```

```
    117A ->130A        0.57358
    121A ->131A       -0.10962
    124A ->132A       -0.21700
    124A ->133A        0.19059
    126A ->132A       -0.21506
    127A ->132A       -0.23198
    127A ->133A        0.29081
    128A ->134A       -0.17343
    117B ->130B        0.29746
    125B ->131B       -0.12487
    126B ->131B        0.15954
    126B ->132B       -0.23452
    127B ->132B        0.14804

 Excited state symmetry could not be determined.
 Excited State  66:  3.227-?Sym    4.4276 eV  280.02 nm  f=0.0003
<S**2>=2.353
    117A ->130A        0.28576
    121A ->131A        0.36970
    122A ->131A        0.27435
    128A ->131A        0.13753
    128A ->134A        0.22377
    129A ->131A       -0.13265
    129A ->134A       -0.13929
    117B ->130B        0.23224
    121B ->131B        0.17687
    123B ->131B        0.18351
    125B ->131B        0.39651
    125B ->132B        0.19585
    126B ->132B        0.10672
    128B ->131B       -0.19039
    128B ->134B        0.26945

 Excited state symmetry could not be determined.
 Excited State  67:  2.563-?Sym    4.4686 eV  277.46 nm  f=0.0054
<S**2>=1.392
    116A ->130A        0.43192
    126A ->131A       -0.14134
    114B ->130B       -0.18939
    116B ->130B        0.58368
    125B ->131B       -0.25624
    125B ->132B        0.38560
    126B ->131B        0.14867
    128B ->132B       -0.16337

 Excited state symmetry could not be determined.
 Excited State  68:  2.909-?Sym    4.4727 eV  277.20 nm  f=0.0034
<S**2>=1.865
    116A ->130A        0.18915
    121A ->132A       -0.14372
```

```
    122A ->132A       -0.16699
    123A ->137A       -0.12014
    124A ->131A        0.20286
    126A ->131A        0.11646
    127A ->134A       -0.14652
    128A ->133A       -0.10641
    114B ->130B       -0.12330
    116B ->130B        0.49497
    121B ->132B       -0.10252
    122B ->137B        0.13019
    123B ->132B       -0.14724
    125B ->131B        0.26481
    125B ->132B       -0.42517
    126B ->131B       -0.11655
    128B ->132B        0.16752
    128B ->135B       -0.14564

 Excited state symmetry could not be determined.
 Excited State  69:  2.626-?Sym    4.4861 eV  276.38 nm  f=0.0211
<S**2>=1.474
    116A ->130A       -0.10655
    121A ->132A       -0.13994
    122A ->132A       -0.13413
    124A ->131A       -0.44286
    124A ->134A       -0.11146
    126A ->131A       -0.42131
    126A ->134A       -0.11359
    127A ->131A        0.19702
    127A ->134A        0.48246
    115B ->129B        0.13783
    125B ->132B       -0.13903
    126B ->131B        0.27265
    126B ->132B        0.12528

 Excited state symmetry could not be determined.
 Excited State  70:  2.768-?Sym    4.5035 eV  275.30 nm  f=0.0021
<S**2>=1.665
    121A ->131A       -0.27665
    122A ->131A       -0.12446
    124A ->132A       -0.18253
    127A ->133A        0.13370
    128A ->134A       -0.31754
    120B ->131B        0.11096
    121B ->131B       -0.15789
    123B ->131B       -0.12667
    125B ->131B        0.50448
    125B ->132B        0.34760
    125B ->134B       -0.12261
    126B ->131B       -0.17127
    126B ->132B        0.32923
```

```
    127B ->132B       -0.13139

 Excited state symmetry could not be determined.
 Excited State  71:  3.248-?Sym    4.5314 eV  273.61 nm  f=0.0120
<S**2>=2.388
    113A ->130A        0.32502
    114A ->130A        0.39223
    116A ->130A       -0.36195
    122A ->133A       -0.14584
    123A ->137A       -0.12210
    124A ->134A        0.12429
    125A ->135A       -0.10476
    125A ->138A       -0.12867
    127A ->134A       -0.11535
    128A ->133A       -0.21704
    113B ->130B        0.29078
    114B ->130B       -0.15288
    115B ->129B       -0.12099
    122B ->137B        0.11839
    125B ->131B       -0.10212
    125B ->132B        0.21820
    127B ->134B        0.10403

 Excited state symmetry could not be determined.
 Excited State  72:  3.357-?Sym    4.5482 eV  272.60 nm  f=0.0046
<S**2>=2.567
    119A ->131A       -0.10516
    120A ->132A        0.13097
    122A ->134A       -0.10972
    122A ->137A       -0.12763
    123A ->133A        0.15825
    123A ->135A        0.13531
    123A ->138A        0.14096
    124A ->132A        0.13431
    125A ->131A       -0.19041
    125A ->137A        0.18426
    126A ->132A       -0.23255
    126A ->133A       -0.22477
    127A ->132A        0.15243
    128A ->136A       -0.10141
    129A ->134A        0.16803
    129A ->136A        0.12933
    116B ->129B       -0.11515
    118B ->131B        0.10183
    119B ->131B       -0.12238
    119B ->132B        0.11771
    121B ->131B        0.11181
    121B ->137B       -0.15699
    122B ->133B       -0.16402
    122B ->135B        0.12484
```

```
    122B ->138B       -0.14854
    123B ->131B        0.27540
    123B ->137B        0.16569
    124B ->131B        0.11716
    124B ->132B       -0.18799
    124B ->133B        0.11737
    125B ->134B        0.14062
    127B ->133B       -0.11755
    128B ->136B        0.14267
    128B ->137B       -0.10921

 Excited state symmetry could not be determined.
 Excited State  73:  3.152-?Sym    4.5570 eV  272.07 nm  f=0.0003
<S**2>=2.233
    113A ->130A        0.12347
    114A ->130A        0.19360
    119A ->132A       -0.10776
    120A ->131A        0.18914
    121A ->132A        0.23436
    124A ->131A        0.23612
    124A ->134A       -0.10584
    126A ->131A       -0.20818
    110B ->129B        0.11572
    113B ->130B        0.13799
    114B ->130B       -0.13515
    115B ->129B        0.36932
    118B ->132B        0.11892
    119B ->131B        0.16258
    119B ->132B        0.13002
    120B ->132B       -0.10237
    121B ->131B       -0.11280
    121B ->132B        0.22911
    123B ->131B       -0.13575
    123B ->132B        0.24489
    124B ->131B       -0.13737
    124B ->132B       -0.18197
    125B ->132B       -0.10766
    126B ->131B       -0.15558
    126B ->132B       -0.12670
    126B ->134B        0.18432
    127B ->134B       -0.11037

 Excited state symmetry could not be determined.
 Excited State  74:  3.341-?Sym    4.5838 eV  270.49 nm  f=0.0154
<S**2>=2.540
    113A ->130A        0.21705
    114A ->130A        0.18566
    116A ->130A        0.11348
    118A ->132A       -0.15878
    120A ->131A       -0.28114
```

```
    121A ->132A        0.11350
    122A ->132A        0.10500
    124A ->131A       -0.25358
    124A ->134A       -0.12952
    126A ->131A        0.33553
    127A ->134A        0.15485
    128A ->133A        0.16595
    129A ->135A        0.10124
    113B ->130B        0.26464
    114B ->130B       -0.10661
    115B ->129B        0.11337
    117B ->129B       -0.12702
    118B ->132B       -0.12895
    119B ->131B       -0.24583
    119B ->132B       -0.13373
    124B ->131B        0.26352
    124B ->132B        0.13206
    126B ->134B        0.15892
    127B ->134B       -0.11213

 Excited state symmetry could not be determined.
 Excited State  75:  2.719-?Sym    4.6000 eV  269.53 nm  f=0.0284
<S**2>=1.598
    121A ->133A        0.11847
    124A ->132A       -0.13284
    124A ->134A        0.16163
    125A ->133A        0.12718
    126A ->134A        0.14005
    127A ->131A       -0.12043
    127A ->133A        0.10145
    127A ->134A       -0.11007
    129A ->133A       -0.13899
    115B ->129B        0.64653
    117B ->129B       -0.12175
    121B ->132B       -0.16659
    123B ->131B        0.10285
    123B ->132B       -0.21135
    123B ->133B        0.11762
    126B ->134B       -0.11185
    127B ->134B        0.12260

 Excited state symmetry could not be determined.
 Excited State  76:  2.815-?Sym    4.6022 eV  269.40 nm  f=0.0088
<S**2>=1.731
    121A ->134A       -0.10428
    122A ->134A       -0.14651
    123A ->138A        0.11243
    124A ->132A        0.34212
    124A ->133A        0.21720
    126A ->132A        0.27054
```

```
    127A ->132A       -0.15658
    127A ->133A       -0.32385
    128A ->134A       -0.24694
    129A ->134A        0.15881
    113B ->129B       -0.15734
    115B ->129B        0.19165
    121B ->131B        0.12787
    122B ->138B       -0.10013
    123B ->131B        0.14129
    124B ->132B        0.10819
    125B ->131B        0.18732
    126B ->131B        0.11984
    126B ->132B       -0.18777
    128B ->137B        0.11861

 Excited state symmetry could not be determined.
 Excited State  77:  2.415-?Sym    4.6166 eV  268.56 nm  f=0.0145
<S**2>=1.208
    121A ->131A        0.16558
    122A ->131A        0.18647
    123A ->138A        0.10796
    124A ->132A        0.11122
    125A ->137A        0.13388
    126A ->133A       -0.14614
    128A ->134A        0.11324
    129A ->134A       -0.13543
    111B ->129B       -0.11738
    113B ->129B        0.24067
    114B ->129B        0.63880
    115B ->130B       -0.18141
    116B ->129B        0.26386
    122B ->138B       -0.10510
    123B ->137B        0.10138
    128B ->134B       -0.20414
    128B ->136B        0.11062

 Excited state symmetry could not be determined.
 Excited State  78:  2.783-?Sym    4.6183 eV  268.46 nm  f=0.0164
<S**2>=1.687
    113A ->130A       -0.12006
    114A ->130A       -0.18153
    120A ->131A       -0.12105
    121A ->132A       -0.14528
    121A ->133A       -0.21043
    122A ->133A       -0.10122
    123A ->131A        0.11823
    123A ->137A       -0.10385
    125A ->133A       -0.18595
    126A ->131A        0.17565
    128A ->133A       -0.28024
```

```
    128A ->135A        0.11823
    129A ->135A       -0.11091
    113B ->130B       -0.12838
    114B ->130B        0.10071
    115B ->129B        0.47416
    117B ->129B       -0.11214
    122B ->137B        0.12083
    123B ->132B        0.11970
    123B ->133B       -0.18782
    125B ->131B       -0.13771
    125B ->132B        0.24034
    128B ->133B        0.12832
    128B ->135B       -0.13516

 Excited state symmetry could not be determined.
 Excited State  79:  3.240-?Sym    4.6290 eV  267.84 nm  f=0.0002
<S**2>=2.374
    120A ->132A       -0.17130
    121A ->134A       -0.13081
    123A ->132A        0.21877
    123A ->133A        0.22340
    124A ->132A        0.11611
    125A ->134A       -0.14663
    125A ->136A       -0.14524
    126A ->132A        0.31268
    126A ->135A        0.11242
    126A ->138A        0.17340
    128A ->137A       -0.18269
    129A ->137A        0.17917
    113B ->129B       -0.13549
    114B ->129B        0.10984
    118B ->131B       -0.10843
    119B ->132B       -0.18344
    121B ->134B        0.11619
    122B ->132B        0.12521
    122B ->133B       -0.20310
    123B ->134B       -0.10748
    123B ->136B        0.10735
    124B ->132B        0.14312
    124B ->138B       -0.16023
    125B ->137B        0.14059
    127B ->133B       -0.12709
    128B ->137B       -0.23647

 Excited state symmetry could not be determined.
 Excited State  80:  3.157-?Sym    4.6319 eV  267.68 nm  f=0.0145
<S**2>=2.242
    121A ->133A       -0.13131
    121A ->135A        0.11880
    122A ->133A       -0.13097
```

123A ->134A	-0.17180
123A ->137A	0.11448
124A ->134A	-0.19977
125A ->132A	0.18654
125A ->133A	0.30892
125A ->140A	-0.10002
126A ->131A	0.22220
126A ->136A	0.10218
128A ->132A	-0.10146
128A ->133A	-0.26048
128A ->138A	-0.15184
129A ->138A	0.15616
113B ->130B	-0.12971
121B ->131B	-0.11206
121B ->132B	0.15131
121B ->133B	-0.16719
122B ->134B	0.13917
122B ->137B	-0.11564
123B ->132B	0.10406
123B ->133B	0.12645
124B ->134B	-0.10979
124B ->137B	-0.10809
125B ->133B	-0.10905
126B ->134B	0.15218
126B ->136B	0.10882
127B ->134B	-0.14887
128B ->133B	0.10881
128B ->138B	-0.21170

Table S34. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 1^-(*S*=1/2)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  2.941-?Sym    0.4533 eV 2734.92 nm  f=0.0007
<S**2>=1.913
    123A ->130A       -0.13064
    129A ->130A        0.66144
    120B ->130B        0.11290
    121B ->130B        0.11380
    122B ->129B        0.15958
    123B ->129B        0.17174
    125B ->129B        0.32426
    126B ->130B        0.19577
    127B ->129B        0.46122
    128B ->130B       -0.55096
    129A <-130A        0.30184
    126B <-130B        0.14820
    127B <-129B        0.10738
    128B <-130B       -0.27854
 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 symmetry could not be determined.
 Excited State   2:  2.020-?Sym    0.4804 eV 2580.60 nm  f=0.0017
<S**2>=0.770
    120B ->129B       -0.39976
    121B ->129B        0.41666
    124B ->129B        0.27081
    126B ->129B        0.23328
    128B ->129B        0.72225

 Excited state symmetry could not be determined.
 Excited State   3:  2.494-?Sym    0.7047 eV 1759.48 nm  f=0.0009
<S**2>=1.306
    129A ->130A       -0.45480
    122B ->129B        0.17034
    123B ->129B        0.19479
    125B ->129B        0.42327
    127B ->129B        0.61355
    128B ->130B        0.36919
    129A <-130A       -0.11958

 Excited state symmetry could not be determined.
 Excited State   4:  3.414-?Sym    1.2848 eV  964.99 nm  f=0.0029
<S**2>=2.664
    122A ->130A       -0.33791
```

```
    127A ->130A       -0.48612
    122B ->130B        0.17339
    123B ->130B        0.19209
    125B ->130B        0.30368
    127B ->130B        0.69010

 Excited state symmetry could not be determined.
 Excited State   5:  2.065-?Sym    1.4296 eV  867.27 nm  f=0.0021
<S**2>=0.816
    122A ->130A       -0.14538
    127A ->130A       -0.31166
    120B ->129B       -0.15544
    121B ->129B        0.27280
    124B ->129B        0.19860
    126B ->129B        0.65494
    127B ->130B       -0.12959
    128B ->129B       -0.52739

 Excited state symmetry could not be determined.
 Excited State   6:  2.677-?Sym    1.4611 eV  848.59 nm  f=0.0441
<S**2>=1.541
    128A ->130A        0.41870
    129A ->130A        0.34377
    120B ->130B       -0.12794
    121B ->130B        0.21302
    123B ->129B       -0.13057
    124B ->130B        0.15255
    125B ->129B       -0.31076
    126B ->130B        0.25055
    127B ->129B        0.31233
    128B ->130B        0.56708

 Excited state symmetry could not be determined.
 Excited State   7:  2.360-?Sym    1.4860 eV  834.37 nm  f=0.0102
<S**2>=1.143
    128A ->130A        0.46280
    121B ->130B        0.10111
    122B ->129B        0.17288
    123B ->129B        0.27005
    125B ->129B        0.56838
    127B ->129B       -0.52500
    128B ->130B        0.18702

 Excited state symmetry could not be determined.
 Excited State   8:  2.120-?Sym    1.5243 eV  813.40 nm  f=0.0170
<S**2>=0.874
    128A ->130A        0.75381
    129A ->130A       -0.32416
    121B ->130B       -0.11382
    125B ->129B       -0.14142
```

```
    126B ->130B       -0.19920
    127B ->129B        0.19736
    128B ->130B       -0.41984

 Excited state symmetry could not be determined.
 Excited State   9:  2.034-?Sym    1.5969 eV  776.39 nm  f=0.0245
<S**2>=0.784
    120B ->129B        0.44578
    121B ->129B       -0.41663
    124B ->129B       -0.23452
    126B ->129B        0.62605
    128B ->129B        0.38579

 Excited state symmetry could not be determined.
 Excited State  10:  2.023-?Sym    1.7436 eV  711.09 nm  f=0.0301
<S**2>=0.773
    127A ->130A        0.69502
    123B ->130B       -0.11052
    125B ->130B       -0.14532
    126B ->129B        0.23130
    127B ->130B        0.61323
    128B ->129B       -0.17537

 Excited state symmetry could not be determined.
 Excited State  11:  2.615-?Sym    1.8826 eV  658.59 nm  f=0.1366
<S**2>=1.459
    121A ->130A       -0.26041
    125A ->130A        0.11667
    129A ->130A       -0.43273
    121B ->130B        0.25976
    124B ->130B        0.23396
    126B ->130B        0.73478
    128B ->130B       -0.22692

 Excited state symmetry could not be determined.
 Excited State  12:  3.423-?Sym    1.9409 eV  638.78 nm  f=0.0020
<S**2>=2.679
    122A ->130A       -0.44461
    127A ->130A        0.41623
    122B ->130B        0.24684
    123B ->130B        0.24887
    125B ->130B        0.59662
    127B ->130B       -0.33232

 Excited state symmetry could not be determined.
 Excited State  13:  3.030-?Sym    1.9808 eV  625.93 nm  f=0.0045
<S**2>=2.045
    123A ->130A        0.33971
    125A ->130A       -0.38677
    121B ->130B       -0.29744
```

```
    122B ->129B       -0.33875
    123B ->129B       -0.36033
    124B ->130B       -0.30184
    125B ->129B        0.27028
    126B ->130B        0.41465

 Excited state symmetry could not be determined.
 Excited State  14:  3.420-?Sym    1.9942 eV  621.71 nm  f=0.0009
<S**2>=2.674
    122A ->130A       -0.16668
    124A ->130A        0.16316
    126A ->130A        0.74427
    122B ->130B        0.34159
    123B ->130B        0.30314
    125B ->130B       -0.36728

 Excited state symmetry could not be determined.
 Excited State  15:  2.588-?Sym    2.0669 eV  599.86 nm  f=0.0019
<S**2>=1.425
    121A ->130A        0.11586
    123A ->130A        0.18312
    125A ->130A       -0.33463
    119B ->129B        0.21960
    121B ->130B       -0.21625
    122B ->129B        0.51300
    123B ->129B        0.43936
    124B ->130B       -0.25570
    125B ->129B       -0.37913
    126B ->130B        0.24823

 Excited state symmetry could not be determined.
 Excited State  16:  2.716-?Sym    2.2007 eV  563.38 nm  f=0.0042
<S**2>=1.594
    121A ->130A        0.11488
    123A ->130A       -0.34383
    125A ->130A        0.48266
    120B ->130B        0.48745
    121B ->130B       -0.32949
    123B ->129B       -0.13805
    124B ->130B       -0.38015
    126B ->130B        0.24627
    128B ->130B        0.17434

 Excited state symmetry could not be determined.
 Excited State  17:  2.244-?Sym    2.2193 eV  558.67 nm  f=0.0001
<S**2>=1.009
    122A ->130A       -0.16902
    124A ->130A       -0.22079
    126A ->130A       -0.12649
    118B ->129B        0.11851
```

```
    120B ->129B        0.32511
    121B ->129B       -0.18157
    122B ->130B       -0.16810
    123B ->130B        0.17899
    124B ->129B        0.81529
    126B ->129B       -0.10805

 Excited state symmetry could not be determined.
 Excited State  18:  2.795-?Sym    2.2491 eV  551.27 nm  f=0.0021
<S**2>=1.703
    123A ->130A        0.41914
    125A ->130A        0.46385
    121B ->130B       -0.33015
    122B ->129B       -0.43062
    123B ->129B        0.50832
    124B ->130B        0.14720

 Excited state symmetry could not be determined.
 Excited State  19:  2.945-?Sym    2.2597 eV  548.68 nm  f=0.0002
<S**2>=1.918
    124A ->130A        0.73920
    126A ->130A       -0.43881
    120B ->129B        0.17964
    121B ->129B        0.12548
    122B ->130B        0.28338
    123B ->130B       -0.12015
    124B ->129B        0.10301
    125B ->130B       -0.28133

 Excited state symmetry could not be determined.
 Excited State  20:  2.619-?Sym    2.2883 eV  541.82 nm  f=0.0071
<S**2>=1.464
    121A ->130A       -0.19511
    123A ->130A        0.47670
    125A ->130A        0.43053
    119B ->129B        0.21646
    120B ->130B       -0.25267
    122B ->129B        0.46759
    123B ->129B       -0.43231

 Excited state symmetry could not be determined.
 Excited State  21:  2.379-?Sym    2.3322 eV  531.61 nm  f=0.0007
<S**2>=1.165
    122A ->130A        0.24565
    124A ->130A        0.44980
    126A ->130A        0.40926
    121B ->129B       -0.22754
    122B ->130B       -0.15050
    123B ->130B       -0.40018
    124B ->129B        0.30809
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    125B ->130B        0.46463

 Excited state symmetry could not be determined.
 Excited State  22:  2.645-?Sym    2.3938 eV  517.95 nm  f=0.0325
<S**2>=1.499
    121A ->130A        0.77211
    119B ->129B        0.16331
    121B ->130B       -0.15663
    122B ->129B        0.11369
    123B ->129B       -0.13581
    124B ->130B        0.50592
    126B ->130B        0.10100

 Excited state symmetry could not be determined.
 Excited State  23:  2.077-?Sym    2.4005 eV  516.48 nm  f=0.0009
<S**2>=0.828
    122A ->130A        0.23249
    124A ->130A        0.24000
    126A ->130A       -0.14805
    118B ->129B       -0.17748
    120B ->129B       -0.49906
    121B ->129B       -0.51702
    123B ->130B        0.52347
    125B ->130B       -0.10780

 Excited state symmetry could not be determined.
 Excited State  24:  2.384-?Sym    2.4251 eV  511.25 nm  f=0.0205
<S**2>=1.171
    121A ->130A        0.20944
    123A ->130A       -0.20876
    125A ->130A        0.16083
    119B ->129B        0.50509
    120B ->130B       -0.47544
    121B ->130B        0.27284
    122B ->129B       -0.23447
    123B ->129B        0.14467
    124B ->130B       -0.45813

 Excited state symmetry could not be determined.
 Excited State  25:  2.100-?Sym    2.4282 eV  510.59 nm  f=0.0054
<S**2>=0.853
    121A ->130A       -0.33510
    125A ->130A       -0.20474
    119B ->129B        0.74942
    120B ->130B        0.26159
    121B ->130B       -0.21875
    122B ->129B       -0.17813
    124B ->130B        0.30471
    125B ->129B        0.11887
```

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 Excited state symmetry could not be determined.
 Excited State  26:  2.266-?Sym    2.4565 eV  504.72 nm  f=0.0004
<S**2>=1.034
    124A ->130A       -0.31041
    120B ->129B       -0.24118
    121B ->129B       -0.32526
    122B ->130B        0.70835
    123B ->130B       -0.42232
    124B ->129B        0.18447

 Excited state symmetry could not be determined.
 Excited State  27:  2.280-?Sym    2.5733 eV  481.81 nm  f=0.0157
<S**2>=1.050
    119A ->130A       -0.16912
    121A ->130A        0.24931
    123A ->130A        0.48601
    119B ->129B        0.14586
    120B ->130B        0.51833
    121B ->130B        0.57337
    124B ->130B       -0.13010

 Excited state symmetry could not be determined.
 Excited State  28:  2.100-?Sym    2.7027 eV  458.74 nm  f=0.0489
<S**2>=0.852
    120A ->130A       -0.21464
    122A ->130A       -0.27172
    129A ->131A       -0.11105
    118B ->129B        0.79599
    120B ->129B       -0.30734
    121B ->129B       -0.20928
    122B ->130B       -0.12314
    123B ->130B       -0.11596

 Excited state symmetry could not be determined.
 Excited State  29:  2.156-?Sym    2.7107 eV  457.40 nm  f=0.1072
<S**2>=0.912
    120A ->130A        0.30431
    121A ->131A       -0.10760
    122A ->130A        0.58181
    118B ->129B        0.46515
    119B ->130B        0.14536
    120B ->129B        0.13468
    121B ->129B        0.17993
    122B ->130B        0.26121
    123B ->130B        0.26987
    125B ->130B        0.19849
    128B ->131B        0.11542

 Excited state symmetry could not be determined.
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 Excited State  30:  3.400-?Sym    2.7562 eV  449.84 nm  f=0.0026
<S**2>=2.640
    119A ->131A        0.14906
    121A ->131A       -0.43720
    128A ->131A        0.34900
    129A ->131A       -0.30729
    118B ->129B       -0.20582
    119B ->130B       -0.14103
    120B ->131B       -0.29346
    121B ->131B        0.30666
    124B ->131B        0.19890
    126B ->131B        0.17292
    128B ->131B        0.44264

 Excited state symmetry could not be determined.
 Excited State  31:  3.408-?Sym    2.8195 eV  439.73 nm  f=0.0117
<S**2>=2.654
    120A ->130A       -0.65484
    119B ->130B        0.68777
    122B ->130B        0.12296
    123B ->130B        0.11486

 Excited state symmetry could not be determined.
 Excited State  32:  3.453-?Sym    2.8402 eV  436.53 nm  f=0.0001
<S**2>=2.730
    117A ->131A       -0.10179
    120A ->131A        0.10730
    122A ->131A       -0.46644
    126A ->131A       -0.14836
    127A ->131A       -0.46314
    122B ->131B        0.17440
    123B ->131B        0.19838
    125B ->131B        0.40075
    127B ->131B        0.47165

 Excited state symmetry could not be determined.
 Excited State  33:  2.613-?Sym    2.8788 eV  430.68 nm  f=0.0026
<S**2>=1.457
    116A ->130A       -0.16315
    118A ->130A        0.32334
    119A ->130A        0.84400
    120B ->130B        0.23021

 Excited state symmetry could not be determined.
 Excited State  34:  3.464-?Sym    2.9785 eV  416.26 nm  f=0.0001
<S**2>=2.749
    119A ->130A        0.10966
    119A ->132A        0.16908
    121A ->132A       -0.42366
    128A ->132A        0.34106
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    129A ->132A       -0.31864
    120B ->132B       -0.28578
    120B ->135B        0.11160
    121B ->132B        0.30344
    124B ->132B        0.18811
    126B ->132B        0.12044
    128B ->132B        0.44598
    128B ->135B       -0.11975

 Excited state symmetry could not be determined.
 Excited State  35:  2.035-?Sym    3.0015 eV  413.07 nm  f=0.0997
<S**2>=0.786
    120A ->130A        0.60142
    122A ->130A       -0.20612
    128A ->131A        0.11277
    129A ->131A        0.11777
    119B ->130B        0.65522
    122B ->130B       -0.16892
    123B ->130B       -0.14275

 Excited state symmetry could not be determined.
 Excited State  36:  2.084-?Sym    3.0430 eV  407.45 nm  f=0.0039
<S**2>=0.836
    118A ->131A        0.25258
    119A ->131A        0.21626
    120A ->130A       -0.12982
    121A ->131A        0.22684
    122A ->132A        0.12372
    123A ->131A       -0.17933
    128A ->131A        0.59473
    129A ->131A        0.53957
    118B ->129B        0.13284
    119B ->130B       -0.16211

 Excited state symmetry could not be determined.
 Excited State  37:  3.347-?Sym    3.1793 eV  389.97 nm  f=0.0010
<S**2>=2.550
    127A ->133A        0.41082
    127A ->134A        0.18379
    128A ->133A        0.22421
    128A ->134A        0.44210
    117B ->129B       -0.18418
    118B ->130B        0.14374
    125B ->133B        0.10686
    126B ->133B        0.13238
    126B ->134B        0.25348
    127B ->133B       -0.43788
    127B ->134B       -0.18616
    128B ->133B        0.16361
    128B ->134B        0.30183
```

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 Excited state symmetry could not be determined.
 Excited State  38:  3.383-?Sym    3.1827 eV  389.55 nm  f=0.0002
<S**2>=2.611
    127A ->133A       -0.18475
    127A ->134A        0.41943
    128A ->133A        0.46778
    128A ->134A       -0.20620
    125B ->134B        0.11357
    126B ->133B        0.26245
    126B ->134B       -0.12729
    127B ->133B        0.18626
    127B ->134B       -0.45379
    128B ->133B        0.31487
    128B ->134B       -0.14684

 Excited state symmetry could not be determined.
 Excited State  39:  2.880-?Sym    3.2151 eV  385.63 nm  f=0.0019
<S**2>=1.823
    118A ->130A       -0.36186
    117B ->129B        0.57084
    118B ->130B        0.69086

 Excited state symmetry could not be determined.
 Excited State  40:  2.540-?Sym    3.2400 eV  382.67 nm  f=0.0022
<S**2>=1.363
    118A ->130A        0.18945
    122A ->131A       -0.16336
    127A ->131A       -0.16755
    127A ->133A        0.13917
    128A ->132A       -0.12893
    128A ->134A        0.15320
    129A ->132A       -0.13720
    117B ->129B        0.67551
    118B ->130B       -0.48661
    127B ->131B       -0.15452
    127B ->133B       -0.12340
    128B ->134B        0.11485

 Excited state symmetry could not be determined.
 Excited State  41:  2.055-?Sym    3.2587 eV  380.47 nm  f=0.0007
<S**2>=0.806
    118A ->130A       -0.13029
    119A ->130A        0.14224
    122A ->131A        0.29979
    126A ->131A        0.10083
    127A ->131A        0.46305
    128A ->132A        0.10641
    129A ->132A        0.22316
    117B ->129B        0.27750
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    118B ->130B       -0.27154
    122B ->131B        0.13123
    123B ->131B        0.14555
    125B ->131B        0.31041
    127B ->131B        0.45510

 Excited state symmetry could not be determined.
 Excited State  42:  3.447-?Sym    3.2765 eV  378.40 nm  f=0.0007
<S**2>=2.721
    120A ->132A       -0.11891
    122A ->132A        0.40899
    126A ->132A        0.16998
    127A ->132A        0.46155
    129A ->131A       -0.13676
    122B ->132B       -0.12441
    123B ->132B       -0.16331
    125B ->132B       -0.38611
    125B ->135B        0.11231
    127B ->132B       -0.45806
    127B ->135B        0.12168

 Excited state symmetry could not be determined.
 Excited State  43:  2.340-?Sym    3.3143 eV  374.09 nm  f=0.0091
<S**2>=1.119
    118A ->130A        0.79507
    119A ->130A       -0.37114
    127A ->131A        0.11958
    117B ->129B        0.13423
    118B ->130B        0.32298
    127B ->131B        0.12741

 Excited state symmetry could not be determined.
 Excited State  44:  2.069-?Sym    3.3948 eV  365.21 nm  f=0.0013
<S**2>=0.820
    121A ->131A       -0.16796
    128A ->131A        0.54345
    129A ->131A       -0.36146
    114B ->129B       -0.14136
    116B ->129B        0.37345
    120B ->131B        0.15942
    121B ->131B       -0.17530
    124B ->131B       -0.13051
    126B ->131B       -0.18785
    128B ->131B       -0.47756

 Excited state symmetry could not be determined.
 Excited State  45:  2.103-?Sym    3.4007 eV  364.59 nm  f=0.0098
<S**2>=0.856
    118A ->132A        0.18106
    119A ->132A        0.23695
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    121A ->132A       -0.19900
    125A ->132A        0.10053
    127A ->131A       -0.12949
    128A ->132A        0.69331
    128A ->135A       -0.10065
    129A ->132A        0.14237
    117B ->129B        0.12287
    120B ->132B        0.17037
    121B ->132B       -0.18834
    124B ->132B       -0.12610
    126B ->132B       -0.12745
    128B ->132B       -0.37895

 Excited state symmetry could not be determined.
 Excited State  46:  2.095-?Sym    3.4614 eV  358.19 nm  f=0.0000
<S**2>=0.847
    117A ->130A        0.10291
    128A ->131A       -0.14173
    129A ->131A        0.25043
    114B ->129B       -0.20460
    116B ->129B        0.84254
    126B ->131B        0.14365
    128B ->131B        0.21780

 Excited state symmetry could not be determined.
 Excited State  47:  2.861-?Sym    3.4909 eV  355.16 nm  f=0.0134
<S**2>=1.796
    111A ->130A       -0.10409
    114A ->130A        0.15529
    116A ->130A        0.42448
    119A ->130A        0.11901
    121A ->132A        0.17735
    127A ->131A       -0.19331
    128A ->132A        0.10490
    129A ->132A        0.50027
    129A ->135A       -0.15509
    114B ->130B       -0.23677
    116B ->130B       -0.27948
    118B ->130B        0.13952
    120B ->132B       -0.17166
    121B ->135B       -0.10451
    127B ->131B       -0.14041
    128B ->132B        0.21004

 Excited state symmetry could not be determined.
 Excited State  48:  2.847-?Sym    3.4984 eV  354.40 nm  f=0.0209
<S**2>=1.777
    111A ->130A        0.10111
    114A ->130A       -0.14998
    116A ->130A       -0.34926
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    118A ->130A       -0.16198
    119A ->130A       -0.15266
    121A ->132A        0.15727
    127A ->131A       -0.21497
    129A ->132A        0.50661
    129A ->135A        0.11374
    114B ->130B        0.22167
    116B ->130B        0.31173
    118B ->130B       -0.19209
    120B ->132B       -0.14512
    121B ->132B        0.13906
    127B ->131B       -0.12962
    128B ->132B        0.16244
    128B ->135B       -0.18692

 Excited state symmetry could not be determined.
 Excited State  49:  3.395-?Sym    3.6128 eV  343.18 nm  f=0.0022
<S**2>=2.631
    110A ->130A       -0.12191
    113A ->130A       -0.14244
    115A ->130A        0.53484
    117A ->130A       -0.35459
    129A ->136A       -0.14191
    129A ->139A        0.11675
    110B ->130B        0.10913
    113B ->130B        0.10999
    114B ->129B       -0.16149
    115B ->130B       -0.51327
    117B ->130B        0.24771
    128B ->136B        0.11843
    128B ->139B       -0.10211

 Excited state symmetry could not be determined.
 Excited State  50:  3.441-?Sym    3.7068 eV  334.48 nm  f=0.0001
<S**2>=2.710
    117A ->130A        0.16706
    121A ->131A        0.26017
    123A ->131A       -0.14637
    123A ->137A        0.11755
    124A ->135A        0.10110
    124A ->138A        0.18730
    125A ->137A        0.18701
    126A ->132A        0.22016
    126A ->138A       -0.10325
    126A ->140A        0.14490
    129A ->131A       -0.21032
    129A ->136A       -0.23583
    129A ->139A       -0.12342
    117B ->130B       -0.20174
    120B ->131B        0.10384
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    121B ->137B       -0.10563
    122B ->132B        0.17453
    122B ->138B        0.12121
    123B ->132B        0.12308
    123B ->138B       -0.16063
    124B ->137B        0.19462
    125B ->140B       -0.12131
    126B ->131B       -0.22823
    126B ->136B       -0.12613
    128B ->131B        0.29715
    128B ->136B        0.18148

 Excited state symmetry could not be determined.
 Excited State  51:  3.339-?Sym    3.7147 eV  333.77 nm  f=0.0003
<S**2>=2.537
    121A ->132A        0.31077
    123A ->132A       -0.22875
    124A ->137A       -0.22027
    125A ->138A       -0.20325
    126A ->131A        0.19440
    126A ->136A        0.17572
    126A ->139A        0.13457
    127A ->131A       -0.20428
    128A ->132A        0.14129
    129A ->135A       -0.21082
    129A ->140A       -0.15761
    120B ->132B        0.12986
    122B ->137B       -0.17545
    123B ->137B        0.13940
    124B ->138B       -0.19696
    125B ->131B       -0.10580
    125B ->136B       -0.13451
    125B ->139B       -0.10039
    126B ->132B       -0.30417
    128B ->132B        0.30897
    128B ->135B        0.12362
    128B ->140B        0.11434

 Excited state symmetry could not be determined.
 Excited State  52:  2.445-?Sym    3.7791 eV  328.08 nm  f=0.0025
<S**2>=1.244
    117A ->130A        0.17254
    122A ->132A        0.19820
    127A ->132A        0.54823
    129A ->131A       -0.18126
    117B ->130B       -0.43263
    125B ->132B        0.22024
    126B ->131B        0.17929
    127B ->132B        0.43311
    128B ->131B       -0.16235
```

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 Excited state symmetry could not be determined.
 Excited State  53:  3.201-?Sym    3.7976 eV  326.48 nm  f=0.0007
<S**2>=2.312
    115A ->130A       -0.29882
    117A ->130A       -0.49345
    121A ->131A        0.14403
    127A ->132A        0.25650
    129A ->131A       -0.19156
    115B ->130B        0.23630
    117B ->130B        0.52340
    125B ->132B        0.12214
    127B ->132B        0.29606

 Excited state symmetry could not be determined.
 Excited State  54:  3.327-?Sym    3.8131 eV  325.15 nm  f=0.0007
<S**2>=2.517
    122A ->131A        0.57104
    126A ->131A        0.16147
    127A ->131A       -0.54120
    123B ->131B       -0.15265
    125B ->131B       -0.21222
    126B ->132B        0.13178
    127B ->131B        0.39868

 Excited state symmetry could not be determined.
 Excited State  55:  2.821-?Sym    3.9246 eV  315.91 nm  f=0.0020
<S**2>=1.739
    117A ->130A        0.42690
    119A ->131A        0.17317
    121A ->131A       -0.38253
    125A ->131A        0.10986
    127A ->132A        0.22539
    128A ->131A       -0.21557
    129A ->131A        0.24994
    117B ->130B        0.42834
    120B ->131B       -0.11145
    121B ->131B        0.14337
    126B ->131B       -0.21336
    128B ->131B       -0.24797

 Excited state symmetry could not be determined.
 Excited State  56:  2.715-?Sym    3.9445 eV  314.32 nm  f=0.0049
<S**2>=1.592
    115A ->130A        0.11754
    117A ->130A        0.55021
    121A ->131A        0.26364
    128A ->131A        0.13633
    129A ->131A       -0.18145
    116B ->129B       -0.12137
```

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    117B ->130B        0.43914
    120B ->131B        0.19824
    121B ->131B       -0.19836
    124B ->131B       -0.10078
    126B ->131B        0.25653
    128B ->131B        0.30395

 Excited state symmetry could not be determined.
 Excited State  57:  2.199-?Sym    3.9906 eV  310.69 nm  f=0.0005
<S**2>=0.959
    122A ->131A        0.32117
    126A ->131A        0.16391
    127A ->131A       -0.25614
    129A ->132A       -0.10267
    122B ->131B        0.14545
    123B ->131B        0.26974
    125B ->131B        0.58751
    127B ->131B       -0.53813

 Excited state symmetry could not be determined.
 Excited State  58:  3.316-?Sym    4.0156 eV  308.76 nm  f=0.0000
<S**2>=2.499
    118A ->131A       -0.13356
    119A ->131A       -0.12788
    121A ->131A       -0.12980
    123A ->131A        0.11390
    124A ->138A        0.12483
    125A ->137A        0.12535
    126A ->132A        0.14698
    127A ->132A       -0.12037
    128A ->131A        0.12255
    129A ->131A        0.21912
    129A ->136A       -0.10553
    114B ->129B       -0.11670
    120B ->131B        0.16149
    123B ->138B       -0.10254
    124B ->137B        0.12701
    125B ->132B       -0.11924
    126B ->131B        0.71182
    126B ->136B       -0.11624
    128B ->131B       -0.23781

 Excited state symmetry could not be determined.
 Excited State  59:  2.355-?Sym    4.0304 eV  307.62 nm  f=0.0103
<S**2>=1.136
    116A ->130A        0.39699
    122A ->131A        0.11626
    114B ->130B       -0.19675
    115B ->129B       -0.13493
    116B ->130B        0.83721
```

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 Excited state symmetry could not be determined.
 Excited State  60:  3.225-?Sym    4.1097 eV  301.69 nm  f=0.0103
<S**2>=2.350
    114A ->130A       -0.21877
    116A ->130A        0.57712
    121A ->132A       -0.12243
    123A ->135A       -0.17568
    125A ->138A       -0.11132
    126A ->131A        0.11743
    129A ->134A       -0.11220
    129A ->135A        0.32940
    129A ->140A       -0.14460
    114B ->130B        0.20594
    115B ->129B        0.11006
    120B ->135B        0.12842
    121B ->132B        0.12191
    121B ->135B        0.13132
    124B ->138B       -0.11392
    128B ->132B       -0.16197
    128B ->135B       -0.22290

 Excited state symmetry could not be determined.
 Excited State  61:  2.231-?Sym    4.1268 eV  300.43 nm  f=0.0132
<S**2>=0.994
    117A ->130A        0.11171
    119A ->131A        0.12321
    121A ->131A        0.22381
    122A ->132A        0.10270
    123A ->131A       -0.15604
    127A ->132A       -0.12831
    129A ->131A       -0.19941
    111B ->129B       -0.10706
    114B ->129B        0.61436
    115B ->130B       -0.14069
    116B ->129B        0.20313
    117B ->130B        0.10479
    120B ->131B       -0.13111
    121B ->131B        0.20339
    124B ->131B        0.13857
    126B ->131B        0.21873
    127B ->134B       -0.12713
    128B ->131B       -0.28914
    128B ->133B       -0.24585

 Excited state symmetry could not be determined.
 Excited State  62:  2.596-?Sym    4.1433 eV  299.24 nm  f=0.0001
<S**2>=1.435
    118A ->131A       -0.13773
    119A ->131A       -0.14107
```

```
    121A ->131A       -0.19851
    122A ->132A       -0.26633
    123A ->131A        0.19785
    125A ->131A       -0.13622
    126A ->132A       -0.15090
    127A ->132A        0.37069
    128A ->131A        0.13767
    129A ->131A        0.16402
    114B ->129B        0.57731
    116B ->129B        0.12759
    120B ->131B        0.16280
    121B ->131B       -0.16601
    124B ->131B       -0.11519
    128B ->131B        0.16014
    128B ->133B        0.20916

 Excited state symmetry could not be determined.
 Excited State  63:  2.550-?Sym    4.1528 eV  298.56 nm  f=0.0215
<S**2>=1.376
    114A ->130A       -0.14453
    116A ->130A        0.18875
    121A ->132A        0.24871
    124A ->137A        0.11592
    125A ->138A        0.12290
    126A ->131A       -0.12841
    128A ->132A        0.14410
    129A ->132A       -0.23514
    115B ->129B        0.75698
    124B ->138B        0.11362
    128B ->132B        0.11765
    128B ->134B        0.10829

 Excited state symmetry could not be determined.
 Excited State  64:  3.041-?Sym    4.1815 eV  296.51 nm  f=0.0005
<S**2>=2.061
    121A ->131A        0.14828
    123A ->131A       -0.12516
    127A ->134A       -0.10515
    129A ->131A       -0.12847
    129A ->133A       -0.31064
    121B ->131B        0.10873
    127B ->132B       -0.10054
    127B ->134B        0.38521
    128B ->133B        0.72506

 Excited state symmetry could not be determined.
 Excited State  65:  2.987-?Sym    4.1867 eV  296.14 nm  f=0.0013
<S**2>=1.980
    114A ->130A        0.20873
    116A ->130A       -0.17031
```

```
    121A ->132A       -0.34359
    124A ->137A       -0.10792
    125A ->138A       -0.10912
    128A ->132A       -0.25134
    129A ->132A        0.24041
    129A ->135A       -0.10931
    114B ->130B       -0.25520
    115B ->129B        0.40130
    124B ->138B       -0.10595
    127B ->133B        0.18534
    128B ->132B       -0.14444
    128B ->134B        0.44526

 Excited state symmetry could not be determined.
 Excited State  66:  3.003-?Sym    4.1937 eV  295.64 nm  f=0.0045
<S**2>=2.005
    121A ->132A        0.19900
    127A ->133A       -0.11044
    128A ->132A        0.15512
    129A ->132A       -0.11592
    115B ->129B       -0.34316
    127B ->132B       -0.13427
    127B ->133B        0.43734
    128B ->132B        0.12226
    128B ->134B        0.65395

 Excited state symmetry could not be determined.
 Excited State  67:  3.121-?Sym    4.1953 eV  295.53 nm  f=0.0002
<S**2>=2.186
    121A ->131A       -0.20896
    122A ->132A        0.43758
    123A ->131A        0.10455
    126A ->132A        0.16177
    127A ->132A       -0.30631
    128A ->133A       -0.13481
    114B ->129B        0.19610
    121B ->131B       -0.13424
    125B ->132B       -0.26802
    126B ->131B       -0.13835
    127B ->132B        0.52283
    127B ->133B        0.11541
    128B ->133B        0.20159
    128B ->134B        0.12875

 Excited state symmetry could not be determined.
 Excited State  68:  2.368-?Sym    4.2329 eV  292.91 nm  f=0.0005
<S**2>=1.151
    127A ->134A       -0.14845
    129A ->133A        0.90388
    127B ->134B        0.10663
```

```
    128B ->133B        0.26547

 Excited state symmetry could not be determined.
 Excited State  69:  2.838-?Sym    4.2519 eV  291.60 nm  f=0.0042
<S**2>=1.763
    114A ->130A       -0.28610
    120A ->131A       -0.15169
    121A ->132A       -0.32859
    128A ->132A       -0.18964
    128A ->134A        0.26203
    129A ->132A        0.17886
    129A ->134A        0.25149
    129A ->135A       -0.21535
    114B ->130B        0.30116
    120B ->135B       -0.10279
    121B ->132B       -0.14618
    125B ->133B        0.14226
    126B ->132B       -0.13869
    127B ->133B        0.35098
    128B ->132B        0.16961
    128B ->135B        0.19344

 Excited state symmetry could not be determined.
 Excited State  70:  2.483-?Sym    4.2683 eV  290.47 nm  f=0.0042
<S**2>=1.292
    121A ->134A        0.10620
    127A ->133A       -0.17731
    129A ->134A        0.92022
    127B ->133B       -0.12815
    128B ->134B        0.13355

 Excited state symmetry could not be determined.
 Excited State  71:  2.739-?Sym    4.2884 eV  289.12 nm  f=0.0342
<S**2>=1.625
    114A ->130A        0.12845
    116A ->130A       -0.12277
    119A ->132A       -0.14036
    121A ->132A        0.12269
    125A ->132A       -0.11531
    128A ->132A        0.16370
    128A ->134A        0.46560
    129A ->135A        0.11672
    110B ->129B       -0.16367
    113B ->129B        0.10239
    114B ->130B       -0.23738
    115B ->129B        0.13714
    125B ->133B        0.21640
    126B ->132B        0.20890
    127B ->133B        0.41854
    128B ->132B       -0.11611
```

```
    128B ->134B       -0.29040
    128B ->135B       -0.11323

 Excited state symmetry could not be determined.
 Excited State  72:  2.743-?Sym    4.3008 eV  288.28 nm  f=0.0034
<S**2>=1.631
    118A ->131A       -0.11639
    123A ->131A        0.15277
    125A ->131A       -0.16642
    127A ->134A       -0.19217
    128A ->133A        0.63847
    129A ->133A       -0.11481
    107B ->129B       -0.11079
    125B ->134B        0.20820
    127B ->132B        0.12438
    127B ->134B        0.48424
    128B ->133B       -0.20674

 Excited state symmetry could not be determined.
 Excited State  73:  3.340-?Sym    4.3273 eV  286.51 nm  f=0.0015
<S**2>=2.539
    114A ->130A       -0.14372
    119A ->132A       -0.14634
    120A ->131A        0.10740
    123A ->132A        0.10602
    124A ->137A       -0.18519
    125A ->132A       -0.24254
    125A ->138A       -0.13656
    126A ->131A       -0.28168
    128A ->132A        0.16794
    128A ->134A       -0.12226
    129A ->132A        0.10330
    129A ->135A       -0.18339
    114B ->130B        0.25561
    122B ->137B       -0.14729
    123B ->137B        0.11768
    124B ->135B       -0.11910
    124B ->138B       -0.12867
    126B ->132B        0.54512
    126B ->135B       -0.14709
    128B ->135B        0.19498

 Excited state symmetry could not be determined.
 Excited State  74:  2.274-?Sym    4.3351 eV  286.00 nm  f=0.0004
<S**2>=1.043
    118A ->131A        0.16500
    119A ->131A        0.32657
    121A ->131A       -0.26235
    123A ->131A       -0.24260
    125A ->131A        0.46035
```

```
    128A ->131A       -0.17498
    128A ->133A        0.20495
    112B ->129B        0.10156
    120B ->131B        0.30161
    121B ->131B       -0.33484
    124B ->131B       -0.19399
    125B ->134B        0.12314
    126B ->131B        0.21965
    127B ->134B        0.16070
    128B ->131B        0.13519

 Excited state symmetry could not be determined.
 Excited State  75:  3.110-?Sym    4.3411 eV  285.60 nm  f=0.0255
<S**2>=2.167
    120A ->131A       -0.23723
    122A ->131A       -0.28307
    124A ->131A        0.15554
    126A ->131A        0.61104
    127A ->133A       -0.24536
    128A ->134A        0.11534
    129A ->135A       -0.10386
    116B ->130B        0.14283
    119B ->131B        0.23013
    122B ->131B        0.11997
    125B ->131B       -0.12605
    126B ->132B        0.35615
    127B ->133B       -0.11077

 Excited state symmetry could not be determined.
 Excited State  76:  2.770-?Sym    4.3635 eV  284.14 nm  f=0.0007
<S**2>=1.668
    120A ->131A       -0.10297
    124A ->131A        0.10673
    125A ->132A       -0.11074
    126A ->131A        0.19716
    127A ->133A        0.60255
    128A ->134A       -0.42357
    129A ->134A        0.16036
    129A ->135A        0.13581
    114B ->130B       -0.15135
    120B ->132B        0.20323
    121B ->132B       -0.15736
    124B ->132B       -0.12014
    126B ->132B        0.13173
    127B ->133B        0.15300
    128B ->132B        0.24077

 Excited state symmetry could not be determined.
 Excited State  77:  2.562-?Sym    4.3713 eV  283.63 nm  f=0.0315
<S**2>=1.391
```

```
    114A ->130A        0.18942
    121A ->132A       -0.18705
    127A ->133A       -0.38304
    128A ->134A        0.20379
    129A ->132A        0.11199
    129A ->135A        0.20073
    120B ->132B        0.32254
    121B ->132B       -0.32327
    121B ->135B        0.15035
    124B ->132B       -0.23086
    126B ->132B        0.11028
    127B ->133B       -0.19906
    128B ->132B        0.47607
    128B ->135B       -0.10754

 Excited state symmetry could not be determined.
 Excited State  78:  2.257-?Sym    4.3950 eV  282.10 nm  f=0.0006
<S**2>=1.023
    122A ->132A       -0.15990
    127A ->134A        0.69592
    128A ->133A       -0.28510
    129A ->133A        0.12065
    125B ->132B       -0.14784
    125B ->134B        0.17408
    126B ->133B        0.11037
    127B ->134B        0.44732

 Excited state symmetry could not be determined.
 Excited State  79:  2.222-?Sym    4.4164 eV  280.74 nm  f=0.0032
<S**2>=0.984
    115A ->130A        0.15424
    121A ->131A       -0.12217
    122A ->132A        0.43454
    124A ->132A        0.11585
    125A ->131A       -0.21307
    126A ->132A        0.13628
    127A ->132A       -0.16430
    127A ->134A        0.18667
    114B ->129B        0.11875
    115B ->130B        0.13532
    122B ->132B        0.18597
    123B ->132B        0.16700
    125B ->132B        0.53467
    125B ->135B       -0.11675
    126B ->133B        0.10506
    127B ->132B       -0.30056
    127B ->134B        0.14097

 Excited state symmetry could not be determined.
```

```
 Excited State  80:  3.235-?Sym    4.4425 eV  279.09 nm  f=0.0052
<S**2>=2.366
    111A ->130A       -0.24684
    112A ->130A        0.60350
    114A ->130A       -0.14244
    115A ->130A       -0.18844
    120A ->131A        0.12679
    111B ->130B        0.14240
    112B ->130B       -0.42780
    113B ->129B       -0.16126
    114B ->130B       -0.15276
    115B ->130B       -0.16971
    119B ->131B       -0.11748
```

Table S35. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 2^{2+}(*S*=0)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    1.4707 eV  843.05 nm
f=0.0118  <S**2>=0.000
     154 ->158         0.18122
     156 ->158        -0.19443
     157 ->158         0.65016
 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 symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    1.7127 eV  723.90 nm
f=0.0055  <S**2>=0.000
     154 ->158         0.10133
     156 ->158         0.66697
     157 ->158         0.17412

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    2.4330 eV  509.59 nm
f=0.1750  <S**2>=0.000
     154 ->158         0.62879
     155 ->158         0.23147
     157 ->158        -0.19309

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    2.5579 eV  484.72 nm
f=0.2328  <S**2>=0.000
     153 ->158         0.14664
     154 ->158        -0.22971
     155 ->158         0.60670
     157 ->160        -0.12157

 Excited state symmetry could not be determined.
 Excited State   5:      Singlet-?Sym    2.7883 eV  444.66 nm
f=0.0413  <S**2>=0.000
     153 ->158         0.65793
     155 ->158        -0.13659
     157 ->159        -0.14307

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    2.8251 eV  438.87 nm
f=0.0152  <S**2>=0.000
     148 ->158        -0.11546
     151 ->158         0.11438
     152 ->158         0.54612
```

```
     155 ->158         0.10413
     157 ->159        -0.37788

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    2.8360 eV  437.17 nm
f=0.0038  <S**2>=0.000
     152 ->158         0.39832
     153 ->158         0.16571
     157 ->159         0.50889
     157 ->160        -0.15244

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    2.8538 eV  434.45 nm
f=0.0041  <S**2>=0.000
     154 ->160         0.10254
     156 ->160        -0.15467
     157 ->159         0.19106
     157 ->160         0.62984

 Excited state symmetry could not be determined.
 Excited State   9:      Singlet-?Sym    2.9123 eV  425.72 nm
f=0.0145  <S**2>=0.000
     151 ->158         0.68848

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    3.0336 eV  408.70 nm
f=0.0050  <S**2>=0.000
     148 ->158         0.14401
     150 ->158         0.68215

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    3.0380 eV  408.11 nm
f=0.0020  <S**2>=0.000
     148 ->158         0.64020
     149 ->158         0.19516
     150 ->158        -0.15497

 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    3.0704 eV  403.80 nm
f=0.0022  <S**2>=0.000
     148 ->158        -0.19662
     149 ->158         0.66824

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    3.1438 eV  394.37 nm
f=0.0489  <S**2>=0.000
     156 ->159         0.68236
     157 ->159         0.10070

 Excited state symmetry could not be determined.
```

```
 Excited State  14:      Singlet-?Sym    3.2693 eV  379.24 nm
f=0.0191  <S**2>=0.000
     155 ->159        -0.26768
     156 ->160         0.61035
     157 ->160         0.11218

 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    3.4037 eV  364.26 nm
f=0.0178  <S**2>=0.000
     155 ->159        -0.18137
     155 ->160         0.60425
     156 ->165        -0.10791
     157 ->165         0.16033

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    3.4381 eV  360.62 nm
f=0.0046  <S**2>=0.000
     154 ->166         0.17068
     154 ->167         0.10993
     155 ->159         0.26575
     155 ->160        -0.10768
     155 ->165        -0.11056
     156 ->160         0.18352
     157 ->160         0.15494
     157 ->166         0.38120
     157 ->167         0.23480
     157 ->169         0.14751

 Excited state symmetry could not be determined.
 Excited State  17:      Singlet-?Sym    3.4568 eV  358.67 nm
f=0.0030  <S**2>=0.000
     155 ->159         0.54321
     155 ->160         0.26711
     156 ->160         0.16080
     157 ->166        -0.19752
     157 ->167        -0.11920

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    3.6015 eV  344.25 nm
f=0.0116  <S**2>=0.000
     155 ->160         0.15865
     155 ->166         0.12009
     156 ->165         0.45917
     156 ->170         0.18692
     156 ->174         0.15907
     157 ->165        -0.25821
     157 ->166         0.14582

 Excited state symmetry could not be determined.
```

```
 Excited State  19:      Singlet-?Sym    3.6952 eV  335.53 nm
f=0.0172  <S**2>=0.000
     154 ->159         0.64778
     154 ->160         0.21541
     157 ->159        -0.10475

 Excited state symmetry could not be determined.
 Excited State  20:      Singlet-?Sym    3.7317 eV  332.25 nm
f=0.0032  <S**2>=0.000
     154 ->165         0.17007
     155 ->166        -0.23517
     155 ->167        -0.14602
     156 ->165         0.29524
     156 ->166        -0.14647
     156 ->170         0.11837
     156 ->174         0.10560
     157 ->165         0.35823
     157 ->170         0.10884

 Excited state symmetry could not be determined.
 Excited State  21:      Singlet-?Sym    3.7531 eV  330.35 nm
f=0.0036  <S**2>=0.000
     154 ->159        -0.20793
     154 ->160         0.61513

 Excited state symmetry could not be determined.
 Excited State  22:      Singlet-?Sym    3.7791 eV  328.08 nm
f=0.0055  <S**2>=0.000
     157 ->161         0.67633

 Excited state symmetry could not be determined.
 Excited State  23:      Singlet-?Sym    3.9429 eV  314.45 nm
f=0.0024  <S**2>=0.000
     156 ->166        -0.14870
     157 ->162         0.63451

 Excited state symmetry could not be determined.
 Excited State  24:      Singlet-?Sym    4.0483 eV  306.26 nm
f=0.0011  <S**2>=0.000
     153 ->159        -0.15118
     153 ->160        -0.19461
     157 ->163         0.60492
     157 ->164         0.15966

 Excited state symmetry could not be determined.
 Excited State  25:      Singlet-?Sym    4.0707 eV  304.57 nm
f=0.0059  <S**2>=0.000
     153 ->159        -0.19123
     153 ->160        -0.13088
     156 ->161         0.16907
```

```
     157 ->163        -0.22376
     157 ->164         0.56028

 Excited state symmetry could not be determined.
 Excited State  26:      Singlet-?Sym    4.0752 eV  304.24 nm
f=0.0112  <S**2>=0.000
     152 ->159         0.16162
     152 ->160         0.11967
     153 ->159         0.25267
     153 ->160         0.27656
     155 ->166         0.10110
     156 ->161         0.49781
     157 ->163         0.13074

 Excited state symmetry could not be determined.
 Excited State  27:      Singlet-?Sym    4.0858 eV  303.45 nm
f=0.0155  <S**2>=0.000
     152 ->160         0.12399
     153 ->159         0.36800
     153 ->160         0.20570
     155 ->166        -0.12642
     156 ->161        -0.29939
     156 ->166        -0.18585
     156 ->167        -0.11025
     157 ->164         0.26223
     157 ->165        -0.13021

 Excited state symmetry could not be determined.
 Excited State  28:      Singlet-?Sym    4.1019 eV  302.26 nm
f=0.0111  <S**2>=0.000
     152 ->159         0.13020
     155 ->166         0.14365
     156 ->161        -0.24693
     156 ->166         0.34180
     156 ->167         0.20761
     156 ->169         0.12429
     157 ->162         0.13994
     157 ->164         0.23363
     157 ->165         0.20720

 Excited state symmetry could not be determined.
 Excited State  29:      Singlet-?Sym    4.1133 eV  301.42 nm
f=0.0035  <S**2>=0.000
     151 ->159         0.11698
     151 ->160        -0.18036
     152 ->159         0.57481
     153 ->159        -0.20241
     153 ->160         0.10993
     156 ->161        -0.12165
```

```
 Excited state symmetry could not be determined.
 Excited State  30:      Singlet-?Sym    4.1440 eV  299.19 nm
f=0.0021  <S**2>=0.000
     151 ->159         0.49337
     152 ->160        -0.40851
     153 ->159         0.26532

 Excited state symmetry could not be determined.
 Excited State  31:      Singlet-?Sym    4.1647 eV  297.70 nm
f=0.0013  <S**2>=0.000
     151 ->160         0.14972
     152 ->159        -0.12256
     152 ->160        -0.31065
     153 ->159        -0.26266
     153 ->160         0.50564

 Excited state symmetry could not be determined.
 Excited State  32:      Singlet-?Sym    4.2024 eV  295.03 nm
f=0.0243  <S**2>=0.000
     149 ->159         0.10664
     150 ->159         0.17735
     150 ->160         0.13774
     155 ->165         0.18340
     155 ->166         0.33276
     155 ->167         0.21728
     155 ->169         0.12953
     156 ->164        -0.17527
     156 ->166        -0.22628
     156 ->167        -0.11942
     157 ->165         0.21541

 Excited state symmetry could not be determined.
 Excited State  33:      Singlet-?Sym    4.2292 eV  293.16 nm
f=0.0340  <S**2>=0.000
     149 ->159        -0.16294
     149 ->160         0.11411
     150 ->159         0.45239
     155 ->161         0.22104
     156 ->162        -0.16266
     156 ->163        -0.27473
     156 ->166         0.13819
     157 ->162         0.13642

 Excited state symmetry could not be determined.
 Excited State  34:      Singlet-?Sym    4.2383 eV  292.54 nm
f=0.0017  <S**2>=0.000
     149 ->159         0.14663
     149 ->160        -0.10015
     150 ->159         0.20950
     150 ->160        -0.15064
```

```
     151 ->159         0.38402
     151 ->160        -0.16012
     152 ->159        -0.23619
     152 ->160         0.32291
     153 ->159        -0.17528
     153 ->160         0.13395

 Excited state symmetry could not be determined.
 Excited State  35:      Singlet-?Sym    4.2502 eV  291.71 nm
f=0.0133  <S**2>=0.000
     150 ->159         0.18467
     155 ->166        -0.11097
     156 ->162         0.61602

 Excited state symmetry could not be determined.
 Excited State  36:      Singlet-?Sym    4.2713 eV  290.27 nm
f=0.0611  <S**2>=0.000
     149 ->159         0.45061
     150 ->159         0.17077
     151 ->159        -0.18916
     152 ->160        -0.16610
     155 ->161        -0.14681
     155 ->162        -0.11126
     156 ->161         0.12074
     156 ->162        -0.16092
     156 ->164        -0.22955

 Excited state symmetry could not be determined.
 Excited State  37:      Singlet-?Sym    4.2776 eV  289.84 nm
f=0.0507  <S**2>=0.000
     149 ->160         0.17998
     150 ->159        -0.29221
     150 ->160         0.38723
     151 ->160        -0.29412
     152 ->159        -0.14865
     156 ->164        -0.19143

 Excited state symmetry could not be determined.
 Excited State  38:      Singlet-?Sym    4.2947 eV  288.69 nm
f=0.0047  <S**2>=0.000
     141 ->158        -0.10940
     145 ->158        -0.14896
     146 ->158         0.17125
     147 ->158         0.61396
     151 ->160        -0.14553

 Excited state symmetry could not be determined.
 Excited State  39:      Singlet-?Sym    4.2980 eV  288.47 nm
f=0.0382  <S**2>=0.000
     147 ->158         0.17000
```

```
     149 ->160        -0.19381
     150 ->160         0.32761
     151 ->159         0.13045
     151 ->160         0.42260
     152 ->160         0.19089
     156 ->164        -0.18012

 Excited state symmetry could not be determined.
 Excited State  40:      Singlet-?Sym    4.3335 eV  286.10 nm
f=0.0008  <S**2>=0.000
     149 ->159         0.24498
     149 ->160         0.51754
     150 ->160        -0.16795
     151 ->159         0.10389
     151 ->160         0.27306
     152 ->160         0.11155
     155 ->161         0.11548

 Excited state symmetry could not be determined.
 Excited State  41:      Singlet-?Sym    4.3777 eV  283.22 nm
f=0.0029  <S**2>=0.000
     145 ->158        -0.12053
     146 ->158         0.22231
     147 ->158        -0.10467
     148 ->159         0.32475
     149 ->159         0.12839
     149 ->160        -0.14980
     155 ->161         0.45697
     156 ->163         0.14353

 Excited state symmetry could not be determined.
 Excited State  42:      Singlet-?Sym    4.3935 eV  282.20 nm
f=0.0104  <S**2>=0.000
     142 ->158        -0.10350
     146 ->158        -0.42526
     147 ->158         0.15516
     148 ->159         0.46838
     151 ->160         0.10239

 Excited state symmetry could not be determined.
 Excited State  43:      Singlet-?Sym    4.4023 eV  281.64 nm
f=0.0026  <S**2>=0.000
     140 ->158        -0.13917
     142 ->158         0.18126
     144 ->158        -0.15243
     145 ->158         0.45539
     146 ->158         0.31171
     148 ->159         0.23338
     155 ->161        -0.18048
```

```
 Excited state symmetry could not be determined.
 Excited State  44:      Singlet-?Sym    4.4083 eV  281.25 nm
f=0.0126  <S**2>=0.000
     144 ->158         0.13584
     145 ->158        -0.29290
     146 ->158         0.22094
     147 ->158        -0.17830
     148 ->159         0.18441
     155 ->161        -0.26328
     155 ->165         0.30544
     155 ->166        -0.10329
     157 ->166         0.12660

 Excited state symmetry could not be determined.
 Excited State  45:      Singlet-?Sym    4.4190 eV  280.57 nm
f=0.0676  <S**2>=0.000
     145 ->158         0.25022
     148 ->159        -0.14806
     148 ->160        -0.11832
     155 ->161         0.14957
     155 ->162        -0.27117
     155 ->165         0.33202
     155 ->166        -0.10087
     156 ->162        -0.13620
     156 ->164         0.22093
     157 ->166         0.10975

 Excited state symmetry could not be determined.
 Excited State  46:      Singlet-?Sym    4.4530 eV  278.43 nm
f=0.0493  <S**2>=0.000
     148 ->159         0.10046
     148 ->160         0.30249
     149 ->159         0.11680
     150 ->160         0.13840
     155 ->162        -0.26119
     155 ->165        -0.16383
     156 ->164         0.42671
     156 ->166        -0.10723

 Excited state symmetry could not be determined.
 Excited State  47:      Singlet-?Sym    4.4606 eV  277.95 nm
f=0.0205  <S**2>=0.000
     148 ->160         0.58408
     155 ->161         0.15469
     155 ->165         0.15426
     156 ->164        -0.18352

 Excited state symmetry could not be determined.
 Excited State  48:      Singlet-?Sym    4.4827 eV  276.58 nm
f=0.0065  <S**2>=0.000
```

```
     140 ->158         0.35778
     142 ->158        -0.31578
     144 ->158         0.35392
     145 ->158         0.26019
     146 ->158         0.20178

 Excited state symmetry could not be determined.
 Excited State  49:      Singlet-?Sym    4.5072 eV  275.08 nm
f=0.2065  <S**2>=0.000
     148 ->160         0.10697
     149 ->159        -0.13868
     149 ->160         0.24926
     150 ->159         0.13997
     150 ->160         0.11442
     154 ->161         0.10561
     155 ->163         0.16182
     156 ->163         0.52645

 Excited state symmetry could not be determined.
 Excited State  50:      Singlet-?Sym    4.5211 eV  274.23 nm
f=0.0062  <S**2>=0.000
     140 ->158        -0.29747
     142 ->158         0.26804
     144 ->158         0.51272
     145 ->158         0.10885
     146 ->158        -0.13073
     155 ->162         0.11424

 Excited state symmetry could not be determined.
 Excited State  51:      Singlet-?Sym    4.5660 eV  271.54 nm
f=0.2341  <S**2>=0.000
     144 ->158        -0.12408
     149 ->159         0.16842
     150 ->160         0.17423
     154 ->161         0.33536
     155 ->162         0.46609
     156 ->164         0.19236

 Excited state symmetry could not be determined.
 Excited State  52:      Singlet-?Sym    4.6066 eV  269.15 nm
f=0.0074  <S**2>=0.000
     141 ->158         0.25228
     143 ->158         0.59090
     144 ->158         0.13495
     154 ->161        -0.16678

 Excited state symmetry could not be determined.
 Excited State  53:      Singlet-?Sym    4.6182 eV  268.47 nm
f=0.0426  <S**2>=0.000
     154 ->161         0.26569
```

```
     155 ->162        -0.18003
     155 ->163         0.55112
     155 ->165        -0.12659
     156 ->163        -0.14408

 Excited state symmetry could not be determined.
 Excited State  54:      Singlet-?Sym    4.6347 eV  267.51 nm
f=0.1917  <S**2>=0.000
     143 ->158         0.16844
     149 ->159        -0.14126
     150 ->160        -0.14496
     154 ->161         0.49074
     155 ->162        -0.15346
     155 ->163        -0.32811
     156 ->164        -0.12151

 Excited state symmetry could not be determined.
 Excited State  55:      Singlet-?Sym    4.6556 eV  266.31 nm
f=0.0094  <S**2>=0.000
     154 ->162        -0.10502
     155 ->164         0.66650

 Excited state symmetry could not be determined.
 Excited State  56:      Singlet-?Sym    4.6858 eV  264.59 nm
f=0.0015  <S**2>=0.000
     157 ->165        -0.10530
     157 ->166        -0.36458
     157 ->167         0.54010

 Excited state symmetry could not be determined.
 Excited State  57:      Singlet-?Sym    4.7357 eV  261.81 nm
f=0.0078  <S**2>=0.000
     141 ->158         0.57476
     143 ->158        -0.25083
     157 ->168        -0.15877
     157 ->170        -0.12575

 Excited state symmetry could not be determined.
 Excited State  58:      Singlet-?Sym    4.7876 eV  258.97 nm
f=0.0009  <S**2>=0.000
     139 ->158         0.11014
     154 ->162         0.63695
     157 ->168        -0.13313

 Excited state symmetry could not be determined.
 Excited State  59:      Singlet-?Sym    4.8341 eV  256.48 nm
f=0.0256  <S**2>=0.000
     138 ->158        -0.10747
     140 ->158         0.43852
     142 ->158         0.48681
```

```
 Excited state symmetry could not be determined.
 Excited State  60:      Singlet-?Sym    4.8518 eV  255.54 nm
f=0.0077  <S**2>=0.000
     138 ->158        -0.11506
     139 ->158        -0.23060
     141 ->158         0.15583
     143 ->158        -0.11984
     154 ->162         0.10456
     154 ->163         0.48251
     154 ->164         0.11012
     154 ->165         0.15942
     157 ->165        -0.11884
     157 ->168         0.15625

 Excited state symmetry could not be determined.
 Excited State  61:      Singlet-?Sym    4.8736 eV  254.40 nm
f=0.0089  <S**2>=0.000
     138 ->158         0.12153
     139 ->158         0.31026
     143 ->158         0.10623
     153 ->161         0.16223
     154 ->163         0.37367
     154 ->164         0.20765
     154 ->165        -0.17645
     157 ->165         0.12522
     157 ->168        -0.20019
     157 ->170        -0.10330

 Excited state symmetry could not be determined.
 Excited State  62:      Singlet-?Sym    4.9010 eV  252.98 nm
f=0.0168  <S**2>=0.000
     137 ->158         0.33913
     138 ->158         0.49470
     142 ->158         0.11265
     154 ->164        -0.22634
     154 ->165         0.10988

 Excited state symmetry could not be determined.
 Excited State  63:      Singlet-?Sym    4.9149 eV  252.26 nm
f=0.0369  <S**2>=0.000
     137 ->158         0.10696
     138 ->158         0.17574
     154 ->163        -0.20922
     154 ->164         0.58918

 Excited state symmetry could not be determined.
 Excited State  64:      Singlet-?Sym    4.9795 eV  248.99 nm
f=0.0203  <S**2>=0.000
     137 ->158         0.10224
```

```
     139 ->158         0.26801
     153 ->161         0.10806
     154 ->166         0.11370
     157 ->166        -0.10091
     157 ->167        -0.17131
     157 ->168         0.47915
     157 ->169         0.15500
     157 ->170        -0.18500

 Excited state symmetry could not be determined.
 Excited State  65:      Singlet-?Sym    4.9833 eV  248.80 nm
f=0.0011  <S**2>=0.000
     151 ->161        -0.10054
     152 ->161         0.20554
     153 ->161         0.57676
     157 ->169         0.10968

 Excited state symmetry could not be determined.
 Excited State  66:      Singlet-?Sym    5.0165 eV  247.15 nm
f=0.0079  <S**2>=0.000
     139 ->158         0.17339
     152 ->161         0.51207
     153 ->161        -0.22881
     154 ->163         0.11465
     154 ->165         0.11415
     157 ->169         0.15540

 Excited state symmetry could not be determined.
 Excited State  67:      Singlet-?Sym    5.0321 eV  246.39 nm
f=0.0084  <S**2>=0.000
     139 ->158        -0.10081
     152 ->161         0.36126
     154 ->165        -0.19125
     154 ->166        -0.16965
     154 ->167        -0.10426
     157 ->165         0.10075
     157 ->167         0.16818
     157 ->168         0.27241
     157 ->169        -0.25392
     157 ->170        -0.13921

 Excited state symmetry could not be determined.
 Excited State  68:      Singlet-?Sym    5.0357 eV  246.21 nm
f=0.0751  <S**2>=0.000
     137 ->158        -0.29676
     138 ->158         0.24642
     139 ->158        -0.24706
     154 ->165        -0.15949
     154 ->166         0.14775
     157 ->165         0.10065
```

```
     157 ->166        -0.17542
     157 ->169         0.30025
     157 ->173        -0.10588

 Excited state symmetry could not be determined.
 Excited State  69:      Singlet-?Sym    5.0462 eV  245.70 nm
f=0.0168  <S**2>=0.000
     137 ->158         0.34011
     138 ->158        -0.17548
     139 ->158        -0.20560
     153 ->161        -0.11953
     154 ->165        -0.17474
     154 ->166         0.11137
     156 ->166        -0.24035
     156 ->167         0.32103

 Excited state symmetry could not be determined.
 Excited State  70:      Singlet-?Sym    5.0686 eV  244.61 nm
f=0.0517  <S**2>=0.000
     137 ->158         0.25023
     138 ->158        -0.13891
     139 ->158        -0.16020
     151 ->161         0.42339
     156 ->166         0.16568
     156 ->167        -0.30664

 Excited state symmetry could not be determined.
 Excited State  71:      Singlet-?Sym    5.0801 eV  244.06 nm
f=0.0057  <S**2>=0.000
     137 ->158        -0.15919
     139 ->158         0.11313
     151 ->161         0.46666
     152 ->163        -0.10188
     156 ->166        -0.19608
     156 ->167         0.31943
     157 ->170         0.11466

 Excited state symmetry could not be determined.
 Excited State  72:      Singlet-?Sym    5.1097 eV  242.64 nm
f=0.0205  <S**2>=0.000
     147 ->159         0.16028
     149 ->161        -0.10337
     150 ->161         0.61890

 Excited state symmetry could not be determined.
 Excited State  73:      Singlet-?Sym    5.1385 eV  241.29 nm
f=0.0431  <S**2>=0.000
     144 ->159         0.11678
     147 ->160         0.11027
     149 ->161         0.58061
```

```
     150 ->161         0.11574
     150 ->162        -0.10558
     151 ->161         0.11494
     154 ->166        -0.12415
     157 ->169         0.11389

 Excited state symmetry could not be determined.
 Excited State  74:      Singlet-?Sym    5.1563 eV  240.45 nm
f=0.0347  <S**2>=0.000
     149 ->161         0.19897
     153 ->162        -0.20444
     154 ->165         0.12800
     154 ->166         0.39473
     154 ->167         0.12878
     157 ->169        -0.37823
     157 ->170        -0.11232

 Excited state symmetry could not be determined.
 Excited State  75:      Singlet-?Sym    5.1611 eV  240.23 nm
f=0.0073  <S**2>=0.000
     153 ->162         0.61732
     154 ->166         0.17459
     157 ->169        -0.13695

 Excited state symmetry could not be determined.
 Excited State  76:      Singlet-?Sym    5.2006 eV  238.40 nm
f=0.0020  <S**2>=0.000
     147 ->159        -0.14224
     149 ->162        -0.10400
     149 ->163        -0.11255
     150 ->164        -0.10945
     151 ->165        -0.10002
     152 ->162         0.44246
     152 ->163         0.16985
     156 ->165        -0.13413
     156 ->168         0.26940
     156 ->170         0.10302

 Excited state symmetry could not be determined.
 Excited State  77:      Singlet-?Sym    5.2035 eV  238.27 nm
f=0.0029  <S**2>=0.000
     148 ->161         0.17199
     151 ->165        -0.10847
     152 ->162        -0.33683
     154 ->165         0.11279
     156 ->165        -0.18877
     156 ->168         0.35498
     156 ->170         0.17135
     157 ->170        -0.14955
```

```
 Excited state symmetry could not be determined.
 Excited State  78:      Singlet-?Sym    5.2233 eV  237.37 nm
f=0.0136  <S**2>=0.000
     147 ->159         0.17516
     149 ->162         0.17015
     149 ->163         0.21415
     149 ->164        -0.11638
     150 ->164         0.11204
     151 ->161        -0.12231
     151 ->162        -0.16014
     152 ->162         0.31007
     152 ->163        -0.16494
     152 ->164         0.15380
     153 ->162         0.14944
     153 ->163         0.20187

 Excited state symmetry could not be determined.
 Excited State  79:      Singlet-?Sym    5.2354 eV  236.82 nm
f=0.0564  <S**2>=0.000
     148 ->161         0.15859
     152 ->162         0.10382
     154 ->165        -0.27776
     155 ->166         0.21845
     155 ->167        -0.28221
     155 ->169        -0.10750
     156 ->168         0.18925
     157 ->169        -0.10315
     157 ->170         0.28778

 Excited state symmetry could not be determined.
 Excited State  80:      Singlet-?Sym    5.2400 eV  236.61 nm
f=0.0032  <S**2>=0.000
     147 ->160        -0.16170
     148 ->161         0.22836
     150 ->162        -0.12409
     150 ->163        -0.20720
     150 ->164        -0.20976
     151 ->162         0.14915
     152 ->163         0.16210
     152 ->164         0.21110
     153 ->162        -0.11556
     153 ->163         0.11862
     153 ->164         0.21453
     156 ->168        -0.16705
```

Table S36. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 2^{3+}(*S*=1/2)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  2.015-?Sym    0.5225 eV 2372.68 nm  f=0.0020
<S**2>=0.765
    142B ->157B        0.16082
    148B ->157B        0.13899
    149B ->157B        0.23081
    150B ->157B        0.66187
    153B ->157B        0.14323
    154B ->157B        0.15999
    155B ->157B        0.53474
    156B ->157B        0.33087
 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 symmetry could not be determined.
 Excited State   2:  2.177-?Sym    0.6763 eV 1833.35 nm  f=0.0005
<S**2>=0.935
    157A ->158A        0.32023
    140B ->157B        0.11608
    148B ->157B        0.21066
    149B ->157B        0.74548
    150B ->157B       -0.33148
    151B ->157B        0.14050
    153B ->157B        0.18456
    154B ->157B        0.25903
    156B ->157B       -0.13482
    156B ->158B       -0.22777
    156B <-158B       -0.17693

 Excited state symmetry could not be determined.
 Excited State   3:  2.020-?Sym    0.7901 eV 1569.28 nm  f=0.0238
<S**2>=0.770
    149A ->158A        0.14324
    149B ->158B        0.11275
    150B ->157B       -0.26825
    155B ->157B       -0.21037
    156B ->157B        0.90341

 Excited state symmetry could not be determined.
 Excited State   4:  2.766-?Sym    0.9804 eV 1264.65 nm  f=0.0112
<S**2>=1.663
    151A ->158A        0.10973
    157A ->158A        0.77428
    148B ->158B        0.11460
```

```
    149B ->157B       -0.30963
    150B ->157B        0.12587
    156B ->158B       -0.46397

 Excited state symmetry could not be determined.
 Excited State   5:  2.113-?Sym    1.4671 eV  845.10 nm  f=0.0325
<S**2>=0.866
    151A ->158A       -0.10265
    148B ->158B       -0.11972
    149B ->157B       -0.15807
    150B ->157B       -0.44022
    152B ->157B        0.48334
    153B ->157B       -0.12521
    155B ->157B        0.66011
    156B ->158B        0.16484

 Excited state symmetry could not be determined.
 Excited State   6:  2.075-?Sym    1.5116 eV  820.21 nm  f=0.0023
<S**2>=0.827
    152B ->157B       -0.11077
    153B ->157B       -0.59324
    154B ->157B        0.75834

 Excited state symmetry could not be determined.
 Excited State   7:  2.053-?Sym    1.5450 eV  802.49 nm  f=0.0021
<S**2>=0.804
    150B ->157B        0.13494
    151B ->157B       -0.46168
    152B ->157B        0.56016
    153B ->157B        0.40530
    154B ->157B        0.37341
    155B ->157B       -0.34884

 Excited state symmetry could not be determined.
 Excited State   8:  2.061-?Sym    1.5772 eV  786.11 nm  f=0.0008
<S**2>=0.811
    149B ->157B       -0.37652
    151B ->157B        0.55439
    152B ->157B       -0.18489
    153B ->157B        0.57932
    154B ->157B        0.36791

 Excited state symmetry could not be determined.
 Excited State   9:  2.044-?Sym    1.5797 eV  784.88 nm  f=0.0006
<S**2>=0.795
    150B ->157B        0.29113
    151B ->157B        0.63826
    152B ->157B        0.61299
    153B ->157B       -0.21133
    154B ->157B       -0.14919
```

```
    155B ->157B       -0.20011

 Excited state symmetry could not be determined.
 Excited State  10:  2.610-?Sym    1.7333 eV  715.31 nm  f=0.0225
<S**2>=1.453
    149A ->158A       -0.20032
    150A ->158A        0.12939
    151A ->158A       -0.10869
    153A ->158A       -0.38008
    156A ->158A        0.24835
    157A ->158A       -0.12646
    148B ->157B        0.70039
    149B ->157B       -0.23870
    149B ->158B        0.11544
    155B ->158B       -0.23339
    156B ->158B       -0.18779

 Excited state symmetry could not be determined.
 Excited State  11:  2.353-?Sym    1.7899 eV  692.70 nm  f=0.1986
<S**2>=1.134
    157A ->158A        0.46179
    148B ->157B        0.32203
    150B ->158B        0.11055
    155B ->157B       -0.12703
    156B ->158B        0.78300

 Excited state symmetry could not be determined.
 Excited State  12:  3.168-?Sym    1.8713 eV  662.56 nm  f=0.0229
<S**2>=2.259
    149A ->158A       -0.41547
    150A ->158A        0.18279
    152A ->158A       -0.10971
    153A ->158A       -0.18562
    155A ->158A       -0.11538
    156A ->158A        0.19841
    157A ->158A        0.12465
    148B ->157B       -0.40707
    148B ->158B        0.10162
    149B ->157B        0.11094
    149B ->158B        0.53995
    150B ->158B       -0.15432
    151B ->158B        0.14527
    153B ->158B        0.10620
    154B ->158B        0.13143
    155B ->158B       -0.21272
    156B ->158B        0.19289

 Excited state symmetry could not be determined.
 Excited State  13:  3.367-?Sym    1.9812 eV  625.79 nm  f=0.0019
<S**2>=2.585
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    149A ->158A       -0.29876
    151A ->158A       -0.37004
    152A ->158A       -0.10132
    153A ->158A        0.39793
    154A ->158A        0.22898
    156A ->158A       -0.14298
    148B ->157B        0.23602
    149B ->158B        0.29504
    150B ->158B        0.17602
    153B ->158B        0.10655
    154B ->158B        0.24020
    155B ->158B        0.47974
    156B ->158B       -0.10728

 Excited state symmetry could not be determined.
 Excited State  14:  3.238-?Sym    2.0866 eV  594.20 nm  f=0.0117
<S**2>=2.371
    149A ->158A        0.20763
    150A ->158A        0.28525
    152A ->158A       -0.20274
    154A ->158A        0.70068
    155A ->158A        0.19996
    156A ->158A        0.21787
    157A ->158A        0.11917
    148B ->158B       -0.26687
    150B ->158B       -0.10207
    153B ->158B       -0.22823
    154B ->158B        0.12599

 Excited state symmetry could not be determined.
 Excited State  15:  2.964-?Sym    2.1292 eV  582.30 nm  f=0.0053
<S**2>=1.946
    149A ->158A        0.19602
    150A ->158A       -0.12697
    153A ->158A       -0.47110
    156A ->158A        0.17002
    148B ->157B       -0.17303
    150B ->158B        0.70131
    152B ->158B       -0.23943
    155B ->158B        0.24763

 Excited state symmetry could not be determined.
 Excited State  16:  2.673-?Sym    2.1478 eV  577.25 nm  f=0.0000
<S**2>=1.536
    150A ->158A        0.47001
    151A ->158A        0.45138
    152A ->158A        0.20599
    153A ->158A        0.10543
    154A ->158A       -0.15006
    155A ->158A        0.31807
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    156A ->158A        0.39801
    152B ->158B        0.13069
    153B ->158B        0.10538
    154B ->158B        0.10701
    155B ->158B        0.39531

 Excited state symmetry could not be determined.
 Excited State  17:  3.115-?Sym    2.1687 eV  571.69 nm  f=0.0044
<S**2>=2.176
    149A ->158A       -0.21168
    150A ->158A       -0.23287
    152A ->158A        0.72273
    154A ->158A        0.48034
    148B ->158B        0.18259
    151B ->158B       -0.20386

 Excited state symmetry could not be determined.
 Excited State  18:  3.074-?Sym    2.2287 eV  556.30 nm  f=0.0128
<S**2>=2.113
    149A ->158A       -0.20049
    150A ->158A       -0.20151
    151A ->158A        0.54624
    152A ->158A       -0.47239
    153A ->158A       -0.19954
    154A ->158A        0.33261
    156A ->158A       -0.14377
    157A ->158A       -0.13932
    148B ->158B        0.33930
    155B ->158B        0.14461

 Excited state symmetry could not be determined.
 Excited State  19:  2.811-?Sym    2.2698 eV  546.25 nm  f=0.0021
<S**2>=1.726
    150A ->158A       -0.25372
    152A ->158A       -0.19334
    153A ->158A        0.39410
    155A ->158A       -0.37778
    156A ->158A        0.73325
    149B ->158B       -0.12877
    154B ->158B       -0.12753

 Excited state symmetry could not be determined.
 Excited State  20:  2.821-?Sym    2.3069 eV  537.45 nm  f=0.0029
<S**2>=1.739
    148A ->158A       -0.10947
    149A ->158A       -0.15364
    150A ->158A       -0.33248
    151A ->158A       -0.21098
    152A ->158A       -0.13886
    155A ->158A        0.81392
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    156A ->158A        0.16053
    148B ->158B        0.17570
    154B ->158B       -0.12804
    155B ->158B       -0.15403

 Excited state symmetry could not be determined.
 Excited State  21:  2.536-?Sym    2.3907 eV  518.60 nm  f=0.0130
<S**2>=1.358
    150A ->158A       -0.29676
    151A ->158A        0.12604
    154A ->158A       -0.22610
    151B ->158B        0.10377
    152B ->158B       -0.11373
    153B ->158B       -0.60726
    154B ->158B        0.63245

 Excited state symmetry could not be determined.
 Excited State  22:  2.433-?Sym    2.4404 eV  508.06 nm  f=0.0054
<S**2>=1.230
    152A ->158A        0.26324
    151B ->158B        0.87393
    152B ->158B       -0.24688
    153B ->158B        0.11204
    154B ->158B       -0.16931
    155B ->158B        0.12062

 Excited state symmetry could not be determined.
 Excited State  23:  2.259-?Sym    2.4991 eV  496.11 nm  f=0.0069
<S**2>=1.026
    149A ->158A        0.11146
    150A ->158A       -0.29219
    151A ->158A       -0.20253
    153A ->158A       -0.38876
    156A ->158A        0.17019
    148B ->158B       -0.18390
    150B ->158B       -0.33657
    152B ->158B        0.58504
    155B ->158B        0.36595

 Excited state symmetry could not be determined.
 Excited State  24:  2.854-?Sym    2.5061 eV  494.73 nm  f=0.0053
<S**2>=1.787
    149A ->158A        0.11546
    149B ->158B       -0.17886
    150B ->158B        0.15303
    151B ->158B        0.12109
    152B ->158B        0.23630
    153B ->158B        0.59726
    154B ->158B        0.60602
    155B ->158B       -0.34643
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 Excited state symmetry could not be determined.
 Excited State  25:  2.700-?Sym    2.5445 eV  487.27 nm  f=0.0007
<S**2>=1.573
    150A ->158A        0.14347
    148B ->158B        0.10710
    149B ->158B        0.12797
    150B ->158B        0.46093
    151B ->158B        0.27296
    152B ->158B        0.63348
    153B ->158B       -0.36079
    154B ->158B       -0.15584
    155B ->158B       -0.28554

 Excited state symmetry could not be determined.
 Excited State  26:  2.487-?Sym    2.5745 eV  481.59 nm  f=0.0554
<S**2>=1.296
    143A ->158A        0.11777
    148A ->158A       -0.46529
    149A ->158A        0.21474
    150A ->158A        0.24058
    151A ->158A       -0.36169
    153A ->158A       -0.11636
    148B ->158B        0.58287
    149B ->158B       -0.22969
    150B ->158B       -0.15863
    151B ->158B        0.11255
    154B ->158B        0.14818
    156B ->158B        0.12726

 Excited state symmetry could not be determined.
 Excited State  27:  2.213-?Sym    2.7493 eV  450.96 nm  f=0.0367
<S**2>=0.974
    143A ->158A       -0.14331
    148A ->158A        0.73547
    149A ->158A       -0.20836
    150A ->158A        0.18916
    151A ->158A       -0.18557
    148B ->158B        0.35337
    149B ->158B       -0.38003

 Excited state symmetry could not be determined.
 Excited State  28:  2.030-?Sym    2.7916 eV  444.13 nm  f=0.0026
<S**2>=0.781
    148A ->158A       -0.10094
    145B ->157B        0.14530
    147B ->157B        0.96136

 Excited state symmetry could not be determined.
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 Excited State  29:  2.049-?Sym    2.8583 eV  433.76 nm  f=0.2093
<S**2>=0.799
    148A ->158A        0.32358
    149A ->158A        0.51487
    153A ->158A        0.12970
    144B ->157B        0.24359
    146B ->157B        0.25271
    147B ->157B        0.14402
    148B ->157B        0.15120
    148B ->158B        0.35217
    149B ->158B        0.46316
    150B ->158B       -0.10075
    156B ->157B       -0.16098

 Excited state symmetry could not be determined.
 Excited State  30:  2.127-?Sym    2.9491 eV  420.41 nm  f=0.0155
<S**2>=0.881
    149A ->158A       -0.12309
    155A ->159A       -0.11126
    142B ->157B       -0.13419
    144B ->157B       -0.13552
    145B ->157B        0.27945
    146B ->157B        0.87120
    147B ->157B       -0.12052
    149B ->158B       -0.11267

 Excited state symmetry could not be determined.
 Excited State  31:  2.147-?Sym    2.9746 eV  416.80 nm  f=0.0142
<S**2>=0.903
    155A ->159A        0.11450
    144B ->157B       -0.18678
    145B ->157B        0.87937
    146B ->157B       -0.25174
    147B ->157B       -0.13242

 Excited state symmetry could not be determined.
 Excited State  32:  3.325-?Sym    2.9991 eV  413.40 nm  f=0.0049
<S**2>=2.513
    155A ->159A        0.57142
    155A ->160A        0.12552
    155A ->163A       -0.12362
    144B ->157B        0.16215
    146B ->157B        0.21799
    151B ->159B        0.10582
    152B ->159B        0.39500
    153B ->159B       -0.32561
    154B ->159B       -0.25577
    156B ->159B       -0.17560

 Excited state symmetry could not be determined.
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 Excited State  33:  3.390-?Sym    3.0071 eV  412.31 nm  f=0.0021
<S**2>=2.623
    153A ->160A        0.20243
    156A ->159A       -0.11001
    156A ->160A        0.56730
    156A ->163A       -0.10294
    144B ->157B       -0.13664
    145B ->157B        0.10155
    146B ->157B       -0.13024
    152B ->160B        0.28651
    153B ->160B        0.19305
    154B ->160B        0.37549
    155B ->160B       -0.30094
    156B ->160B       -0.22373

 Excited state symmetry could not be determined.
 Excited State  34:  2.138-?Sym    3.0721 eV  403.58 nm  f=0.0139
<S**2>=0.893
    149A ->158A       -0.14837
    155A ->159A       -0.12974
    143B ->157B        0.10987
    144B ->157B        0.86574
    145B ->157B        0.28016
    149B ->158B       -0.11946

 Excited state symmetry could not be determined.
 Excited State  35:  2.054-?Sym    3.1706 eV  391.05 nm  f=0.0065
<S**2>=0.805
    141B ->157B        0.25735
    143B ->157B        0.92886
    144B ->157B       -0.18092

 Excited state symmetry could not be determined.
 Excited State  36:  3.456-?Sym    3.2358 eV  383.16 nm  f=0.0001
<S**2>=2.737
    142A ->161A       -0.13634
    149A ->161A       -0.22995
    150A ->161A       -0.33986
    151A ->161A       -0.36419
    153A ->161A        0.19876
    156A ->161A       -0.13153
    142B ->161B        0.12058
    148B ->161B        0.12392
    149B ->161B        0.25310
    150B ->161B        0.38280
    150B ->162B        0.15629
    153B ->161B        0.10835
    154B ->161B        0.12546
    155B ->161B        0.32108
    155B ->162B        0.12477
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    156B ->161B        0.14956

 Excited state symmetry could not be determined.
 Excited State  37:  2.107-?Sym    3.2724 eV  378.87 nm  f=0.0021
<S**2>=0.860
    139B ->157B       -0.32230
    142B ->157B        0.87263
    146B ->157B        0.17922
    150B ->157B       -0.14600

 Excited state symmetry could not be determined.
 Excited State  38:  2.130-?Sym    3.3402 eV  371.19 nm  f=0.0020
<S**2>=0.884
    157A ->159A        0.15988
    138B ->157B        0.10391
    141B ->157B        0.88862
    143B ->157B       -0.26264

 Excited state symmetry could not be determined.
 Excited State  39:  3.402-?Sym    3.3601 eV  368.99 nm  f=0.0006
<S**2>=2.643
    142A ->162A       -0.14206
    149A ->162A       -0.11085
    150A ->162A       -0.37146
    150A ->168A       -0.11074
    151A ->162A       -0.35629
    153A ->162A        0.19722
    156A ->162A       -0.14027
    141B ->157B       -0.18213
    142B ->163B        0.12532
    149B ->163B        0.12036
    150B ->163B        0.43996
    150B ->168B        0.16584
    155B ->163B        0.31874
    155B ->168B        0.10271
    156B ->163B        0.13453

 Excited state symmetry could not be determined.
 Excited State  40:  2.299-?Sym    3.3656 eV  368.38 nm  f=0.0016
<S**2>=1.071
    148A ->161A        0.20175
    149A ->161A       -0.19871
    151A ->161A        0.12578
    157A ->159A        0.64382
    157A ->160A       -0.42529
    157A ->161A        0.29954
    138B ->157B       -0.11235
    141B ->157B       -0.16430
    149B ->161B        0.10034
    156B ->159B        0.12567
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    156B ->160B       -0.11107
    156B ->161B        0.14969

 Excited state symmetry could not be determined.
 Excited State  41:  2.423-?Sym    3.4242 eV  362.08 nm  f=0.0007
<S**2>=1.217
    149A ->161A        0.12509
    157A ->159A        0.66793
    157A ->160A        0.65278
    157A ->161A       -0.15803

 Excited state symmetry could not be determined.
 Excited State  42:  3.130-?Sym    3.4451 eV  359.88 nm  f=0.0014
<S**2>=2.199
    143A ->158A        0.13847
    149A ->161A       -0.41369
    150A ->161A        0.21636
    157A ->159A       -0.15794
    157A ->160A        0.41470
    157A ->161A        0.14462
    140B ->157B       -0.23686
    149B ->161B        0.33731
    149B ->162B        0.14231
    150B ->161B       -0.26731
    150B ->162B       -0.11061
    154B ->161B        0.10457

 Excited state symmetry could not be determined.
 Excited State  43:  3.039-?Sym    3.4560 eV  358.75 nm  f=0.0016
<S**2>=2.059
    149A ->161A        0.10728
    157A ->159A       -0.16839
    157A ->160A        0.34403
    138B ->157B       -0.17060
    149B ->161B       -0.11609
    156B ->159B        0.60618
    156B ->160B       -0.44040
    156B ->161B        0.21027
    156B ->163B       -0.10098

 Excited state symmetry could not be determined.
 Excited State  44:  2.843-?Sym    3.4777 eV  356.52 nm  f=0.0126
<S**2>=1.771
    137A ->158A       -0.15879
    142A ->158A        0.18168
    143A ->158A       -0.28226
    149A ->161A       -0.19346
    157A ->160A        0.15242
    157A ->161A        0.11830
    137B ->157B       -0.20166
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    137B ->158B        0.14250
    138B ->158B       -0.16494
    139B ->157B        0.15478
    140B ->157B        0.56825
    142B ->158B       -0.10928
    144B ->158B        0.18118
    149B ->161B        0.14357
    150B ->161B       -0.10240
    156B ->159B       -0.10012
    156B ->160B       -0.17211

 Excited state symmetry could not be determined.
 Excited State  45:  2.764-?Sym    3.4883 eV  355.43 nm  f=0.0102
<S**2>=1.661
    136A ->158A       -0.10020
    138A ->158A        0.18943
    139A ->158A        0.18277
    144A ->158A       -0.19157
    145A ->158A        0.31862
    146A ->158A       -0.10582
    135B ->157B       -0.12384
    138B ->157B        0.56232
    139B ->157B        0.22669
    140B ->158B       -0.22212
    143B ->158B        0.11380
    144B ->157B        0.11189
    145B ->158B       -0.20629
    156B ->159B        0.24688
    156B ->160B       -0.17402

 Excited state symmetry could not be determined.
 Excited State  46:  2.584-?Sym    3.5128 eV  352.95 nm  f=0.0031
<S**2>=1.419
    145A ->158A       -0.16279
    147A ->158A       -0.31245
    139B ->157B        0.62842
    142B ->157B        0.29661
    156B ->159B       -0.33131
    156B ->160B       -0.37703

 Excited state symmetry could not be determined.
 Excited State  47:  2.762-?Sym    3.5188 eV  352.34 nm  f=0.0073
<S**2>=1.658
    147A ->158A       -0.15019
    139B ->157B        0.45111
    140B ->157B        0.12172
    142B ->157B        0.17980
    156B ->159B        0.53963
    156B ->160B        0.49383
    156B ->161B       -0.10071
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 Excited state symmetry could not be determined.
 Excited State  48:  2.415-?Sym    3.5435 eV  349.90 nm  f=0.0043
<S**2>=1.208
    143A ->161A       -0.12352
    147A ->158A       -0.24153
    148A ->161A        0.28990
    149A ->162A       -0.10484
    150A ->161A       -0.18961
    151A ->161A        0.13458
    157A ->159A       -0.10848
    157A ->160A        0.19590
    157A ->161A        0.46036
    137B ->157B        0.18713
    138B ->157B        0.26352
    149B ->161B       -0.16096
    150B ->161B        0.11990
    156B ->159B       -0.13942
    156B ->160B        0.40075
    156B ->161B        0.16002

 Excited state symmetry could not be determined.
 Excited State  49:  2.504-?Sym    3.5559 eV  348.68 nm  f=0.0014
<S**2>=1.317
    138A ->158A       -0.10535
    144A ->158A        0.11902
    145A ->158A       -0.15362
    147A ->158A        0.51731
    137B ->157B        0.58353
    138B ->157B        0.42265
    140B ->158B        0.11621
    141B ->157B       -0.10274
    145B ->158B        0.13049
    156B ->160B       -0.10511

 Excited state symmetry could not be determined.
 Excited State  50:  2.567-?Sym    3.5583 eV  348.43 nm  f=0.0025
<S**2>=1.397
    147A ->158A        0.70138
    148A ->161A        0.11695
    157A ->161A        0.19472
    137B ->157B       -0.24915
    138B ->157B       -0.27572
    139B ->157B        0.34120
    140B ->157B       -0.20152
    142B ->157B        0.11702
    156B ->160B        0.18096

 Excited state symmetry could not be determined.
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 Excited State  51:  2.787-?Sym    3.6444 eV  340.20 nm  f=0.0074
<S**2>=1.692
    142A ->158A       -0.17075
    143A ->158A        0.32430
    145A ->158A        0.12311
    146A ->158A       -0.32033
    148A ->158A        0.15292
    157A ->162A        0.21315
    157A ->167A       -0.15038
    137B ->157B        0.13787
    138B ->157B       -0.11226
    138B ->158B        0.11915
    140B ->157B        0.58477
    144B ->158B       -0.18118
    146B ->158B       -0.11521
    156B ->161B       -0.15802

 Excited state symmetry could not be determined.
 Excited State  52:  2.913-?Sym    3.6480 eV  339.87 nm  f=0.0030
<S**2>=1.872
    145A ->158A        0.16506
    148A ->162A        0.13495
    149A ->161A       -0.14362
    151A ->161A       -0.10314
    153A ->167A        0.10537
    153A ->171A       -0.10264
    154A ->170A        0.15650
    157A ->162A        0.62016
    140B ->157B       -0.22240
    149B ->163B        0.11031
    153B ->170B       -0.10473
    155B ->163B        0.10010
    156B ->163B       -0.25592

 Excited state symmetry could not be determined.
 Excited State  53:  3.127-?Sym    3.6897 eV  336.03 nm  f=0.0035
<S**2>=2.194
    143A ->158A        0.11006
    145A ->158A       -0.25356
    149A ->162A       -0.20380
    150A ->162A        0.13869
    152A ->169A        0.11222
    153A ->162A        0.12016
    154A ->170A        0.10289
    157A ->161A       -0.30339
    137B ->157B       -0.25634
    138B ->157B        0.13957
    139B ->157B       -0.10485
    140B ->157B        0.16383
    149B ->159B       -0.10422
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    149B ->163B        0.24595
    150B ->159B        0.11129
    150B ->163B       -0.15739
    154B ->163B        0.11976
    155B ->163B        0.11215
    156B ->160B        0.10288
    156B ->161B        0.37110
    156B ->163B       -0.10530

 Excited state symmetry could not be determined.
 Excited State  54:  2.833-?Sym    3.7036 eV  334.77 nm  f=0.0042
<S**2>=1.757
    144A ->158A       -0.10120
    145A ->158A        0.33931
    146A ->158A       -0.31075
    149A ->161A        0.11203
    151A ->161A        0.10678
    151A ->162A        0.10407
    157A ->161A       -0.19329
    157A ->167A        0.10097
    137B ->157B        0.43520
    138B ->157B       -0.29315
    139B ->157B        0.11261
    145B ->158B       -0.10739
    156B ->160B        0.12756
    156B ->161B        0.31139
    156B ->162B        0.13285
    156B ->163B        0.20434

 Excited state symmetry could not be determined.
 Excited State  55:  2.848-?Sym    3.7255 eV  332.80 nm  f=0.0008
<S**2>=1.778
    143A ->158A        0.18666
    145A ->158A        0.23104
    146A ->158A        0.85813
    137B ->157B        0.11326
    138B ->157B       -0.10644
    140B ->157B        0.15116
    144B ->158B       -0.10193

 Excited state symmetry could not be determined.
 Excited State  56:  3.280-?Sym    3.7490 eV  330.71 nm  f=0.0017
<S**2>=2.440
    145A ->158A        0.10835
    147A ->159A        0.10047
    147A ->166A        0.11019
    149A ->162A       -0.15475
    150A ->159A       -0.24049
    150A ->161A        0.10157
    151A ->159A       -0.20655
```

```
    151A ->160A        0.10050
    153A ->159A        0.10092
    155A ->159A        0.11739
    137B ->157B        0.12138
    138B ->157B       -0.11378
    147B ->158B        0.15710
    147B ->159B       -0.11214
    147B ->166B       -0.10097
    149B ->163B        0.11658
    150B ->159B        0.41153
    150B ->160B       -0.23019
    150B ->165B        0.11112
    155B ->159B        0.27293
    155B ->160B       -0.14158
    156B ->161B       -0.12611
    156B ->163B        0.20196

 Excited state symmetry could not be determined.
 Excited State  57:  2.655-?Sym    3.7635 eV  329.44 nm  f=0.0041
<S**2>=1.512
    142A ->162A        0.10000
    145A ->158A       -0.14737
    148A ->162A        0.24931
    151A ->162A        0.32838
    153A ->162A       -0.16063
    157A ->162A        0.30381
    157A ->168A        0.11354
    137B ->157B       -0.20165
    138B ->157B        0.10645
    149B ->160B        0.10625
    149B ->161B       -0.14954
    150B ->160B        0.11796
    155B ->160B        0.15613
    156B ->159B        0.10086
    156B ->163B        0.50197

 Excited state symmetry could not be determined.
 Excited State  58:  3.090-?Sym    3.7804 eV  327.96 nm  f=0.0017
<S**2>=2.138
    145A ->158A        0.15206
    150A ->160A       -0.14810
    151A ->160A       -0.18633
    153A ->160A        0.12840
    147B ->158B        0.64936
    149B ->160B        0.12253
    150B ->159B        0.14395
    150B ->160B        0.28102
    153B ->160B        0.14200
    154B ->160B        0.10691
    155B ->159B        0.12946
```

```
    155B ->160B        0.22535
    156B ->163B       -0.10366

 Excited state symmetry could not be determined.
 Excited State  59:  3.108-?Sym    3.7901 eV  327.13 nm  f=0.0008
<S**2>=2.164
    149A ->162A        0.16832
    150A ->160A        0.11253
    151A ->160A        0.15253
    147B ->158B        0.65649
    149B ->160B       -0.13526
    149B ->163B       -0.12374
    150B ->159B       -0.20895
    150B ->160B       -0.20470
    153B ->160B       -0.11126
    155B ->159B       -0.16958
    155B ->160B       -0.20598
    156B ->161B        0.15773

 Excited state symmetry could not be determined.
 Excited State  60:  3.325-?Sym    3.8176 eV  324.77 nm  f=0.0006
<S**2>=2.514
    145A ->158A        0.11139
    149A ->162A        0.43692
    149A ->168A        0.11776
    150A ->162A       -0.18701
    151A ->159A       -0.10883
    157A ->162A        0.10376
    147B ->158B       -0.19893
    148B ->163B       -0.10931
    149B ->163B       -0.34559
    149B ->168B       -0.11094
    150B ->159B        0.20436
    150B ->163B        0.12270
    155B ->159B        0.17642
    156B ->161B        0.30611

 Excited state symmetry could not be determined.
 Excited State  61:  2.681-?Sym    3.8314 eV  323.60 nm  f=0.0069
<S**2>=1.547
    138A ->158A       -0.11146
    139A ->158A       -0.15662
    140A ->158A        0.10631
    144A ->158A        0.39106
    145A ->158A        0.63746
    137B ->157B       -0.15424
    138B ->157B        0.15489
    140B ->158B        0.17525
    143B ->158B       -0.14425
    145B ->158B        0.31789
```

```
    146B ->158B        0.15048
    147B ->158B       -0.11826

 Excited state symmetry could not be determined.
 Excited State  62:  2.281-?Sym    3.8565 eV  321.50 nm  f=0.0035
<S**2>=1.050
    143A ->162A        0.10001
    148A ->162A       -0.13410
    150A ->161A        0.17302
    150A ->162A        0.40788
    150A ->168A        0.10039
    151A ->162A        0.19049
    152A ->169A       -0.10087
    153A ->161A       -0.12213
    153A ->162A       -0.15558
    156A ->162A        0.17145
    142B ->163B        0.11006
    149B ->161B        0.11070
    150B ->161B        0.10218
    150B ->163B        0.45979
    150B ->168B        0.14377
    155B ->163B        0.27630
    155B ->168B        0.10392

 Excited state symmetry could not be determined.
 Excited State  63:  3.198-?Sym    3.8898 eV  318.74 nm  f=0.0010
<S**2>=2.306
    148A ->159A       -0.11200
    148A ->160A        0.11132
    149A ->159A        0.12495
    149A ->161A        0.19675
    150A ->160A       -0.10074
    150A ->162A       -0.10285
    155A ->163A       -0.11551
    156A ->159A       -0.10001
    156A ->160A        0.13843
    156A ->163A        0.19692
    156A ->164A       -0.18803
    156A ->165A       -0.10211
    146B ->158B        0.25980
    149B ->159B       -0.15288
    149B ->160B       -0.21026
    149B ->161B        0.16766
    150B ->160B        0.13597
    152B ->160B        0.11200
    152B ->164B       -0.14348
    153B ->162B        0.12802
    154B ->162B        0.15538
    155B ->160B       -0.15745
    155B ->163B       -0.12268
```

```
    155B ->164B        0.10520

 Excited state symmetry could not be determined.
 Excited State  64:  2.651-?Sym    3.9072 eV  317.32 nm  f=0.0001
<S**2>=1.507
    144A ->158A        0.13636
    149A ->160A       -0.11695
    149A ->161A        0.42501
    149A ->162A       -0.15740
    151A ->162A       -0.11239
    153A ->161A       -0.10729
    155A ->159A        0.10061
    155A ->163A        0.13903
    157A ->162A        0.19212
    137B ->157B       -0.10856
    146B ->158B       -0.12192
    149B ->159B        0.28959
    149B ->161B        0.27022
    149B ->162B        0.19171
    152B ->159B        0.12938
    154B ->159B        0.11256
    154B ->161B        0.12577
    156B ->163B        0.13773

 Excited state symmetry could not be determined.
 Excited State  65:  3.250-?Sym    3.9131 eV  316.84 nm  f=0.0020
<S**2>=2.390
    144A ->158A       -0.17093
    145A ->164A       -0.11628
    148A ->159A        0.10645
    149A ->159A       -0.18632
    149A ->161A       -0.11169
    155A ->159A        0.15323
    155A ->163A        0.19938
    155A ->164A        0.14221
    156A ->163A        0.17833
    156A ->164A       -0.13541
    144B ->159B       -0.10008
    145B ->164B        0.10472
    146B ->158B        0.20456
    149B ->159B        0.24941
    149B ->161B       -0.13287
    149B ->164B        0.14335
    151B ->159B        0.14550
    152B ->162B        0.22549
    153B ->164B       -0.10233
    154B ->161B       -0.10156
    154B ->164B       -0.10914
    156B ->161B       -0.13489
```

```
 Excited state symmetry could not be determined.
 Excited State  66:  2.829-?Sym    3.9277 eV  315.66 nm  f=0.0118
<S**2>=1.751
    141A ->158A       -0.10859
    143A ->158A        0.14895
    144A ->158A       -0.54589
    156A ->163A       -0.10718
    145B ->158B        0.17320
    146B ->158B        0.61783
    155B ->160B        0.11616
    156B ->161B        0.10234

 Excited state symmetry could not be determined.
 Excited State  67:  2.737-?Sym    3.9396 eV  314.72 nm  f=0.0095
<S**2>=1.622
    141A ->158A        0.19115
    143A ->158A        0.34657
    144A ->158A        0.51307
    144B ->158B        0.14096
    145B ->158B       -0.40889
    146B ->158B        0.52361

 Excited state symmetry could not be determined.
 Excited State  68:  2.905-?Sym    3.9455 eV  314.24 nm  f=0.0123
<S**2>=1.859
    141A ->158A        0.10890
    144A ->158A        0.17348
    149A ->159A       -0.11503
    149A ->161A       -0.15892
    149A ->162A        0.11537
    151A ->161A       -0.21272
    152A ->169A       -0.16406
    153A ->162A       -0.12087
    154A ->170A       -0.14957
    155A ->163A        0.13460
    157A ->161A       -0.15977
    157A ->167A       -0.17776
    157A ->171A        0.10837
    148B ->161B       -0.14008
    149B ->161B       -0.13275
    149B ->163B        0.12804
    151B ->169B        0.15773
    153B ->170B        0.11051
    155B ->161B       -0.12914
    156B ->161B        0.31523
    156B ->162B        0.16152
    156B ->163B       -0.17551
    156B ->167B        0.17320

 Excited state symmetry could not be determined.
```

```
 Excited State  69:  2.571-?Sym    3.9828 eV  311.30 nm  f=0.0022
<S**2>=1.402
    140A ->158A       -0.21586
    142A ->158A        0.21586
    143A ->158A        0.56699
    139B ->158B        0.10677
    144B ->158B        0.43153
    145B ->158B        0.38924
    146B ->158B       -0.32212

 Excited state symmetry could not be determined.
 Excited State  70:  2.989-?Sym    4.0089 eV  309.27 nm  f=0.0089
<S**2>=1.984
    150A ->159A        0.10005
    155A ->163A       -0.24481
    155A ->165A       -0.14331
    156A ->159A        0.13356
    148B ->159B        0.11429
    149B ->159B        0.35327
    149B ->161B       -0.11223
    149B ->163B        0.10342
    150B ->159B        0.11869
    150B ->160B        0.10231
    152B ->162B       -0.15420
    153B ->159B        0.23859
    153B ->162B        0.12662
    154B ->159B        0.32042
    155B ->159B        0.46325

 Excited state symmetry could not be determined.
 Excited State  71:  2.933-?Sym    4.0243 eV  308.09 nm  f=0.0087
<S**2>=1.900
    138A ->158A       -0.17408
    139A ->158A       -0.12233
    140A ->158A        0.24817
    141A ->158A       -0.28037
    142A ->158A       -0.22326
    143A ->158A        0.17885
    144A ->158A       -0.11111
    136B ->157B        0.13168
    139B ->158B       -0.12536
    140B ->158B        0.22279
    141B ->158B        0.16316
    143B ->158B       -0.14723
    144B ->158B        0.43776
    145B ->158B       -0.42984
    146B ->158B       -0.11069
    147B ->158B        0.12092
    155B ->160B       -0.12743
```

```
 Excited state symmetry could not be determined.
 Excited State  72:  3.021-?Sym    4.0440 eV  306.59 nm  f=0.0017
<S**2>=2.032
    136A ->158A       -0.10916
    137A ->158A       -0.10710
    138A ->158A        0.17215
    139A ->158A        0.11151
    140A ->158A        0.43429
    141A ->158A        0.23255
    142A ->158A       -0.34381
    135B ->157B       -0.20852
    137B ->157B        0.13197
    139B ->158B       -0.18724
    140B ->158B       -0.11614
    144B ->158B        0.37254
    145B ->158B        0.27130
    155B ->160B        0.21690

 Excited state symmetry could not be determined.
 Excited State  73:  2.795-?Sym    4.0575 eV  305.57 nm  f=0.0033
<S**2>=1.704
    140A ->158A        0.12286
    148A ->159A       -0.11632
    150A ->159A        0.22081
    150A ->160A       -0.12690
    153A ->159A       -0.10169
    155A ->159A        0.13555
    155A ->163A        0.15203
    156A ->159A        0.65331
    149B ->159B       -0.13391
    149B ->160B       -0.12353
    150B ->159B        0.11549
    150B ->160B        0.12396
    150B ->161B        0.14775
    153B ->160B        0.10487
    155B ->160B       -0.16348

 Excited state symmetry could not be determined.
 Excited State  74:  2.728-?Sym    4.0652 eV  304.99 nm  f=0.0186
<S**2>=1.610
    150A ->160A        0.13835
    151A ->160A        0.17985
    153A ->160A       -0.14932
    156A ->159A        0.21493
    156A ->160A        0.24801
    156A ->164A       -0.10777
    156A ->165A        0.10586
    156A ->166A       -0.10927
    145B ->158B       -0.20410
    149B ->159B       -0.14519
```

```
    150B ->159B        0.10255
    150B ->160B        0.14633
    154B ->160B        0.23457
    155B ->160B        0.56527

 Excited state symmetry could not be determined.
 Excited State  75:  3.061-?Sym    4.0741 eV  304.32 nm  f=0.0019
<S**2>=2.093
    150A ->159A        0.14663
    150A ->160A        0.16216
    151A ->159A        0.13449
    153A ->159A       -0.19137
    153A ->160A       -0.10353
    154A ->159A       -0.15605
    154A ->160A        0.20636
    156A ->163A        0.15398
    156A ->165A       -0.10629
    143B ->158B        0.14761
    145B ->158B        0.13329
    149B ->160B        0.30920
    150B ->160B       -0.33399
    151B ->159B       -0.10181
    152B ->159B       -0.11574
    152B ->162B        0.11459
    154B ->159B       -0.10690
    154B ->160B        0.38261
    155B ->159B        0.28478

 Excited state symmetry could not be determined.
 Excited State  76:  2.481-?Sym    4.0875 eV  303.33 nm  f=0.0047
<S**2>=1.288
    139A ->158A        0.11923
    141A ->158A       -0.24146
    142A ->158A       -0.15571
    144A ->158A        0.15630
    134B ->157B       -0.18911
    136B ->157B        0.67452
    141B ->158B        0.19139
    143B ->158B        0.38211
    145B ->158B        0.13907

 Excited state symmetry could not be determined.
 Excited State  77:  3.176-?Sym    4.1047 eV  302.05 nm  f=0.0169
<S**2>=2.272
    150A ->160A        0.10782
    151A ->159A        0.12441
    151A ->160A        0.13232
    152A ->159A        0.16384
    153A ->159A       -0.17545
    153A ->160A       -0.20627
```

```
    154A ->160A       -0.14453
    155A ->160A        0.17967
    155A ->163A        0.12561
    155A ->164A        0.12956
    156A ->159A       -0.29833
    156A ->160A        0.11831
    156A ->164A        0.13201
    149B ->160B       -0.16699
    150B ->160B        0.18276
    151B ->159B       -0.19414
    152B ->164B        0.14713
    154B ->159B       -0.27251
    154B ->160B       -0.29051
    154B ->162B       -0.10484
    155B ->159B        0.33983

 Excited state symmetry could not be determined.
 Excited State  78:  3.107-?Sym    4.1116 eV  301.55 nm  f=0.0086
<S**2>=2.163
    140A ->158A       -0.10831
    142A ->158A       -0.16118
    154A ->159A        0.10221
    154A ->160A       -0.44834
    156A ->159A        0.11077
    135B ->157B        0.25899
    144B ->158B        0.19423
    149B ->160B        0.22727
    150B ->160B       -0.18045
    151B ->160B        0.19549
    153B ->160B        0.45121
    154B ->159B       -0.14253
    154B ->160B       -0.11008
    156B ->163B        0.18776

 Excited state symmetry could not be determined.
 Excited State  79:  2.846-?Sym    4.1229 eV  300.72 nm  f=0.0058
<S**2>=1.775
    137A ->158A       -0.12379
    140A ->158A        0.17939
    141A ->158A       -0.10568
    142A ->158A        0.16759
    143A ->158A        0.18622
    154A ->160A        0.14308
    156A ->160A        0.11727
    135B ->157B       -0.21208
    138B ->158B       -0.10747
    139B ->158B       -0.11847
    144B ->158B       -0.31261
    151B ->160B        0.14881
    152B ->159B        0.13291
```

```
    153B ->160B        0.51316
    154B ->159B        0.13907
    154B ->160B       -0.31914

 Excited state symmetry could not be determined.
 Excited State  80:  2.439-?Sym    4.1249 eV  300.57 nm  f=0.0017
<S**2>=1.237
    137A ->158A        0.10065
    140A ->158A       -0.14639
    141A ->158A        0.11631
    143A ->158A       -0.13689
    152A ->159A       -0.10384
    152A ->160A        0.10216
    154A ->159A       -0.17023
    154A ->160A        0.66057
    155A ->159A       -0.12888
    155A ->160A        0.16853
    156A ->160A        0.14682
    144B ->158B        0.19550
    153B ->159B       -0.12530
    153B ->160B        0.25585
    154B ->159B       -0.13049
    154B ->160B       -0.28923
```

Table S37. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 2^+(*S*=1/2)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  2.016-?Sym    1.3096 eV  946.75 nm  f=0.0293
<S**2>=0.766
    158A ->160A       -0.11252
    157B ->158B        0.95187
    157B ->159B        0.20626
 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 symmetry could not be determined.
 Excited State   2:  2.036-?Sym    1.3709 eV  904.37 nm  f=0.0037
<S**2>=0.786
    158A ->159A        0.98147

 Excited state symmetry could not be determined.
 Excited State   3:  2.038-?Sym    1.4317 eV  866.02 nm  f=0.0014
<S**2>=0.788
    158A ->159A        0.11021
    158A ->160A        0.97829
    157B ->158B        0.10583

 Excited state symmetry could not be determined.
 Excited State   4:  2.078-?Sym    1.9188 eV  646.15 nm  f=0.0066
<S**2>=0.829
    155B ->158B        0.11594
    156B ->158B        0.91721
    156B ->159B        0.26966
    157B ->158B        0.11492
    157B ->159B       -0.16725

 Excited state symmetry could not be determined.
 Excited State   5:  3.078-?Sym    1.9816 eV  625.66 nm  f=0.0029
<S**2>=2.119
    157A ->159A       -0.15390
    157A ->160A        0.14454
    154B ->159B        0.15011
    154B ->160B       -0.11834
    156B ->158B        0.18767
    157B ->158B       -0.16413
    157B ->159B        0.74287
    157B ->160B       -0.51387

 Excited state symmetry could not be determined.
```

```
 Excited State   6:  3.039-?Sym    2.0154 eV  615.18 nm  f=0.0020
<S**2>=2.058
    157A ->160A       -0.16120
    154B ->160B        0.16009
    157B ->158B       -0.11364
    157B ->159B        0.52971
    157B ->160B        0.77173

 Excited state symmetry could not be determined.
 Excited State   7:  2.110-?Sym    2.1428 eV  578.60 nm  f=0.1027
<S**2>=0.863
    156A ->160A       -0.10621
    157A ->159A        0.14158
    157A ->160A       -0.24049
    158A ->161A        0.30825
    155B ->158B        0.83358
    155B ->159B        0.20245
    156B ->158B       -0.10491

 Excited state symmetry could not be determined.
 Excited State   8:  2.521-?Sym    2.2443 eV  552.44 nm  f=0.0048
<S**2>=1.339
    156A ->159A       -0.12845
    156A ->160A        0.10363
    157A ->159A        0.80351
    157A ->160A       -0.34254
    158A ->161A       -0.30311
    155B ->158B       -0.13550
    157B ->159B        0.15771
    157B ->160B       -0.13697

 Excited state symmetry could not be determined.
 Excited State   9:  2.506-?Sym    2.2719 eV  545.73 nm  f=0.0026
<S**2>=1.320
    156A ->160A       -0.11315
    157A ->159A        0.46657
    157A ->160A        0.67225
    158A ->161A        0.48430
    157B ->160B        0.12711

 Excited state symmetry could not be determined.
 Excited State  10:  2.170-?Sym    2.2921 eV  540.92 nm  f=0.0241
<S**2>=0.928
    156A ->160A        0.16475
    157A ->160A       -0.45789
    158A ->161A        0.73145
    155B ->158B       -0.39924
    157B ->160B       -0.15103

 Excited state symmetry could not be determined.
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 Excited State  11:  3.417-?Sym    2.3696 eV  523.22 nm  f=0.0034
<S**2>=2.670
    156A ->159A        0.14792
    156A ->160A       -0.56220
    155B ->158B       -0.11993
    156B ->159B       -0.17281
    156B ->160B        0.71268

 Excited state symmetry could not be determined.
 Excited State  12:  2.088-?Sym    2.3899 eV  518.78 nm  f=0.0371
<S**2>=0.840
    158A ->162A        0.15442
    153B ->158B        0.10483
    154B ->158B        0.92443
    154B ->159B        0.17894
    157B ->159B       -0.11379

 Excited state symmetry could not be determined.
 Excited State  13:  2.102-?Sym    2.4232 eV  511.65 nm  f=0.0006
<S**2>=0.855
    158A ->162A        0.93240
    158A ->163A        0.16294
    154B ->158B       -0.17672
    155B ->160B        0.12085
    156B ->159B        0.11859

 Excited state symmetry could not be determined.
 Excited State  14:  3.358-?Sym    2.4569 eV  504.64 nm  f=0.0025
<S**2>=2.568
    156A ->159A       -0.48587
    156A ->160A       -0.14989
    158A ->162A       -0.14931
    158A ->163A       -0.11484
    155B ->159B        0.11010
    155B ->160B        0.11491
    156B ->158B       -0.22504
    156B ->159B        0.73103
    156B ->160B        0.15289

 Excited state symmetry could not be determined.
 Excited State  15:  2.182-?Sym    2.5586 eV  484.57 nm  f=0.0021
<S**2>=0.941
    158A ->162A       -0.13255
    158A ->163A        0.89712
    158A ->165A        0.15763
    155B ->159B        0.13388
    155B ->160B       -0.24741
    156B ->159B        0.16324

 Excited state symmetry could not be determined.
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 Excited State  16:  2.405-?Sym    2.5661 eV  483.16 nm  f=0.0020
<S**2>=1.196
    156A ->159A       -0.13456
    158A ->161A        0.14133
    158A ->163A        0.17965
    158A ->164A        0.75654
    155B ->158B        0.16368
    155B ->159B       -0.51738
    156B ->160B        0.10306

 Excited state symmetry could not be determined.
 Excited State  17:  2.556-?Sym    2.5803 eV  480.50 nm  f=0.0036
<S**2>=1.383
    156A ->159A       -0.35111
    158A ->162A       -0.17403
    158A ->163A        0.24218
    158A ->164A       -0.39943
    155B ->159B       -0.28824
    155B ->160B        0.64984
    156B ->159B       -0.25022

 Excited state symmetry could not be determined.
 Excited State  18:  2.746-?Sym    2.5995 eV  476.96 nm  f=0.0010
<S**2>=1.636
    155A ->159A       -0.10269
    156A ->159A       -0.17261
    156A ->160A       -0.18675
    158A ->163A        0.10417
    158A ->164A        0.45537
    155B ->158B       -0.13333
    155B ->159B        0.63204
    155B ->160B        0.35498
    156B ->159B       -0.21217
    156B ->160B       -0.26403

 Excited state symmetry could not be determined.
 Excited State  19:  2.481-?Sym    2.6626 eV  465.64 nm  f=0.0543
<S**2>=1.288
    156A ->159A        0.68571
    157A ->159A        0.16197
    158A ->165A        0.16282
    155B ->160B        0.46800
    156B ->159B        0.39054
    156B ->160B       -0.13708

 Excited state symmetry could not be determined.
 Excited State  20:  2.325-?Sym    2.7037 eV  458.56 nm  f=0.0365
<S**2>=1.101
    154A ->165A       -0.10304
    155A ->165A        0.16397
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    156A ->159A       -0.14658
    157A ->166A       -0.12810
    158A ->163A       -0.16853
    158A ->165A        0.81229
    158A ->172A       -0.16981
    158A ->174A       -0.11977
    158A ->175A        0.11074
    155B ->165B       -0.10375
    156B ->159B       -0.10239

 Excited state symmetry could not be determined.
 Excited State  21:  2.561-?Sym    2.7746 eV  446.86 nm  f=0.0010
<S**2>=1.389
    154A ->171A       -0.11768
    155A ->166A        0.12321
    155A ->167A       -0.11419
    155A ->171A        0.18329
    156A ->160A       -0.15966
    157A ->165A       -0.25173
    157A ->172A        0.10442
    158A ->166A        0.50385
    158A ->167A       -0.32801
    158A ->168A       -0.23842
    158A ->170A       -0.14118
    158A ->171A        0.33128
    158A ->173A       -0.14451
    155B ->160B       -0.17304
    155B ->171B       -0.12819
    157B ->165B        0.15046

 Excited state symmetry could not be determined.
 Excited State  22:  2.383-?Sym    2.8081 eV  441.53 nm  f=0.0220
<S**2>=1.169
    154A ->159A        0.10254
    155A ->159A       -0.16092
    156A ->160A        0.62367
    157A ->160A        0.12282
    158A ->166A        0.12379
    154B ->160B       -0.15653
    155B ->159B        0.25267
    156B ->160B        0.50383
    157B ->160B        0.15963
    157B ->162B        0.16380

 Excited state symmetry could not be determined.
 Excited State  23:  3.336-?Sym    2.8782 eV  430.77 nm  f=0.0030
<S**2>=2.532
    155A ->171A       -0.10355
    156A ->160A       -0.14004
    156A ->165A        0.15274
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    157A ->160A       -0.10723
    157A ->165A       -0.26006
    157A ->166A       -0.15644
    157A ->167A        0.14380
    157A ->168A        0.14951
    157A ->170A        0.10722
    157A ->171A       -0.25566
    157A ->172A        0.18655
    158A ->165A       -0.13635
    158A ->166A       -0.12596
    154B ->165B        0.11479
    154B ->166B        0.11419
    154B ->171B        0.19567
    156B ->160B       -0.10919
    156B ->165B       -0.17463
    156B ->171B       -0.14233
    156B ->172B        0.10986
    157B ->165B        0.26022
    157B ->166B        0.21076
    157B ->167B       -0.14491
    157B ->168B       -0.17708
    157B ->171B        0.31536
    157B ->172B       -0.15214

 Excited state symmetry could not be determined.
 Excited State  24:  3.000-?Sym    2.9065 eV  426.57 nm  f=0.0059
<S**2>=2.000
    155A ->160A        0.10066
    154B ->158B        0.12254
    154B ->159B       -0.20978
    154B ->161B        0.13003
    157B ->159B        0.11324
    157B ->161B        0.84826
    157B ->164B       -0.11290

 Excited state symmetry could not be determined.
 Excited State  25:  3.237-?Sym    2.9379 eV  422.01 nm  f=0.0018
<S**2>=2.369
    156A ->165A        0.16177
    157A ->160A        0.10172
    157A ->165A       -0.27831
    157A ->166A        0.12055
    157A ->167A       -0.10140
    157A ->171A        0.11688
    157A ->173A       -0.10838
    157A ->174A        0.10601
    158A ->165A        0.15635
    158A ->166A       -0.17241
    158A ->167A        0.12093
    158A ->171A       -0.11943
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    154B ->159B       -0.10173
    154B ->160B        0.17695
    154B ->165B        0.14137
    154B ->171B       -0.11763
    156B ->165B       -0.20074
    156B ->172B        0.10450
    156B ->173B       -0.10140
    157B ->161B        0.21660
    157B ->162B       -0.20783
    157B ->165B        0.35362
    157B ->166B       -0.16644
    157B ->167B        0.12052
    157B ->171B       -0.18336
    157B ->172B       -0.13000
    157B ->173B        0.15023

 Excited state symmetry could not be determined.
 Excited State  26:  2.982-?Sym    2.9934 eV  414.20 nm  f=0.0003
<S**2>=1.973
    148A ->160A        0.12846
    149A ->159A       -0.14089
    154A ->159A       -0.25805
    155A ->159A        0.43279
    155A ->160A        0.10463
    157A ->171A        0.12072
    148B ->160B       -0.13516
    149B ->159B        0.15431
    154B ->159B        0.11477
    154B ->160B       -0.41323
    154B ->162B        0.10039
    155B ->159B        0.20251
    157B ->160B        0.14015
    157B ->161B        0.15123
    157B ->162B        0.33343
    157B ->163B        0.11657

 Excited state symmetry could not be determined.
 Excited State  27:  2.971-?Sym    3.0105 eV  411.84 nm  f=0.0007
<S**2>=1.957
    148A ->159A       -0.16284
    149A ->160A        0.17826
    154A ->159A       -0.12074
    154A ->160A        0.18259
    155A ->160A       -0.37584
    148B ->159B        0.14205
    149B ->160B       -0.17786
    154B ->158B       -0.12824
    154B ->159B        0.61573
    155B ->160B       -0.17894
    157B ->159B       -0.11755
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    157B ->161B        0.36007

 Excited state symmetry could not be determined.
 Excited State  28:  2.272-?Sym    3.0469 eV  406.93 nm  f=0.0156
<S**2>=1.040
    157A ->166A        0.10511
    152B ->158B       -0.44421
    153B ->158B        0.75896
    153B ->159B        0.11863
    154B ->158B       -0.11739

 Excited state symmetry could not be determined.
 Excited State  29:  2.664-?Sym    3.0962 eV  400.44 nm  f=0.0016
<S**2>=1.524
    155A ->159A       -0.13411
    155A ->160A       -0.16788
    158A ->166A       -0.26748
    158A ->171A        0.15171
    152B ->158B       -0.41231
    153B ->158B       -0.32450
    154B ->159B       -0.17753
    154B ->160B        0.13561
    157B ->162B        0.57503
    157B ->163B        0.12993

 Excited state symmetry could not be determined.
 Excited State  30:  2.661-?Sym    3.1031 eV  399.55 nm  f=0.0017
<S**2>=1.521
    158A ->166A        0.24892
    158A ->167A        0.11123
    158A ->171A       -0.16972
    152B ->158B        0.45034
    153B ->158B        0.26515
    154B ->159B       -0.18582
    154B ->160B        0.37333
    157B ->162B        0.49894
    157B ->163B        0.23522

 Excited state symmetry could not be determined.
 Excited State  31:  2.749-?Sym    3.1246 eV  396.80 nm  f=0.0242
<S**2>=1.639
    154A ->160A       -0.25208
    155A ->160A        0.52053
    153B ->158B       -0.13261
    154B ->159B        0.55021
    154B ->160B        0.33574
    157B ->162B        0.14406
    157B ->163B        0.13006
    157B ->164B       -0.21424
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 Excited state symmetry could not be determined.
 Excited State  32:  2.845-?Sym    3.1408 eV  394.75 nm  f=0.0018
<S**2>=1.773
    154A ->159A       -0.12844
    155A ->159A        0.42175
    155A ->160A       -0.15062
    156A ->160A        0.16335
    157A ->161A       -0.14149
    152B ->158B       -0.17122
    154B ->159B       -0.12082
    154B ->160B        0.40366
    154B ->163B        0.10068
    155B ->159B        0.11954
    157B ->162B       -0.26416
    157B ->163B        0.46785
    157B ->164B       -0.14239

 Excited state symmetry could not be determined.
 Excited State  33:  3.065-?Sym    3.1656 eV  391.66 nm  f=0.0002
<S**2>=2.098
    148A ->159A        0.27417
    148A ->160A       -0.19776
    149A ->159A        0.11894
    155A ->159A        0.42569
    155A ->160A       -0.24545
    157A ->159A       -0.10430
    157A ->161A       -0.33257
    148B ->158B        0.10041
    148B ->159B       -0.24439
    148B ->160B        0.19916
    149B ->159B       -0.10597
    154B ->159B        0.18162
    157B ->162B        0.12196
    157B ->163B       -0.31937
    157B ->164B       -0.17898

 Excited state symmetry could not be determined.
 Excited State  34:  2.920-?Sym    3.1956 eV  387.98 nm  f=0.0016
<S**2>=1.882
    148A ->159A        0.21395
    148A ->160A       -0.14737
    154A ->159A       -0.13758
    155A ->159A        0.21928
    157A ->161A        0.65287
    148B ->159B       -0.21705
    148B ->160B        0.16471
    157B ->161B        0.11210
    157B ->162B       -0.11749
    157B ->163B        0.17824
    157B ->164B        0.34889
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 Excited state symmetry could not be determined.
 Excited State  35:  3.362-?Sym    3.2084 eV  386.44 nm  f=0.0027
<S**2>=2.576
    156A ->165A        0.48669
    156A ->172A       -0.23883
    156A ->174A       -0.15572
    156A ->175A        0.14986
    157A ->161A        0.12877
    157A ->165A        0.14277
    158A ->166A        0.11973
    154B ->160B        0.11627
    154B ->165B       -0.19062
    154B ->172B        0.11306
    156B ->165B       -0.40328
    156B ->172B        0.20646
    156B ->173B       -0.15259
    157B ->165B       -0.31087
    157B ->172B        0.11059

 Excited state symmetry could not be determined.
 Excited State  36:  2.298-?Sym    3.2174 eV  385.36 nm  f=0.0203
<S**2>=1.071
    154A ->160A        0.14950
    155A ->159A       -0.15027
    155A ->160A       -0.12355
    158A ->166A        0.56280
    158A ->167A        0.33039
    158A ->168A        0.17459
    158A ->170A        0.10670
    158A ->171A       -0.19418
    152B ->158B       -0.40327
    153B ->158B       -0.21078
    154B ->160B       -0.13754
    157B ->163B        0.17352
    157B ->164B       -0.27845

 Excited state symmetry could not be determined.
 Excited State  37:  2.915-?Sym    3.2213 eV  384.89 nm  f=0.0147
<S**2>=1.875
    148A ->159A        0.18065
    149A ->160A       -0.18905
    154A ->159A        0.10795
    154A ->160A        0.26176
    155A ->159A       -0.29212
    155A ->160A       -0.24013
    157A ->162A       -0.17141
    158A ->166A       -0.27301
    158A ->167A       -0.16799
    148B ->159B       -0.17693
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    149B ->160B        0.18741
    152B ->158B        0.21286
    153B ->158B        0.10597
    154B ->160B       -0.19303
    157B ->162B       -0.11269
    157B ->163B        0.40663
    157B ->164B       -0.25614

 Excited state symmetry could not be determined.
 Excited State  38:  2.886-?Sym    3.2299 eV  383.87 nm  f=0.0231
<S**2>=1.832
    155A ->160A        0.12695
    157A ->161A       -0.55107
    157B ->163B        0.31256
    157B ->164B        0.69181

 Excited state symmetry could not be determined.
 Excited State  39:  3.175-?Sym    3.2380 eV  382.90 nm  f=0.0021
<S**2>=2.271
    148A ->160A       -0.15789
    149A ->159A        0.28909
    149A ->160A        0.29300
    154A ->159A       -0.17326
    154A ->160A       -0.17195
    155A ->160A        0.25059
    156A ->160A       -0.11868
    157A ->161A       -0.12040
    148B ->160B        0.16175
    149B ->158B        0.10870
    149B ->159B       -0.28347
    149B ->160B       -0.28349
    154B ->160B       -0.29671
    156B ->164B        0.10475
    157B ->162B       -0.13189
    157B ->163B        0.33089
    157B ->164B       -0.24306

 Excited state symmetry could not be determined.
 Excited State  40:  2.791-?Sym    3.3155 eV  373.95 nm  f=0.0072
<S**2>=1.698
    154A ->159A        0.82075
    154A ->160A        0.11075
    155A ->159A        0.38411
    157A ->159A       -0.12054
    157A ->161A        0.13829
    157A ->162A       -0.17465
    156B ->161B        0.10715

 Excited state symmetry could not be determined.
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 Excited State  41:  2.713-?Sym    3.3372 eV  371.52 nm  f=0.0014
<S**2>=1.590
    154A ->159A        0.12970
    154A ->160A       -0.43440
    155A ->160A       -0.23787
    156A ->166A       -0.12294
    156A ->167A        0.10182
    156A ->171A       -0.13306
    157A ->160A        0.14890
    157A ->162A        0.45925
    157A ->163A       -0.17753
    157A ->171A        0.12783
    158A ->167A       -0.13244
    154B ->160B       -0.10165
    154B ->171B        0.13688
    155B ->161B       -0.11642
    157B ->163B        0.20267
    157B ->166B        0.19884
    157B ->167B       -0.12951
    157B ->168B       -0.11107
    157B ->171B        0.17861

 Excited state symmetry could not be determined.
 Excited State  42:  3.322-?Sym    3.3495 eV  370.16 nm  f=0.0007
<S**2>=2.510
    154A ->160A        0.22742
    155A ->160A        0.13035
    156A ->166A       -0.26411
    156A ->167A        0.23080
    156A ->168A        0.17433
    156A ->170A        0.13907
    156A ->171A       -0.33442
    156A ->173A        0.15064
    157A ->162A       -0.13343
    154B ->171B        0.10426
    155B ->161B        0.11111
    155B ->171B        0.10653
    156B ->162B        0.11972
    156B ->166B        0.28543
    156B ->167B       -0.19894
    156B ->168B       -0.20331
    156B ->171B        0.39056

 Excited state symmetry could not be determined.
 Excited State  43:  2.229-?Sym    3.3731 eV  367.57 nm  f=0.0433
<S**2>=0.992
    154A ->160A        0.11839
    157A ->163A        0.13221
    158A ->165A        0.19733
    158A ->167A       -0.55629
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    158A ->168A        0.57466
    158A ->171A       -0.10521
    158A ->172A        0.28015
    158A ->173A       -0.13629
    147B ->158B        0.10991
    150B ->158B        0.15422
    152B ->158B       -0.11334
    155B ->165B        0.12854

 Excited state symmetry could not be determined.
 Excited State  44:  2.844-?Sym    3.3825 eV  366.55 nm  f=0.0006
<S**2>=1.773
    154A ->159A        0.10119
    154A ->160A        0.44655
    155A ->160A        0.27054
    156A ->161A        0.16788
    157A ->162A        0.60445
    157A ->163A        0.23925
    157A ->164A       -0.15513
    155B ->161B       -0.21258
    156B ->161B       -0.26086
    157B ->163B        0.11505

 Excited state symmetry could not be determined.
 Excited State  45:  3.261-?Sym    3.3857 eV  366.20 nm  f=0.0017
<S**2>=2.409
    154A ->159A       -0.10419
    154A ->160A        0.25139
    156A ->161A       -0.42582
    156A ->164A       -0.10876
    157A ->162A        0.24042
    157A ->163A        0.18564
    157A ->164A        0.16052
    156B ->161B        0.66898

 Excited state symmetry could not be determined.
 Excited State  46:  2.345-?Sym    3.4454 eV  359.86 nm  f=0.0049
<S**2>=1.125
    154A ->165A        0.10124
    156A ->161A       -0.13312
    156A ->165A       -0.17670
    157A ->162A       -0.20668
    157A ->163A        0.29833
    157A ->164A       -0.23490
    157A ->165A        0.35668
    157A ->168A       -0.12803
    157A ->171A        0.18465
    157A ->172A       -0.17534
    155B ->165B       -0.10330
    155B ->166B       -0.12126
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    155B ->171B       -0.18249
    156B ->165B       -0.29504
    156B ->172B        0.14260
    156B ->173B       -0.10329
    157B ->165B        0.31366
    157B ->166B        0.15186
    157B ->171B        0.12436

 Excited state symmetry could not be determined.
 Excited State  47:  2.693-?Sym    3.4503 eV  359.35 nm  f=0.0030
<S**2>=1.563
    154A ->160A       -0.34258
    155A ->160A       -0.18056
    156A ->163A       -0.11654
    157A ->162A       -0.14386
    157A ->163A        0.56754
    157A ->166A       -0.15557
    157A ->167A        0.11445
    157A ->171A       -0.15787
    154B ->160B       -0.13597
    155B ->161B       -0.26696
    155B ->165B        0.14384
    156B ->162B       -0.13089
    156B ->163B        0.21811
    157B ->163B        0.10091
    157B ->166B       -0.12687
    157B ->171B       -0.13458

 Excited state symmetry could not be determined.
 Excited State  48:  2.574-?Sym    3.4704 eV  357.27 nm  f=0.0243
<S**2>=1.406
    154A ->166A        0.10898
    155A ->165A       -0.20124
    155A ->166A        0.13511
    157A ->162A       -0.12826
    157A ->164A       -0.12318
    157A ->165A       -0.15110
    157A ->171A        0.12102
    158A ->165A        0.20207
    158A ->167A        0.29105
    158A ->168A       -0.23780
    158A ->169A       -0.16850
    158A ->172A        0.41400
    158A ->173A       -0.18470
    153B ->158B        0.16581
    155B ->165B        0.20731
    157B ->165B       -0.15722
    157B ->166B        0.25768

 Excited state symmetry could not be determined.
```

```
 Excited State  49:  2.769-?Sym    3.4864 eV  355.62 nm  f=0.0083
<S**2>=1.666
    156A ->162A       -0.10807
    156A ->163A        0.12478
    157A ->162A        0.10158
    157A ->164A        0.73754
    157A ->165A        0.17410
    158A ->168A       -0.13643
    158A ->172A        0.12640
    155B ->165B        0.12886
    156B ->161B       -0.25023
    156B ->162B        0.12988
    156B ->163B       -0.17635
    156B ->165B       -0.12261
    157B ->165B        0.13610

 Excited state symmetry could not be determined.
 Excited State  50:  2.609-?Sym    3.5084 eV  353.39 nm  f=0.0090
<S**2>=1.451
    156A ->162A        0.12983
    156A ->163A       -0.15425
    157A ->162A       -0.16397
    157A ->163A        0.32779
    157A ->164A        0.38258
    157A ->165A       -0.18504
    157A ->166A        0.24003
    157A ->167A       -0.18031
    157A ->168A       -0.10214
    157A ->171A        0.20033
    157A ->173A       -0.12128
    155B ->162B        0.12937
    155B ->165B       -0.28395
    155B ->172B        0.11689
    155B ->173B       -0.10977
    156B ->163B        0.15113
    156B ->165B        0.13674
    157B ->165B       -0.15409
    157B ->166B        0.14477
    157B ->171B        0.14708

 Excited state symmetry could not be determined.
 Excited State  51:  2.420-?Sym    3.5177 eV  352.46 nm  f=0.0083
<S**2>=1.214
    158A ->167A        0.35522
    158A ->168A        0.53638
    158A ->169A       -0.11013
    158A ->170A       -0.20781
    158A ->171A        0.34895
    151B ->158B       -0.32030
    152B ->158B        0.16707
```

```
    155B ->161B       -0.13154
    155B ->166B       -0.13455
    155B ->171B       -0.16037

 Excited state symmetry could not be determined.
 Excited State  52:  2.860-?Sym    3.5491 eV  349.34 nm  f=0.0107
<S**2>=1.795
    154A ->160A        0.12934
    156A ->160A        0.10358
    156A ->161A        0.37172
    156A ->162A        0.26832
    156A ->163A       -0.26455
    157A ->163A       -0.35610
    157A ->164A        0.27369
    155B ->161B       -0.27823
    155B ->162B       -0.13167
    156B ->161B        0.31842
    156B ->162B       -0.24964
    156B ->163B        0.13458
    156B ->164B       -0.12241
    156B ->165B       -0.16615

 Excited state symmetry could not be determined.
 Excited State  53:  2.514-?Sym    3.5548 eV  348.78 nm  f=0.0076
<S**2>=1.330
    156A ->161A        0.65508
    156A ->162A       -0.16710
    156A ->163A        0.21544
    156A ->165A       -0.10812
    157A ->163A        0.27064
    155B ->161B        0.14140
    156B ->161B        0.42304
    156B ->162B        0.12444
    156B ->163B       -0.25434

 Excited state symmetry could not be determined.
 Excited State  54:  2.972-?Sym    3.5681 eV  347.48 nm  f=0.0014
<S**2>=1.959
    156A ->163A       -0.15769
    156A ->164A        0.10897
    157A ->162A        0.17953
    155B ->161B        0.76847
    156B ->162B       -0.16245
    156B ->163B        0.36765
    156B ->164B       -0.16297

 Excited state symmetry could not be determined.
 Excited State  55:  2.160-?Sym    3.5973 eV  344.66 nm  f=0.0027
<S**2>=0.917
    158A ->167A        0.13944
```

```
    158A ->168A        0.23913
    158A ->171A        0.13145
    150B ->158B       -0.20380
    151B ->158B        0.86953

 Excited state symmetry could not be determined.
 Excited State  56:  2.110-?Sym    3.6042 eV  344.00 nm  f=0.0004
<S**2>=0.863
    158A ->167A        0.19436
    150B ->158B        0.91840
    151B ->158B        0.16072

 Excited state symmetry could not be determined.
 Excited State  57:  2.484-?Sym    3.6332 eV  341.25 nm  f=0.0037
<S**2>=1.293
    156A ->163A        0.14989
    156A ->165A        0.37455
    156A ->172A       -0.15779
    156A ->174A       -0.11384
    156A ->175A        0.10411
    157A ->165A        0.13442
    158A ->171A       -0.13101
    150B ->158B       -0.13249
    151B ->158B       -0.15786
    155B ->162B       -0.23196
    155B ->164B        0.10422
    155B ->166B       -0.15437
    155B ->167B        0.10956
    155B ->168B        0.11883
    155B ->171B       -0.22652
    156B ->162B       -0.31732
    156B ->164B        0.11098
    156B ->165B        0.39649
    156B ->172B       -0.16622
    156B ->173B        0.11693
    157B ->165B        0.19485

 Excited state symmetry could not be determined.
 Excited State  58:  3.040-?Sym    3.6439 eV  340.25 nm  f=0.0038
<S**2>=2.060
    156A ->161A        0.15594
    156A ->162A       -0.18921
    156A ->163A       -0.14781
    156A ->165A        0.16985
    158A ->169A        0.10291
    158A ->171A       -0.10121
    158A ->172A       -0.10910
    155B ->161B       -0.12735
    155B ->171B       -0.12641
    156B ->162B        0.66058
```

```
    156B ->163B        0.40450
    156B ->165B        0.12819

 Excited state symmetry could not be determined.
 Excited State  59:  3.180-?Sym    3.6616 eV  338.61 nm  f=0.0092
<S**2>=2.278
    148A ->159A        0.12553
    149A ->160A       -0.14483
    156A ->164A       -0.34699
    156A ->165A       -0.12908
    157A ->164A        0.10913
    155B ->161B        0.11772
    155B ->162B       -0.45432
    155B ->163B       -0.16670
    155B ->164B        0.19116
    156B ->161B       -0.13055
    156B ->164B        0.47892
    156B ->165B       -0.14162
    157B ->165B       -0.14718

 Excited state symmetry could not be determined.
 Excited State  60:  2.969-?Sym    3.6726 eV  337.59 nm  f=0.0076
<S**2>=1.954
    151A ->168A        0.14495
    153A ->166A        0.15505
    155A ->165A        0.18519
    156A ->163A       -0.14182
    157A ->173A        0.10210
    158A ->169A       -0.17617
    158A ->170A       -0.19820
    158A ->171A        0.14169
    158A ->172A        0.25999
    158A ->173A        0.18684
    158A ->174A       -0.21563
    146B ->158B        0.13873
    147B ->158B        0.15213
    151B ->158B       -0.15153
    151B ->168B        0.15440
    152B ->158B       -0.10056
    153B ->165B        0.14686
    153B ->166B       -0.13761
    154B ->165B       -0.13341
    155B ->165B       -0.16121
    156B ->162B        0.21259
    156B ->163B        0.17158
    156B ->164B        0.15823
    157B ->165B        0.14150
    157B ->167B        0.12324

 Excited state symmetry could not be determined.
```

```
 Excited State  61:  2.833-?Sym    3.7038 eV  334.75 nm  f=0.0068
<S**2>=1.757
    150A ->167A       -0.12340
    152A ->165A        0.12988
    152A ->166A        0.11767
    154A ->165A        0.13127
    154A ->173A        0.10285
    156A ->162A        0.18209
    157A ->166A        0.17091
    157A ->173A       -0.12454
    158A ->165A        0.12075
    158A ->168A        0.14253
    158A ->169A       -0.21737
    158A ->170A       -0.10191
    158A ->171A        0.14674
    158A ->173A        0.36280
    158A ->174A        0.18977
    158A ->175A       -0.15350
    147B ->158B       -0.29428
    150B ->167B        0.13288
    152B ->165B       -0.13918
    152B ->166B       -0.13167
    155B ->162B       -0.15422
    155B ->165B        0.19003
    155B ->172B       -0.11307
    155B ->173B        0.10140
    157B ->168B       -0.13200
    157B ->171B        0.11312
    157B ->173B        0.10049

 Excited state symmetry could not be determined.
 Excited State  62:  3.071-?Sym    3.7160 eV  333.65 nm  f=0.0285
<S**2>=2.108
    156A ->161A        0.27650
    156A ->162A       -0.15789
    156A ->163A       -0.13780
    156A ->164A       -0.20741
    157A ->164A       -0.11922
    153B ->159B       -0.10330
    155B ->162B        0.58879
    155B ->163B        0.18878
    156B ->162B       -0.23857
    156B ->163B        0.10052
    156B ->164B        0.45567

 Excited state symmetry could not be determined.
 Excited State  63:  2.481-?Sym    3.7408 eV  331.44 nm  f=0.0053
<S**2>=1.289
    156A ->162A        0.70628
    156A ->163A        0.28784
```

```
    156A ->164A       -0.11712
    155B ->161B        0.16016
    155B ->162B        0.25938
    155B ->163B        0.17017
    155B ->164B        0.20648
    156B ->162B        0.28139
    156B ->163B        0.11158

 Excited state symmetry could not be determined.
 Excited State  64:  2.978-?Sym    3.7502 eV  330.61 nm  f=0.0008
<S**2>=1.967
    156A ->162A       -0.12681
    152B ->159B        0.13257
    152B ->160B        0.12208
    153B ->158B       -0.10393
    153B ->159B        0.76014
    153B ->160B        0.51586
    155B ->162B        0.10262
    156B ->164B        0.13600

 Excited state symmetry could not be determined.
 Excited State  65:  2.986-?Sym    3.7786 eV  328.12 nm  f=0.0028
<S**2>=1.979
    150A ->167A        0.10591
    156A ->165A        0.10074
    157A ->165A        0.10305
    157A ->166A        0.11446
    158A ->165A        0.10999
    158A ->173A       -0.10372
    150B ->167B       -0.11688
    152B ->158B        0.12878
    152B ->159B       -0.32237
    152B ->160B        0.15991
    152B ->165B        0.13172
    153B ->159B        0.15661
    153B ->160B       -0.11537
    154B ->166B        0.10226
    155B ->162B       -0.27444
    155B ->163B        0.42315
    155B ->164B       -0.28198
    155B ->165B        0.12485
    155B ->166B        0.11480
    155B ->171B        0.15870
    157B ->166B       -0.14036
    157B ->171B        0.13860

 Excited state symmetry could not be determined.
 Excited State  66:  2.856-?Sym    3.7879 eV  327.32 nm  f=0.0047
<S**2>=1.789
    156A ->163A        0.17600
```

```
    158A ->165A       -0.11170
    158A ->169A        0.10316
    158A ->171A        0.13104
    158A ->172A       -0.15012
    152B ->159B        0.47256
    152B ->160B       -0.17427
    153B ->159B       -0.10471
    153B ->160B        0.15376
    155B ->162B       -0.13516
    155B ->163B        0.32866
    155B ->164B       -0.34335
    155B ->166B        0.14458
    155B ->168B       -0.10471
    155B ->171B        0.20443
    156B ->163B        0.10998
    156B ->164B        0.17364
    157B ->165B        0.10610
    157B ->166B        0.14021

 Excited state symmetry could not be determined.
 Excited State  67:  2.922-?Sym    3.8080 eV  325.59 nm  f=0.0013
<S**2>=1.884
    156A ->162A       -0.18474
    156A ->163A       -0.22122
    157A ->165A       -0.10921
    152B ->159B        0.49410
    152B ->160B       -0.19252
    155B ->162B       -0.10670
    155B ->163B        0.40680
    155B ->164B        0.36489
    156B ->164B       -0.10537
    157B ->165B       -0.12930
    157B ->166B       -0.10684

 Excited state symmetry could not be determined.
 Excited State  68:  2.853-?Sym    3.8200 eV  324.56 nm  f=0.0030
<S**2>=1.784
    153A ->159A       -0.33797
    153A ->160A       -0.23703
    156A ->162A       -0.10443
    156A ->163A       -0.12443
    157A ->166A       -0.10027
    158A ->165A       -0.10021
    158A ->173A        0.13850
    152B ->159B       -0.39926
    155B ->163B        0.49310
    155B ->164B        0.27954
    155B ->165B       -0.14097
    157B ->166B        0.14019
    157B ->171B       -0.11596
```

```
 Excited state symmetry could not be determined.
 Excited State  69:  2.716-?Sym    3.8302 eV  323.70 nm  f=0.0034
<S**2>=1.594
    153A ->159A        0.63647
    153A ->160A        0.35072
    156A ->162A        0.11541
    156A ->163A       -0.17410
    157A ->165A       -0.12974
    158A ->170A        0.10382
    158A ->171A       -0.10727
    158A ->173A        0.11341
    153B ->160B        0.11675
    155B ->162B       -0.11337
    155B ->163B        0.28081
    155B ->165B       -0.13656
    155B ->166B       -0.11074
    155B ->171B       -0.13653
    156B ->163B       -0.12242
    157B ->165B       -0.14773

 Excited state symmetry could not be determined.
 Excited State  70:  2.475-?Sym    3.8398 eV  322.89 nm  f=0.0068
<S**2>=1.281
    153A ->159A        0.19516
    156A ->164A        0.61979
    158A ->169A        0.18171
    158A ->170A       -0.16381
    148B ->158B       -0.10265
    149B ->158B        0.11867
    153B ->159B       -0.10641
    155B ->164B        0.46484
    155B ->166B        0.11474
    155B ->171B        0.14904
    156B ->164B        0.26839

 Excited state symmetry could not be determined.
 Excited State  71:  2.356-?Sym    3.8432 eV  322.61 nm  f=0.0054
<S**2>=1.138
    152A ->159A       -0.29165
    153A ->160A        0.13702
    156A ->164A       -0.13582
    158A ->169A        0.73499
    158A ->170A       -0.14516
    158A ->171A        0.15449
    152B ->159B       -0.12490
    153B ->159B        0.21213
    153B ->160B       -0.16345
    154B ->165B       -0.10568
    155B ->165B        0.13970
```

```
    157B ->166B        0.13574

 Excited state symmetry could not be determined.
 Excited State  72:  2.525-?Sym    3.8502 eV  322.02 nm  f=0.0168
<S**2>=1.344
    152A ->159A       -0.37672
    152A ->160A        0.13689
    153A ->159A       -0.36312
    156A ->162A        0.11545
    156A ->164A        0.37059
    157A ->165A       -0.15640
    158A ->169A       -0.10285
    158A ->170A        0.19738
    148B ->158B       -0.12052
    153B ->160B       -0.11927
    155B ->164B       -0.16969
    155B ->166B       -0.14618
    155B ->167B        0.10276
    155B ->168B        0.10878
    155B ->171B       -0.19343
    156B ->164B        0.40718
    157B ->165B       -0.17723

 Excited state symmetry could not be determined.
 Excited State  73:  2.754-?Sym    3.8665 eV  320.66 nm  f=0.0023
<S**2>=1.647
    152A ->159A        0.55953
    152A ->160A       -0.15100
    156A ->163A        0.16341
    156A ->164A        0.11896
    152B ->159B        0.13912
    152B ->160B       -0.13493
    153B ->159B        0.37766
    153B ->160B       -0.55382
    156B ->163B        0.13274

 Excited state symmetry could not be determined.
 Excited State  74:  2.679-?Sym    3.8758 eV  319.89 nm  f=0.0060
<S**2>=1.544
    152A ->159A        0.50141
    152A ->160A       -0.14435
    153A ->160A       -0.21383
    158A ->169A        0.36495
    158A ->170A       -0.10344
    158A ->172A        0.14702
    158A ->173A        0.13462
    149B ->158B        0.14007
    153B ->159B       -0.28631
    153B ->160B        0.38059
    155B ->164B       -0.19178
```

```
    155B ->171B       -0.11376
    156B ->163B       -0.12768
    156B ->164B        0.17192

 Excited state symmetry could not be determined.
 Excited State  75:  2.576-?Sym    3.9054 eV  317.47 nm  f=0.0090
<S**2>=1.408
    153A ->159A       -0.13031
    155A ->161A       -0.12095
    156A ->162A        0.18212
    156A ->163A       -0.22106
    157A ->165A        0.10658
    158A ->170A       -0.12863
    148B ->158B        0.16144
    149B ->158B        0.57661
    152B ->159B        0.25366
    152B ->160B        0.34494
    153B ->160B       -0.26585
    156B ->163B       -0.25077

 Excited state symmetry could not be determined.
 Excited State  76:  2.300-?Sym    3.9081 eV  317.25 nm  f=0.0066
<S**2>=1.073
    152A ->159A        0.14682
    156A ->163A       -0.10908
    158A ->166A       -0.12712
    158A ->170A        0.66610
    158A ->171A        0.34860
    158A ->172A       -0.18274
    158A ->173A       -0.20614
    148B ->158B        0.12944
    149B ->158B        0.13018
    154B ->165B       -0.11405
    156B ->163B       -0.10137
    157B ->165B        0.14124
    157B ->166B        0.12557

 Excited state symmetry could not be determined.
 Excited State  77:  2.901-?Sym    3.9125 eV  316.89 nm  f=0.0004
<S**2>=1.854
    153A ->159A        0.11618
    153A ->160A       -0.12490
    149B ->158B       -0.35600
    151B ->159B       -0.11281
    152B ->159B        0.24166
    152B ->160B        0.76151
    153B ->159B       -0.11458
    154B ->161B       -0.17692

 Excited state symmetry could not be determined.
```

```
 Excited State  78:  2.516-?Sym    3.9275 eV  315.69 nm  f=0.0190
<S**2>=1.333
    152A ->159A       -0.10192
    153A ->159A        0.24874
    153A ->160A       -0.32326
    156A ->162A       -0.11845
    156A ->163A        0.28630
    156A ->164A       -0.12576
    158A ->171A       -0.11750
    158A ->172A       -0.12649
    149B ->158B        0.59066
    149B ->159B        0.13308
    153B ->160B        0.13317
    154B ->161B       -0.20783
    156B ->162B       -0.11137
    156B ->163B        0.20358

 Excited state symmetry could not be determined.
 Excited State  79:  2.737-?Sym    3.9349 eV  315.09 nm  f=0.0061
<S**2>=1.622
    154A ->161A       -0.18398
    154A ->162A        0.10181
    155A ->161A        0.15454
    156A ->163A        0.10480
    156A ->164A       -0.10009
    158A ->172A        0.11410
    158A ->173A       -0.15582
    148B ->158B       -0.34457
    149B ->158B        0.16770
    152B ->160B        0.28969
    154B ->161B        0.56597
    154B ->162B       -0.10446
    155B ->162B       -0.15151
    155B ->165B       -0.16947

 Excited state symmetry could not be determined.
 Excited State  80:  2.608-?Sym    3.9397 eV  314.70 nm  f=0.0042
<S**2>=1.451
    152A ->159A        0.16405
    153A ->159A       -0.31495
    153A ->160A        0.59921
    158A ->173A       -0.15710
    148B ->158B       -0.29838
    154B ->161B       -0.42026
    155B ->165B       -0.13333
    157B ->166B       -0.12769
```

Table S38. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 2 (*S*=0)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    0.8794 eV 1409.88 nm
f=0.0083  <S**2>=0.000
     158 ->159         0.66315
     158 ->160        -0.23367
 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 symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    1.0784 eV 1149.75 nm
f=0.0737  <S**2>=0.000
     158 ->159         0.23726
     158 ->160         0.66445

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    1.7195 eV  721.07 nm
f=0.0041  <S**2>=0.000
     157 ->159         0.68727

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    1.7230 eV  719.57 nm
f=0.0033  <S**2>=0.000
     157 ->160         0.13762
     158 ->161         0.68108

 Excited state symmetry could not be determined.
 Excited State   5:      Singlet-?Sym    1.7563 eV  705.93 nm
f=0.0075  <S**2>=0.000
     155 ->160         0.10893
     156 ->160        -0.11807
     157 ->160         0.66262
     158 ->161        -0.14398

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    1.9256 eV  643.87 nm
f=0.0021  <S**2>=0.000
     158 ->162         0.67889
     158 ->164        -0.16226

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    2.0111 eV  616.51 nm
f=0.0029  <S**2>=0.000
     158 ->162         0.11076
     158 ->163         0.67521
```

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     158 ->164         0.13197

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    2.1017 eV  589.93 nm
f=0.0357  <S**2>=0.000
     158 ->162         0.14192
     158 ->163        -0.15416
     158 ->164         0.66626

 Excited state symmetry could not be determined.
 Excited State   9:      Singlet-?Sym    2.3273 eV  532.73 nm
f=0.0006  <S**2>=0.000
     155 ->160         0.15125
     156 ->159         0.40466
     156 ->160         0.54468

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    2.4269 eV  510.87 nm
f=0.0280  <S**2>=0.000
     155 ->159        -0.15790
     156 ->159         0.52894
     156 ->160        -0.36796
     157 ->159         0.10991

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    2.5807 eV  480.43 nm
f=0.0079  <S**2>=0.000
     154 ->159         0.10885
     155 ->160         0.59729
     156 ->160        -0.12605
     157 ->160        -0.13310
     157 ->161         0.23568

 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    2.6169 eV  473.78 nm
f=0.0114  <S**2>=0.000
     154 ->159        -0.13204
     154 ->160         0.20921
     155 ->159         0.60265
     157 ->161        -0.11534
     158 ->165        -0.18719

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    2.6241 eV  472.48 nm
f=0.0203  <S**2>=0.000
     155 ->159         0.10932
     155 ->160        -0.22537
     156 ->159         0.12621
     157 ->161         0.63187
```

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 Excited state symmetry could not be determined.
 Excited State  14:      Singlet-?Sym    2.6885 eV  461.16 nm
f=0.1552  <S**2>=0.000
     155 ->159         0.18199
     158 ->165         0.62015

 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    2.7348 eV  453.35 nm
f=0.0289  <S**2>=0.000
     154 ->159         0.65747
     155 ->159         0.10201

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    2.8218 eV  439.39 nm
f=0.0151  <S**2>=0.000
     154 ->160         0.28008
     157 ->162         0.60255
     157 ->163         0.11350
     157 ->164        -0.13659

 Excited state symmetry could not be determined.
 Excited State  17:      Singlet-?Sym    2.8880 eV  429.31 nm
f=0.0080  <S**2>=0.000
     154 ->160         0.17091
     155 ->160        -0.11626
     157 ->162        -0.23269
     157 ->163         0.59023
     157 ->164        -0.11192

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    2.9150 eV  425.33 nm
f=0.0257  <S**2>=0.000
     154 ->160        -0.30857
     157 ->163         0.20985
     157 ->164         0.24846
     158 ->166         0.38555
     158 ->167         0.21649
     158 ->168        -0.16044

 Excited state symmetry could not be determined.
 Excited State  19:      Singlet-?Sym    2.9325 eV  422.79 nm
f=0.0523  <S**2>=0.000
     154 ->160        -0.15804
     157 ->162         0.18016
     157 ->163         0.21993
     157 ->164         0.39829
     158 ->166        -0.39132
     158 ->167        -0.13743

 Excited state symmetry could not be determined.
```

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 Excited State  20:      Singlet-?Sym    2.9869 eV  415.09 nm
f=0.0028  <S**2>=0.000
     154 ->160         0.15708
     157 ->164         0.24106
     158 ->166         0.41351
     158 ->167        -0.36207
     158 ->168         0.24188

 Excited state symmetry could not be determined.
 Excited State  21:      Singlet-?Sym    3.0355 eV  408.44 nm
f=0.0215  <S**2>=0.000
     154 ->160         0.36607
     155 ->159        -0.12446
     157 ->163        -0.13222
     157 ->164         0.41511
     158 ->167         0.24583
     158 ->168        -0.13109

 Excited state symmetry could not be determined.
 Excited State  22:      Singlet-?Sym    3.1599 eV  392.37 nm
f=0.0013  <S**2>=0.000
     158 ->167         0.43325
     158 ->168         0.50296
     158 ->169        -0.16028

 Excited state symmetry could not be determined.
 Excited State  23:      Singlet-?Sym    3.2953 eV  376.25 nm
f=0.0084  <S**2>=0.000
     156 ->161        -0.45435
     158 ->168         0.14383
     158 ->169         0.49455

 Excited state symmetry could not be determined.
 Excited State  24:      Singlet-?Sym    3.3112 eV  374.44 nm
f=0.0091  <S**2>=0.000
     156 ->161         0.47999
     156 ->163         0.12108
     158 ->168         0.10157
     158 ->169         0.45742

 Excited state symmetry could not be determined.
 Excited State  25:      Singlet-?Sym    3.3727 eV  367.61 nm
f=0.0139  <S**2>=0.000
     156 ->162         0.17510
     156 ->165         0.14208
     157 ->165        -0.32622
     158 ->167        -0.12320
     158 ->168         0.21454
     158 ->170         0.40020
     158 ->171         0.13102
```

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 Excited state symmetry could not be determined.
 Excited State  26:      Singlet-?Sym    3.4175 eV  362.79 nm
f=0.0029  <S**2>=0.000
     156 ->161         0.13292
     156 ->165        -0.17436
     156 ->172         0.10241
     157 ->165         0.27121
     157 ->167         0.13610
     157 ->168        -0.15964
     157 ->172        -0.16270
     158 ->170         0.42854

 Excited state symmetry could not be determined.
 Excited State  27:      Singlet-?Sym    3.4555 eV  358.81 nm
f=0.0010  <S**2>=0.000
     153 ->159         0.67157
     153 ->160        -0.11742

 Excited state symmetry could not be determined.
 Excited State  28:      Singlet-?Sym    3.4840 eV  355.87 nm
f=0.0025  <S**2>=0.000
     155 ->161         0.60879
     156 ->162        -0.30769

 Excited state symmetry could not be determined.
 Excited State  29:      Singlet-?Sym    3.4979 eV  354.45 nm
f=0.0090  <S**2>=0.000
     153 ->160        -0.20824
     156 ->162        -0.15824
     157 ->165        -0.19501
     157 ->167         0.16994
     157 ->168        -0.12596
     157 ->171         0.10038
     158 ->168         0.15145
     158 ->170        -0.24348
     158 ->171         0.28166
     158 ->172        -0.15014

 Excited state symmetry could not be determined.
 Excited State  30:      Singlet-?Sym    3.5104 eV  353.19 nm
f=0.0155  <S**2>=0.000
     155 ->161         0.29265
     156 ->162         0.53294
     156 ->163         0.12426
     158 ->170        -0.15286

 Excited state symmetry could not be determined.
 Excited State  31:      Singlet-?Sym    3.5216 eV  352.07 nm
f=0.0011  <S**2>=0.000
```

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     153 ->159         0.15224
     153 ->160         0.61157
     156 ->162        -0.15221
     157 ->165        -0.15248

 Excited state symmetry could not be determined.
 Excited State  32:      Singlet-?Sym    3.5593 eV  348.33 nm
f=0.0450  <S**2>=0.000
     155 ->163         0.17697
     156 ->163         0.51923
     158 ->171         0.10679
     158 ->172        -0.23607

 Excited state symmetry could not be determined.
 Excited State  33:      Singlet-?Sym    3.5924 eV  345.13 nm
f=0.0583  <S**2>=0.000
     153 ->160        -0.10078
     154 ->161         0.12271
     156 ->163         0.34269
     156 ->164         0.35007
     157 ->165        -0.14878
     158 ->170         0.13978
     158 ->171        -0.14673
     158 ->172         0.28563

 Excited state symmetry could not be determined.
 Excited State  34:      Singlet-?Sym    3.6250 eV  342.02 nm
f=0.0061  <S**2>=0.000
     154 ->161         0.65532
     158 ->172        -0.10051

 Excited state symmetry could not be determined.
 Excited State  35:      Singlet-?Sym    3.6623 eV  338.54 nm
f=0.0029  <S**2>=0.000
     152 ->159         0.65754
     152 ->160         0.18162
     153 ->160        -0.11599

 Excited state symmetry could not be determined.
 Excited State  36:      Singlet-?Sym    3.6822 eV  336.71 nm
f=0.1054  <S**2>=0.000
     152 ->159        -0.10228
     152 ->160         0.19707
     154 ->165         0.13876
     156 ->165         0.15535
     157 ->165         0.19586
     157 ->166        -0.14466
     158 ->171         0.41122
     158 ->172         0.22973
     158 ->173        -0.17989
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     158 ->177        -0.11069

 Excited state symmetry could not be determined.
 Excited State  37:      Singlet-?Sym    3.6950 eV  335.54 nm
f=0.0501  <S**2>=0.000
     152 ->159         0.12254
     152 ->160        -0.23942
     153 ->160         0.10992
     154 ->161        -0.11255
     155 ->162        -0.11297
     155 ->163        -0.25676
     155 ->164         0.14023
     156 ->164         0.41849
     157 ->165         0.12205
     158 ->171         0.20684
     158 ->172        -0.12081

 Excited state symmetry could not be determined.
 Excited State  38:      Singlet-?Sym    3.7073 eV  334.44 nm
f=0.0524  <S**2>=0.000
     152 ->159        -0.12629
     152 ->160         0.58726
     155 ->163        -0.12867
     155 ->164         0.10027
     156 ->164         0.18811
     156 ->165        -0.10586
     158 ->172        -0.13538

 Excited state symmetry could not be determined.
 Excited State  39:      Singlet-?Sym    3.7298 eV  332.42 nm
f=0.0311  <S**2>=0.000
     155 ->162         0.60119
     155 ->163        -0.27526

 Excited state symmetry could not be determined.
 Excited State  40:      Singlet-?Sym    3.7834 eV  327.71 nm
f=0.0296  <S**2>=0.000
     154 ->162        -0.18356
     154 ->163         0.17662
     155 ->162         0.21403
     155 ->163         0.36810
     156 ->163        -0.13482
     156 ->165        -0.28110
     158 ->171         0.17974
     158 ->172         0.16660
     158 ->173         0.10982

 Excited state symmetry could not be determined.
 Excited State  41:      Singlet-?Sym    3.8112 eV  325.31 nm
f=0.0128  <S**2>=0.000
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```
     154 ->162         0.37640
     155 ->164         0.49609
     156 ->164        -0.14357
     158 ->171         0.15058
     158 ->173         0.12366

 Excited state symmetry could not be determined.
 Excited State  42:      Singlet-?Sym    3.8266 eV  324.01 nm
f=0.0201  <S**2>=0.000
     154 ->162        -0.25021
     155 ->163         0.29030
     155 ->164         0.30334
     156 ->165         0.24432
     157 ->165         0.13544
     157 ->166         0.24528
     158 ->171        -0.10045
     158 ->172        -0.18516

 Excited state symmetry could not be determined.
 Excited State  43:      Singlet-?Sym    3.8584 eV  321.33 nm
f=0.0048  <S**2>=0.000
     154 ->162         0.35083
     154 ->163         0.46537
     155 ->163         0.12627
     155 ->164        -0.19644
     156 ->164         0.11660
     156 ->165         0.13424
     157 ->166         0.11580

 Excited state symmetry could not be determined.
 Excited State  44:      Singlet-?Sym    3.8648 eV  320.81 nm
f=0.0144  <S**2>=0.000
     154 ->163        -0.12234
     155 ->164        -0.15936
     157 ->166         0.56302
     158 ->171         0.16194
     158 ->172         0.17686
     158 ->173         0.19354

 Excited state symmetry could not be determined.
 Excited State  45:      Singlet-?Sym    3.8851 eV  319.13 nm
f=0.0011  <S**2>=0.000
     150 ->159        -0.32015
     150 ->160         0.15338
     151 ->159         0.55390
     151 ->160        -0.21202

 Excited state symmetry could not be determined.
 Excited State  46:      Singlet-?Sym    3.9451 eV  314.28 nm
f=0.0425  <S**2>=0.000
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     149 ->160        -0.14181
     150 ->159         0.10981
     154 ->162         0.12352
     154 ->163        -0.17409
     154 ->164         0.47611
     155 ->163         0.12789
     157 ->166        -0.10082
     158 ->173         0.24036

 Excited state symmetry could not be determined.
 Excited State  47:      Singlet-?Sym    3.9536 eV  313.60 nm
f=0.0454  <S**2>=0.000
     154 ->163         0.10444
     154 ->164         0.41243
     155 ->164         0.15972
     156 ->165        -0.19806
     157 ->166         0.13884
     157 ->167        -0.11931
     158 ->173        -0.29694

 Excited state symmetry could not be determined.
 Excited State  48:      Singlet-?Sym    3.9989 eV  310.05 nm
f=0.0053  <S**2>=0.000
     150 ->159         0.50375
     150 ->160         0.16979
     151 ->159         0.35423
     151 ->160         0.22612

 Excited state symmetry could not be determined.
 Excited State  49:      Singlet-?Sym    4.0154 eV  308.77 nm
f=0.0402  <S**2>=0.000
     150 ->159        -0.12813
     154 ->162        -0.22721
     154 ->163         0.31560
     154 ->164         0.13824
     156 ->164        -0.15273
     156 ->165         0.12966
     157 ->167         0.31292
     158 ->172         0.12246
     158 ->173         0.18448
     158 ->174         0.11698
     158 ->175        -0.11463

 Excited state symmetry could not be determined.
 Excited State  50:      Singlet-?Sym    4.0480 eV  306.28 nm
f=0.0005  <S**2>=0.000
     150 ->159        -0.29111
     150 ->160         0.40970
     151 ->159        -0.10387
     151 ->160         0.42598
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     157 ->167         0.10853
     157 ->168         0.11488

 Excited state symmetry could not be determined.
 Excited State  51:      Singlet-?Sym    4.0847 eV  303.53 nm
f=0.0157  <S**2>=0.000
     150 ->160        -0.27762
     157 ->167         0.36710
     157 ->168         0.35407
     158 ->173        -0.15945
     158 ->174        -0.18628

 Excited state symmetry could not be determined.
 Excited State  52:      Singlet-?Sym    4.1119 eV  301.53 nm
f=0.0385  <S**2>=0.000
     150 ->160         0.24586
     154 ->162        -0.14727
     154 ->163         0.12181
     155 ->167        -0.10721
     155 ->168         0.12330
     156 ->164        -0.14395
     156 ->167        -0.18555
     156 ->168         0.16485
     156 ->171        -0.12036
     156 ->172         0.15312
     156 ->174        -0.10058
     157 ->165        -0.16420
     157 ->167        -0.15932
     157 ->169         0.13386
     158 ->172        -0.11270
     158 ->173        -0.14240
     158 ->174        -0.10990

 Excited state symmetry could not be determined.
 Excited State  53:      Singlet-?Sym    4.1161 eV  301.22 nm
f=0.0102  <S**2>=0.000
     150 ->159        -0.15063
     150 ->160        -0.35489
     151 ->159         0.17121
     151 ->160         0.44108
     157 ->167        -0.23948
     157 ->168        -0.14746

 Excited state symmetry could not be determined.
 Excited State  54:      Singlet-?Sym    4.1943 eV  295.60 nm
f=0.0116  <S**2>=0.000
     155 ->165         0.13872
     156 ->168         0.11866
     158 ->172         0.11301
     158 ->174         0.57597
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     158 ->175         0.12956

 Excited state symmetry could not be determined.
 Excited State  55:      Singlet-?Sym    4.1962 eV  295.47 nm
f=0.0050  <S**2>=0.000
     157 ->168         0.20691
     157 ->169         0.62133
     158 ->173         0.11429
     158 ->175         0.11316

 Excited state symmetry could not be determined.
 Excited State  56:      Singlet-?Sym    4.2531 eV  291.52 nm
f=0.0310  <S**2>=0.000
     154 ->165         0.13035
     155 ->165        -0.18316
     157 ->167        -0.15802
     157 ->168         0.32506
     157 ->169        -0.23148
     157 ->170         0.25436
     157 ->171         0.10563
     157 ->172        -0.11172
     158 ->173         0.21181
     158 ->176         0.23074
     158 ->177        -0.10453

 Excited state symmetry could not be determined.
 Excited State  57:      Singlet-?Sym    4.2744 eV  290.06 nm
f=0.0094  <S**2>=0.000
     149 ->159         0.38763
     149 ->160        -0.17828
     155 ->165         0.10412
     157 ->170         0.25537
     158 ->173        -0.13637
     158 ->175        -0.38496
     158 ->176        -0.14994
     158 ->177         0.14436

 Excited state symmetry could not be determined.
 Excited State  58:      Singlet-?Sym    4.2767 eV  289.91 nm
f=0.0034  <S**2>=0.000
     149 ->159         0.50555
     149 ->160        -0.20932
     155 ->165        -0.10568
     157 ->170        -0.26767
     158 ->173         0.12454
     158 ->175         0.19480
     158 ->176         0.13999
     158 ->177        -0.12426

 Excited state symmetry could not be determined.
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 Excited State  59:      Singlet-?Sym    4.3084 eV  287.77 nm
f=0.0034  <S**2>=0.000
     153 ->161         0.23626
     157 ->170         0.25450
     158 ->175         0.42262
     158 ->176        -0.32486
     158 ->177         0.15271

 Excited state symmetry could not be determined.
 Excited State  60:      Singlet-?Sym    4.3202 eV  286.98 nm
f=0.0086  <S**2>=0.000
     153 ->161         0.64483
     158 ->175        -0.18494
     158 ->176         0.13563

 Excited state symmetry could not be determined.
 Excited State  61:      Singlet-?Sym    4.3538 eV  284.78 nm
f=0.0059  <S**2>=0.000
     154 ->165        -0.17241
     155 ->165         0.30976
     157 ->170         0.19299
     158 ->174        -0.14567
     158 ->175         0.15893
     158 ->176         0.46807

 Excited state symmetry could not be determined.
 Excited State  62:      Singlet-?Sym    4.3774 eV  283.24 nm
f=0.0019  <S**2>=0.000
     155 ->165        -0.14649
     155 ->172         0.10528
     157 ->168        -0.19515
     157 ->170         0.36638
     157 ->171        -0.22143
     157 ->172         0.21652
     158 ->177        -0.31914

 Excited state symmetry could not be determined.
 Excited State  63:      Singlet-?Sym    4.4064 eV  281.37 nm
f=0.0520  <S**2>=0.000
     148 ->159         0.48447
     148 ->160         0.43380
     149 ->160        -0.14094
     154 ->165         0.10506

 Excited state symmetry could not be determined.
 Excited State  64:      Singlet-?Sym    4.4203 eV  280.49 nm
f=0.0386  <S**2>=0.000
     149 ->159         0.11874
     149 ->160         0.29258
     154 ->165         0.28987
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     155 ->165         0.17655
     156 ->166         0.10015
     156 ->167         0.11451
     156 ->168        -0.11525
     157 ->165        -0.16382
     157 ->171        -0.17165
     157 ->173         0.15473
     158 ->177        -0.14638

 Excited state symmetry could not be determined.
 Excited State  65:      Singlet-?Sym    4.4596 eV  278.01 nm
f=0.3632  <S**2>=0.000
     148 ->160         0.36579
     149 ->159         0.16416
     149 ->160         0.41314
     154 ->164         0.14156
     154 ->165        -0.12640
     155 ->165        -0.12998
     158 ->177         0.11966

 Excited state symmetry could not be determined.
 Excited State  66:      Singlet-?Sym    4.4861 eV  276.37 nm
f=0.4382  <S**2>=0.000
     148 ->159         0.34758
     148 ->160        -0.31261
     149 ->160         0.24255
     153 ->162         0.10214
     154 ->165        -0.20139
     158 ->177        -0.22121

 Excited state symmetry could not be determined.
 Excited State  67:      Singlet-?Sym    4.4978 eV  275.66 nm
f=0.1816  <S**2>=0.000
     148 ->159         0.23622
     148 ->160        -0.22667
     152 ->161         0.18122
     153 ->162         0.10986
     154 ->165         0.21532
     155 ->165        -0.22181
     157 ->171        -0.11576
     157 ->172         0.10396
     158 ->176         0.12300
     158 ->177         0.36005

 Excited state symmetry could not be determined.
 Excited State  68:      Singlet-?Sym    4.5143 eV  274.65 nm
f=0.0021  <S**2>=0.000
     152 ->161         0.65172
     153 ->163         0.10247
     158 ->177        -0.11036
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 Excited state symmetry could not be determined.
 Excited State  69:      Singlet-?Sym    4.5346 eV  273.42 nm
f=0.0382  <S**2>=0.000
     148 ->159        -0.11710
     153 ->161        -0.10418
     153 ->162         0.65051
     153 ->163         0.15042

 Excited state symmetry could not be determined.
 Excited State  70:      Singlet-?Sym    4.5994 eV  269.57 nm
f=0.0315  <S**2>=0.000
     153 ->163         0.23908
     154 ->167         0.12516
     154 ->168        -0.10775
     155 ->166        -0.14363
     155 ->167        -0.19898
     155 ->168         0.17333
     155 ->172         0.10240
     156 ->166         0.12394
     156 ->167         0.13491
     156 ->168        -0.10467
     157 ->171         0.38880

 Excited state symmetry could not be determined.
 Excited State  71:      Singlet-?Sym    4.6322 eV  267.66 nm
f=0.0161  <S**2>=0.000
     152 ->161        -0.11251
     153 ->162        -0.14101
     153 ->163         0.60336
     153 ->164         0.11048
     156 ->166        -0.11133
     157 ->171        -0.16768

 Excited state symmetry could not be determined.
 Excited State  72:      Singlet-?Sym    4.6678 eV  265.61 nm
f=0.0075  <S**2>=0.000
     154 ->165        -0.17410
     155 ->165        -0.10819
     156 ->165         0.16495
     156 ->166         0.47975
     157 ->171        -0.25658
     157 ->172        -0.28017

 Excited state symmetry could not be determined.
 Excited State  73:      Singlet-?Sym    4.6806 eV  264.89 nm
f=0.0081  <S**2>=0.000
     154 ->165         0.13112
     154 ->166        -0.10194
     154 ->167        -0.13929
```

```
     154 ->168         0.13553
     156 ->166         0.42564
     156 ->167        -0.19334
     156 ->169        -0.10332
     157 ->171         0.21906
     157 ->172         0.22342

 Excited state symmetry could not be determined.
 Excited State  74:      Singlet-?Sym    4.7008 eV  263.75 nm
f=0.0018  <S**2>=0.000
     151 ->161         0.10399
     152 ->162         0.35674
     153 ->164         0.57813

 Excited state symmetry could not be determined.
 Excited State  75:      Singlet-?Sym    4.7245 eV  262.43 nm
f=0.0054  <S**2>=0.000
     150 ->161        -0.10172
     151 ->161         0.20032
     152 ->162         0.52107
     152 ->164        -0.15843
     153 ->164        -0.34808

 Excited state symmetry could not be determined.
 Excited State  76:      Singlet-?Sym    4.7439 eV  261.35 nm
f=0.0269  <S**2>=0.000
     154 ->166         0.20037
     154 ->167         0.23269
     154 ->168        -0.22149
     154 ->171         0.10840
     154 ->172        -0.11668
     155 ->165         0.18345
     156 ->167        -0.14421
     157 ->171        -0.16604
     157 ->172         0.33745
     157 ->173        -0.19808

 Excited state symmetry could not be determined.
 Excited State  77:      Singlet-?Sym    4.7494 eV  261.05 nm
f=0.0090  <S**2>=0.000
     150 ->161        -0.26635
     151 ->161         0.54080
     151 ->162         0.10151
     152 ->162        -0.26086
     152 ->163        -0.16973

 Excited state symmetry could not be determined.
 Excited State  78:      Singlet-?Sym    4.8073 eV  257.91 nm
f=0.0025  <S**2>=0.000
     150 ->161        -0.12364
```

```
     151 ->161         0.11892
     152 ->163         0.62767
     152 ->164         0.18874

 Excited state symmetry could not be determined.
 Excited State  79:      Singlet-?Sym    4.8232 eV  257.06 nm
f=0.0063  <S**2>=0.000
     146 ->160        -0.12247
     147 ->159         0.53191
     147 ->160         0.22359
     155 ->166         0.20510
     156 ->168        -0.13099
     156 ->169        -0.12695

 Excited state symmetry could not be determined.
 Excited State  80:      Singlet-?Sym    4.8290 eV  256.75 nm
f=0.0037  <S**2>=0.000
     147 ->160         0.21023
     150 ->161         0.12323
     152 ->164         0.13208
     155 ->166         0.11354
     156 ->167         0.32362
     156 ->168         0.36582
     156 ->169         0.27229
     157 ->172         0.11528
     157 ->173         0.15293
```

Table S39. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 2 (*S*=1)

```
     Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  3.008-?Sym    0.3615 eV 3429.32 nm  f=0.0366
<S**2>=2.012
    159A ->160A        1.03311
    159A <-160A       -0.27800
 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 symmetry could not be determined.
 Excited State   2:  3.021-?Sym    1.1436 eV 1084.18 nm  f=0.0014
<S**2>=2.031
    159A ->161A        0.97513
    159A ->162A       -0.17736

 Excited state symmetry could not be determined.
 Excited State   3:  3.015-?Sym    1.1975 eV 1035.32 nm  f=0.0179
<S**2>=2.023
    158A ->160A       -0.37167
    154B ->158B        0.11390
    157B ->158B        0.90212

 Excited state symmetry could not be determined.
 Excited State   4:  3.022-?Sym    1.2745 eV  972.84 nm  f=0.0026
<S**2>=2.033
    155A ->160A        0.10109
    158A ->160A        0.91015
    156B ->158B       -0.12092
    157B ->158B        0.36395

 Excited state symmetry could not be determined.
 Excited State   5:  3.022-?Sym    1.3490 eV  919.06 nm  f=0.0040
<S**2>=2.034
    159A ->161A        0.14965
    159A ->162A        0.74021
    159A ->163A       -0.62440
    159A ->164A        0.15470

 Excited state symmetry could not be determined.
 Excited State   6:  3.023-?Sym    1.4167 eV  875.15 nm  f=0.0161
<S**2>=2.034
    159A ->162A        0.61857
    159A ->163A        0.63855
    159A ->164A       -0.43140
```

```
 Excited state symmetry could not be determined.
 Excited State   7:  3.023-?Sym    1.4614 eV  848.40 nm  f=0.0095
<S**2>=2.035
    159A ->161A        0.11227
    159A ->162A        0.15737
    159A ->163A        0.42887
    159A ->164A        0.87227

 Excited state symmetry could not be determined.
 Excited State   8:  3.015-?Sym    1.6947 eV  731.62 nm  f=0.0039
<S**2>=2.023
    155B ->158B       -0.19343
    156B ->158B        0.95149
    156B ->159B       -0.10242
    157B ->158B        0.11778

 Excited state symmetry could not be determined.
 Excited State   9:  3.610-?Sym    1.8981 eV  653.20 nm  f=0.0564
<S**2>=3.008
    154A ->160A        0.14867
    157A ->160A        0.79388
    155B ->158B       -0.51849
    157B ->160B       -0.14693

 Excited state symmetry could not be determined.
 Excited State  10:  3.183-?Sym    1.9961 eV  621.12 nm  f=0.0344
<S**2>=2.282
    156A ->160A       -0.24367
    157A ->160A        0.30323
    159A ->165A        0.73569
    159A ->166A        0.17329
    155B ->158B        0.46554
    157B ->160B       -0.10770

 Excited state symmetry could not be determined.
 Excited State  11:  3.257-?Sym    1.9998 eV  619.99 nm  f=0.0552
<S**2>=2.402
    156A ->160A        0.31384
    157A ->160A       -0.36472
    159A ->165A        0.60505
    159A ->166A        0.15293
    155B ->158B       -0.55171
    156B ->158B       -0.11864
    157B ->160B        0.11689

 Excited state symmetry could not be determined.
 Excited State  12:  3.015-?Sym    2.1516 eV  576.24 nm  f=0.0003
<S**2>=2.022
    159A ->165A       -0.22430
    159A ->166A        0.92061
```

```
    159A ->168A        0.23626
    159A ->169A       -0.12561

 Excited state symmetry could not be determined.
 Excited State  13:  3.345-?Sym    2.1674 eV  572.04 nm  f=0.0095
<S**2>=2.547
    156A ->160A        0.41984
    154B ->158B       -0.14333
    154B ->159B        0.15281
    155B ->158B        0.14072
    156B ->160B       -0.10958
    157B ->159B        0.80330
    157B ->160B       -0.23485

 Excited state symmetry could not be determined.
 Excited State  14:  3.615-?Sym    2.2190 eV  558.73 nm  f=0.0099
<S**2>=3.018
    156A ->160A        0.63463
    154B ->158B        0.15522
    154B ->160B       -0.12878
    155B ->158B        0.24549
    156B ->159B        0.22395
    156B ->160B       -0.22662
    157B ->159B       -0.46340
    157B ->160B       -0.33771

 Excited state symmetry could not be determined.
 Excited State  15:  3.016-?Sym    2.2789 eV  544.05 nm  f=0.0011
<S**2>=2.023
    159A ->166A       -0.23937
    159A ->167A        0.76052
    159A ->168A        0.56743
    154B ->158B        0.10378

 Excited state symmetry could not be determined.
 Excited State  16:  3.026-?Sym    2.3020 eV  538.60 nm  f=0.0046
<S**2>=2.039
    159A ->166A       -0.11523
    159A ->167A       -0.59221
    159A ->168A        0.62865
    154B ->158B        0.42491

 Excited state symmetry could not be determined.
 Excited State  17:  3.070-?Sym    2.3197 eV  534.48 nm  f=0.0420
<S**2>=2.106
    159A ->167A        0.21823
    159A ->168A       -0.38805
    154B ->158B        0.80098
    157B ->159B        0.18400
    157B ->160B       -0.17504
```

```
 Excited state symmetry could not be determined.
 Excited State  18:  3.340-?Sym    2.3635 eV  524.58 nm  f=0.0023
<S**2>=2.540
    156A ->160A        0.20078
    157A ->160A        0.23141
    154B ->158B        0.22330
    154B ->160B        0.10188
    155B ->158B        0.15277
    156B ->159B        0.11090
    156B ->160B       -0.32834
    157B ->159B        0.12317
    157B ->160B        0.79861

 Excited state symmetry could not be determined.
 Excited State  19:  3.033-?Sym    2.5265 eV  490.74 nm  f=0.0049
<S**2>=2.049
    158A ->161A        0.96228
    156B ->159B       -0.12944

 Excited state symmetry could not be determined.
 Excited State  20:  3.084-?Sym    2.6306 eV  471.32 nm  f=0.0215
<S**2>=2.128
    156A ->160A       -0.12526
    159A ->169A        0.32466
    159A ->170A       -0.10192
    153B ->160B        0.10410
    155B ->159B       -0.34376
    156B ->159B        0.77758
    156B ->160B        0.15889
    157B ->159B        0.14281

 Excited state symmetry could not be determined.
 Excited State  21:  3.041-?Sym    2.6343 eV  470.65 nm  f=0.0431
<S**2>=2.062
    158A ->162A        0.29323
    159A ->168A        0.16629
    159A ->169A        0.73565
    159A ->170A       -0.21837
    159A ->172A        0.13973
    159A ->173A        0.19425
    155B ->159B        0.12840
    156B ->159B       -0.32094

 Excited state symmetry could not be determined.
 Excited State  22:  3.439-?Sym    2.6653 eV  465.18 nm  f=0.0031
<S**2>=2.707
    155A ->160A        0.23938
    158A ->161A        0.12167
    158A ->162A       -0.34283
```

```
    159A ->169A        0.15487
    155B ->159B        0.72890
    155B ->160B       -0.30620
    156B ->159B        0.26658
    156B ->160B        0.12853

 Excited state symmetry could not be determined.
 Excited State  23:  3.063-?Sym    2.6989 eV  459.39 nm  f=0.0308
<S**2>=2.095
    155A ->160A       -0.11773
    158A ->162A        0.69647
    158A ->163A       -0.20297
    158A ->165A       -0.31907
    159A ->169A       -0.22875
    159A ->170A        0.10246
    155B ->159B        0.36261
    156B ->159B        0.21571
    156B ->160B        0.15939

 Excited state symmetry could not be determined.
 Excited State  24:  3.141-?Sym    2.7257 eV  454.88 nm  f=0.0248
<S**2>=2.216
    155A ->160A        0.13872
    158A ->162A        0.41133
    158A ->163A        0.55470
    158A ->164A       -0.24461
    158A ->165A        0.41878
    158A ->166A        0.24038
    158A ->175A        0.10284
    159A ->169A       -0.10347
    159A ->170A        0.17576
    155B ->160B       -0.13376

 Excited state symmetry could not be determined.
 Excited State  25:  3.073-?Sym    2.7319 eV  453.84 nm  f=0.0442
<S**2>=2.110
    158A ->162A       -0.11907
    158A ->165A       -0.24641
    159A ->168A        0.15195
    159A ->169A        0.11098
    159A ->170A        0.76671
    159A ->171A       -0.13855
    159A ->172A        0.21069
    159A ->173A        0.26577
    155B ->159B       -0.18109

 Excited state symmetry could not be determined.
 Excited State  26:  3.164-?Sym    2.7519 eV  450.54 nm  f=0.0201
<S**2>=2.252
    155A ->160A       -0.14490
```

```
    158A ->163A       -0.27995
    158A ->165A        0.32983
    159A ->169A        0.13567
    159A ->170A        0.42274
    159A ->171A        0.58639
    159A ->173A       -0.14367
    155B ->160B        0.23163

 Excited state symmetry could not be determined.
 Excited State  27:  3.166-?Sym    2.7877 eV  444.75 nm  f=0.0091
<S**2>=2.255
    156A ->160A        0.16186
    158A ->161A       -0.10725
    158A ->163A        0.62422
    158A ->164A        0.22941
    158A ->165A       -0.24618
    158A ->166A       -0.10182
    159A ->171A        0.28434
    159A ->173A       -0.11750
    155B ->160B        0.27036
    156B ->160B        0.42706

 Excited state symmetry could not be determined.
 Excited State  28:  3.431-?Sym    2.7958 eV  443.47 nm  f=0.0035
<S**2>=2.693
    155A ->160A       -0.30387
    158A ->162A       -0.19104
    158A ->165A        0.29003
    159A ->171A       -0.46775
    159A ->173A        0.20759
    155B ->159B        0.20035
    155B ->160B        0.52080
    156B ->160B        0.30854

 Excited state symmetry could not be determined.
 Excited State  29:  3.083-?Sym    2.8598 eV  433.53 nm  f=0.0075
<S**2>=2.126
    157A ->165A       -0.10669
    158A ->162A        0.19408
    158A ->164A        0.80098
    158A ->165A        0.29170
    158A ->166A       -0.14912
    158A ->168A       -0.10870
    159A ->169A        0.14026
    159A ->171A       -0.16103
    155B ->160B       -0.20352

 Excited state symmetry could not be determined.
 Excited State  30:  3.222-?Sym    2.8815 eV  430.27 nm  f=0.0131
<S**2>=2.346
```

```
    154A ->160A       -0.13694
    155A ->160A        0.25481
    156A ->160A        0.31584
    157A ->160A        0.11559
    158A ->163A       -0.35636
    155B ->159B       -0.24321
    155B ->160B       -0.25584
    156B ->159B       -0.12879
    156B ->160B        0.58295
    157B ->160B        0.17795

 Excited state symmetry could not be determined.
 Excited State  31:  3.649-?Sym    2.9057 eV  426.69 nm  f=0.0013
<S**2>=3.079
    155A ->160A       -0.17547
    156A ->165A       -0.12904
    157A ->165A        0.31814
    157A ->166A        0.12184
    157A ->172A        0.14058
    157A ->175A        0.16653
    158A ->164A        0.36253
    158A ->166A        0.33457
    158A ->168A        0.18432
    158A ->173A       -0.11591
    159A ->169A       -0.12195
    159A ->171A        0.23862
    156B ->160B       -0.15011
    156B ->165B        0.14644
    157B ->165B       -0.33041
    157B ->173B       -0.13551
    157B ->176B       -0.10283

 Excited state symmetry could not be determined.
 Excited State  32:  3.118-?Sym    2.9431 eV  421.27 nm  f=0.0086
<S**2>=2.181
    154A ->160A       -0.10848
    155A ->160A        0.73154
    156A ->160A       -0.10427
    158A ->162A        0.10892
    158A ->164A        0.15298
    155B ->160B        0.53746

 Excited state symmetry could not be determined.
 Excited State  33:  3.542-?Sym    2.9659 eV  418.03 nm  f=0.0117
<S**2>=2.887
    155A ->160A        0.11907
    156A ->165A        0.15003
    157A ->165A       -0.18502
    157A ->172A       -0.14817
    157A ->173A       -0.11264
```

```
    157A ->175A       -0.11674
    158A ->164A        0.18816
    158A ->165A       -0.18773
    158A ->166A        0.52445
    158A ->168A        0.23315
    158A ->173A       -0.15665
    159A ->172A       -0.20792
    154B ->165B        0.11323
    156B ->165B       -0.18492
    157B ->165B        0.23811
    157B ->171B       -0.19147

 Excited state symmetry could not be determined.
 Excited State  34:  3.126-?Sym    2.9919 eV  414.39 nm  f=0.0079
<S**2>=2.193
    157A ->165A       -0.10494
    158A ->165A        0.18648
    159A ->169A       -0.27445
    159A ->170A       -0.17440
    159A ->171A        0.22556
    159A ->172A        0.74115
    159A ->173A        0.24288
    159A ->174A       -0.20734
    159A ->175A        0.12319
    157B ->165B        0.13766

 Excited state symmetry could not be determined.
 Excited State  35:  3.975-?Sym    3.0278 eV  409.49 nm  f=0.0032
<S**2>=3.699
    157A ->163A        0.10186
    157A ->164A       -0.10268
    157A ->166A        0.18082
    157A ->168A        0.20684
    157A ->169A       -0.19576
    157A ->171A        0.15064
    157A ->173A       -0.29642
    157A ->176A       -0.11457
    158A ->166A       -0.21293
    159A ->171A       -0.13111
    159A ->172A        0.13966
    159A ->173A       -0.10909
    154B ->169B        0.15710
    154B ->171B       -0.12263
    156B ->169B       -0.11397
    157B ->161B        0.13423
    157B ->163B       -0.14697
    157B ->164B        0.11751
    157B ->166B       -0.21276
    157B ->168B       -0.25398
    157B ->169B        0.30062
```

```
    157B ->171B       -0.23371
    157B ->173B       -0.16153

 Excited state symmetry could not be determined.
 Excited State  36:  3.119-?Sym    3.0921 eV  400.96 nm  f=0.0010
<S**2>=2.182
    158A ->166A       -0.38383
    158A ->169A       -0.13090
    159A ->169A       -0.19074
    159A ->170A       -0.11118
    159A ->171A        0.25516
    159A ->172A       -0.25677
    159A ->173A        0.59136
    159A ->174A        0.11218
    159A ->175A       -0.17997
    152B ->158B        0.33928

 Excited state symmetry could not be determined.
 Excited State  37:  3.252-?Sym    3.1109 eV  398.55 nm  f=0.0148
<S**2>=2.395
    159A ->171A       -0.11004
    159A ->172A        0.25053
    159A ->173A       -0.21003
    150B ->158B       -0.23240
    152B ->158B        0.72414
    157B ->161B       -0.22733

 Excited state symmetry could not be determined.
 Excited State  38:  3.190-?Sym    3.1376 eV  395.16 nm  f=0.0046
<S**2>=2.294
    155A ->173A        0.13857
    158A ->165A       -0.12984
    158A ->166A        0.34764
    158A ->167A       -0.22218
    158A ->168A       -0.40789
    158A ->169A        0.28081
    158A ->170A        0.10514
    158A ->171A       -0.20266
    158A ->172A        0.11920
    158A ->173A        0.22313
    159A ->173A        0.47287
    151B ->158B       -0.11428
    157B ->161B        0.17820

 Excited state symmetry could not be determined.
 Excited State  39:  3.735-?Sym    3.1537 eV  393.14 nm  f=0.0129
<S**2>=3.237
    154A ->160A        0.13359
    155A ->160A       -0.10431
    157A ->161A       -0.17395
```

```
    159A ->173A       -0.11704
    152B ->158B        0.27835
    154B ->159B        0.22254
    154B ->161B        0.12685
    157B ->159B       -0.10610
    157B ->161B        0.79216
    157B ->163B        0.11157

 Excited state symmetry could not be determined.
 Excited State  40:  3.873-?Sym    3.2009 eV  387.34 nm  f=0.0048
<S**2>=3.500
    150A ->160A        0.27491
    154A ->160A        0.63909
    157A ->160A       -0.14343
    157A ->162A       -0.10100
    150B ->159B        0.15962
    151B ->159B       -0.15728
    153B ->159B        0.12466
    154B ->159B        0.22756
    154B ->160B       -0.18813
    155B ->159B       -0.11463
    157B ->160B        0.11483
    157B ->161B       -0.30480
    157B ->162B        0.20009
    157B ->163B        0.10380

 Excited state symmetry could not be determined.
 Excited State  41:  3.178-?Sym    3.2256 eV  384.37 nm  f=0.0169
<S**2>=2.275
    156A ->165A       -0.12061
    158A ->166A        0.26096
    158A ->168A       -0.21058
    150B ->158B        0.40804
    151B ->158B        0.62014
    152B ->158B        0.27510
    153B ->158B        0.27579

 Excited state symmetry could not be determined.
 Excited State  42:  3.474-?Sym    3.2491 eV  381.60 nm  f=0.0081
<S**2>=2.768
    150A ->160A        0.17996
    151A ->160A       -0.24325
    152A ->160A        0.18644
    153A ->160A        0.13797
    154A ->160A       -0.33954
    155A ->160A       -0.22012
    158A ->167A        0.12885
    150B ->159B        0.17601
    151B ->159B       -0.13601
    153B ->160B       -0.22271
```

```
    154B ->159B        0.56331
    154B ->160B        0.10174
    157B ->161B       -0.22013
    157B ->162B       -0.14755

 Excited state symmetry could not be determined.
 Excited State  43:  3.220-?Sym    3.2578 eV  380.57 nm  f=0.0140
<S**2>=2.343
    154A ->160A        0.10153
    156A ->165A       -0.15728
    158A ->165A       -0.16454
    158A ->167A        0.83167
    158A ->168A       -0.13664
    158A ->172A        0.15139
    159A ->174A       -0.15837
    156B ->165B        0.11799
    157B ->161B        0.11849
    157B ->165B        0.10929

 Excited state symmetry could not be determined.
 Excited State  44:  3.516-?Sym    3.2684 eV  379.35 nm  f=0.0015
<S**2>=2.840
    156A ->165A       -0.28472
    156A ->166A       -0.10670
    156A ->172A       -0.14560
    156A ->175A       -0.16681
    158A ->167A       -0.10038
    159A ->172A        0.19490
    159A ->174A        0.66170
    150B ->158B       -0.11328
    151B ->158B       -0.16232
    154B ->159B        0.11047
    154B ->165B        0.10237
    156B ->165B        0.25465
    156B ->173B        0.13632
    157B ->165B        0.20538

 Excited state symmetry could not be determined.
 Excited State  45:  3.455-?Sym    3.2719 eV  378.93 nm  f=0.0070
<S**2>=2.735
    156A ->165A        0.26402
    156A ->166A        0.10154
    156A ->172A        0.13402
    156A ->175A        0.15208
    158A ->167A        0.29041
    158A ->168A       -0.13487
    159A ->172A        0.16562
    159A ->174A        0.65063
    152B ->158B       -0.11548
    156B ->165B       -0.24021
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    156B ->173B       -0.12509
    157B ->165B       -0.20960

 Excited state symmetry could not be determined.
 Excited State  46:  3.501-?Sym    3.3244 eV  372.95 nm  f=0.0063
<S**2>=2.813
    150A ->160A        0.31860
    154A ->160A       -0.29785
    157A ->161A        0.61037
    157A ->164A        0.11253
    150B ->159B        0.20807
    150B ->160B       -0.11353
    151B ->159B       -0.19621
    153B ->158B        0.12361
    153B ->159B        0.14662
    154B ->159B       -0.25486
    154B ->160B       -0.10411
    157B ->161B        0.17649
    157B ->162B        0.10391

 Excited state symmetry could not be determined.
 Excited State  47:  3.569-?Sym    3.3278 eV  372.58 nm  f=0.0065
<S**2>=2.934
    150A ->160A       -0.23842
    151A ->160A        0.16737
    152A ->160A       -0.10755
    154A ->160A       -0.12532
    157A ->161A        0.27031
    157A ->162A       -0.17538
    150B ->159B       -0.18462
    151B ->159B        0.14234
    153B ->160B        0.11337
    154B ->159B        0.55344
    154B ->160B       -0.17155
    157B ->162B        0.42305
    157B ->163B       -0.18699

 Excited state symmetry could not be determined.
 Excited State  48:  3.529-?Sym    3.3361 eV  371.65 nm  f=0.0085
<S**2>=2.864
    150A ->160A       -0.18299
    151A ->160A       -0.20880
    152A ->160A        0.25347
    154A ->160A        0.36295
    157A ->161A        0.53150
    157A ->163A        0.15043
    159A ->171A        0.10452
    153B ->158B       -0.27971
    153B ->159B       -0.22517
    153B ->160B       -0.30196
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    156B ->160B        0.10921
    157B ->161B        0.12102
    157B ->163B       -0.11358

 Excited state symmetry could not be determined.
 Excited State  49:  3.773-?Sym    3.3472 eV  370.42 nm  f=0.0094
<S**2>=3.309
    151A ->160A       -0.17254
    152A ->160A        0.16009
    153A ->160A        0.10272
    154A ->160A       -0.21870
    157A ->161A       -0.26572
    157A ->162A       -0.29387
    153B ->158B       -0.20936
    153B ->160B       -0.15731
    154B ->159B       -0.28532
    154B ->162B        0.10032
    157B ->162B        0.63565
    157B ->163B        0.21868

 Excited state symmetry could not be determined.
 Excited State  50:  3.151-?Sym    3.3901 eV  365.72 nm  f=0.0094
<S**2>=2.232
    158A ->165A        0.13275
    158A ->167A        0.12253
    158A ->172A       -0.20823
    159A ->172A       -0.24864
    159A ->173A        0.12636
    159A ->175A        0.74503
    152B ->158B        0.11129
    153B ->158B       -0.30042
    154B ->160B       -0.13803
    155B ->165B        0.13062

 Excited state symmetry could not be determined.
 Excited State  51:  3.287-?Sym    3.3972 eV  364.95 nm  f=0.0035
<S**2>=2.452
    151A ->160A       -0.13442
    152A ->160A        0.13287
    158A ->168A        0.27691
    158A ->169A        0.14873
    159A ->175A        0.14914
    151B ->158B       -0.10434
    153B ->158B        0.67606
    153B ->159B       -0.10640
    153B ->160B       -0.13024
    157B ->162B        0.18580
    157B ->163B       -0.32213

 Excited state symmetry could not be determined.
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 Excited State  52:  3.418-?Sym    3.4119 eV  363.39 nm  f=0.0070
<S**2>=2.670
    150A ->160A       -0.12712
    157A ->161A        0.22233
    157A ->162A       -0.11006
    157A ->169A       -0.10374
    157A ->173A       -0.11626
    158A ->168A       -0.10558
    159A ->175A        0.33341
    153B ->158B        0.35890
    154B ->159B        0.12333
    154B ->160B        0.33772
    157B ->163B        0.56953
    157B ->164B       -0.11037

 Excited state symmetry could not be determined.
 Excited State  53:  3.406-?Sym    3.4208 eV  362.44 nm  f=0.0154
<S**2>=2.650
    156A ->168A       -0.12055
    156A ->169A        0.10845
    156A ->173A        0.15699
    158A ->168A        0.51183
    158A ->169A        0.23835
    158A ->171A       -0.13023
    158A ->173A        0.15320
    159A ->176A       -0.14144
    150B ->158B        0.19110
    151B ->158B        0.26084
    153B ->158B       -0.20344
    154B ->160B        0.13607
    156B ->161B       -0.12567
    156B ->168B        0.13189
    156B ->169B       -0.15783
    156B ->171B        0.10670
    157B ->163B        0.16477
    157B ->165B       -0.18165

 Excited state symmetry could not be determined.
 Excited State  54:  3.574-?Sym    3.4529 eV  359.08 nm  f=0.0149
<S**2>=2.943
    155A ->165A        0.10699
    156A ->161A        0.14302
    156A ->163A       -0.11116
    156A ->166A       -0.10067
    157A ->161A       -0.16102
    157A ->163A        0.13521
    157A ->165A        0.18664
    158A ->167A       -0.14835
    158A ->169A       -0.18209
    158A ->172A        0.37843
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    159A ->175A        0.28105
    147B ->158B       -0.10137
    152B ->158B       -0.13335
    155B ->165B       -0.12227
    156B ->161B       -0.19834
    156B ->163B        0.10864
    156B ->165B       -0.14472
    156B ->171B        0.10687
    157B ->163B       -0.32820
    157B ->164B       -0.19698
    157B ->165B        0.12601
    157B ->166B        0.22131

 Excited state symmetry could not be determined.
 Excited State  55:  3.655-?Sym    3.4572 eV  358.63 nm  f=0.0150
<S**2>=3.091
    156A ->161A       -0.19199
    156A ->163A        0.15928
    156A ->168A        0.10830
    156A ->169A       -0.11261
    156A ->173A       -0.15584
    157A ->163A       -0.12164
    158A ->168A        0.35624
    158A ->169A        0.13019
    158A ->171A       -0.17853
    158A ->172A        0.29774
    159A ->175A        0.27682
    154B ->160B       -0.11735
    155B ->165B       -0.21088
    155B ->171B        0.10666
    156B ->161B        0.23372
    156B ->163B       -0.15790
    156B ->169B        0.15232
    156B ->171B       -0.12631
    157B ->162B       -0.12326
    157B ->163B        0.12130
    157B ->164B        0.11425
    157B ->169B        0.10681

 Excited state symmetry could not be determined.
 Excited State  56:  3.215-?Sym    3.4658 eV  357.73 nm  f=0.0047
<S**2>=2.334
    156A ->165A        0.11187
    157A ->162A        0.28535
    157A ->165A       -0.24127
    157A ->166A       -0.10059
    157A ->172A       -0.10741
    159A ->175A        0.11183
    159A ->176A        0.58105
    153B ->158B       -0.10327
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    154B ->160B        0.29955
    156B ->161B        0.12770
    156B ->165B        0.16978
    157B ->162B        0.22977
    157B ->163B       -0.13606
    157B ->165B       -0.20118

 Excited state symmetry could not be determined.
 Excited State  57:  3.285-?Sym    3.4713 eV  357.17 nm  f=0.0016
<S**2>=2.447
    156A ->173A        0.13293
    157A ->162A       -0.20675
    157A ->165A        0.18009
    159A ->173A       -0.10644
    159A ->175A       -0.11919
    159A ->176A        0.68934
    154B ->160B       -0.23437
    156B ->165B       -0.15487
    156B ->168B        0.12049
    156B ->169B       -0.12711
    156B ->171B        0.17302
    157B ->162B       -0.16189
    157B ->165B        0.11440

 Excited state symmetry could not be determined.
 Excited State  58:  3.462-?Sym    3.4901 eV  355.24 nm  f=0.0114
<S**2>=2.746
    156A ->161A       -0.13450
    156A ->165A       -0.15437
    156A ->172A       -0.11464
    156A ->173A       -0.11578
    157A ->162A        0.16751
    157A ->163A        0.23312
    157A ->164A       -0.15927
    157A ->165A        0.22325
    157A ->166A        0.16073
    158A ->168A        0.10341
    158A ->169A        0.16870
    158A ->173A        0.10381
    159A ->176A        0.10230
    150B ->158B        0.12731
    154B ->160B        0.37873
    155B ->165B        0.10755
    155B ->169B       -0.10633
    156B ->165B       -0.21591
    156B ->173B       -0.13733
    157B ->162B        0.27383
    157B ->164B       -0.11545
    157B ->165B        0.22885
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 Excited state symmetry could not be determined.
 Excited State  59:  3.520-?Sym    3.5170 eV  352.53 nm  f=0.0029
<S**2>=2.848
    154A ->160A       -0.15503
    156A ->161A        0.13712
    156A ->164A       -0.12034
    156A ->173A       -0.11361
    157A ->162A       -0.24674
    157A ->163A        0.47142
    157A ->166A        0.10713
    157A ->168A        0.13776
    157A ->169A       -0.10452
    157A ->173A       -0.14202
    159A ->176A        0.24337
    154B ->160B       -0.22641
    156B ->161B       -0.15644
    156B ->165B        0.12618
    156B ->169B        0.10517
    156B ->171B       -0.13787
    157B ->162B       -0.18741
    157B ->164B       -0.37280
    157B ->165B       -0.10758

 Excited state symmetry could not be determined.
 Excited State  60:  3.826-?Sym    3.5255 eV  351.68 nm  f=0.0011
<S**2>=3.410
    156A ->161A       -0.44395
    157A ->162A       -0.16629
    157A ->163A        0.17297
    159A ->176A       -0.22345
    150B ->158B       -0.20292
    151B ->158B        0.18391
    155B ->165B        0.10256
    156B ->161B        0.54234
    157B ->163B       -0.25541
    157B ->164B       -0.13519
    157B ->166B        0.10022
    157B ->168B        0.10424

 Excited state symmetry could not be determined.
 Excited State  61:  3.465-?Sym    3.5352 eV  350.72 nm  f=0.0040
<S**2>=2.751
    157A ->162A       -0.38479
    157A ->163A       -0.22872
    157A ->164A        0.21618
    150B ->158B        0.10373
    154B ->160B        0.46058
    155B ->161B        0.16884
    155B ->165B       -0.11147
    156B ->161B        0.11306
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    157B ->162B       -0.14343
    157B ->163B       -0.19948
    157B ->164B       -0.39072
    157B ->165B       -0.12271
    157B ->166B       -0.19134
    157B ->168B       -0.14221

 Excited state symmetry could not be determined.
 Excited State  62:  3.154-?Sym    3.5551 eV  348.75 nm  f=0.0002
<S**2>=2.237
    156A ->161A       -0.12409
    157A ->162A       -0.10679
    150B ->158B        0.70405
    151B ->158B       -0.54508
    152B ->158B        0.16230
    156B ->161B        0.11587
    157B ->164B        0.14333

 Excited state symmetry could not be determined.
 Excited State  63:  3.660-?Sym    3.5778 eV  346.54 nm  f=0.0118
<S**2>=3.099
    152A ->160A       -0.12217
    156A ->161A        0.11867
    156A ->163A       -0.18560
    157A ->162A       -0.44771
    157A ->163A        0.39398
    157A ->164A       -0.15147
    154B ->160B        0.21639
    155B ->161B        0.15104
    157B ->164B        0.58478

 Excited state symmetry could not be determined.
 Excited State  64:  3.451-?Sym    3.6072 eV  343.71 nm  f=0.0060
<S**2>=2.728
    156A ->161A       -0.15537
    157A ->162A        0.22014
    157A ->163A        0.53948
    157A ->164A        0.48026
    157A ->166A       -0.10972
    157A ->168A       -0.13628
    157A ->169A        0.12198
    157A ->171A       -0.10235
    157A ->173A        0.16220
    155B ->161B       -0.16116
    155B ->163B       -0.10885
    155B ->165B       -0.16546
    156B ->161B        0.11263
    157B ->163B        0.20711
    157B ->166B       -0.15172
    157B ->168B       -0.12876
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 Excited state symmetry could not be determined.
 Excited State  65:  3.617-?Sym    3.6441 eV  340.23 nm  f=0.0102
<S**2>=3.021
    148A ->167A        0.11121
    153A ->166A        0.13217
    154A ->165A       -0.11332
    155A ->165A       -0.12096
    156A ->163A        0.15692
    156A ->165A       -0.11651
    157A ->164A        0.27489
    158A ->169A       -0.25823
    158A ->170A       -0.20069
    158A ->172A        0.15685
    158A ->173A        0.18249
    158A ->174A        0.18881
    145B ->158B        0.12622
    147B ->158B       -0.10364
    148B ->167B       -0.11365
    152B ->165B       -0.12228
    154B ->165B        0.10500
    155B ->162B       -0.10988
    155B ->165B        0.28615
    155B ->169B       -0.11170
    155B ->173B        0.13651
    156B ->162B        0.12205
    156B ->163B       -0.11342
    157B ->164B        0.23092
    157B ->165B       -0.10737

 Excited state symmetry could not be determined.
 Excited State  66:  3.284-?Sym    3.6625 eV  338.52 nm  f=0.0201
<S**2>=2.447
    156A ->161A       -0.30752
    156A ->165A        0.32168
    156A ->166A        0.12051
    156A ->172A        0.11377
    156A ->175A        0.14901
    157A ->164A       -0.21398
    157A ->165A        0.14649
    158A ->169A       -0.19251
    158A ->170A       -0.12688
    158A ->173A        0.15466
    154B ->165B        0.11165
    155B ->161B       -0.19036
    155B ->162B        0.10158
    155B ->165B       -0.15980
    155B ->168B        0.11363
    155B ->169B       -0.15105
    155B ->171B        0.16862
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    156B ->161B       -0.28635
    156B ->164B       -0.12184
    156B ->165B        0.25725
    157B ->165B        0.12254

 Excited state symmetry could not be determined.
 Excited State  67:  3.619-?Sym    3.6681 eV  338.01 nm  f=0.0022
<S**2>=3.024
    156A ->161A       -0.27517
    156A ->162A       -0.21352
    156A ->163A        0.20198
    156A ->164A       -0.19373
    157A ->162A        0.16367
    157A ->164A        0.20268
    155B ->161B        0.58539
    156B ->161B       -0.24480
    156B ->162B        0.24771
    156B ->163B       -0.11569
    156B ->165B        0.11672
    157B ->164B        0.12322
    157B ->165B        0.10871

 Excited state symmetry could not be determined.
 Excited State  68:  3.704-?Sym    3.6791 eV  336.99 nm  f=0.0019
<S**2>=3.180
    156A ->161A        0.40899
    156A ->163A        0.37634
    156A ->164A       -0.10773
    157A ->164A       -0.19615
    158A ->169A       -0.14166
    158A ->172A       -0.10904
    158A ->173A        0.14021
    158A ->175A        0.12813
    147B ->158B        0.14958
    155B ->161B       -0.29262
    155B ->165B       -0.17968
    155B ->171B        0.10152
    156B ->161B        0.17388
    156B ->162B        0.20532
    156B ->163B       -0.20793

 Excited state symmetry could not be determined.
 Excited State  69:  3.373-?Sym    3.6877 eV  336.21 nm  f=0.0106
<S**2>=2.595
    154A ->165A        0.13327
    156A ->161A        0.32227
    156A ->164A       -0.10519
    156A ->165A        0.22894
    156A ->172A        0.13007
    156A ->175A        0.12680
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    157A ->164A        0.15312
    157A ->165A        0.20978
    158A ->169A        0.13915
    158A ->173A       -0.21236
    158A ->175A       -0.13576
    147B ->158B       -0.15282
    148B ->158B        0.10305
    154B ->160B        0.11759
    156B ->161B        0.26538
    156B ->165B        0.26995
    156B ->173B        0.13551
    157B ->165B        0.22905

 Excited state symmetry could not be determined.
 Excited State  70:  3.506-?Sym    3.7042 eV  334.71 nm  f=0.0067
<S**2>=2.824
    156A ->161A        0.16938
    156A ->163A       -0.20501
    156A ->165A        0.10770
    157A ->163A       -0.11232
    157A ->164A        0.41924
    157A ->165A        0.10332
    157A ->166A        0.22355
    157A ->173A       -0.16706
    158A ->169A       -0.11584
    158A ->173A        0.20050
    158A ->175A        0.14681
    147B ->158B        0.13969
    155B ->169B       -0.11044
    155B ->171B        0.10708
    156B ->161B        0.25599
    156B ->162B       -0.28485
    156B ->163B        0.20164
    157B ->164B        0.11397
    157B ->165B        0.13953
    157B ->168B        0.11474
    157B ->169B       -0.13104

 Excited state symmetry could not be determined.
 Excited State  71:  3.494-?Sym    3.7107 eV  334.13 nm  f=0.0012
<S**2>=2.802
    150A ->160A       -0.13092
    156A ->161A        0.20603
    156A ->162A       -0.14920
    157A ->162A        0.21318
    157A ->163A        0.12149
    157A ->164A       -0.35067
    157A ->173A        0.10035
    154B ->160B       -0.12036
    155B ->161B        0.50619
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    156B ->161B        0.33572
    156B ->163B        0.26857
    157B ->163B        0.10676
    157B ->164B       -0.17174
    157B ->166B       -0.13070

 Excited state symmetry could not be determined.
 Excited State  72:  3.087-?Sym    3.7522 eV  330.43 nm  f=0.0015
<S**2>=2.132
    148B ->158B       -0.21113
    149B ->158B        0.93181

 Excited state symmetry could not be determined.
 Excited State  73:  3.938-?Sym    3.7593 eV  329.80 nm  f=0.0013
<S**2>=3.627
    150A ->160A        0.10405
    156A ->161A        0.11584
    156A ->162A        0.44530
    156A ->163A        0.28798
    156A ->164A        0.20330
    159A ->177A       -0.20631
    149B ->158B        0.11386
    150B ->159B        0.11664
    155B ->161B        0.31895
    156B ->162B       -0.38388
    156B ->163B       -0.32354
    156B ->164B       -0.17341
    157B ->166B        0.10766

 Excited state symmetry could not be determined.
 Excited State  74:  3.436-?Sym    3.7666 eV  329.16 nm  f=0.0059
<S**2>=2.702
    148A ->168A        0.10293
    149A ->167A        0.13145
    153A ->165A       -0.10275
    157A ->166A       -0.12144
    158A ->165A        0.12241
    158A ->172A       -0.16830
    158A ->173A        0.17737
    148B ->158B        0.67039
    149B ->158B        0.12402
    149B ->167B        0.11981
    151B ->165B        0.11049
    154B ->166B       -0.11886
    157B ->166B        0.21818
    157B ->167B        0.10508
    157B ->169B        0.14592

 Excited state symmetry could not be determined.
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 Excited State  75:  3.472-?Sym    3.7829 eV  327.75 nm  f=0.0220
<S**2>=2.765
    154A ->166A       -0.10006
    157A ->166A        0.15707
    158A ->165A       -0.10918
    158A ->167A       -0.11368
    158A ->169A       -0.10836
    158A ->172A        0.21014
    159A ->177A        0.11000
    148B ->158B        0.61648
    149B ->158B        0.15515
    150B ->158B       -0.10826
    152B ->158B        0.14380
    154B ->166B        0.11752
    156B ->162B       -0.15151
    156B ->163B       -0.11432
    157B ->166B       -0.38394
    157B ->169B       -0.17006
    157B ->171B        0.12350

 Excited state symmetry could not be determined.
 Excited State  76:  3.114-?Sym    3.8055 eV  325.80 nm  f=0.0006
<S**2>=2.174
    156A ->164A        0.12580
    159A ->177A        0.94017
    156B ->162B       -0.11630
    156B ->164B       -0.10766

 Excited state symmetry could not be determined.
 Excited State  77:  3.969-?Sym    3.8321 eV  323.54 nm  f=0.0011
<S**2>=3.688
    151A ->160A       -0.10727
    152A ->160A        0.12295
    153A ->160A        0.18331
    156A ->162A       -0.48201
    156A ->164A        0.53401
    159A ->177A       -0.11668
    153B ->159B       -0.11856
    153B ->162B        0.13163
    155B ->162B       -0.14740
    155B ->164B        0.15735
    156B ->162B        0.10803
    156B ->164B       -0.37002

 Excited state symmetry could not be determined.
 Excited State  78:  3.438-?Sym    3.8492 eV  322.11 nm  f=0.0023
<S**2>=2.705
    153A ->160A       -0.24799
    156A ->162A        0.31438
    156A ->163A        0.19427
```

```
    156A ->164A        0.21397
    158A ->173A       -0.15474
    150B ->159B        0.12016
    153B ->160B       -0.10681
    155B ->162B        0.41378
    155B ->163B        0.20182
    155B ->169B       -0.10381
    156B ->162B        0.44019
    156B ->163B        0.28956
    156B ->164B       -0.18116

 Excited state symmetry could not be determined.
 Excited State  79:  3.398-?Sym    3.8577 eV  321.40 nm  f=0.0246
<S**2>=2.637
    156A ->162A       -0.34537
    158A ->169A        0.12152
    158A ->172A       -0.18247
    158A ->173A       -0.20776
    148B ->158B        0.14446
    154B ->165B        0.10233
    155B ->162B        0.41203
    155B ->163B        0.25364
    155B ->165B       -0.22306
    155B ->171B        0.12104
    156B ->162B       -0.24562
    156B ->163B       -0.23748
    156B ->164B        0.13619
    157B ->165B       -0.14165
    157B ->166B        0.19322

 Excited state symmetry could not be determined.
 Excited State  80:  3.651-?Sym    3.8662 eV  320.69 nm  f=0.0045
<S**2>=3.083
    151A ->160A        0.27133
    152A ->160A       -0.15404
    153A ->160A        0.67482
    157A ->165A       -0.10717
    158A ->169A       -0.14171
    158A ->170A       -0.11494
    158A ->173A        0.10607
    148B ->158B       -0.14663
    154B ->165B       -0.11898
    155B ->162B        0.33712
    155B ->163B        0.14917
    157B ->166B       -0.10153
```

Table S40. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 3^+ (*S*=1/2)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  2.052-?Sym    0.5498 eV 2255.22 nm  f=0.0047
<S**2>=0.802
    172A ->173A        0.99211
 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 symmetry could not be determined.
 Excited State   2:  2.067-?Sym    0.6225 eV 1991.69 nm  f=0.0018
<S**2>=0.818
    172A ->174A        0.98808

 Excited state symmetry could not be determined.
 Excited State   3:  2.718-?Sym    1.2857 eV  964.31 nm  f=0.0144
<S**2>=1.597
    170B ->172B        0.16887
    171B ->172B        0.95948
    171B ->174B       -0.17420

 Excited state symmetry could not be determined.
 Excited State   4:  3.259-?Sym    1.3014 eV  952.69 nm  f=0.0019
<S**2>=2.405
    168A ->174A       -0.13028
    171A ->174A       -0.32810
    168B ->173B        0.17385
    170B ->173B        0.26540
    171B ->173B        0.86579

 Excited state symmetry could not be determined.
 Excited State   5:  2.721-?Sym    1.4357 eV  863.59 nm  f=0.0299
<S**2>=1.601
    170A ->173A        0.13849
    171A ->173A       -0.50001
    170B ->172B        0.10092
    171B ->174B        0.82146

 Excited state symmetry could not be determined.
 Excited State   6:  2.521-?Sym    1.5809 eV  784.25 nm  f=0.0058
<S**2>=1.339
    170A ->174A       -0.48937
    171A ->174A        0.76316
    171B ->173B        0.36529

 Excited state symmetry could not be determined.
```

```
 Excited State   7:  2.375-?Sym    1.6200 eV  765.33 nm  f=0.0056
<S**2>=1.160
    170A ->173A       -0.33633
    171A ->173A        0.75868
    171B ->172B        0.14007
    171B ->174B        0.50479

 Excited state symmetry could not be determined.
 Excited State   8:  3.331-?Sym    1.6624 eV  745.83 nm  f=0.0007
<S**2>=2.524
    164A ->173A       -0.10545
    166A ->174A        0.23553
    168A ->174A        0.28295
    169A ->173A        0.10193
    170A ->174A        0.41380
    171A ->174A        0.35559
    163B ->172B        0.12868
    166B ->173B       -0.24985
    168B ->173B       -0.24626
    169B ->172B       -0.15197
    170B ->173B        0.59524

 Excited state symmetry could not be determined.
 Excited State   9:  3.391-?Sym    1.8195 eV  681.42 nm  f=0.0003
<S**2>=2.625
    164A ->174A       -0.12100
    166A ->173A        0.21232
    168A ->173A        0.17038
    169A ->174A        0.11521
    170A ->173A        0.48851
    171A ->173A        0.24867
    163B ->173B        0.14260
    166B ->172B       -0.20490
    168B ->172B       -0.12441
    169B ->173B       -0.25273
    170B ->172B        0.62326
    170B ->174B        0.11599

 Excited state symmetry could not be determined.
 Excited State  10:  3.061-?Sym    2.0340 eV  609.55 nm  f=0.0000
<S**2>=2.092
    167A ->174A       -0.13296
    169A ->174A       -0.20624
    170A ->173A       -0.11578
    167B ->173B        0.23885
    169B ->173B        0.79758
    170B ->172B        0.41194

 Excited state symmetry could not be determined.
```

```
 Excited State  11:  3.099-?Sym    2.0772 eV  596.89 nm  f=0.0009
<S**2>=2.151
    167A ->173A       -0.11752
    169A ->173A       -0.21185
    167B ->172B        0.17861
    169B ->172B        0.86010
    169B ->174B        0.14665
    170B ->173B        0.29838
    171B ->173B       -0.10197

 Excited state symmetry could not be determined.
 Excited State  12:  2.333-?Sym    2.1436 eV  578.39 nm  f=0.0191
<S**2>=1.111
    167A ->174A       -0.11506
    169A ->174A       -0.15049
    170A ->173A        0.67521
    171A ->173A        0.23747
    169B ->173B        0.28368
    170B ->172B       -0.54554
    171B ->172B        0.11732

 Excited state symmetry could not be determined.
 Excited State  13:  2.408-?Sym    2.2282 eV  556.43 nm  f=0.0097
<S**2>=1.200
    167A ->173A        0.10119
    169A ->173A        0.14976
    170A ->174A       -0.51721
    171A ->174A       -0.16650
    166B ->173B        0.13194
    168B ->173B        0.29135
    169B ->172B       -0.22026
    170B ->173B        0.62974
    171B ->173B       -0.28062

 Excited state symmetry could not be determined.
 Excited State  14:  2.491-?Sym    2.3320 eV  531.67 nm  f=0.0176
<S**2>=1.301
    165A ->173A        0.16096
    167A ->173A        0.36358
    169A ->173A        0.62810
    172A ->175A       -0.14892
    168B ->173B       -0.21004
    169B ->172B        0.35770
    169B ->174B       -0.37387

 Excited state symmetry could not be determined.
 Excited State  15:  3.413-?Sym    2.3620 eV  524.91 nm  f=0.0000
<S**2>=2.662
    162A ->174A       -0.29910
    163A ->174A       -0.10264
```

```
    164A ->173A       -0.36548
    165A ->173A       -0.33357
    166A ->174A        0.15264
    168A ->174A       -0.10920
    169A ->173A        0.26610
    170A ->174A       -0.17782
    162B ->173B        0.30523
    163B ->172B        0.47496
    165B ->172B        0.20707
    166B ->173B       -0.15123
    167B ->172B        0.10969
    170B ->173B       -0.15992

 Excited state symmetry could not be determined.
 Excited State  16:  2.275-?Sym    2.3725 eV  522.58 nm  f=0.0057
<S**2>=1.044
    165A ->174A        0.10363
    167A ->174A        0.29231
    169A ->174A        0.45686
    162B ->174B       -0.11823
    168B ->172B       -0.33497
    169B ->173B        0.23098
    170B ->172B       -0.12466
    170B ->174B        0.66078

 Excited state symmetry could not be determined.
 Excited State  17:  2.772-?Sym    2.3960 eV  517.47 nm  f=0.0081
<S**2>=1.671
    162A ->173A        0.15607
    164A ->174A        0.12203
    166A ->173A       -0.16898
    167A ->174A       -0.25384
    169A ->174A       -0.40697
    170A ->173A        0.14516
    162B ->172B       -0.15337
    162B ->174B       -0.10422
    163B ->173B       -0.17306
    166B ->172B        0.25714
    168B ->172B        0.26926
    168B ->174B        0.11280
    169B ->173B       -0.16921
    170B ->172B        0.11040
    170B ->174B        0.59227

 Excited state symmetry could not be determined.
 Excited State  18:  3.170-?Sym    2.4398 eV  508.17 nm  f=0.0045
<S**2>=2.262
    162A ->173A       -0.33333
    163A ->173A       -0.12556
    164A ->174A       -0.26704
```

```
    165A ->174A       -0.27479
    166A ->173A        0.22307
    167A ->174A       -0.12291
    168A ->173A       -0.12755
    170A ->173A       -0.22739
    162B ->172B        0.34768
    163B ->173B        0.31037
    165B ->173B        0.13178
    166B ->172B       -0.18635
    168B ->172B        0.19682
    169B ->173B       -0.12564
    170B ->172B       -0.22201
    170B ->174B        0.35085

 Excited state symmetry could not be determined.
 Excited State  19:  2.762-?Sym    2.4719 eV  501.58 nm  f=0.0114
<S**2>=1.658
    166A ->174A       -0.17210
    168A ->174A       -0.27782
    169A ->173A        0.24830
    170A ->174A        0.33200
    171A ->174A        0.24131
    172A ->175A        0.58241
    172A ->177A        0.25831
    166B ->173B        0.18053
    168B ->173B        0.35840
    169B ->174B       -0.17040

 Excited state symmetry could not be determined.
 Excited State  20:  3.107-?Sym    2.4827 eV  499.38 nm  f=0.0100
<S**2>=2.163
    159A ->173A        0.10385
    166A ->173A       -0.18040
    167A ->174A        0.13400
    168A ->173A       -0.39351
    169A ->174A        0.48289
    170A ->173A        0.21358
    171A ->173A        0.17892
    166B ->172B        0.16858
    167B ->173B        0.14798
    168B ->172B        0.58043

 Excited state symmetry could not be determined.
 Excited State  21:  2.438-?Sym    2.4851 eV  498.91 nm  f=0.0137
<S**2>=1.236
    168A ->174A        0.20361
    170A ->174A       -0.25847
    171A ->174A       -0.18562
    172A ->175A        0.74309
    172A ->177A       -0.20033
```

```
    166B ->173B       -0.11664
    168B ->173B       -0.32174
    169B ->174B        0.29492

 Excited state symmetry could not be determined.
 Excited State  22:  2.548-?Sym    2.5416 eV  487.82 nm  f=0.0038
<S**2>=1.373
    166A ->174A        0.15820
    167A ->173A        0.10654
    168A ->174A        0.24897
    169A ->173A       -0.36004
    170A ->174A       -0.17491
    171A ->174A       -0.15294
    172A ->175A        0.17371
    172A ->177A        0.64000
    167B ->172B       -0.26250
    169B ->174B       -0.29744

 Excited state symmetry could not be determined.
 Excited State  23:  2.060-?Sym    2.5444 eV  487.28 nm  f=0.0014
<S**2>=0.811
    172A ->176A        0.98563

 Excited state symmetry could not be determined.
 Excited State  24:  2.860-?Sym    2.5978 eV  477.27 nm  f=0.0315
<S**2>=1.795
    157A ->173A       -0.10123
    158A ->173A        0.11408
    159A ->174A        0.14020
    167A ->173A       -0.26654
    169A ->173A        0.14736
    172A ->175A       -0.15203
    172A ->177A        0.50659
    154B ->172B       -0.10650
    158B ->173B       -0.12511
    159B ->172B        0.13451
    167B ->172B        0.47179
    167B ->174B        0.11646
    168B ->173B       -0.21514
    169B ->174B        0.35002

 Excited state symmetry could not be determined.
 Excited State  25:  2.501-?Sym    2.6427 eV  469.15 nm  f=0.0711
<S**2>=1.314
    166A ->174A       -0.11259
    167A ->173A        0.17512
    168A ->174A       -0.25610
    169A ->173A        0.23211
    172A ->175A       -0.10568
    172A ->177A        0.21849
```

```
    159B ->172B       -0.10484
    167B ->172B       -0.56726
    167B ->174B        0.10717
    169B ->174B        0.58305

 Excited state symmetry could not be determined.
 Excited State  26:  2.323-?Sym    2.6610 eV  465.93 nm  f=0.0516
<S**2>=1.099
    166A ->173A        0.17586
    167A ->174A        0.21539
    168A ->173A        0.58252
    167B ->173B       -0.15289
    168B ->172B        0.53737
    168B ->174B       -0.39368
    169B ->173B        0.15114

 Excited state symmetry could not be determined.
 Excited State  27:  3.370-?Sym    2.7007 eV  459.07 nm  f=0.0034
<S**2>=2.589
    157A ->174A       -0.12617
    158A ->174A        0.15872
    159A ->173A        0.23242
    160A ->173A       -0.12741
    167A ->174A       -0.37700
    168A ->173A        0.35848
    169A ->174A        0.13248
    154B ->173B       -0.14593
    156B ->172B       -0.10853
    158B ->172B       -0.21771
    159B ->173B        0.18232
    160B ->172B        0.13293
    164B ->172B        0.10166
    167B ->173B        0.54802
    168B ->174B       -0.18241

 Excited state symmetry could not be determined.
 Excited State  28:  2.258-?Sym    2.7379 eV  452.84 nm  f=0.0009
<S**2>=1.025
    158A ->173A       -0.11720
    159A ->174A       -0.11565
    167A ->173A        0.71720
    168A ->174A       -0.24466
    169A ->173A       -0.26992
    167B ->172B        0.46164
    167B ->174B       -0.11473
    169B ->174B        0.13812

 Excited state symmetry could not be determined.
 Excited State  29:  2.455-?Sym    2.7545 eV  450.11 nm  f=0.0141
<S**2>=1.257
```

```
    167A ->178A        0.15261
    167A ->185A        0.10390
    168A ->173A       -0.17220
    169A ->178A        0.17143
    170A ->177A       -0.11705
    171A ->177A        0.22647
    172A ->178A        0.69193
    172A ->179A        0.16857
    172A ->181A        0.22287
    172A ->185A        0.18480
    172A ->188A        0.15323
    168B ->174B       -0.24189
    171B ->177B       -0.13785

 Excited state symmetry could not be determined.
 Excited State  30:  2.111-?Sym    2.7962 eV  443.41 nm  f=0.0225
<S**2>=0.864
    166A ->173A        0.11577
    168A ->173A        0.35732
    169A ->174A        0.14196
    172A ->178A        0.27413
    166B ->172B        0.18648
    168B ->174B        0.77881

 Excited state symmetry could not be determined.
 Excited State  31:  2.086-?Sym    2.8530 eV  434.58 nm  f=0.0028
<S**2>=0.838
    158A ->174A       -0.10183
    159A ->173A       -0.11131
    166A ->173A        0.15786
    167A ->174A        0.54370
    169A ->174A       -0.30591
    166B ->172B        0.31188
    167B ->173B        0.59392
    169B ->173B       -0.16295

 Excited state symmetry could not be determined.
 Excited State  32:  3.291-?Sym    2.9164 eV  425.13 nm  f=0.0021
<S**2>=2.458
    162A ->173A       -0.14044
    166A ->173A       -0.20390
    167A ->174A       -0.16858
    168A ->173A        0.13715
    169A ->174A        0.15139
    170A ->177A       -0.26332
    171A ->177A        0.30208
    172A ->178A       -0.20219
    158B ->172B        0.11210
    162B ->172B        0.15137
    166B ->172B        0.42320
```

```
    168B ->172B       -0.13662
    170B ->177B       -0.29583
    170B ->188B       -0.11743
    171B ->177B       -0.35853

 Excited state symmetry could not be determined.
 Excited State  33:  2.314-?Sym    2.9264 eV  423.67 nm  f=0.0029
<S**2>=1.089
    166A ->174A       -0.11160
    168A ->174A       -0.36715
    165B ->172B        0.13213
    166B ->173B        0.19269
    167B ->174B        0.60351
    168B ->173B       -0.49075
    169B ->174B       -0.28412

 Excited state symmetry could not be determined.
 Excited State  34:  3.171-?Sym    2.9357 eV  422.33 nm  f=0.0113
<S**2>=2.264
    162A ->173A       -0.12590
    165A ->174A       -0.12561
    166A ->173A       -0.14562
    167A ->174A       -0.23057
    169A ->174A        0.17093
    170A ->177A        0.18950
    171A ->177A       -0.24432
    172A ->178A        0.17793
    158B ->172B        0.13711
    162B ->172B        0.18740
    163B ->173B        0.12891
    166B ->172B        0.49960
    168B ->172B       -0.15538
    168B ->174B       -0.19651
    170B ->177B        0.25130
    170B ->188B        0.10197
    171B ->177B        0.31937

 Excited state symmetry could not be determined.
 Excited State  35:  3.368-?Sym    2.9577 eV  419.19 nm  f=0.0000
<S**2>=2.585
    158A ->173A       -0.13737
    159A ->174A       -0.15755
    160A ->174A        0.25615
    161A ->173A       -0.45523
    166A ->174A       -0.13108
    167A ->173A       -0.23991
    168A ->174A        0.16817
    169A ->173A        0.18898
    154B ->172B        0.10390
    158B ->173B        0.15282
```

```
    159B ->172B       -0.14956
    160B ->173B       -0.24654
    161B ->172B        0.46844
    164B ->173B       -0.10802
    165B ->172B       -0.11312
    166B ->173B        0.17903
    167B ->172B        0.22026
    167B ->174B       -0.13352

 Excited state symmetry could not be determined.
 Excited State  36:  2.537-?Sym    2.9683 eV  417.69 nm  f=0.0216
<S**2>=1.359
    158A ->174A        0.10395
    159A ->173A        0.17958
    160A ->173A       -0.19963
    161A ->174A        0.13509
    162A ->173A        0.13742
    166A ->173A        0.61634
    168A ->173A       -0.21061
    160B ->172B        0.17838
    161B ->173B       -0.10983
    164B ->172B        0.10015
    166B ->172B        0.40202
    166B ->174B       -0.19236
    167B ->173B       -0.31996
    169B ->173B        0.12228

 Excited state symmetry could not be determined.
 Excited State  37:  3.318-?Sym    3.0081 eV  412.16 nm  f=0.0046
<S**2>=2.503
    160A ->173A        0.35352
    161A ->174A       -0.21752
    163A ->173A        0.21289
    165A ->174A        0.14368
    166A ->173A        0.44080
    167A ->174A       -0.29338
    168A ->173A       -0.16526
    169A ->174A        0.19060
    160B ->172B       -0.37246
    161B ->173B        0.21568
    164B ->172B       -0.37532
    165B ->173B       -0.13901
    167B ->173B        0.17230

 Excited state symmetry could not be determined.
 Excited State  38:  3.411-?Sym    3.0098 eV  411.93 nm  f=0.0002
<S**2>=2.659
    168A ->178A       -0.11171
    170A ->178A        0.29517
    170A ->181A        0.10226
```

```
    170A ->185A        0.14642
    170A ->188A        0.10817
    171A ->178A       -0.36501
    171A ->181A       -0.12329
    171A ->185A       -0.17484
    171A ->188A       -0.12263
    172A ->177A        0.10281
    168B ->173B        0.13431
    168B ->178B        0.12874
    170B ->178B        0.32972
    170B ->179B        0.11829
    170B ->181B        0.15984
    170B ->185B        0.16242
    170B ->187B        0.16299
    171B ->178B        0.38305
    171B ->179B        0.13621
    171B ->181B        0.17924
    171B ->185B        0.16676
    171B ->187B        0.15813

 Excited state symmetry could not be determined.
 Excited State  39:  3.341-?Sym    3.0274 eV  409.54 nm  f=0.0008
<S**2>=2.541
    159A ->174A       -0.13034
    161A ->173A        0.22627
    165A ->173A       -0.29713
    166A ->174A       -0.34483
    168A ->174A        0.25223
    158B ->173B        0.12207
    159B ->172B       -0.11379
    161B ->172B       -0.22450
    165B ->172B        0.44417
    166B ->173B        0.45538
    167B ->174B       -0.24188
    168B ->173B       -0.15538

 Excited state symmetry could not be determined.
 Excited State  40:  2.168-?Sym    3.0449 eV  407.18 nm  f=0.0063
<S**2>=0.925
    165A ->173A       -0.46187
    166A ->174A       -0.33597
    167A ->173A        0.21783
    168A ->174A        0.34330
    165B ->172B       -0.35607
    166B ->173B       -0.14373
    167B ->172B        0.10726
    167B ->174B        0.47726
    168B ->173B        0.19800

 Excited state symmetry could not be determined.
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 Excited State  41:  2.828-?Sym    3.0494 eV  406.58 nm  f=0.0019
<S**2>=1.749
    160A ->173A        0.26184
    161A ->174A       -0.18277
    165A ->174A        0.13432
    160B ->172B       -0.21837
    161B ->173B        0.16671
    163B ->173B       -0.22557
    164B ->172B        0.80809
    165B ->173B        0.14001

 Excited state symmetry could not be determined.
 Excited State  42:  2.736-?Sym    3.0544 eV  405.92 nm  f=0.0070
<S**2>=1.621
    160A ->174A        0.10640
    161A ->173A       -0.25613
    168A ->174A        0.18379
    161B ->172B        0.16800
    163B ->172B       -0.24628
    164B ->173B        0.27433
    165B ->172B        0.68883
    166B ->173B       -0.20715
    167B ->174B        0.25932
    168B ->173B        0.22943

 Excited state symmetry could not be determined.
 Excited State  43:  2.872-?Sym    3.0748 eV  403.22 nm  f=0.0021
<S**2>=1.812
    159A ->173A       -0.10511
    161A ->174A        0.11535
    162A ->173A        0.20155
    163A ->173A        0.76366
    164A ->174A       -0.37618
    169A ->174A        0.10398
    160B ->172B        0.14174
    161B ->173B       -0.10990
    162B ->172B       -0.15550
    163B ->173B        0.15745
    164B ->172B        0.16040
    165B ->173B        0.14389

 Excited state symmetry could not be determined.
 Excited State  44:  2.505-?Sym    3.0870 eV  401.63 nm  f=0.0414
<S**2>=1.318
    159A ->174A       -0.11555
    162A ->174A       -0.10718
    163A ->174A        0.16238
    165A ->173A        0.57197
    166A ->174A       -0.14514
    168A ->174A        0.22446
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    161B ->172B       -0.18168
    162B ->173B       -0.15852
    163B ->172B        0.58966
    164B ->173B       -0.14031
    167B ->174B        0.24117
    168B ->173B        0.13688

 Excited state symmetry could not be determined.
 Excited State  45:  2.515-?Sym    3.0926 eV  400.91 nm  f=0.0095
<S**2>=1.331
    161A ->173A       -0.11622
    162A ->174A       -0.10137
    163A ->174A       -0.36564
    164A ->173A        0.77648
    165A ->173A       -0.19460
    166A ->174A        0.11896
    161B ->172B        0.13455
    163B ->172B        0.34662

 Excited state symmetry could not be determined.
 Excited State  46:  3.358-?Sym    3.1144 eV  398.10 nm  f=0.0024
<S**2>=2.568
    160A ->173A       -0.19770
    162A ->173A       -0.38773
    163A ->173A        0.35396
    165A ->174A        0.35845
    167A ->174A       -0.11130
    160B ->172B        0.22272
    162B ->172B        0.47956
    163B ->173B       -0.29795
    165B ->173B       -0.24226

 Excited state symmetry could not be determined.
 Excited State  47:  2.303-?Sym    3.1187 eV  397.54 nm  f=0.0136
<S**2>=1.075
    160A ->173A       -0.10863
    162A ->173A       -0.22624
    164A ->174A        0.10656
    165A ->174A        0.12695
    166A ->173A        0.19947
    170A ->177A        0.11888
    172A ->185A       -0.14672
    158B ->172B        0.10779
    162B ->172B       -0.20721
    162B ->174B        0.20670
    163B ->173B        0.11628
    166B ->172B        0.11766
    166B ->174B        0.75232

 Excited state symmetry could not be determined.
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 Excited State  48:  2.054-?Sym    3.1588 eV  392.50 nm  f=0.0165
<S**2>=0.805
    162A ->173A        0.52589
    164A ->174A       -0.18042
    165A ->174A       -0.35125
    162B ->172B        0.47986
    162B ->174B        0.10104
    163B ->173B       -0.32746
    165B ->173B       -0.24202
    166B ->174B        0.31219

 Excited state symmetry could not be determined.
 Excited State  49:  2.340-?Sym    3.1633 eV  391.95 nm  f=0.0035
<S**2>=1.119
    162A ->174A       -0.24811
    163A ->174A       -0.12384
    166A ->174A        0.54176
    168A ->174A        0.16162
    162B ->173B        0.14900
    163B ->172B       -0.15779
    166B ->173B        0.53880
    167B ->174B        0.21646
    169B ->174B        0.11921
    170B ->176B       -0.10069
    171B ->176B       -0.28737

 Excited state symmetry could not be determined.
 Excited State  50:  3.320-?Sym    3.1772 eV  390.24 nm  f=0.0000
<S**2>=2.505
    157A ->173A       -0.10370
    158A ->173A        0.17866
    159A ->174A        0.19468
    161A ->173A       -0.15316
    162A ->174A        0.43750
    164A ->173A       -0.25903
    165A ->173A       -0.18803
    167A ->173A        0.15001
    154B ->172B       -0.11597
    158B ->173B       -0.16121
    159B ->172B        0.16640
    161B ->172B        0.18867
    162B ->173B       -0.42252
    163B ->172B        0.29230
    166B ->173B        0.34035
    167B ->172B       -0.10830

 Excited state symmetry could not be determined.
 Excited State  51:  3.384-?Sym    3.1980 eV  387.69 nm  f=0.0007
<S**2>=2.613
    157A ->173A        0.13184
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    158A ->173A       -0.10332
    159A ->174A       -0.17533
    161A ->173A        0.15572
    162A ->174A        0.24766
    163A ->174A        0.25728
    164A ->173A        0.16454
    165A ->173A       -0.21182
    166A ->174A        0.42052
    168A ->174A       -0.17758
    169A ->173A        0.15806
    154B ->172B        0.11333
    156B ->173B        0.10112
    158B ->173B        0.17217
    159B ->172B       -0.15659
    162B ->173B       -0.29018
    164B ->173B       -0.33642
    165B ->172B        0.18683
    166B ->173B       -0.15056
    167B ->172B        0.14748
    167B ->174B        0.10498
    168B ->173B        0.17414

 Excited state symmetry could not be determined.
 Excited State  52:  3.429-?Sym    3.2151 eV  385.63 nm  f=0.0003
<S**2>=2.690
    157A ->174A       -0.12959
    158A ->174A        0.21073
    159A ->173A        0.32648
    160A ->173A        0.18293
    161A ->174A       -0.11227
    162A ->173A       -0.15292
    163A ->173A        0.18819
    164A ->174A       -0.19936
    165A ->174A        0.11773
    166A ->173A       -0.17616
    167A ->174A        0.20758
    169A ->174A       -0.19014
    154B ->173B       -0.15674
    155B ->172B        0.15924
    156B ->172B       -0.12337
    158B ->172B       -0.31933
    159B ->173B        0.22865
    160B ->172B       -0.14085
    163B ->173B        0.13121
    164B ->172B       -0.17354
    166B ->172B        0.15104
    166B ->174B        0.12725
    167B ->173B       -0.24620
    171B ->175B        0.10368
```

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 Excited state symmetry could not be determined.
 Excited State  53:  2.018-?Sym    3.2422 eV  382.41 nm  f=0.0069
<S**2>=0.768
    160A ->174A       -0.13518
    161A ->173A        0.65815
    161B ->172B        0.67692

 Excited state symmetry could not be determined.
 Excited State  54:  2.728-?Sym    3.2452 eV  382.06 nm  f=0.0660
<S**2>=1.611
    162A ->173A       -0.13207
    164A ->174A       -0.19485
    165A ->174A       -0.27870
    160B ->172B        0.10535
    162B ->172B       -0.28330
    163B ->173B       -0.15333
    165B ->173B       -0.14424
    171B ->175B        0.80514

 Excited state symmetry could not be determined.
 Excited State  55:  2.797-?Sym    3.2702 eV  379.13 nm  f=0.0049
<S**2>=1.706
    160A ->173A       -0.13296
    160B ->172B       -0.19246
    162B ->172B        0.11365
    163B ->173B       -0.32776
    164B ->172B       -0.25126
    164B ->174B        0.17183
    165B ->173B        0.81319
    171B ->175B        0.19041

 Excited state symmetry could not be determined.
 Excited State  56:  2.127-?Sym    3.2704 eV  379.11 nm  f=0.0194
<S**2>=0.881
    159A ->174A       -0.10438
    161A ->173A        0.16819
    162A ->174A        0.11084
    163A ->174A        0.47601
    164A ->173A        0.18141
    161B ->172B        0.11882
    163B ->172B        0.15327
    164B ->173B        0.73406
    165B ->172B       -0.17546
    165B ->174B        0.12876

 Excited state symmetry could not be determined.
 Excited State  57:  2.449-?Sym    3.2765 eV  378.41 nm  f=0.0008
<S**2>=1.250
    160A ->173A        0.56999
    161A ->174A       -0.16200
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    163A ->173A        0.12718
    164A ->174A        0.30729
    165A ->174A       -0.30961
    160B ->172B        0.53903
    161B ->173B       -0.15954
    163B ->173B       -0.12989
    164B ->172B       -0.10574
    165B ->173B        0.14706
    171B ->175B       -0.14178

 Excited state symmetry could not be determined.
 Excited State  58:  2.502-?Sym    3.2901 eV  376.84 nm  f=0.0000
<S**2>=1.316
    160A ->173A       -0.23766
    161A ->174A        0.15491
    162A ->173A       -0.15210
    163A ->173A        0.33591
    164A ->174A        0.59404
    165A ->174A       -0.50214
    167A ->174A        0.10199
    160B ->172B       -0.33875
    165B ->173B       -0.12727

 Excited state symmetry could not be determined.
 Excited State  59:  3.274-?Sym    3.3054 eV  375.10 nm  f=0.0082
<S**2>=2.430
    158A ->173A        0.18774
    162A ->174A       -0.13295
    163A ->174A        0.62362
    164A ->173A        0.21425
    172A ->183A        0.11986
    155B ->173B        0.13186
    158B ->173B       -0.12476
    159B ->172B        0.22858
    162B ->173B        0.37910
    164B ->173B       -0.35646
    165B ->174B       -0.12676

 Excited state symmetry could not be determined.
 Excited State  60:  3.124-?Sym    3.3189 eV  373.57 nm  f=0.0019
<S**2>=2.190
    156A ->174A       -0.12290
    158A ->173A        0.12956
    162A ->174A       -0.15041
    168A ->174A        0.13643
    171A ->176A       -0.24128
    172A ->183A       -0.13474
    155B ->173B        0.11027
    157B ->172B       -0.16134
    163B ->172B       -0.11660
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    166B ->173B        0.14223
    168B ->176B        0.10439
    171B ->176B        0.77580

 Excited state symmetry could not be determined.
 Excited State  61:  2.405-?Sym    3.3277 eV  372.58 nm  f=0.3825
<S**2>=1.197
    159A ->173A       -0.10331
    162A ->173A        0.38316
    164A ->174A        0.32645
    165A ->174A        0.21511
    171A ->175A       -0.19870
    172A ->181A        0.10044
    160B ->172B        0.12714
    162B ->172B        0.24886
    163B ->173B        0.54171
    171B ->175B        0.38245

 Excited state symmetry could not be determined.
 Excited State  62:  2.285-?Sym    3.3498 eV  370.13 nm  f=0.0514
<S**2>=1.055
    162A ->174A        0.60706
    163A ->174A       -0.24195
    165A ->173A        0.15229
    172A ->182A       -0.15182
    172A ->183A        0.29434
    172A ->186A       -0.13323
    162B ->173B        0.50028
    165B ->174B       -0.13953
    171B ->176B        0.15671

 Excited state symmetry could not be determined.
 Excited State  63:  2.172-?Sym    3.3542 eV  369.64 nm  f=0.0974
<S**2>=0.929
    162A ->174A       -0.29908
    172A ->177A        0.13703
    172A ->180A        0.12688
    172A ->182A       -0.32908
    172A ->183A        0.57872
    172A ->186A       -0.22797
    172A ->187A       -0.17788
    162B ->173B       -0.35340
    164B ->173B        0.19240
    165B ->172B       -0.10310
    165B ->174B       -0.23086

 Excited state symmetry could not be determined.
 Excited State  64:  3.361-?Sym    3.3806 eV  366.75 nm  f=0.0030
<S**2>=2.573
    156A ->173A       -0.19045
```

```
    157A ->174A        0.14592
    158A ->174A        0.11158
    160A ->173A        0.39075
    161A ->174A        0.59849
    165A ->174A        0.14961
    155B ->172B        0.14407
    156B ->172B        0.13468
    157B ->173B       -0.16512
    160B ->172B       -0.23720
    161B ->173B       -0.37610
    171B ->175B        0.14848

 Excited state symmetry could not be determined.
 Excited State  65:  3.336-?Sym    3.4006 eV  364.60 nm  f=0.0009
<S**2>=2.532
    156A ->174A       -0.24942
    157A ->173A        0.25549
    158A ->173A        0.25135
    160A ->174A        0.40633
    161A ->173A        0.14971
    163A ->174A       -0.13407
    155B ->173B        0.18175
    156B ->173B        0.16993
    157B ->172B       -0.31758
    159B ->172B        0.13813
    160B ->173B       -0.35110
    161B ->172B       -0.13354
    164B ->173B        0.10800
    171B ->176B       -0.36104

 Excited state symmetry could not be determined.
 Excited State  66:  2.620-?Sym    3.4062 eV  364.00 nm  f=0.0707
<S**2>=1.466
    161A ->174A       -0.17856
    170A ->177A       -0.28539
    171A ->186A        0.10146
    172A ->181A       -0.33732
    172A ->184A       -0.11373
    172A ->185A        0.40029
    172A ->188A        0.12784
    164B ->174B       -0.37176
    166B ->174B        0.26900
    168B ->177B        0.12899
    170B ->177B       -0.13955
    171B ->177B        0.35660

 Excited state symmetry could not be determined.
 Excited State  67:  2.109-?Sym    3.4257 eV  361.92 nm  f=0.0035
<S**2>=0.862
    160A ->173A        0.18088
```

```
    161A ->174A        0.57491
    172A ->181A       -0.12782
    160B ->172B        0.22876
    161B ->173B        0.69426

 Excited state symmetry could not be determined.
 Excited State  68:  2.429-?Sym    3.4325 eV  361.20 nm  f=0.0058
<S**2>=1.225
    170A ->177A       -0.21292
    172A ->184A        0.20781
    172A ->185A        0.11488
    164B ->174B        0.80448
    165B ->173B       -0.14745
    166B ->174B        0.21513
    171B ->177B        0.23642

 Excited state symmetry could not be determined.
 Excited State  69:  2.369-?Sym    3.4463 eV  359.76 nm  f=0.0041
<S**2>=1.153
    160A ->174A       -0.32267
    161A ->173A       -0.11127
    172A ->180A        0.19135
    172A ->183A        0.12125
    172A ->186A       -0.14280
    163B ->174B       -0.32753
    165B ->174B        0.76887

 Excited state symmetry could not be determined.
 Excited State  70:  3.060-?Sym    3.4489 eV  359.49 nm  f=0.0043
<S**2>=2.092
    156A ->174A        0.17316
    157A ->173A       -0.20394
    158A ->173A       -0.14890
    160A ->174A        0.66571
    161A ->173A        0.27524
    172A ->180A        0.20590
    156B ->173B       -0.14027
    157B ->172B        0.24465
    158B ->173B       -0.12523
    160B ->173B       -0.12012
    161B ->172B       -0.14341
    164B ->173B       -0.12171
    165B ->174B        0.29099
    171B ->176B        0.12905

 Excited state symmetry could not be determined.
 Excited State  71:  2.888-?Sym    3.4589 eV  358.45 nm  f=0.0332
<S**2>=1.835
    156A ->173A       -0.24562
    157A ->174A        0.15231
```

```
    158A ->174A        0.17461
    160A ->173A       -0.11721
    161A ->174A       -0.14260
    170A ->177A       -0.15143
    171A ->175A        0.13514
    171A ->177A        0.13662
    172A ->179A        0.23639
    172A ->181A        0.38730
    172A ->185A       -0.19270
    172A ->188A       -0.11641
    155B ->172B        0.19625
    156B ->172B        0.14346
    157B ->173B       -0.21044
    160B ->172B        0.18487
    161B ->173B        0.37915
    163B ->173B       -0.11820
    164B ->174B       -0.17325
    171B ->177B        0.21382

 Excited state symmetry could not be determined.
 Excited State  72:  2.380-?Sym    3.4742 eV  356.87 nm  f=0.0058
<S**2>=1.167
    157A ->173A        0.14116
    159A ->174A       -0.13889
    160A ->174A        0.33481
    160B ->173B        0.83329
    161B ->172B        0.22435

 Excited state symmetry could not be determined.
 Excited State  73:  2.803-?Sym    3.4862 eV  355.65 nm  f=0.0506
<S**2>=1.714
    156A ->173A        0.21885
    157A ->174A       -0.18882
    158A ->174A       -0.12545
    159A ->173A        0.12983
    161A ->174A        0.15183
    164A ->174A       -0.10126
    170A ->177A       -0.28135
    171A ->177A        0.25867
    172A ->181A        0.20419
    172A ->184A        0.10906
    172A ->185A       -0.28616
    155B ->172B       -0.16720
    156B ->172B       -0.16992
    157B ->173B        0.19537
    160B ->172B       -0.10104
    161B ->173B       -0.16382
    164B ->174B       -0.13073
    169B ->178B        0.15823
    171B ->175B       -0.15586
```

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    171B ->177B        0.36042

 Excited state symmetry could not be determined.
 Excited State  74:  2.257-?Sym    3.5018 eV  354.06 nm  f=0.0153
<S**2>=1.024
    156A ->173A        0.12846
    157A ->174A       -0.10142
    172A ->178A       -0.39442
    172A ->179A        0.74140
    172A ->181A        0.28260
    172A ->185A        0.23799
    155B ->172B       -0.10332
    161B ->173B       -0.10946

 Excited state symmetry could not be determined.
 Excited State  75:  2.139-?Sym    3.5092 eV  353.31 nm  f=0.0016
<S**2>=0.894
    172A ->177A       -0.14438
    172A ->180A        0.89416
    172A ->183A       -0.23335
    165B ->174B       -0.22204

 Excited state symmetry could not be determined.
 Excited State  76:  2.238-?Sym    3.5239 eV  351.84 nm  f=0.0027
<S**2>=1.002
    168A ->178A        0.11095
    170A ->178A       -0.28726
    170A ->185A       -0.12246
    171A ->176A       -0.10381
    171A ->178A        0.41875
    171A ->179A        0.10941
    171A ->181A        0.13072
    171A ->185A        0.18564
    171A ->188A        0.12517
    160B ->173B       -0.12748
    167B ->177B        0.10410
    168B ->178B        0.14221
    169B ->177B        0.31988
    169B ->188B        0.10048
    170B ->178B        0.13742
    171B ->178B        0.41701
    171B ->179B        0.14738
    171B ->181B        0.18574
    171B ->185B        0.11896
    171B ->187B        0.11630

 Excited state symmetry could not be determined.
 Excited State  77:  2.620-?Sym    3.5419 eV  350.05 nm  f=0.0001
<S**2>=1.466
    159A ->173A       -0.15076
```

```
    168A ->177A        0.20483
    171A ->175A        0.29075
    171A ->177A        0.43388
    171A ->186A        0.11951
    172A ->179A        0.10424
    172A ->181A       -0.26247
    172A ->184A       -0.34155
    172A ->189A        0.11730
    164B ->174B        0.16631
    168B ->177B       -0.13021
    169B ->178B        0.13128
    169B ->185B        0.10367
    170B ->177B        0.36197
    170B ->188B        0.10804
    171B ->177B        0.11260

 Excited state symmetry could not be determined.
 Excited State  78:  2.405-?Sym    3.5863 eV  345.72 nm  f=0.0019
<S**2>=1.196
    156A ->173A        0.10914
    158A ->174A       -0.14526
    159A ->173A       -0.16834
    171A ->175A        0.44605
    172A ->178A       -0.15135
    172A ->179A       -0.35889
    172A ->181A        0.45712
    172A ->184A        0.30367
    172A ->185A        0.25458
    158B ->172B       -0.18329
    164B ->174B       -0.14465

 Excited state symmetry could not be determined.
 Excited State  79:  2.506-?Sym    3.6019 eV  344.22 nm  f=0.0084
<S**2>=1.320
    156A ->173A        0.11632
    158A ->174A       -0.20470
    159A ->173A       -0.22560
    168A ->177A       -0.16441
    171A ->175A        0.41683
    171A ->177A       -0.23500
    172A ->178A        0.14051
    172A ->179A        0.22382
    172A ->181A       -0.18410
    172A ->184A       -0.11383
    172A ->185A       -0.27710
    154B ->173B       -0.12346
    156B ->172B       -0.15232
    158B ->172B       -0.34194
    159B ->173B        0.14112
    162B ->174B        0.11034
```

```
    168B ->177B        0.11995
    170B ->177B       -0.22240

 Excited state symmetry could not be determined.
 Excited State  80:  2.126-?Sym    3.6097 eV  343.47 nm  f=0.0002
<S**2>=0.880
    171A ->176A       -0.11666
    163B ->174B        0.87030
    165B ->174B        0.34513
```

Table S41. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 3^{2+} (*S*=0)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:      Singlet-?Sym    1.6577 eV  747.91 nm
f=0.0295  <S**2>=0.000
     170 ->172        -0.27036
     171 ->172         0.63317
 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 symmetry could not be determined.
 Excited State   2:      Singlet-?Sym    1.9952 eV  621.40 nm
f=0.0556  <S**2>=0.000
     170 ->172        -0.34594
     170 ->173        -0.22588
     171 ->172        -0.21011
     171 ->173         0.50266

 Excited state symmetry could not be determined.
 Excited State   3:      Singlet-?Sym    2.0248 eV  612.33 nm
f=0.0153  <S**2>=0.000
     170 ->174        -0.30400
     171 ->174         0.61756

 Excited state symmetry could not be determined.
 Excited State   4:      Singlet-?Sym    2.0330 eV  609.85 nm
f=0.0258  <S**2>=0.000
     163 ->172         0.11776
     170 ->172         0.49239
     171 ->172         0.15918
     171 ->173         0.42404

 Excited state symmetry could not be determined.
 Excited State   5:      Singlet-?Sym    2.4239 eV  511.52 nm
f=0.0277  <S**2>=0.000
     167 ->173        -0.10043
     170 ->172        -0.12124
     170 ->173         0.62908
     171 ->173         0.21244

 Excited state symmetry could not be determined.
 Excited State   6:      Singlet-?Sym    2.5204 eV  491.93 nm
f=0.0275  <S**2>=0.000
     166 ->172        -0.20523
     166 ->173        -0.11205
     170 ->174         0.57676
```

```
     171 ->174         0.28498

 Excited state symmetry could not be determined.
 Excited State   7:      Singlet-?Sym    2.5617 eV  483.99 nm
f=0.0310  <S**2>=0.000
     166 ->172        -0.32831
     169 ->172         0.59729
     170 ->174        -0.11566

 Excited state symmetry could not be determined.
 Excited State   8:      Singlet-?Sym    2.5632 eV  483.71 nm
f=0.1002  <S**2>=0.000
     161 ->172         0.21568
     163 ->172         0.29292
     165 ->172         0.50757
     167 ->172         0.15699
     168 ->174         0.10244
     170 ->172        -0.11073
     171 ->172        -0.15985

 Excited state symmetry could not be determined.
 Excited State   9:      Singlet-?Sym    2.5909 eV  478.54 nm
f=0.0931  <S**2>=0.000
     166 ->172         0.43447
     166 ->173        -0.20499
     168 ->172        -0.16691
     168 ->173         0.24183
     169 ->172         0.27447
     169 ->173        -0.29444

 Excited state symmetry could not be determined.
 Excited State  10:      Singlet-?Sym    2.6568 eV  466.67 nm
f=0.0087  <S**2>=0.000
     165 ->172         0.18136
     166 ->174         0.32179
     168 ->174        -0.34658
     169 ->174         0.45515

 Excited state symmetry could not be determined.
 Excited State  11:      Singlet-?Sym    2.6820 eV  462.29 nm
f=0.0067  <S**2>=0.000
     166 ->172         0.28408
     168 ->172         0.59474
     169 ->172         0.15793
     169 ->173         0.13198

 Excited state symmetry could not be determined.
 Excited State  12:      Singlet-?Sym    2.6931 eV  460.38 nm
f=0.0158  <S**2>=0.000
     160 ->172         0.10095
```

```
     161 ->172         0.16863
     163 ->172         0.12296
     165 ->172        -0.30764
     167 ->172         0.58277

 Excited state symmetry could not be determined.
 Excited State  13:      Singlet-?Sym    2.7138 eV  456.87 nm
f=0.0521  <S**2>=0.000
     162 ->172        -0.12648
     163 ->174        -0.11934
     164 ->172        -0.21924
     165 ->174        -0.11006
     166 ->172         0.20296
     166 ->173         0.11695
     168 ->172        -0.28209
     168 ->173        -0.19781
     169 ->173         0.41810
     170 ->174         0.12179
     171 ->174         0.12389

 Excited state symmetry could not be determined.
 Excited State  14:      Singlet-?Sym    2.7657 eV  448.30 nm
f=0.0057  <S**2>=0.000
     161 ->172         0.28534
     163 ->172         0.43608
     165 ->172        -0.30099
     167 ->172        -0.32882
     170 ->172        -0.14552

 Excited state symmetry could not be determined.
 Excited State  15:      Singlet-?Sym    2.7792 eV  446.12 nm
f=0.0737  <S**2>=0.000
     162 ->172         0.29106
     164 ->172         0.57526
     168 ->172        -0.11980
     169 ->172         0.12561
     169 ->173         0.16804

 Excited state symmetry could not be determined.
 Excited State  16:      Singlet-?Sym    2.8999 eV  427.55 nm
f=0.0013  <S**2>=0.000
     162 ->172         0.14617
     164 ->173         0.12658
     166 ->173         0.43167
     167 ->174         0.13023
     168 ->173        -0.28971
     169 ->173        -0.35949

 Excited state symmetry could not be determined.
```

```
 Excited State  17:      Singlet-?Sym    2.9282 eV  423.41 nm
f=0.0228  <S**2>=0.000
     160 ->172        -0.25719
     163 ->173        -0.19597
     165 ->173        -0.12146
     166 ->174        -0.27558
     167 ->173        -0.31330
     168 ->174         0.26244
     169 ->174         0.32065

 Excited state symmetry could not be determined.
 Excited State  18:      Singlet-?Sym    2.9366 eV  422.21 nm
f=0.0001  <S**2>=0.000
     160 ->172         0.62711
     163 ->173        -0.11851
     165 ->173        -0.11944
     166 ->174        -0.11577
     169 ->174         0.13916

 Excited state symmetry could not be determined.
 Excited State  19:      Singlet-?Sym    2.9449 eV  421.02 nm
f=0.0046  <S**2>=0.000
     162 ->172         0.58682
     164 ->172        -0.31876
     168 ->173         0.12647
     169 ->173         0.10086

 Excited state symmetry could not be determined.
 Excited State  20:      Singlet-?Sym    2.9803 eV  416.01 nm
f=0.0060  <S**2>=0.000
     161 ->172         0.50508
     163 ->172        -0.37826
     163 ->173         0.19793
     167 ->173        -0.14231
     168 ->174         0.12443
     169 ->174         0.11862

 Excited state symmetry could not be determined.
 Excited State  21:      Singlet-?Sym    2.9835 eV  415.56 nm
f=0.0128  <S**2>=0.000
     162 ->172        -0.10383
     166 ->173         0.41356
     167 ->174        -0.24776
     168 ->173         0.46156

 Excited state symmetry could not be determined.
 Excited State  22:      Singlet-?Sym    2.9935 eV  414.18 nm
f=0.0793  <S**2>=0.000
     161 ->172        -0.19230
     161 ->173         0.22175
```

```
     163 ->172         0.11966
     163 ->173         0.29878
     165 ->173         0.40890
     167 ->173        -0.28715
     169 ->174         0.10207
     170 ->173        -0.10991

 Excited state symmetry could not be determined.
 Excited State  23:      Singlet-?Sym    3.0241 eV  409.98 nm
f=0.0140  <S**2>=0.000
     164 ->174         0.13574
     165 ->173        -0.33694
     166 ->174         0.40399
     167 ->173        -0.24831
     168 ->174         0.26879
     169 ->174        -0.16078

 Excited state symmetry could not be determined.
 Excited State  24:      Singlet-?Sym    3.0913 eV  401.07 nm
f=0.0039  <S**2>=0.000
     162 ->172        -0.11019
     162 ->173        -0.43806
     163 ->174         0.14088
     164 ->173         0.49246
     166 ->173        -0.12011

 Excited state symmetry could not be determined.
 Excited State  25:      Singlet-?Sym    3.0950 eV  400.59 nm
f=0.0506  <S**2>=0.000
     161 ->172        -0.13752
     161 ->173        -0.24639
     162 ->174        -0.12478
     163 ->173         0.47190
     164 ->174         0.14743
     165 ->173        -0.13390
     166 ->174        -0.12670
     167 ->173         0.25250
     168 ->174         0.10197
     169 ->174         0.20472

 Excited state symmetry could not be determined.
 Excited State  26:      Singlet-?Sym    3.1229 eV  397.01 nm
f=0.1130  <S**2>=0.000
     161 ->174        -0.11973
     162 ->173        -0.23898
     164 ->173        -0.21781
     165 ->174         0.24871
     166 ->173         0.15691
     167 ->174         0.47240
     168 ->173         0.17438
```

```
     169 ->173         0.13470
     170 ->174         0.12527

 Excited state symmetry could not be determined.
 Excited State  27:      Singlet-?Sym    3.1382 eV  395.08 nm
f=0.0307  <S**2>=0.000
     162 ->173         0.38782
     164 ->173         0.25058
     165 ->174        -0.28844
     167 ->174         0.38460
     168 ->173         0.17312

 Excited state symmetry could not be determined.
 Excited State  28:      Singlet-?Sym    3.1413 eV  394.69 nm
f=0.0516  <S**2>=0.000
     161 ->173         0.37049
     162 ->174         0.29941
     163 ->173         0.20806
     165 ->173        -0.33370
     166 ->174        -0.23083
     168 ->174        -0.21816

 Excited state symmetry could not be determined.
 Excited State  29:      Singlet-?Sym    3.2093 eV  386.33 nm
f=0.0132  <S**2>=0.000
     161 ->173         0.32879
     162 ->174        -0.37745
     163 ->173        -0.12455
     164 ->174         0.47332

 Excited state symmetry could not be determined.
 Excited State  30:      Singlet-?Sym    3.2195 eV  385.11 nm
f=0.4717  <S**2>=0.000
     160 ->173         0.11445
     161 ->173         0.30266
     162 ->174         0.16431
     164 ->174        -0.14926
     166 ->174         0.16705
     167 ->173         0.36757
     168 ->174         0.34373
     169 ->174         0.18953

 Excited state symmetry could not be determined.
 Excited State  31:      Singlet-?Sym    3.2269 eV  384.22 nm
f=0.0093  <S**2>=0.000
     161 ->174        -0.28953
     163 ->174         0.58665
     164 ->173        -0.16799
     168 ->173        -0.10843
```

```
 Excited state symmetry could not be determined.
 Excited State  32:      Singlet-?Sym    3.2583 eV  380.52 nm
f=0.0002  <S**2>=0.000
     162 ->173         0.25924
     163 ->174         0.11656
     164 ->173         0.27883
     165 ->174         0.52686

 Excited state symmetry could not be determined.
 Excited State  33:      Singlet-?Sym    3.3144 eV  374.08 nm
f=0.0288  <S**2>=0.000
     161 ->173        -0.15020
     162 ->174         0.46461
     164 ->174         0.43558
     165 ->173         0.21611
     168 ->174         0.10757

 Excited state symmetry could not be determined.
 Excited State  34:      Singlet-?Sym    3.3357 eV  371.69 nm
f=0.0030  <S**2>=0.000
     161 ->174         0.59030
     162 ->173        -0.11673
     163 ->174         0.21114
     164 ->173        -0.10409
     165 ->174        -0.12768

 Excited state symmetry could not be determined.
 Excited State  35:      Singlet-?Sym    3.4102 eV  363.57 nm
f=0.0768  <S**2>=0.000
     158 ->173         0.16907
     160 ->173         0.63213
     161 ->173        -0.10842

 Excited state symmetry could not be determined.
 Excited State  36:      Singlet-?Sym    3.4961 eV  354.63 nm
f=0.0225  <S**2>=0.000
     157 ->173        -0.14772
     158 ->174         0.17919
     159 ->173         0.11590
     160 ->174         0.62909

 Excited state symmetry could not be determined.
 Excited State  37:      Singlet-?Sym    3.5077 eV  353.47 nm
f=0.0048  <S**2>=0.000
     161 ->174         0.10115
     165 ->178         0.13011
     166 ->177         0.11114
     167 ->178         0.13123
     169 ->177         0.11054
     170 ->178        -0.27969
```

```
     171 ->178         0.48456
     171 ->181         0.10100

 Excited state symmetry could not be determined.
 Excited State  38:      Singlet-?Sym    3.5667 eV  347.62 nm
f=0.0001  <S**2>=0.000
     160 ->177        -0.12455
     166 ->178         0.13494
     167 ->177         0.12324
     168 ->178        -0.10985
     169 ->178         0.12531
     170 ->177        -0.39094
     171 ->177         0.42228

 Excited state symmetry could not be determined.
 Excited State  39:      Singlet-?Sym    3.5946 eV  344.92 nm
f=0.0087  <S**2>=0.000
     156 ->173        -0.16515
     157 ->174        -0.26447
     158 ->172        -0.20623
     158 ->173         0.44722
     159 ->174         0.23211
     160 ->173        -0.22069
     166 ->174         0.12965

 Excited state symmetry could not be determined.
 Excited State  40:      Singlet-?Sym    3.6377 eV  340.83 nm
f=0.0034  <S**2>=0.000
     156 ->174        -0.14311
     157 ->173        -0.32048
     158 ->174         0.36029
     159 ->172        -0.10806
     159 ->173         0.26442
     160 ->174        -0.28645
     163 ->174         0.13377
     166 ->173         0.10898

 Excited state symmetry could not be determined.
 Excited State  41:      Singlet-?Sym    3.7632 eV  329.47 nm
f=0.0025  <S**2>=0.000
     158 ->172         0.65474
     158 ->173         0.17716

 Excited state symmetry could not be determined.
 Excited State  42:      Singlet-?Sym    3.7857 eV  327.51 nm
f=0.0299  <S**2>=0.000
     158 ->172         0.10171
     160 ->177         0.11192
     161 ->177         0.20024
     163 ->177         0.24368
```

```
     165 ->177         0.20130
     170 ->177         0.34860
     171 ->177         0.34165

 Excited state symmetry could not be determined.
 Excited State  43:      Singlet-?Sym    3.8266 eV  324.01 nm
f=0.0169  <S**2>=0.000
     157 ->172        -0.29967
     159 ->172         0.61092
     159 ->173         0.10247

 Excited state symmetry could not be determined.
 Excited State  44:      Singlet-?Sym    3.9160 eV  316.61 nm
f=0.0013  <S**2>=0.000
     157 ->172         0.62161
     159 ->172         0.32230

 Excited state symmetry could not be determined.
 Excited State  45:      Singlet-?Sym    3.9908 eV  310.67 nm
f=0.0013  <S**2>=0.000
     156 ->172         0.68942

 Excited state symmetry could not be determined.
 Excited State  46:      Singlet-?Sym    4.0335 eV  307.39 nm
f=0.0770  <S**2>=0.000
     159 ->174         0.14045
     170 ->175        -0.10243
     171 ->175         0.66141

 Excited state symmetry could not be determined.
 Excited State  47:      Singlet-?Sym    4.1074 eV  301.86 nm
f=0.0001  <S**2>=0.000
     157 ->173        -0.12198
     159 ->173        -0.18106
     170 ->178         0.12753
     171 ->176         0.63110

 Excited state symmetry could not be determined.
 Excited State  48:      Singlet-?Sym    4.1308 eV  300.15 nm
f=0.0309  <S**2>=0.000
     157 ->174         0.35072
     158 ->173         0.41316
     159 ->174        -0.40701
     171 ->175         0.14592

 Excited state symmetry could not be determined.
 Excited State  49:      Singlet-?Sym    4.1399 eV  299.49 nm
f=0.0005  <S**2>=0.000
     156 ->174        -0.16242
     157 ->173         0.38206
```

```
     158 ->174         0.46727
     159 ->173        -0.28074

 Excited state symmetry could not be determined.
 Excited State  50:      Singlet-?Sym    4.1625 eV  297.86 nm
f=0.0054  <S**2>=0.000
     166 ->178         0.35124
     168 ->178        -0.29847
     169 ->178         0.35305
     171 ->177        -0.27835

 Excited state symmetry could not be determined.
 Excited State  51:      Singlet-?Sym    4.2414 eV  292.32 nm
f=0.0050  <S**2>=0.000
     156 ->174         0.22674
     157 ->173         0.30901
     159 ->173         0.46586
     166 ->177         0.11386
     168 ->177        -0.13450
     169 ->177         0.16185
     170 ->178         0.12221
     171 ->176         0.15132

 Excited state symmetry could not be determined.
 Excited State  52:      Singlet-?Sym    4.2852 eV  289.33 nm
f=0.0041  <S**2>=0.000
     156 ->173         0.41562
     157 ->174         0.34515
     158 ->173         0.14954
     159 ->174         0.41187

 Excited state symmetry could not be determined.
 Excited State  53:      Singlet-?Sym    4.3115 eV  287.56 nm
f=0.0013  <S**2>=0.000
     157 ->173        -0.23705
     158 ->174        -0.11502
     159 ->173        -0.14268
     166 ->177         0.33573
     168 ->177        -0.25462
     169 ->177         0.32895
     170 ->178         0.10364
     171 ->176        -0.12240
     171 ->178        -0.15452

 Excited state symmetry could not be determined.
 Excited State  54:      Singlet-?Sym    4.3752 eV  283.38 nm
f=0.0008  <S**2>=0.000
     160 ->178         0.11362
     161 ->178         0.15038
     163 ->178         0.18672
```

```
     165 ->178         0.13731
     170 ->176        -0.13610
     170 ->178         0.45905
     171 ->176        -0.18732
     171 ->178         0.27965

 Excited state symmetry could not be determined.
 Excited State  55:      Singlet-?Sym    4.4304 eV  279.85 nm
f=0.0818  <S**2>=0.000
     156 ->173        -0.15671
     157 ->174         0.18519
     159 ->174         0.15899
     170 ->175         0.60583

 Excited state symmetry could not be determined.
 Excited State  56:      Singlet-?Sym    4.4417 eV  279.14 nm
f=0.0127  <S**2>=0.000
     155 ->172         0.62447
     156 ->174        -0.18664
     170 ->176        -0.16635

 Excited state symmetry could not be determined.
 Excited State  57:      Singlet-?Sym    4.4477 eV  278.76 nm
f=0.0429  <S**2>=0.000
     156 ->173         0.47701
     157 ->174        -0.32477
     159 ->174        -0.16709
     170 ->175         0.25972
     171 ->175         0.11152

 Excited state symmetry could not be determined.
 Excited State  58:      Singlet-?Sym    4.4727 eV  277.20 nm
f=0.0179  <S**2>=0.000
     155 ->172         0.23532
     156 ->174         0.54044
     157 ->173        -0.12915
     158 ->174         0.20139
     159 ->173        -0.13963
     169 ->175        -0.11676

 Excited state symmetry could not be determined.
 Excited State  59:      Singlet-?Sym    4.5068 eV  275.11 nm
f=0.0130  <S**2>=0.000
     154 ->172         0.68247

 Excited state symmetry could not be determined.
 Excited State  60:      Singlet-?Sym    4.5240 eV  274.06 nm
f=0.0023  <S**2>=0.000
     154 ->174        -0.10132
     155 ->172         0.12064
```

```
     155 ->173         0.16427
     156 ->174        -0.15840
     170 ->176         0.60306

 Excited state symmetry could not be determined.
 Excited State  61:      Singlet-?Sym    4.6981 eV  263.90 nm
f=0.0079  <S**2>=0.000
     150 ->172         0.65960
     151 ->172        -0.10290

 Excited state symmetry could not be determined.
 Excited State  62:      Singlet-?Sym    4.6985 eV  263.88 nm
f=0.0051  <S**2>=0.000
     154 ->174        -0.11557
     155 ->173         0.47938
     166 ->175         0.16844
     167 ->176         0.10165
     168 ->175        -0.36239
     169 ->175         0.15139
     170 ->176        -0.10370

 Excited state symmetry could not be determined.
 Excited State  63:      Singlet-?Sym    4.7360 eV  261.79 nm
f=0.0028  <S**2>=0.000
     155 ->173        -0.26230
     166 ->175         0.16445
     169 ->175         0.57146
     170 ->176         0.14630

 Excited state symmetry could not be determined.
 Excited State  64:      Singlet-?Sym    4.7440 eV  261.35 nm
f=0.0157  <S**2>=0.000
     154 ->173        -0.12737
     155 ->174         0.10171
     161 ->177        -0.18873
     163 ->177        -0.23596
     165 ->175        -0.10937
     165 ->177        -0.25964
     166 ->176        -0.10201
     168 ->176         0.17898
     169 ->176        -0.13745
     170 ->177         0.23535
     171 ->177         0.26763
     171 ->179        -0.18495

 Excited state symmetry could not be determined.
 Excited State  65:      Singlet-?Sym    4.7567 eV  260.65 nm
f=0.0402  <S**2>=0.000
     154 ->173        -0.30278
     155 ->174         0.37920
```

```
     163 ->177         0.12150
     165 ->177         0.12998
     166 ->176        -0.11527
     167 ->175        -0.16091
     168 ->176         0.30667
     170 ->177        -0.11850
     171 ->177        -0.13002

 Excited state symmetry could not be determined.
 Excited State  66:      Singlet-?Sym    4.7765 eV  259.57 nm
f=0.0726  <S**2>=0.000
     154 ->173        -0.21312
     155 ->174         0.18231
     166 ->176         0.22724
     168 ->176        -0.12879
     169 ->176         0.55993

 Excited state symmetry could not be determined.
 Excited State  67:      Singlet-?Sym    4.8089 eV  257.82 nm
f=0.0006  <S**2>=0.000
     153 ->172         0.57595
     171 ->178        -0.12537
     171 ->180         0.10043
     171 ->181         0.23293

 Excited state symmetry could not be determined.
 Excited State  68:      Singlet-?Sym    4.8569 eV  255.27 nm
f=0.0002  <S**2>=0.000
     152 ->172         0.62339
     152 ->173        -0.12492
     154 ->174         0.18987
     155 ->173         0.15784

 Excited state symmetry could not be determined.
 Excited State  69:      Singlet-?Sym    4.8718 eV  254.50 nm
f=0.0020  <S**2>=0.000
     152 ->174        -0.12215
     154 ->173         0.50921
     155 ->174         0.44294

 Excited state symmetry could not be determined.
 Excited State  70:      Singlet-?Sym    4.8770 eV  254.22 nm
f=0.0046  <S**2>=0.000
     152 ->172        -0.25129
     154 ->174         0.24073
     155 ->173         0.29820
     166 ->175        -0.19871
     168 ->175         0.36038
     169 ->175         0.20805
     171 ->180         0.10742
```

```
 Excited state symmetry could not be determined.
 Excited State  71:      Singlet-?Sym    4.9003 eV  253.01 nm
f=0.0341  <S**2>=0.000
     151 ->172        -0.35890
     165 ->177        -0.17887
     170 ->177         0.13897
     171 ->179         0.50635

 Excited state symmetry could not be determined.
 Excited State  72:      Singlet-?Sym    4.9324 eV  251.37 nm
f=0.0065  <S**2>=0.000
     154 ->174         0.28777
     166 ->175         0.55466
     168 ->175         0.13078
     169 ->175        -0.19923

 Excited state symmetry could not be determined.
 Excited State  73:      Singlet-?Sym    4.9359 eV  251.19 nm
f=0.0084  <S**2>=0.000
     163 ->175        -0.17499
     165 ->175        -0.11323
     166 ->176        -0.16975
     167 ->175         0.48782
     168 ->176         0.31526
     169 ->176         0.21071

 Excited state symmetry could not be determined.
 Excited State  74:      Singlet-?Sym    4.9718 eV  249.38 nm
f=0.0407  <S**2>=0.000
     151 ->172         0.55903
     171 ->179         0.35174

 Excited state symmetry could not be determined.
 Excited State  75:      Singlet-?Sym    4.9768 eV  249.12 nm
f=0.0034  <S**2>=0.000
     152 ->173         0.14071
     154 ->174         0.43822
     166 ->175        -0.22380
     167 ->176        -0.31410
     168 ->175        -0.30635

 Excited state symmetry could not be determined.
 Excited State  76:      Singlet-?Sym    4.9887 eV  248.53 nm
f=0.0173  <S**2>=0.000
     152 ->174        -0.13982
     154 ->173        -0.10466
     155 ->174         0.14491
     163 ->175         0.14825
     165 ->175         0.29296
```

```
     166 ->176         0.28138
     167 ->175         0.35879
     169 ->176        -0.22010
     171 ->182         0.20627

 Excited state symmetry could not be determined.
 Excited State  77:      Singlet-?Sym    4.9912 eV  248.41 nm
f=0.0281  <S**2>=0.000
     153 ->172        -0.24528
     161 ->178         0.19018
     163 ->178         0.22446
     165 ->178         0.29215
     166 ->177        -0.10749
     167 ->176         0.17297
     167 ->178         0.11111
     168 ->175         0.14758
     171 ->178        -0.28588
     171 ->181         0.17942

 Excited state symmetry could not be determined.
 Excited State  78:      Singlet-?Sym    5.0057 eV  247.68 nm
f=0.1083  <S**2>=0.000
     161 ->175         0.16562
     163 ->175         0.25392
     165 ->175         0.44061
     166 ->176        -0.31873
     168 ->176         0.15343
     169 ->176         0.19073

 Excited state symmetry could not be determined.
 Excited State  79:      Singlet-?Sym    5.0200 eV  246.98 nm
f=0.0001  <S**2>=0.000
     152 ->173         0.49184
     153 ->173         0.15262
     154 ->174         0.11113
     167 ->176         0.27940
     168 ->177         0.13180
     169 ->177         0.21448
     171 ->180        -0.10821

 Excited state symmetry could not be determined.
 Excited State  80:      Singlet-?Sym    5.0299 eV  246.49 nm
f=0.0546  <S**2>=0.000
     152 ->173        -0.22575
     166 ->177        -0.18193
     167 ->176        -0.16350
     168 ->177         0.32692
     169 ->177         0.45789
     171 ->180        -0.11924
```

Table S42. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 3 (*S*=1)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  3.035-?Sym    0.5006 eV 2476.79 nm  f=0.0133
<S**2>=2.053
    169A ->174A        0.15353
    172A ->174A        0.56005
    173A ->174A        0.80795
 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 symmetry could not be determined.
 Excited State   2:  3.028-?Sym    0.6538 eV 1896.49 nm  f=0.0193
<S**2>=2.042
    172A ->174A        0.80278
    173A ->174A       -0.57543

 Excited state symmetry could not be determined.
 Excited State   3:  3.812-?Sym    1.2392 eV 1000.55 nm  f=0.0008
<S**2>=3.383
    168A ->174A        0.16373
    170A ->174A       -0.43735
    171A ->174A        0.84891
    170B ->174B        0.11643
    171B ->174B       -0.14882

 Excited state symmetry could not be determined.
 Excited State   4:  3.041-?Sym    1.4388 eV  861.72 nm  f=0.0447
<S**2>=2.062
    171B ->172B       -0.49940
    171B ->173B        0.84652

 Excited state symmetry could not be determined.
 Excited State   5:  3.980-?Sym    1.6087 eV  770.72 nm  f=0.0184
<S**2>=3.711
    168A ->174A        0.31259
    170A ->174A        0.72959
    171A ->174A        0.28716
    168B ->174B       -0.28223
    169B ->173B       -0.15961
    170B ->174B       -0.25602
    171B ->174B       -0.29751

 Excited state symmetry could not be determined.
 Excited State   6:  3.055-?Sym    1.6929 eV  732.40 nm  f=0.0054
<S**2>=2.083
```

```
    170B ->172B       -0.23587
    170B ->173B       -0.19347
    171B ->172B        0.81199
    171B ->173B        0.46259

 Excited state symmetry could not be determined.
 Excited State   7:  3.390-?Sym    1.8831 eV  658.41 nm  f=0.0135
<S**2>=2.624
    171A ->174A        0.24163
    170B ->174B       -0.43788
    171B ->174B        0.84010

 Excited state symmetry could not be determined.
 Excited State   8:  3.514-?Sym    2.0790 eV  596.35 nm  f=0.0113
<S**2>=2.837
    166A ->174A        0.12680
    169A ->174A        0.64233
    172A ->174A       -0.15363
    169B ->174B       -0.23491
    170B ->172B        0.22185
    170B ->173B       -0.62612

 Excited state symmetry could not be determined.
 Excited State   9:  3.420-?Sym    2.1276 eV  582.75 nm  f=0.0194
<S**2>=2.675
    167A ->174A       -0.20999
    169A ->174A        0.46361
    167B ->174B       -0.11363
    168B ->172B        0.10061
    169B ->174B       -0.25486
    170B ->172B        0.26206
    170B ->173B        0.68328
    171B ->172B        0.19752
    171B ->173B        0.18604

 Excited state symmetry could not be determined.
 Excited State  10:  3.236-?Sym    2.1445 eV  578.15 nm  f=0.0262
<S**2>=2.367
    166A ->174A       -0.18840
    167A ->174A       -0.12855
    169A ->174A       -0.35940
    167B ->174B       -0.10945
    168B ->173B        0.13906
    170B ->172B        0.83211
    170B ->173B       -0.15109
    171B ->172B        0.15630

 Excited state symmetry could not be determined.
 Excited State  11:  3.136-?Sym    2.2749 eV  545.00 nm  f=0.0063
<S**2>=2.209
```

```
    173A ->175A       -0.24718
    167B ->172B        0.13462
    169B ->172B        0.59956
    169B ->173B        0.65679
    170B ->174B       -0.24863
    171B ->174B       -0.11062

 Excited state symmetry could not be determined.
 Excited State  12:  3.072-?Sym    2.3224 eV  533.86 nm  f=0.1086
<S**2>=2.109
    168A ->174A        0.12034
    173A ->175A        0.32115
    169B ->172B        0.76023
    169B ->173B       -0.50615

 Excited state symmetry could not be determined.
 Excited State  13:  3.098-?Sym    2.3317 eV  531.73 nm  f=0.0009
<S**2>=2.150
    172A ->175A       -0.10573
    173A ->175A        0.88717
    169B ->172B       -0.11709
    169B ->173B        0.33339
    170B ->174B       -0.14349

 Excited state symmetry could not be determined.
 Excited State  14:  3.100-?Sym    2.4173 eV  512.90 nm  f=0.0055
<S**2>=2.152
    173A ->176A        0.95979
    169B ->174B       -0.11147

 Excited state symmetry could not be determined.
 Excited State  15:  3.148-?Sym    2.4547 eV  505.08 nm  f=0.0043
<S**2>=2.227
    165A ->174A        0.15290
    168A ->174A       -0.40137
    170A ->174A        0.44267
    171A ->174A        0.27953
    172A ->175A       -0.10764
    167B ->172B       -0.14030
    169B ->172B        0.15272
    169B ->173B        0.15341
    170B ->174B        0.60940
    171B ->174B        0.25340

 Excited state symmetry could not be determined.
 Excited State  16:  3.246-?Sym    2.4628 eV  503.43 nm  f=0.0058
<S**2>=2.385
    166A ->174A        0.10061
    169A ->174A        0.31710
    168B ->173B       -0.12596
```

```
    169B ->174B        0.90036
    170B ->172B        0.10091

 Excited state symmetry could not be determined.
 Excited State  17:  3.350-?Sym    2.5941 eV  477.95 nm  f=0.0080
<S**2>=2.555
    164A ->174A       -0.14785
    165A ->174A       -0.31034
    169A ->177A       -0.10930
    172A ->177A       -0.34594
    173A ->177A       -0.41970
    173A ->183A       -0.10420
    164B ->174B        0.11385
    165B ->174B        0.22524
    167B ->172B        0.51392
    167B ->173B        0.22288
    169B ->173B       -0.13784
    170B ->174B        0.19197

 Excited state symmetry could not be determined.
 Excited State  18:  3.741-?Sym    2.6032 eV  476.28 nm  f=0.0000
<S**2>=3.248
    166A ->174A        0.29775
    167A ->174A        0.58920
    173A ->176A       -0.13275
    164B ->172B        0.11828
    165B ->172B        0.34316
    165B ->173B        0.16248
    167B ->174B        0.39312
    168B ->172B       -0.16012
    168B ->173B       -0.16077
    169B ->174B       -0.11047
    170B ->172B        0.28941
    170B ->173B        0.11559

 Excited state symmetry could not be determined.
 Excited State  19:  3.580-?Sym    2.6160 eV  473.95 nm  f=0.0008
<S**2>=2.954
    164A ->174A        0.12946
    165A ->174A        0.20845
    168A ->174A        0.49180
    169A ->177A       -0.10454
    171A ->174A       -0.12697
    172A ->175A       -0.16487
    172A ->177A       -0.44847
    173A ->177A       -0.27692
    165B ->174B       -0.11825
    166B ->172B        0.11890
    167B ->172B       -0.28997
    167B ->173B       -0.18660
```

```
    168B ->174B       -0.17658
    169B ->173B        0.11750
    170B ->174B        0.14433
    171B ->174B        0.16965

 Excited state symmetry could not be determined.
 Excited State  20:  3.063-?Sym    2.6359 eV  470.37 nm  f=0.0073
<S**2>=2.096
    169A ->174A        0.13730
    165B ->173B        0.15108
    168B ->172B       -0.51535
    168B ->173B        0.79741

 Excited state symmetry could not be determined.
 Excited State  21:  3.616-?Sym    2.6551 eV  466.97 nm  f=0.0000
<S**2>=3.020
    165A ->174A       -0.19865
    168A ->174A        0.47565
    169A ->177A        0.10706
    171A ->174A       -0.13856
    172A ->175A       -0.33646
    172A ->177A        0.35010
    173A ->177A        0.23689
    165B ->174B        0.10219
    167B ->172B        0.22767
    167B ->173B        0.11570
    168B ->174B       -0.23612
    169B ->173B        0.15302
    170B ->174B        0.36369
    171B ->174B        0.20016

 Excited state symmetry could not be determined.
 Excited State  22:  3.185-?Sym    2.6922 eV  460.54 nm  f=0.0023
<S**2>=2.286
    168A ->174A        0.16529
    172A ->175A        0.90188
    168B ->174B       -0.20502
    169B ->173B        0.17681
    170B ->174B        0.19280
    171B ->174B        0.14071

 Excited state symmetry could not be determined.
 Excited State  23:  3.147-?Sym    2.7557 eV  449.92 nm  f=0.0057
<S**2>=2.225
    166A ->174A        0.11322
    167A ->174A       -0.14596
    169A ->174A       -0.10568
    172A ->176A        0.84095
    172A ->178A        0.12029
    168B ->172B       -0.33683
```

```
    168B ->173B       -0.15994

 Excited state symmetry could not be determined.
 Excited State  24:  3.296-?Sym    2.7801 eV  445.97 nm  f=0.0217
<S**2>=2.465
    158A ->174A       -0.12966
    166A ->174A       -0.24400
    167A ->174A        0.19198
    169A ->174A        0.12165
    172A ->176A        0.40557
    172A ->178A        0.13226
    173A ->178A        0.11046
    158B ->174B        0.14506
    159B ->172B       -0.18162
    164B ->172B        0.10065
    165B ->172B        0.14690
    166B ->174B        0.17893
    167B ->174B        0.13009
    168B ->172B        0.56072
    168B ->173B        0.34430

 Excited state symmetry could not be determined.
 Excited State  25:  3.147-?Sym    2.8267 eV  438.62 nm  f=0.0169
<S**2>=2.226
    159A ->174A       -0.11969
    172A ->177A       -0.50826
    173A ->177A        0.61216
    173A ->180A        0.14286
    173A ->186A        0.10881
    158B ->172B       -0.15096
    159B ->174B        0.16450
    166B ->172B       -0.17072
    166B ->173B       -0.34760

 Excited state symmetry could not be determined.
 Excited State  26:  3.562-?Sym    2.8632 eV  433.03 nm  f=0.0228
<S**2>=2.923
    158A ->174A        0.20984
    166A ->174A        0.62811
    167A ->174A       -0.29085
    169A ->174A       -0.13388
    171A ->177A       -0.13827
    172A ->176A        0.11471
    172A ->178A       -0.13793
    165B ->173B        0.10994
    166B ->174B       -0.12224
    167B ->174B        0.10875
    168B ->172B        0.40110
    168B ->173B        0.25174
```

```
 Excited state symmetry could not be determined.
 Excited State  27:  3.509-?Sym    2.8810 eV  430.35 nm  f=0.0027
<S**2>=2.828
    158A ->174A        0.10375
    166A ->174A        0.24591
    167A ->174A       -0.25986
    169A ->178A        0.12457
    169A ->185A        0.17700
    169A ->189A        0.10634
    170A ->177A       -0.12545
    171A ->177A        0.26662
    172A ->176A       -0.29474
    172A ->178A        0.39046
    172A ->179A       -0.17424
    172A ->185A        0.24383
    172A ->189A        0.14357
    173A ->178A        0.29240
    173A ->179A       -0.10518
    173A ->181A       -0.10574
    173A ->185A        0.19479
    170B ->177B        0.11719
    171B ->177B       -0.17559

 Excited state symmetry could not be determined.
 Excited State  28:  3.218-?Sym    2.8900 eV  429.02 nm  f=0.0002
<S**2>=2.340
    159A ->174A        0.17395
    162A ->174A       -0.10990
    173A ->177A        0.20956
    158B ->172B        0.21318
    158B ->173B        0.10524
    159B ->174B       -0.21361
    166B ->172B        0.74477
    166B ->173B       -0.29376
    167B ->172B        0.22229
    167B ->173B       -0.13029
    168B ->174B        0.14072

 Excited state symmetry could not be determined.
 Excited State  29:  3.195-?Sym    2.9597 eV  418.91 nm  f=0.0030
<S**2>=2.302
    159A ->174A        0.15827
    172A ->177A       -0.27246
    173A ->177A        0.36107
    158B ->172B        0.17508
    159B ->174B       -0.17802
    166B ->173B        0.70976
    167B ->173B        0.26392
    168B ->174B       -0.10787
```

```
 Excited state symmetry could not be determined.
 Excited State  30:  3.900-?Sym    2.9979 eV  413.57 nm  f=0.0106
<S**2>=3.553
    169A ->185A        0.10021
    170A ->177A        0.27356
    170A ->186A        0.13224
    170A ->190A        0.12267
    171A ->177A       -0.34999
    171A ->180A       -0.11921
    171A ->186A       -0.16412
    171A ->190A       -0.15134
    172A ->178A        0.23896
    172A ->179A       -0.10157
    172A ->185A        0.15161
    173A ->178A        0.23788
    173A ->179A       -0.13619
    173A ->185A        0.16057
    170B ->177B       -0.31808
    170B ->180B       -0.10063
    170B ->186B       -0.18587
    171B ->177B        0.35433
    171B ->180B        0.10180
    171B ->186B        0.17154

 Excited state symmetry could not be determined.
 Excited State  31:  3.214-?Sym    3.0627 eV  404.81 nm  f=0.0127
<S**2>=2.332
    167A ->174A       -0.26652
    172A ->178A       -0.26620
    173A ->178A        0.26409
    173A ->181A       -0.18828
    173A ->184A       -0.18325
    173A ->185A        0.12568
    158B ->174B        0.14132
    159B ->172B       -0.19225
    159B ->173B       -0.10343
    162B ->173B       -0.18498
    164B ->172B        0.26393
    164B ->173B       -0.27463
    165B ->173B        0.49568
    166B ->174B        0.17839
    167B ->174B        0.10752
    168B ->173B       -0.16495

 Excited state symmetry could not be determined.
 Excited State  32:  3.178-?Sym    3.0837 eV  402.06 nm  f=0.0359
<S**2>=2.274
    166A ->174A       -0.12777
    167A ->174A       -0.34237
    172A ->185A       -0.14155
```

```
    173A ->178A        0.16261
    173A ->179A        0.44700
    173A ->181A       -0.22079
    173A ->184A       -0.17385
    162B ->173B        0.12743
    164B ->173B        0.28049
    165B ->172B        0.46399
    165B ->173B       -0.21625
    167B ->174B        0.12609
    168B ->172B       -0.16518

 Excited state symmetry could not be determined.
 Excited State  33:  3.210-?Sym    3.0975 eV  400.28 nm  f=0.0048
<S**2>=2.326
    165A ->174A        0.37647
    165B ->174B       -0.10676
    166B ->172B       -0.13681
    166B ->173B        0.27057
    167B ->172B        0.61710
    167B ->173B       -0.56927

 Excited state symmetry could not be determined.
 Excited State  34:  3.184-?Sym    3.0992 eV  400.05 nm  f=0.0119
<S**2>=2.284
    161A ->174A       -0.11077
    166A ->174A       -0.36514
    167A ->174A        0.10151
    169A ->174A        0.10140
    173A ->178A        0.14987
    173A ->179A        0.42649
    173A ->181A       -0.12011
    158B ->174B       -0.22661
    159B ->172B        0.31497
    159B ->173B        0.15558
    160B ->172B       -0.14934
    162B ->172B        0.25904
    164B ->173B       -0.11821
    165B ->173B        0.19342
    166B ->174B       -0.39524
    168B ->172B        0.14991

 Excited state symmetry could not be determined.
 Excited State  35:  3.409-?Sym    3.1217 eV  397.16 nm  f=0.0325
<S**2>=2.655
    159A ->174A       -0.25406
    162A ->174A        0.15022
    165A ->174A        0.51790
    168A ->174A        0.23305
    172A ->177A       -0.11372
    173A ->183A       -0.11892
```

```
    167B ->172B        0.16927
    167B ->173B        0.47800
    168B ->174B        0.42957

 Excited state symmetry could not be determined.
 Excited State  36:  3.227-?Sym    3.1508 eV  393.51 nm  f=0.0034
<S**2>=2.353
    159A ->174A       -0.12476
    162A ->174A        0.17129
    164A ->174A       -0.22271
    165A ->174A       -0.35887
    168A ->174A        0.27231
    170A ->174A        0.17436
    166B ->173B        0.19548
    167B ->172B       -0.10193
    167B ->173B       -0.43994
    168B ->174B        0.55425

 Excited state symmetry could not be determined.
 Excited State  37:  4.050-?Sym    3.1613 eV  392.20 nm  f=0.0006
<S**2>=3.850
    165A ->174A       -0.11170
    168A ->185A        0.10273
    170A ->178A       -0.16945
    170A ->185A       -0.21786
    170A ->189A       -0.11916
    171A ->176A        0.10552
    171A ->178A        0.28418
    171A ->179A       -0.13542
    171A ->185A        0.34633
    171A ->189A        0.19971
    172A ->177A       -0.14304
    172A ->180A        0.10482
    168B ->174B       -0.15722
    168B ->178B       -0.10664
    168B ->185B       -0.13611
    170B ->178B        0.22880
    170B ->179B       -0.10645
    170B ->185B        0.27991
    171B ->178B       -0.26948
    171B ->179B        0.12123
    171B ->185B       -0.31183

 Excited state symmetry could not be determined.
 Excited State  38:  3.147-?Sym    3.1897 eV  388.70 nm  f=0.0147
<S**2>=2.225
    166A ->174A        0.11436
    172A ->178A        0.33796
    172A ->179A       -0.16948
    172A ->185A        0.10261
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    173A ->178A       -0.26270
    173A ->179A        0.57389
    173A ->181A        0.16265
    173A ->184A        0.23440
    173A ->185A       -0.15424
    158B ->174B        0.14463
    159B ->172B       -0.19639
    159B ->173B       -0.10213
    164B ->173B       -0.12734
    165B ->172B       -0.25881
    166B ->174B        0.22760
    167B ->174B        0.17200

 Excited state symmetry could not be determined.
 Excited State  39:  3.251-?Sym    3.2209 eV  384.94 nm  f=0.0112
<S**2>=2.393
    159A ->174A        0.16275
    162A ->174A       -0.14425
    164A ->174A        0.10364
    169A ->177A        0.11885
    172A ->177A       -0.22231
    172A ->180A        0.51849
    172A ->182A        0.28773
    172A ->183A        0.15981
    172A ->186A        0.22688
    173A ->177A       -0.15756
    173A ->180A        0.45396
    173A ->182A       -0.13472
    173A ->186A        0.11960
    166B ->172B       -0.13637
    171B ->178B        0.12844

 Excited state symmetry could not be determined.
 Excited State  40:  3.298-?Sym    3.2276 eV  384.14 nm  f=0.0145
<S**2>=2.469
    159A ->174A        0.13646
    160A ->174A        0.24756
    162A ->174A       -0.23865
    172A ->180A        0.15259
    173A ->180A       -0.35761
    173A ->182A        0.58351
    173A ->183A       -0.12056
    160B ->174B        0.14039
    161B ->172B        0.26726
    161B ->173B        0.13436
    162B ->174B       -0.11867
    163B ->172B        0.13004
    166B ->172B       -0.29525
    166B ->173B       -0.13114
    168B ->174B        0.14911
```

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 Excited state symmetry could not be determined.
 Excited State  41:  3.279-?Sym    3.2354 eV  383.21 nm  f=0.0030
<S**2>=2.438
    172A ->178A       -0.14884
    173A ->178A        0.24143
    173A ->181A       -0.11553
    173A ->184A       -0.11160
    164B ->172B       -0.13239
    165B ->172B       -0.55973
    165B ->173B       -0.34547
    167B ->174B        0.61742

 Excited state symmetry could not be determined.
 Excited State  42:  3.100-?Sym    3.2377 eV  382.94 nm  f=0.0460
<S**2>=2.153
    161A ->174A       -0.12210
    166A ->174A        0.20536
    167A ->174A        0.21547
    172A ->178A       -0.24134
    173A ->178A        0.56304
    173A ->179A        0.25363
    173A ->181A        0.22083
    173A ->184A        0.34991
    173A ->185A        0.25199
    160B ->172B       -0.13532
    164B ->172B       -0.11521
    165B ->173B       -0.11944
    166B ->174B        0.11564
    167B ->174B       -0.27659

 Excited state symmetry could not be determined.
 Excited State  43:  3.441-?Sym    3.2600 eV  380.32 nm  f=0.0019
<S**2>=2.710
    159A ->174A       -0.36104
    160A ->174A       -0.15937
    162A ->174A        0.36709
    164A ->174A       -0.19853
    172A ->180A        0.29518
    172A ->182A        0.11552
    172A ->186A        0.12295
    173A ->177A       -0.10726
    173A ->180A       -0.14116
    173A ->182A        0.39969
    173A ->183A        0.15906
    159B ->174B        0.12441
    166B ->172B        0.32494
    166B ->173B        0.16233
    168B ->174B       -0.26431
```

```
 Excited state symmetry could not be determined.
 Excited State  44:  3.572-?Sym    3.2909 eV  376.74 nm  f=0.0088
<S**2>=2.939
    160A ->174A       -0.23274
    164A ->174A        0.70106
    165A ->174A       -0.29940
    173A ->183A        0.35288
    164B ->174B       -0.13427
    165B ->174B       -0.25641
    167B ->172B        0.16771
    167B ->173B        0.13703
    168B ->174B        0.14200

 Excited state symmetry could not be determined.
 Excited State  45:  3.269-?Sym    3.3211 eV  373.32 nm  f=0.0069
<S**2>=2.421
    159A ->174A        0.16014
    162A ->174A       -0.15101
    164A ->174A       -0.44925
    165A ->174A        0.14275
    173A ->183A        0.72613
    173A ->186A       -0.15447
    165B ->174B       -0.18508
    166B ->172B       -0.12492
    167B ->172B        0.12795

 Excited state symmetry could not be determined.
 Excited State  46:  3.281-?Sym    3.3252 eV  372.86 nm  f=0.0542
<S**2>=2.441
    161A ->174A       -0.18925
    170A ->177A        0.11817
    172A ->178A        0.31183
    172A ->181A        0.13950
    172A ->184A        0.17106
    172A ->185A       -0.36671
    172A ->188A       -0.15140
    173A ->178A        0.13614
    173A ->179A       -0.11405
    164B ->173B        0.28636
    165B ->172B       -0.28365
    165B ->173B        0.43389
    166B ->174B        0.12275
    171B ->175B        0.10492
    171B ->177B       -0.19509

 Excited state symmetry could not be determined.
 Excited State  47:  3.624-?Sym    3.3428 eV  370.90 nm  f=0.0470
<S**2>=3.033
    161A ->174A        0.68327
    163A ->174A       -0.37806
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    173A ->178A        0.20254
    173A ->179A        0.19316
    160B ->172B        0.25687
    160B ->173B        0.12391
    161B ->174B        0.13903
    162B ->172B       -0.11434
    166B ->174B       -0.16661
    167B ->174B       -0.22818

 Excited state symmetry could not be determined.
 Excited State  48:  3.177-?Sym    3.3666 eV  368.28 nm  f=0.0052
<S**2>=2.274
    159A ->174A       -0.12548
    160A ->174A        0.20779
    165A ->174A       -0.12165
    172A ->180A       -0.24254
    172A ->182A       -0.13208
    173A ->177A       -0.21077
    173A ->180A        0.67133
    173A ->182A        0.32820
    173A ->187A       -0.13567
    157B ->172B       -0.10474
    161B ->172B        0.15001
    165B ->174B       -0.23206

 Excited state symmetry could not be determined.
 Excited State  49:  3.114-?Sym    3.3841 eV  366.37 nm  f=0.2098
<S**2>=2.174
    161A ->174A        0.14984
    166A ->174A       -0.18002
    167A ->174A       -0.21269
    171A ->175A        0.11155
    172A ->178A        0.15459
    172A ->181A        0.25884
    172A ->185A       -0.13301
    173A ->178A        0.17218
    173A ->179A       -0.15414
    173A ->181A        0.48205
    173A ->184A        0.24711
    162B ->173B       -0.13319
    164B ->172B       -0.21906
    164B ->173B       -0.11771
    165B ->172B        0.27076
    165B ->173B        0.15413
    166B ->174B       -0.21496
    167B ->174B        0.30803
    171B ->175B       -0.17458

 Excited state symmetry could not be determined.
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 Excited State  50:  3.158-?Sym    3.4016 eV  364.48 nm  f=0.0312
<S**2>=2.244
    172A ->178A        0.25980
    172A ->181A        0.31535
    172A ->185A       -0.11889
    173A ->181A        0.12813
    173A ->184A       -0.10881
    159B ->172B        0.12019
    162B ->172B        0.26174
    162B ->173B       -0.18871
    164B ->172B        0.54660
    164B ->173B       -0.17075
    165B ->173B       -0.39847
    166B ->174B        0.24622

 Excited state symmetry could not be determined.
 Excited State  51:  3.179-?Sym    3.4242 eV  362.08 nm  f=0.0276
<S**2>=2.276
    161A ->174A       -0.18222
    172A ->179A        0.14257
    172A ->181A        0.47500
    172A ->184A       -0.33000
    172A ->185A        0.21880
    173A ->181A        0.12042
    173A ->184A       -0.41492
    162B ->173B       -0.10963
    164B ->172B       -0.31595
    164B ->173B        0.28031
    167B ->174B       -0.10599

 Excited state symmetry could not be determined.
 Excited State  52:  3.544-?Sym    3.4303 eV  361.44 nm  f=0.0006
<S**2>=2.889
    159A ->174A       -0.34078
    160A ->174A        0.65611
    164A ->174A        0.20964
    173A ->180A       -0.15517
    173A ->182A       -0.37283
    173A ->183A        0.21901
    158B ->172B       -0.10153
    159B ->174B        0.12475
    161B ->172B        0.23010
    161B ->173B        0.12126
    163B ->172B        0.13829
    166B ->172B        0.10877

 Excited state symmetry could not be determined.
 Excited State  53:  3.243-?Sym    3.4378 eV  360.65 nm  f=0.0417
<S**2>=2.380
    162A ->174A        0.31326
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    164A ->174A        0.17030
    165A ->174A        0.20676
    172A ->180A       -0.14027
    173A ->180A        0.11468
    173A ->182A        0.17530
    173A ->183A        0.29530
    158B ->172B        0.24692
    158B ->173B        0.12313
    159B ->174B       -0.26000
    161B ->172B        0.12321
    165B ->174B        0.61175
    166B ->172B       -0.20291

 Excited state symmetry could not be determined.
 Excited State  54:  3.255-?Sym    3.4444 eV  359.96 nm  f=0.1939
<S**2>=2.398
    158A ->174A        0.11201
    161A ->174A        0.19190
    163A ->174A       -0.20035
    171A ->175A        0.17834
    172A ->178A       -0.16267
    172A ->184A       -0.12024
    172A ->185A        0.18023
    173A ->178A       -0.15946
    173A ->181A        0.27855
    173A ->184A        0.11671
    173A ->185A        0.21972
    156B ->172B       -0.12392
    159B ->172B        0.13637
    159B ->173B        0.12703
    162B ->173B        0.22885
    164B ->172B        0.20356
    164B ->173B        0.46779
    165B ->173B        0.13349
    166B ->174B        0.25453
    167B ->174B        0.18054

 Excited state symmetry could not be determined.
 Excited State  55:  3.484-?Sym    3.4727 eV  357.03 nm  f=0.0009
<S**2>=2.785
    161A ->174A        0.24642
    163A ->174A        0.77596
    173A ->178A        0.12888
    173A ->181A        0.28314
    173A ->184A       -0.17786
    173A ->185A       -0.10564
    160B ->173B        0.14448
    162B ->172B       -0.15308
    162B ->173B        0.16575
    164B ->172B        0.19609
```

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 Excited state symmetry could not be determined.
 Excited State  56:  3.615-?Sym    3.4875 eV  355.51 nm  f=0.0072
<S**2>=3.016
    161A ->174A        0.26092
    163A ->174A        0.37129
    171A ->175A        0.29933
    172A ->181A        0.20329
    173A ->178A       -0.16227
    173A ->181A       -0.34593
    173A ->184A        0.29368
    173A ->185A        0.18085
    166B ->174B       -0.11478
    168B ->175B        0.11560
    171B ->175B        0.49159

 Excited state symmetry could not be determined.
 Excited State  57:  3.469-?Sym    3.4991 eV  354.33 nm  f=0.0104
<S**2>=2.758
    161A ->174A       -0.25515
    163A ->174A       -0.15594
    171A ->175A        0.23988
    171A ->177A        0.11884
    172A ->181A       -0.16715
    172A ->184A        0.10223
    173A ->181A        0.40436
    173A ->184A       -0.23723
    160B ->173B        0.13520
    162B ->172B       -0.35189
    164B ->172B        0.14603
    166B ->174B       -0.31737
    171B ->175B        0.41089

 Excited state symmetry could not be determined.
 Excited State  58:  3.197-?Sym    3.5050 eV  353.73 nm  f=0.0008
<S**2>=2.306
    162A ->174A        0.11251
    169A ->177A        0.11077
    172A ->180A       -0.43652
    172A ->182A        0.18153
    172A ->183A        0.45170
    172A ->186A        0.28985
    173A ->186A        0.11764
    161B ->172B       -0.16695
    161B ->173B        0.17790
    163B ->172B        0.26412
    163B ->173B       -0.37178
    165B ->174B       -0.16609
    169B ->177B       -0.13082
    171B ->178B        0.12021
```

```
 Excited state symmetry could not be determined.
 Excited State  59:  3.433-?Sym    3.5244 eV  351.79 nm  f=0.0058
<S**2>=2.697
    158A ->174A        0.20119
    161A ->174A       -0.11271
    170A ->177A       -0.37605
    170A ->180A       -0.11743
    170A ->186A       -0.15005
    170A ->190A       -0.13428
    171A ->177A        0.19032
    173A ->181A       -0.15855
    173A ->184A        0.21054
    160B ->172B        0.16547
    160B ->173B        0.10079
    162B ->172B       -0.15810
    164B ->173B        0.18748
    168B ->177B        0.14778
    169B ->178B        0.13916
    169B ->185B        0.15563
    171B ->175B       -0.13815
    171B ->177B        0.52854
    171B ->186B        0.12348

 Excited state symmetry could not be determined.
 Excited State  60:  3.404-?Sym    3.5285 eV  351.38 nm  f=0.0057
<S**2>=2.647
    161A ->174A        0.18377
    170A ->177A       -0.12230
    172A ->179A       -0.10107
    172A ->181A       -0.17076
    172A ->184A        0.10299
    173A ->181A        0.11854
    173A ->184A       -0.22951
    173A ->185A       -0.19450
    159B ->172B        0.10425
    160B ->172B       -0.17230
    162B ->172B        0.28798
    162B ->173B        0.11946
    164B ->172B       -0.35414
    164B ->173B       -0.18755
    166B ->174B        0.39723
    171B ->175B        0.44307
    171B ->177B        0.12591

 Excited state symmetry could not be determined.
 Excited State  61:  3.485-?Sym    3.5293 eV  351.30 nm  f=0.0368
<S**2>=2.786
    159A ->174A        0.31481
    160A ->174A        0.21415
```

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    162A ->174A        0.68895
    172A ->180A        0.21769
    172A ->183A       -0.15086
    173A ->182A       -0.12200
    173A ->183A       -0.15363
    158B ->172B        0.14112
    159B ->174B       -0.12477
    162B ->174B       -0.10249
    163B ->172B        0.11810
    165B ->174B       -0.34946
    166B ->172B       -0.11101
    166B ->173B       -0.12682

 Excited state symmetry could not be determined.
 Excited State  62:  3.651-?Sym    3.5343 eV  350.80 nm  f=0.0347
<S**2>=3.083
    156A ->174A        0.15411
    160A ->174A        0.26232
    164A ->174A        0.15485
    168A ->176A        0.10224
    171A ->176A        0.25037
    173A ->180A        0.16613
    173A ->182A        0.19774
    173A ->186A       -0.13616
    173A ->187A        0.17736
    156B ->174B       -0.16715
    157B ->172B        0.18087
    161B ->172B       -0.27793
    163B ->173B       -0.15864
    164B ->174B        0.14666
    165B ->174B        0.16530
    168B ->176B        0.13671
    171B ->176B        0.50530

 Excited state symmetry could not be determined.
 Excited State  63:  3.086-?Sym    3.5466 eV  349.59 nm  f=0.0006
<S**2>=2.131
    163A ->174A       -0.13101
    172A ->178A        0.17247
    172A ->179A        0.14488
    172A ->181A        0.33393
    172A ->184A       -0.11949
    173A ->181A       -0.11090
    160B ->172B       -0.34144
    160B ->173B        0.15883
    162B ->172B       -0.32965
    162B ->173B        0.62962
    164B ->173B       -0.28619

 Excited state symmetry could not be determined.
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 Excited State  64:  3.272-?Sym    3.5518 eV  349.07 nm  f=0.0084
<S**2>=2.427
    156A ->174A        0.10051
    159A ->174A       -0.15114
    160A ->174A       -0.43769
    162A ->174A       -0.12857
    171A ->176A        0.14375
    172A ->180A        0.12628
    173A ->180A        0.11012
    173A ->182A       -0.19856
    161B ->172B        0.34465
    161B ->173B        0.24007
    162B ->174B       -0.10778
    163B ->172B        0.59033
    171B ->176B        0.14544

 Excited state symmetry could not be determined.
 Excited State  65:  3.248-?Sym    3.5605 eV  348.22 nm  f=0.0048
<S**2>=2.387
    162A ->174A        0.12741
    171A ->176A        0.16574
    172A ->180A       -0.32272
    172A ->182A        0.10720
    172A ->183A        0.23852
    173A ->182A       -0.10515
    161B ->172B        0.35390
    161B ->173B       -0.14353
    163B ->172B       -0.30929
    163B ->173B        0.58041
    165B ->174B       -0.11268
    171B ->176B        0.30323

 Excited state symmetry could not be determined.
 Excited State  66:  3.314-?Sym    3.5703 eV  347.27 nm  f=0.0372
<S**2>=2.496
    158A ->174A        0.23594
    161A ->174A       -0.26275
    166A ->174A       -0.10841
    171A ->175A        0.15455
    171A ->177A       -0.29892
    172A ->185A        0.10000
    173A ->178A        0.13578
    173A ->184A        0.27993
    173A ->185A       -0.25392
    156B ->172B        0.11492
    160B ->172B        0.37521
    160B ->173B        0.15321
    161B ->174B        0.11459
    162B ->172B       -0.14116
    166B ->174B        0.10807
```

```
    169B ->178B       -0.11664
    169B ->185B       -0.13333
    170B ->177B        0.22932
    170B ->186B        0.12078
    171B ->175B        0.15665
    171B ->177B       -0.17661

 Excited state symmetry could not be determined.
 Excited State  67:  3.086-?Sym    3.5909 eV  345.27 nm  f=0.0030
<S**2>=2.130
    158A ->174A        0.12463
    172A ->178A        0.29911
    172A ->179A        0.77539
    172A ->181A       -0.37617
    172A ->184A       -0.11957
    172A ->185A       -0.10542
    173A ->179A        0.12756
    173A ->184A       -0.11341
    173A ->185A        0.13774
    164B ->172B       -0.13402

 Excited state symmetry could not be determined.
 Excited State  68:  3.291-?Sym    3.6043 eV  343.99 nm  f=0.0346
<S**2>=2.458
    157A ->174A        0.11749
    158A ->174A        0.33305
    172A ->179A       -0.27863
    172A ->181A        0.15411
    172A ->184A        0.10337
    172A ->185A       -0.10776
    173A ->178A       -0.14544
    173A ->179A        0.15604
    173A ->184A       -0.15068
    173A ->185A        0.40529
    173A ->188A       -0.12837
    156B ->172B       -0.14349
    157B ->174B        0.10672
    159B ->172B        0.14072
    160B ->172B        0.20039
    160B ->173B        0.13124
    162B ->172B       -0.17861
    164B ->172B       -0.28435
    164B ->173B       -0.32035
    166B ->174B        0.19632
    171B ->175B       -0.17863

 Excited state symmetry could not be determined.
 Excited State  69:  3.598-?Sym    3.6126 eV  343.20 nm  f=0.0001
<S**2>=2.987
    156A ->174A       -0.20929
```

```
    171A ->176A        0.17000
    172A ->180A        0.13265
    173A ->180A       -0.17870
    173A ->186A        0.24271
    173A ->187A       -0.30430
    173A ->190A       -0.17583
    156B ->174B        0.20276
    157B ->172B       -0.25461
    157B ->173B       -0.13051
    162B ->174B        0.10583
    163B ->173B       -0.18814
    164B ->174B       -0.10710
    171B ->176B        0.54919

 Excited state symmetry could not be determined.
 Excited State  70:  3.350-?Sym    3.6315 eV  341.41 nm  f=0.0094
<S**2>=2.555
    159A ->174A        0.30648
    162A ->174A        0.11710
    170A ->178A        0.13126
    171A ->176A       -0.25220
    171A ->178A       -0.15028
    171A ->185A       -0.21625
    171A ->189A       -0.10795
    173A ->183A        0.11340
    158B ->172B       -0.18622
    158B ->173B       -0.11004
    159B ->174B        0.17907
    163B ->172B        0.28304
    163B ->173B        0.21793
    164B ->174B        0.18704
    168B ->185B       -0.11030
    169B ->177B       -0.28053
    169B ->186B       -0.12748
    171B ->178B       -0.28942
    171B ->179B        0.12997
    171B ->185B       -0.16170

 Excited state symmetry could not be determined.
 Excited State  71:  3.404-?Sym    3.6526 eV  339.44 nm  f=0.0235
<S**2>=2.647
    171A ->178A        0.18634
    171A ->185A        0.13301
    172A ->182A        0.23111
    172A ->183A        0.20282
    172A ->187A        0.18298
    161B ->172B       -0.25788
    161B ->173B       -0.22265
    163B ->172B        0.34473
    163B ->173B        0.29539
```

```
    164B ->174B        0.14933
    166B ->177B        0.14721
    169B ->177B        0.34334
    169B ->180B        0.10530
    169B ->186B        0.19994
    171B ->185B        0.12558

 Excited state symmetry could not be determined.
 Excited State  72:  3.432-?Sym    3.6535 eV  339.35 nm  f=0.0162
<S**2>=2.694
    158A ->174A       -0.17786
    161A ->174A       -0.12184
    168A ->177A        0.12475
    170A ->177A        0.13342
    171A ->175A        0.12995
    171A ->177A        0.27161
    172A ->181A        0.13614
    159B ->172B        0.15574
    159B ->173B        0.13537
    160B ->172B        0.40312
    160B ->173B        0.21381
    161B ->174B        0.11520
    162B ->172B        0.27680
    162B ->173B        0.28847
    166B ->174B        0.14409
    168B ->177B       -0.13027
    170B ->177B       -0.33185
    170B ->186B       -0.14421

 Excited state symmetry could not be determined.
 Excited State  73:  3.537-?Sym    3.6583 eV  338.91 nm  f=0.0136
<S**2>=2.877
    158A ->174A        0.42619
    171A ->175A       -0.24172
    171A ->177A        0.15023
    172A ->181A        0.16026
    172A ->185A        0.10656
    172A ->188A        0.17672
    155B ->172B        0.10668
    155B ->173B       -0.10487
    160B ->172B       -0.24208
    160B ->173B       -0.12688
    162B ->172B       -0.28543
    162B ->173B       -0.24233
    163B ->174B        0.11046
    165B ->173B        0.10064
    166B ->174B        0.10896
    166B ->178B        0.10767
    170B ->177B       -0.25528
    171B ->175B        0.20151
```

```
 Excited state symmetry could not be determined.
 Excited State  74:  3.305-?Sym    3.6643 eV  338.36 nm  f=0.0111
<S**2>=2.481
    159A ->174A        0.40238
    162A ->174A        0.13663
    172A ->183A        0.12370
    158B ->172B       -0.26166
    158B ->173B       -0.11345
    159B ->174B        0.20006
    161B ->172B        0.43388
    161B ->173B        0.18683
    162B ->174B        0.22670
    163B ->172B       -0.23045
    163B ->173B       -0.23649
    165B ->174B        0.10573
    166B ->172B        0.10636
    169B ->177B        0.27112
    169B ->186B        0.14109

 Excited state symmetry could not be determined.
 Excited State  75:  3.246-?Sym    3.7056 eV  334.59 nm  f=0.2131
<S**2>=2.384
    157A ->174A        0.12968
    167A ->174A        0.10644
    171A ->175A        0.57021
    172A ->179A       -0.13177
    172A ->184A       -0.12788
    172A ->188A        0.17142
    173A ->178A        0.14814
    173A ->184A       -0.10334
    173A ->185A       -0.34217
    173A ->189A       -0.14610
    155B ->173B       -0.11347
    160B ->172B       -0.14057
    162B ->172B       -0.11173
    162B ->173B       -0.10851
    164B ->172B       -0.13078
    169B ->176B        0.11036
    171B ->175B       -0.36243

 Excited state symmetry could not be determined.
 Excited State  76:  3.402-?Sym    3.7069 eV  334.47 nm  f=0.0000
<S**2>=2.644
    159A ->174A       -0.20789
    163A ->180A       -0.10332
    166A ->177A       -0.13900
    170A ->178A        0.14230
    171A ->176A        0.14561
    171A ->185A       -0.12627
```

```
    172A ->182A        0.38008
    172A ->187A        0.23375
    172A ->190A       -0.13101
    173A ->186A       -0.13286
    173A ->187A        0.10161
    158B ->172B        0.18056
    159B ->174B       -0.14860
    161B ->172B        0.13028
    163B ->172B       -0.21273
    163B ->173B       -0.28020
    166B ->173B       -0.13067
    166B ->177B        0.14372
    171B ->176B       -0.20448
    171B ->178B       -0.25458
    171B ->179B        0.11560

 Excited state symmetry could not be determined.
 Excited State  77:  3.453-?Sym    3.7115 eV  334.05 nm  f=0.0230
<S**2>=2.732
    157A ->174A       -0.10858
    171A ->175A        0.30647
    171A ->177A        0.18446
    171A ->187A       -0.11073
    172A ->178A       -0.17422
    172A ->184A       -0.15938
    172A ->188A       -0.25054
    172A ->189A        0.17452
    173A ->189A        0.17938
    155B ->172B       -0.15792
    155B ->173B        0.25434
    156B ->172B        0.12333
    157B ->174B       -0.11281
    159B ->172B        0.23485
    159B ->173B       -0.19094
    160B ->172B       -0.22297
    162B ->172B       -0.12530
    162B ->173B       -0.11676
    164B ->172B        0.13154
    170B ->177B       -0.18011
    171B ->175B       -0.12450
    171B ->177B       -0.11162
    171B ->180B        0.11195
    171B ->186B        0.11913
    171B ->187B        0.13226

 Excited state symmetry could not be determined.
 Excited State  78:  3.234-?Sym    3.7323 eV  332.19 nm  f=0.0204
<S**2>=2.364
    157A ->174A       -0.10437
    158A ->174A        0.52873
```

```
    171A ->175A        0.23512
    172A ->184A        0.10834
    173A ->184A       -0.10808
    173A ->185A        0.12623
    156B ->172B        0.14531
    158B ->174B        0.15576
    159B ->172B       -0.43465
    159B ->173B       -0.17889
    162B ->172B        0.32576
    162B ->173B        0.19257
    165B ->172B       -0.10536
    166B ->174B       -0.19023

 Excited state symmetry could not be determined.
 Excited State  79:  3.271-?Sym    3.7477 eV  330.83 nm  f=0.0125
<S**2>=2.425
    157A ->174A       -0.14515
    158A ->174A       -0.25254
    171A ->175A        0.22732
    172A ->179A        0.17347
    172A ->181A        0.21041
    172A ->184A        0.58228
    172A ->189A       -0.11440
    173A ->185A        0.29200
    173A ->188A        0.15022
    173A ->189A        0.17284
    156B ->172B        0.13596
    157B ->174B       -0.11408
    159B ->172B        0.16702
    159B ->173B        0.11384
    160B ->172B       -0.10108
    162B ->172B       -0.13946
    162B ->173B       -0.13756

 Excited state symmetry could not be determined.
 Excited State  80:  3.113-?Sym    3.7519 eV  330.46 nm  f=0.0014
<S**2>=2.173
    169A ->177A       -0.12781
    171A ->178A       -0.12616
    171A ->185A       -0.10195
    172A ->177A        0.13002
    172A ->180A        0.23947
    172A ->182A       -0.46302
    172A ->183A        0.68341
    173A ->186A       -0.18855
    171B ->178B       -0.13389
    171B ->185B       -0.12659
```

Table S43. TD-DFT (B3LYP/CPCM/CH_3CN) Predicted Electronic Transitions for 3^- (*S*=3/2)

```
Excitation energies and oscillator strengths:

 Excited state symmetry could not be determined.
 Excited State   1:  4.019-?Sym    1.0012 eV 1238.34 nm  f=0.0105
<S**2>=3.787
    170B ->172B       -0.21185
    171B ->172B        0.92722
    171B ->173B        0.24984
 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 symmetry could not be determined.
 Excited State   2:  4.022-?Sym    1.4031 eV  883.66 nm  f=0.0134
<S**2>=3.793
    166B ->172B        0.10910
    170B ->172B        0.90402
    170B ->173B        0.28835
    171B ->172B        0.24467

 Excited state symmetry could not be determined.
 Excited State   3:  4.034-?Sym    1.6350 eV  758.33 nm  f=0.0073
<S**2>=3.818
    168B ->173B        0.12414
    170B ->172B        0.17278
    170B ->173B       -0.22983
    171B ->172B       -0.23773
    171B ->173B        0.91185

 Excited state symmetry could not be determined.
 Excited State   4:  4.029-?Sym    1.6711 eV  741.93 nm  f=0.0272
<S**2>=3.808
    168B ->174B        0.15092
    169B ->172B       -0.22557
    170B ->174B       -0.32062
    171B ->174B        0.88946

 Excited state symmetry could not be determined.
 Excited State   5:  4.020-?Sym    1.8188 eV  681.70 nm  f=0.1231
<S**2>=3.791
    169B ->172B        0.90860
    169B ->173B        0.17036
    170B ->174B       -0.30106
    171B ->174B        0.13870

 Excited state symmetry could not be determined.
```

```
 Excited State   6:  4.029-?Sym    1.9917 eV  622.52 nm  f=0.0521
<S**2>=3.809
    168B ->173B        0.10561
    170B ->172B       -0.27760
    170B ->173B        0.90194
    171B ->173B        0.25184

 Excited state symmetry could not be determined.
 Excited State   7:  4.032-?Sym    2.1058 eV  588.79 nm  f=0.0017
<S**2>=3.814
    173A ->175A       -0.15820
    174A ->176A        0.25430
    169B ->172B        0.26369
    169B ->173B       -0.43622
    170B ->174B        0.73011
    171B ->174B        0.27722

 Excited state symmetry could not be determined.
 Excited State   8:  4.039-?Sym    2.1788 eV  569.06 nm  f=0.0002
<S**2>=3.829
    173A ->175A       -0.34190
    174A ->176A        0.48335
    169B ->172B       -0.13232
    169B ->173B        0.74238
    170B ->174B        0.20560

 Excited state symmetry could not be determined.
 Excited State   9:  4.047-?Sym    2.1796 eV  568.84 nm  f=0.0004
<S**2>=3.845
    172A ->176A        0.11147
    173A ->176A       -0.33077
    174A ->175A        0.72370
    168B ->172B       -0.14109
    169B ->174B       -0.53936

 Excited state symmetry could not be determined.
 Excited State  10:  4.038-?Sym    2.2302 eV  555.93 nm  f=0.0625
<S**2>=3.827
    174A ->175A        0.20529
    168B ->172B        0.92535
    168B ->173B        0.15483

 Excited state symmetry could not be determined.
 Excited State  11:  4.044-?Sym    2.2483 eV  551.45 nm  f=0.0063
<S**2>=3.838
    173A ->176A       -0.19879
    174A ->175A        0.44736
    168B ->172B       -0.16971
    169B ->174B        0.82384
```

```
 Excited state symmetry could not be determined.
 Excited State  12:  4.058-?Sym    2.3193 eV  534.58 nm  f=0.0123
<S**2>=3.867
    172A ->175A        0.20435
    173A ->175A       -0.35758
    174A ->176A        0.57250
    169B ->173B       -0.44610
    170B ->174B       -0.42283
    170B ->176B        0.10720
    171B ->174B       -0.23933

 Excited state symmetry could not be determined.
 Excited State  13:  4.129-?Sym    2.3669 eV  523.83 nm  f=0.0036
<S**2>=4.012
    170A ->177A        0.15350
    174A ->177A        0.75834
    174A ->179A        0.31134
    174A ->183A       -0.21576
    174A ->185A        0.23466
    174A ->187A       -0.17872
    174A ->191A        0.19990

 Excited state symmetry could not be determined.
 Excited State  14:  4.116-?Sym    2.6082 eV  475.37 nm  f=0.0071
<S**2>=3.985
    169A ->177A        0.10439
    171A ->186A        0.12246
    172A ->177A        0.48035
    172A ->179A        0.13295
    173A ->177A        0.53111
    173A ->179A        0.16231
    173A ->183A       -0.12457
    174A ->178A       -0.22320
    174A ->180A       -0.12890
    174A ->186A        0.19251
    165B ->172B        0.18699
    167B ->172B        0.25163
    167B ->173B       -0.13409

 Excited state symmetry could not be determined.
 Excited State  15:  4.044-?Sym    2.6412 eV  469.43 nm  f=0.0003
<S**2>=3.838
    172A ->177A       -0.12276
    173A ->175A        0.60854
    174A ->176A        0.45020
    174A ->178A        0.14249
    174A ->181A       -0.11495
    174A ->184A       -0.11806
    166B ->174B       -0.13780
    167B ->172B        0.45047
```

```
    167B ->173B       -0.28762

 Excited state symmetry could not be determined.
 Excited State  16:  4.054-?Sym    2.6708 eV  464.22 nm  f=0.0067
<S**2>=3.858
    172A ->177A       -0.10072
    173A ->175A       -0.54899
    174A ->176A       -0.31090
    174A ->178A        0.18825
    174A ->184A       -0.18130
    174A ->186A       -0.11304
    166B ->174B       -0.12802
    167B ->172B        0.58602
    167B ->173B       -0.27720

 Excited state symmetry could not be determined.
 Excited State  17:  4.050-?Sym    2.6954 eV  459.98 nm  f=0.0005
<S**2>=3.851
    173A ->176A        0.87327
    174A ->175A        0.42906

 Excited state symmetry could not be determined.
 Excited State  18:  4.115-?Sym    2.7227 eV  455.38 nm  f=0.0000
<S**2>=3.984
    167A ->186A       -0.11010
    172A ->177A        0.26729
    173A ->177A        0.31778
    174A ->178A        0.50672
    174A ->180A        0.25252
    174A ->184A       -0.22612
    174A ->186A       -0.38777
    174A ->189A       -0.18837
    165B ->172B        0.10924
    167B ->172B       -0.31333

 Excited state symmetry could not be determined.
 Excited State  19:  4.645-?Sym    2.7520 eV  450.52 nm  f=0.0027
<S**2>=5.144
    169A ->186A        0.10035
    171A ->177A        0.39422
    171A ->179A        0.20356
    171A ->183A       -0.14353
    171A ->185A        0.19476
    171A ->187A       -0.16846
    171A ->191A        0.19903
    172A ->178A       -0.18922
    172A ->186A        0.10673
    173A ->176A        0.10114
    173A ->178A       -0.19871
    173A ->184A        0.14267
```

```
    173A ->186A        0.10767
    174A ->183A        0.13580
    166B ->172B       -0.15809
    166B ->173B        0.20458
    167B ->174B        0.20759
    170B ->177B        0.13652
    170B ->185B       -0.11012
    170B ->187B       -0.11900
    171B ->177B       -0.29913
    171B ->180B        0.17658
    171B ->185B        0.13526
    171B ->187B        0.15340

 Excited state symmetry could not be determined.
 Excited State  20:  4.063-?Sym    2.7866 eV  444.93 nm  f=0.0010
<S**2>=3.877
    172A ->175A        0.11700
    172A ->177A        0.15320
    173A ->183A        0.19454
    174A ->180A        0.14679
    174A ->181A        0.23724
    174A ->184A        0.13300
    174A ->186A       -0.11553
    166B ->174B        0.22442
    167B ->172B        0.52110
    167B ->173B        0.65483

 Excited state symmetry could not be determined.
 Excited State  21:  4.261-?Sym    2.8100 eV  441.22 nm  f=0.0176
<S**2>=4.288
    171A ->177A       -0.18761
    171A ->185A       -0.10569
    171A ->191A       -0.10744
    173A ->181A        0.16920
    173A ->184A        0.17649
    174A ->183A        0.31225
    166B ->172B       -0.28546
    166B ->173B        0.36584
    167B ->174B        0.44409
    168B ->173B        0.33685
    170B ->177B       -0.10666
    171B ->177B        0.15888

 Excited state symmetry could not be determined.
 Excited State  22:  4.038-?Sym    2.8128 eV  440.78 nm  f=0.0016
<S**2>=3.827
    172A ->175A        0.94189
    174A ->176A       -0.20306

 Excited state symmetry could not be determined.
```

```
 Excited State  23:  4.133-?Sym    2.8777 eV  430.85 nm  f=0.0084
<S**2>=4.019
    169A ->186A       -0.10546
    172A ->176A        0.73759
    172A ->178A        0.26818
    172A ->180A        0.11493
    173A ->176A        0.11533
    173A ->178A        0.22725
    173A ->180A        0.19079
    173A ->186A       -0.15692
    174A ->183A        0.10833
    166B ->172B        0.12725
    170B ->177B        0.10238

 Excited state symmetry could not be determined.
 Excited State  24:  4.080-?Sym    2.8893 eV  429.11 nm  f=0.0005
<S**2>=3.912
    173A ->177A       -0.25260
    158B ->173B        0.11686
    164B ->174B        0.13914
    165B ->172B        0.87075
    167B ->173B       -0.10254

 Excited state symmetry could not be determined.
 Excited State  25:  4.048-?Sym    2.8894 eV  429.11 nm  f=0.0085
<S**2>=3.847
    172A ->176A        0.30445
    172A ->178A       -0.17443
    173A ->178A       -0.12484
    173A ->180A       -0.12509
    173A ->181A       -0.11737
    173A ->186A        0.10470
    174A ->183A       -0.17613
    164B ->173B       -0.10157
    165B ->174B        0.12090
    166B ->172B        0.21540
    166B ->173B       -0.18360
    167B ->174B       -0.17938
    168B ->172B       -0.16298
    168B ->173B        0.73264
    171B ->173B       -0.10568

 Excited state symmetry could not be determined.
 Excited State  26:  4.050-?Sym    2.9103 eV  426.02 nm  f=0.0001
<S**2>=3.852
    172A ->177A       -0.43465
    173A ->177A        0.26108
    173A ->179A        0.22859
    173A ->182A        0.20927
    174A ->178A       -0.29365
```

```
    174A ->180A        0.37318
    174A ->181A        0.46915
    164B ->174B        0.16637
    165B ->173B       -0.26442

 Excited state symmetry could not be determined.
 Excited State  27:  4.139-?Sym    2.9132 eV  425.59 nm  f=0.0420
<S**2>=4.032
    169A ->186A        0.13824
    172A ->176A        0.52114
    172A ->178A       -0.31020
    172A ->180A       -0.13052
    172A ->186A        0.15090
    173A ->178A       -0.32408
    173A ->180A       -0.12856
    173A ->186A        0.19507
    166B ->172B       -0.10220
    168B ->173B       -0.44626
    170B ->177B       -0.11471
    171B ->177B        0.11022

 Excited state symmetry could not be determined.
 Excited State  28:  4.791-?Sym    2.9541 eV  419.71 nm  f=0.0002
<S**2>=5.488
    170A ->186A        0.13253
    171A ->178A        0.24906
    171A ->180A        0.13389
    171A ->184A       -0.16070
    171A ->186A       -0.39070
    171A ->189A       -0.24231
    173A ->177A        0.23514
    174A ->178A       -0.18393
    174A ->180A       -0.12167
    166B ->186B       -0.10606
    168B ->174B       -0.10842
    168B ->186B        0.12384
    170B ->178B        0.10860
    170B ->179B        0.10241
    170B ->184B       -0.10004
    170B ->186B       -0.26683
    171B ->178B       -0.20719
    171B ->179B       -0.18607
    171B ->184B        0.16228
    171B ->186B        0.42041
    171B ->191B        0.12440

 Excited state symmetry could not be determined.
 Excited State  29:  4.049-?Sym    2.9555 eV  419.51 nm  f=0.0190
<S**2>=3.848
    172A ->176A       -0.10561
```

```
    173A ->178A       -0.14510
    173A ->184A        0.10619
    174A ->179A        0.16510
    174A ->183A        0.11610
    166B ->172B        0.85226
    166B ->173B        0.21984
    167B ->174B        0.16894
    170B ->172B       -0.11418

 Excited state symmetry could not be determined.
 Excited State  30:  4.044-?Sym    2.9743 eV  416.85 nm  f=0.0042
<S**2>=3.838
    173A ->178A       -0.11113
    173A ->180A        0.27441
    173A ->181A        0.13431
    174A ->177A       -0.41173
    174A ->179A        0.65423
    174A ->182A        0.34823
    174A ->183A       -0.10164
    164B ->173B        0.11416
    166B ->172B       -0.15352
    166B ->173B       -0.10474
    167B ->174B       -0.10752
    168B ->173B        0.14905

 Excited state symmetry could not be determined.
 Excited State  31:  4.057-?Sym    2.9753 eV  416.72 nm  f=0.0571
<S**2>=3.865
    172A ->177A        0.44719
    173A ->177A       -0.31798
    173A ->182A        0.15632
    174A ->178A       -0.21180
    174A ->180A        0.43645
    174A ->181A        0.31549
    158B ->173B       -0.12325
    164B ->174B       -0.14442
    165B ->172B       -0.16464
    165B ->173B        0.26861
    167B ->173B       -0.30302
    168B ->174B        0.11162

 Excited state symmetry could not be determined.
 Excited State  32:  4.073-?Sym    3.0162 eV  411.06 nm  f=0.0061
<S**2>=3.897
    172A ->178A       -0.11253
    172A ->180A       -0.10387
    173A ->181A        0.28661
    174A ->177A        0.28815
    174A ->179A       -0.34693
    174A ->182A        0.41079
```

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    174A ->183A        0.15102
    158B ->174B        0.16125
    162B ->174B       -0.10004
    163B ->173B       -0.10253
    164B ->172B       -0.22075
    164B ->173B        0.36604
    165B ->174B       -0.30696
    168B ->173B        0.14617

 Excited state symmetry could not be determined.
 Excited State  33:  4.052-?Sym    3.0448 eV  407.20 nm  f=0.0003
<S**2>=3.855
    173A ->180A        0.16590
    173A ->181A        0.25670
    173A ->184A       -0.11876
    174A ->177A        0.13957
    174A ->179A       -0.12335
    174A ->182A        0.47804
    158B ->174B       -0.21036
    159B ->173B       -0.13329
    161B ->173B        0.17616
    164B ->172B        0.33593
    164B ->173B       -0.39096
    165B ->174B        0.37160
    168B ->173B       -0.12441

 Excited state symmetry could not be determined.
 Excited State  34:  4.040-?Sym    3.0507 eV  406.42 nm  f=0.0170
<S**2>=3.830
    172A ->177A       -0.38976
    172A ->179A        0.13020
    173A ->177A        0.17459
    173A ->179A        0.17843
    158B ->173B       -0.21623
    164B ->174B       -0.29930
    165B ->172B        0.27166
    165B ->173B        0.59791
    168B ->174B        0.26005

 Excited state symmetry could not be determined.
 Excited State  35:  4.056-?Sym    3.0686 eV  404.04 nm  f=0.0104
<S**2>=3.862
    172A ->179A       -0.15878
    173A ->177A        0.21540
    173A ->179A       -0.27291
    173A ->183A        0.13157
    174A ->178A        0.17208
    174A ->180A       -0.36676
    174A ->181A        0.42471
    167B ->173B       -0.18331
```

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    168B ->174B        0.59174
    171B ->174B       -0.11519

 Excited state symmetry could not be determined.
 Excited State  36:  4.097-?Sym    3.0864 eV  401.71 nm  f=0.0018
<S**2>=3.946
    172A ->179A        0.33366
    172A ->183A       -0.15406
    172A ->185A        0.15451
    173A ->177A       -0.27422
    173A ->179A        0.34397
    173A ->185A        0.11175
    174A ->180A        0.13035
    174A ->181A       -0.21546
    174A ->184A        0.11727
    158B ->173B        0.10318
    164B ->174B        0.13221
    165B ->173B       -0.24732
    168B ->174B        0.56124
    171B ->174B       -0.10318

 Excited state symmetry could not be determined.
 Excited State  37:  4.289-?Sym    3.1074 eV  399.00 nm  f=0.0093
<S**2>=4.349
    167A ->177A        0.11445
    169A ->186A        0.11460
    170A ->177A       -0.17727
    171A ->185A        0.10224
    172A ->178A        0.37497
    172A ->180A        0.14783
    172A ->184A        0.14229
    172A ->186A        0.20594
    173A ->178A       -0.11679
    173A ->184A        0.12740
    173A ->186A        0.30143
    174A ->182A        0.17182
    174A ->183A       -0.12630
    159B ->172B        0.11495
    163B ->172B       -0.36227
    164B ->172B       -0.21297
    164B ->173B       -0.16289
    166B ->172B       -0.16223
    170B ->177B        0.11418
    171B ->177B        0.25766

 Excited state symmetry could not be determined.
 Excited State  38:  4.072-?Sym    3.1268 eV  396.52 nm  f=0.0104
<S**2>=3.895
    172A ->179A        0.31429
    172A ->183A       -0.17112
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    172A ->185A        0.13393
    173A ->177A       -0.20096
    173A ->179A        0.14397
    173A ->185A        0.11261
    174A ->178A        0.40553
    174A ->180A       -0.28445
    174A ->181A        0.45981
    174A ->184A        0.19946
    174A ->186A        0.11504
    165B ->173B        0.13419
    167B ->173B       -0.17378
    168B ->174B       -0.30012

 Excited state symmetry could not be determined.
 Excited State  39:  4.118-?Sym    3.1694 eV  391.20 nm  f=0.1639
<S**2>=3.989
    172A ->178A        0.13875
    172A ->180A        0.14596
    173A ->178A       -0.33977
    173A ->180A        0.10101
    174A ->177A        0.18687
    174A ->179A        0.22045
    174A ->182A       -0.27071
    174A ->183A        0.51945
    166B ->173B       -0.10738
    167B ->174B       -0.40045
    171B ->175B        0.35379

 Excited state symmetry could not be determined.
 Excited State  40:  4.064-?Sym    3.1778 eV  390.16 nm  f=0.0610
<S**2>=3.880
    172A ->179A       -0.13083
    173A ->177A        0.17588
    173A ->182A       -0.32945
    173A ->183A        0.32018
    174A ->180A        0.27411
    174A ->181A       -0.12585
    174A ->184A        0.60193
    174A ->186A       -0.14137
    166B ->174B        0.17916
    167B ->173B       -0.32600
    171B ->176B        0.16113

 Excited state symmetry could not be determined.
 Excited State  41:  4.095-?Sym    3.2269 eV  384.23 nm  f=0.0178
<S**2>=3.943
    172A ->178A       -0.28349
    172A ->180A        0.40827
    172A ->181A       -0.24223
    173A ->178A       -0.30846
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    173A ->180A        0.49720
    173A ->181A       -0.23284
    174A ->182A       -0.10097
    174A ->183A       -0.12259
    166B ->173B       -0.15018
    167B ->174B        0.30100
    171B ->175B       -0.22271

 Excited state symmetry could not be determined.
 Excited State  42:  4.100-?Sym    3.2381 eV  382.89 nm  f=0.0050
<S**2>=3.953
    170A ->186A        0.10789
    172A ->179A       -0.11390
    173A ->177A        0.12631
    173A ->179A       -0.16159
    173A ->182A        0.24068
    173A ->183A       -0.13007
    174A ->178A        0.45244
    174A ->180A        0.40062
    174A ->181A       -0.15709
    174A ->184A        0.18557
    174A ->186A        0.51837
    174A ->189A        0.15182
    167B ->173B        0.10961
    168B ->174B        0.10608
    170B ->186B       -0.12120

 Excited state symmetry could not be determined.
 Excited State  43:  4.151-?Sym    3.2431 eV  382.30 nm  f=0.0228
<S**2>=4.058
    171A ->175A        0.12317
    171A ->177A       -0.10074
    172A ->178A       -0.19821
    172A ->180A        0.15420
    172A ->181A       -0.13010
    173A ->180A        0.18881
    174A ->177A       -0.10389
    174A ->179A       -0.20019
    174A ->183A       -0.28354
    164B ->172B       -0.15165
    166B ->173B        0.56376
    167B ->174B       -0.40491
    171B ->175B        0.27497
    171B ->177B       -0.11405

 Excited state symmetry could not be determined.
 Excited State  44:  4.087-?Sym    3.2623 eV  380.06 nm  f=0.0793
<S**2>=3.925
    172A ->178A        0.37566
    172A ->180A        0.19414
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    173A ->178A       -0.32826
    173A ->180A       -0.16454
    173A ->181A       -0.23870
    174A ->182A        0.19570
    174A ->183A       -0.12190
    174A ->187A        0.10788
    163B ->172B        0.26827
    164B ->172B        0.37530
    164B ->173B        0.21422
    165B ->174B       -0.11544
    166B ->173B        0.28915
    171B ->175B       -0.28101

 Excited state symmetry could not be determined.
 Excited State  45:  4.054-?Sym    3.2677 eV  379.43 nm  f=0.0114
<S**2>=3.858
    172A ->178A        0.34283
    172A ->180A       -0.13258
    173A ->178A       -0.25893
    173A ->180A        0.25648
    173A ->181A        0.53773
    174A ->179A       -0.21049
    174A ->182A       -0.41434
    174A ->183A       -0.27296
    164B ->172B        0.15366
    166B ->173B       -0.18856
    171B ->177B       -0.10038

 Excited state symmetry could not be determined.
 Excited State  46:  4.101-?Sym    3.2827 eV  377.69 nm  f=0.0404
<S**2>=3.955
    169A ->186A        0.10518
    172A ->180A        0.13871
    172A ->181A       -0.12104
    172A ->184A        0.17360
    172A ->186A        0.29423
    173A ->178A        0.46081
    173A ->180A        0.28383
    173A ->184A        0.12377
    173A ->186A        0.12933
    163B ->172B        0.16774
    164B ->172B        0.52684
    164B ->173B        0.14497
    171B ->175B        0.15947
    171B ->177B        0.19136

 Excited state symmetry could not be determined.
 Excited State  47:  4.359-?Sym    3.3036 eV  375.30 nm  f=0.0210
<S**2>=4.501
    171A ->175A        0.17754
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    172A ->178A        0.14420
    172A ->180A        0.26361
    173A ->180A       -0.14408
    173A ->181A       -0.14937
    173A ->184A        0.16021
    174A ->177A       -0.10631
    174A ->179A       -0.16042
    174A ->182A        0.25818
    174A ->185A        0.11409
    166B ->173B       -0.33162
    167B ->174B        0.31457
    170B ->177B       -0.12641
    171B ->175B        0.53835
    171B ->177B       -0.19035

 Excited state symmetry could not be determined.
 Excited State  48:  4.056-?Sym    3.3097 eV  374.61 nm  f=0.0003
<S**2>=3.863
    172A ->179A       -0.27857
    172A ->182A       -0.14032
    172A ->183A        0.10800
    172A ->185A       -0.15261
    173A ->179A        0.64396
    173A ->182A        0.43756
    173A ->183A        0.28393
    174A ->178A        0.13217
    174A ->180A       -0.23568
    174A ->181A       -0.16750

 Excited state symmetry could not be determined.
 Excited State  49:  4.460-?Sym    3.3367 eV  371.58 nm  f=0.1233
<S**2>=4.723
    171A ->175A        0.32090
    171A ->177A        0.10005
    172A ->180A       -0.10054
    172A ->186A       -0.11641
    173A ->180A       -0.11419
    173A ->184A       -0.13391
    174A ->179A        0.16627
    174A ->183A       -0.35836
    174A ->185A       -0.13207
    166B ->173B        0.10424
    167B ->174B        0.24770
    170B ->177B        0.21275
    170B ->180B       -0.11727
    171B ->175B        0.36803
    171B ->177B        0.35799
    171B ->180B       -0.15397

 Excited state symmetry could not be determined.
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 Excited State  50:  4.272-?Sym    3.3375 eV  371.49 nm  f=0.0008
<S**2>=4.312
    171A ->176A       -0.14791
    172A ->179A       -0.36057
    172A ->182A        0.11843
    173A ->177A       -0.12817
    173A ->179A        0.23922
    173A ->182A       -0.30569
    173A ->183A       -0.27192
    173A ->187A       -0.10239
    174A ->181A        0.17877
    174A ->189A        0.10445
    166B ->174B       -0.39978
    167B ->173B        0.20109
    171B ->176B        0.47485

 Excited state symmetry could not be determined.
 Excited State  51:  4.540-?Sym    3.3491 eV  370.20 nm  f=0.0147
<S**2>=4.902
    171A ->176A       -0.30737
    172A ->183A       -0.15191
    172A ->185A        0.11436
    173A ->179A       -0.23012
    173A ->182A        0.29403
    174A ->181A       -0.13427
    174A ->184A       -0.10965
    166B ->174B        0.27899
    171B ->176B        0.68685

 Excited state symmetry could not be determined.
 Excited State  52:  4.238-?Sym    3.3679 eV  368.14 nm  f=0.0039
<S**2>=4.239
    169A ->177A       -0.11303
    170A ->178A       -0.10171
    171A ->176A       -0.13135
    172A ->179A        0.57394
    172A ->182A       -0.11181
    172A ->183A        0.28938
    172A ->185A       -0.21762
    173A ->177A        0.11343
    173A ->179A        0.10642
    173A ->182A       -0.23014
    173A ->183A        0.17821
    173A ->185A       -0.17405
    174A ->184A       -0.11149
    174A ->186A        0.11428
    158B ->172B        0.14782
    165B ->172B       -0.11275
    169B ->177B        0.15309
    171B ->176B        0.20072
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    171B ->178B        0.18549

 Excited state symmetry could not be determined.
 Excited State  53:  4.149-?Sym    3.3746 eV  367.40 nm  f=0.0068
<S**2>=4.053
    171A ->175A       -0.10967
    171A ->177A       -0.43639
    171A ->179A       -0.17843
    171A ->183A        0.12601
    171A ->185A       -0.15278
    171A ->187A        0.12710
    171A ->191A       -0.14351
    172A ->178A       -0.14654
    173A ->180A       -0.15490
    173A ->181A        0.11975
    166B ->173B       -0.12328
    169B ->186B       -0.13910
    170B ->177B        0.43822
    170B ->180B       -0.25884
    170B ->183B       -0.12819
    170B ->185B       -0.21145
    170B ->187B       -0.21946
    170B ->189B       -0.12167
    170B ->193B       -0.11148
    171B ->177B       -0.21232

 Excited state symmetry could not be determined.
 Excited State  54:  4.085-?Sym    3.3993 eV  364.73 nm  f=0.0358
<S**2>=3.922
    171A ->175A       -0.11618
    171A ->177A        0.10532
    171A ->179A        0.10189
    172A ->178A       -0.15823
    172A ->180A        0.52953
    172A ->181A       -0.27417
    173A ->180A       -0.46254
    173A ->181A        0.46980
    167B ->174B       -0.10165
    171B ->175B       -0.13152
    171B ->177B        0.16606

 Excited state symmetry could not be determined.
 Excited State  55:  4.062-?Sym    3.4293 eV  361.55 nm  f=0.0952
<S**2>=3.875
    172A ->179A       -0.20591
    173A ->179A        0.17364
    173A ->182A       -0.37729
    173A ->183A       -0.19331
    174A ->184A       -0.37095
    174A ->186A        0.22349
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    166B ->174B        0.65932
    167B ->173B       -0.11976

 Excited state symmetry could not be determined.
 Excited State  56:  4.102-?Sym    3.4408 eV  360.34 nm  f=0.0392
<S**2>=3.956
    172A ->178A        0.11323
    173A ->178A        0.22233
    173A ->184A        0.17862
    173A ->186A        0.19332
    174A ->179A        0.10338
    174A ->185A       -0.15369
    174A ->187A        0.11714
    159B ->172B       -0.10942
    161B ->172B        0.23368
    163B ->172B        0.56667
    163B ->173B        0.10899
    164B ->172B       -0.44043
    164B ->173B       -0.15333
    165B ->174B        0.14796

 Excited state symmetry could not be determined.
 Excited State  57:  4.212-?Sym    3.4609 eV  358.25 nm  f=0.0006
<S**2>=4.185
    170A ->186A       -0.10551
    171A ->178A       -0.27316
    171A ->180A       -0.14203
    171A ->184A        0.15393
    171A ->186A        0.35917
    171A ->189A        0.19953
    173A ->182A       -0.10488
    168B ->174B        0.10906
    168B ->186B        0.16962
    169B ->177B        0.24916
    169B ->180B       -0.14446
    169B ->185B       -0.10432
    169B ->187B       -0.12747
    171B ->178B       -0.33912
    171B ->179B       -0.30735
    171B ->184B        0.16347
    171B ->186B        0.37685
    171B ->191B        0.10031

 Excited state symmetry could not be determined.
 Excited State  58:  4.155-?Sym    3.4840 eV  355.87 nm  f=0.0527
<S**2>=4.065
    171A ->175A        0.39043
    171A ->177A       -0.11820
    172A ->180A        0.14511
    172A ->184A        0.17435
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    173A ->178A        0.10968
    173A ->181A        0.14753
    173A ->184A       -0.37091
    173A ->186A        0.15114
    174A ->179A        0.19125
    174A ->182A       -0.17879
    174A ->185A       -0.32624
    174A ->187A        0.22499
    163B ->172B       -0.18915
    170B ->177B       -0.18849
    170B ->180B        0.12186
    171B ->177B       -0.28591

 Excited state symmetry could not be determined.
 Excited State  59:  4.085-?Sym    3.4867 eV  355.59 nm  f=0.0184
<S**2>=3.922
    172A ->183A       -0.26519
    173A ->182A       -0.18290
    173A ->183A        0.66806
    173A ->185A        0.12411
    174A ->184A       -0.43618
    174A ->186A        0.18176
    174A ->189A        0.14369
    166B ->174B       -0.22576
    169B ->177B       -0.10739

 Excited state symmetry could not be determined.
 Excited State  60:  4.099-?Sym    3.5089 eV  353.34 nm  f=0.0755
<S**2>=3.950
    172A ->178A       -0.17537
    172A ->181A        0.24456
    172A ->184A       -0.16764
    172A ->186A       -0.16417
    173A ->178A        0.10314
    173A ->180A        0.16505
    173A ->181A        0.13189
    173A ->184A        0.53650
    173A ->188A       -0.12634
    173A ->189A       -0.15576
    174A ->179A        0.12534
    174A ->183A       -0.11493
    174A ->185A       -0.18934
    174A ->187A        0.32451
    156B ->173B       -0.17710
    157B ->174B        0.13688
    163B ->172B       -0.24985
    164B ->173B        0.10335
    166B ->173B       -0.17045

 Excited state symmetry could not be determined.
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 Excited State  61:  4.232-?Sym    3.5384 eV  350.40 nm  f=0.0130
<S**2>=4.226
    168A ->183A       -0.11869
    171A ->176A        0.25249
    171A ->178A       -0.10020
    172A ->187A        0.14238
    173A ->179A       -0.15498
    173A ->182A        0.18541
    173A ->187A       -0.26041
    173A ->190A       -0.12175
    173A ->191A       -0.12531
    174A ->181A       -0.10069
    174A ->186A       -0.19372
    174A ->188A        0.24556
    174A ->189A        0.36931
    156B ->174B        0.20693
    157B ->173B       -0.22800
    158B ->172B        0.14888
    162B ->172B       -0.15776
    162B ->173B        0.11750
    166B ->174B        0.12055
    166B ->184B       -0.12039
    167B ->183B       -0.13660
    169B ->177B        0.10423
    170B ->186B       -0.15346
    171B ->176B        0.15309

 Excited state symmetry could not be determined.
 Excited State  62:  4.044-?Sym    3.5479 eV  349.45 nm  f=0.0058
<S**2>=3.838
    172A ->180A        0.39164
    172A ->181A        0.82325
    172A ->184A        0.14555
    173A ->181A        0.14294
    174A ->187A       -0.10916

 Excited state symmetry could not be determined.
 Excited State  63:  4.115-?Sym    3.5573 eV  348.53 nm  f=0.2211
<S**2>=3.983
    171A ->175A        0.60078
    174A ->177A       -0.11625
    174A ->179A       -0.11537
    174A ->183A        0.21946
    174A ->185A        0.36707
    174A ->190A        0.13281
    174A ->191A        0.19352
    166B ->173B       -0.15205
    169B ->176B        0.15145
    170B ->175B        0.13827
    170B ->177B        0.15102
```

```
    171B ->175B       -0.30477
    171B ->177B        0.12937

 Excited state symmetry could not be determined.
 Excited State  64:  4.302-?Sym    3.5912 eV  345.24 nm  f=0.0293
<S**2>=4.376
    171A ->175A        0.24357
    172A ->188A       -0.17214
    173A ->184A        0.35170
    173A ->186A       -0.17070
    173A ->189A        0.18055
    174A ->185A       -0.14300
    174A ->187A       -0.24834
    174A ->190A       -0.12777
    174A ->191A       -0.13494
    154B ->172B       -0.11284
    156B ->173B        0.11821
    163B ->172B       -0.13724
    164B ->173B       -0.10844
    165B ->174B       -0.16478
    169B ->176B        0.11320
    170B ->175B        0.48906
    171B ->177B       -0.20935
    171B ->180B       -0.11558
    171B ->185B       -0.10968

 Excited state symmetry could not be determined.
 Excited State  65:  4.336-?Sym    3.5961 eV  344.78 nm  f=0.0195
<S**2>=4.451
    161A ->179A       -0.10474
    165A ->177A        0.13465
    170A ->178A        0.12103
    171A ->176A        0.15879
    172A ->179A        0.10959
    172A ->183A        0.36813
    172A ->185A       -0.27573
    172A ->187A       -0.11508
    172A ->191A        0.10035
    173A ->185A       -0.14931
    173A ->187A       -0.15395
    174A ->189A        0.10371
    158B ->172B       -0.28180
    158B ->173B       -0.12919
    159B ->179B       -0.11460
    160B ->172B       -0.25947
    162B ->172B        0.27015
    165B ->172B        0.12943
    165B ->177B       -0.12865
    169B ->185B        0.10669
    171B ->176B        0.13100
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    171B ->179B       -0.18260

 Excited state symmetry could not be determined.
 Excited State  66:  4.600-?Sym    3.6164 eV  342.84 nm  f=0.0541
<S**2>=5.041
    170A ->175A        0.17520
    171A ->175A       -0.32815
    173A ->184A       -0.16514
    173A ->186A        0.10304
    174A ->187A        0.10900
    156B ->173B       -0.10169
    164B ->173B        0.11315
    167B ->174B        0.11919
    167B ->176B       -0.14626
    170B ->175B        0.73529
    171B ->175B        0.11524

 Excited state symmetry could not be determined.
 Excited State  67:  4.155-?Sym    3.6408 eV  340.54 nm  f=0.0004
<S**2>=4.067
    171A ->176A        0.46935
    173A ->183A       -0.10981
    174A ->189A       -0.13545
    157B ->173B        0.10330
    158B ->172B       -0.16544
    158B ->173B        0.13639
    162B ->172B        0.15816
    162B ->173B       -0.13333
    164B ->174B        0.39191
    165B ->173B        0.35021
    169B ->175B       -0.23820
    170B ->176B       -0.30856
    171B ->176B        0.21199

 Excited state symmetry could not be determined.
 Excited State  68:  4.362-?Sym    3.6455 eV  340.10 nm  f=0.0302
<S**2>=4.507
    167A ->185A       -0.11865
    171A ->175A        0.19139
    171A ->177A       -0.17900
    171A ->185A        0.12269
    172A ->180A       -0.10114
    172A ->186A        0.17747
    172A ->188A        0.30286
    172A ->189A       -0.16293
    173A ->184A        0.25163
    173A ->186A       -0.19793
    173A ->188A        0.25802
    174A ->185A       -0.10694
    174A ->191A       -0.14169
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    152B ->172B       -0.12820
    154B ->172B        0.19174
    164B ->173B        0.14646
    165B ->174B        0.22239
    171B ->177B        0.12114
    171B ->180B        0.21853
    171B ->183B        0.11078
    171B ->185B        0.18945

 Excited state symmetry could not be determined.
 Excited State  69:  4.419-?Sym    3.6459 eV  340.06 nm  f=0.0021
<S**2>=4.632
    170A ->176A       -0.14643
    171A ->176A        0.56332
    172A ->183A        0.13459
    158B ->172B        0.19812
    160B ->172B        0.13895
    162B ->172B       -0.17407
    164B ->174B       -0.22085
    165B ->173B       -0.22899
    169B ->175B       -0.14742
    169B ->177B       -0.18363
    169B ->180B        0.11726
    170B ->176B        0.43217
    171B ->176B        0.21765

 Excited state symmetry could not be determined.
 Excited State  70:  4.091-?Sym    3.6716 eV  337.68 nm  f=0.0017
<S**2>=3.934
    171A ->177A        0.10370
    172A ->188A       -0.14871
    174A ->187A       -0.11349
    163B ->172B       -0.11344
    164B ->173B        0.57028
    165B ->174B        0.69141
    171B ->180B       -0.11881

 Excited state symmetry could not be determined.
 Excited State  71:  4.451-?Sym    3.6726 eV  337.59 nm  f=0.0135
<S**2>=4.704
    170A ->176A       -0.13755
    172A ->182A        0.11031
    172A ->183A       -0.17784
    158B ->172B       -0.24654
    160B ->172B       -0.23160
    162B ->172B        0.34146
    164B ->174B        0.13341
    165B ->173B        0.15538
    166B ->174B        0.16547
    167B ->175B       -0.14438
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    169B ->175B        0.11910
    169B ->177B        0.22167
    169B ->180B       -0.12978
    169B ->185B       -0.10474
    170B ->176B        0.61382

 Excited state symmetry could not be determined.
 Excited State  72:  4.114-?Sym    3.6972 eV  335.35 nm  f=0.0027
<S**2>=3.981
    171A ->176A        0.13872
    172A ->179A        0.10514
    172A ->182A        0.74820
    172A ->183A       -0.25571
    172A ->185A       -0.10712
    173A ->179A        0.10270
    173A ->182A        0.16579
    173A ->185A       -0.15884
    173A ->187A        0.10150
    164B ->174B       -0.19733
    165B ->173B       -0.15817
    169B ->175B       -0.10602
    169B ->177B        0.17348
    170B ->176B       -0.14863

 Excited state symmetry could not be determined.
 Excited State  73:  4.096-?Sym    3.7033 eV  334.79 nm  f=0.0007
<S**2>=3.945
    172A ->182A        0.41136
    172A ->183A        0.35724
    173A ->182A        0.15391
    158B ->173B        0.13864
    160B ->172B        0.33438
    161B ->174B       -0.11394
    162B ->172B       -0.29581
    164B ->174B        0.40061
    165B ->173B        0.30910
    169B ->175B        0.12510
    169B ->177B       -0.13279
    170B ->176B        0.16058

 Excited state symmetry could not be determined.
 Excited State  74:  4.340-?Sym    3.7267 eV  332.69 nm  f=0.0112
<S**2>=4.459
    170A ->177A       -0.10682
    171A ->177A       -0.10515
    172A ->180A       -0.13916
    172A ->181A        0.11936
    172A ->186A       -0.17627
    172A ->188A       -0.20878
    173A ->188A       -0.12161
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    174A ->185A       -0.12018
    159B ->172B        0.49783
    160B ->179B        0.10102
    163B ->172B        0.29419
    164B ->173B        0.11155
    168B ->177B       -0.19410
    169B ->186B       -0.18343
    171B ->177B        0.25293
    171B ->180B        0.26636
    171B ->183B        0.13388
    171B ->185B        0.11400
    171B ->187B        0.12440

 Excited state symmetry could not be determined.
 Excited State  75:  4.180-?Sym    3.7399 eV  331.52 nm  f=0.0002
<S**2>=4.117
    171A ->178A        0.12239
    172A ->182A       -0.34826
    172A ->183A       -0.33379
    172A ->185A       -0.11512
    173A ->185A       -0.17074
    158B ->172B       -0.30839
    160B ->172B        0.58323
    162B ->172B       -0.20062
    169B ->177B        0.14591
    171B ->186B       -0.11197

 Excited state symmetry could not be determined.
 Excited State  76:  4.133-?Sym    3.7523 eV  330.42 nm  f=0.0001
<S**2>=4.021
    172A ->182A        0.10552
    172A ->183A        0.33105
    172A ->185A        0.22218
    173A ->185A        0.19516
    158B ->172B       -0.34093
    158B ->173B       -0.13681
    160B ->172B        0.46876
    162B ->172B        0.41614
    164B ->174B       -0.24211
    165B ->173B       -0.14054
    169B ->175B       -0.12837
    171B ->179B        0.18474

 Excited state symmetry could not be determined.
 Excited State  77:  4.181-?Sym    3.7699 eV  328.88 nm  f=0.0002
<S**2>=4.120
    172A ->188A        0.10516
    174A ->185A        0.12602
    159B ->172B        0.75526
    159B ->173B        0.10644
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    161B ->172B        0.23999
    168B ->177B        0.10237
    169B ->186B        0.15475
    171B ->177B       -0.25895
    171B ->180B       -0.31349

 Excited state symmetry could not be determined.
 Excited State  78:  4.093-?Sym    3.7765 eV  328.30 nm  f=0.0078
<S**2>=3.937
    172A ->182A        0.13658
    172A ->183A       -0.13967
    172A ->185A       -0.20573
    173A ->185A       -0.10552
    158B ->172B        0.47995
    160B ->172B        0.31971
    161B ->174B        0.11441
    162B ->172B        0.46632
    162B ->173B       -0.40339
    163B ->174B       -0.10181
    164B ->174B        0.12134
    169B ->175B        0.15183
    169B ->177B       -0.10485
    171B ->179B       -0.16334

 Excited state symmetry could not be determined.
 Excited State  79:  4.071-?Sym    3.7869 eV  327.40 nm  f=0.0162
<S**2>=3.894
    172A ->184A        0.10199
    173A ->186A       -0.11582
    159B ->172B       -0.14378
    161B ->172B        0.69640
    161B ->173B       -0.33460
    162B ->174B        0.17631
    163B ->172B       -0.25236
    163B ->173B        0.32841
    171B ->177B        0.12919
    171B ->180B        0.15322

 Excited state symmetry could not be determined.
 Excited State  80:  4.077-?Sym    3.7976 eV  326.48 nm  f=0.0011
<S**2>=3.906
    172A ->184A        0.68147
    172A ->186A        0.11356
    172A ->189A        0.14283
    173A ->184A        0.14928
    173A ->186A       -0.50324
    173A ->189A       -0.17079
    174A ->187A        0.19285
    161B ->172B       -0.12846
```