Supporting Information

Electronic Effects of *Para*-phenolate Substitution in an Extended Series of Neutral and Oxidized Chromium Salen Nitrides

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Table S1: Key crystallographic information for **CrNSal^{NO2}**, **CrNSal^{H}**, **CrNSal^{OMe}** and **CrNSal^{OiPr}**.

Complex	**CrNSal^{NO2}**	**CrNSal^{H}**	**CrNSal^{OMe}**	**CrNSal^{OiPr}**
Formula	$C_{28}H_{34}CrN_5O_6$	$C_{28}H_{36}CrN_3O_2$	$C_{30}H_{40}CrN_3O_4$	$C_{34}H_{48}CrN_3O_4$
Formula weight	588.61	498.61	558.66	614.77
Space group	P 1 21/c 1	P 1 21/n 1	P-1	I 2
a **(Å)**	11.34(5)	13.14(3)	11.19(1)	14.90(7)
b (Å)	23.91(4)	12.80(5)	11.40(5)	13.44(0)
c (Å)	10.82(5)	15.45(5)	13.41(1)	21.26(4)
α (deg)	90	90	87.71(6)	90
β (deg)	104.66(1)	99.91(5)	69.85(6)	99.15(5)
γ (deg)	90	90	82.00(9)	90
V **(Å^3)**	2841.17(17)	2562.20(8)	1591.3(2)	4206.0(4)
Z	4	33	2	2

T (K)	296	296	296	210
ρ_{calcd} (g cm^{-3})	1.376	1.293	1.252	1.142
λ (Å)	1.54178	1.54178	1.54178	0.71073
μ (cm^{-1})	3.735	3.898	3.282	0.315
R indices[a] with I > 2.0σ(I) (data)	0.0604	0.0318	0.0491	0.0831
wR_2	0.1472	0.0924	0.1449	0.2707
R_1	0.0604	0.0318	0.0491	0.0831
Goodness-of-fit on F^2	1.053	1.046	1.094	1.100

Table S2: Key metrical parameters including distances (Å) and angles (°) for **CrNSal^{NO2}**, **CrNSal^{H}**, **CrNSal^{OMe}** and **CrNSal^{OiPr}**.

Parameter	**CrNSal^{NO2}**	**CrNSal^{H}**	**CrNSal^{OMe}**	**CrNSal^{OiPr}**
Cr(1)--O1	1.910(2)	1.896(1)	1.907(3)	1.839(6)
Cr(1)--O(2)	1.906(2)	1.915(1)	1.911(3)	1.823(6)
Cr(1)--N(1)	2.015(3)	2.008(1)	2.010(3)	2.036(6)
Cr(1)--N(2)	2.002(3)	2.031(1)	2.006(5)	2.051(6)
Cr(1)--N(3)	1.560(4)	1.549(2)	1.556(5)	1.538(1)
O(1)--C(1)	1.314(4)	1.317(2)	1.317(5)	1.340(9)
O(2)--C(2)	1.314(4)	1.316(2)	1.318(6)	1.340(9)
O(1)--Cr(1)--O(2)	89.1(5)	87.8(1)	89.5(1)	92.0(2)
O(1)--Cr(1)--N(1)	88.0(6)	88.3(5)	88.6(3)	89.9(6)
O(1)--Cr(1)--N(2)	152.4(4)	141.5(8)	147.0(8)	153.5(5)
O(1)--Cr(1)--N(3)	104.8(7)	111.9(3)	108.9(8)	101.3(8)
O(2)--Cr(1)--N(2)	89.2(7)	88.7(7)	86.7(6)	89.9(8)
O(2)--Cr(1)--N(1)	149.3(9)	156.4(7)	152.7(4)	157.8(6)
O(2)--Cr(1)--N(3)	107.6(8)	104.5(7)	105.0(4)	98.5(0)

N(1)--Cr(1)--N(2)	79.5(0)	79.9(7)	80.2(2)	78.7(5)
N(1)--Cr(1)--N(3)	102.4(7)	98.3(8)	101.2(1)	102.7(1)
N(2)--Cr(1)--N(3)	101.8(0)	105.9(7)	103.5(5)	104.3(9)
τ_5 parameter[1]	0.05	0.25	0.03	0.13
Cr -Sal^{R} mean plane	0.48	0.52	0.50	0.46

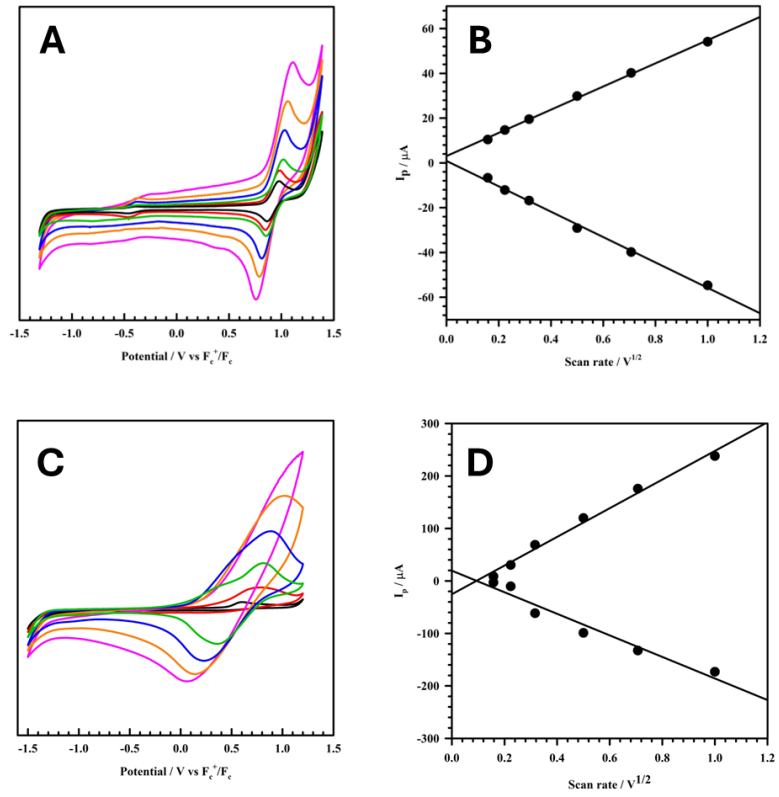

Figure S1: Scan rate dependence for A) **CrNSal^{NO2}**, C) **CrNSal^{H}**. Conditions: 0.1 M TBAP; CH_2Cl_2; 1 mM complex; T = 298 K; Scan rate 25 mV/s (black), 50 mV/s (red), 100 mV/s (green), 250 mV/s (blue), 500 mV/s (orange), 1000 mV/S (purple). Randles–Sevcik plots for B) **CrNSal^{NO2}** and D) **CrNSal^{H}** obtained from the cyclic voltammetry.

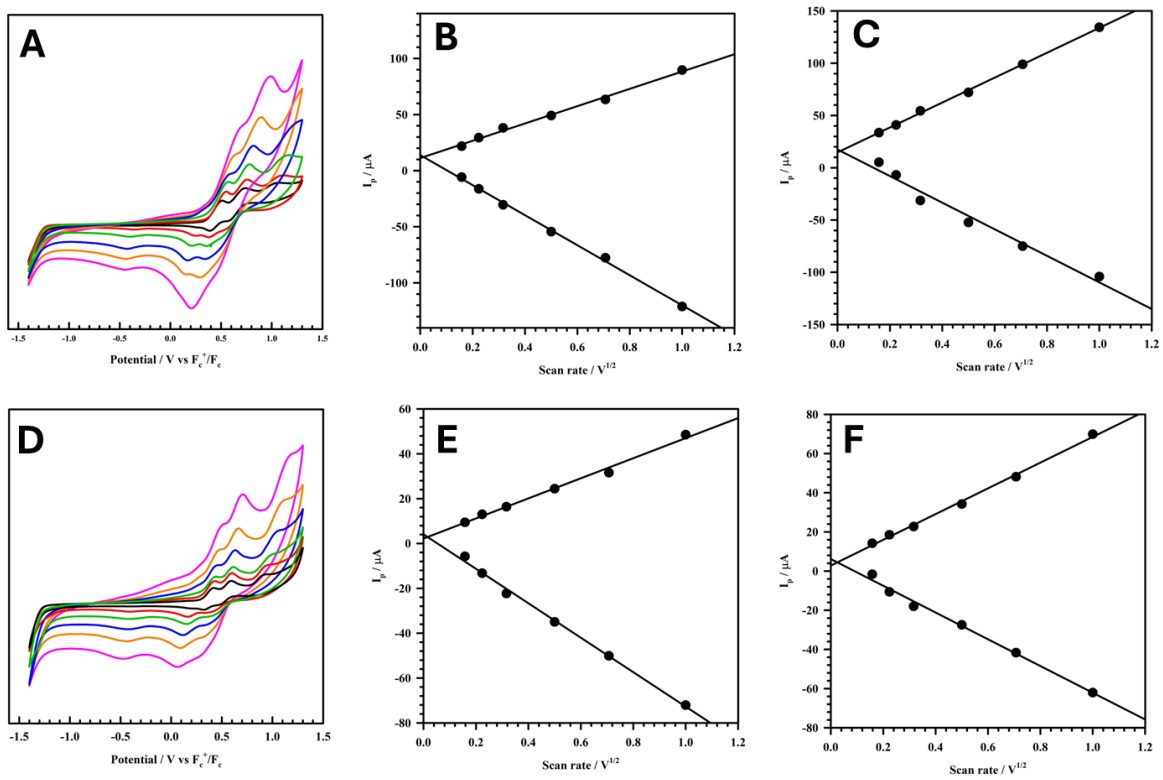

Figure S2: Scan rate dependence for A) **CrNSal^{OMe}**, D) **CrNSal^{OiPr}**. Conditions: 0.1 M TBAP; CH_2Cl_2; 1 mM complex; T = 298 K; Scan rate 25 mV/s (black), 50 mV/s (red), 100 mV/s (green), 250 mV/s (blue), 500 mV/s (orange), 1000 mV/S (purple). Randles–Sevcik plots for **CrNSal^{OMe}** (B and C) **CrNSal^{H}** obtained from the cyclic voltammetry.

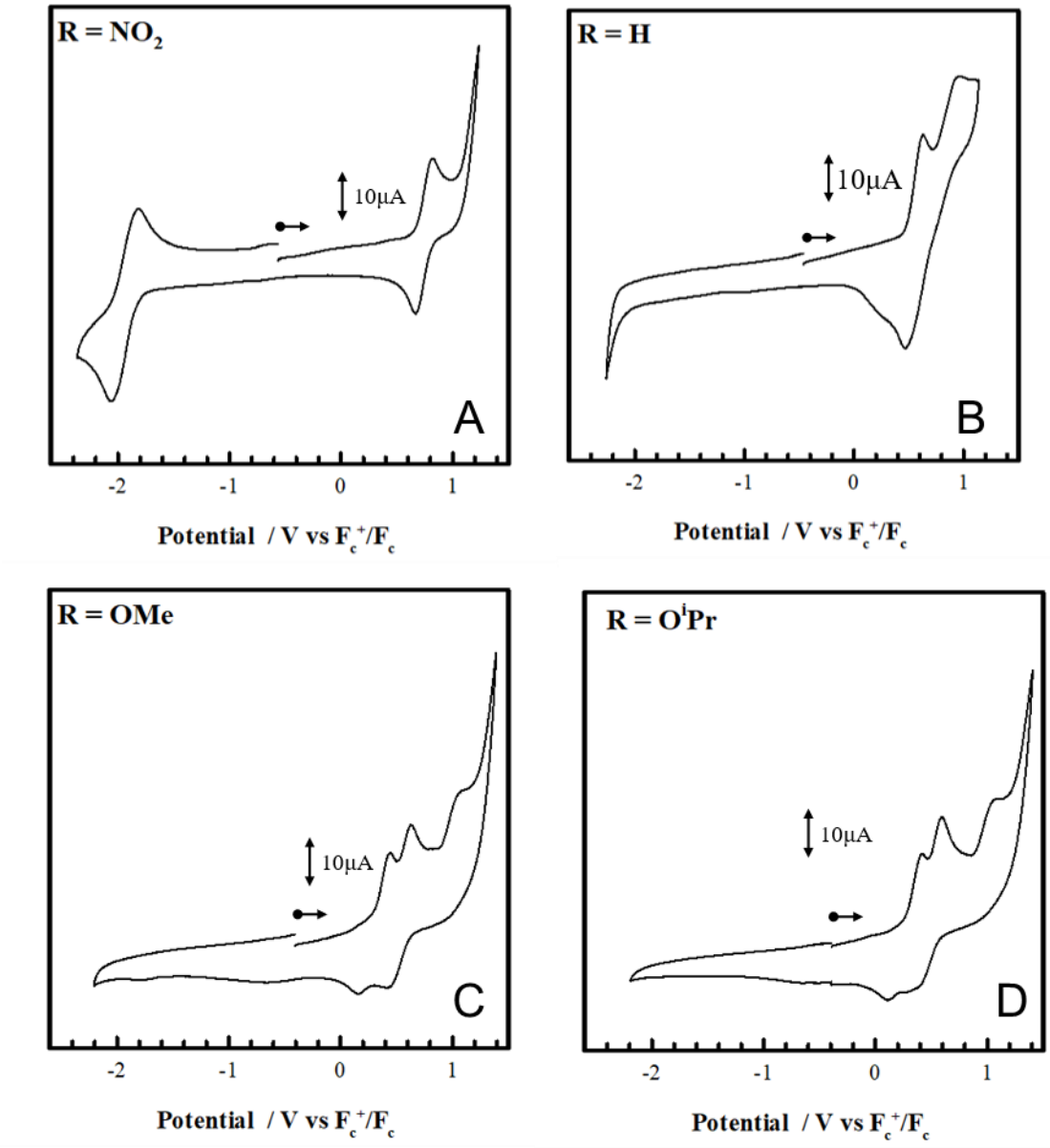

Figure S3: Full scan window cyclic voltammogram for A) **CrNSal^{NO2}**, B) **CrNSal^{H}**, C) **CrNSal^{OMe}**, D) **CrNSal^{OiPr}**. Conditions: 0.1 M TBAP; CH_2Cl_2; 1 mM complex; T = 298 K; scan rate = 100 mV/s.

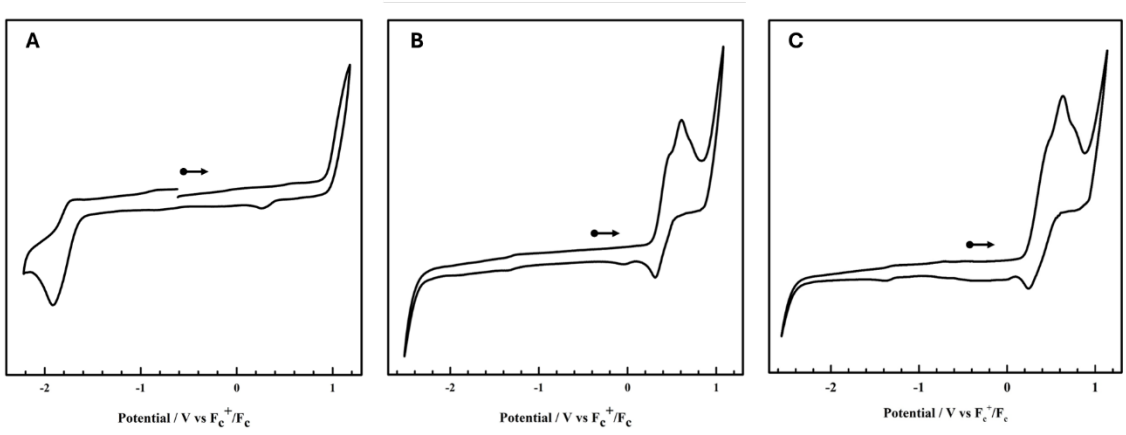

Figure S4: Full scan window cyclic voltammogram for A) **H_2Sal^{NO2}**, B) **H_2Sal^{OMe}**, C) **H_2Sal^{OiPr}**. Conditions: 0.1 M TBAP; CH_2Cl_2; 1 mM complex; T = 298 K; scan rate = 100 mV/s.

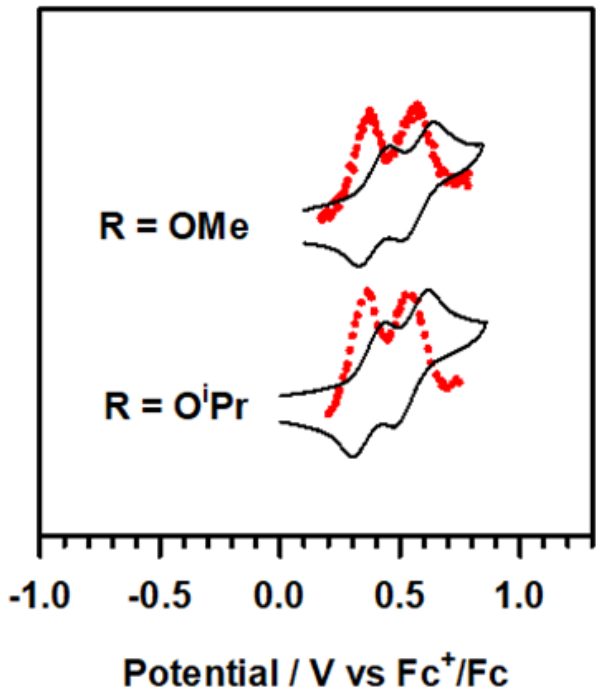

Figure S5: Stacked plots of cyclic voltammograms (black) and differential pulse voltammograms (red) for **$CrNSal^{OMe}$** and **$CrNSal^{OiPr}$**. Conditions: 0.1 M TBAP; CH_2Cl_2; 1 mM complex; T = 298 K; scan rate = 100 mV/s (CV).

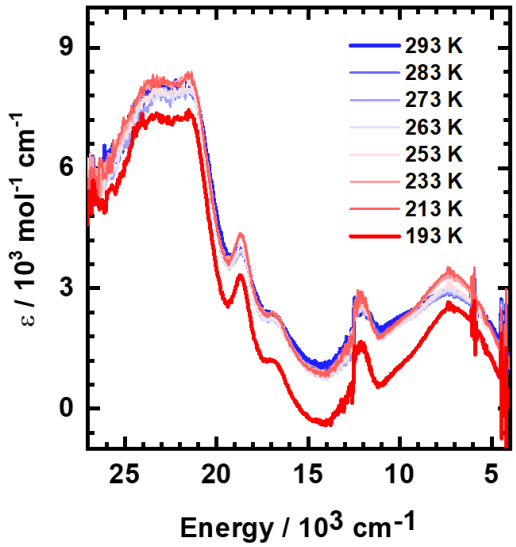

Figure S6: Variable temperature (VT) UV-vis-NIR spectra for oxidized **[CrNSal^{OiPr}]$^{+}$** derivative. Conditions: 0.45 mM; CH_2Cl_2. Note: Baseline is not corrected.

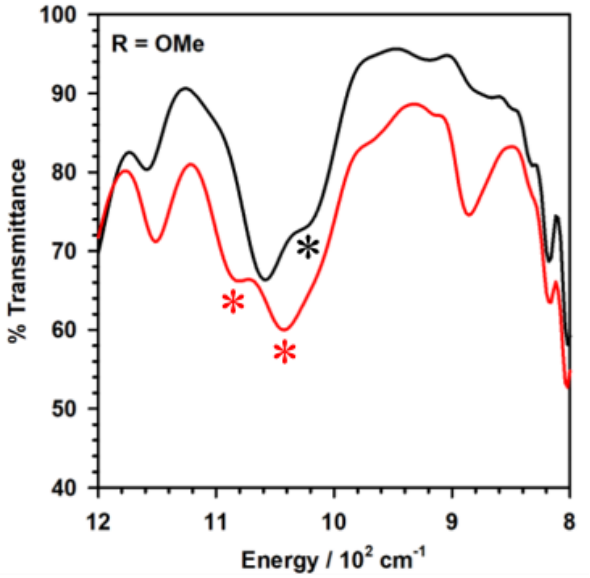

Figure S7: Solution IR spectra for neutral (black) and chemically oxidized with magic green (red) for **CrNSal^{OMe}**. * – ν(**Cr≡N**). Conditions: 5 mM complex; T = 298 K; CH_2Cl_2.

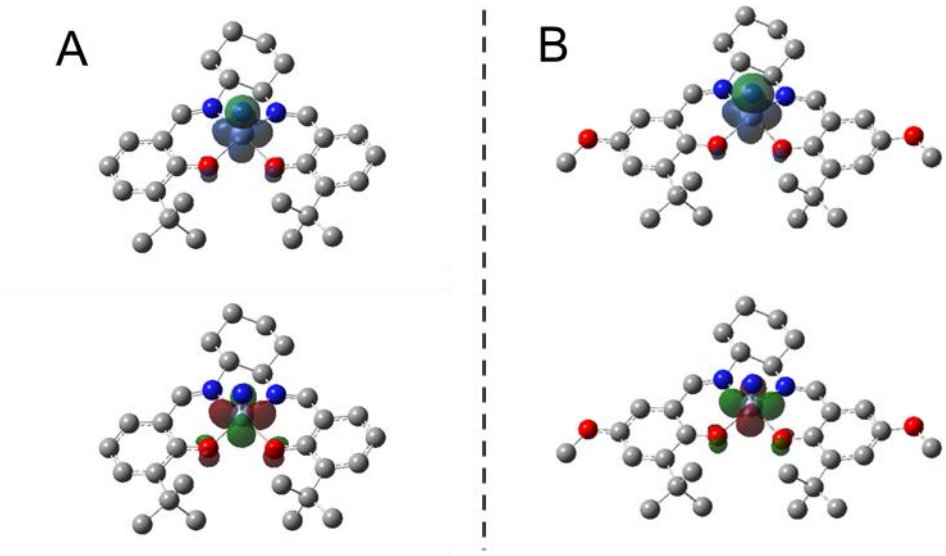

Figure S8: Spin density (top) and SOMO (bottom) plots for A) **CrNSal^{H}** B) **CrNSal^{OMe}**.

Table S3: A comparison of the spin density distribution versus σ_p for the **CrNSal^{R}** complexes. Using two different functionals we observe a small decrease in Cr-centered spin density as the substituent becomes more donating. The trend is continuous and small in magnitude for both functionals, indicating a gradual, yet limited spin delocalization over the ligand framework rather than a threshold-type behaviour that would signal a switch from metal to ligand-centered oxidation.

R =	σ_p	UBLYP	UM06L
NO_2	0.78	Cr = 94.30%, L = 5.70	Cr = 96.36%, L = 3.64%
CF_3	0.54	Cr = 94.26%, L = 5.74%	Cr = 95.80%, L = 4.20%
H	0.00	Cr = 93.99%, L = 6.01%	Cr = 95.77%, L = 4.23%
tBu	-0.20	Cr = 94.23%, L = 5.77%	Cr = 95.75%, L = 4.25%
OMe	-0.27	Cr = 93.91%, L = 6.07%	Cr = 95.63%, L = 4.37%
OiPr	-0.45	Cr = 93.88%, L = 6.12%	Cr = 95.49%, L = 4.51%
NMe_2	-0.83	Cr = 93.35%, L = 6.65%	Cr = 95.37% , L = 4.63%

Table S4: Computed relative energies (kcal/mol) of singlet (s), broken-symmetry singlet (bss), and triplet (t) states for **[CrNSal^{R}]$^{+}$** (R = tBu, OMe, OiPr, NMe_2) using UBLYP, UM06L, and UMN15L functionals with the def2-TZVP basis set. Zero indicates the lowest-energy spin state for each functional.

	UBLYP/Def2TZVP			UM06L/Def2TZVP			UMN15L/Def2TZVP		
	s	**bss**	**t**	**s**	**bss**	**t**	**s**	**bss**	**t**

$[CrNSal^{tBu}]^+$	**0**	2.9	7.7	**0**	3.3	6.9	**0**	1.3	5.0
$[CrNSal^{OMe}]^+$	**0**	0.6	3.4	0.2	**0**	2.1	2.8	**0**	2.4
$[CrNSal^{OiPr}]^+$	**0**	0.4	3.3	0.4	**0**	2.3	2.8	**0**	2.5
$[CrNSal^{NMe2}]^+$	2.3	**0**	1.35	3.9	**0**	+1.2	7.3	**0**	1.4

Table S5: Computed relative energies (kcal/mol) of singlet (s), broken-symmetry singlet (bss), and triplet (t) states for $[\mathbf{CrNSal^R}]^+$ (R = tBu, OMe, OiPr, NMe_2) using UBLYP/def2-TZVP/PCM(DCM) single-point calculations on geometries optimized at the UB3LYP/6-31G*/PCM(DCM) level.

Complex	Singlet	BSS	Triplet
$[CrNSal^{tBu}]^+$	**0**	2.8	6.4
$[CrNSal^{OMe}]^+$	**0**	1.9	2.3
$[CrNSal^{OiPr}]^+$	**0**	0.3	2.5
$[CrNSal^{NMe2}]^+$	2.3	**0**	0.6

Table S6: Computed relative energies (kcal/mol) of singlet (s), broken-symmetry singlet (bss), and triplet (t) states for $\mathbf{[CrNSal^R]^+}$ (R = tBu, OMe, OiPr, NMe_2) using UBLYP/def2-TZVP/PCM(DCM) single-point calculations on geometries optimized at the UB3LYP-GD3/6-31G*/PCM(DCM) level, to evaluate the influence of dispersion corrections.

Complex	Singlet	BSS	Triplet
$[CrNSal^{tBu}]^+$	**0**	2.9	7.7
$[CrNSal^{OMe}]^+$	**0**	0.6	3.4
$[CrNSal^{OiPr}]^+$	**0**	0.4	3.3
$[CrNSal^{NMe2}]^+$	2.3	**0**	1.35

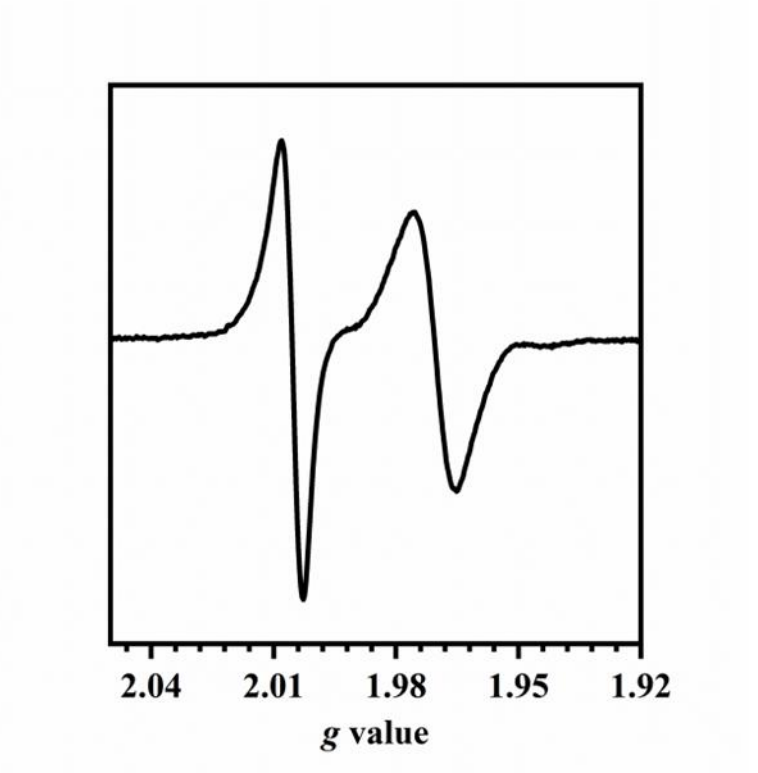

Figure S9: X-band EPR spectra for bis-oxidized in frozen CH2Cl2 at 0.4 mM. Conditions: frequency = 9.38 GHz, power = 2.0 mW, modulation frequency = 100 kHz, modulation amplitude = 0.6 mT, and T = −173 °C.

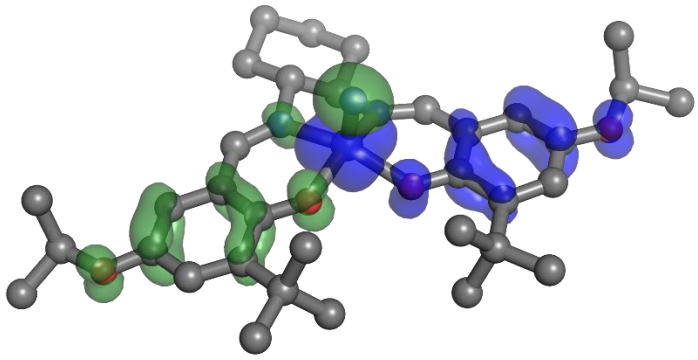

Figure S10: Computed spin density for the doublet Cr(V) bis-phenoxyl radical dication **[CrNSal^{OiPr}]$^{2+}$**. See calculation section for further details.

Optimized DFT co-ordinates:

Oxidized $[CrN(Sal)^{NO2}]^{+}$, singlet

H	3.03726900	-5.24187100	-0.27810600
H	-3.25658900	-5.19213600	0.63526000
H	-1.14569700	-4.31783100	-0.34637300
H	4.18360900	-4.29159000	0.67200500
H	1.15502200	-4.22635700	0.91667300
C	3.59143300	-4.29825900	-0.24994500
H	-4.19947900	-4.33398400	-0.58547200
H	4.27483900	-4.29238400	-1.10631200
H	1.24343800	-4.20922100	-1.62945800
C	-3.76286400	-4.24683500	0.41565700
H	-2.06839700	-3.40680500	-1.55727200
H	-4.57389000	-4.12895200	1.14323500
H	-1.68747200	-4.09101800	2.12700900
C	-1.63806100	-3.36108300	-0.55054400
H	2.24869600	-3.19518800	1.85817900
C	1.66345300	-3.25644200	0.93386500
C	1.78459200	-3.25691300	-1.61747100
C	2.58780900	-3.12966600	-0.30096800
H	2.46060300	-3.23764200	-2.47959200
C	-2.73785600	-3.09964200	0.50361700
H	-0.87368800	-2.58382100	-0.54007300
C	-2.13801800	-3.11180000	1.93096100
H	0.89723900	-2.48210700	0.96325400
H	5.30096900	-2.54933000	-0.16757900
H	1.05584600	-2.45343300	-1.73694900
H	-5.35149500	-2.49433100	-0.21750900
H	-2.92077000	-2.94179900	2.67864100
H	-1.36487400	-2.35319600	2.06297100
C	3.29806000	-1.76727400	-0.27336100
C	4.68484300	-1.66288100	-0.20939200
C	-3.38473500	-1.73685800	0.21321800
C	-4.72213700	-1.61885100	-0.14774900
O	1.24283100	-0.52990800	-0.39152900
C	2.57498100	-0.54354100	-0.29415800
O	-1.36122800	-0.54454500	0.62788500
C	-2.63245000	-0.52688000	0.25965100
C	5.33688600	-0.42356900	-0.20070600
N	6.80128700	-0.39041900	-0.14458700
C	-5.31139000	-0.37761200	-0.42693400
N	-6.72942700	-0.32846400	-0.79155500

Cr	0.07774700	0.54039300	0.48210700
N	0.63261200	0.63458900	1.87512300
C	3.24182900	0.71368300	-0.28297600
C	4.64196300	0.76761000	-0.25389400
C	-3.23708100	0.73114900	-0.02205900
C	-4.59630800	0.79997600	-0.35954300
H	5.16833300	1.71431600	-0.26328200
H	-5.07615000	1.74933200	-0.56375600
C	2.50534700	1.94965300	-0.40642200
C	-2.50585600	1.96165000	0.12253900
N	1.23175400	2.08603300	-0.24264400
N	-1.24644100	2.07650900	0.40018400
H	3.09121100	2.82539200	-0.67841400
H	-3.09317100	2.87095200	0.01303300
C	0.55252500	3.38352100	-0.45200700
H	0.11531800	3.34412600	-1.45911500
C	-0.60258200	3.39810600	0.55717000
H	-0.17485700	3.39993300	1.56811000
H	1.93249600	4.61516300	0.65547100
C	1.42661100	4.63542400	-0.31879800
H	2.19788500	4.65033100	-1.09554300
H	-2.28659900	4.63407100	1.12943000
C	-1.47962500	4.63843900	0.38847500
H	-1.93696500	4.64482000	-0.60980500
C	-0.60676800	5.89470300	0.55611200
C	0.55799200	5.89997100	-0.44132800
H	-0.21727900	5.93251200	1.58206000
H	0.16370200	5.96998100	-1.46383100
H	1.18936700	6.78072200	-0.28490300
H	-1.22812300	6.78547500	0.41843100
O	-7.22391800	0.77442600	-1.03346900
O	-7.35165600	-1.39073400	-0.83731100
O	7.35191400	0.71213400	-0.13539100
O	7.40326500	-1.46461800	-0.11077200

Oxidized $[CrN(Sal)^{H}]^{+}$, singlet

O	0.70290700	-1.33474300	0.49538700
N	-1.91763700	-1.40215400	0.27526800
C	0.77493000	-2.57300600	0.00876100
O	0.50262000	1.29507500	-0.39766400
N	-2.10960200	1.08846100	-0.25576100
C	2.03064100	-3.23061200	-0.10002700
C	2.00023300	-4.54329800	-0.57578700

H	2.93328600	-5.08035300	-0.69260800
C	0.81535400	-5.22035400	-0.90920600
C	-0.39925500	-4.57956900	-0.77358000
H	-1.32996800	-5.08877900	-1.00646500
C	-0.43431000	-3.24336700	-0.32450000
C	3.34568300	-2.50964300	0.23683300
C	3.33316000	-2.02743700	1.70798600
H	4.27838700	-1.52136700	1.93550900
H	3.23065600	-2.87887600	2.39053600
H	2.51941300	-1.32789300	1.90519800
C	3.51367300	-1.30940300	-0.72224900
H	2.68106200	-0.61045600	-0.64283900
H	3.57800600	-1.65048800	-1.76207500
H	4.43369600	-0.76366900	-0.48537600
C	4.56880600	-3.43017500	0.05889700
H	5.47481400	-2.87127600	0.31537100
H	4.67831100	-3.77548100	-0.97526700
H	4.52247400	-4.30582400	0.71623600
C	-1.70959500	-2.62335500	-0.11136900
H	-2.57503300	-3.26383500	-0.26995500
C	-3.28017400	-0.86744200	0.46410000
H	-3.31093100	-0.48091300	1.49109600
C	-4.45663900	-1.82299200	0.26440200
H	-4.38711000	-2.65944900	0.96870200
H	-4.44099400	-2.23715500	-0.75218700
C	-5.77091900	-1.05105500	0.47343100
H	-6.61714200	-1.72783400	0.31557800
H	-5.82921400	-0.70461200	1.51401600
C	-5.86556900	0.14874200	-0.47791600
H	-6.79012400	0.70698800	-0.29654000
H	-5.91071500	-0.21142400	-1.51469900
C	-4.66643800	1.10102400	-0.32478900
H	-4.74202000	1.90058800	-1.06906900
H	-4.67733600	1.56826400	0.66888300
C	-3.35389100	0.32877200	-0.49578100
H	-3.29086400	-0.06460700	-1.52022500
C	-2.06579000	2.37836900	-0.35176400
H	-2.98399600	2.91122100	-0.59347000
C	-0.89255200	3.19482500	-0.18583200
C	-1.04825100	4.59227000	-0.08877500
H	-2.04726800	5.01822900	-0.07651800
C	0.06989300	5.39622900	0.00630400
C	1.34721800	4.81629400	-0.02920200
H	2.20044500	5.47876200	0.04658200

C	1.56725600	3.44155200	-0.16092600
C	0.40959300	2.62542800	-0.22497400
C	2.98170500	2.84103900	-0.21552400
C	3.17674300	1.86107800	0.96655200
H	3.07237500	2.38993600	1.92088700
H	4.18097800	1.42459100	0.92780700
H	2.45807900	1.04217100	0.95110400
C	3.17911100	2.12522200	-1.57304900
H	3.11743400	2.84723200	-2.39543900
H	2.42911600	1.35096900	-1.74165900
H	4.16762000	1.65343700	-1.60669400
C	4.07368100	3.92303000	-0.09897300
H	4.02106000	4.65128500	-0.91594700
H	5.05655700	3.44268300	-0.14903000
H	4.01845300	4.46245800	0.85334700
Cr	-0.48505300	0.02394400	0.42631700
N	-0.60425100	0.51905000	1.84248100
H	0.86251700	-6.24449000	-1.26394000
H	-0.03031300	6.47216000	0.10360300

Oxidized [CrN(Sal)^{OMe}]$^{+}$, singlet

H	-3.38212600	-5.06058300	0.90247700
H	2.98889100	-5.21023700	-0.22380300
H	-1.88699300	-3.88712500	2.38762100
H	1.16016100	-4.15278900	1.03037200
H	1.15092700	-4.18803400	-1.51185900
H	-1.19996200	-4.31833100	-0.02607000
C	-3.84937800	-4.12767700	0.57064600
H	-4.70320300	-3.93242500	1.22957100
C	3.55258300	-4.27138500	-0.23250000
H	-4.22248300	-4.29382600	-0.44624100
H	4.20162700	-4.28576100	-1.11544200
H	4.18210900	-4.25783700	0.66448000
C	-2.28746000	-2.91235500	2.08647200
C	1.68753700	-3.19252000	1.01326500
C	1.70145300	-3.24078300	-1.54049000
H	-3.10429900	-2.65518400	2.77058300
C	-1.64980000	-3.36632900	-0.32944300
H	2.34259800	-3.24560000	-2.42959700
H	2.31639500	-3.13358800	1.90906500
H	-2.01785900	-3.47534600	-1.35627800
C	-2.80442900	-2.99625000	0.62916400
C	2.56002200	-3.09209400	-0.26171700

H	-1.49535300	-2.17084300	2.19926500
H	0.94121100	-2.39999400	1.06875500
H	0.97800100	-2.43124400	-1.64504900
H	-0.86681100	-2.60857300	-0.32465400
H	-5.30641800	-2.42704900	-0.32804300
H	5.24494900	-2.55121800	-0.23440200
H	-7.52616900	-1.75693000	-0.21167600
H	-6.97787800	-2.09961300	-1.88404200
H	7.32891100	-2.09919100	-1.13376100
H	7.31856300	-2.06510700	0.65791100
C	-3.39132400	-1.64358800	0.19245200
C	3.27418900	-1.72971300	-0.28201200
C	-4.69684000	-1.53661800	-0.28606400
C	4.66885400	-1.63819200	-0.26334600
C	-7.38080000	-1.33243600	-1.21214400
C	7.50808000	-1.47686800	-0.24834100
H	-8.33612200	-0.97669700	-1.59887900
H	8.54423000	-1.13653800	-0.24873300
O	-1.36017100	-0.47957400	0.66533200
O	1.20330100	-0.50582600	-0.36158300
C	-2.60454000	-0.45755400	0.20103300
C	2.54570500	-0.51433600	-0.28838800
C	-5.26364800	-0.31738400	-0.71050100
C	5.35824900	-0.41132000	-0.28263900
O	-6.53234900	-0.18225800	-1.16910800
O	6.71320500	-0.29106100	-0.27526800
Cr	0.08082700	0.61140500	0.52327100
N	0.66230200	0.69011800	1.91070000
C	-3.17434500	0.78280000	-0.20995500
C	3.23188800	0.73149200	-0.29800100
C	-4.50337800	0.84402400	-0.65248700
C	4.63515800	0.77263200	-0.31734200
H	-4.95111900	1.79013500	-0.93850900
H	5.16183600	1.72105800	-0.34880600
C	-2.46229800	2.01963800	-0.03269100
C	2.51507300	1.97685100	-0.41066300
N	1.24519700	2.13486600	-0.22338700
N	-1.23758600	2.14003400	0.37516300
H	3.11099300	2.84288000	-0.69434600
H	-3.03548500	2.92492400	-0.22476300
H	0.16955900	3.42515400	-1.44914800
C	0.58534900	3.44100600	-0.43161200
C	-0.59726300	3.45726000	0.54949200
H	-0.19113400	3.45522300	1.56917500

H	-1.88369900	4.73170600	-0.64475900
H	2.25754600	4.70576600	-1.01240100
C	1.46433100	4.68495200	-0.25813700
C	-1.46018900	4.70539700	0.36777800
H	-2.29320300	4.69539500	1.07963700
H	1.94469800	4.64575500	0.72840200
H	0.24387900	6.04571800	-1.41720000
C	0.61049000	5.95922000	-0.38537800
C	-0.58309300	5.95203400	0.57852500
H	-0.22183900	5.97220800	1.61550700
H	1.24370900	6.83350700	-0.20079700
H	-1.19081900	6.85171600	0.43576200

Oxidized [CrN(Sal)^{OIPr}]$^{+}$, singlet

O	-1.33585200	-0.68474600	0.76579700
N	-1.24189300	1.93433000	0.49529200
C	-2.59649300	-0.66607900	0.35891000
O	1.18755500	-0.68629700	-0.35304300
N	1.21961100	1.95497000	-0.18508800
C	-3.37931200	-1.86196700	0.38749300
C	-4.69681300	-1.75178700	-0.02827900
H	-5.33834000	-2.62339900	-0.05482500
C	-5.29795700	-0.53576900	-0.43286500
C	-4.54694300	0.63024000	-0.41147400
H	-4.97395200	1.59162200	-0.66788900
C	-3.19159500	0.56772300	-0.02581200
C	-2.76683300	-3.21101500	0.79573600
C	-2.18419200	-3.12667700	2.22786800
H	-1.76841600	-4.10079000	2.50981000
H	-2.96940800	-2.87180200	2.94893000
H	-1.38922400	-2.38348200	2.30477900
C	-1.65553800	-3.57466200	-0.21509600
H	-0.87534500	-2.81444500	-0.24419300
H	-2.06957300	-3.68300100	-1.22428300
H	-1.18916500	-4.52564600	0.06558700
C	-3.81099500	-4.34421100	0.78205100
H	-3.32776800	-5.27730700	1.08978600
H	-4.23038200	-4.50669800	-0.21707100
H	-4.63432500	-4.15076200	1.47903100
C	-2.48044600	1.80537400	0.12744600
H	-3.06368400	2.70873000	-0.04219300
C	-0.60885900	3.25682300	0.65491400
H	-0.17326900	3.25558700	1.66232700

C	-1.48754000	4.49815600	0.50348900
H	-2.30132700	4.47695600	1.23712200
H	-1.93825000	4.52633700	-0.49747500
C	-0.61595800	5.75107800	0.70022900
H	-1.23427900	6.64659300	0.57810500
H	-0.23040200	5.76771900	1.72848400
C	0.55420900	5.77537800	-0.29189900
H	1.18494500	6.65303300	-0.11481000
H	0.16190900	5.86832800	-1.31361400
C	1.42055100	4.50648100	-0.19854200
H	2.19279200	4.54017200	-0.97393100
H	1.92819600	4.46170200	0.77407200
C	0.54578800	3.25799800	-0.36019300
H	0.10094500	3.25126800	-1.36536100
C	2.48532100	1.80383900	-0.41310100
H	3.06761600	2.67730600	-0.70287400
C	3.20967400	0.56192500	-0.34444300
C	4.61943800	0.61677700	-0.41864900
H	5.10299500	1.58552100	-0.44510800
C	5.34173500	-0.56494400	-0.44307000
C	4.64735400	-1.79513500	-0.42367600
H	5.26471900	-2.68432200	-0.44112300
C	3.26313300	-1.90165800	-0.38981900
C	2.52817600	-0.68313400	-0.33687700
C	2.55603100	-3.26648000	-0.36564500
C	1.74622300	-3.39675600	0.94747700
H	2.41710000	-3.35175700	1.81309100
H	1.22509700	-4.36027000	0.97063500
H	0.99950200	-2.60964400	1.05412800
C	1.63721300	-3.39426800	-1.60403200
H	2.23396100	-3.37419700	-2.52335800
H	0.90295200	-2.58930600	-1.65481000
H	1.09643100	-4.34691500	-1.56944500
C	3.55640800	-4.43835000	-0.40859800
H	4.16445000	-4.42628400	-1.32014000
H	3.00013500	-5.38162700	-0.39527200
H	4.22704000	-4.43891500	0.45797700
Cr	0.09386400	0.42388800	0.58320200
N	0.72749700	0.48961700	1.94852800
C	-7.35989700	0.52726900	-1.18273700
H	-6.73384300	1.16515400	-1.81986900
C	7.53362600	0.49981200	-0.46413400
H	7.10267800	1.26128500	-1.12755000
O	-6.59238400	-0.64687300	-0.80957100

O	6.69300700	-0.67951800	-0.50568100
C	-8.53098700	-0.00012200	-1.99951700
H	-9.14300500	-0.67563200	-1.39236500
H	-9.15829500	0.83223300	-2.33359800
H	-8.17404700	-0.54541800	-2.87832600
C	-7.80257600	1.28280900	0.06802700
H	-8.43762100	0.63932100	0.68591500
H	-6.94900600	1.60503000	0.67189800
H	-8.37671300	2.17090300	-0.21572100
C	7.63302200	1.02791400	0.96539500
H	8.08168600	0.26664000	1.61243000
H	8.26251100	1.92351500	0.99167700
H	6.65045000	1.28739200	1.37055200
C	8.87817100	0.05588700	-1.02344800
H	9.57463200	0.90010900	-1.04086900
H	9.30583600	-0.73559000	-0.39866200
H	8.76434300	-0.32632600	-2.04238100

Oxidized $[CrN(Sal)^{H}]^{+}$, bss

O	0.79570800	-1.32115900	0.27212800
N	-1.95337200	-1.45390200	0.20190000
C	0.81390400	-2.55938400	-0.04698800
O	0.57123600	1.33108500	-0.17468300
N	-2.14011600	1.12802200	-0.15301400
C	2.09627600	-3.25139100	-0.13100300
C	2.06494400	-4.58507500	-0.51655300
H	2.98950200	-5.14043400	-0.60443700
C	0.86805500	-5.26448000	-0.80025000
C	-0.36699500	-4.61602400	-0.69008000
H	-1.28505500	-5.16006500	-0.89095600
C	-0.42181300	-3.27857100	-0.31620400
C	3.40072200	-2.51640500	0.18551500
C	3.36371300	-1.98125100	1.64173500
H	4.31037300	-1.47518300	1.86068900
H	3.24651700	-2.80585800	2.35390700
H	2.55331700	-1.26783600	1.79567800
C	3.58645600	-1.34212100	-0.80859200
H	2.77957900	-0.61597200	-0.72759800
H	3.63068700	-1.70895200	-1.84051200
H	4.52914300	-0.82870900	-0.59004100
C	4.62391600	-3.44500100	0.05668400
H	5.52663300	-2.87580400	0.29956800
H	4.74310300	-3.83025400	-0.96215700

H	4.57207300	-4.29287100	0.74892300
C	-1.72654000	-2.67105600	-0.15981000
H	-2.56862400	-3.33540100	-0.34746100
C	-3.32171600	-0.92402000	0.38110900
H	-3.38016500	-0.64373100	1.44145800
C	-4.49015700	-1.85323800	0.05218900
H	-4.43945100	-2.75732600	0.66936800
H	-4.43854100	-2.16323800	-1.00026600
C	-5.81595200	-1.11655200	0.31037500
H	-6.65259300	-1.77332400	0.04954300
H	-5.90461000	-0.89901600	1.38321800
C	-5.89591500	0.19054700	-0.48775400
H	-6.82671400	0.71983400	-0.25729700
H	-5.91953700	-0.03904800	-1.56195800
C	-4.70212000	1.11646600	-0.19747800
H	-4.77381900	2.00262300	-0.83589900
H	-4.72542700	1.45854000	0.84567000
C	-3.38254500	0.37654400	-0.44788400
H	-3.32729800	0.08927800	-1.50771600
C	-2.07472900	2.41837600	-0.27736200
H	-2.98364400	2.96331200	-0.53008300
C	-0.89038900	3.21978500	-0.14299600
C	-1.04442500	4.62258100	-0.13419600
H	-2.04443600	5.04733100	-0.15268800
C	0.06731800	5.43785800	-0.09331200
C	1.35208800	4.86267800	-0.10369400
H	2.19993200	5.53652200	-0.08287000
C	1.57618700	3.48938800	-0.14647600
C	0.42179200	2.63926300	-0.13879800
C	2.99392500	2.89624200	-0.21041100
C	3.23699800	1.93982300	0.98293100
H	3.14466500	2.48190100	1.93153200
H	4.25137600	1.52755700	0.92645800
H	2.53237500	1.10921000	0.99040200
C	3.16009500	2.14696000	-1.55534800
H	3.07673800	2.84745100	-2.39462800
H	2.40434300	1.37018700	-1.67957400
H	4.14856500	1.67503700	-1.60259700
C	4.08095300	3.98781600	-0.15090300
H	4.00964900	4.68881900	-0.99021400
H	5.06661200	3.51295300	-0.20329800
H	4.03805800	4.55883600	0.78369500
Cr	-0.59906900	0.02208900	0.51284100
N	-0.67066000	0.26380000	2.01259900

H	0.90284500	-6.30728400	-1.09719500
H	-0.03930400	6.51739200	-0.06548400

Oxidized $[CrN(Sal)^{OMe}]^{+}$, bss

H	-3.26236100	-5.20012100	0.31927600
H	3.13679700	-5.19711500	-0.17096700
H	-1.67211900	-4.13655800	1.82898200
H	1.21661800	-4.21806600	0.94617100
H	1.36805700	-4.18124100	-1.58427500
H	-1.21989500	-4.31606000	-0.66800600
C	-3.78136900	-4.25089300	0.15391500
H	-4.57201100	-4.17334900	0.90901000
C	3.68116800	-4.24701100	-0.14170300
H	-4.24500000	-4.29920700	-0.83802700
H	4.37958700	-4.24422100	-0.98648200
H	4.26020800	-4.22706700	0.78894700
C	-2.13491200	-3.15495200	1.67896200
C	1.70371500	-3.23621700	0.98227900
C	1.90138300	-3.22359900	-1.55413300
H	-2.90507700	-3.02140900	2.44708900
C	-1.67145700	-3.32894000	-0.81550600
H	2.59846700	-3.19559600	-2.40007400
H	2.25415900	-3.16620500	1.92808900
H	-2.10735200	-3.30211600	-1.82092200
C	-2.76164700	-3.10052600	0.26125000
C	2.67000800	-3.08569500	-0.21759100
H	-1.36721300	-2.39287200	1.81620700
H	0.92924000	-2.47059300	0.97530100
H	1.17300800	-2.42154200	-1.68062900
H	-0.88086000	-2.58314800	-0.75356000
H	-5.38703600	-2.49477500	-0.26667800
H	5.34001100	-2.49937400	-0.11581200
H	-7.57817300	-1.85390500	0.23650200
H	-7.28237300	-1.96314300	-1.53375200
H	7.43893500	-2.02582400	-0.94426800
H	7.37740700	-1.97283700	0.84482600
C	-3.42121400	-1.73353400	0.04542000
C	3.35800600	-1.70864000	-0.18037900
C	-4.77238900	-1.60882700	-0.20828800
C	4.74754200	-1.59656700	-0.14624800
C	-7.57501200	-1.30526000	-0.71009400
C	7.58376400	-1.38983800	-0.06169400
H	-8.56023500	-0.88327300	-0.90111300

H	8.61605800	-1.03770600	-0.03685500
O	-1.36722800	-0.59981200	0.32460800
O	1.26656200	-0.55584800	-0.23500800
C	-2.62273300	-0.51174900	0.10978000
C	2.59037100	-0.50492700	-0.19115000
C	-5.39074200	-0.34792900	-0.39113300
C	5.41857300	-0.35711100	-0.15479000
O	-6.68854500	-0.17134200	-0.63127100
O	6.77639000	-0.21648400	-0.12359000
Cr	0.08939200	0.69190400	0.53710300
N	0.39233700	0.72493400	2.02652700
C	-3.26999100	0.77675400	-0.06685400
C	3.27121000	0.75291400	-0.21104400
C	-4.62735000	0.83796400	-0.31389500
C	4.67795800	0.81111300	-0.20912300
H	-5.13621800	1.78763900	-0.44360200
H	5.19126600	1.76756300	-0.23681900
C	-2.55152300	2.03602600	0.03884100
C	2.55672200	1.99491200	-0.34334200
N	1.28166900	2.15428700	-0.16975800
N	-1.29777400	2.16649900	0.29855200
H	3.15754800	2.85680500	-0.63186100
H	-3.16530800	2.92518000	-0.09981700
H	0.26186100	3.38066300	-1.50457300
C	0.60562400	3.43928000	-0.46150500
C	-0.65258800	3.49169500	0.42968800
H	-0.31723400	3.54145500	1.47452400
H	-1.87699700	4.67095600	-0.90936500
H	2.30629300	4.69528200	-0.96788100
C	1.45031600	4.70697200	-0.28589200
C	-1.50570400	4.72319400	0.12314700
H	-2.37551300	4.75716800	0.78863400
H	1.84530900	4.73207200	0.73839100
H	0.31366500	5.96939900	-1.62508100
C	0.60122600	5.95832600	-0.56462000
C	-0.66107000	5.99577600	0.30502500
H	-0.37740200	6.09312600	1.36159200
H	1.20888200	6.85319600	-0.39224900
H	-1.26877800	6.87269600	0.05753800

Oxidized [CrN(Sal)^{OiPr}]$^{+}$, bss

O	-1.35947800	-0.79173800	0.37327100
N	-1.29695200	1.96652600	0.34261900

C	-2.61945400	-0.71023000	0.18177200
O	1.26620900	-0.75062300	-0.22398000
N	1.27030100	1.95860600	-0.17346700
C	-3.41516700	-1.93492900	0.14305500
C	-4.76023300	-1.80443100	-0.09808200
H	-5.41026100	-2.66839000	-0.14637300
C	-5.39610300	-0.54519400	-0.29375800
C	-4.64030400	0.64200000	-0.22950400
H	-5.11086600	1.60922900	-0.35433300
C	-3.27391000	0.57404700	0.00645300
C	-2.75262000	-3.29914400	0.37048700
C	-2.09964300	-3.33162300	1.77619800
H	-1.63916500	-4.31275200	1.93668100
H	-2.85406800	-3.17904000	2.55645100
H	-1.32511600	-2.57147700	1.88493800
C	-1.68334100	-3.54720800	-0.72152400
H	-0.89281600	-2.79928000	-0.68827600
H	-2.13789400	-3.53891400	-1.71903100
H	-1.22681400	-4.53082900	-0.56527300
C	-3.77852000	-4.44658200	0.30083600
H	-3.26126800	-5.39557300	0.47398900
H	-4.25986900	-4.50866100	-0.68173500
H	-4.55629000	-4.35032000	1.06690200
C	-2.55515300	1.83198300	0.09995200
H	-3.16940100	2.72182600	-0.03164400
C	-0.65374100	3.29363800	0.45984100
H	-0.29789200	3.34609700	1.49774100
C	-1.51511000	4.52296900	0.16825100
H	-2.37179300	4.55631700	0.85068300
H	-1.90642200	4.46907000	-0.85673400
C	-0.66899300	5.79718800	0.33136000
H	-1.28291700	6.67290800	0.09518200
H	-0.36384700	5.89635300	1.38176200
C	0.57538600	5.76038100	-0.56367900
H	1.18420100	6.65719600	-0.40604200
H	0.26619000	5.76802200	-1.61809800
C	1.43271900	4.51159900	-0.29890700
H	2.27521300	4.50046200	-0.99756700
H	1.84756800	4.54010300	0.71742400
C	0.58750600	3.24174700	-0.45542000
H	0.22297300	3.18141700	-1.49145100
C	2.54367100	1.80043200	-0.37433400
H	3.13445200	2.66584800	-0.67331600
C	3.26467700	0.56317100	-0.26452600

C	4.67896300	0.63068600	-0.30920500
H	5.15232200	1.60466500	-0.34604700
C	5.41615000	-0.53815800	-0.28891100
C	4.73729900	-1.77911300	-0.26196100
H	5.36896800	-2.65877600	-0.25769800
C	3.35729200	-1.90232500	-0.25039300
C	2.58663500	-0.69265600	-0.22803800
C	2.67033500	-3.27897000	-0.26993200
C	1.74567500	-3.43670500	0.96147800
H	2.32744900	-3.36623700	1.88831300
H	1.26320800	-4.42117500	0.93902300
H	0.96679400	-2.67564800	0.98315500
C	1.85744400	-3.41242800	-1.58038600
H	2.52564900	-3.38012600	-2.44913800
H	1.12367000	-2.61134700	-1.67934800
H	1.32489000	-4.37074100	-1.59609400
C	3.68835400	-4.43578400	-0.23318900
H	4.35871800	-4.42422900	-1.10008400
H	3.14780900	-5.38842100	-0.24899400
H	4.29805200	-4.41603500	0.67748400
Cr	0.09618100	0.50011800	0.56125600
N	0.42631400	0.53896700	2.04526400
C	-7.53595600	0.58152500	-0.70084800
H	-6.97902200	1.29492400	-1.31753500
C	7.59530200	0.55167300	-0.27680300
H	7.17296500	1.29592700	-0.96525900
O	-6.70257400	-0.61397400	-0.52569200
O	6.77433300	-0.63815200	-0.31833700
C	-8.76215300	0.09914400	-1.45867300
H	-9.30317300	-0.65035100	-0.87230300
H	-9.43082000	0.94457600	-1.64688200
H	-8.47590100	-0.34106200	-2.41808900
C	-7.85866500	1.16746500	0.66878200
H	-8.39368700	0.42984700	1.27515100
H	-6.95416400	1.46861400	1.20580300
H	-8.49579800	2.04888100	0.54728400
C	7.65026800	1.10982900	1.14424400
H	8.09470000	0.36891600	1.81750800
H	8.26393600	2.01652700	1.16921100
H	6.65311300	1.35944500	1.51848500
C	8.96159700	0.11840400	-0.79101100
H	9.64724600	0.97163400	-0.80351800
H	9.38226200	-0.65667700	-0.14124500
H	8.88177400	-0.28274500	-1.80596700

Oxidized $[CrN(Sal)^{NO2}]^{+}$, triplet

H	3.16116900	-5.26306100	-0.23785700
H	-3.25764000	-5.26399800	0.29743100
H	-1.23616300	-4.37135500	-0.71581800
H	4.29263800	-4.31413000	0.73338100
H	1.26585000	-4.32807100	0.94120500
C	3.70167700	-4.31210400	-0.18966100
H	-4.26246200	-4.34975500	-0.82979400
H	4.38754400	-4.28173500	-1.04369000
H	1.36181800	-4.21222000	-1.59322900
C	-3.78007200	-4.31363600	0.15326900
H	-2.13847500	-3.34267400	-1.84416900
H	-4.55474100	-4.24413700	0.92478400
H	-1.63212800	-4.21502200	1.78414100
C	-1.68497600	-3.38129800	-0.84766800
H	2.29576300	-3.27733400	1.93114300
C	1.73529200	-3.33893700	0.99115300
C	1.89523400	-3.25594000	-1.54906000
C	2.68319900	-3.15564300	-0.21937800
H	2.57897200	-3.20729000	-2.40428600
C	-2.75689300	-3.16602700	0.25361500
H	-0.89079400	-2.63923200	-0.79058200
C	-2.09966700	-3.23269000	1.65980600
H	0.94607000	-2.58868200	1.00887000
H	5.38552300	-2.54307100	-0.14214200
H	1.16381500	-2.45215100	-1.64684600
H	-5.42620700	-2.53559100	-0.21853900
H	-2.85355200	-3.11168800	2.44510100
H	-1.33061100	-2.47053100	1.79074700
C	3.37463200	-1.78450500	-0.16313000
C	4.75472700	-1.66615700	-0.15166400
C	-3.41876000	-1.80365200	0.06618900
C	-4.78270700	-1.67015500	-0.15675200
O	1.30421200	-0.62151300	-0.11578900
C	2.60714100	-0.56583000	-0.13688900
O	-1.37243200	-0.65449100	0.30036700
C	-2.62902900	-0.56965100	0.13067100
C	5.39427400	-0.41457800	-0.15874900
N	6.85291300	-0.36150900	-0.15202300
C	-5.37011300	-0.41212300	-0.30742900
N	-6.82213400	-0.33468000	-0.55273900
Cr	0.06971200	0.65924200	0.55314100
N	0.28208200	0.71418900	2.05162400

C	3.27990100	0.70603000	-0.17157200
C	4.67920200	0.76639300	-0.19276800
C	-3.28254400	0.72788900	-0.00843000
C	-4.64597500	0.78320000	-0.23336800
H	5.19676900	1.71754400	-0.22996800
H	-5.16103900	1.72902500	-0.35000100
C	2.56098700	1.94978000	-0.29306300
C	-2.56777300	1.99095100	0.07803500
N	1.28597000	2.10606700	-0.13335100
N	-1.30715000	2.12629100	0.29767700
H	3.16491900	2.81314900	-0.56813100
H	-3.18952700	2.87656400	-0.04254100
C	0.61534800	3.39718100	-0.42964600
H	0.29665000	3.33677300	-1.47992000
C	-0.66258600	3.45209900	0.43260300
H	-0.35246100	3.50554500	1.48520200
H	1.82619100	4.68900200	0.80099000
C	1.45823200	4.66247700	-0.23308100
H	2.33053300	4.64973900	-0.89365900
H	-2.39124100	4.72097600	0.74951900
C	-1.50980800	4.68096900	0.10048400
H	-1.86010000	4.62014400	-0.93872800
C	-0.66895600	5.95450900	0.29567800
C	0.61652600	5.91314300	-0.53856200
H	-0.41545400	6.05942700	1.35897100
H	0.35974600	5.92147000	-1.60666300
H	1.22039500	6.80717500	-0.35102700
H	-1.27065300	6.82841100	0.02517800
O	-7.30794400	0.78288000	-0.72251000
O	-7.45407600	-1.38823700	-0.57413000
O	7.39359800	0.74830200	-0.16259500
O	7.47351100	-1.42790300	-0.13616400

Oxidized $[CrN(Sal)^{H}]^{+}$, triplet

O	0.82642600	-1.30213600	0.16640600
N	-1.94689200	-1.47949900	0.18477300
C	0.84757300	-2.55897800	-0.04394400
O	0.54731400	1.35058000	-0.15317100
N	-2.15202300	1.11660400	-0.13718200
C	2.14128700	-3.24015500	-0.14012700
C	2.11736900	-4.60228200	-0.41275800
H	3.04632500	-5.15061500	-0.49670500
C	0.92162900	-5.31595600	-0.58306100

C	-0.32237400	-4.67398900	-0.47255100
H	-1.23670500	-5.24580600	-0.59935300
C	-0.38787600	-3.31666000	-0.20026400
C	3.44275400	-2.46834800	0.07814800
C	3.45355000	-1.87042400	1.51094400
H	4.39195200	-1.32643900	1.66368800
H	3.39482700	-2.66582700	2.26232800
H	2.62807300	-1.17573600	1.67066900
C	3.56654200	-1.33553500	-0.97316500
H	2.75913900	-0.61140700	-0.88385000
H	3.56560900	-1.74668400	-1.98901000
H	4.51476600	-0.80863900	-0.82124500
C	4.67725400	-3.38029500	-0.06162900
H	5.57831100	-2.78186600	0.10473600
H	4.75326800	-3.81814800	-1.06321600
H	4.67894500	-4.18942300	0.67708400
C	-1.70375400	-2.71440300	-0.08414300
H	-2.53487000	-3.40343800	-0.22761200
C	-3.32195400	-0.95786800	0.34524300
H	-3.39905600	-0.69231200	1.40869800
C	-4.47636400	-1.89387400	-0.01439400
H	-4.43567300	-2.80007300	0.59994900
H	-4.39426700	-2.19953600	-1.06622000
C	-5.81511800	-1.17241400	0.21819300
H	-6.63837000	-1.83505700	-0.06917900
H	-5.93144700	-0.96715800	1.29088800
C	-5.88930400	0.14244500	-0.56683800
H	-6.83078200	0.65982300	-0.35318700
H	-5.88400700	-0.07430300	-1.64393100
C	-4.71214600	1.07502000	-0.23550500
H	-4.77775400	1.96962200	-0.86253700
H	-4.76316100	1.40202000	0.81148500
C	-3.37921200	0.35241300	-0.46581300
H	-3.29856400	0.08114200	-1.52848000
C	-2.10151000	2.40875400	-0.25370500
H	-3.01577600	2.94285900	-0.51029900
C	-0.92925300	3.22489700	-0.10774600
C	-1.09991100	4.62603400	-0.07714600
H	-2.10506300	5.03920200	-0.08781100
C	0.00249900	5.45274100	-0.02375000
C	1.29282300	4.89067000	-0.04406700
H	2.13393900	5.57287300	-0.01686100
C	1.53156400	3.51998500	-0.10442500
C	0.38707200	2.65776000	-0.10635700

C	2.95551200	2.94386800	-0.19046200
C	3.21912400	1.96269700	0.97742400
H	3.12261200	2.47829900	1.94030500
H	4.23954800	1.56759400	0.90621600
H	2.52657800	1.12244800	0.96415100
C	3.11755200	2.22311400	-1.55123100
H	3.01660800	2.93775400	-2.37658200
H	2.36915800	1.43983000	-1.68101800
H	4.11089000	1.76379200	-1.61808100
C	4.03154700	4.04525800	-0.11677700
H	3.94749200	4.76191900	-0.94155700
H	5.02187200	3.58206300	-0.18477600
H	3.98857500	4.59745800	0.82912500
Cr	-0.60313300	0.01133600	0.51199000
N	-0.65845800	0.16512600	2.02014000
H	0.95794400	-6.37894600	-0.79627400
H	-0.11530000	6.53062200	0.02013100

Oxidized $[CrN(Sal)^{OMe}]^{+}$, triplet

H	-3.25210400	-5.21144800	0.17484700
H	3.15753600	-5.19418100	-0.17657900
H	-1.62921900	-4.18178000	1.68825800
H	1.22153400	-4.22769100	0.92332100
H	1.40406100	-4.17004600	-1.60371500
H	-1.24191900	-4.29707800	-0.82358700
C	-3.77813100	-4.25960100	0.05257000
H	-4.55189300	-4.21118100	0.82711300
C	3.69963000	-4.24324900	-0.13382900
H	-4.26340900	-4.27639000	-0.93006900
H	4.40766500	-4.23266100	-0.97051800
H	4.26814300	-4.22925700	0.80342300
C	-2.10632900	-3.20172700	1.57868000
C	1.70557300	-3.24481700	0.97293000
C	1.93423800	-3.21117600	-1.55858100
H	-2.86311600	-3.10188500	2.36493100
C	-1.68990900	-3.30290900	-0.92844200
H	2.64020400	-3.17291800	-2.39675300
H	2.24210300	-3.17962800	1.92706200
H	-2.14340500	-3.23879700	-1.92435400
C	-2.76028600	-3.10914900	0.17520200
C	2.68743100	-3.08311600	-0.21229500
H	-1.34488300	-2.43510600	1.72567600
H	0.92978500	-2.48067900	0.95876700

H	1.20476400	-2.40992900	-1.68485600
H	-0.89401500	-2.56412200	-0.85377300
H	-5.40497300	-2.49636800	-0.23821300
H	5.35549000	-2.49256100	-0.07917400
H	-7.58094000	-1.87799100	0.33496300
H	-7.33873700	-1.92216000	-1.44648400
H	7.46185100	-2.01314000	-0.88351900
H	7.38178400	-1.96662500	0.90482700
C	-3.42916900	-1.73911300	0.01750700
C	3.37233700	-1.70497900	-0.15665900
C	-4.78895000	-1.61138800	-0.18008000
C	4.76183600	-1.59051400	-0.11042100
C	-7.60691900	-1.29574600	-0.59070100
C	7.59663900	-1.37973400	0.00266300
H	-8.59685900	-0.86697800	-0.73613100
H	8.62851400	-1.02715400	0.03943900
O	-1.36772900	-0.60909600	0.25070600
O	1.27889100	-0.55492100	-0.22190300
C	-2.62965100	-0.51585400	0.09374600
C	2.60293800	-0.50318500	-0.16997700
C	-5.41389000	-0.34695600	-0.30488500
C	5.43088000	-0.35027000	-0.10867800
O	-6.71707600	-0.16435800	-0.49760100
O	6.78920700	-0.20726500	-0.06343900
Cr	0.08417400	0.69107200	0.52350400
N	0.33198600	0.72467900	2.02048300
C	-3.28488500	0.77670100	-0.02051600
C	3.28171000	0.75478700	-0.18568600
C	-4.64837600	0.84000500	-0.22168900
C	4.68884000	0.81616000	-0.16885800
H	-5.16326700	1.79058000	-0.31658400
H	5.20008700	1.77393700	-0.19004800
C	-2.56335600	2.03782200	0.06773200
C	2.56514000	1.99401800	-0.32813000
N	1.28755400	2.15095400	-0.16997800
N	-1.30099200	2.16897000	0.27418500
H	3.16671000	2.85666100	-0.61283800
H	-3.18411300	2.92632000	-0.04111800
H	0.27948100	3.36440300	-1.52556500
C	0.61249400	3.43306900	-0.47960700
C	-0.65364100	3.49413500	0.39838800
H	-0.32782100	3.55192900	1.44605800
H	-1.87108100	4.65873500	-0.95857200
H	2.31754900	4.68447500	-0.98217700

C	1.45502700	4.70298100	-0.30871800
C	-1.50402500	4.72349200	0.07481500
H	-2.37654800	4.76693800	0.73600100
H	1.84025400	4.73875900	0.71901400
H	0.33090400	5.95093900	-1.67177700
C	0.60892100	5.95129900	-0.60875500
C	-0.66085700	5.99804200	0.24902400
H	-0.38642400	6.10714800	1.30691300
H	1.21511000	6.84796800	-0.44051600
H	-1.26670100	6.87197600	-0.01322900

Oxidized [CrN(Sal)^{OiPr}]$^{+}$, triplet.

O	-1.36141700	-0.80058100	0.26544900
N	-1.30014000	1.97167900	0.27835100
C	-2.62662800	-0.71345100	0.13227000
O	1.28125900	-0.75042900	-0.23015200
N	1.28079800	1.95388800	-0.19839300
C	-3.42327500	-1.93974400	0.07928200
C	-4.77643800	-1.80534200	-0.10399900
H	-5.42769100	-2.66823700	-0.15334600
C	-5.41941300	-0.54132700	-0.23505900
C	-4.66045800	0.64683500	-0.16540200
H	-5.13669500	1.61539900	-0.25323700
C	-3.28839800	0.57582900	0.02058400
C	-2.75169200	-3.30795400	0.24634300
C	-2.07387400	-3.38064400	1.63879400
H	-1.59729400	-4.36005200	1.75688600
H	-2.81649200	-3.26545900	2.43651300
H	-1.30765300	-2.61403300	1.76065100
C	-1.70125500	-3.51931200	-0.87187300
H	-0.90574000	-2.77765000	-0.82378200
H	-2.17219500	-3.47234400	-1.86067600
H	-1.24853800	-4.51058300	-0.75906000
C	-3.77509400	-4.45637300	0.15855900
H	-3.25071100	-5.40862600	0.28610900
H	-4.27792800	-4.48473400	-0.81480100
H	-4.53577400	-4.39173600	0.94465400
C	-2.56624300	1.83622200	0.09246200
H	-3.18748900	2.72507100	-0.01050200
C	-0.65425000	3.29876600	0.38548100
H	-0.31522300	3.36453800	1.42853700
C	-1.51045700	4.52466200	0.06403400
H	-2.37474200	4.57173200	0.73572800

H	-1.89038700	4.45237200	-0.96420000
C	-0.66689300	5.80154900	0.21883700
H	-1.27699900	6.67289000	-0.04222800
H	-0.37971600	5.91852700	1.27249800
C	0.59247400	5.75034100	-0.65387400
H	1.19903000	6.64931800	-0.49975100
H	0.30150200	5.74159400	-1.71340400
C	1.44400900	4.50547200	-0.35497700
H	2.29849900	4.48364600	-1.03855600
H	1.84143700	4.54902000	0.66782000
C	0.60130600	3.23327300	-0.50754600
H	0.25485800	3.15941700	-1.54890800
C	2.55803500	1.79666000	-0.37564200
H	3.15208200	2.66149400	-0.66976300
C	3.27971600	0.56223000	-0.24667400
C	4.69528300	0.63209100	-0.26365800
H	5.16739800	1.60698000	-0.29348900
C	5.43315100	-0.53510900	-0.22522500
C	4.75502000	-1.77616100	-0.20994100
H	5.38706300	-2.65550500	-0.19463500
C	3.37453200	-1.90094700	-0.22303900
C	2.60254300	-0.69277900	-0.21535400
C	2.68982200	-3.27846900	-0.26170500
C	1.73821400	-3.44188900	0.94775700
H	2.29797600	-3.37312600	1.88819900
H	1.25765100	-4.42697100	0.91131400
H	0.95856800	-2.68143400	0.95205900
C	1.90355100	-3.40684500	-1.58879300
H	2.58833600	-3.36762600	-2.44428900
H	1.16978100	-2.60679300	-1.69680200
H	1.37372600	-4.36635100	-1.62066600
C	3.70786500	-4.43451900	-0.20888700
H	4.39565200	-4.41892800	-1.06198600
H	3.16878700	-5.38768100	-0.23927900
H	4.29917700	-4.41762300	0.71391300
Cr	0.08931700	0.50020200	0.51862300
N	0.35311700	0.54148700	2.01298300
C	-7.57600000	0.59529400	-0.52099700
H	-7.04388100	1.33329600	-1.13023200
C	7.60961100	0.55786600	-0.17055700
H	7.20106100	1.29980300	-0.86993100
O	-6.73174800	-0.60298100	-0.41949200
O	6.79324700	-0.63357300	-0.22718200
C	-8.82645700	0.13445600	-1.25160000

H	-9.34274000	-0.63927500	-0.67459000
H	-9.50461900	0.98299700	-1.38333800
H	-8.57339600	-0.26765900	-2.23668700
C	-7.84902500	1.12676800	0.88096800
H	-8.36186100	0.36573900	1.47742000
H	-6.92533600	1.40816200	1.39574400
H	-8.48990100	2.01144100	0.81639700
C	7.63299700	1.12074700	1.24968100
H	8.06535300	0.38322200	1.93448100
H	8.24328700	2.02942400	1.28493500
H	6.62748300	1.36842100	1.60220700
C	8.98825600	0.12738200	-0.65353100
H	9.67204000	0.98223800	-0.65247400
H	9.39633000	-0.64546300	0.00689200
H	8.93195500	-0.27602800	-1.66918600

Predicted TD-DFT transitions:

Oxidized $[CrN(Sal)^{OiPr}]^{+}$, triplet:

Excited State 1: 3.113-A 2.0375 eV 608.51 nm f=0.0239 <S**2>=2.173
159B -> 164B 0.18413
160B -> 164B 0.71615
161B -> 164B 0.42077
163B -> 164B 0.44385
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2834.11886744
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.124-A 2.1699 eV 571.39 nm f=0.0227 <S**2>=2.190
165A -> 167A -0.11250
159B -> 164B -0.32438
160B -> 164B -0.34197
161B -> 164B -0.12432
163B -> 164B 0.83034
163B -> 166B -0.11468

Excited State 3: 4.112-A 2.3261 eV 533.01 nm f=0.0018 <S**2>=3.977
163A -> 167A -0.12096
165A -> 167A 0.66201
162B -> 166B -0.11254
163B -> 164B 0.15842

163B -> 165B 0.23168
163B -> 166B 0.60797

Excited State 4: 3.085-A 2.6018 eV 476.53 nm f=0.0047 <S**2>=2.130
152A -> 171A -0.13198
154A -> 171A -0.17462
155A -> 171A -0.16017
158A -> 171A 0.18242
159A -> 167A -0.12467
159A -> 169A -0.16788
159A -> 171A -0.27046
162A -> 167A -0.27671
162A -> 169A -0.31879
162A -> 170A 0.12770
162A -> 171A -0.50483
162A -> 172A 0.16475
162A -> 173A 0.11971
165A -> 171A 0.12130

Excited State 5: 3.122-A 2.7019 eV 458.87 nm f=0.0060 <S**2>=2.186
133B -> 164B -0.10805
135B -> 164B 0.10287
137B -> 164B -0.12192
148B -> 164B 0.14732
153B -> 164B -0.13098
156B -> 164B 0.24871
157B -> 164B 0.72236
157B -> 165B 0.12295
158B -> 164B -0.32978
159B -> 164B 0.22411
163B -> 164B 0.18362

Excited State 6: 3.351-A 2.8274 eV 438.51 nm f=0.2020 <S**2>=2.558
156A -> 169A -0.10623
160A -> 166A 0.13576
161A -> 166A 0.22307
164A -> 166A -0.15854
164A -> 168A -0.10886
149B -> 164B 0.12637
153B -> 164B -0.13368
157B -> 164B 0.39035
158B -> 164B 0.57809
159B -> 164B -0.29621
160B -> 165B -0.13301

161B -> 164B 0.11718
163B -> 164B -0.10400

Excited State 7: 3.875-A 2.9900 eV 414.66 nm f=0.0360 <S**2>=3.504
143A -> 169A -0.11842
151A -> 170A 0.10451
156A -> 169A -0.25491
156A -> 170A -0.10100
157A -> 170A 0.10520
158A -> 169A 0.13769
158A -> 170A -0.15343
160A -> 170A 0.11824
161A -> 169A -0.12156
162A -> 169A 0.22253
163A -> 167A -0.10871
164A -> 166A 0.21415
164A -> 170A -0.13768
145B -> 169B -0.10727
149B -> 164B -0.13101
151B -> 168B -0.11157
151B -> 170B 0.13494
154B -> 169B -0.11046
155B -> 169B -0.10980
156B -> 169B -0.11294
158B -> 164B -0.23516
159B -> 164B 0.10684
159B -> 170B 0.10438
161B -> 169B 0.13074
162B -> 166B -0.10531

Excited State 8: 3.413-A 3.1461 eV 394.09 nm f=0.0123 <S**2>=2.663
161A -> 166A 0.16643
162A -> 169A 0.10553
163A -> 167A 0.19512
164A -> 166A 0.72855
165A -> 166A 0.24420
165A -> 167A -0.12657
165A -> 173A -0.10144
160B -> 165B -0.13427
162B -> 166B 0.17278
163B -> 166B 0.23925

Excited State 9: 4.017-A 3.1821 eV 389.64 nm f=0.0120 <S**2>=3.783
163A -> 167A 0.44777

163A -> 173A -0.12489
164A -> 166A -0.27559
165A -> 166A -0.11399
165A -> 171A -0.13650
165A -> 173A -0.26144
162B -> 165B 0.14946
162B -> 166B 0.44326
163B -> 166B 0.14600
163B -> 167B 0.13210
163B -> 171B -0.17298
163B -> 173B 0.20499

Excited State 10: 3.127-A 3.2837 eV 377.58 nm f=0.1432 <S**2>=2.195
163A -> 167A 0.10972
164A -> 166A 0.20476
165A -> 167A 0.66507
162B -> 166B 0.10521
163B -> 165B -0.24964
163B -> 166B -0.58257

Excited State 11: 3.146-A 3.3179 eV 373.69 nm f=0.0107 <S**2>=2.225
152A -> 170A 0.12537
154A -> 170A 0.14697
155A -> 170A 0.14591
158A -> 170A -0.10424
159A -> 168A 0.15394
159A -> 170A 0.23640
162A -> 166A 0.17808
162A -> 167A -0.13571
162A -> 168A 0.37618
162A -> 170A 0.55515
162A -> 171A 0.13775
164A -> 166A 0.19497
164A -> 170A -0.11337
165A -> 168A -0.14248
165A -> 170A -0.20749

Excited State 12: 3.205-A 3.4053 eV 364.10 nm f=0.0011 <S**2>=2.318
152A -> 169A 0.13670
154A -> 169A 0.15927
155A -> 169A 0.14727
158A -> 169A -0.14521
159A -> 169A 0.25335
159A -> 170A 0.10997

162A -> 166A -0.15240
162A -> 169A 0.54540
162A -> 170A 0.15907
162A -> 171A -0.21129
162A -> 172A 0.17149
164A -> 166A -0.17378
164A -> 169A -0.11270
165A -> 169A -0.20663
165A -> 171A 0.10865
163B -> 167B 0.10152

Excited State 13: 3.208-A 3.6326 eV 341.31 nm f=0.0007 <S**2>=2.323
156A -> 169A -0.12113
151B -> 164B 0.11637
155B -> 164B -0.14256
156B -> 164B -0.16610
159B -> 164B 0.10563
159B -> 167B 0.12408
161B -> 164B 0.19954
162B -> 164B 0.72506
163B -> 167B -0.40068

Excited State 14: 3.198-A 3.6550 eV 339.22 nm f=0.0123 <S**2>=2.308
163A -> 167A -0.10363
156B -> 164B -0.10486
159B -> 167B -0.19516
161B -> 164B 0.15215
161B -> 167B 0.14148
162B -> 164B 0.41592
162B -> 166B -0.10133
163B -> 167B 0.74077

Excited State 15: 3.727-A 3.7527 eV 330.39 nm f=0.0140 <S**2>=3.223
156A -> 169A -0.25042
158A -> 169A 0.21428
159A -> 169A -0.17567
160A -> 169A 0.10517
160A -> 170A -0.13266
161A -> 166A 0.22251
161A -> 169A -0.16522
162A -> 169A -0.10920
164A -> 166A -0.19713
164A -> 168A 0.17478
165A -> 166A 0.20335

165A -> 168A 0.12623
165A -> 169A -0.16903
165A -> 170A 0.14877
158B -> 164B -0.12623
160B -> 165B -0.12438
161B -> 165B -0.13147
162B -> 164B -0.23029
163B -> 165B -0.16431
163B -> 167B 0.18040

Excited State 16: 3.843-A 3.7797 eV 328.02 nm f=0.0011 <S**2>=3.442
150A -> 169A -0.15650
151A -> 169A -0.15394
156A -> 168A 0.13137
156A -> 170A 0.21743
157A -> 169A -0.12702
158A -> 167A 0.10123
158A -> 168A -0.11667
158A -> 169A 0.13791
158A -> 170A -0.19028
159A -> 169A 0.10353
159A -> 170A 0.12344
160A -> 166A 0.16421
160A -> 169A -0.21491
161A -> 166A 0.13326
161A -> 169A 0.13688
161A -> 170A 0.13265
163A -> 169A -0.12933
164A -> 168A 0.12845
164A -> 169A 0.13020
165A -> 166A -0.11604
165A -> 169A 0.22692
160B -> 165B -0.11378
161B -> 164B -0.21205
163B -> 167B -0.11624

Excited State 17: 3.721-A 3.8551 eV 321.61 nm f=0.0228 <S**2>=3.212
156A -> 170A -0.13055
158A -> 166A 0.10028
158A -> 169A -0.14686
158A -> 170A 0.11883
160A -> 166A 0.20675
160A -> 170A 0.12041
161A -> 166A 0.29947

161A -> 168A -0.12844
161A -> 170A -0.10974
164A -> 166A -0.19529
164A -> 168A 0.30279
164A -> 170A -0.19153
165A -> 170A -0.22439
158B -> 164B -0.22076
160B -> 165B -0.26060
161B -> 165B -0.12845
162B -> 164B -0.12065

Excited State 18: 3.397-A 3.9333 eV 315.21 nm f=0.0024 <S**2>=2.635
152A -> 169A -0.11183
153A -> 169A -0.13597
156A -> 169A -0.11833
160A -> 169A -0.11128
165A -> 166A -0.28437
165A -> 169A 0.18409
153B -> 164B 0.18346
155B -> 164B -0.10434
160B -> 164B -0.28671
161B -> 164B 0.57456
162B -> 164B -0.33031

Excited State 19: 3.720-A 3.9619 eV 312.94 nm f=0.0088 <S**2>=3.209
153A -> 170A -0.10019
156A -> 169A 0.19049
157A -> 170A 0.10195
158A -> 168A -0.18227
158A -> 170A -0.26187
164A -> 166A -0.11136
164A -> 170A -0.17376
165A -> 166A 0.37862
165A -> 168A 0.15285
165A -> 170A 0.14800
165A -> 171A 0.16541
149B -> 164B -0.10699
160B -> 164B -0.20359
161B -> 164B 0.38844
162B -> 166B 0.10819
163B -> 171B 0.11163

Excited State 20: 4.048-A 4.0027 eV 309.75 nm f=0.0021 <S**2>=3.846
156A -> 169A -0.10013

163A -> 167A 0.28937
165A -> 169A 0.23166
165A -> 171A 0.26654
165A -> 173A 0.40254
165A -> 177A 0.10186
161B -> 164B -0.17443
162B -> 165B 0.10861
162B -> 166B 0.29743
163B -> 167B 0.10201
163B -> 169B -0.12683
163B -> 171B 0.29935
163B -> 172B 0.14734
163B -> 173B -0.27639

Excited State 21: 3.796-A 4.0855 eV 303.47 nm f=0.0009 <S**2>=3.352
150A -> 170A 0.11205
152A -> 168A 0.11356
152A -> 170A 0.18292
153A -> 168A 0.13202
153A -> 170A 0.20512
156A -> 168A 0.11010
156A -> 169A 0.10853
156A -> 170A 0.14100
157A -> 169A -0.10407
158A -> 169A 0.21526
158A -> 170A 0.13571
160A -> 170A 0.12851
164A -> 169A 0.15557
164A -> 170A 0.14565
165A -> 166A 0.35820
165A -> 168A -0.10475
165A -> 169A -0.13324
165A -> 170A -0.23914
165A -> 171A 0.15905
149B -> 164B 0.18968
149B -> 169B 0.12561
154B -> 164B 0.11876
158B -> 169B -0.11580
161B -> 164B 0.15923

Excited State 22: 3.732-A 4.1574 eV 298.23 nm f=0.0122 <S**2>=3.231
150A -> 169A -0.13055
152A -> 169A -0.19179
153A -> 169A -0.20475

158A -> 169A -0.23812
160A -> 166A -0.10267
160A -> 169A -0.13944
163A -> 167A -0.11589
164A -> 166A -0.11816
164A -> 169A -0.12169
165A -> 166A 0.51030
165A -> 169A 0.18588
165A -> 171A 0.10448
165A -> 173A -0.17715
163B -> 165B 0.13854
163B -> 171B -0.12401
163B -> 172B -0.11050
163B -> 173B 0.11650

Excited State 23: 3.138-A 4.1951 eV 295.55 nm f=0.0012 <S**2>=2.212
127B -> 164B 0.13793
130B -> 164B -0.18245
133B -> 164B 0.11278
135B -> 164B -0.10118
137B -> 164B 0.11862
142B -> 164B -0.34418
143B -> 164B -0.10517
146B -> 164B 0.10389
147B -> 164B 0.17160
148B -> 164B 0.61940
149B -> 164B 0.16008
152B -> 164B -0.16815
155B -> 164B -0.15536
156B -> 164B 0.25498
157B -> 164B -0.12810
163B -> 165B 0.16053

Excited State 24: 3.487-A 4.2536 eV 291.48 nm f=0.0002 <S**2>=2.789
161A -> 166A 0.12965
164A -> 168A 0.20958
165A -> 169A -0.15658
142B -> 164B 0.13753
148B -> 164B -0.13856
149B -> 164B -0.12243
151B -> 164B -0.11375
152B -> 164B 0.10324
155B -> 164B 0.20237
156B -> 164B 0.10085

159B -> 165B -0.16726
163B -> 165B 0.58101
163B -> 166B -0.23157
163B -> 168B 0.20935
163B -> 169B -0.13340
163B -> 173B -0.13105

Excited State 25: 3.302-A 4.3201 eV 286.99 nm f=0.0152 <S**2>=2.477
158A -> 170A 0.20485
164A -> 168A 0.21841
165A -> 169A 0.20732
165A -> 170A -0.14601
165A -> 171A 0.11428
165A -> 172A -0.11372
143B -> 164B -0.10932
145B -> 164B 0.14838
149B -> 164B -0.19237
151B -> 164B -0.15097
152B -> 164B 0.20004
153B -> 164B -0.13001
155B -> 164B 0.33125
156B -> 164B 0.31250
157B -> 164B -0.12369
158B -> 164B 0.12016
160B -> 164B -0.13604
163B -> 165B -0.15822

Oxidized [CrN(Sal)^{OiPr}]$^{+}$, broken symmetry singlet:

Excited State 1: 2.337-A 1.9689 eV 629.73 nm f=0.0517 <S**2>=1.115
160A -> 165A 0.14938
161A -> 165A 0.59782
162A -> 165A -0.34627
164A -> 165A 0.65553
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2834.12194056
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.423-A 2.1267 eV 582.99 nm f=0.0194 <S**2>=1.218
160A -> 165A -0.38871
161A -> 165A -0.57364
164A -> 165A 0.65608
164A -> 167A 0.13048

164B -> 166B 0.11431

Excited State 3: 2.122-A 2.2566 eV 549.43 nm f=0.0015 <S**2>=0.876
153A -> 165A -0.11794
154A -> 165A -0.13484
159A -> 165A 0.49934
160A -> 165A -0.16641
161A -> 165A 0.32811
162A -> 165A 0.64367
164A -> 165A 0.15017

Excited State 4: 3.586-A 2.3303 eV 532.06 nm f=0.0035 <S**2>=2.965
163A -> 167A -0.11480
164A -> 165A -0.18899
164A -> 166A -0.19140
164A -> 167A 0.62534
162B -> 166B -0.11873
164B -> 165B 0.11817
164B -> 166B 0.64651

Excited State 5: 2.365-A 2.6555 eV 466.90 nm f=0.0062 <S**2>=1.148
152A -> 170A -0.10307
153A -> 170A -0.13196
154A -> 167A -0.10560
154A -> 170A -0.23377
157A -> 170A 0.18088
159A -> 167A -0.10260
159A -> 168A -0.10234
159A -> 169A -0.10362
159A -> 170A -0.24395
162A -> 167A -0.26699
162A -> 168A -0.23259
162A -> 169A -0.21751
162A -> 170A -0.52050
162A -> 171A 0.16791
162A -> 172A 0.14481
162A -> 173A 0.13358
164A -> 170A 0.12090

Excited State 6: 2.577-A 2.7942 eV 443.73 nm f=0.2143 <S**2>=1.411
135A -> 165A -0.12204
146A -> 165A 0.10571
155A -> 165A -0.10783
157A -> 165A -0.11272

158A -> 165A 0.66019
160A -> 165A -0.39283
161A -> 166A -0.13869
162A -> 165A -0.18630
163A -> 165A -0.11680
164A -> 165A -0.18081
159B -> 165B 0.10711
160B -> 165B 0.23601
163B -> 165B -0.17710

Excited State 7: 3.443-A 3.0393 eV 407.94 nm f=0.0182 <S**2>=2.713
143A -> 168A -0.12545
145A -> 169A 0.10334
151A -> 169A -0.15678
155A -> 168A -0.15536
156A -> 169A -0.12816
157A -> 166A -0.11053
157A -> 168A 0.12116
157A -> 169A 0.23216
158A -> 165A 0.13424
160A -> 168A 0.16906
160A -> 169A -0.12429
161A -> 168A -0.10939
162A -> 166A -0.12006
162A -> 168A 0.14725
162A -> 169A 0.20615
162A -> 170A -0.10877
163A -> 167A -0.15824
164A -> 168A -0.10635
151B -> 170B -0.19034
155B -> 169B -0.15988
155B -> 170B 0.14520
156B -> 165B 0.10024
156B -> 169B 0.15498
156B -> 170B 0.14328
156B -> 172B -0.12678
159B -> 170B -0.11095
162B -> 166B -0.14761

Excited State 8: 3.546-A 3.1825 eV 389.59 nm f=0.0087 <S**2>=2.893
163A -> 166A -0.13026
163A -> 167A 0.46272
163A -> 169A -0.11062
163A -> 173A -0.14143

164A -> 168A -0.13424
164A -> 171A 0.11133
164A -> 173A -0.27304
162B -> 166B 0.47547
163B -> 165B -0.14541
164B -> 166B 0.23575
164B -> 167B 0.13387
164B -> 171B -0.18926
164B -> 173B 0.23177

Excited State 9: 2.534-A 3.1895 eV 388.72 nm f=0.0126 <S**2>=1.355
161A -> 166A -0.14550
164A -> 167A -0.23748
160B -> 165B 0.16833
163B -> 165B 0.81427
164B -> 165B 0.22321
164B -> 166B 0.21898

Excited State 10: 2.478-A 3.2876 eV 377.12 nm f=0.1554 <S**2>=1.285
163A -> 167A 0.12492
164A -> 166A -0.24611
164A -> 167A 0.58823
162B -> 166B 0.11535
163B -> 165B 0.29744
164B -> 166B -0.58497

Excited State 11: 2.495-A 3.3346 eV 371.81 nm f=0.0055 <S**2>=1.306
143A -> 169A -0.10046
152A -> 169A 0.14386
153A -> 169A 0.16646
154A -> 169A 0.19394
159A -> 169A 0.21569
162A -> 166A -0.26535
162A -> 168A -0.32200
162A -> 169A 0.56536
162A -> 171A 0.10326
164A -> 166A 0.10143
164A -> 167A 0.15272
164A -> 168A 0.13689
164A -> 169A -0.25537
164B -> 166B -0.10771

Excited State 12: 2.299-A 3.3917 eV 365.55 nm f=0.0036 <S**2>=1.072
147A -> 165A 0.11928

149A -> 165A -0.10569
151A -> 165A -0.19677
153A -> 165A 0.28062
154A -> 165A 0.31060
154A -> 168A 0.12205
159A -> 165A -0.35014
159A -> 168A 0.12448
162A -> 165A 0.47395
162A -> 166A -0.10745
162A -> 168A 0.29531
162A -> 170A -0.13084
162A -> 171A 0.11163
163A -> 165A -0.17175

Excited State 13: 2.460-A 3.4191 eV 362.62 nm f=0.0019 <S**2>=1.263
151A -> 168A -0.13108
153A -> 165A -0.18224
154A -> 165A -0.16856
154A -> 168A 0.21713
157A -> 165A 0.10140
159A -> 165A 0.20360
159A -> 168A 0.23336
162A -> 165A -0.27758
162A -> 168A 0.53448
162A -> 169A 0.12056
162A -> 170A -0.17451
162A -> 172A 0.11533
164A -> 168A -0.15157
160B -> 165B -0.10610

Excited State 14: 2.527-A 3.5884 eV 345.51 nm f=0.0025 <S**2>=1.346
153A -> 165A 0.13319
157A -> 165A -0.27855
160A -> 165A 0.11097
161A -> 166A -0.14032
163A -> 165A 0.80742
160B -> 165B 0.16186

Excited State 15: 2.557-A 3.6482 eV 339.85 nm f=0.0066 <S**2>=1.384
160A -> 169A -0.11187
163A -> 167A -0.12996
164A -> 166A -0.11679
159B -> 167B -0.22854
160B -> 167B 0.13309

161B -> 167B 0.11674
162B -> 166B -0.11083
164B -> 165B -0.11433
164B -> 167B 0.81724

Excited State 16: 3.152-A 3.7564 eV 330.06 nm f=0.0105 <S**2>=2.234
150A -> 169A -0.11458
154A -> 169A 0.12769
155A -> 169A 0.11434
157A -> 168A -0.21162
157A -> 169A -0.16744
158A -> 165A -0.12597
159A -> 169A 0.14866
160A -> 166A 0.13357
160A -> 169A -0.25189
161A -> 166A -0.16559
161A -> 169A 0.13651
162A -> 169A 0.12492
163A -> 165A -0.20809
164A -> 166A -0.24165
164A -> 167A -0.10077
164A -> 169A 0.25517
160B -> 165B 0.12392
163B -> 165B -0.16509
163B -> 168B 0.13797
164B -> 165B 0.22829
164B -> 167B -0.24180

Excited State 17: 3.191-A 3.8058 eV 325.77 nm f=0.0093 <S**2>=2.296
150A -> 168A -0.10442
151A -> 169A -0.11771
152A -> 169A -0.12812
153A -> 169A -0.11810
154A -> 165A 0.11435
155A -> 168A 0.13486
156A -> 169A -0.10986
157A -> 165A -0.11687
157A -> 168A -0.16379
157A -> 169A 0.24434
158A -> 165A 0.13355
159A -> 168A 0.12739
160A -> 165A -0.12898
160A -> 166A 0.11586
160A -> 168A -0.22756

161A -> 166A 0.18572
161A -> 168A 0.14161
162A -> 166A -0.10678
163A -> 165A 0.24061
163A -> 169A -0.12254
164A -> 168A 0.20157
164A -> 169A 0.11376
156B -> 170B 0.10975
159B -> 165B -0.11972
160B -> 165B -0.22807
163B -> 165B 0.12646
163B -> 168B -0.19581

Excited State 18: 3.178-A 3.8440 eV 322.54 nm f=0.0118 <S**2>=2.275
150A -> 168A -0.10033
152A -> 168A -0.11924
153A -> 165A -0.10741
153A -> 168A -0.10454
157A -> 166A -0.10822
157A -> 169A 0.29327
158A -> 165A -0.24194
158A -> 166A -0.10764
160A -> 168A -0.17842
161A -> 166A -0.20924
161A -> 169A -0.15715
163A -> 165A -0.15274
164A -> 168A 0.20955
164A -> 169A -0.17882
159B -> 165B 0.12453
160B -> 165B 0.28623
163B -> 165B -0.16546
163B -> 168B 0.27631

Excited State 19: 3.110-A 3.9719 eV 312.15 nm f=0.0034 <S**2>=2.168
149A -> 169A -0.17819
152A -> 169A -0.10190
154A -> 165A -0.22645
155A -> 165A -0.12719
155A -> 169A -0.14487
156A -> 165A -0.17623
157A -> 165A 0.35370
157A -> 168A 0.19378
158A -> 169A -0.24213
160A -> 165A 0.12866

160A -> 168A -0.10058
162A -> 169A 0.12806
163A -> 165A 0.22470
164A -> 166A -0.20041
164A -> 169A 0.14442
160B -> 165B 0.12633
164B -> 165B 0.22609

Excited State 20: 3.519-A 3.9931 eV 310.50 nm f=0.0002 <S**2>=2.846
158A -> 168A -0.11233
163A -> 167A 0.28294
164A -> 168A 0.25903
164A -> 169A 0.14748
164A -> 170A 0.16711
164A -> 171A -0.20388
164A -> 173A 0.37886
162B -> 166B 0.31614
164B -> 165B -0.16121
164B -> 171B 0.31608
164B -> 172B 0.13103
164B -> 173B -0.28872

Excited State 21: 3.000-A 4.0474 eV 306.33 nm f=0.0014 <S**2>=2.000
146A -> 165A -0.14603
147A -> 165A 0.24514
149A -> 168A 0.14652
149A -> 169A -0.13977
152A -> 168A 0.10059
154A -> 165A 0.28017
155A -> 165A 0.26708
155A -> 169A -0.12552
156A -> 165A 0.14549
157A -> 165A -0.17768
157A -> 168A 0.21821
158A -> 168A 0.24380
158A -> 169A -0.17398
159A -> 165A 0.18285
160A -> 165A -0.12662
164A -> 168A -0.22769
164A -> 169A 0.11627
164A -> 170A 0.11648
164A -> 173A 0.11623
152B -> 170B 0.10452
163B -> 168B 0.11933

Excited State 22: 2.767-A 4.0534 eV 305.88 nm f=0.0126 <S**2>=1.665

161A -> 166A	0.10632
164A -> 166A	0.17681
164A -> 167A	0.11391
164A -> 169A	-0.14664
164A -> 173A	0.10021
159B -> 165B	-0.17832
163B -> 165B	-0.10794
164B -> 165B	0.77637
164B -> 166B	-0.15072
164B -> 167B	0.18270
164B -> 169B	0.18225
164B -> 170B	0.13938
164B -> 173B	-0.11936

Excited State 23: 3.051-A 4.1013 eV 302.30 nm f=0.0024 <S**2>=2.078

149A -> 165A	0.24022
149A -> 168A	0.20078
152A -> 165A	0.13786
152A -> 168A	0.16534
153A -> 168A	0.10823
154A -> 165A	-0.18193
155A -> 168A	0.16729
156A -> 165A	-0.14656
157A -> 165A	0.30573
157A -> 169A	0.15920
158A -> 165A	0.15210
158A -> 166A	-0.12417
158A -> 168A	0.25632
158A -> 169A	0.15302
160A -> 165A	0.13823
164A -> 166A	0.15035
164A -> 168A	-0.17814
164A -> 170A	0.10313
155B -> 169B	0.13754
163B -> 168B	0.10807

Excited State 24: 2.643-A 4.2079 eV 294.65 nm f=0.0020 <S**2>=1.497

129A -> 165A	-0.11838
130A -> 165A	-0.10907
142A -> 165A	-0.15510
143A -> 165A	-0.10621
144A -> 165A	0.10400

145A -> 165A 0.13136
146A -> 165A -0.10955
147A -> 165A 0.45545
148A -> 165A 0.15796
149A -> 165A -0.12665
152A -> 165A -0.18620
157A -> 165A 0.42859
163A -> 165A 0.16416
164A -> 166A 0.25215
164A -> 168A 0.10737
160B -> 165B 0.14080
163B -> 168B 0.21401

Excited State 25: 2.977-A 4.2570 eV 291.25 nm f=0.0009 <S**2>=1.965
142A -> 165A 0.17651
146A -> 165A 0.14787
147A -> 165A -0.30852
149A -> 165A 0.16251
150A -> 165A -0.10083
151A -> 165A -0.13514
152A -> 169A -0.13263
153A -> 169A -0.10980
156A -> 165A -0.13260
157A -> 165A -0.15314
158A -> 169A -0.12337
162A -> 166A -0.10594
164A -> 166A 0.45669
164A -> 167A 0.13566
164A -> 170A 0.22074
164A -> 173A -0.11357
163B -> 168B 0.11287

Mono-oxidized [CrN(Sal)^{OiPr}]$^{+}$, singlet:

Excited State 1: 2.345-A 0.8273 eV 1498.66 nm f=0.0670
161A -> 165A -0.17869
164A -> 165A 0.97405
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2834.14173997
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.371-A 1.5197 eV 815.86 nm f=0.0070
160A -> 165A -0.67176
161A -> 165A 0.68369

Excited State 3: 1.936-A 1.7213 eV 720.30 nm f=0.0083
158A -> 165A 0.20322
159A -> 165A 0.48075
160A -> 165A -0.17666
161A -> 165A -0.20630
162A -> 165A 0.69744
163A -> 165A -0.18280

Excited State 4: 3.639-A 2.0291 eV 611.04 nm f=0.0005
164A -> 167A -0.66070
164A -> 169A -0.13253
164A -> 170A 0.11169
164B -> 166B 0.67110

Excited State 5: 2.496-A 2.4056 eV 515.40 nm f=0.2092
152A -> 165A 0.10056
158A -> 165A 0.61709
159A -> 165A -0.34806
160A -> 165A 0.34069
161A -> 165A 0.26742
161A -> 166A -0.11734
162A -> 165A 0.24663
159B -> 165B -0.15306
160B -> 165B 0.19821

Excited State 6: 2.365-A 2.6560 eV 466.81 nm f=0.0041
147A -> 165A 0.12681
151A -> 165A 0.15194
152A -> 165A 0.11867
152A -> 170A -0.12787
153A -> 165A 0.14628
155A -> 165A 0.18888
156A -> 165A -0.16714
156A -> 170A 0.12368
157A -> 165A 0.11042
158A -> 165A -0.22571
158A -> 168A -0.11456
158A -> 170A -0.14749
158A -> 171A 0.11287
158A -> 172A 0.11490
159A -> 168A -0.12399
159A -> 170A -0.16029
159A -> 171A 0.14134

159A -> 172A 0.13429
162A -> 166A 0.14859
162A -> 167A -0.12963
162A -> 168A -0.22770
162A -> 169A -0.12329
162A -> 170A -0.29023
162A -> 171A 0.23199
162A -> 172A 0.22740

Excited State 7: 2.396-A 2.8740 eV 431.39 nm f=0.0276
147A -> 165A 0.11970
149A -> 165A -0.12387
151A -> 165A 0.23721
153A -> 165A 0.19603
155A -> 165A 0.32386
156A -> 165A -0.11241
157A -> 165A 0.15016
158A -> 165A -0.24671
159A -> 165A -0.21614
159A -> 166A -0.11077
160A -> 165A 0.14776
161A -> 165A 0.12104
162A -> 165A 0.49707
162A -> 166A -0.12905
162A -> 169A 0.10160
162A -> 170A 0.10220
162A -> 171A -0.15392
163A -> 165A -0.14896

Excited State 8: 2.385-A 2.9579 eV 419.17 nm f=0.0541
156A -> 165A -0.14457
163A -> 165A 0.50017
164A -> 166A 0.14872
164A -> 167A 0.52778
164B -> 165B 0.24839
164B -> 166B 0.50377

Excited State 9: 3.197-A 3.0027 eV 412.91 nm f=0.0157
150A -> 168A -0.13489
154A -> 169A 0.11165
155A -> 168A -0.15649
156A -> 169A 0.15121
159A -> 165A 0.16821
160A -> 168A -0.12802

161A -> 166A -0.10792
161A -> 168A -0.11728
161A -> 169A 0.15419
162A -> 169A 0.10275
163A -> 165A 0.39134
164A -> 166A 0.11887
164A -> 167A -0.13959
164A -> 168A 0.13507
164A -> 169A -0.20721
150B -> 170B -0.10174
151B -> 170B -0.11026
154B -> 170B -0.12359
156B -> 169B 0.15401
160B -> 169B 0.11300
162B -> 165B 0.15989
164B -> 165B -0.24802
164B -> 166B -0.12567
164B -> 169B -0.10396

Excited State 10: 2.659-A 3.0262 eV 409.71 nm f=0.0465
154A -> 165A -0.10296
156A -> 165A -0.19598
156A -> 169A -0.10344
161A -> 166A 0.12580
161A -> 169A -0.10891
162A -> 165A 0.16253
163A -> 165A 0.59410
164A -> 166A -0.18181
164A -> 167A -0.35752
164B -> 166B -0.33872
164B -> 167B -0.11787

Excited State 11: 2.680-A 3.1104 eV 398.61 nm f=0.0092
163A -> 167A 0.13083
164A -> 173A 0.18454
159B -> 167B -0.13316
160B -> 165B -0.10138
160B -> 167B -0.14685
162B -> 165B -0.15980
163B -> 166B -0.12490
164B -> 165B 0.36895
164B -> 166B -0.25202
164B -> 167B 0.63589
164B -> 168B 0.27683

164B -> 173B 0.13957
164B -> 174B -0.10713

Excited State 12: 3.492-A 3.1672 eV 391.46 nm f=0.0041
163A -> 165A 0.15677
163A -> 167A 0.26994
163A -> 173A 0.11475
164A -> 166A 0.14239
164A -> 168A -0.13331
164A -> 171A 0.17741
164A -> 173A 0.42229
162B -> 165B 0.13714
163B -> 166B -0.28425
164B -> 165B -0.29988
164B -> 167B -0.14388
164B -> 170B 0.10488
164B -> 171B -0.20508
164B -> 172B 0.13150
164B -> 173B 0.29929
164B -> 174B -0.25760

Excited State 13: 2.927-A 3.2181 eV 385.27 nm f=0.0124
151A -> 165A 0.15050
152A -> 165A -0.12938
154A -> 165A 0.18224
156A -> 165A 0.22077
158A -> 165A -0.13950
160A -> 168A 0.11340
161A -> 166A -0.18201
162A -> 165A 0.11756
162A -> 168A -0.12083
163A -> 165A 0.13131
163A -> 167A -0.12475
164A -> 166A 0.15990
164A -> 168A -0.12834
164A -> 173A -0.11905
160B -> 165B 0.15215
162B -> 165B 0.24938
163B -> 166B 0.10518
164B -> 165B -0.21442
164B -> 167B 0.45964
164B -> 168B 0.11849

Excited State 14: 2.655-A 3.2884 eV 377.04 nm f=0.0307

156A -> 165A 0.18751
160A -> 166A -0.13231
164A -> 166A 0.59719
164A -> 167A -0.18433
164A -> 168A -0.16086
164A -> 169A -0.33602
164A -> 171A 0.11421
162B -> 165B -0.32313
164B -> 165B 0.23950
164B -> 166B -0.15388
164B -> 167B -0.21373

Excited State 15: 2.880-A 3.3208 eV 373.36 nm f=0.0018
143A -> 165A 0.10631
150A -> 165A 0.10691
151A -> 165A 0.10935
152A -> 165A -0.25672
154A -> 165A 0.27497
156A -> 165A 0.43759
158A -> 165A -0.12405
159A -> 165A 0.11029
160A -> 165A 0.11963
161A -> 165A 0.20849
162A -> 168A -0.10432
163A -> 165A 0.15510
164A -> 166A -0.29466
164A -> 168A 0.20883
164A -> 169A 0.18023
164B -> 165B 0.35803
164B -> 167B -0.17924

Bis-oxidized [CrN(Sal)^{OiPr}]$^{+}$, doublet:

Excited State 1: 2.987-A 2.0245 eV 612.43 nm f=0.0077 <S**2>=1.980
163A -> 165A -0.12707
161B -> 164B 0.17008
162B -> 164B 0.93331
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2833.64893010
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.986-A 2.0710 eV 598.66 nm f=0.0144 <S**2>=1.978
161A -> 165A 0.18056
162A -> 165A 0.15000

163A -> 165A 0.91617
164A -> 165A -0.10205
162B -> 164B 0.12703

Excited State 3: 2.835-A 2.6220 eV 472.87 nm f=0.0396 <S**2>=1.759
153A -> 171A 0.10409
154A -> 170A 0.10899
154A -> 171A 0.13528
156A -> 165A -0.16683
159A -> 165A 0.28656
160A -> 165A 0.11729
161A -> 165A 0.69962
161A -> 167A 0.18199
161A -> 170A 0.18250
161A -> 171A 0.23205

Excited State 4: 3.044-A 2.6921 eV 460.55 nm f=0.4163 <S**2>=2.067
160A -> 165A 0.56823
162A -> 165A -0.12892
162A -> 166A -0.17155
163A -> 167A -0.12379
164A -> 165A -0.32438
164A -> 166A 0.10177
160B -> 164B -0.44323
161B -> 165B 0.17890
162B -> 166B 0.11864
163B -> 164B -0.28226
163B -> 165B 0.12489

Excited State 5: 2.931-A 2.7705 eV 447.52 nm f=0.0102 <S**2>=1.898
150A -> 170A -0.12196
150A -> 171A -0.12998
153A -> 170A -0.14818
153A -> 171A -0.16031
154A -> 170A -0.19231
154A -> 171A -0.20718
156A -> 165A -0.11470
159A -> 165A 0.19620
161A -> 165A 0.38647
161A -> 166A 0.14332
161A -> 167A -0.11888
161A -> 168A 0.11190
161A -> 170A -0.35373
161A -> 171A -0.36656

161A -> 172A 0.16237
163A -> 171A 0.10154

Excited State 6: 2.990-A 2.7851 eV 445.16 nm f=0.0036 <S**2>=1.985
160A -> 165A 0.44625
162A -> 165A -0.11552
162A -> 166A 0.21613
164A -> 165A -0.29920
160B -> 164B 0.53393
161B -> 164B -0.10716
161B -> 165B 0.16086
162B -> 166B -0.13054
163B -> 164B 0.39413

Excited State 7: 2.960-A 2.8729 eV 431.57 nm f=0.0019 <S**2>=1.941
140B -> 164B 0.15805
154B -> 164B 0.15378
156B -> 164B -0.22585
158B -> 164B 0.17042
159B -> 164B 0.84667
159B -> 166B 0.13198
163B -> 164B 0.15256

Excited State 8: 2.712-A 2.9912 eV 414.49 nm f=0.0217 <S**2>=1.589
160A -> 165A -0.13879
162A -> 166A -0.10593
164A -> 165A -0.45448
164A -> 166A 0.24989
157B -> 164B 0.10212
159B -> 164B -0.10460
160B -> 164B -0.31413
163B -> 164B 0.59840
163B -> 165B -0.14579

Excited State 9: 3.274-A 3.0036 eV 412.79 nm f=0.0006 <S**2>=2.430
148A -> 168A -0.14752
149A -> 169A -0.15809
155A -> 168A 0.11182
155A -> 169A -0.11765
160A -> 168A -0.10492
162A -> 166A -0.14647
164A -> 165A 0.32936
164A -> 166A -0.18215
148B -> 170B 0.11674

149B -> 169B 0.12964
153B -> 169B 0.11381
159B -> 164B -0.10209
160B -> 164B -0.13735
162B -> 166B 0.10077
163B -> 164B 0.52197
163B -> 165B -0.15326

Excited State 10: 3.052-A 3.0420 eV 407.58 nm f=0.0519 <S**2>=2.079
148A -> 168A 0.11533
149A -> 169A 0.11778
160A -> 165A 0.32331
160A -> 168A 0.10062
164A -> 165A 0.60550
160B -> 164B -0.17122
161B -> 165B 0.10066
163B -> 164B 0.21291
163B -> 165B 0.16890

Excited State 11: 3.151-A 3.1450 eV 394.22 nm f=0.0273 <S**2>=2.232
163A -> 167A 0.15142
164A -> 166A 0.27639
161B -> 165B -0.19543
163B -> 164B 0.15686
163B -> 165B 0.81510
163B -> 166B -0.13180

Excited State 12: 3.164-A 3.1783 eV 390.10 nm f=0.0783 <S**2>=2.253
162A -> 166A 0.20450
164A -> 165A 0.25333
164A -> 166A 0.78587
164A -> 167A -0.10005
162B -> 166B -0.17390
163B -> 165B -0.26495

Excited State 13: 3.225-A 3.5839 eV 345.94 nm f=0.0007 <S**2>=2.350
147A -> 169A -0.14115
149A -> 168A 0.14325
150A -> 168A 0.10261
150A -> 169A -0.12133
153A -> 168A 0.11482
154A -> 167A 0.11661
154A -> 168A 0.22029
154A -> 169A -0.19230

157A -> 169A 0.14600
160A -> 168A 0.16281
161A -> 167A 0.23744
161A -> 168A 0.39268
161A -> 169A -0.34308
161A -> 170A 0.13236
162A -> 168A -0.13301
163A -> 167A -0.16061
163A -> 168A -0.11030
163A -> 169A 0.13087
164A -> 167A 0.12949
164A -> 169A -0.16864

Excited State 14: 3.234-A 3.6108 eV 343.37 nm f=0.0028 <S**2>=2.365
148A -> 168A -0.16130
149A -> 169A 0.14922
150A -> 168A 0.12351
150A -> 169A 0.11241
153A -> 168A 0.11077
153A -> 169A 0.10021
154A -> 168A 0.19684
154A -> 169A 0.23719
157A -> 168A -0.11537
160A -> 169A 0.12444
161A -> 166A -0.12445
161A -> 168A 0.41023
161A -> 169A 0.42379
162A -> 169A -0.13108
163A -> 168A -0.19268
163A -> 169A -0.14059
164A -> 168A 0.17224

Excited State 15: 3.510-A 3.7346 eV 331.98 nm f=0.0388 <S**2>=2.830
147A -> 168A 0.12181
147A -> 169A -0.10476
148A -> 169A -0.11966
149A -> 169A 0.11505
153A -> 168A -0.14719
155A -> 169A 0.12881
157A -> 169A 0.10676
158A -> 168A -0.12005
160A -> 168A -0.10737
161A -> 168A -0.18606
161A -> 169A -0.16452

162A -> 166A 0.31556
164A -> 166A -0.22833
164A -> 167A 0.10173
164A -> 168A 0.17299
164A -> 169A -0.12335
164A -> 170A -0.14033
164A -> 171A 0.12246
148B -> 169B 0.11560
149B -> 164B -0.11648
153B -> 164B -0.16019
160B -> 164B -0.21741
160B -> 166B -0.12369
161B -> 165B -0.11378
162B -> 166B -0.25241

Excited State 16: 3.468-A 3.7556 eV 330.14 nm f=0.0190 <S**2>=2.757
148A -> 168A -0.10199
148A -> 169A 0.17763
153A -> 168A -0.17376
154A -> 168A -0.10119
155A -> 168A 0.17906
160A -> 165A -0.22287
160A -> 167A -0.16489
160A -> 169A 0.14981
161A -> 165A 0.12756
161A -> 167A -0.11315
161A -> 168A -0.22529
162A -> 165A 0.10459
163A -> 167A -0.25072
161B -> 165B 0.32195
163B -> 165B 0.21940
163B -> 168B -0.29404

Excited State 17: 3.570-A 3.8314 eV 323.60 nm f=0.0236 <S**2>=2.937
147A -> 169A 0.14174
148A -> 168A 0.12624
149A -> 169A -0.11923
153A -> 168A 0.11266
155A -> 168A -0.13189
157A -> 169A -0.13199
160A -> 165A -0.15009
160A -> 168A 0.10340
160A -> 169A -0.10390
161A -> 168A 0.11017

162A -> 166A 0.29780
162A -> 167A -0.11989
162A -> 169A 0.11930
163A -> 167A -0.12673
164A -> 166A -0.21079
164A -> 170A -0.29404
164A -> 171A 0.13087
164A -> 172A -0.11002
160B -> 164B -0.23802
161B -> 165B 0.20155
162B -> 166B -0.22762
163B -> 168B -0.17063

Excited State 18: 3.636-A 3.8472 eV 322.27 nm f=0.0147 <S**2>=3.055
147A -> 168A -0.16811
148A -> 169A 0.20857
149A -> 168A 0.16100
153A -> 169A 0.16676
155A -> 167A 0.11284
155A -> 168A 0.11240
155A -> 169A -0.23982
157A -> 168A 0.15854
160A -> 165A 0.14997
160A -> 168A 0.11486
160A -> 169A 0.12957
161A -> 169A 0.15002
162A -> 166A 0.10250
162A -> 168A -0.11855
163A -> 167A 0.18015
164A -> 170A -0.11815
149B -> 169B 0.10902
161B -> 165B -0.23216
163B -> 165B -0.11615
163B -> 168B 0.20528

Excited State 19: 3.526-A 3.9705 eV 312.26 nm f=0.0007 <S**2>=2.858
147A -> 169A 0.10815
148A -> 167A -0.15674
148A -> 168A -0.19046
148A -> 169A 0.20363
149A -> 165A -0.16045
150A -> 165A -0.18100
151A -> 169A -0.12697
153A -> 165A -0.13695

153A -> 167A 0.12612
153A -> 169A -0.26966
154A -> 165A -0.15050
155A -> 165A -0.11754
155A -> 169A 0.11612
156A -> 165A -0.16761
158A -> 167A 0.10624
158A -> 169A -0.20374
159A -> 165A 0.23066
161A -> 165A -0.20001
161A -> 167A 0.10951
161A -> 169A -0.11753
162A -> 165A 0.11807
164A -> 169A 0.11068
148B -> 169B -0.10394
148B -> 170B 0.11108

Excited State 20: 3.058-A 4.0119 eV 309.04 nm f=0.0008 <S**2>=2.087
133A -> 165A 0.10964
148A -> 167A 0.10293
148A -> 168A 0.12806
148A -> 169A -0.17602
149A -> 165A -0.14336
150A -> 165A -0.32760
153A -> 165A -0.29705
153A -> 169A 0.13865
154A -> 165A -0.20709
156A -> 165A -0.33701
158A -> 169A 0.11568
159A -> 165A 0.33890
161A -> 165A -0.26994
161A -> 169A 0.10608
161A -> 172A -0.10724
163B -> 168B -0.11790

Excited State 21: 3.740-A 4.0411 eV 306.81 nm f=0.0047 <S**2>=3.247
142A -> 168A 0.10360
147A -> 168A -0.13306
148A -> 165A 0.16937
148A -> 168A -0.35735
148A -> 169A -0.21692
148A -> 170A -0.12252
151A -> 168A 0.13762
153A -> 168A 0.25408

153A -> 169A 0.11948
154A -> 168A -0.15783
157A -> 165A 0.11236
158A -> 168A 0.23490
158A -> 169A 0.13067
160A -> 168A -0.17821
164A -> 168A -0.17893
148B -> 164B 0.16269
148B -> 169B -0.14180
148B -> 170B -0.16637

Excited State 22: 2.971-A 4.1130 eV 301.44 nm f=0.0006 <S**2>=1.957
133B -> 164B 0.17504
135B -> 164B 0.20206
140B -> 164B 0.15395
143B -> 164B -0.10530
146B -> 164B -0.21682
147B -> 164B -0.35106
148B -> 164B -0.11471
149B -> 164B -0.16443
150B -> 164B -0.24087
151B -> 164B -0.11659
152B -> 164B -0.37350
154B -> 164B -0.22611
155B -> 164B 0.25213
156B -> 164B 0.39868
157B -> 164B 0.10388
158B -> 164B -0.12233
159B -> 164B 0.14197
161B -> 164B 0.10206

Excited State 23: 2.925-A 4.1970 eV 295.41 nm f=0.0011 <S**2>=1.889
133A -> 165A -0.15050
135A -> 165A -0.12884
146A -> 165A -0.29199
148A -> 165A 0.12111
149A -> 165A 0.23105
150A -> 165A 0.27222
151A -> 165A 0.13000
154A -> 165A -0.32065
156A -> 165A 0.35539
157A -> 165A 0.15551
158A -> 165A 0.12569
159A -> 165A 0.45069

161A -> 165A -0.16692
163B -> 167B 0.14659

Excited State 24: 2.972-A 4.2369 eV 292.63 nm f=0.0370 <S**2>=1.958
162A -> 166A 0.10277
164A -> 169A -0.11315
164A -> 170A -0.20685
164A -> 171A 0.14214
149B -> 164B 0.14685
150B -> 167B -0.10051
153B -> 164B 0.30501
153B -> 167B -0.11635
154B -> 164B 0.16194
155B -> 167B -0.14834
160B -> 166B 0.12054
163B -> 166B 0.19953
163B -> 167B 0.51363
163B -> 168B 0.12445

Excited State 25: 2.940-A 4.2646 eV 290.73 nm f=0.0063 <S**2>=1.911
164A -> 168A -0.14408
164A -> 170A 0.22524
164A -> 171A -0.13858
149B -> 164B -0.19548
153B -> 164B -0.35107
154B -> 164B -0.11687
155B -> 167B -0.16300
156B -> 164B -0.17353
160B -> 167B 0.13851
161B -> 164B 0.28867
163B -> 166B 0.11635
163B -> 167B 0.49108

Bis-oxidized [CrN(Sal)^{OiPr}]$^{+}$, quartet:

Excited State 1: 4.105-A 2.0230 eV 612.88 nm f=0.0064 <S**2>=3.962
161B -> 163B 0.33779
161B -> 164B 0.44722
162B -> 163B 0.66168
162B -> 164B 0.40909
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -2833.64826313
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 4.105-A 2.0681 eV 599.52 nm f=0.0118 <S**2>=3.964

161B -> 163B	0.59451
161B -> 164B	-0.47706
162B -> 163B	-0.29278
162B -> 164B	0.50002

Excited State 3: 4.090-A 2.7010 eV 459.03 nm f=0.0886 <S**2>=3.931

150A -> 170A	-0.13840
150A -> 172A	-0.13383
153A -> 170A	-0.13889
153A -> 172A	-0.13037
154A -> 170A	-0.21310
154A -> 172A	-0.19917
158A -> 170A	0.10646
161A -> 167A	0.19739
161A -> 168A	0.12095
161A -> 170A	-0.40681
161A -> 171A	-0.16913
161A -> 172A	-0.35332
161A -> 173A	0.12650
162A -> 167A	-0.14867
162A -> 170A	0.12623
162A -> 172A	0.14795
158B -> 164B	-0.12264
159B -> 164B	0.11517
160B -> 163B	-0.22129

Excited State 4: 4.209-A 2.7716 eV 447.34 nm f=0.3909 <S**2>=4.179

161A -> 167A	0.12108
161A -> 170A	-0.10839
161A -> 172A	-0.14298
162A -> 167A	0.15157
162A -> 170A	0.11024
163A -> 166A	0.19269
164A -> 167A	0.11286
165A -> 166A	0.11347
157B -> 164B	0.21530
158B -> 164B	0.29850
159B -> 164B	-0.30223
160B -> 163B	0.61137
160B -> 164B	-0.14369
161B -> 166B	-0.12165
162B -> 165B	-0.13093

Excited State 5: 4.403-A 2.8001 eV 442.78 nm f=0.0076 <S**2>=4.596
149A -> 169A 0.10897
162A -> 166A 0.21776
163A -> 167A 0.21008
165A -> 168A 0.10308
147B -> 168B 0.14405
149B -> 169B -0.10510
157B -> 163B 0.25483
158B -> 163B 0.35588
158B -> 164B 0.13747
159B -> 163B -0.24361
160B -> 164B 0.51136
161B -> 165B -0.13318
162B -> 166B -0.12694

Excited State 6: 4.114-A 2.8704 eV 431.94 nm f=0.0094 <S**2>=3.981
140B -> 163B 0.13607
140B -> 164B 0.11469
154B -> 163B 0.11983
155B -> 163B -0.11816
156B -> 163B -0.12783
156B -> 164B -0.10290
158B -> 163B 0.42084
158B -> 164B 0.35918
159B -> 163B 0.51002
159B -> 164B 0.39881

Excited State 7: 4.136-A 2.9399 eV 421.74 nm f=0.0157 <S**2>=4.028
154B -> 163B 0.10382
154B -> 164B -0.12130
155B -> 163B -0.17921
155B -> 164B 0.18140
157B -> 163B -0.48319
157B -> 164B 0.54482
157B -> 165B 0.10094
158B -> 163B 0.24894
158B -> 164B -0.18539
159B -> 163B -0.19717
159B -> 164B 0.14309

Excited State 8: 4.619-A 2.9629 eV 418.45 nm f=0.0048 <S**2>=5.085
147A -> 168A 0.16035
149A -> 168A -0.11859
149A -> 169A 0.16756

151A -> 168A -0.11296
155A -> 168A -0.14289
155A -> 169A 0.11953
159A -> 168A 0.17079
159A -> 169A 0.10183
162A -> 169A -0.14400
164A -> 166A -0.13073
165A -> 167A -0.18249
165A -> 168A 0.13785
147B -> 164B 0.10778
147B -> 168B 0.22260
148B -> 163B 0.10163
149B -> 165B 0.10625
149B -> 169B -0.15979
153B -> 165B 0.10315
153B -> 168B -0.12332
153B -> 169B -0.13562
157B -> 163B -0.23640
157B -> 164B 0.13385
158B -> 163B -0.12493
159B -> 163B 0.16331
160B -> 164B -0.25331
160B -> 168B 0.13159

Excited State 9: 4.247-A 3.0982 eV 400.18 nm f=0.0073 <S**2>=4.259
162A -> 167A -0.13719
163A -> 166A -0.15548
164A -> 166A -0.13973
164A -> 167A 0.50477
165A -> 166A 0.70989
165A -> 167A -0.14191
161B -> 166B 0.11674
162B -> 165B 0.13083

Excited State 10: 4.278-A 3.1689 eV 391.25 nm f=0.1006 <S**2>=4.324
162A -> 166A -0.14507
163A -> 167A -0.15332
164A -> 166A 0.54111
164A -> 167A 0.23952
165A -> 167A 0.62897
161B -> 165B 0.12007
162B -> 166B 0.14923

Excited State 11: 4.272-A 3.5608 eV 348.19 nm f=0.0047 <S**2>=4.313

147A -> 168A 0.11594
150A -> 169A -0.13434
151A -> 169A -0.12627
154A -> 169A -0.26334
156A -> 169A 0.10545
158A -> 169A 0.14014
159A -> 168A 0.12698
159A -> 169A 0.12055
161A -> 166A 0.19897
161A -> 169A -0.50722
161A -> 171A -0.14690
162A -> 166A -0.14391
162A -> 169A 0.25100
163A -> 169A -0.12825
165A -> 168A 0.12476
165A -> 169A 0.24169

Excited State 12: 4.278-A 3.5691 eV 347.39 nm f=0.0003 <S**2>=4.325
147A -> 169A 0.11497
149A -> 168A 0.10927
149A -> 169A 0.10634
150A -> 168A 0.14408
153A -> 168A 0.12435
154A -> 168A 0.25208
156A -> 168A -0.15209
157A -> 168A 0.10320
158A -> 168A -0.13605
159A -> 169A 0.14386
161A -> 168A 0.53662
161A -> 170A 0.15365
162A -> 168A -0.27254
163A -> 168A 0.12163
164A -> 167A 0.11590
165A -> 168A -0.20440
165A -> 169A 0.14303

Excited State 13: 4.524-A 3.7113 eV 334.07 nm f=0.0182 <S**2>=4.866
147A -> 168A -0.15150
147A -> 169A 0.11590
149A -> 169A 0.13063
150A -> 168A -0.15430
153A -> 168A -0.20348
153A -> 170A -0.10584
154A -> 168A -0.15512

155A -> 168A 0.18081
158A -> 169A 0.11486
159A -> 166A -0.11218
159A -> 168A -0.16305
159A -> 169A 0.15242
161A -> 168A -0.31945
162A -> 166A 0.11300
163A -> 166A 0.13252
163A -> 167A 0.10289
164A -> 167A 0.18660
165A -> 168A -0.15449
165A -> 169A 0.18890
147B -> 168B -0.13647
149B -> 169B -0.10286
162B -> 165B -0.12509

Excited State 14: 4.523-A 3.7470 eV 330.89 nm f=0.0122 <S**2>=4.865
147A -> 169A -0.12327
148A -> 168A 0.10922
149A -> 168A -0.19764
149A -> 169A 0.15003
150A -> 169A -0.15832
153A -> 168A 0.10853
153A -> 169A -0.12175
154A -> 169A -0.18082
155A -> 166A -0.10652
155A -> 168A -0.15966
155A -> 169A 0.19084
161A -> 166A 0.14016
161A -> 169A -0.26695
162A -> 166A 0.17560
163A -> 167A 0.15287
164A -> 166A 0.12254
164A -> 171A -0.11083
165A -> 167A 0.12663
165A -> 168A -0.13489
165A -> 169A -0.13585
165A -> 172A -0.11766
147B -> 169B 0.12768
149B -> 168B -0.11827
153B -> 168B -0.10219
160B -> 164B -0.16786
161B -> 165B -0.17451
162B -> 166B -0.13592

Excited State 15: 4.530-A 3.8011 eV 326.18 nm f=0.0280 <S**2>=4.880

147A -> 168A	0.10616
159A -> 168A	0.10983
161A -> 168A	0.10350
162A -> 167A	0.27559
163A -> 166A	0.26883
163A -> 167A	0.17485
164A -> 166A	0.12028
164A -> 167A	0.14317
164A -> 168A	-0.12601
164A -> 170A	0.21654
164A -> 172A	-0.13911
165A -> 166A	0.16613
165A -> 170A	0.19180
165A -> 171A	-0.19207
165A -> 173A	0.10907
159B -> 164B	0.13857
160B -> 163B	-0.21488
161B -> 166B	-0.18797
162B -> 165B	-0.23147
162B -> 166B	-0.13207

Excited State 16: 4.535-A 3.8411 eV 322.79 nm f=0.0289 <S**2>=4.891

149A -> 168A	0.13517
149A -> 169A	-0.11606
153A -> 169A	0.14783
155A -> 168A	0.11136
155A -> 169A	-0.16453
159A -> 168A	0.10261
161A -> 169A	0.14407
162A -> 166A	0.20803
162A -> 167A	-0.13502
163A -> 166A	-0.16982
163A -> 167A	0.21318
164A -> 166A	0.18363
164A -> 169A	0.13606
164A -> 171A	-0.19461
165A -> 166A	-0.11250
165A -> 170A	0.14687
165A -> 171A	0.23715
165A -> 172A	-0.15643
158B -> 163B	-0.10562
159B -> 163B	0.11833

160B -> 163B 0.13051
160B -> 164B -0.14160
161B -> 165B -0.16277
161B -> 166B 0.13239
162B -> 165B 0.11344
162B -> 166B -0.15457

Excited State 17: 4.722-A 3.9578 eV 313.27 nm f=0.0018 <S**2>=5.324
148A -> 166A -0.14634
148A -> 168A -0.21538
148A -> 169A 0.27764
153A -> 166A 0.12122
153A -> 168A 0.19620
153A -> 169A -0.26223
154A -> 168A -0.12640
154A -> 169A 0.12660
156A -> 166A -0.10049
156A -> 168A -0.14476
156A -> 169A 0.20494
157A -> 168A 0.11180
157A -> 169A -0.16099
163A -> 167A 0.10504
164A -> 166A 0.13278
164A -> 168A 0.14412
164A -> 169A -0.19275
164A -> 171A -0.10779
148B -> 165B -0.16780
148B -> 168B 0.17902
148B -> 169B 0.19749
149B -> 163B -0.11196
153B -> 163B -0.13326

Excited State 18: 4.699-A 4.0185 eV 308.53 nm f=0.0139 <S**2>=5.269
142A -> 168A -0.10347
148A -> 168A 0.28054
148A -> 169A 0.18929
148A -> 170A 0.12425
150A -> 168A 0.10119
153A -> 168A -0.24437
153A -> 169A -0.17303
154A -> 168A 0.20806
154A -> 169A 0.12004
156A -> 168A 0.17170
156A -> 169A 0.12114

157A -> 168A -0.14681
157A -> 169A -0.10251
164A -> 168A -0.22864
164A -> 169A -0.13624
147B -> 163B -0.18587
148B -> 164B -0.17770
148B -> 168B -0.22558
148B -> 169B 0.17414

Excited State 19: 4.100-A 4.1073 eV 301.86 nm f=0.0006 <S**2>=3.953
132B -> 163B -0.11409
134B -> 163B 0.11718
135B -> 163B 0.11002
135B -> 164B 0.14094
140B -> 163B 0.14101
145B -> 163B 0.28050
145B -> 164B 0.24120
146B -> 163B -0.10713
147B -> 163B 0.17598
147B -> 164B 0.10203
149B -> 164B -0.11950
150B -> 163B -0.19295
150B -> 164B -0.29270
152B -> 163B 0.20952
152B -> 164B 0.22127
154B -> 163B -0.17741
155B -> 163B 0.41858
155B -> 164B 0.18377
156B -> 163B 0.12455
158B -> 163B 0.10822

Excited State 20: 4.090-A 4.1430 eV 299.26 nm f=0.0011 <S**2>=3.932
132B -> 164B -0.14790
134B -> 164B 0.11820
135B -> 163B 0.14798
140B -> 164B 0.10037
145B -> 163B 0.10821
146B -> 163B 0.24561
146B -> 164B -0.28594
147B -> 164B 0.14510
149B -> 163B -0.19210
149B -> 164B 0.13916
150B -> 163B -0.34910
150B -> 164B 0.24088

152B -> 163B 0.18142
154B -> 163B 0.11506
154B -> 164B -0.19872
155B -> 163B -0.23535
155B -> 164B 0.36840
156B -> 164B 0.10198
158B -> 164B 0.12027

Excited State 21: 4.285-A 4.2287 eV 293.20 nm f=0.0198 <S**2>=4.339
148A -> 169A 0.13069
164A -> 170A -0.20566
164A -> 171A 0.10245
165A -> 170A -0.16834
165A -> 172A 0.10451
149B -> 163B 0.20411
149B -> 164B 0.10560
153B -> 163B 0.29043
153B -> 164B 0.16446
154B -> 163B 0.28672
154B -> 164B 0.13649
155B -> 163B 0.11130
155B -> 164B 0.12149
159B -> 163B -0.10687
161B -> 163B -0.28437
162B -> 164B 0.29864

Excited State 22: 4.151-A 4.2475 eV 291.90 nm f=0.0059 <S**2>=4.058
147B -> 163B 0.17128
150B -> 163B 0.10162
154B -> 163B 0.12774
158B -> 163B -0.15118
158B -> 164B -0.17197
159B -> 164B 0.17567
160B -> 163B 0.18125
160B -> 164B 0.11171
161B -> 163B 0.31645
161B -> 164B 0.50142
162B -> 163B -0.46916
162B -> 164B -0.15671

Excited State 23: 4.148-A 4.2755 eV 289.99 nm f=0.0253 <S**2>=4.051
164A -> 170A 0.10480
165A -> 169A 0.16620
165A -> 171A -0.12335

149B -> 164B -0.14408
152B -> 163B 0.10486
153B -> 164B -0.18861
154B -> 164B -0.19808
159B -> 163B -0.15506
159B -> 164B 0.10392
160B -> 164B -0.11668
161B -> 163B -0.35258
161B -> 164B 0.27097
162B -> 163B -0.31402
162B -> 164B 0.53353

Excited State 24: 4.292-A 4.3556 eV 284.66 nm f=0.1538 <S**2>=4.355
149A -> 168A -0.10007
159A -> 166A -0.12309
164A -> 167A 0.20728
164A -> 169A 0.13801
164A -> 170A -0.17717
164A -> 171A -0.15400
164A -> 172A 0.13388
165A -> 166A -0.10089
165A -> 171A 0.36369
144B -> 163B -0.16693
144B -> 164B 0.12543
147B -> 164B -0.10422
147B -> 167B -0.12608
149B -> 163B -0.10409
153B -> 163B -0.20240
154B -> 163B -0.13253
156B -> 163B 0.15584
157B -> 163B 0.17146
160B -> 163B -0.12198
160B -> 164B -0.15848
160B -> 167B -0.10566
162B -> 165B -0.11323

Excited State 25: 4.376-A 4.3989 eV 281.85 nm f=0.0029 <S**2>=4.537
147A -> 169A 0.10931
148A -> 168A 0.12569
149A -> 168A -0.26910
149A -> 169A -0.18761
149A -> 170A -0.12101
153A -> 168A 0.12765
153A -> 169A 0.11870

155A -> 168A	-0.21915
155A -> 169A	-0.19829
155A -> 170A	-0.10999
158A -> 168A	-0.10224
159A -> 168A	-0.12652
159A -> 169A	0.13255
162A -> 168A	0.17877
164A -> 167A	0.16536
165A -> 166A	-0.17265
165A -> 168A	-0.16959
165A -> 169A	0.31258
153B -> 163B	0.15049
161B -> 163B	0.12060
162B -> 164B	-0.15051

References:

1. Addison, A. W., Rao, T. N., Reedijk, J., Rijn, J., Verschoor, G. C. *J. Chem. Soc. Dalton Trans.* **1984**, 7, 1349-1356.