

## **Cyclopentadienyl chromium diimine and pyridine-imine complexes: ligand-based radicals and metal-based redox chemistry**

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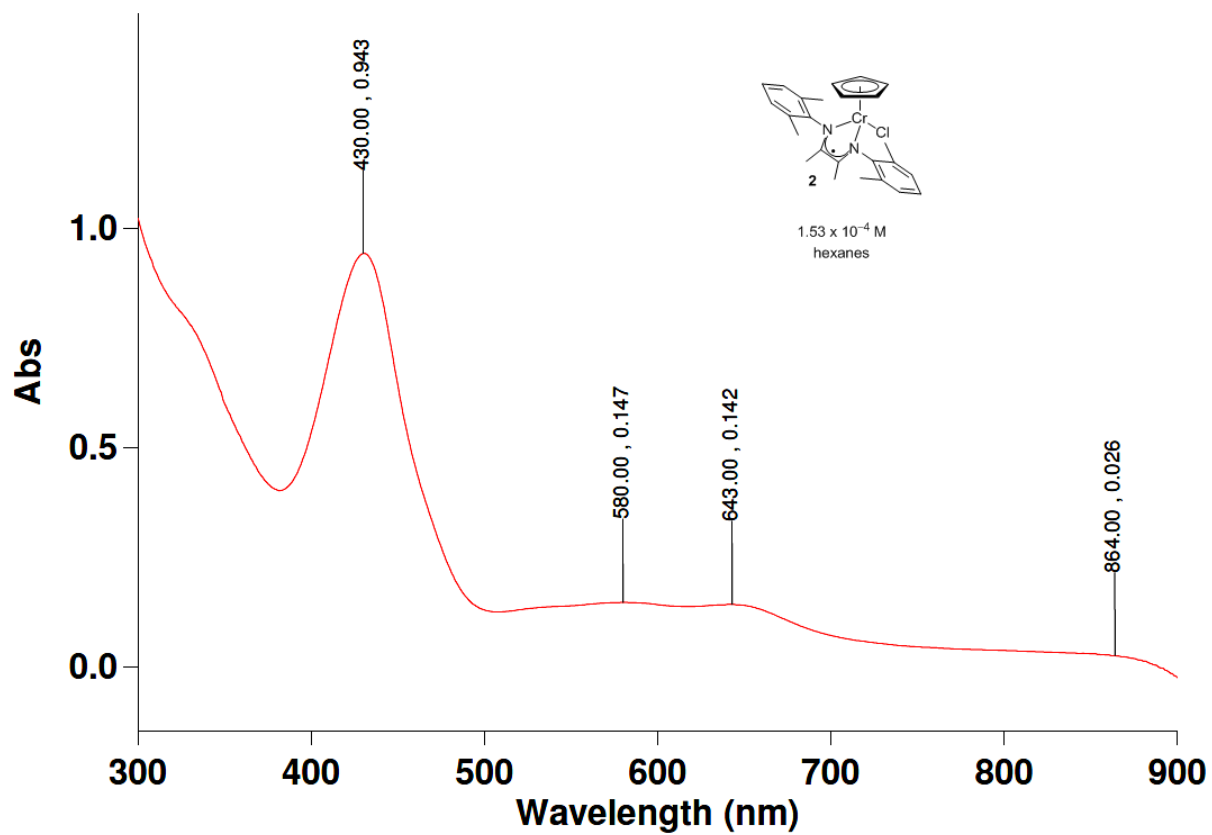
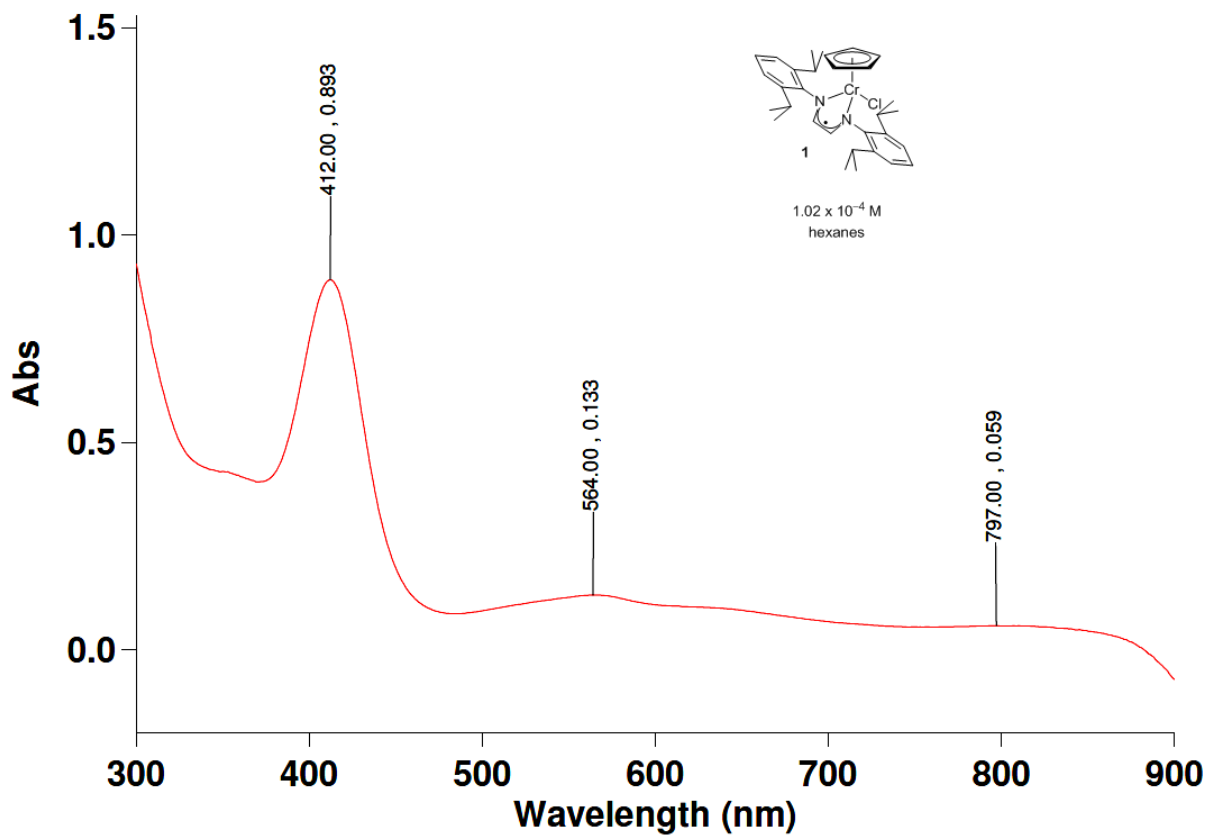
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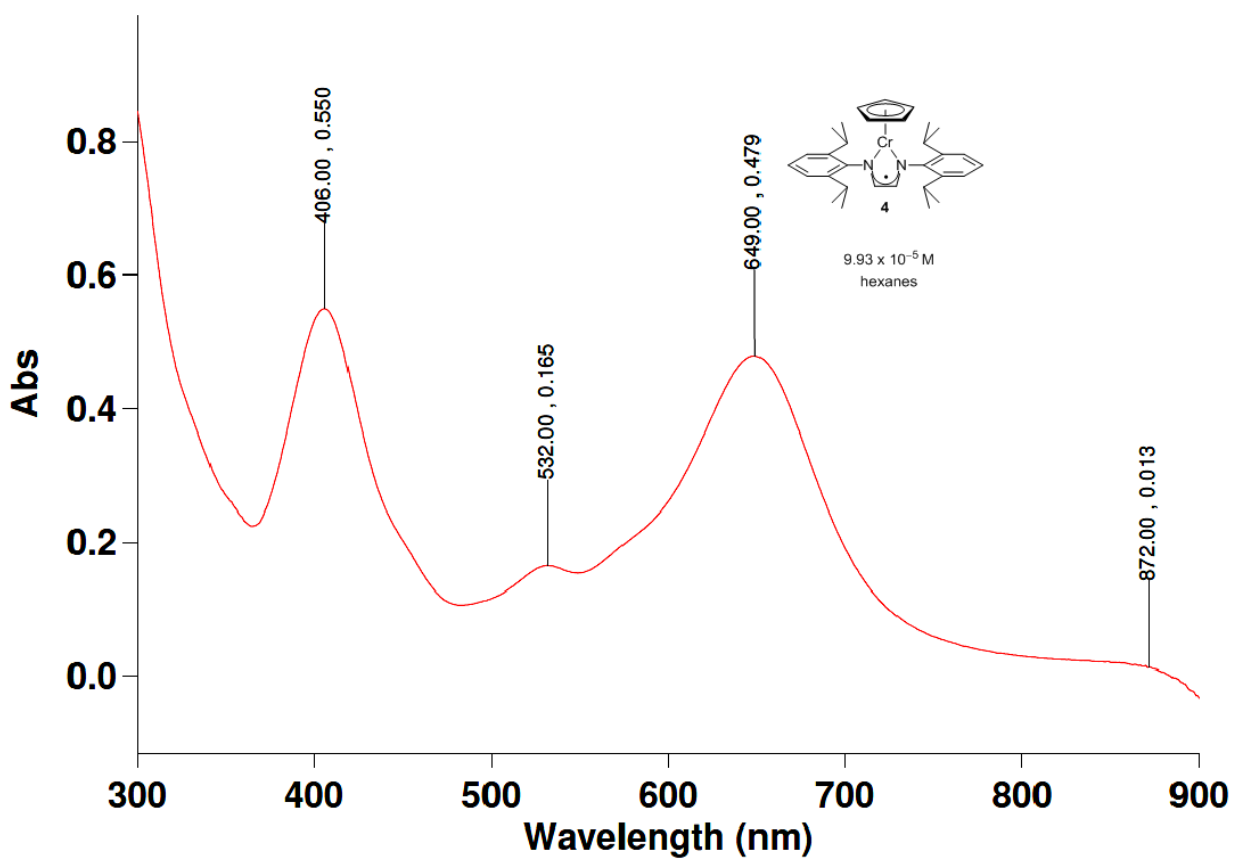
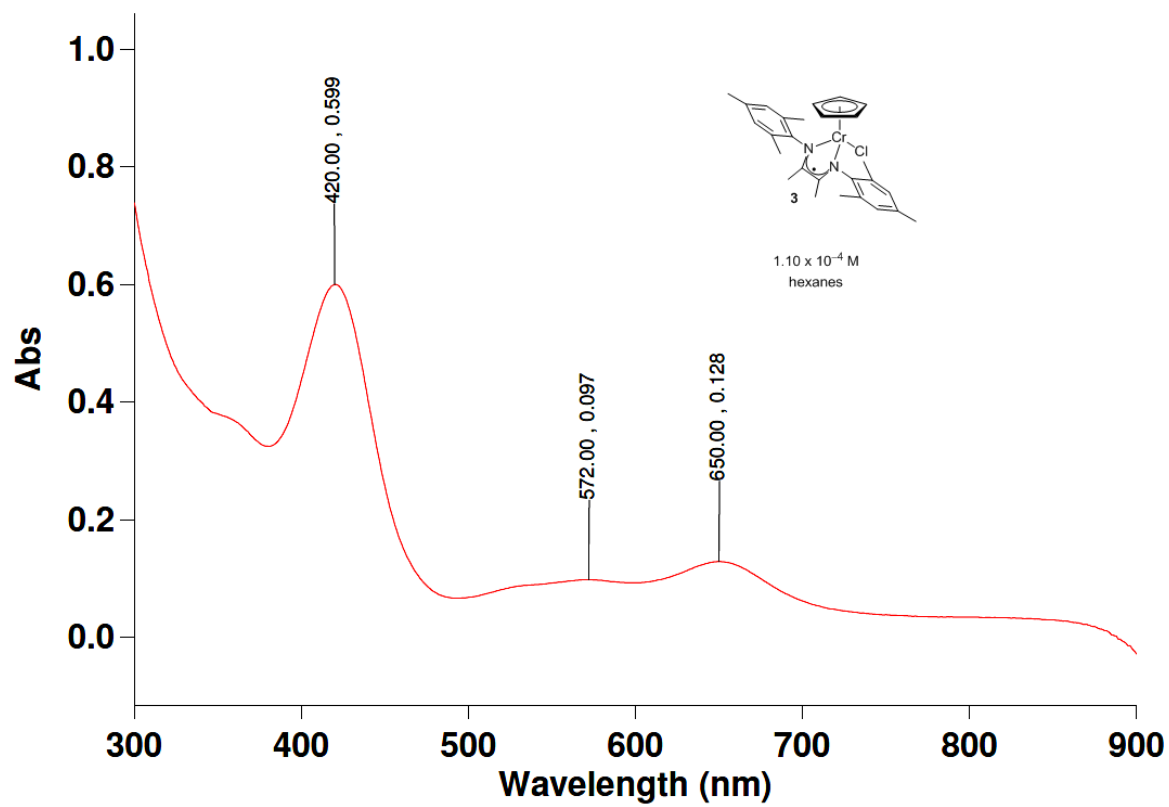
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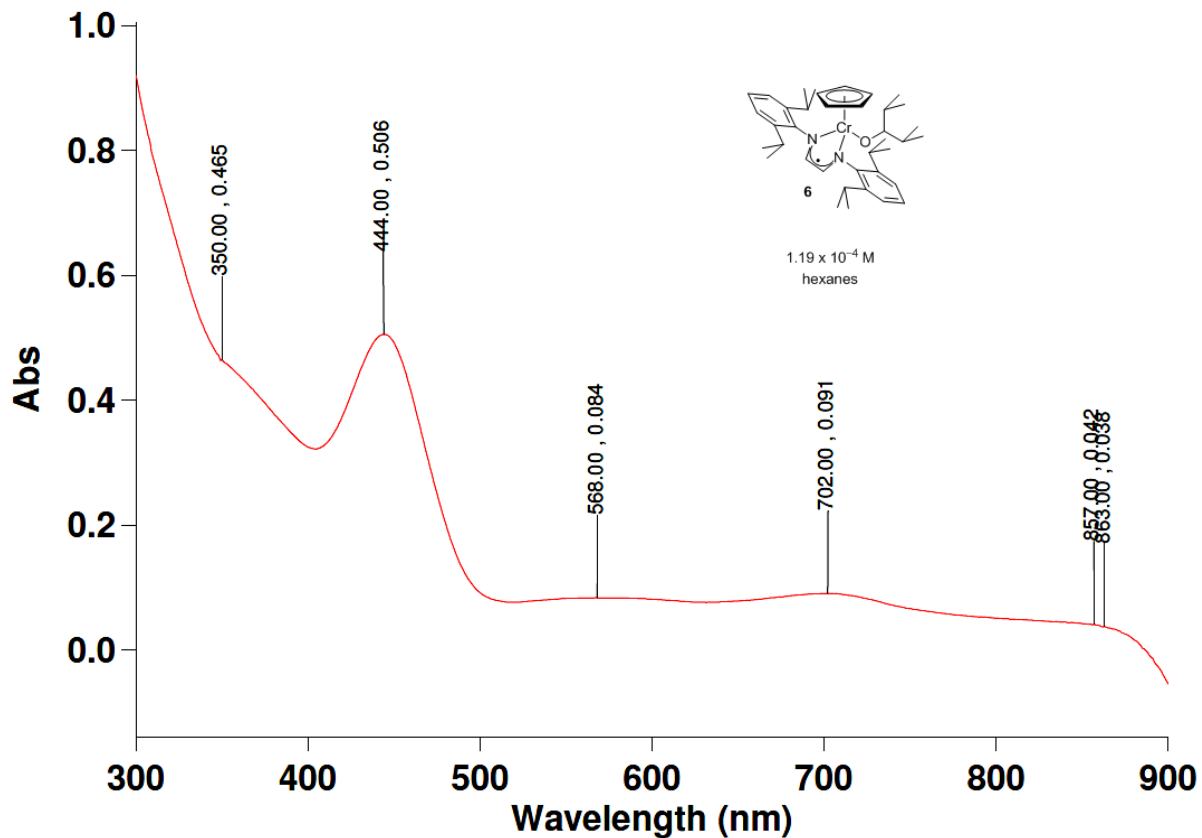
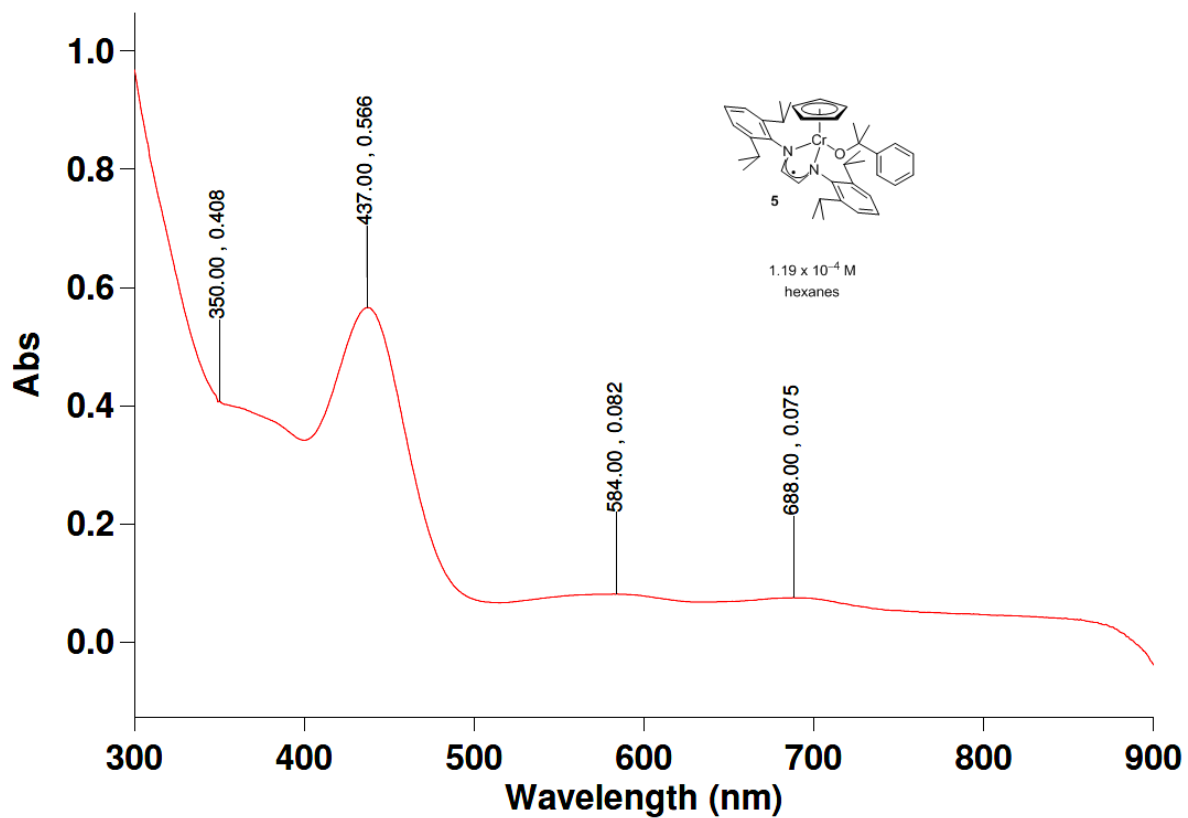
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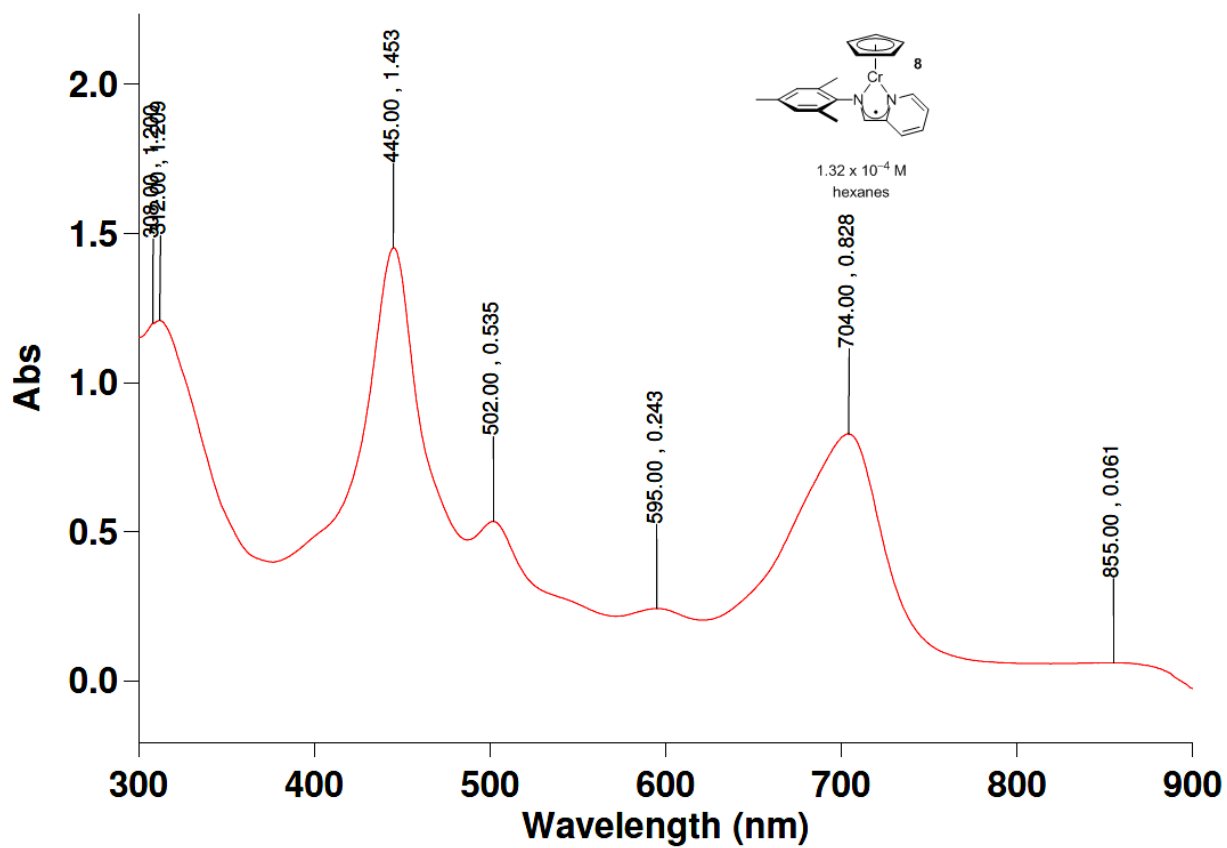
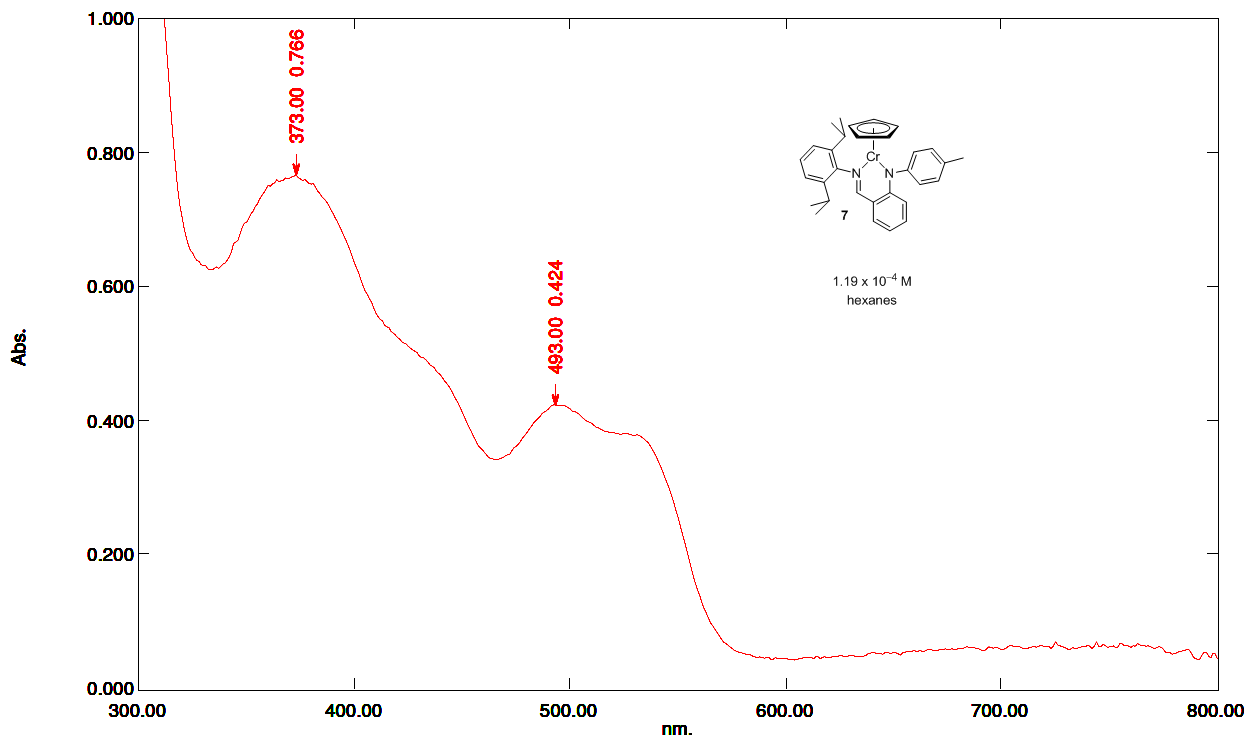
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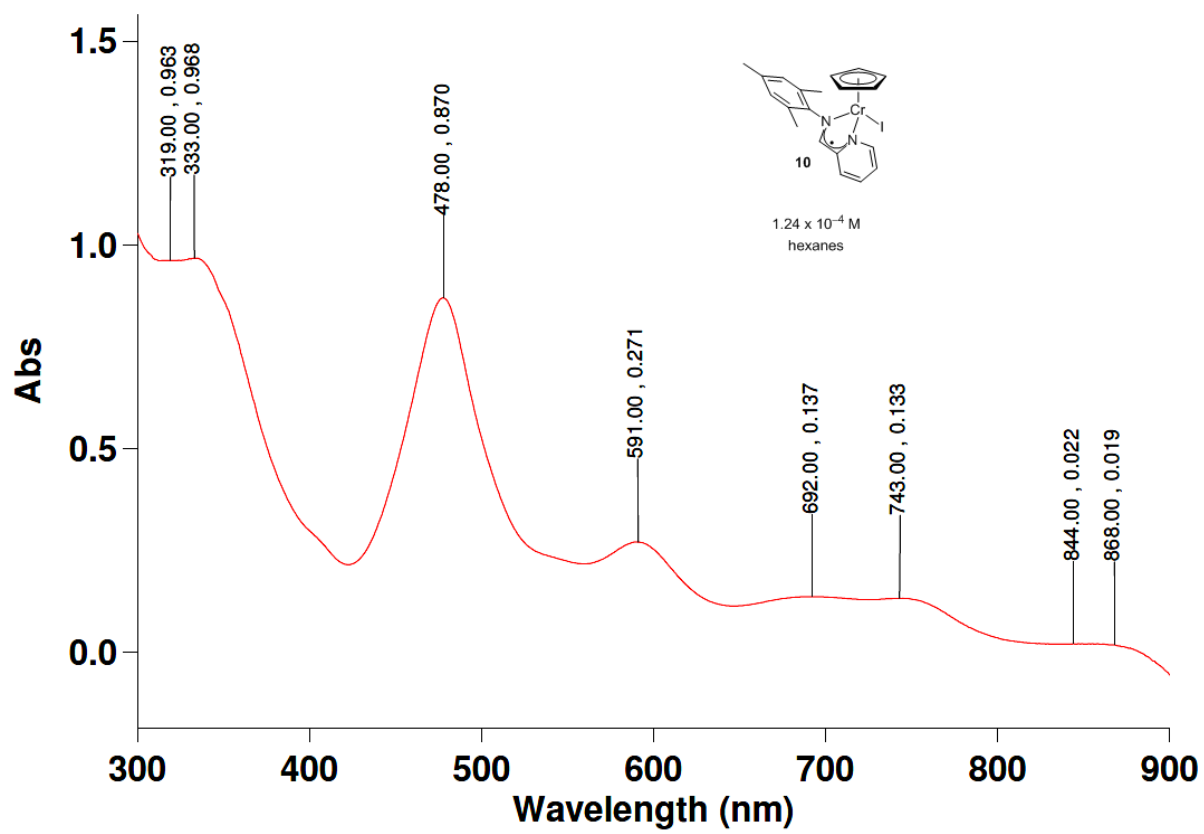
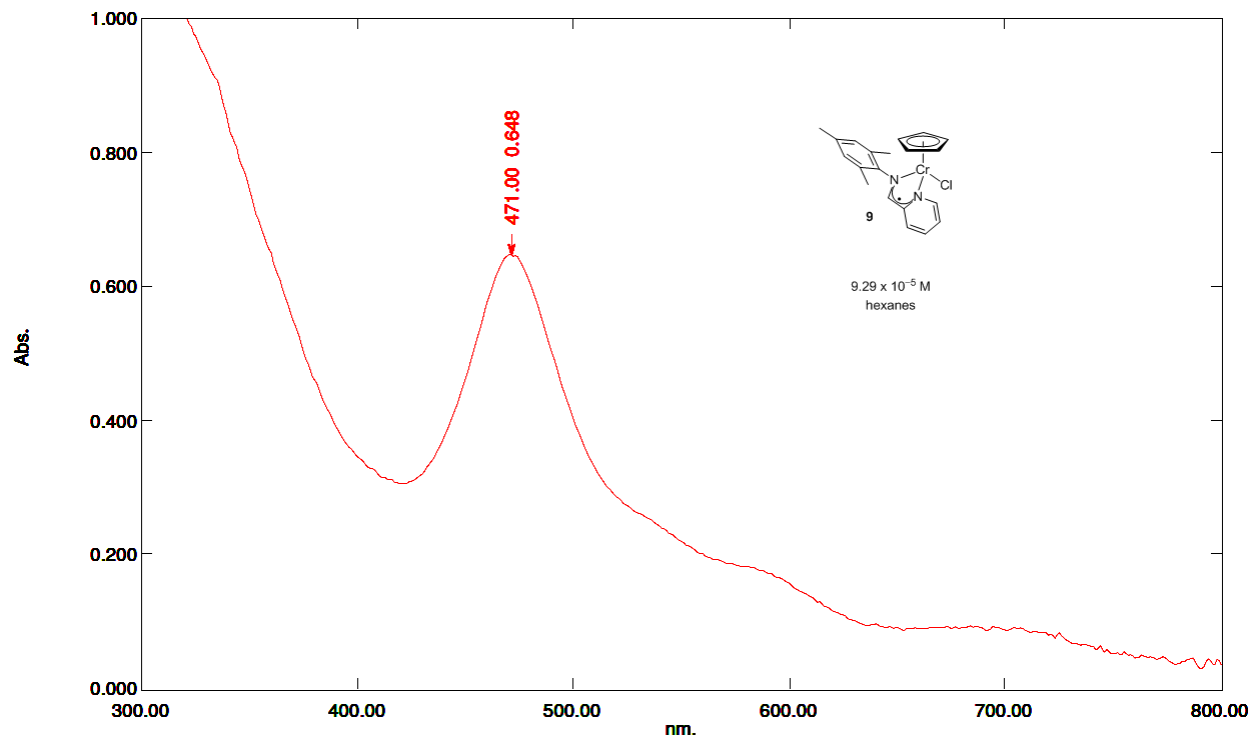
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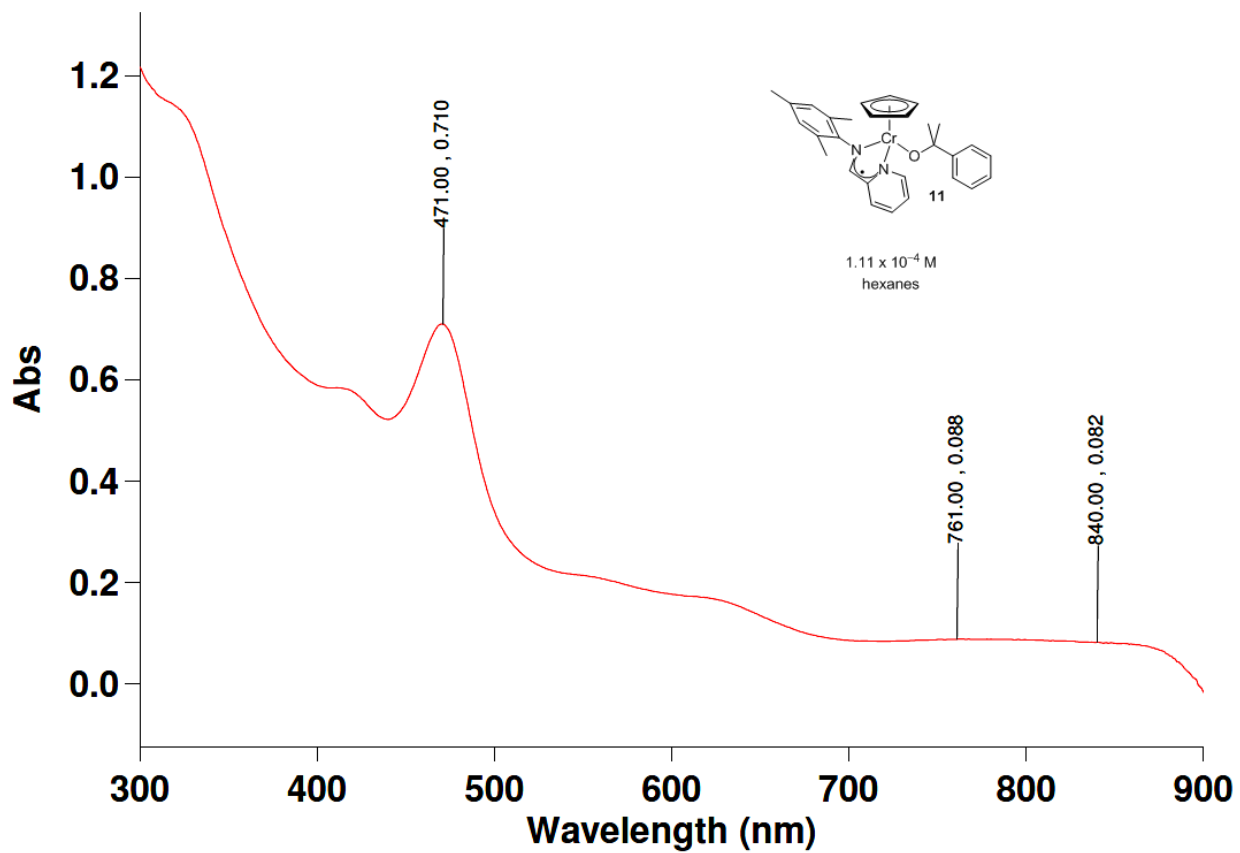




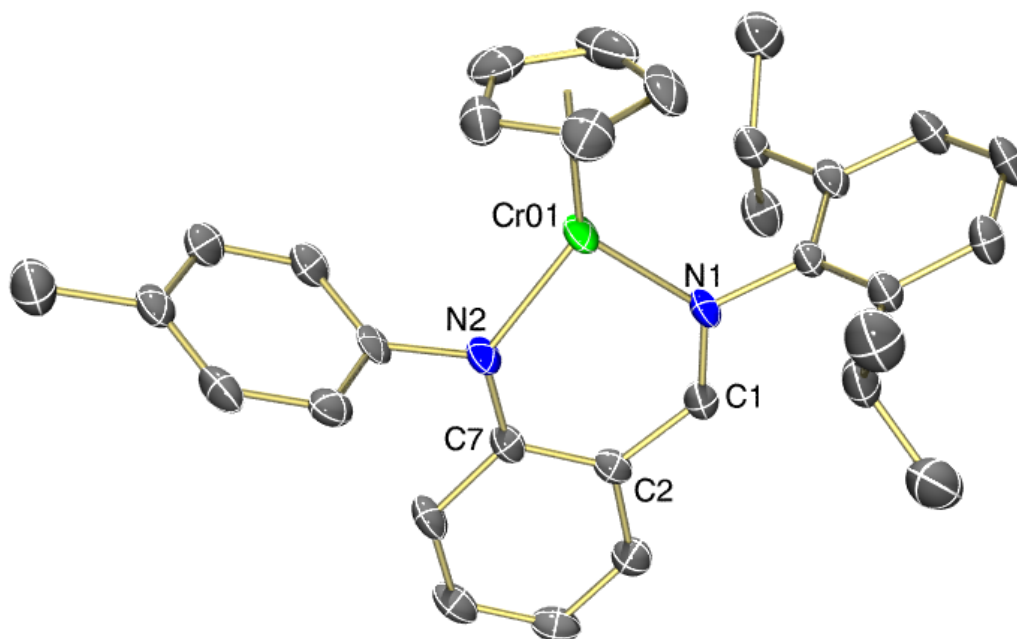




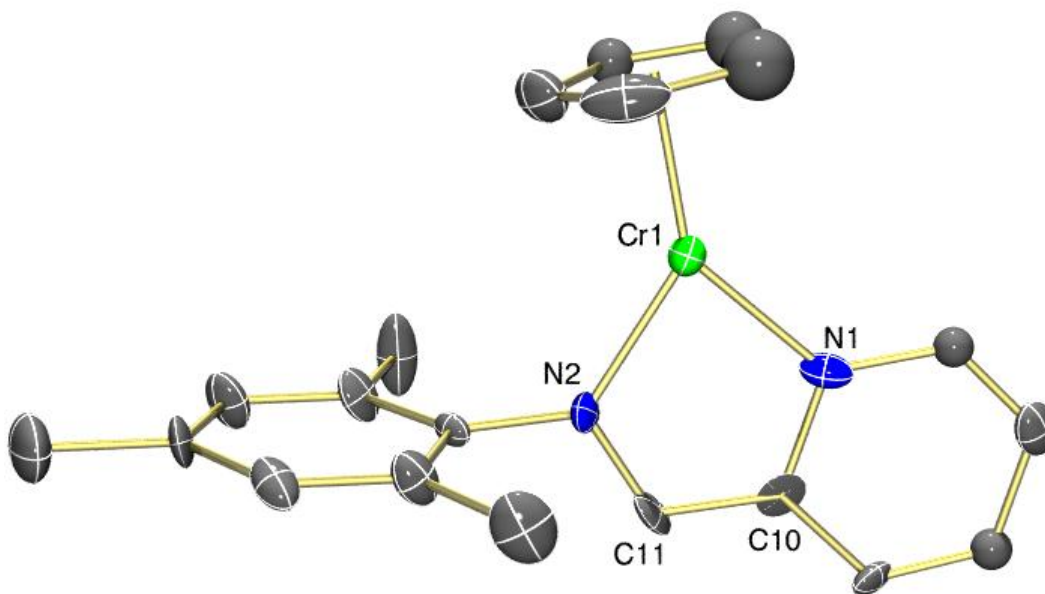




### X-ray Crystallography



**Figure S1.** Thermal ellipsoid diagram (50 %) of **7**. All H atoms are omitted for clarity



**Figure S2.** Thermal ellipsoid diagram (50 %) of **8**. All H atoms are omitted for clarity



**Table S1.** X-ray crystallographic data for complexes **1**, **2**, **4**, **5** and **6**.

	<b>1</b>	<b>2</b>	<b>4</b>	<b>5</b>	<b>6</b>
Formula	C <sub>31</sub> H <sub>41</sub> ClCrN <sub>2</sub>	C <sub>25</sub> H <sub>29</sub> N <sub>2</sub> ClCr	C <sub>31</sub> H <sub>41</sub> N <sub>2</sub> Cr	C <sub>40</sub> H <sub>52</sub> N <sub>2</sub> Ocr	C <sub>38</sub> H <sub>56</sub> N <sub>2</sub> ClO
M(g/mol)	529.11	444.95	493.66	628.84	608.85
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	Pbnm	P2 <sub>1</sub> /n	P2 <sub>1</sub>	P-1	P 2 <sub>1</sub> /c
a/Å	10.5374(2)	8.1510(4)	22.2076(14)	12.1823(7)	11.2842(3)
b/Å	13.0276(2)	13.9425(7)	10.7791(6)	12.3521(7)	27.0693(9)
c/Å	20.7603(4)	19.9028(10)	37.7205(23)	13.2389(8)	12.1378(4)
α(°)	90.00	90.00	90.00	111.688(3)	90.00
β(°)	90.00	94.522(3)	105.701(2)	106.727(3)	111.777(10)
γ(°)	90.00	90.00	90.00	91.867(3)	90.00
V/Å <sup>3</sup>	2849.91(9)	2254.82(19)	8692.54(52)	1751.06(18)	3442.97(19)
Z	4	4	12	2	4
ρ <sub>c</sub> /Mg m <sup>-3</sup>	1.233	1.311	1.13	1.19	1.175
T/K	173(2)	173(2)	173(2)	173(2)	173(2)
Radiation, λ/Å	0.71073	0.71073	0.71073	0.71073	0.71073
F(000)	1128	936	3180	675.9	1320
range, deg	2.486 to 28.068	3.439 to 27.870	2.517 to 25.481	2.866 to 27.951	2.352 to 27.892
Reflns collected/unique	25342/3540	53834/5394	88464/39600	45684/8362	47576/8191
R <sub>int</sub>	0.041	0.149	0.0453	0.0304	0.0454
Final R1 (I>2σI)	0.0320; 0.0801	0.0700; 0.1626	0.0537; 0.0972	0.0355; 0.0937	0.0419; 0.1032
R1 (all data)	0.0463; 0.0876	0.0966; 0.1727	0.0966; 0.1118	0.0427; 0.0989	0.0616; 0.1148

Complex **4** has a Flack parameter of 0.49(1).

**Table S2.** X-ray crystallographic data for complexes **7**, **8**, **10** and **11**.

	<b>7</b>	<b>8</b>	<b>10</b>	<b>11</b>
Formula	C <sub>31</sub> H <sub>34</sub> CrN <sub>2</sub>	C <sub>20</sub> H <sub>21</sub> CrN <sub>2</sub>	C <sub>20</sub> H <sub>21</sub> N <sub>2</sub> CrI	C <sub>29</sub> H <sub>32</sub> N <sub>2</sub> CrO
M(g/mol)	486.60	341.39	468.29	476.57
Crystal system	Triclinic	Monoclinic	Orthorhombic	Triclinic
Space group	P-1	P2 <sub>1</sub>	Pbca	P-1
<i>a</i> /Å	9.2266(14)	13.1264(14)	10.0652(5)	8.2157(7)
<i>b</i> /Å	11.0286(16)	7.0886(8)	17.6932(9)	8.8464(8)
<i>c</i> /Å	13.5053(19)	18.898(2)	20.9964(11)	16.8445(15)
α(°)	81.930(7)	90	90.00	89.077(2)
β(°)	82.478(7)	100.821(6)	90.00	89.842(2)
γ(°)	72.311(7)	90	90.00	77.669(2)
<i>V</i> /Å <sup>3</sup>	1290.6(3)	1727.2(3)	20.9960(11)	1195.80(18)
<i>Z</i>	2	4	8	2
<i>P</i> <sub>c</sub> /Mg m <sup>-3</sup>	1.25	1.313	1.664	1.324
T/K	173(2)	173(2)	173(2)	173(2)
Radiation, λ/Å	0.71073	0.71073	0.71073	0.71073
F(000)	515.9	716	1856	504
range, deg	2.5645 to 22.783	2.193 to 22.759	3.012 to 27.894	2.419 to 30.168
Reflns collected/unique	11493/3422	12684/2546	26941/4465	33519/7055
R <sub>int</sub>	0.0392	0.088	0.0224	0.0325
Final R1 (I>2σI)	0.0452; 0.1259	0.0816;0.1988	0.0169; 0.0414	0.0337; 0.0811
R1 (all data)	0.0639; 0.1259	0.1022;0.2161	0.0216; 0.0442	0.0458; 0.0867

Complex **8** has a Flack parameter of 0.14(8).

### Computed Metrical Parameters

#### 1) Compound 8 broken symmetry (S = 3/2):

Cr	1.05531929	0.94164235	-0.02694522
N	2.43622398	-0.53389230	0.01689854
N	-0.16705919	-0.62562603	0.04029942
C	3.79236374	-0.43833088	0.00251069
C	4.63413693	-1.52542733	0.03873687
C	4.06503004	-2.82869118	0.09488390
C	2.70029683	-2.96315460	0.11006049
C	1.86606234	-1.81116944	0.07000244
C	0.46724463	-1.82223120	0.07863722
C	-1.59504134	-0.61596218	0.03020774
C	-2.28921517	-0.72262169	-1.19215738
C	-3.68655185	-0.67430749	-1.17870478
C	-4.41282882	-0.52569083	0.00678012
C	-3.69854227	-0.41667980	1.20327108
C	-2.30100770	-0.45964373	1.23963886
C	-1.54004148	-0.87457802	-2.49470136
C	-5.92418815	-0.50911297	-0.00410330
C	-1.56377521	-0.34090027	2.55230038
C	1.88174139	2.91651160	-0.91756403
C	2.02960178	2.97370817	0.50198945
C	0.73503199	2.96806446	1.08190834
C	-0.21190189	2.86447333	0.02457032
C	0.49650845	2.86475200	-1.21229561
H	4.18747684	0.57334077	-0.04014790
H	4.70655009	-3.70478430	0.12521721
H	2.23087237	-3.94228353	0.15240755
H	5.70884486	-1.37973112	0.02481464
H	-4.22139649	-0.75318500	-2.12376898
H	-4.24244182	-0.29481700	2.13841007
H	-0.81583745	-0.06270127	-2.63488639
H	-2.22958056	-0.87009902	-3.34455230
H	-0.96645152	-1.80841956	-2.52827798
H	-6.31405282	-0.05503598	-0.92179654
H	-6.32574520	0.05167573	0.84680737
H	-6.33637843	-1.52575486	0.05370096
H	-0.96714375	-1.23628642	2.76333933
H	-2.26259853	-0.19446958	3.38171768
H	-0.86227978	0.50225871	2.54175557
H	2.68894860	2.92395473	-1.64009971
H	2.96799623	3.03730266	1.03986862
H	0.50794434	3.01258397	2.13978407
H	-1.28817896	2.81991653	0.13749350
H	0.05274912	2.81860914	-2.19903750
H	-0.10065896	-2.74891057	0.11772156

#### 2) Compound 8 high spin (S = 5/2):

Cr	1.09985530	0.95993900	-0.04856633
N	2.47938219	-0.58101651	0.09227788
N	-0.22331864	-0.61093540	0.16390143
C	3.82387653	-0.54485441	0.07325964
C	4.62420629	-1.67176265	0.15784533

C	3.98912831	-2.93389136	0.27054036
C	2.61541133	-3.00270774	0.29297812
C	1.84105791	-1.81432205	0.20276527
C	0.42957236	-1.78573475	0.22105316
C	-1.64306227	-0.60409339	0.10931114
C	-2.32281697	-1.02134668	-1.05544666
C	-3.72021141	-0.96205229	-1.07774328
C	-4.46364550	-0.49975464	0.01151505
C	-3.76532562	-0.07882875	1.14763317
C	-2.37056261	-0.12352877	1.21895386
C	-1.56538488	-1.48628663	-2.27798035
C	-5.97423641	-0.47388318	-0.02933008
C	-1.65165733	0.31549546	2.47196813
C	1.93142507	2.80955685	-1.22747509
C	2.17713180	3.01543342	0.16786195
C	0.92755489	3.14644230	0.82346158
C	-0.09002250	2.95046088	-0.15146276
C	0.53289306	2.78720320	-1.42589968
H	4.26381174	0.44541930	-0.01510674
H	4.58351578	-3.84087380	0.33893166
H	2.10258045	-3.95658015	0.37927671
H	5.70393658	-1.57759910	0.13714361
H	-4.24103198	-1.27610322	-1.98083491
H	-4.32131992	0.29119776	2.00753286
H	-0.76747861	-0.78217122	-2.54295564
H	-2.23771932	-1.58198042	-3.13629052
H	-1.08179865	-2.45882616	-2.12559133
H	-6.34576027	-0.36953209	-1.05452160
H	-6.37816121	0.35541110	0.56185892
H	-6.40285315	-1.39981353	0.37810659
H	-1.11056460	-0.51775746	2.93720009
H	-2.35570088	0.71581947	3.20828752
H	-0.90362030	1.08808188	2.25655992
H	2.68924787	2.70206166	-1.99445547
H	3.15247533	3.10930461	0.63117708
H	0.77458279	3.32802328	1.88015494
H	-1.15789405	2.97468162	0.02951882
H	0.01971876	2.64612138	-2.36918185
H	-0.12693072	-2.71902646	0.30267305

### 3) Compound 8 ( $S=1/2$ )

Cr	1.05776400	0.97521900	-0.03111900
N	2.45794900	-0.52199100	0.01676400
N	-0.17933500	-0.59723900	0.04231100
C	3.80666300	-0.44364400	-0.00109900
C	4.63812900	-1.54628400	0.03770700
C	4.04958000	-2.83351200	0.10034700
C	2.67730200	-2.94653600	0.11879200
C	1.87209900	-1.78212400	0.07511600
C	0.46051000	-1.78004700	0.08456700
C	-1.60793200	-0.59977000	0.03167000
C	-2.30013400	-0.71285400	-1.19131800
C	-3.69750000	-0.66853900	-1.17910200
C	-4.42551200	-0.51745400	0.00512400
C	-3.71260900	-0.40067000	1.20155400

C	-2.31492200	-0.44012400	1.23999300
C	-1.54893400	-0.86367700	-2.49255400
C	-5.93693300	-0.50447800	-0.00749000
C	-1.57899900	-0.31400300	2.55216100
C	1.88709500	2.85866200	-0.93633400
C	2.06885300	2.91549000	0.46919400
C	0.78832600	2.87884700	1.08842200
C	-0.18474200	2.81856700	0.05165800
C	0.49101600	2.79258000	-1.19852800
H	4.21406200	0.56239600	-0.04870200
H	4.67489600	-3.72118400	0.13320500
H	2.19371100	-3.91826700	0.16598700
H	5.71465600	-1.41668700	0.02074100
H	-4.23095300	-0.75120000	-2.12468300
H	-4.25745300	-0.27429300	2.13560000
H	-0.79878300	-0.07220200	-2.61013600
H	-2.23383400	-0.82437100	-3.34537600
H	-1.00381300	-1.81431400	-2.54258200
H	-6.32691400	-0.04740000	-0.92370100
H	-6.34068100	0.05195000	0.84524700
H	-6.34717800	-1.52222600	0.04552900
H	-1.05362900	-1.24121100	2.81322200
H	-2.27018500	-0.07820800	3.36746000
H	-0.81353700	0.46946800	2.50293000
H	2.67215700	2.85789000	-1.68282000
H	3.01917800	2.96141900	0.98789500
H	0.59150500	2.93819900	2.15119300
H	-1.25737000	2.76204700	0.19213500
H	0.02773100	2.75861400	-2.17642700
H	-0.09833700	-2.71365400	0.12732600

#### 4) Compound 8 Structure A CH2 backbone (S=2)

Cr	1.03069962	0.94856279	-0.04961365
N	2.47531277	-0.53386512	0.07447774
N	-0.16248098	-0.62306207	0.09864495
C	3.81641474	-0.36238758	0.11360815
C	4.70590146	-1.42098079	0.19628981
C	4.19194326	-2.72106556	0.24075781
C	2.81428325	-2.90078653	0.19884553
C	1.96929229	-1.79030829	0.11481822
C	0.46712447	-1.91817431	0.04835413
C	-1.57691007	-0.62452434	0.07222659
C	-2.30509341	-0.94834627	-1.09879063
C	-3.70478620	-0.91129728	-1.07772864
C	-4.42238197	-0.55517912	0.06469010
C	-3.69260090	-0.22408070	1.21234495
C	-2.29692259	-0.25718558	1.23833498
C	-1.59132028	-1.29413762	-2.38423463
C	-5.93384743	-0.53332583	0.07069297
C	-1.55921918	0.08946667	2.51037074
C	1.70759092	2.88260460	-1.21811132
C	2.01775577	3.06371290	0.16571230
C	0.79913960	3.10466993	0.89256984
C	-0.25714868	2.87784254	-0.02994420
C	0.30322136	2.77606192	-1.33967569

H	4.16042648	0.66630333	0.07710069
H	4.85751076	-3.57690094	0.30742825
H	2.37889134	-3.89519326	0.23048183
H	0.24119422	-2.50317173	-0.86866391
H	0.15144775	-2.58083754	0.87962837
H	5.77364240	-1.23113633	0.22615873
H	-4.24801484	-1.15374119	-1.99052157
H	-4.22773382	0.05968333	2.11799201
H	-0.65079933	-0.73795220	-2.46444040
H	-2.21369032	-1.06002876	-3.25480196
H	-1.34097057	-2.36281711	-2.44853376
H	-6.33808662	-0.62299694	-0.94322960
H	-6.32301655	0.39581316	0.50501203
H	-6.34845675	-1.36032929	0.66322327
H	-0.90741702	-0.73087712	2.83368788
H	-2.26110060	0.30926563	3.32212201
H	-0.90921399	0.96251377	2.37695919
H	2.42515926	2.84413388	-2.02942557
H	3.00928924	3.21312311	0.57844958
H	0.69534990	3.25121703	1.96061708
H	-1.31222999	2.82556483	0.20913909
H	-0.25341260	2.62587534	-2.25630056

**5) Compound 10 high spin (S=2)**

Cr	-0.70434101	-0.23050984	0.75087477
I	-2.09434346	-1.85077613	-0.93809125
N	-1.75560809	1.41682057	0.13832434
N	0.73870465	0.62513586	-0.43904653
C	-3.03191009	1.74307291	0.41769683
H	-3.53728497	1.10536778	1.13697464
C	-3.68313695	2.81444466	-0.16502381
H	-4.70879450	3.03870004	0.10412965
C	-2.98042944	3.58805651	-1.12313762
H	-3.46581502	4.43172147	-1.60537839
C	-1.68475993	3.25754855	-1.44498231
H	-1.12598537	3.82269082	-2.18510721
C	-1.05559156	2.15420638	-0.80843342
C	0.26146878	1.72793134	-1.05583660
H	0.89899390	2.28476067	-1.73903627
C	2.14535350	0.40207081	-0.43786804
C	2.66630012	-0.80245791	-0.97014216
C	4.04548071	-1.01879822	-0.93374843
H	4.43563400	-1.94307590	-1.35649501
C	4.93654900	-0.08643725	-0.39079516
C	4.40207371	1.09560325	0.12224387
H	5.07228612	1.83688805	0.55388355
C	3.02742199	1.36449888	0.11146828
C	2.54345279	2.67074227	0.70588713
H	3.29222656	3.07408195	1.39570127
H	1.60167604	2.55447922	1.25104893
H	2.36561771	3.43651898	-0.05958484
C	6.42321515	-0.35619994	-0.36544357
H	6.66031905	-1.24849560	0.22803892
H	6.97482406	0.48551344	0.06557949
H	6.81642560	-0.53073877	-1.37488754

C	1.76604237	-1.83536721	-1.60148160
H	2.35511494	-2.56474943	-2.16659435
H	1.03441654	-1.37969085	-2.27462862
H	1.18248545	-2.39031283	-0.85695008
C	-0.60086832	-1.92288294	2.28710547
H	-0.80932772	-2.93947627	1.98408842
C	0.65829579	-1.28057287	2.24265112
H	1.59122283	-1.71851973	1.91257629
C	0.47702463	0.06837428	2.67178189
H	1.25197097	0.81942916	2.73615950
C	-0.89347143	0.24699206	2.99032475
H	-1.35204915	1.17314090	3.31284772
C	-1.56954859	-0.97375140	2.73025090
H	-2.62901840	-1.16100194	2.84542576

**6) Compounds 10 broken symmetry (S = 1)**

Cr	-0.67256229	-0.20727333	0.77356039
I	-2.06096006	-1.84321983	-0.92430613
N	-1.72037867	1.39689664	0.14432832
N	0.69571196	0.62773855	-0.42095368
C	-2.97458198	1.76274968	0.50255750
H	-3.42905555	1.17852353	1.29636152
C	-3.65623232	2.79835924	-0.09938119
H	-4.65802657	3.04936946	0.23097728
C	-3.03175729	3.50223684	-1.15979351
H	-3.55281556	4.31348429	-1.65949792
C	-1.76474096	3.14061984	-1.55235214
H	-1.25728847	3.65091181	-2.36567764
C	-1.09579460	2.08111307	-0.88859070
C	0.21685731	1.65158648	-1.15153548
H	0.84725861	2.15154163	-1.88214700
C	2.11102445	0.40426851	-0.43858032
C	2.64322416	-0.77048503	-1.01357505
C	4.02774032	-0.96519604	-0.97989895
H	4.43422948	-1.86579559	-1.43634049
C	4.90078469	-0.04326315	-0.39484540
C	4.34920472	1.11691225	0.15239976
H	5.00736075	1.85667074	0.60456719
C	2.97212935	1.36654342	0.13825336
C	2.45528013	2.65886452	0.73355400
H	3.19140560	3.08348621	1.42396085
H	1.51451764	2.51728192	1.27428035
H	2.25957845	3.41495953	-0.03715200
C	6.38858002	-0.30331608	-0.34443542
H	6.65215760	-0.95543535	0.49927675
H	6.95457880	0.62671401	-0.22651239
H	6.73963520	-0.79960309	-1.25610572
C	1.76309226	-1.79440338	-1.68781438
H	2.36727123	-2.48028620	-2.29015237
H	1.01531698	-1.32849958	-2.33557937
H	1.19963564	-2.39664472	-0.96601922
C	-0.68642237	-1.90385826	2.30849243
H	-0.99202577	-2.89968154	2.02079032
C	0.62651726	-1.37700536	2.22604436
H	1.50740024	-1.90305418	1.88207241

C	0.58006250	-0.01773015	2.65106215
H	1.42149964	0.65938902	2.69473721
C	-0.76300577	0.28747159	2.99691051
H	-1.12623057	1.25142814	3.33023257
C	-1.55062013	-0.87345892	2.77464181
H	-2.61940881	-0.96405026	2.91840053

**7) Compounds 10 low spin (S = 0)**

Cr	-0.66300801	-0.19436842	0.74423998
I	-2.10302832	-1.90223543	-0.81449330
N	-1.65522851	1.35695239	0.01184673
N	0.71441979	0.67726781	-0.41596595
C	-2.94933178	1.65896663	0.29831762
H	-3.43394267	1.00736562	1.01649306
C	-3.62446526	2.70613717	-0.29196927
H	-4.65953603	2.89261928	-0.02543631
C	-2.96180659	3.51450103	-1.24230702
H	-3.47831953	4.34279724	-1.71742432
C	-1.65127323	3.22533821	-1.55732688
H	-1.09911751	3.81129158	-2.28615928
C	-1.01324544	2.13835131	-0.92333849
C	0.32473793	1.72783392	-1.12415389
H	1.00663650	2.26056172	-1.78255012
C	2.12622381	0.38730639	-0.43808094
C	2.59718278	-0.81733951	-1.00333643
C	3.96953441	-1.08014069	-0.96743471
H	4.32952486	-2.00342388	-1.41722940
C	4.88755484	-0.20111808	-0.38463135
C	4.39489583	0.99001588	0.14882903
H	5.08880983	1.69963636	0.59547326
C	3.03265737	1.31386842	0.12496504
C	2.60325688	2.65294600	0.68906957
H	3.30451913	2.98181244	1.46317790
H	1.60131124	2.62580332	1.12340293
H	2.59357769	3.43278268	-0.08393566
C	6.35914020	-0.53854947	-0.32567050
H	6.57581770	-1.23404182	0.49622763
H	6.96975227	0.35622912	-0.16593831
H	6.69767208	-1.01884052	-1.25064872
C	1.67219383	-1.80610837	-1.66894729
H	2.24275718	-2.49754788	-2.29704713
H	0.91956379	-1.31444797	-2.29125633
H	1.11674180	-2.40478086	-0.93852699
C	-0.54972231	-1.71219574	2.30828082
H	-0.68526035	-2.76164315	2.08561186
C	0.67948879	-0.98897886	2.25119717
H	1.65702965	-1.39035258	2.01977331
C	0.38921764	0.35906499	2.61559945
H	1.10383708	1.16696458	2.68341498
C	-0.99888894	0.45453883	2.91021434
H	-1.52488326	1.36069505	3.18478779
C	-1.57778224	-0.81815790	2.72840004
H	-2.62554848	-1.06738281	2.83695162



### TD-DFT calculations

#### 1) Compound 8 broken symmetry (S = 3/2):

Excited State 1: 4.475-A 1.8134 eV 683.73 nm f=0.0251 <S\*\*2>=4.755  
91A -> 92A 0.19550

91A -> 94A 0.12965

88B -> 89B 0.94901

88B -> 92B 0.13893

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

Total Energy, E(TD-HF/TD-KS) = -1929.05335693

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

Excited State 2: 4.510-A 1.8650 eV 664.79 nm f=0.0000 <S\*\*2>=4.835

83A -> 93A 0.17362

91A -> 93A 0.85751

91A -> 94A -0.23770

91A -> 96A -0.36876

Excited State 3: 4.243-A 2.0493 eV 605.00 nm f=0.0947 <S\*\*2>=4.250

91A -> 92A 0.95072

88B -> 89B -0.20880

88B -> 92B 0.11348

88B -> 97B 0.10307

Excited State 4: 4.120-A 2.3437 eV 529.01 nm f=0.0007 <S\*\*2>=3.994

88B -> 90B 0.92838

88B -> 91B 0.33561

88B -> 94B 0.12336

Excited State 5: 4.126-A 2.4434 eV 507.42 nm f=0.0001 <S\*\*2>=4.005

90A -> 93A 0.11465

88B -> 90B -0.34623

88B -> 91B 0.90303

88B -> 94B 0.13212

Excited State 6: 4.268-A 2.5078 eV 494.40 nm f=0.0264 <S\*\*2>=4.304

88A -> 93A -0.16041

89A -> 92A -0.14806

89A -> 93A -0.24220

89A -> 94A 0.10065

89A -> 96A 0.12181

90A -> 92A -0.20553

90A -> 93A 0.18031

91A -> 92A -0.11209

88B -> 92B 0.85479

Excited State 7: 4.258-A 2.5902 eV 478.67 nm f=0.0054 <S\*\*2>=4.283

88A -> 93A 0.26205

88A -> 96A -0.12831

89A -> 92A 0.30842

89A -> 93A 0.44932

89A -> 94A -0.13188

89A -> 96A -0.21295

90A -> 92A 0.41366

90A -> 93A -0.31376

90A -> 96A	0.13892
88B -> 89B	-0.10628
88B -> 92B	0.44674
Excited State 8: 4.304-A	2.6366 eV 470.24 nm f=0.0003 <S**2>=4.382
82A -> 93A	-0.10638
85A -> 93A	0.30464
85A -> 96A	-0.15735
86A -> 92A	0.14556
88A -> 92A	-0.13901
89A -> 92A	-0.18855
89A -> 93A	0.44539
89A -> 94A	-0.10664
89A -> 96A	-0.20344
90A -> 92A	0.13608
90A -> 93A	0.58623
90A -> 94A	-0.17159
90A -> 96A	-0.27245
88B -> 91B	-0.16896
Excited State 9: 4.335-A	2.7465 eV 451.43 nm f=0.0003 <S**2>=4.448
86A -> 93A	0.82844
86A -> 94A	-0.22971
86A -> 96A	-0.41686
88A -> 93A	-0.20571
Excited State 10: 4.061-A	2.7933 eV 443.87 nm f=0.0002 <S**2>=3.873
88A -> 92A	0.29421
89A -> 92A	0.74028
89A -> 93A	0.11002
90A -> 92A	-0.52956
90A -> 93A	0.16362
Excited State 11: 4.248-A	2.8830 eV 430.05 nm f=0.0188 <S**2>=4.262
86A -> 93A	-0.11187
88A -> 93A	-0.19268
88A -> 96A	0.10890
89A -> 92A	0.46075
89A -> 93A	-0.39086
89A -> 96A	0.16039
90A -> 92A	0.61065
90A -> 93A	0.25597
90A -> 96A	-0.11141
91A -> 94A	0.18427
Excited State 12: 4.462-A	3.1266 eV 396.54 nm f=0.0035 <S**2>=4.726
88B -> 91B	-0.16122
88B -> 93B	0.45084
88B -> 94B	0.86509
Excited State 13: 4.472-A	3.1776 eV 390.19 nm f=0.0008 <S**2>=4.751
90A -> 92A	-0.12599
91A -> 93A	0.21454
91A -> 94A	0.76741
88B -> 89B	-0.11623
88B -> 93B	-0.42753

88B -> 94B	0.23529				
88B -> 95B	-0.23870				
Excited State 14:	4.472-A	3.1909 eV	388.56 nm	f=0.0027	<S**2>=4.750
91A -> 93A	0.11623				
91A -> 94A	0.43591				
88B -> 93B	0.77445				
88B -> 94B	-0.38364				
Excited State 15:	4.398-A	3.4805 eV	356.23 nm	f=0.0154	<S**2>=4.586
85A -> 92A	-0.25057				
86A -> 92A	-0.39548				
88A -> 92A	0.63273				
89A -> 92A	-0.14674				
90A -> 92A	0.11848				
90A -> 93A	0.10501				
87B -> 94B	-0.10064				
88B -> 95B	0.46272				
Excited State 16:	4.466-A	3.4978 eV	354.46 nm	f=0.0591	<S**2>=4.735
85A -> 92A	-0.32096				
86A -> 92A	0.33559				
88A -> 92A	-0.38017				
90A -> 92A	-0.11540				
90A -> 94A	0.10608				
91A -> 94A	0.13258				
91A -> 98A	0.13934				
88B -> 95B	0.66748				
88B -> 97B	-0.11415				
Excited State 17:	4.923-A	3.5581 eV	348.46 nm	f=0.0004	<S**2>=5.809
86A -> 92A	0.47190				
87A -> 95A	0.34471				
88A -> 93A	0.32926				
88A -> 96A	0.25791				
89A -> 93A	-0.15509				
89A -> 96A	-0.11415				
90A -> 96A	0.15885				
86B -> 93B	-0.32734				
87B -> 90B	0.14293				
87B -> 91B	0.26103				
87B -> 94B	-0.36346				
Excited State 18:	4.434-A	3.6301 eV	341.55 nm	f=0.0046	<S**2>=4.664
86A -> 92A	0.67872				
87A -> 95A	-0.14177				
88A -> 92A	0.56685				
88A -> 93A	-0.11621				
88A -> 96A	-0.10388				
89A -> 92A	-0.16558				
90A -> 92A	0.17897				
90A -> 93A	-0.10318				
86B -> 93B	0.13446				
87B -> 91B	-0.10180				
87B -> 94B	0.14412				

Excited State 19: 4.253-A 3.8644 eV 320.84 nm f=0.0970 <S\*\*2>=4.273  
83A -> 92A 0.10104  
85A -> 92A 0.37123  
91A -> 92A -0.12356  
91A -> 94A 0.16582  
83B -> 89B -0.12791  
88B -> 95B 0.35188  
88B -> 97B 0.77216  
88B -> 101B 0.13708

Excited State 20: 4.539-A 3.9453 eV 314.25 nm f=0.0007 <S\*\*2>=4.900  
91A -> 95A 0.86185  
91A -> 96A 0.15479  
88B -> 96B -0.44126  
88B -> 99B 0.10153

Excited State 21: 4.494-A 3.9488 eV 313.98 nm f=0.0012 <S\*\*2>=4.800  
91A -> 95A 0.47818  
88B -> 96B 0.84236  
88B -> 99B -0.18112

Excited State 22: 4.547-A 3.9986 eV 310.07 nm f=0.0002 <S\*\*2>=4.918  
91A -> 93A 0.38394  
91A -> 94A -0.10505  
91A -> 95A -0.12741  
91A -> 96A 0.88101  
88B -> 96B 0.15598

Excited State 23: 4.501-A 4.1005 eV 302.37 nm f=0.0807 <S\*\*2>=4.814  
85A -> 92A -0.41022  
87A -> 92A 0.81095  
91A -> 98A -0.13613  
88B -> 95B -0.13340  
88B -> 97B 0.29341

Excited State 24: 4.501-A 4.1328 eV 300.00 nm f=0.1319 <S\*\*2>=4.814  
85A -> 92A 0.62787  
87A -> 92A 0.57163  
91A -> 98A 0.18086  
88B -> 95B 0.16358  
88B -> 97B -0.38120

Excited State 25: 4.747-A 4.2650 eV 290.70 nm f=0.0536 <S\*\*2>=5.383  
85A -> 92A 0.10751  
85A -> 94A -0.18146  
89A -> 93A 0.12967  
89A -> 94A 0.45841  
90A -> 93A 0.19435  
90A -> 94A 0.69445  
83B -> 89B 0.31270  
83B -> 92B 0.11326  
88B -> 97B 0.15547

Excited State 26: 4.530-A 4.3118 eV 287.55 nm f=0.0005 <S\*\*2>=4.880  
84A -> 92A -0.13140  
91A -> 97A -0.33001

88B -> 96B	0.18356
88B -> 98B	0.12059
88B -> 99B	0.86119
88B ->102B	-0.18155
Excited State 27: 4.472-A	4.3266 eV 286.56 nm f=0.0013 <S**2>=4.749
91A -> 97A	0.91886
88B -> 99B	0.32591
Excited State 28: 4.949-A	4.3482 eV 285.14 nm f=0.0002 <S**2>=5.873
84A -> 92A	0.52671
87A -> 93A	-0.19450
87A -> 96A	-0.14489
88A -> 95A	-0.38741
89A -> 95A	0.20396
90A -> 95A	-0.22747
86B -> 91B	-0.12671
86B -> 94B	0.17447
87B -> 89B	-0.18787
87B -> 92B	0.10766
87B -> 93B	0.46545
Excited State 29: 4.716-A	4.3522 eV 284.88 nm f=0.0006 <S**2>=5.311
84A -> 92A	0.73088
87A -> 93A	0.13891
88A -> 95A	0.25093
89A -> 95A	-0.13405
90A -> 95A	0.14837
91A ->100A	-0.13786
85B -> 90B	0.13363
85B -> 91B	-0.11625
86B -> 91B	0.10930
87B -> 89B	0.22521
87B -> 92B	-0.12830
87B -> 93B	-0.29800
88B -> 99B	0.10336
Excited State 30: 4.989-A	4.4078 eV 281.28 nm f=0.0153 <S**2>=5.973
87A -> 95A	0.44826
88A -> 93A	-0.30650
89A -> 93A	0.11554
90A -> 93A	-0.13985
91A -> 99A	-0.30776
91A ->103A	0.10897
85B -> 89B	0.22450
85B -> 90B	-0.11629
85B -> 92B	-0.25839
86B -> 93B	-0.44387
87B -> 89B	-0.11604
87B -> 90B	-0.16227
87B -> 91B	-0.14352
87B -> 94B	0.17923

**2) Compound 8 high spin (S = 5/2):**

Excited State 1: 6.010-A 1.1414 eV 1086.29 nm f=0.0003 <S\*\*2>=8.780  
83A -> 94A 0.16634  
84A -> 94A 0.11011  
91A -> 94A 0.47082  
91A -> 96A -0.15863  
92A -> 94A 0.80004  
92A -> 96A -0.20674

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

Total Energy, E(TD-HF/TD-KS) = -1929.06320358

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

Excited State 2: 6.021-A 1.6064 eV 771.81 nm f=0.0073 <S\*\*2>=8.815  
92A -> 93A 0.98327

Excited State 3: 6.002-A 2.3977 eV 517.09 nm f=0.0002 <S\*\*2>=8.757  
86A -> 94A 0.23108  
88A -> 94A -0.13194  
89A -> 94A 0.30701  
90A -> 94A 0.80513  
90A -> 96A -0.25730  
91A -> 94A -0.20566  
92A -> 94A 0.12852

Excited State 4: 6.005-A 2.4655 eV 502.88 nm f=0.0012 <S\*\*2>=8.764  
84A -> 94A -0.12441  
88A -> 94A 0.52763  
88A -> 96A -0.18181  
89A -> 94A 0.62903  
89A -> 96A -0.19786  
90A -> 94A -0.25172  
91A -> 94A -0.27287  
92A -> 94A 0.19456

Excited State 5: 6.003-A 2.4866 eV 498.61 nm f=0.0001 <S\*\*2>=8.758  
86A -> 94A 0.86813  
86A -> 96A -0.29866  
86A -> 98A 0.10736  
88A -> 94A 0.11856  
89A -> 94A -0.21161  
90A -> 94A -0.18066

Excited State 6: 6.013-A 2.5939 eV 477.99 nm f=0.0100 <S\*\*2>=8.789  
83A -> 94A 0.15165  
86A -> 94A 0.16484  
88A -> 94A 0.19863  
89A -> 94A 0.29813  
89A -> 96A -0.11742  
90A -> 94A 0.11191  
91A -> 94A 0.61123  
91A -> 96A -0.14430  
92A -> 94A -0.52504  
92A -> 96A -0.28967

Excited State 7: 6.023-A 2.7999 eV 442.82 nm f=0.0091 <S\*\*2>=8.818  
91A -> 93A 0.10600  
91A -> 94A 0.16099

92A -> 95A	0.75396
92A -> 96A	0.37752
92A -> 97A	-0.25174
92A -> 98A	0.13740
83B -> 88B	-0.18827
84B -> 88B	0.13061
87B -> 88B	-0.29825
Excited State 8: 6.025-A	2.8636 eV 432.96 nm f=0.0068 <S**2>=8.825
91A -> 94A	-0.22425
92A -> 95A	0.63116
92A -> 96A	-0.60550
92A -> 97A	0.19898
92A -> 98A	-0.10131
83B -> 88B	0.13802
84B -> 88B	-0.10168
87B -> 88B	0.26603
Excited State 9: 6.017-A	2.9873 eV 415.04 nm f=0.0568 <S**2>=8.800
91A -> 94A	0.17880
92A -> 95A	0.13829
92A -> 96A	0.54309
92A -> 97A	0.34917
92A -> 98A	-0.14206
83B -> 88B	0.13536
84B -> 88B	-0.10388
87B -> 88B	0.66865
Excited State 10: 6.055-A	3.0954 eV 400.54 nm f=0.0313 <S**2>=8.915
91A -> 93A	-0.32670
91A -> 94A	0.11955
92A -> 96A	0.13438
92A -> 97A	0.65346
92A -> 98A	-0.13100
83B -> 88B	0.22195
84B -> 88B	-0.11339
87B -> 88B	-0.52838
Excited State 11: 6.086-A	3.2147 eV 385.68 nm f=0.0316 <S**2>=9.010
91A -> 93A	0.88175
92A -> 93A	0.10066
92A -> 97A	0.20992
83B -> 88B	0.23369
84B -> 88B	-0.14652
87B -> 88B	-0.19794
Excited State 12: 6.032-A	3.3145 eV 374.07 nm f=0.0006 <S**2>=8.846
92A -> 97A	0.36573
92A -> 98A	0.88044
83B -> 88B	-0.15209
84B -> 88B	0.10095
Excited State 13: 6.568-A	3.6088 eV 343.56 nm f=0.0010 <S**2>=10.536
87A -> 95A	0.38714
88A -> 94A	-0.27282
88A -> 96A	-0.25626

89A -> 94A	0.17940				
89A -> 96A	0.17543				
90A -> 94A	-0.14283				
90A -> 96A	-0.16693				
92A -> 98A	0.11450				
83B -> 94B	0.10664				
84B -> 88B	0.14390				
85B -> 93B	-0.15159				
86B -> 93B	-0.33220				
87B -> 88B	0.18649				
87B -> 90B	0.10196				
87B -> 91B	0.27319				
87B -> 93B	-0.13818				
87B -> 94B	-0.37402				
Excited State 14:	6.027-A	3.6408 eV	340.54 nm	f=0.0549	$\langle S^{*2} \rangle = 8.832$
92A -> 97A	-0.15922				
92A -> 98A	0.14898				
83B -> 88B	0.19548				
84B -> 88B	-0.24581				
85B -> 88B	-0.11893				
86B -> 88B	0.89382				
Excited State 15:	6.030-A	3.6720 eV	337.65 nm	f=0.1725	$\langle S^{*2} \rangle = 8.839$
91A -> 93A	0.11682				
92A -> 97A	0.30002				
92A -> 98A	-0.27503				
82B -> 89B	0.11943				
83B -> 88B	-0.41149				
84B -> 88B	0.64050				
86B -> 88B	0.40203				
Excited State 16:	6.018-A	3.7119 eV	334.01 nm	f=0.0015	$\langle S^{*2} \rangle = 8.805$
85B -> 88B	0.98479				
86B -> 88B	0.12200				
Excited State 17:	6.026-A	3.8245 eV	324.18 nm	f=0.0253	$\langle S^{*2} \rangle = 8.828$
92A -> 97A	-0.11974				
83B -> 88B	0.72527				
84B -> 88B	0.63597				
Excited State 18:	6.088-A	3.9819 eV	311.37 nm	f=0.0046	$\langle S^{*2} \rangle = 9.016$
91A -> 100A	0.17220				
91A -> 101A	0.15675				
92A -> 99A	-0.46016				
92A -> 100A	0.62479				
92A -> 101A	0.45950				
85B -> 90B	0.13366				
85B -> 92B	-0.13808				
Excited State 19:	6.080-A	4.0005 eV	309.92 nm	f=0.0092	$\langle S^{*2} \rangle = 8.991$
91A -> 100A	0.12061				
91A -> 101A	-0.10628				
91A -> 102A	-0.15200				
92A -> 99A	0.52811				
92A -> 100A	0.58949				



92A ->101A	-0.35631
92A ->102A	-0.25893
92A ->104A	-0.14697
85B -> 92B	-0.13909
Excited State 20: 6.033-A	4.0517 eV 306.00 nm f=0.0009 <S**2>=8.848
88A -> 93A	-0.18759
89A -> 93A	0.10055
90A -> 93A	0.96691
Excited State 21: 6.096-A	4.1295 eV 300.24 nm f=0.0004 <S**2>=9.041
88A -> 93A	0.15380
89A -> 93A	0.47550
92A -> 99A	0.31754
92A ->100A	0.18698
92A ->101A	0.17011
92A ->102A	0.65808
82B -> 88B	0.11093
83B -> 89B	-0.11514
87B -> 89B	-0.13364
Excited State 22: 6.186-A	4.1405 eV 299.44 nm f=0.0044 <S**2>=9.318
83A -> 93A	-0.10065
84A -> 93A	0.12443
88A -> 93A	0.20387
89A -> 93A	0.64957
92A -> 99A	-0.25688
92A ->100A	-0.14695
92A ->101A	-0.10689
92A ->102A	-0.44001
82B -> 88B	0.14988
83B -> 89B	-0.20988
84B -> 89B	0.13075
87B -> 89B	-0.23956
Excited State 23: 6.296-A	4.2086 eV 294.60 nm f=0.0005 <S**2>=9.660
82A -> 93A	0.18984
83A -> 93A	0.10308
84A -> 93A	-0.22530
88A -> 93A	0.22557
89A -> 93A	0.17518
91A -> 93A	0.16699
91A -> 95A	0.24280
91A -> 96A	0.36672
92A ->104A	0.10408
82B -> 88B	0.32925
82B -> 89B	-0.18805
83B -> 89B	0.34013
84B -> 89B	-0.19334
87B -> 89B	0.39759
Excited State 24: 6.044-A	4.2307 eV 293.06 nm f=0.0002 <S**2>=8.882
92A -> 99A	0.44265
92A ->100A	-0.17054
92A ->101A	0.35441
92A ->102A	-0.28640

92A ->103A	0.67492				
Excited State 25:	6.167-A	4.2715 eV	290.26 nm	f=0.0075	<S**2>=9.257
82A -> 93A	-0.11436				
84A -> 93A	0.11177				
88A -> 93A	-0.10630				
88A -> 95A	0.11144				
91A -> 94A	0.12740				
91A -> 95A	0.67578				
91A -> 96A	0.42297				
91A -> 97A	-0.11101				
92A ->101A	-0.12192				
92A ->103A	-0.12712				
82B -> 88B	-0.26838				
82B -> 89B	0.11480				
83B -> 89B	-0.13570				
87B -> 89B	-0.20369				
87B -> 93B	0.14465				
Excited State 26:	6.159-A	4.2971 eV	288.53 nm	f=0.0055	<S**2>=9.232
87A -> 95A	0.10051				
88A -> 95A	-0.15074				
89A -> 95A	0.10035				
91A -> 94A	0.20458				
91A -> 95A	-0.50778				
91A -> 96A	0.68591				
92A ->100A	0.11875				
82B -> 88B	-0.13919				
86B -> 93B	-0.10414				
87B -> 93B	-0.18190				
Excited State 27:	6.519-A	4.3607 eV	284.32 nm	f=0.0002	<S**2>=10.373
87A -> 94A	-0.20000				
87A -> 95A	0.11438				
87A -> 96A	-0.17035				
88A -> 94A	0.10696				
88A -> 95A	0.34969				
89A -> 95A	-0.26414				
90A -> 95A	0.27897				
91A -> 95A	-0.36069				
92A ->104A	0.11506				
83B -> 93B	-0.11574				
86B -> 91B	-0.14105				
86B -> 94B	0.16507				
87B -> 90B	-0.13573				
87B -> 91B	0.11241				
87B -> 93B	0.53729				
Excited State 28:	6.075-A	4.3698 eV	283.73 nm	f=0.0046	<S**2>=8.976
88A -> 94A	0.12029				
91A -> 96A	-0.19707				
92A ->100A	0.23922				
92A ->101A	-0.20643				
92A ->103A	0.14614				
92A ->104A	0.80763				
85B -> 89B	-0.10161				

85B -> 92B 0.13833  
87B -> 93B -0.10291

Excited State 29: 6.536-A 4.4026 eV 281.61 nm f=0.0091 <S\*\*2>=10.429

87A -> 95A 0.50324  
88A -> 94A 0.31953  
89A -> 94A -0.22241  
90A -> 94A 0.17617  
91A -> 95A 0.24243  
92A -> 104A -0.18541  
85B -> 93B -0.19669  
86B -> 93B -0.44584  
87B -> 91B -0.21730  
87B -> 94B 0.21677

Excited State 30: 6.050-A 4.4982 eV 275.63 nm f=0.0036 <S\*\*2>=8.901

91A -> 97A 0.54315  
91A -> 98A 0.13164  
92A -> 99A -0.22069  
92A -> 101A -0.42778  
92A -> 102A 0.30928  
92A -> 103A 0.36994  
92A -> 104A -0.13845  
92A -> 105A 0.16611  
92A -> 106A 0.15431  
82B -> 88B 0.16960  
87B -> 89B -0.16126

### 3) Compound 8 Structure A CH2 backbone (S=2)

Excited State 1: 5.022-A 1.1997 eV 1033.49 nm f=0.0005 <S\*\*2>=6.055

84A -> 95A 0.20540  
91A -> 95A -0.13590  
92A -> 95A 0.90280  
92A -> 97A -0.12615  
92A -> 98A 0.25277

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

Total Energy, E(TD-HF/TD-KS) = -1929.66701545

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

Excited State 2: 5.107-A 1.3831 eV 896.41 nm f=0.0066 <S\*\*2>=6.270

92A -> 93A 0.99405

Excited State 3: 5.117-A 1.9306 eV 642.20 nm f=0.0006 <S\*\*2>=6.296

92A -> 94A 0.99535

Excited State 4: 5.117-A 2.3969 eV 517.26 nm f=0.0005 <S\*\*2>=6.295

86A -> 95A 0.19676  
89A -> 95A -0.18719  
90A -> 95A 0.74373  
90A -> 97A -0.12142  
90A -> 98A 0.22021  
91A -> 93A 0.22555  
88B -> 89B -0.44495

Excited State 5: 5.203-A 2.4567 eV 504.67 nm f=0.0061 <S\*\*2>=6.519

86A -> 95A	0.30768
86A -> 98A	0.10426
89A -> 95A	0.19197
90A -> 95A	0.31964
91A -> 93A	-0.17248
91A -> 95A	0.44273
91A -> 98A	0.12881
88B -> 89B	0.65857
Excited State 6: 5.114-A	2.4900 eV 497.93 nm f=0.0116 <S**2>=6.289
86A -> 95A	0.13139
87A -> 95A	-0.25987
88A -> 95A	-0.13356
89A -> 95A	0.42674
89A -> 98A	0.13882
90A -> 95A	-0.26384
91A -> 95A	0.52591
91A -> 98A	0.13636
88B -> 89B	-0.50163
Excited State 7: 5.005-A	2.5658 eV 483.21 nm f=0.0010 <S**2>=6.012
86A -> 95A	0.53454
86A -> 98A	0.17900
87A -> 95A	0.66605
87A -> 97A	-0.11308
87A -> 98A	0.21835
88A -> 95A	0.21330
89A -> 95A	0.19927
90A -> 95A	-0.16642
Excited State 8: 5.088-A	2.8103 eV 441.17 nm f=0.0927 <S**2>=6.222
90A -> 93A	0.37882
91A -> 93A	0.84938
88B -> 89B	0.27318
Excited State 9: 5.040-A	2.8487 eV 435.23 nm f=0.0099 <S**2>=6.100
89A -> 93A	-0.26024
90A -> 93A	0.89179
91A -> 93A	-0.34036
Excited State 10: 5.486-A	3.1368 eV 395.26 nm f=0.0053 <S**2>=7.273
91A -> 94A	-0.27385
87B -> 90B	-0.12062
88B -> 90B	0.93711
Excited State 11: 5.241-A	3.1845 eV 389.33 nm f=0.0068 <S**2>=6.618
89A -> 95A	0.11625
92A -> 95A	-0.20505
92A -> 96A	0.80366
92A -> 97A	-0.38192
92A -> 98A	0.18625
88B -> 92B	-0.14454
88B -> 95B	-0.10345
Excited State 12: 5.086-A	3.2682 eV 379.37 nm f=0.0004 <S**2>=6.216
89A -> 94A	0.12179

90A -> 94A	0.11300				
91A -> 94A	0.93547				
88B -> 90B	0.27607				
Excited State 13:	5.261-A	3.2736 eV	378.74 nm	f=0.0037	<S**2>=6.669
88A -> 96A	0.11488				
89A -> 95A	-0.13295				
91A -> 95A	0.11825				
92A -> 95A	0.14519				
92A -> 96A	0.55456				
92A -> 97A	0.67820				
92A -> 98A	-0.20421				
86B -> 94B	0.10836				
87B -> 95B	0.10148				
88B -> 92B	0.13405				
88B -> 95B	0.12157				
Excited State 14:	5.416-A	3.4117 eV	363.41 nm	f=0.0054	<S**2>=7.082
89A -> 93A	0.17716				
91A -> 93A	-0.10460				
92A -> 97A	-0.14362				
87B -> 89B	0.94589				
88B -> 89B	0.10328				
Excited State 15:	5.284-A	3.4310 eV	361.36 nm	f=0.0015	<S**2>=6.731
88A -> 96A	-0.15597				
89A -> 93A	-0.15859				
89A -> 95A	0.17487				
89A -> 97A	0.10140				
91A -> 95A	-0.15674				
92A -> 95A	-0.10291				
92A -> 97A	0.54178				
92A -> 98A	0.53502				
86B -> 94B	-0.15837				
87B -> 89B	0.19850				
87B -> 95B	-0.14219				
88B -> 91B	-0.10322				
88B -> 92B	-0.25327				
88B -> 95B	-0.14935				
Excited State 16:	5.210-A	3.4485 eV	359.53 nm	f=0.0040	<S**2>=6.536
86A -> 93A	0.22265				
89A -> 93A	0.87630				
90A -> 93A	0.19284				
91A -> 93A	-0.17694				
92A -> 97A	0.12579				
92A -> 98A	0.16874				
87B -> 89B	-0.16164				
Excited State 17:	5.045-A	3.5015 eV	354.09 nm	f=0.0006	<S**2>=6.113
89A -> 94A	-0.16829				
90A -> 94A	0.97294				
Excited State 18:	5.260-A	3.5774 eV	346.57 nm	f=0.0109	<S**2>=6.667
87A -> 93A	0.14369				
88A -> 96A	0.19210				

89A -> 95A	-0.16635
89A -> 97A	-0.12477
89A -> 98A	0.11845
92A -> 95A	-0.21495
92A -> 98A	0.63938
86B -> 94B	0.20608
87B -> 95B	0.16327
88B -> 91B	0.24745
88B -> 92B	0.38198
88B -> 95B	0.13950
Excited State 19: 5.056-A	3.6113 eV 343.33 nm f=0.0006 <S**2>=6.140
86A -> 93A	0.36297
87A -> 93A	0.83675
88A -> 93A	0.33485
92A -> 98A	-0.13398
Excited State 20: 5.176-A	3.6674 eV 338.07 nm f=0.0015 <S**2>=6.449
88A -> 96A	-0.11588
89A -> 95A	0.12022
92A -> 98A	-0.11845
86B -> 94B	-0.10997
87B -> 91B	-0.15191
87B -> 92B	-0.11312
88B -> 91B	0.90807
Excited State 21: 5.166-A	3.7615 eV 329.61 nm f=0.0048 <S**2>=6.421
88A -> 96A	-0.14205
89A -> 95A	0.15454
86B -> 94B	-0.13754
87B -> 92B	-0.23646
88B -> 91B	-0.22774
88B -> 92B	0.82155
88B -> 93B	-0.16302
88B -> 95B	-0.20231
Excited State 22: 5.254-A	3.8487 eV 322.15 nm f=0.0026 <S**2>=6.650
86A -> 93A	0.81105
87A -> 93A	-0.18985
88A -> 93A	-0.33556
89A -> 93A	-0.22858
83B -> 89B	-0.12694
85B -> 89B	0.16521
86B -> 89B	0.17547
88B -> 93B	0.13422
Excited State 23: 5.341-A	3.8642 eV 320.86 nm f=0.0007 <S**2>=6.882
86A -> 93A	-0.19947
92A -> 101A	0.12596
85B -> 89B	0.53081
85B -> 93B	-0.10231
86B -> 89B	0.77871
Excited State 24: 5.300-A	3.9106 eV 317.05 nm f=0.0002 <S**2>=6.773
92A -> 101A	0.19400
92A -> 104A	-0.10700

85B -> 89B	0.74435				
85B -> 93B	-0.13332				
86B -> 89B	-0.59403				
Excited State 25:	5.619-A	3.9773 eV	311.73 nm	f=0.0012	<S**2>=7.644
79A -> 93A	0.18858				
80A -> 93A	0.13940				
83A -> 93A	-0.16835				
83A -> 94A	-0.49431				
86A -> 94A	-0.16286				
87A -> 94A	0.15729				
88A -> 94A	0.10446				
89A -> 93A	-0.11003				
89A -> 94A	-0.10500				
91A -> 93A	-0.10446				
80B -> 89B	-0.15601				
81B -> 89B	-0.20044				
83B -> 89B	0.13203				
83B -> 90B	0.51391				
87B -> 90B	0.40107				
88B -> 90B	0.11756				
Excited State 26:	5.341-A	3.9872 eV	310.96 nm	f=0.0019	<S**2>=6.881
89A -> 94A	0.92360				
90A -> 94A	0.14260				
91A -> 94A	-0.15253				
83B -> 89B	0.10370				
Excited State 27:	5.339-A	4.0089 eV	309.27 nm	f=0.0091	<S**2>=6.875
86A -> 95A	-0.27443				
87A -> 95A	0.25650				
88A -> 95A	0.15877				
88A -> 96A	-0.12683				
89A -> 94A	0.19074				
89A -> 95A	-0.20403				
91A -> 95A	0.44460				
92A -> 95A	0.10667				
92A -> 98A	0.15878				
92A -> 99A	-0.22468				
92A ->101A	-0.26180				
92A ->102A	-0.14477				
92A ->103A	0.28909				
84B -> 89B	0.31332				
85B -> 91B	0.10348				
86B -> 94B	-0.15248				
Excited State 28:	5.272-A	4.0280 eV	307.81 nm	f=0.0009	<S**2>=6.699
92A -> 99A	0.22374				
92A ->101A	0.33848				
92A ->102A	0.10132				
92A ->103A	-0.19862				
84B -> 89B	0.82801				
85B -> 89B	-0.13404				
88B -> 93B	-0.12231				
Excited State 29:	5.306-A	4.0487 eV	306.23 nm	f=0.0049	<S**2>=6.789

86A -> 95A	-0.22433
87A -> 95A	0.21261
88A -> 95A	0.17147
89A -> 95A	-0.17976
91A -> 95A	0.32963
92A -> 98A	0.11596
92A -> 99A	0.27964
92A ->100A	0.11198
92A ->101A	0.44231
92A ->102A	0.11217
92A ->103A	-0.20698
92A ->104A	-0.10681
84B -> 89B	-0.38213
85B -> 89B	-0.15912
85B -> 91B	-0.10884
85B -> 93B	-0.10360
88B -> 94B	-0.15670

Excited State 30: 5.397-A 4.0576 eV 305.56 nm f=0.0069 <S\*\*2>=7.033

87A -> 93A	-0.18300
88A -> 93A	0.45989
89A -> 96A	0.18860
90A -> 96A	0.10796
91A -> 96A	-0.17698
92A -> 99A	0.12166
92A ->101A	0.14193
87B -> 94B	0.16142
88B -> 93B	0.60086
88B -> 94B	0.38172

#### 4) Compound 10 broken symmetry (S = 1)

Excited State 1: 3.249-A 1.5652 eV 792.12 nm f=0.0081 <S\*\*2>=2.389

92B -> 93B	0.95149
92B -> 94B	0.25237

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

Total Energy, E(TD-HF/TD-KS) = -1940.49860814

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

Excited State 2: 3.234-A 1.6866 eV 735.13 nm f=0.0064 <S\*\*2>=2.365

85A -> 96A	0.10018
89A -> 96A	-0.10066
94A -> 96A	-0.29910
92B -> 93B	-0.22118
92B -> 94B	0.86186
92B -> 95B	0.19471

Excited State 3: 3.509-A 1.7321 eV 715.81 nm f=0.0048 <S\*\*2>=2.829

82A -> 96A	-0.10470
83A -> 96A	0.11528
85A -> 96A	-0.21684
86A -> 96A	0.10266
88A -> 96A	-0.19320
89A -> 96A	0.25276
91A -> 96A	-0.19072
91A -> 97A	-0.12431



92A -> 96A -0.19839  
94A -> 96A 0.70497  
94A -> 97A 0.10047  
92B -> 93B -0.15036  
92B -> 94B 0.34010

Excited State 4: 3.662-A 1.9455 eV 637.29 nm f=0.0024 <S\*\*2>=3.102

83A -> 96A -0.21502  
84A -> 96A -0.14223  
86A -> 96A 0.35421  
88A -> 96A 0.15518  
89A -> 96A -0.32264  
89A -> 97A 0.10755  
91A -> 96A -0.43545  
92A -> 96A -0.19452  
93A -> 96A 0.55875  
94A -> 96A -0.13775  
94A -> 97A 0.10587  
92B -> 95B 0.10260  
92B -> 97B 0.10095

Excited State 5: 3.285-A 2.0107 eV 616.62 nm f=0.0299 <S\*\*2>=2.447

92B -> 94B -0.20597  
92B -> 95B 0.94867

Excited State 6: 3.589-A 2.2366 eV 554.35 nm f=0.0065 <S\*\*2>=2.970

83A -> 97A 0.13011  
84A -> 96A 0.11574  
84A -> 97A -0.12304  
85A -> 97A -0.20231  
87A -> 96A 0.15606  
88A -> 97A -0.19290  
89A -> 97A 0.27898  
91A -> 96A 0.10666  
91A -> 97A -0.20004  
92A -> 96A 0.10257  
92A -> 97A -0.24561  
94A -> 95A 0.12405  
94A -> 97A 0.69090  
94A -> 98A -0.10562  
92B -> 96B 0.20740

Excited State 7: 3.557-A 2.3670 eV 523.79 nm f=0.0188 <S\*\*2>=2.913

89A -> 97A -0.12390  
94A -> 97A -0.18803  
92B -> 96B 0.91896

Excited State 8: 3.690-A 2.5492 eV 486.37 nm f=0.0017 <S\*\*2>=3.155

83A -> 97A 0.13967  
84A -> 97A 0.26985  
87A -> 97A 0.34082  
88A -> 97A -0.11296  
89A -> 97A 0.22419  
91A -> 97A 0.46056  
92A -> 97A 0.26927  
93A -> 96A -0.10211

93A -> 97A	-0.34734
94A -> 95A	0.18513
94A -> 96A	0.23415
94A -> 97A	0.10379
92B -> 96B	0.12359
92B -> 97B	-0.12763
92B -> 98B	-0.22472
92B -> 100B	-0.15592

Excited State 9: 3.415-A 2.6397 eV 469.68 nm f=0.0316 <S\*\*2>=2.665

89A -> 95A	0.12507
92A -> 95A	-0.19664
93A -> 97A	0.11335
94A -> 95A	0.90607
92B -> 96B	-0.11723
92B -> 98B	0.10200

Excited State 10: 3.590-A 2.6492 eV 468.00 nm f=0.0027 <S\*\*2>=2.973

84A -> 96A	-0.14253
84A -> 97A	0.11800
85A -> 97A	-0.10165
86A -> 96A	-0.16333
86A -> 97A	0.21522
87A -> 96A	-0.28323
87A -> 97A	0.27466
92A -> 96A	-0.15378
93A -> 96A	-0.25175
93A -> 97A	0.12919
94A -> 96A	-0.13555
94A -> 97A	0.18035
92B -> 97B	0.66204
92B -> 98B	-0.23012

Excited State 11: 3.514-A 2.6911 eV 460.71 nm f=0.0019 <S\*\*2>=2.837

84A -> 97A	-0.18123
85A -> 97A	0.14472
86A -> 97A	-0.35220
87A -> 96A	0.17007
87A -> 97A	-0.42949
89A -> 97A	0.10291
91A -> 96A	0.13397
92A -> 96A	0.15221
93A -> 97A	-0.27297
92B -> 97B	0.53919
92B -> 98B	-0.27782

Excited State 12: 3.633-A 2.7652 eV 448.37 nm f=0.0037 <S\*\*2>=3.049

84A -> 96A	0.19331
84A -> 97A	0.10836
86A -> 96A	0.15062
86A -> 97A	0.24331
87A -> 96A	0.42572
87A -> 97A	0.26720
89A -> 97A	-0.12070
91A -> 96A	0.29557
92A -> 96A	0.34582

93A -> 96A	0.40815
93A -> 97A	0.23463
94A -> 97A	-0.10008
92B -> 97B	0.28263
Excited State 13: 3.562-A	2.8868 eV 429.49 nm f=0.0113 <S**2>=2.921
86A -> 96A	-0.12342
93A -> 95A	0.92878
93A -> 96A	0.16343
92B -> 98B	-0.17810
Excited State 14: 3.537-A	2.9587 eV 419.05 nm f=0.0117 <S**2>=2.878
91A -> 97A	0.14238
92A -> 97A	0.11565
93A -> 95A	0.19887
93A -> 97A	-0.22293
94A -> 96A	0.12455
92B -> 96B	0.10457
92B -> 97B	0.27254
92B -> 98B	0.77886
92B -> 99B	-0.11714
92B -> 100B	0.27479
Excited State 15: 3.730-A	3.0917 eV 401.02 nm f=0.0463 <S**2>=3.227
87A -> 96A	-0.11600
88A -> 95A	-0.14071
89A -> 95A	-0.16703
92A -> 95A	0.85269
92A -> 96A	0.14941
94A -> 95A	0.24067
94A -> 96A	0.11313
92B -> 100B	0.10498
Excited State 16: 3.904-A	3.0956 eV 400.52 nm f=0.0055 <S**2>=3.561
83A -> 96A	0.12945
84A -> 96A	-0.12182
85A -> 96A	0.13073
86A -> 96A	-0.40405
87A -> 96A	-0.32149
89A -> 96A	0.27917
91A -> 96A	0.29559
93A -> 95A	-0.23507
93A -> 96A	0.60842
93A -> 97A	-0.13192
94A -> 97A	0.10126
Excited State 17: 3.962-A	3.2260 eV 384.32 nm f=0.0043 <S**2>=3.674
84A -> 96A	-0.10841
85A -> 96A	0.19948
86A -> 96A	-0.15628
87A -> 96A	-0.30368
88A -> 96A	0.23288
89A -> 96A	-0.36951
91A -> 96A	-0.12355
92A -> 95A	-0.20046
92A -> 96A	0.58043

94A -> 95A	-0.11571				
94A -> 96A	0.40302				
Excited State 18:	3.641-A	3.3543 eV	369.63 nm	f=0.0376	<S**2>=3.064
87A -> 96A	-0.12527				
91A -> 95A	0.71381				
90B -> 93B	-0.11707				
91B -> 93B	0.24144				
92B -> 99B	0.50188				
Excited State 19:	3.708-A	3.3559 eV	369.45 nm	f=0.0178	<S**2>=3.188
90A -> 99A	0.10064				
91A -> 95A	-0.45304				
92A -> 95A	0.10521				
92B -> 98B	0.16398				
92B -> 99B	0.78958				
92B -> 101B	-0.11066				
Excited State 20:	3.728-A	3.4146 eV	363.10 nm	f=0.0047	<S**2>=3.225
89A -> 95A	0.14974				
91A -> 95A	-0.18529				
91A -> 96A	0.11298				
91B -> 93B	0.86900				
91B -> 96B	0.13973				
92B -> 99B	-0.15657				
Excited State 21:	3.944-A	3.4581 eV	358.53 nm	f=0.0136	<S**2>=3.639
89A -> 95A	0.29193				
90A -> 99A	0.21028				
91A -> 95A	0.21010				
91A -> 96A	0.22346				
91A -> 97A	0.22029				
91A -> 100A	0.12094				
92A -> 96A	-0.14630				
92A -> 97A	-0.15920				
92A -> 100A	-0.15365				
88B -> 99B	-0.20257				
89B -> 94B	-0.12982				
89B -> 96B	-0.10160				
89B -> 97B	-0.14934				
89B -> 98B	-0.16614				
89B -> 100B	0.11268				
90B -> 93B	-0.27587				
91B -> 93B	-0.24561				
92B -> 98B	-0.11700				
92B -> 100B	0.46275				
Excited State 22:	3.596-A	3.4729 eV	357.01 nm	f=0.0017	<S**2>=2.982
91B -> 94B	0.96169				
91B -> 95B	0.10694				
Excited State 23:	3.651-A	3.4980 eV	354.44 nm	f=0.0343	<S**2>=3.082
86A -> 96A	-0.10054				
88A -> 95A	-0.13124				
89A -> 95A	-0.15400				
91A -> 95A	0.12695				

92A -> 95A	-0.11090
93A -> 97A	-0.10940
90B -> 93B	0.67201
90B -> 94B	0.10458
90B -> 96B	0.11129
91B -> 93B	0.15460
92B -> 97B	-0.10228
92B -> 98B	-0.13916
92B -> 100B	0.52586
92B -> 101B	0.20884
Excited State 24: 3.711-A	3.5260 eV 351.63 nm f=0.0409 <S**2>=3.192
88A -> 95A	0.16039
89A -> 95A	0.31089
91A -> 95A	0.19234
91A -> 97A	0.12204
92A -> 95A	0.11003
93A -> 97A	0.21169
90B -> 93B	0.56376
90B -> 94B	0.15798
91B -> 93B	-0.12505
92B -> 98B	0.10130
92B -> 99B	-0.14306
92B -> 100B	-0.38052
92B -> 101B	-0.28371
Excited State 25: 3.610-A	3.5558 eV 348.68 nm f=0.0037 <S**2>=3.008
86A -> 96A	0.13803
91A -> 95A	-0.12679
90B -> 94B	0.92370
90B -> 95B	0.17112
Excited State 26: 3.992-A	3.6031 eV 344.10 nm f=0.0018 <S**2>=3.734
84A -> 97A	-0.11917
85A -> 97A	0.12378
86A -> 97A	-0.27718
87A -> 97A	-0.13093
89A -> 95A	-0.11644
89A -> 97A	0.17606
91A -> 97A	0.33131
92A -> 96A	-0.11583
92A -> 97A	0.29726
93A -> 97A	0.68618
92B -> 101B	0.17587
Excited State 27: 3.887-A	3.6626 eV 338.51 nm f=0.0085 <S**2>=3.527
86A -> 96A	0.10016
88A -> 95A	-0.11730
88A -> 96A	0.24004
89A -> 95A	-0.23560
89A -> 96A	-0.29069
91A -> 96A	0.45427
91A -> 97A	-0.11074
92A -> 95A	-0.10689
92A -> 96A	-0.36789
92A -> 97A	-0.11815

93A -> 97A	-0.10859
94A -> 96A	0.20521
90B -> 93B	0.13709
90B -> 94B	-0.14819
91B -> 95B	0.22276
92B -> 98B	0.11392
92B ->100B	-0.28356
92B ->101B	0.18973

Excited State 28: 3.891-A 3.6921 eV 335.81 nm f=0.0041 <S\*\*2>=3.536

86A -> 96A	0.20998
87A -> 96A	-0.22956
88A -> 95A	0.13592
88A -> 96A	0.10997
89A -> 95A	0.29092
89A -> 96A	0.13498
90A -> 99A	-0.13585
91A -> 95A	-0.19310
91A -> 96A	0.10167
91A -> 97A	-0.13583
92A -> 95A	0.17198
92A -> 96A	0.10034
92A -> 97A	0.22772
87B -> 95B	-0.10776
88B -> 99B	0.13651
89B -> 94B	0.14072
90B -> 93B	0.17662
90B -> 94B	-0.15772
90B -> 95B	0.23564
91B -> 95B	0.44948
92B ->100B	0.20037
92B ->101B	-0.11343

Excited State 29: 3.946-A 3.7190 eV 333.38 nm f=0.0004 <S\*\*2>=3.643

85A -> 96A	-0.16341
86A -> 96A	0.13905
87A -> 96A	-0.16720
88A -> 95A	-0.14053
89A -> 95A	-0.21416
89A -> 96A	0.28506
90A -> 99A	0.15956
91A -> 96A	-0.21470
91A -> 97A	0.17674
92A -> 95A	-0.16472
92A -> 96A	0.34210
92A -> 97A	-0.19640
94A -> 96A	-0.15372
88B -> 99B	-0.16046
89B -> 94B	-0.14160
90B -> 95B	0.13270
91B -> 95B	0.40983
91B -> 96B	0.10839
92B -> 98B	0.11949
92B ->100B	-0.17137
92B ->101B	0.15495

Excited State 30: 3.751-A 3.7656 eV 329.26 nm f=0.0031 <S\*\*2>=3.267  
89A -> 97A 0.13994  
90A -> 95A 0.89826  
90A -> 97A -0.10285  
92A -> 97A -0.24324  
94A -> 97A -0.17613

### 5) Compound 10 high spin (S=2)

Excited State 1: 5.010-A 0.2914 eV 4254.20 nm f=0.0005 <S\*\*2>=6.025  
95A -> 96A 0.99879

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

Total Energy, E(TD-HF/TD-KS) = -1939.70133905

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

Excited State 2: 5.014-A 0.5804 eV 2136.15 nm f=0.0019 <S\*\*2>=6.035  
95A -> 97A 0.99737

Excited State 3: 5.021-A 1.5219 eV 814.66 nm f=0.0057 <S\*\*2>=6.053  
95A -> 98A 0.99005

Excited State 4: 5.059-A 1.7346 eV 714.78 nm f=0.0007 <S\*\*2>=6.149  
93A -> 97A -0.15506  
94A -> 96A 0.97112

Excited State 5: 5.077-A 2.0393 eV 607.97 nm f=0.0040 <S\*\*2>=6.195  
89A -> 96A -0.13654  
93A -> 96A -0.66751  
94A -> 97A 0.71333

Excited State 6: 5.085-A 2.1031 eV 589.52 nm f=0.0031 <S\*\*2>=6.215  
92A -> 96A 0.11139  
93A -> 96A 0.70968  
94A -> 97A 0.64595  
91B -> 92B 0.20705

Excited State 7: 5.028-A 2.1613 eV 573.65 nm f=0.0157 <S\*\*2>=6.069  
94A -> 97A -0.17048  
95A -> 100A -0.11231  
90B -> 92B 0.33905  
91B -> 92B 0.90509

Excited State 8: 5.026-A 2.2060 eV 562.04 nm f=0.0135 <S\*\*2>=6.066  
93A -> 96A 0.10311  
90B -> 92B 0.92878  
91B -> 92B -0.32417

Excited State 9: 5.026-A 2.2515 eV 550.67 nm f=0.0003 <S\*\*2>=6.065  
89B -> 92B 0.99564

Excited State 10: 5.022-A 2.3288 eV 532.38 nm f=0.0030 <S\*\*2>=6.055  
95A -> 99A 0.99054

Excited State 11: 5.130-A 2.4535 eV 505.33 nm f=0.0019 <S\*\*2>=6.329  
92A -> 96A 0.16191  
92A -> 97A -0.14824

93A -> 97A	0.92412				
94A -> 96A	0.14537				
95A ->100A	-0.17803				
Excited State 12:	5.029-A	2.4811 eV	499.71 nm	f=0.0796	<S**2>=6.072
93A -> 97A	0.18141				
95A ->100A	0.93722				
91B -> 92B	0.11925				
91B -> 93B	0.12434				
Excited State 13:	5.026-A	2.4918 eV	497.57 nm	f=0.0003	<S**2>=6.065
88B -> 92B	0.99264				
Excited State 14:	5.138-A	2.5621 eV	483.91 nm	f=0.0115	<S**2>=6.351
92A -> 96A	0.88698				
92A -> 97A	-0.26078				
93A -> 97A	-0.17320				
94A -> 97A	-0.11827				
95A ->100A	0.11328				
90B -> 93B	0.12531				
91B -> 93B	-0.14798				
Excited State 15:	5.048-A	2.6079 eV	475.42 nm	f=0.0054	<S**2>=6.121
88A -> 96A	-0.10172				
88A -> 97A	0.11717				
89A -> 97A	-0.18898				
91A -> 96A	0.13995				
91A -> 97A	0.18544				
92A -> 96A	0.18961				
92A -> 97A	0.72960				
93A -> 97A	0.11579				
91B -> 93B	-0.52076				
Excited State 16:	5.207-A	2.6678 eV	464.74 nm	f=0.0010	<S**2>=6.527
91A -> 96A	0.60676				
92A -> 96A	-0.23775				
92A -> 97A	-0.39374				
90B -> 93B	0.23139				
91B -> 93B	-0.57928				
Excited State 17:	5.111-A	2.6813 eV	462.41 nm	f=0.0046	<S**2>=6.281
91A -> 96A	0.41004				
92A -> 97A	0.28263				
90B -> 93B	0.70945				
91B -> 93B	0.47083				
Excited State 18:	5.181-A	2.6951 eV	460.04 nm	f=0.0032	<S**2>=6.462
91A -> 96A	0.64910				
92A -> 96A	0.15018				
90B -> 93B	-0.64566				
91B -> 93B	0.33036				
Excited State 19:	5.037-A	2.7652 eV	448.37 nm	f=0.0005	<S**2>=6.092
89B -> 93B	0.99349				
Excited State 20:	5.323-A	2.8265 eV	438.66 nm	f=0.0013	<S**2>=6.833



89A -> 96A	0.53095				
90A -> 96A	0.76270				
93A -> 96A	-0.13083				
89B -> 94B	0.12012				
91B -> 94B	-0.20771				
Excited State 21:	5.096-A	2.8557 eV	434.16 nm	f=0.0034	<S**2>=6.242
88A -> 96A	-0.12385				
89A -> 96A	0.14624				
90A -> 96A	0.10190				
91A -> 97A	0.18505				
94A -> 98A	-0.10640				
89B -> 94B	0.15040				
90B -> 94B	-0.10413				
91B -> 94B	0.91381				
Excited State 22:	5.057-A	2.8836 eV	429.96 nm	f=0.0013	<S**2>=6.144
89B -> 94B	0.16990				
90B -> 94B	0.97354				
Excited State 23:	5.295-A	2.9055 eV	426.72 nm	f=0.0015	<S**2>=6.758
88A -> 96A	-0.12319				
89A -> 96A	0.59822				
90A -> 96A	-0.53401				
91A -> 97A	0.22905				
94A -> 98A	0.12656				
95A ->101A	0.20948				
87B -> 92B	-0.35960				
89B -> 94B	0.19858				
91B -> 94B	-0.17289				
Excited State 24:	5.104-A	2.9129 eV	425.64 nm	f=0.0036	<S**2>=6.262
89A -> 96A	0.37457				
90A -> 96A	-0.26832				
95A ->101A	-0.45710				
87B -> 92B	0.73860				
Excited State 25:	5.402-A	2.9429 eV	421.30 nm	f=0.0269	<S**2>=7.046
88A -> 96A	-0.26065				
89A -> 96A	-0.26252				
90A -> 96A	0.12923				
91A -> 97A	0.79654				
92A -> 97A	-0.18091				
94A -> 98A	0.10688				
95A ->101A	-0.14764				
87B -> 92B	0.15694				
89B -> 94B	0.10514				
90B -> 94B	-0.10631				
91B -> 94B	-0.18055				
91B -> 95B	-0.13540				
Excited State 26:	5.339-A	2.9915 eV	414.45 nm	f=0.0033	<S**2>=6.877
88A -> 96A	0.78359				
88A -> 97A	0.12400				
89A -> 96A	0.11979				
89A -> 97A	-0.17598				

91A -> 97A	0.36324				
89B -> 94B	-0.34627				
Excited State 27: 5.040-A	3.0092 eV	412.02 nm	f=0.0003	<S**2>=6.099	
88B -> 93B	0.99486				
Excited State 28: 5.129-A	3.0167 eV	410.99 nm	f=0.0146	<S**2>=6.326	
86A -> 96A	0.14408				
88A -> 96A	0.33259				
89A -> 96A	-0.15097				
94A -> 98A	-0.40455				
89B -> 94B	0.78425				
90B -> 94B	-0.10667				
91B -> 94B	-0.11599				
Excited State 29: 5.102-A	3.0582 eV	405.42 nm	f=0.0046	<S**2>=6.258	
88A -> 96A	0.23124				
89A -> 96A	-0.14621				
91A -> 97A	-0.10096				
94A -> 98A	0.86646				
86B -> 92B	-0.14410				
89B -> 94B	0.28594				
91B -> 94B	0.11166				
Excited State 30: 5.316-A	3.1180 eV	397.64 nm	f=0.0013	<S**2>=6.814	
88A -> 96A	0.20055				
88A -> 97A	-0.18414				
89A -> 97A	0.56910				
90A -> 97A	0.68447				
91A -> 97A	0.10927				
92A -> 97A	0.23416				
86B -> 92B	-0.15658				