Characterization of an oxidized Mn(III)bis(phenolate)dipyrrin Radical Complex and Oxidation Catalysis Control via Ligandcentered Redox Activity

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II. Figures ----3.182 -1.281 -650 -600 550 ,// 5 500 450 400 350 300 250 200 150 100 50 F 00'9 17.91 20.25 다 **년1**7 38,55 8 38,55 8 3.85 Å -50 0.0 0.5 10.0 8.5 7.5 6.5 5.0 f1 (ppm) 4.5 3.0 2.5 2.0 1.0 9.5 9.0 8.0 7.0 6.0 5.5 4.0 3.5 1.5 6000 $\bigwedge_{31.696}^{35.410}$ --60.946 -5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 -500

Fig. S1 ¹H and ¹³C NMR spectra of dppHMe₂

200 190 180 170 160 150 140 130 120 110 100 90 80 70 fl(ppm) 30

20 10 0

40

60 50



Fig. S2 $^1\mathrm{H}$ and $^{13}\mathrm{C}$ NMR spectra of dppH_3



Fig. S3 Spin density plot of 1. See experimental section for calculation details.



Fig. S4 Cyclic voltammetry curves of **1** in CH_2Cl_2 solution (containing 0.1 M TBAP) at a carbon electrode (left) and plot of I as a function of the square root of the scan rate (right).



Fig. S5 TD-DFT assignment of the calculated NIR transitions for 1^{2+} . As numerous orbitals contribute to each transition (details in tabulated TD-DFT data), only the major components are shown. See experimental section for computational information.



Fig. S6 X-band EPR spectra of an 8 mM CH_2Cl_2 solution of 1^{2+} in (a) parallel and (b) perpendicular modes. Microwave Freq., (a) 9.39 GHz, (b) 9.64 GHz; power, 0.7 mW; Mod. Amp., 1 mT; Mod. Freq., 100 KHz; *T*, 10 K.



Fig. S7 X-band EPR spectra of an 8 mM CH_2Cl_2 solution of 1^+ SbF₆⁻ (a) before and (b) after 20 min stirring at room temperature in the presence of one molar equivalent of PhIO. Microwave Freq., 9.64 GHz; power, 4 mW; Mod. Amp., 1 mT; Mod. Freq., 100 KHz; *T*, 10 K.

II. Tables

	$1, \mathrm{CH}_2\mathrm{Cl}_2$	[1 ⁺] • SbF ₆ ⁻ , 0.47 CH ₂ Cl ₂
Empirical formula	$C_{57}H_{63}Cl_2MnN_2O_3$	$C_{55.47}H_{61.93}Cl_{0.93}F_6MnN_2O_4Sb$
Formula weight	949.93	1144.32
Temperature/K	473.15	200
Crystal system	monoclinic	orthorhombic
Space group	$P2_1/c$	P2 ₁ 2 ₁ 2
a/Å	22.958(5)	11.451(2)
b/Å	11.988(2)	11.555(2)
c/Å	18.415(4)	20.572(4)
α/°	90.00	90.00
β/°	99.50(3)	90.00
γ/°	90.00	90.00
Volume/Å ³	4998.8(17)	2722.0(9)
Ζ	4	2
$\rho_{calc}mg/mm^3$	1.262	1.396
m/mm ⁻¹	0.417	0.840
F(000)	2008.0	1173.0
Crystal size/mm ³	$0.47 \times 0.16 \times 0.02$	$0.46 \times 0.2 \times 0.18$
2Θ range for data collection	4.3 to 50°	5 to 50.16°
Index ranges	-27 \leq h \leq 27, -14 \leq k \leq 14, -	$-13 \le h \le 13, -13 \le k \le 13, -$
index ranges	$21 \le l \le 21$	$24 \le l \le 24$
Reflections collected	36581	23218
Independent reflections	8743[R(int) = 0.0427]	4837[R(int) = 0.0552]
Data/restraints/parameters	8743/79/606	4837/221/343
Goodness-of-fit on F ²	1.055	1.221
Final R indexes [I>= 2σ (I)]	$R_1 = 0.0717, wR_2 = 0.1838$	$R_1 = 0.0853, wR_2 = 0.2120$
Final R indexes [all data]	$R_1 = 0.0989, wR_2 = 0.2042$	$R_1 = 0.0901, wR_2 = 0.2148$
Largest diff. peak/hole / e Å ⁻³	1.98/-1.31	1.22/-0.84

Table S1. Crystallographic data and structure refinement for 1 and 1^+ SbF₆-

Bond	X-ray	Calc.
Mn-N(1)	1.956	1.977
Mn-N(2)	1.963	1.984
Mn-O(1)	1.870	1.867
Mn-O(2)	1.857	1.873
Mn-MeOH	2.270	2.294

 Table S2. Experimental and calculated coordination sphere bond lengths for 1.

 Table S3. Experimental and calculated coordination sphere bond lengths for 1⁺.

Bond	X-ray	Calc. $(S = 5/2)$	Calc. $(S = 3/2)$	
Mn-N(1)	Mn-N(1) 1.956		1.975	
Mn-N(2)	1.956	1.981	1.980	
Mn-O(1)	1.867	1.895	1.886	
Mn-O(2)	1.867	1.904	1.891	
$Mn-OH_2(1)$	2.295	2.314	2.325	
Mn- OH ₂ (2)	2.295	2.333	2.340	

III. Computational Details

0 -0.9499000 -2.0659000 -0.0541000 1.3314000 1.050000 -0.956000 -0.1520002 -2.052074409 0 1.230400 -0.956000 -0.152000 -0.152017 -0.152017 -0.152017 -0.152117 -0.954137 -0.92375763 -2.74295056 C -0.8571000 -0.3510000 -0.9540000 -0.9540000 -0.9540000 -0.9540000 -0.75556149 -0.9375763 -2.74295056 C -0.9571400 -0.957140 -0.9377563 -2.74295056 -0.27754000 -0.9570400 -0.957144 -0.957147 -0.2377540 -0.948774 -0.957144 -0.957144 -0.957144 -0.957144	a) Optimized XYZ coordinates (Å) for 1	b) Optimized XYZ coordinates (Å) for 1 ⁺			
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$ \begin{array}{c} \mbox{H} & -4.48630000 & -4.87030000 & -0.02670000 \\ \mbox{C} & 5.79270000 & -1.01740000 & -0.17210000 \\ \mbox{C} & 7.88410000 & -1.78240000 & 0.017170000 \\ \mbox{C} & 7.88410000 & -1.87240000 & 0.017170000 \\ \mbox{H} & 7.63880000 & -1.83570000 & 0.83950000 \\ \mbox{H} & 7.63880000 & -1.85270000 & 0.83950000 \\ \mbox{H} & 7.47510000 & -1.69950000 & 1.06320000 \\ \mbox{H} & 7.47510000 & -1.69950000 & 0.06720000 \\ \mbox{H} & 7.32320000 & -0.25710000 \\ \mbox{C} & 7.32320000 & -0.25710000 \\ \mbox{C} & 7.32320000 & -0.25710000 \\ \mbox{C} & 7.32320000 & -0.8700000 & -0.58710000 \\ \mbox{C} & 7.32320000 & -0.8700000 & -0.58710000 \\ \mbox{C} & 7.32320000 & -4.6710000 & 0.288710000 \\ \mbox{C} & 7.32320000 & -4.6710000 & 0.28870000 \\ \mbox{H} & 2.14970000 & -5.47490000 & 0.2880000 \\ \mbox{C} & 7.323220000 & -4.50700000 & 0.129280000 \\ \mbox{H} & 1.64930000 & -4.50700000 & 0.129280000 \\ \mbox{H} & 2.14970000 & -5.8710000 & 0.68810000 \\ \mbox{C} & -0.71680000 & 4.28450000 & 0.17110000 \\ \mbox{C} & -0.71680000 & 4.28450000 & 0.17110000 \\ \mbox{C} & -0.71680000 & -3.82130000 & 0.03810000 \\ \mbox{C} & -0.71680000 & -3.82130000 & 0.03810000 \\ \mbox{C} & -3.0740170 & -4.83273161 & -1.58317007 \\ \mbox{C} & -3.18780000 & -1.25950000 & -0.34610000 \\ \mbox{C} & (Fragment=2) & -0.07740170 & -4.83273161 & -1.58317007 \\ \mbox{C} & -3.18780000 & -0.34510000 & 0.14740000 \\ \mbox{C} & (Fragment=2) & -0.07740170 & -4.83273161 & -1.58317007 \\ \mbox{C} & -3.18780000 & -1.25950000 & -0.34600000 \\ \mbox{C} & (Fragment=2) & -1.0389513 & -5.0585648 & -2.79936132 \\ \mbox{C} & -3.18780000 & -1.25950000 & -0.34590000 \\ \mbox{H} & -5.03730000 & -1.67810000 \\ \mbox{H} & Fragment=2) & -1.0389513 & -3.6712032 & 2.46240278 \\ \mbox{C} & -3.6580000 & -1.2580000 & -1.67810000 \\ \mbox{H} & -7.74390000 & -4.46760000 & -1.89920000 \\ \mbox{C} & (Fragment=2) & -1.0573455 & -1.65905864 & -3.9351498 \\ \mbox{C} & -3.6580000 & -1.92850000 \\ \mbox{C} & Fragment=2) & -0.5714484 & -2.01869306 & -5.83231498 \\ \mbox{C} & -3.6580000 & -1.22850000 \\ \mbox{C} & (Fragm$	C = -4.11530000 - 3.85820000 - 0.12590000	H(Fragment=2) = 3.21786389 - 5.151188886 - 4.54903139			
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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C -6.53920000 -3.20170000 -0.58710000	C(Fragment=2) 0.80487824 -4.76787050 2.16169392			
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H 3.13990000 -4.30700000 1.29280000 H 2.14970000 -5.47490000 0.20500000 K 1.66490000 -3.8213000 0.61880000 C -0.71680000 4.28450000 0.17110000 C 3.32220000 -3.93480000 0.017110000 C(Fragment=2) -0.07740170 -4.83273161 -1.58317007 C -2.74920000 -3.64710000 0.03180000 C(Fragment=2) -0.0554292 -6.21662615 -1.80183071 C -3.18780000 -1.25950000 0.3460000 C(Fragment=2) -0.08793900 -3.97649125 2.90218006 H 5.30780000 1.3180000 0.17470000 H(Fragment=2) -2.34347047 -4.5150218 -3.06555431 C -0.83260000 5.16810000 -0.92730000 C(Fragment=2) -0.95217082 -2.29986424 -4.96957504 C -3.65420000 1.24880000 -0.46260000 H(Fragment=2) -1.17028495 -1.67690080 -5.83231498 C -6.69600000 -4.18920000 -1.76810000 C(Fragment=2) -3.37714484 -2.0156945 -0.2202780 4	C 2.51960000 -4.461/0000 0.40280000	C(Fragment=2) = -2.38943294 - 2.94915212 = 0.00288375 U(Fragment=2) = 2.40561866 - 4.02202118 = 0.04062210			
H 2.14970000 -3.247490000 0.2050000 F(Fragmett=2) -1.43977623 -0.74530790 0.00009023 C -0.71680000 -3.82130000 0.61880000 C(Fragmett=2) -0.07740170 -4.83273161 -1.58317007 C 3.32220000 -3.93480000 0.08081000 C(Fragmett=2) -0.05254292 -6.21662615 -1.80183071 H 5.30780000 1.03160000 0.17470000 C(Fragmett=2) -0.05254292 -6.21662615 -1.80183071 H 5.30780000 1.03160000 0.01490000 C(Fragmett=2) -0.05217930 -3.97649125 2.90218006 H 5.30780000 1.03160000 0.17470000 H(Fragmett=2) -1.03189513 -3.67120332 2.46240278 C -9.93660000 5.16810000 -0.92730000 C(Fragmett=2) -0.50217082 -2.9986424 -4.96957504 C -3.65420000 1.24880000 -0.4520000 C(Fragmett=2) -1.17328495 -1.67690080 -5.83231498 H -6.34360000 -3.7870000 -1.0621000 -0.59580000 H(Fragmett=2) -3.37714484 -2.01869306 0.11380112 <td>H $5.15990000 -4.30700000 -1.29280000$ H $2.14070000 -5.47400000 -0.20500000$</td> <td>H(Fragment=2) = -2.49501800 - 4.02502118 - 0.04905510 N(Fragment=2) = 1.42007822 = 0.74856706 = 0.06660022</td>	H $5.15990000 -4.30700000 -1.29280000$ H $2.14070000 -5.47400000 -0.20500000$	H(Fragment=2) = -2.49501800 - 4.02502118 - 0.04905510 N(Fragment=2) = 1.42007822 = 0.74856706 = 0.06660022			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\Gamma(\text{Fragment}=2) = 1.43337823 = 0.74830790 = 0.00000023$ $\Gamma(\text{Fragment}=2) = 1.13731254 = 2.24440487 = 0.00990430$			
C 3.32220000 -3.93480000 -0.80810000 C -2.74920000 -3.64710000 0.03180000 C -2.74920000 -3.64710000 0.03180000 C 4.91710000 0.03940000 -0.00490000 H 5.30780000 1.03160000 0.17470000 C -3.18780000 -1.25950000 0.34660000 C -0.93660000 4.76110000 1.48590000 C -0.33260000 5.16810000 -0.92730000 C -0.3524000 5.16810000 -0.92730000 C -1.81220000 -3.4890000 0.34590000 C -1.81220000 -2.27030000 C(Fragment=2) -1.00471479 -4.03494948 -3.41419412 H -4.72460000 1.24880000 -0.42620000 C(Fragment=2) -1.7028495 -1.6790080 -5.83231498 C -6.69600000 -4.8920000 -1.76810000 C(Fragment=2) -3.37714484 -2.01869306 0.11380112 H -7.74930000 -4.0570000 -1.07880000 -1.6710000 H(Fragment=2) -5.37251885 -0.43583590 0.2766	C = -0.71680000 + 2.8450000 + 0.010000000	C(Fragment=2) = -0.07740170 - 4.83273161 - 1.58317007			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C 3.32220000 -3.93480000 -0.80810000	C(Fragment=2) -0.05254292 -6.21662615 -1.80183071			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C -2.74920000 -3.64710000 0.03180000	H(Fragment=2) -0.25417833 -6.59585648 -2.79936132			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C 4.91710000 0.03940000 -0.00490000	C(Fragment=2) -0.08793900 -3.97649125 2.90218006			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н 5.30780000 1.03160000 0.17470000	H(Fragment=2) -1.03189513 -3.67120332 2.46240278			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C -3.18780000 -1.25950000 -0.34060000	C(Fragment=2) -1.60471479 -4.03494948 -3.41419412			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C -0.93660000 4.76110000 1.48590000	H(Fragment=2) -2.34347047 -4.75150218 -3.06555431			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C -0.83260000 5.16810000 -0.92730000	C(Fragment=2) -0.95217082 -2.29986424 -4.96957504			
C -3.05420000 1.24880000 -0.46260000 C(Fragment=2) 1.39/26265 -4.02502/80 4.81429841 H -4.72460000 1.20620000 -0.59580000 H(Fragment=2) 1.62262714 -3.74205604 5.83868617 C -6.69600000 -4.18920000 -1.76810000 C(Fragment=2) -3.37714484 -2.01869306 0.11380112 H -6.34360000 -3.73870000 -2.70300000 H(Fragment=2) -4.43761672 -2.21236418 0.16331585 H -7.74930000 -4.6760000 -1.60710000 H(Fragment=2) -5.37251885 -0.43583590 0.27666460 C 4.45740000 -4.94570000 -1.07480000 C(Fragment=2) 0.57034152 -3.01291348 -3.2052254 H 5.08100000 -1.07480000 C(Fragment=2) 0.20600438 -3.61002948 4.21600668 H 5.10740000 -5.98170000 -0.20260000 H(Fragment=2) 0.2060438 -3.61002948 4.21600668 H 7.37090000 0.27810000 0.19810000 C(Fragment=2) 0.28626102 -2.0422591 -4.32529120 H 8.85200	$\begin{array}{c} \begin{array}{c} -1.81220000 & -4.82940000 & 0.34590000 \\ \end{array}$	H(Fragment=2) = -1.1/028495 = -1.6/690080 = -5.83231498			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H 4 72460000 1 20620000 0 50580000	U(Fragment=2) = 1.39/20205 - 4.02502/80 = 4.81429841 H(Fragment=2) = 1.62262714 = 2.74205604 = 5.82869617			
C -6.34360000 -3.73870000 -2.70300000 H -6.34360000 -3.73870000 -2.70300000 H -7.74930000 -4.46760000 -1.89920000 H -6.12590000 -5.11030000 -1.60710000 C 4.45740000 -5.11030000 -1.60710000 C 4.45740000 -4.94570000 -1.07480000 C 4.45740000 -4.94570000 -1.07480000 C 4.45740000 -4.65580000 -1.92850000 H 5.08100000 -4.65580000 -1.92850000 H 5.10740000 -5.92140000 -1.30780000 C 7.75830000 0.57610000 0.19810000 C 7.75830000 0.57610000 0.19810000 H 7.37090000 0.24180000 H(Fragment=2) 0.2060438 -3.61002948 4.21600668 H 7.37090000 0.29480000 1.16250000 C(Fragment=2) 0.28626102 -2.0422591 -4.32529120 H 7.42350000 1.6250000 C(Fragment=2) -3.43927337 0.52219359 0.27884691 C	$\begin{array}{c} 11 & -4.72400000 & 1.20020000 & -0.39380000 \\ C & -6.69600000 & -7.18020000 & 1.76810000 \\ \end{array}$	$\begin{array}{c} \Pi(\text{Fragment}=2) & 1.02202/14 & -5.74203004 & 5.63808017 \\ C(\text{Fragment}=2) & -3.37717787487 & -2.01860306 & 0.11380112 \\ \end{array}$			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H -6 34360000 -3 73870000 -2 70300000	H(Fragment=2) -4.43761672 -2.21236418 -0.16331585			
H -6.12590000 -5.11030000 -1.60710000 H -6.12590000 -5.11030000 -1.60710000 H 5.08100000 -4.94570000 -1.07480000 H 5.08100000 -4.65580000 -1.92850000 H 4.01610000 -5.92140000 -1.30780000 H 5.10740000 -5.08170000 -0.20260000 H 5.10740000 -5.08170000 -0.20260000 H 5.10740000 -5.08170000 -0.20260000 C 7.75830000 0.57610000 0.19810000 C 7.75830000 0.63280000 0.24180000 H 7.37090000 0.92480000 1.16250000 C -5.05330000 0.278604000 -0.40870000 C -5.05330000 -2.84460000 -0.40870000 C -1.12360000 6.52060000 -0.67940000 C -1.12360000 -1.52360000 -1.52360000 C -1.2360000 -1.52360000 -1.67940000	H -7.74930000 -4.46760000 -1.89920000	C(Fragment=2) -4.86019911 -0.51212287 -0.35126193			
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H 5.08100000 -4.65580000 -1.92850000 H 4.01610000 -5.92140000 -1.30780000 H 5.10740000 -5.08170000 -0.20260000 H 5.10740000 -5.08170000 -0.20260000 C 7.75830000 0.57610000 0.19810000 H 8.85200000 0.63280000 0.24180000 H 7.37090000 0.92480000 1.16250000 C -5.05330000 0.27380000 -0.57830000 H 7.42350000 1.27380000 -0.57830000 C -5.05330000 -2.84460000 -0.40870000 C -1.12360000 6.52060000 -0.67940000 C -1.12360000 7.20020000 -1.52360000 H -1.12360000 -1.52360000 -1.52360000	C 4.45740000 -4.94570000 -1.07480000	C(Fragment=2) 0.57034152 -3.01291348 -3.22052254			
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H 8.85200000 0.63280000 0.24180000 H(Fragment=2) 1.05034652 -1.53209844 -4.71022689 H 7.3709000 0.92480000 1.16250000 C(Fragment=2) -3.43927337 0.52219359 0.27884691 H 7.42350000 1.27380000 -0.57830000 C(Fragment=2) 3.18921206 3.27347836 -0.50141097 C -5.05330000 -0.40870000 C(Fragment=2) -2.73337244 1.77621429 0.34939430 C -1.12360000 6.52060000 -0.67940000 C(Fragment=2) -1.89414188 -3.22171025 -4.51128307 H -1.19630000 7.20020000 1.52360000 H(Fragment=7) -2.85412494 -3.31356417 -5.01116790	C 7.75830000 0.57610000 0.19810000	C(Fragment=2) 0.28626102 -2.20422591 -4.32529120			
H 7.57090000 0.92480000 1.16250000 C(Fragment=2) -3.43927337 0.52219359 0.27884691 H 7.42350000 1.27380000 -0.57830000 C(Fragment=2) 3.18921206 3.27347836 -0.50141097 C -5.05330000 -2.84460000 -0.40870000 C(Fragment=2) -2.73337244 1.77621429 0.34939430 C -1.12360000 6.52060000 -0.67940000 C(Fragment=2) -1.89414188 -3.22171025 -4.51128307 H -1.19630000 7.20020000 1.52360000 H(Fragment=7) -2.85412494 -3.31356417 -5.01116790	H 8.8520000 0.63280000 0.24180000	H(Fragment=2) 1.05034652 -1.53209844 -4.71022689			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	H 7.37090000 0.92480000 1.16250000	C(Fragment=2) -3.43927337 0.52219359 0.27884691 0.52219359 0.27884691 0.52219359 0.27884691 0.52219359 0.27884691 0.52219359 0.52219359 0.52219359 0.5284691 0.52515959 0.5284691 0.52515959 0.5284691 0.55515959 0.5551599 0.555199 0.555999 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.5599 0.5599 0.55999 0.55999 0.55999 0.55599 0.55599 0.55599 0.55599 0.55599 0.55999 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55599 0.55999 0.55599 0.55599 0.55999 0.55599 0.55999 0.55999 0.55999 0.55999 0.559990000000000			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccc} H & & /.42350000 & 1.27380000 & -0.57830000 \\ C & & & 5.05220000 & -2.84460000 & 0.40870000 \\ \end{array}$	C(Fragment=2) = 2.72227244 = 1.77621420 = 0.24020420			
$\begin{array}{c} C & -1.12500000 & 0.52000000 & -0.07940000 \\ H & -1.19630000 & 7.20020000 & -1.52360000 \\ H & Fragment=2, -2.85412494 & -3.31356417 & -5.01116790 \\ \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(Fragment=2) = -2.75557244 = 1.77621429 = 0.54939430 C(Fragment=2) = 1.80414189 = 2.22171025 = 4.51128207			
	H -1 19630000 7 2002000 -0.07940000 H -1 19630000 7 20020000 -1 52360000	H(Fragment=2) = -2.85412494 = -3.31356417 = -5.01116790			

C	-7.40550000 -1.96290000 -0.88280000	C(Fragment=2) -2.74709009 -0.71910712 0.16170406
H	-7.09580000 -1.46140000 -1.80690000	C(Fragment=2) -7.12542712 1.69484175 0.58285304
H	-7.36450000 -1.23310000 -0.06580000	C(Fragment=2) -3.48261445 2.98927853 0.54819015
H	-8.45270000 -2.26260000 -1.00460000	C(Fragment=2) = -7.74148405 = 0.28909738 = 0.45729526
C	-0.44410000 2.81/30000 -0.01540000	H(Fragment=2) -8.832/4586 - 0.36048163 - 0.50925512
	-/.0/530000 -3.86300000 0.70520000	H(Fragment=2) -7.41826740 -0.37323437 -1.26885368
H	-8.13330000 -4.12990000 0.58950000	H(Fragment=2) - 7.48951562 - 0.18374345 - 0.49904666
H	-6.98/30000 -3.18100000 1.558/0000	C(Fragment=2) = -7.67277695 = 2.56941340 = 0.57165109
H C	-6.52/80000 -4.//850000 0.95320000	H(Fragment=2) = 7.39142975 = 2.15560172 = 1.34655864 H(Fragment=2) = 7.20064702 = 2.50706702 = 0.52212545
	7.70220000 -1.28240000 -1.40070000	H(Fragment=2) = 7.29904705 = 5.39790702 = 0.32512345 H(Fragment=2) = 8.76684287 = 2.61220475 = 0.52422012
п	9.03810000 -2.51820000 -1.72190000 9.03810000 -1.19420000 -1.42510000	$\Gamma(\text{Fragment}=2) = 5.70084587 = 2.01550473 = 0.32455015$ $\Gamma(\text{Fragment}=2) = 5.50126162 = 1.66457142 = 0.51145053$
н н	7.57750000 0.64070000 2.26070000	C(Fragment-2) = 3.59120102 = 1.00457142 = 0.51145955 C(Fragment-2) = 4.85002806 = 2.88121406 = 0.61732755
	-1 30930000 -0.04070000 -2.20970000	H(Fragment=2) = 5.43214247 = 3.78851317 = 0.75968015
н	-1.52/30000 8.0/750000 0.01440000	C(Fragment=2) = 7.56721325 = 2.9739142 = 1.93806826
C	-1 22880000 6 11590000 1 69070000	H(Fragment=2) = -8.66117585 = 2.32964425 = 1.99684221
Н	-1 39190000 6 47230000 2 70400000	H(Fragment=2) = -7.20117148 = 3.32027423 = 2.07658190
C	-1.03710000 -4.55040000 -1.65570000	H(Fragment=2) -7.20109375 + 1.69347704 + 2.77690909
H	-1.73240000 -4.46970000 2.50030000	C(Fragment=2) -2.05078401 4.68103911 -0.65143834
Н	-0.46950000 -3.62190000 1.58950000	H(Fragment=2) -1.29436595 3.93092217 -0.88443742
Н	-0.34170000 -5.37160000 1.86840000	H(Fragment=2) -1.55817790 5.65734306 -0.57955572
C	-0.84310000 -5.03680000 -0.83900000	H(Fragment=2) -2.76253974 4.72592385 -1.48396831
Н	-0.16550000 -5.87510000 -0.63650000	C(Fragment=2) -2.78909211 4.36008460 0.66942451
Н	-0.24500000 -4.14470000 -1.02070000	C(Fragment=2) -3.79326059 5.50328866 0.92433892
Н	-1.40350000 -5.27020000 -1.75260000	H(Fragment=2) -4.50651641 5.62135731 0.10093633
C	-0.74330000 4.72700000 -2.35380000	H(Fragment=2) -3.24349502 6.44607397 1.01316391
C	0.38360000 4.08110000 -2.88600000	H(Fragment=2) -4.35571050 5.36416071 1.85472485
C	-1.81660000 5.01000000 -3.21600000	C(Fragment=2) -1.80907179 4.34924569 1.86836516
C	0.42750000 3.72090000 -4.23330000	H(Fragment=2) -2.34597928 4.14375597 2.80228905
Н	1.23560000 3.87050000 -2.24990000	H(Fragment=2) -1.32444949 5.32677677 1.96965618
C	-1.77370000 4.64700000 -4.56160000	H(Fragment=2) -1.02587787 3.59949797 1.73904453
H	-2.69890000 5.50540000 -2.81910000	C(Fragment=2) 7.52235106 2.90927977 -1.04411650
C	-0.65000000 3.99850000 -5.07560000	H(Fragment=2) 7.09216700 3.85229576 -1.39806154
H	1.31190000 3.22530000 -4.62480000	H(Fragment=2) 7.38869211 2.16121120 -1.83367713
H	-2.62060000 4.86750000 -5.20610000	H(Fragment=2) = 8.59/83450 = 3.06952028 = -0.90/34524
H	-0.613/0000 3./1320000 -6.12350000	O(Fragment=3) = 0.161/0555 = 0.77908816 = 2.33416408
	-0.95//0000 3.84410000 2.6/220000	H(Fragment=3) 1.0158/562 0.6414/856 2.7324804 H(Fragment=2) 0.18154507 1.02758885 2.65778457
	0.20900000 3.27140000 3.20330000	H(Fragment=3) = 0.18154597 = 1.62758885 = 2.65778457
	-2.18130000 - 3.30820000 - 3.30190000 - 0.14600000 - 2.42240000 - 4.22000000	U(Fragment=4) = 0.2/9/0/20 = 0.48121043 = 2.29831/01 U(Fragment=4) = 0.22208158 = 1.06444421 = 2.77280102
	0.14090000 - 2.45340000 - 4.52090000 - 1.16010000 - 2.48720000 - 2.74680000	H(Fragment-4) = 0.35308138 = 1.00444421 - 2.77289193 H(Fragment-4) = 0.20272001 = 0.26217256 = 2.78701658
	2.24580000 - 2.72790000 - 4.41460000	$\Gamma(\text{Fragment}=4) = -0.29272091 = -0.30517230 = 2.78701058$ $\Gamma(\text{Fragment}=2) = 1.40100804 = 4.08603175 = 0.21387630$
н	3 00100000 / 00500000 2 00160000	H(Fragment=2) = 0.77301711 + 4.20095175 = 0.21587039
C	-1.08190000 -2.15350000 -2.90100000	H(Fragment=2) = 0.77501711 + 2.1204520 = 0.48155575 = 0.93531724 = 5.88495733 = 0.07783619
н	1.06480000 2.02010000 4.73260000	H(Fragment=2) = 2.08740803 + 5.36475755 + 0.07785017 H(Fragment=2) = 2.08740803 + 5.23537046 + 1.10051507
н	-3 20640000 2 52030000 4 87790000	C(Fragment=2) = 2.00740005 = 5.25557040 = 1.10051507
H	-1 12860000 1 50240000 5 79530000	C(Fragment=2) 3 34274340 5 70445073 -1 29232762
Mn	0 12640000 -0 54160000 0 00410000	H(Fragment=2) = 2.73679994 = 6.55105908 = 1.63147905
0	0.13710000 -0.42990000 2.29570000	H(Fragment=2) 4.03915277 5.45456360 -2.10102880
Ĥ	-0.00570000 0.48070000 2.61090000	H(Fragment=2) 3.92248217 6.04926056 -0.42885345
C	1.24810000 -0.99500000 3.00910000	C(Fragment=2) 1.57357206 4.22250023 -2.21079759
Н	2.18150000 -0.47080000 2.77540000	H(Fragment=2) 2.22483489 3.90456470 -3.03424555
Н	1.06050000 -0.96640000 4.08780000	H(Fragment=2) 1.04404394 5.12509497 -2.53580727
Н	1.33050000 -2.03240000 2.68520000	H(Fragment=2) 0.83025394 3.44472051 -2.02737647
c) Opt	timized XYZ coordinates (Å) for 12 ⁺	
Mm	0.05810000 0.55726200 0.02044700	
C	-0.02819000 0.22736200 0.02944700	
	0.19282700 -2.84103400 -0.00711000	
	-1.48320700 1.79517800 $0.219143000.42006200$ 7.06209200 0.95596200	
ц Ц	0.42000200 -7.00200300 -0.83380200	
N	-1 36367100 -0.91526600 -0.09872400	
Ċ	0.73450000 -6.58447900 0.41320300	
H H	1.00943100 -7.27909000 1.20081800	
0	1.18985700 1.96740900 -0.23412400	
Ĭč	-0.37316700 -3.87964900 -2.74297500	
Č	2.22098200 -5.16886300 2.67722800	
H	2.91776600 -5.76851800 2.09714200	
C	2.78450700 -0.37403400 0.15829700	
C	0.28802100 -4.31799700 -0.31542600	
C	3.57195300 -1.60135300 0.17471400	
Н	4.64937800 -1.65669100 0.21174600	
C	4.48527700 3.39328100 -0.36697000	
H	4.97340200 4.33513700 -0.57756900	

C	0.66724400	-5.21442300	0.71255000	
С	5.33226400	2.31579800	0.06210900	
C	6.83188600	2.57123300	0.24227600	
	7.03066600	3.68543500	1.30161800	
п	8 10003500	4.02988800	1.00921100	
H	6 62124100	3 38726500	2 27308900	
C	3.32437400	0.92395100	0.10437500	
č	4.73330600	1.10137300	0.26570900	
Н	5.33015100	0.25212900	0.56570700	
C	2.54447400	-4.80857400	3.98543500	
Н	3.48944100	-5.12966100	4.41387800	
C	2.48258500	2.07880700	-0.21342100	
	2.71184300	-2.64091000	0.07097500	
H C	2.94286600	-3.6940//00	0.02144800	
н	7.38118100	0.95024500	1 68006000	
H	8 64281200	1 54379000	0.83912300	
H	7.51375000	0.49569500	-0.01639000	
C	1.00325400	-4.77048400	2.09852600	
C	1.37193900	-2.08785400	0.03711400	
С	-2.32570700	-3.00601700	0.01943100	
Н	-2.39591600	-4.08282800	-0.02664000	
Ν	1.44825600	-0.71386800	0.09678400	
С	-1.08322700	-2.25928900	-0.00012300	
C	-0.01402900	-4.79668300	-1.61552800	
	0.04615200	-6.17429300	-1.86227800	
H C	-0.1//46200	-6.54205100	-2.85913500	
ч	0.11219300	3 73874600	2.87043400	
C	-1 61676600	-3 99888100	-3 38399700	
н	-2 32345900	-4 74926800	-3 03986800	
C	-1.05109800	-2.21539600	-4.91979100	
H	-1.30500400	-1.58857300	-5.76963900	
С	1.65158000	-4.05068400	4.74523000	
Н	1.89628000	-3.78304700	5.76894900	
C	-3.33154500	-2.10792500	0.12940200	
H	-4.38641200	-2.32862000	0.18654800	
	-4.87740500	0.38300600	0.36685800	
H	-5.3/3/6900	-0.5/234800	0.28518700	
н	1 52814700	-2.92234200	-3.22329000	
C	0 43227800	-3 65830700	4 18792100	
Ĥ	-0.28394900	-3.09960500	4.78454400	
C	0.20222000	-2.09911400	-4.30650800	
Н	0.94383000	-1.41197500	-4.70876100	
C	-3.45413400	0.42563600	0.29369100	
C	3.11466300	3.33352200	-0.52804700	
	-2.//059800	1./1890300	0.30420300	
н	-2 92278300	-3 28416500	-4.43023000	
C	-2 73383200	-0 77943400	0 17411000	
č	-7.15725700	1.52577200	0.60845300	
C	-3.54575000	2.91228100	0.59332100	
C	-7.75219500	0.11347600	0.46111200	
Н	-8.84353100	0.17078900	0.51032500	
H	-7.42683200	-0.55573200	1.26626700	
H	-7.49455000	-0.34208700	-0.50216200	
	-7.70783400	2.41403800	-0.53/14900	
п	-7.42321000	2.01802/00	-1.31809300	
H	-8 80140200	2 44039600	-0.47221700	
Ċ	-5.62752600	1.51875100	0.53881300	
č	-4.91552200	2.75840400	0.66515400	
Н	-5.51314900	3.64519500	0.82852700	
C	-7.60433600	2.10746100	1.97438400	
H	-8.69807400	2.11938800	2.02584600	
H	-7.26087400	3.13616800	2.12539200	
H	-7.23342600	1.49903300	2.80648900	
	-2.188/6200	4.08249300	-0.58383/00	
н п	-1.40/29400	5.9/182600	-0.85/0/800	
	-1./3109300	4 73136400	-0.400//200	
	-2.88772300	4.29790900	0.74198200	
Č	-3.92497800	5.39685700	1.05382600	

Н	-4.65310400	5.52449600 0.2452	2300
Н	-3.40458100	6.35247600 1.1689	7500
Н	-4.46658000	5.20742200 1.9875	6100
C	-1.88250800	4.27884100 1.9204	5800
Н	-2.38976300	4.02314500 2.8583	0700
Н	-1.43727100	5.27135200 2.0454	1000
Н	-1.06837900	3.56976700 1.7519	0600
C	7.43778200	3.02792300 -1.1093	4100
Н	6.98445600	3.95285200 -1.4814	8800
Н	7.31858300	2.25707700 -1.8785	9600
Н	8.50893600	3.21828300 -0.9849	5000
0	0.07800300	0.76558500 2.3348	0400
Н	0.70078500	0.33198700 2.9396	9200
Н	-0.23239900	1.57139600 2.7786	1600
0	-0.28527400	0.48406700 -2.2439	7500
Н	0.08758900	1.18873300 -2.7976	5900
Н	-0.30818900	-0.32580400 -2.7921	7200
C	1.42029500	5.06175600 0.16480	5800
Н	0.71105000	4.29731400 0.48494	4100
Н	0.85171700	5.94251100 -0.1529	0400
Н	2.03246500	5.35334600 1.0257	7800
C	2.31188000	4.56465400 -0.9960	3300
C	3.23609500	5.72928800 -1.4100	6500
Н	2.62070900	6.55936700 -1.7699	4200
Н	3.91699000	5.45186700 -2.2229	0600
Н	3.82865100	6.11214800 -0.5719	6200
C	1.45251800	4.20496800 -2.2334	7300
Н	2.08384600	3.85117600 -3.0573	3700
Н	0.91947800	5.09452900 -2.5846	7700
Н	0.70722200	3.44036100 -2.0026	1500

d) TD-DFT excitation energies and oscillator strengths for 1^+

```
Excited State 1: 4.496-A 0.9410 eV 1317.54 nm f=0.0583 <S**2>=4.804
  231A -> 234A
                 -0.10311
  232A -> 233A
                 0.96249
 229B -> 230B
                 0.21522
Excited State 2: 4.501-A 1.1530 eV 1075.36 nm f=0.0263 <S**2>=4.815
 231A -> 233A 0.98316
Excited State 3: 4.432-A 1.4444 eV 858.39 nm f=0.0242 <S**2>=4.662
 227A -> 233A -0.19730
 229A -> 233A
                 -0.38286
 230A -> 233A
                 0.32898
  231A -> 234A
                 0.14424
 232A -> 233A
                 -0.11495
 229B -> 230B
                 0.80051
Excited State 4: 4.480-A 1.5938 eV 777.91 nm f=0.0181 <S**2>=4.766
 230A -> 233A
                 0.92027
  232A -> 233A
                 0.10714
 229B -> 230B
                 -0.35978
Excited State 5: 4.473-A
                        1.7493 eV 708.77 nm f=0.0573 <S**2>=4.752
 227A -> 233A
                 0.13035
  229A -> 233A
                 0.87557
 230A -> 233A
                 0.19352
  232A -> 233A
                 -0.11426
  227B -> 230B
                 -0.11964
 229B -> 230B
                 0.35335
  229B -> 233B
                 -0.10774
Excited State 6: 4.875-A 1.9733 eV 628.30 nm f=0.0049 <S**2>=5.690
 224A -> 233A
                -0.10407
  227A -> 233A
                 -0.20938
  228A -> 233A
                 0.51618
                 0.11043
 229A -> 233A
 232A -> 234A
                 0.40805
 228B -> 230B
                 0.65888
Excited State 7: 4.705-A 1.9902 eV 622.99 nm f=0.0137 <S**2>=5.283
  227A -> 233A -0.29889
  228A -> 233A
                 0.72975
```

229A -> 233A 0.10377 232A -> 234A -0.29126 228B -> 230B -0.47769 Excited State 8: 4.509-A 2.0638 eV 600.75 nm f=0.0247 <S**2>=4.833 227A -> 233A 0.85779 228A -> 233A 0.41468 229A -> 233A -0.19518 227B -> 230B -0.12963 Excited State 9: 4.828-A 2.1402 eV 579.30 nm f=0.0001 <S**2>=5.578 0.97298 232A -> 235A Excited State 10: 4.482-A 2.1759 eV 569.81 nm f=0.0004 <S**2>=4.773 220A -> 233A 0.15708 221A -> 234A 0.12092 222A -> 233A -0.10100 224A -> 233A 0.88511 226A -> 233A 0.27455 228B -> 230B 0.15215 Excited State 11: 4.312-A 2.2167 eV 559.32 nm f=0.0013 <S**2>=4.398 219A -> 235A 0 10421 221A -> 233A -0.17956 223A -> 233A 0.65471 223A -> 235A 0.11983 224A -> 233A -0.20371225A -> 233A 0.24040 226A -> 233A 0.42436 229B -> 231B 0.41887 Excited State 12: 4.130-A 2.2461 eV 552.01 nm f=0.0014 <S**2>=4.014 221A -> 233A 0.15705 223A -> 233A -0 23068 225A -> 233A -0.13951 226A -> 233A -0.26845 227B -> 231B -0.10893 229B -> 231B 0.88108 Excited State 13: 4.620-A 2.2967 eV 539.84 nm f=0.0335 <S**2>=5.086 -0.39204 219A -> 235A 221A -> 233A 0.29487 223A -> 233A 0.41509 223A -> 235A -0.39573 224A -> 235A 0 18983 227A -> 233A -0.12705 231A -> 234A -0.23574 231A -> 235A 0.11316 232A -> 234A -0.13295 226B -> 230B 0.13556 227B -> 230B -0.40581 Excited State 14: 4.523-A 2.3176 eV 534.97 nm f=0.0172 <S**2>=4.864 219A -> 235A 0.26572 221A -> 233A 0.45633 223A -> 233A 0.43567 223A -> 235A 0.25998 224A -> 233A 0.12516 224A -> 235A -0.10234 225A -> 233A -0.14912 226A -> 233A -0.42864 227A -> 233A 0.13371 231A -> 235A -0.16881 232A -> 234A -0.18376 227B -> 230B 0.23000 228B -> 230B 0.10793 229B -> 231B -0.10296 Excited State 15: 4.843-A 2.3186 eV 534.74 nm f=0.0062 <S**2>=5.613 219A -> 235A -0.31847 223A -> 235A -0.36295 224A -> 235A 0.16202 227A -> 233A 0.12135 229A -> 233A 0.10143 231A -> 234A 0.40821

231A -> 235A 226B -> 230B 227B -> 230B	0.13873 -0.18306 0.62146	
Excited State 16: 208A -> 235A 214A -> 235A 215A -> 235A 223A -> 235A 224A -> 235A	4.722-A 0.14462 -0.10201 -0.15732 0.14386 -0.30259	2.3458 eV 528.54 nm f=0.0006 <s**2>=5.323</s**2>
231A -> 235A Excited State 17:	0.87401 4.564-A	2.3882 eV 519.15 nm f=0.0403 <s**2>=4.957</s**2>
220A -> 233A 221A -> 233A	0.10384	
222A -> 233A	-0.12790	
224A -> 233A	0.11622	
$232A \rightarrow 234A$ $223P \rightarrow 230P$	0.73770	
$225B \rightarrow 230B$ $225B \rightarrow 230B$	-0.13544	
228B -> 230B	-0.47603	
228B -> 233B	0.11413	
Excited State 18:	4.517-A	2.4179 eV 512.77 nm f=0.0109 <s**2>=4.850</s**2>
221A -> 233A	0.44237	
223A -> 233A	-0.18434	
224A -> 233A	-0.15114	
$225A \rightarrow 233A$ $226A \rightarrow 233A$	-0.48853	
$232A \rightarrow 233A$	-0.12796	
228B -> 230B	0.11082	
Excited State 19	4 799-A	2 4878 eV 498 37 nm f=0 0009 <s**2>=5 507</s**2>
220A -> 233A	-0.12502	
221A -> 233A	-0.15192	
222A -> 233A	0.24916	
$225A \rightarrow 233A$ $225B \rightarrow 230B$	-0.15588	
$223B \rightarrow 230B$ $226B \rightarrow 230B$	0.83003	
227B -> 230B	0.28350	
Excited State 20:	4.580-A	2.5031 eV 495.33 nm f=0.0271 <s**2>=4.994</s**2>
220A -> 233A	0.21534	
221A -> 233A	0.33536	
$222A \rightarrow 233A$	-0.44538	
223A -> 233A 224A -> 233A	-0.18/48	
225A -> 233A	0.54250	
223B -> 230B	0.14637	
$225B \rightarrow 230B$	0.11008	
226B -> 230B 227B -> 230B	0.36140	
$228B \rightarrow 230B$ $228B \rightarrow 230B$	0.14290	
229B -> 232B	-0.20059	
Excited State 21	4.529-A	2.5539 eV 485.47 nm f=0.0111 <\$**2>=4.877
220A -> 233A	-0.26641	
221A -> 233A	0.34538	
222A -> 233A	0.55316	
223A -> 233A 225A -> 233A	-0.142/6	
$226A \rightarrow 233A$	0.18281	
223B -> 230B	-0.11851	
225B -> 230B	-0.12238	
226B -> 230B 229B -> 232B	-0.11962	
2270 - 2320	0.20000	
Excited State 22: 222A -> 233A	4.331-A	2.6339 eV 470.73 nm f=0.0003 <s**2>=4.440</s**2>
223B -> 230B	0.13016	
225B -> 230B	0.43054	
226B -> 230B	0.15676	
229B -> 232B	0.83393	
Excited State 23:	4.502-A	2.6745 eV 463.59 nm f=0.0399 <s**2>=4.818</s**2>

221A -> 233A 231A -> 234A 226B -> 230B 227B -> 230B 229B -> 233B	0.15526 0.73695 0.20919 -0.45426 0.36971				
Excited State 24: 222A -> 233A 224A -> 233A 229A -> 234A 230A -> 234A 232A -> 234A 232A -> 234A 225B -> 230B 226B -> 230B 229B -> 232B	4.759-A 0.34695 0.13949 0.23768 -0.16338 0.19373 0.69441 0.11791 -0.39435	2.6838 eV	461.98 nm	f=0.0502 <	S**2>=5.411
Excited State 25: 219A -> 233A 220A -> 233A 222A -> 233A 229A -> 235A 228B -> 235B 229B -> 233B	4.347-A 0.74760 -0.34303 -0.21584 -0.10210 0.26125 0.28639	2.8042 eV	442.14 nm	f=0.0069 <	<\$**2>=4.475
Excited State 26: 219A -> 233A 219A -> 235A 220A -> 233A 222A -> 233A 223A -> 235A 231A -> 234A 228B -> 231B 229B -> 233B	4.455-A -0.14963 0.10420 0.44831 0.28032 -0.10045 -0.20984 0.56241 0.47144	2.8166 eV	440.19 nm	f=0.0370 <	<\$**2>=4.711
Excited State 27: 219A -> 233A 219A -> 235A 220A -> 233A 222A -> 233A 223A -> 235A 231A -> 234A 228B -> 231B 229B -> 233B	4.459-A -0.16011 -0.14464 -0.21919 -0.12228 0.10678 0.18412 0.75319 -0.40195	2.8323 eV	437.75 nm	f=0.0366 <	S**2>=4.721
Excited State 28: 219A -> 233A 220A -> 233A 222A -> 233A 229A -> 235A 231A -> 234A 223B -> 230B 229B -> 233B	4.416-A 0.52666 0.53163 0.29144 -0.10879 0.16872 0.11645 -0.42230	2.8438 eV	435.98 nm	f=0.0361 <	<\$**2>=4.626
Excited State 29: 194A -> 235A 205A -> 235A 219A -> 235A 219A -> 235A 221A -> 235A 226A -> 235A 227A -> 235A 229A -> 235A 230A -> 235A 230A -> 234A 230A -> 235A 223B -> 230B 224B -> 230B 225B -> 230B	4.708-A 0.10215 -0.10413 -0.24848 0.10466 0.26893 -0.10378 -0.24563 -0.18279 -0.37418 0.38950 0.27759 -0.24925 0.35893 0.24011	2.8771 eV	430.93 nm	f=0.0003 <	<\$**2>=5.292
Excited State 30: 194A -> 235A 205A -> 235A 219A -> 233A 220A -> 233A 221A -> 235A	4.715-A -0.10790 0.10426 0.15053 0.19529 -0.27133	2.8819 eV	430.22 nm	f=0.0045 <	S**2>=5.308

226A -> 235A	0.10229
227A -> 235A	0.24466
229A -> 234A	-0.19277
229A -> 235A	0.37327
230A -> 234A	0.44482
230A -> 235A	-0.27322
223B -> 230B	-0.20001
224B -> 230B	0.33487
225B -> 230B	0.22120

e) TD-DFT excitation energies and oscillator strengths for 1^{2+}

Excited State 1: 5.666-A 0.2495 eV 4970.15 nm f=0.0019 <S**2>=7.777 230A -> 233A 0.12288 231A -> 233A -0.55616 232A -> 233A 0.51726 221B -> 229B -0.10168 225B -> 229B 0.21220 226B -> 229B -0.17164227B -> 229B 0.71823 228B -> 229B -0.26132 231A <- 233A -0.27500 232A <- 233A 0.23755 225B <- 229B 0.11315 227B <- 229B 0.34087 228B <- 229B -0.10075 Excited State 2: 5.434-A 0.6454 eV 1920.91 nm f=0.0043 <S**2>=7.131 -0.13095 231A -> 233A 227B -> 229B 0.22584 228B -> 229B 0.94625 Excited State 3: 5.565-A 0.7359 eV 1684.84 nm f=0.0099 <S**2>=7.493 228A -> 233A -0.54466 229A -> 233A 0.19600 232A -> 233A -0.37588 224B -> 229B 0.62284 $225B \rightarrow 229B$ 0.14902 226B -> 229B -0.22031 228B -> 229B -0.18217 Excited State 4: 5.397-A 0.8210 eV 1510.11 nm f=0.0010 <S**2>=7.031 228A -> 233A -0.20850 229A -> 233A 0 12874 231A -> 233A 0.58640 232A -> 233A 0.71969 224B -> 229B 0.25390 Excited State 5: 5.358-A 0.9365 eV 1323.85 nm f=0.0296 <S**2>=6.926 225A -> 233A 0.10080 230A -> 233A -0.15141 231A -> 233A 0.25386 232A -> 233A -0.20663 225B -> 229B -0.42757 226B -> 229B 0 52094 227B -> 229B 0.61452 Excited State 6: 5.295-A 1.0414 eV 1190.52 nm f=0.0462 <S**2>=6.758 0.11120 228A -> 233A 229A -> 233A -0.18597 230A -> 233A 0.31224 231A -> 233A 0 53811 232A -> 233A -0.24569221B -> 229B 0.16286 222B -> 229B 0.11399 $224B \rightarrow 229B$ -0.24614 224B -> 230B 0.10489 225B -> 229B 0.48862 226B -> 229B -0 18851 227B -> 229B 0.33675 Excited State 7: 5.378-A 1.0639 eV 1165.40 nm f=0.0051 <S**2>=6.981 -0 11668 231A -> 233A 224B -> 229B 0.11321

225B -> 229B 0.61539 226B -> 229B 0.74885 227B -> 229B -0.13991 1.1470 eV 1080.98 nm f=0.0140 <S**2>=6.409 Excited State 8: 5.161-A 225A -> 233A -0.12833 229A -> 233A -0.32246 230A -> 233A 0.80693 224B -> 229B 0.26355 225B -> 229B -0.31024 226B -> 229B 0.17549 Excited State 9: 5.080-A 1.1905 eV 1041.48 nm f=0.0223 <S**2>=6.201 228A -> 233A 0.60415 229A -> 233A -0.35271 230A -> 233A -0.31443 224B -> 229B 0.59776 225B -> 229B 0.10561 226B -> 229B -0.12352 Excited State 10: 5.346-A 1.2347 eV 1004.16 nm f=0.0007 <S**2>=6.894 228A -> 233A 0.49091 0 79995 229A -> 233A 0.29764 230A -> 233A 224B -> 229B 0.11644 Excited State 11: 5.575-A 1.4104 eV 879.07 nm f=0.0066 <S**2>=7.521 224A -> 233A 0.12160 225A -> 233A -0.32171 226A -> 233A -0 20565 227A -> 233A -0.15283229A -> 233A 0.13112 220B -> 229B -0.14281 221B -> 229B 0 31058 222B -> 229B 0.29589 223B -> 229B 0.73915 Excited State 12: 5.460-A 1.4700 eV 843.42 nm f=0.0014 <S**2>=7.203 225A -> 233A 0.30480 226A -> 233A 0.19272 220B -> 229B 0.14494 221B -> 229B -0.34488 222B -> 229B -0.49768 223B -> 229B 0.65369 Excited State 13: 5.325-A 1.5892 eV 780.15 nm f=0.0052 <S**2>=6.840 225A -> 233A 0.14552 227A -> 233A 0.61180 220B -> 229B 0.11856 221B -> 229B -0.31322 222B -> 229B 0.67719 223B -> 229B 0.11894 Excited State 14: 5.430-A 1.5992 eV 775.28 nm f=0.0006 <S**2>=7.121 225A -> 233A -0.25852 226A -> 233A -0.11725 227A -> 233A 0.76147 221B -> 229B 0.37866 222B -> 229B -0.41088Excited State 15: 5.466-A 1.7257 eV 718.47 nm f=0.0040 <S**2>=7.219 226A -> 233A -0.48909 231A -> 234A 0.32214 231A -> 235A 0.15430 232A -> 234A -0.33018 232A -> 235A -0.18442 221B -> 229B -0.17245 227B -> 230B 0.49216 228B -> 230B -0.37277 Excited State 16: 5.415-A 1.7407 eV 712.28 nm f=0.0082 <S**2>=7.079 225A -> 233A -0.18885 226A -> 233A 0.74067 231A -> 234A 0.38164 232A -> 234A -0.38591

221B -> 229B 227B -> 230B 228B -> 230B	0.19686 0.16935 -0.15539				
Excited State 17: 226A -> 233A 231A -> 234A 231A -> 235A 232A -> 235A 232A -> 235A 227B -> 230B 228B -> 230B	5.429-A 0.26487 -0.46708 0.20329 0.47448 -0.21658 0.43055 -0.39725	1.7508 eV	708.14 nm	f=0.0044	<\$**2>=7.117
Excited State 18: 224A -> 233A 225A -> 233A 226A -> 233A 217B -> 229B 220B -> 229B 221B -> 229B 228B -> 230B	5.436-A -0.17672 0.16182 -0.13255 0.10615 0.80860 0.40519 -0.24289	1.8148 eV	683.19 nm	f=0.0058	<s**2>=7.138</s**2>
Excited State 19: 225A -> 233A 231A -> 235A 232A -> 235A 220B -> 229B 221B -> 229B 227B -> 230B 228B -> 230B	5.336-A 0.11493 0.14081 -0.12401 0.15676 0.16208 0.51964 0.77369	1.8729 eV	662.01 nm	f=0.0053	<s**2>=6.868</s**2>
Excited State 20: 222A -> 233A 225A -> 233A 231A -> 233A 220B -> 229B 221B -> 229B 224B -> 230B	5.136-A -0.11465 0.71294 -0.10775 -0.41154 0.43542 -0.14451	1.9023 eV	651.74 nm	f=0.1437	<s**2>=6.345</s**2>
Excited State 21: 222A -> 233A 224A -> 233A 225A -> 233A 219B -> 229B 220B -> 229B	5.326-A 0.18326 0.87553 0.19612 -0.26738 0.19219	1.9831 eV	625.20 nm	f=0.0083	<\$**2>=6.843
Excited State 22: 222A -> 233A 224A -> 233A 232A -> 235A 217B -> 229B 219B -> 229B 221B -> 229B	5.614-A -0.54471 0.31217 0.11166 -0.23381 0.63696 -0.10470	2.0445 eV	606.43 nm	f=0.0074	<\$**2>=7.629
Excited State 23: 222A -> 233A 228A -> 234A 228A -> 235A 231A -> 235A 231A -> 235A 232A -> 235A 232A -> 235A 217B -> 229B 224B -> 230B 225B -> 230B 226B -> 230B 227B -> 230B	5.396-A 0.13731 0.16849 0.12160 0.38027 -0.13573 0.44326 0.50676 0.12546 0.36431 0.10493 -0.12208 0.23416	2.1076 eV	588.27 nm	f=0.0216	<\$**2>=7.028
Excited State 24: 221A -> 233A 222A -> 233A 223A -> 233A 228A -> 234A 228A -> 235A 231A -> 234A	5.408-A -0.12956 -0.11138 0.15435 0.11313 -0.11889 0.53988	2.1275 eV	582.76 nm	f=0.0119	<\$**2>=7.061

231A -> 235A 232A -> 234A 232A -> 235A 217B -> 229B 224B -> 230B 227B -> 230B	0.19162 0.52545 -0.27622 -0.16470 -0.30950 -0.20421				
Excited State 25: 220A -> 233A 221A -> 233A 223A -> 233A 224A -> 233A 228A -> 235A 231A -> 235A 232A -> 235A 213B -> 229B 214B -> 229B 214B -> 229B 219B -> 229B 224B -> 230B 225B -> 230B 226B -> 230B 227B -> 230B	5.421-A 0.11165 0.18399 -0.23499 0.12019 -0.16420 -0.14673 0.19905 -0.10333 -0.13414 0.26904 0.12295 -0.43695 -0.24089 0.48321 0.27111	2.1433 eV	578.46 nm	f=0.0200	<\$**2>=7.096
Excited State 26: 223A -> 233A 223A -> 234A 231A -> 234A 232A -> 235A 216B -> 229B 217B -> 229B 224B -> 230B 226B -> 230B 227B -> 230B	5.352-A 0.77819 0.10609 -0.11929 0.43100 0.10278 -0.12679 -0.10732 0.12936 0.12807	2.1760 eV	569.78 nm	f=0.0094	<s**2>=6.912</s**2>
Excited State 27: 223A -> 233A 228A -> 234A 231A -> 235A 232A -> 235A 224B -> 230B 225B -> 230B 226B -> 230B	5.388-A 0.28306 0.15520 -0.25690 -0.42304 0.46053 -0.39784 0.41940	2.1988 eV	563.88 nm	f=0.0039	<\$**2>=7.007
Excited State 28: 212A -> 234A 221A -> 233A 223A -> 233A 223A -> 234A 224A -> 233A 231A -> 235A 232A -> 235A 217B -> 229B 219B -> 229B 224B -> 230B 225B -> 230B 226B -> 230B	5.445-A 0.11299 0.36378 0.30831 0.13013 0.15530 -0.30513 -0.28228 0.38687 0.12844 -0.16251 0.31347 -0.37942	2.2224 eV	557.89 nm	f=0.0022	<\$**2>=7.161
Excited State 29: 212A -> 234A 213A -> 234A 214A -> 234A 216A -> 234A 220A -> 233A 221A -> 234A 223A -> 234A 228A -> 234A 228A -> 234A 229A -> 234A 230A -> 234A 230A -> 234A 231A -> 234A 232A -> 234A 232A -> 234A 231A -> 234A 232A -> 234A 231A -> 234A 232A -> 234A 232B -> 234B -> 229B	5.283-A -0.30077 -0.31651 -0.12718 0.15830 0.26031 -0.10498 0.11315 -0.33154 0.53207 -0.12069 -0.14228 -0.17926 -0.10551 -0.10551 -0.13190	2.2405 eV	553.37 nm	f=0.0017	<\$**2>=6.727

224B -> 230B	-0.18024				
225B -> 230B	0.11735				
Excited State 30:	5.254-A	2.2461 eV	551.99 nm	f=0.0089	<s**2>=6.652</s**2>
203A -> 234A	-0.10389				
212A -> 234A	0.30997				
213A -> 234A	0.20706				
216A -> 234A	-0.14034				
220A -> 233A	-0.14072				
222A -> 234A	-0.12550				
223A -> 233A	-0.13732				
223A -> 234A	0.36110				
228A -> 234A	0.64856				
229A -> 234A	-0.29059				
231A -> 234A	-0.15014				