Supporting Information

Influence of the Chelate Effect on the Electronic Structure of One-electron Oxidized Group 10 Metal(II)-(Disalicylidene)diamine Complexes

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1. Experimental Data

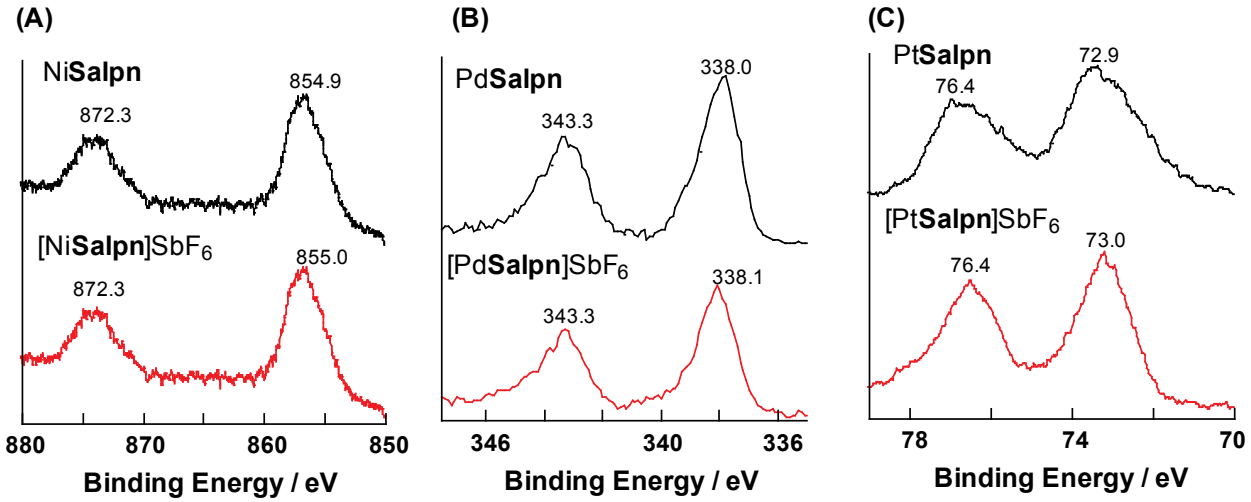

Figure S1. XPS of neutral and one-electron oxidized M**Salpn**; (A) Ni**Salpn**; (B) Pd**Salpn**; (C) Pt**Salpn**.

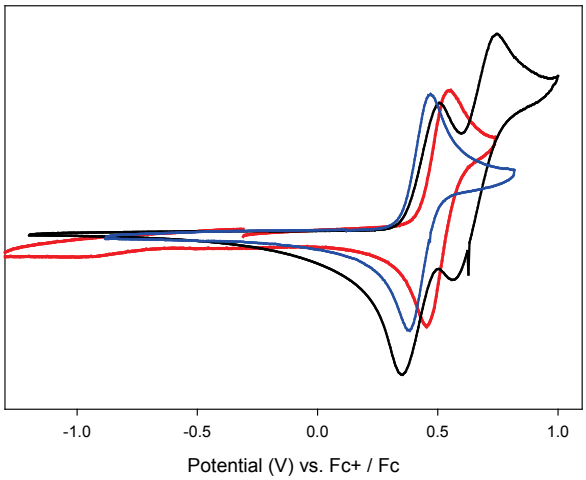

Figure S2. Cyclic Voltammograms of group 10 metal M**Salpn** complexes ; black line: Ni**Salpn** (**1**); red line: Pd**Salpn** (**2**); blue line: Pt**Salpn** (**3**). Conditions; 1 mM complex, 0.1 M NBu_4ClO_4 , scan rate 100 mV/s, CH_2Cl_2 , 298 K.

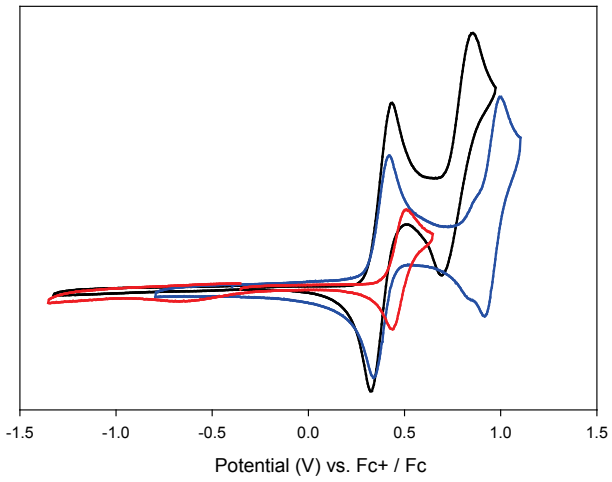

Figure S3. Cyclic Voltammograms of group 10 metal M**Salpn** complexes ; black line: Ni**Salpn** (**1**); red line: Pd**Salpn** (**2**); blue line: Pt**Salpn** (**3**). Conditions; 1 mM complex, 0.1 M NBu_4PF_6 , scan rate 100 mV/s, CH_2Cl_2 , 230 K.

Table S1. Redox potentials for **1**, **2**, and **3** versus Fc^+/Fc (1mM complex, 0.1M NBu_4PF_6, scan rate 100mV/s, CH_2Cl_2, 230 K), and the comproportionation constant (K_c) at 230 K.

Compound	$E_{1/2}^1$ (V)	$E_{1/2}^2$ (V)	ΔE_{ox} ($E_{1/2}^2$ - $E_{1/2}^1$) (V)	K_c
Ni(Salpn) (1)	0.38	0.77	0.39	3.5×10^8
Pd(Salpn) (2)	0.48	-	-	-
Pt(Salpn) (3)	0.39	0.97	0.57	3.1×10^{12}

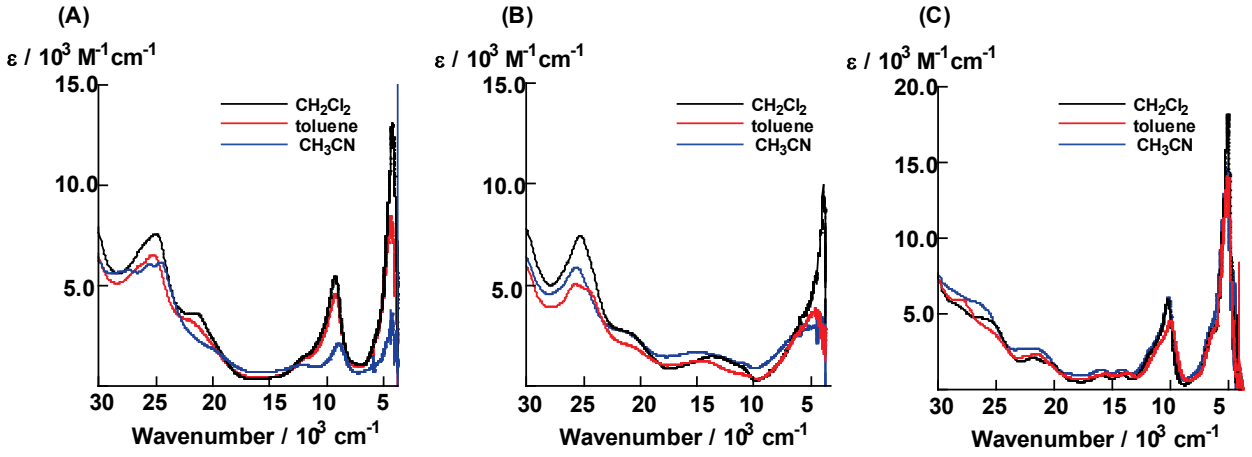

Figure S4 Solvent dependent electronic spectra of oxidized **Salpn** complexes (A) [**1**]$^+$, (B) [**2**]$^+$, and (C) [**3**]$^+$. Conditions for measurements: 0.5 mM, in a 2mm quartz cell at 298 K.

2. Calculation Data

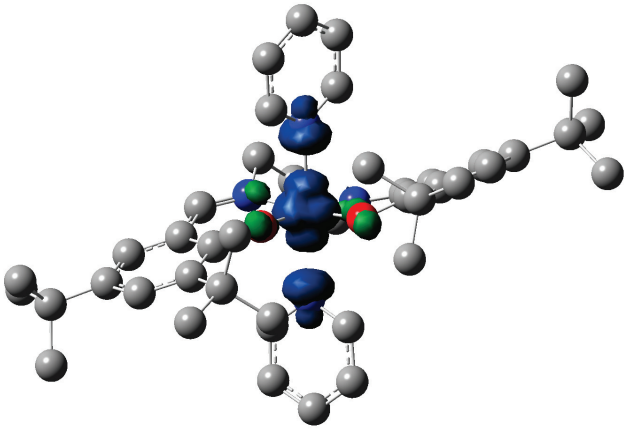

Figure S5 Calculated spin density for [**1**$(py)_2$]$^+$ showing showing ca. 93 % spin density on Ni.

Table S2. Calculated AOMIX[1] orbital breakdown for [**1**]$^+$.

Orbital	AOMIX Orbital Breakdown				
	% Ni	% O	% N	% phenyl rings	% periphery
α-manifold					
αLUMO (148)	54.15	10.51	14.79	5.29	15.25
αHOMO (147)	4.40	17.34	5.39	30.05	42.82
αHOMO-2 (145)	4.10	1.48	11.26	16.52	66.65
β-manifold					
βLUMO (147)	8.39	21.67	7.07	29.62	33.25
βHOMO (146)	2.59	15.71	4.34	35.54	41.82
βHOMO-2 (144)	5.21	0.52	11.25	46.09	36.94

Table S3. Calculated AOMIX[1] orbital breakdown for [**2**]$^+$.

Orbital	AOMIX Orbital Breakdown				
	% Pd	% O	% N	% phenyl rings	% periphery
α-manifold					
αLUMO (148)	1.30	3.27	17.75	37.51	40.17
αHOMO (147)	6.64	17.67	5.70	31.96	38.03
αHOMO-2 (145)	5.40	0.13	10.93	38.33	45.22
β-manifold					
βLUMO (147)	9.11	21.95	7.04	28.80	33.09
βHOMO (146)	2.08	16.35	4.68	36.00	40.89
βHOMO-2 (144)	6.87	0.16	11.16	39.60	42.21

Table S4. Calculated AOMIX[1] orbital breakdown for [**3**]$^+$.

Orbital	AOMIX Orbital Breakdown				
	% Pt	% O	% N	% phenyl rings	% periphery
α-manifold					
αLUMO (148)	1.49	2.96	17.28	37.76	40.51
αHOMO (147)	9.97	17.68	6.27	30.25	35.82
αHOMO-2 (145)	7.77	0.08	10.42	38.90	42.83
β-manifold					
βLUMO (147)	16.28	22.26	7.54	24.99	28.93
βHOMO (146)	2.65	15.82	4.30	36.14	41.10
βHOMO-2 (144)	13.15	0.17	7.65	37.20	41.01

a) TD-DFT excitation energies and oscillator strengths for [1]$^+$.

Excitation energies and oscillator strengths:
Excited State 1: 3.426-A -0.6763 eV -1833.21 nm f=-0.0000 <S**2>=2.684
139A -> 148A 0.10594
142A -> 148A 0.65128
142A -> 149A 0.18668
143A -> 148A 0.25829
140B -> 148B -0.25557
140B -> 150B -0.20399
141B -> 148B -0.31805
141B -> 150B -0.25537
142B -> 148B -0.40134
142B -> 150B -0.32732
142A <- 148A 0.24938
140B <- 148B -0.10530
141B <- 148B -0.12894
141B <- 150B -0.10393
142B <- 148B -0.15766
142B <- 150B -0.13261
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 3.322-A 0.4031 eV 3075.80 nm f=0.0006 <S**2>=2.508
121A -> 148A -0.14577
123A -> 148A -0.11733
128A -> 148A 0.13991
131A -> 148A -0.15666
133A -> 148A -0.18888
136A -> 148A 0.10274
140A -> 148A 0.60130
140A -> 149A 0.16855
141A -> 148A 0.10597
143A -> 148A 0.13134
145A -> 148A 0.23871
146A -> 148A 0.17228
147A -> 148A -0.26423
133B -> 148B 0.11246

139B -> 148B -0.28009
139B -> 150B -0.21250
140B -> 147B 0.10579
140B -> 148B -0.34878
140B -> 150B -0.28826
142B -> 148B 0.15133
142B -> 150B 0.11535
143B -> 148B 0.28062
143B -> 150B 0.22008
144B -> 148B -0.12969
145B -> 148B 0.28756
145B -> 150B 0.22367
146B -> 148B -0.11500
131A <- 148A -0.10170
133A <- 148A -0.12159
140A <- 148A 0.38067
140A <- 149A 0.10495
145A <- 148A 0.14368
147A <- 148A -0.14540
139B <- 148B -0.17936
139B <- 150B -0.13277
140B <- 148B -0.21848
140B <- 150B -0.18701
143B <- 148B 0.18036
143B <- 150B 0.13992
145B <- 148B 0.17936
145B <- 150B 0.13987

Excited State 3: 2.159-A 0.5210 eV 2379.89 nm f=0.1942 <S**2>=0.916
146B -> 147B 0.98708

Excited State 4: 3.129-A 0.8330 eV 1488.43 nm f=0.0013 <S**2>=2.198
121A -> 148A -0.12637
133A -> 148A -0.13027
138A -> 148A -0.13465
139A -> 148A 0.36886
139A -> 149A 0.10824
140A -> 148A -0.21515
141A -> 148A -0.24615
143A -> 148A 0.14471
144A -> 148A -0.21288
147A -> 148A -0.22494
139B -> 148B 0.28372
139B -> 150B 0.21431
140B -> 148B 0.12432
140B -> 150B 0.10426
141B -> 148B -0.20978
141B -> 150B -0.16967
143B -> 147B -0.15518
143B -> 148B 0.21938
143B -> 150B 0.17148
144B -> 148B 0.17274
144B -> 150B 0.14671
145B -> 147B -0.20263
145B -> 148B 0.17716
145B -> 150B 0.13043

146B -> 148B 0.10727
139A <- 148A 0.13770
139B <- 148B 0.10719

Excited State 5: 3.302-A 1.3110 eV 945.71 nm f=0.0005 <S**2>=2.476
105A -> 148A -0.21050
110A -> 148A 0.12621
115A -> 148A -0.19282
121A -> 148A 0.17287
128A -> 148A 0.12259
129A -> 148A -0.31068
130A -> 148A -0.19883
135A -> 148A -0.16859
139A -> 148A -0.11442
143A -> 148A 0.26499
147A -> 148A 0.11626
105B -> 148B 0.15902
105B -> 150B 0.13249
117B -> 148B 0.17533
117B -> 150B 0.14544
129B -> 148B 0.16441
129B -> 150B 0.13304
130B -> 148B 0.27443
130B -> 150B 0.22387
135B -> 148B 0.17580
135B -> 150B 0.14244
141B -> 147B -0.11791
142B -> 147B -0.15117
142B -> 148B -0.14144
142B -> 150B -0.10333
143B -> 148B 0.17720
143B -> 150B 0.14217
145B -> 147B 0.20253

Excited State 6: 2.280-A 1.3382 eV 926.49 nm f=0.0054 <S**2>=1.049
140B -> 147B -0.13521
141B -> 147B -0.29833
142B -> 147B -0.53958
143B -> 147B 0.20527
144B -> 147B 0.21973
145B -> 147B 0.61254

Excited State 7: 2.147-A 1.4372 eV 862.65 nm f=0.0351 <S**2>=0.903
142A -> 148A 0.13171
139B -> 147B 0.24180
140B -> 147B 0.25955
141B -> 147B -0.17606
144B -> 147B 0.81270
145B -> 147B -0.33828
146B -> 147B -0.11430

Excited State 8: 2.166-A 1.5031 eV 824.84 nm f=0.0104 <S**2>=0.923
140B -> 147B 0.28066
141B -> 147B 0.24158
142B -> 147B 0.63134
143B -> 147B 0.10294

144B -> 147B 0.20781
145B -> 147B 0.57411

Excited State 9: 2.160-A 1.7827 eV 695.47 nm f=0.0022 <S**2>=0.917
140A -> 148A -0.13468
129B -> 147B 0.11246
130B -> 147B 0.10044
135B -> 147B 0.11908
140B -> 147B 0.25097
141B -> 147B 0.30574
142B -> 147B -0.19403
143B -> 147B 0.79711
145B -> 147B -0.19627

Excited State 10: 2.129-A 1.9675 eV 630.16 nm f=0.0044 <S**2>=0.883
140A -> 148A -0.11165
142A -> 148A -0.34945
142A -> 149A -0.10522
143A -> 148A -0.12491
147A -> 148A -0.12850
139B -> 147B -0.33689
140B -> 147B -0.32044
140B -> 148B -0.15837
140B -> 150B -0.12511
141B -> 147B 0.41646
141B -> 148B -0.10561
142B -> 148B -0.23135
142B -> 150B -0.19526
144B -> 147B 0.44208

Excited State 11: 2.136-A 2.0512 eV 604.45 nm f=0.0017 <S**2>=0.891
139A -> 148A -0.16804
141A -> 148A 0.14833
143A -> 148A -0.11074
147A -> 148A 0.10907
139B -> 147B -0.10646
139B -> 148B 0.16998
139B -> 150B 0.11209
140B -> 147B -0.37306
141B -> 147B -0.32655
141B -> 148B -0.18040
141B -> 150B -0.14103
142B -> 147B 0.35929
143B -> 147B 0.41059
143B -> 148B 0.13056
144B -> 148B 0.11906
145B -> 147B -0.18551
145B -> 148B 0.15879
145B -> 150B 0.10414
146B -> 148B 0.13505

Excited State 12: 2.189-A 2.1226 eV 584.10 nm f=0.0032 <S**2>=0.948
128A -> 148A -0.10872
133A -> 148A 0.11590
139A -> 148A -0.14482
140A -> 148A -0.12641

142A -> 148A 0.24907
145A -> 148A -0.12252
147A -> 148A 0.38020
147A -> 149A 0.11268
140B -> 147B -0.16991
141B -> 147B 0.38037
142B -> 147B -0.17290
142B -> 148B 0.28872
142B -> 150B 0.20320
143B -> 147B -0.18816
143B -> 148B 0.22583
143B -> 150B 0.19941
145B -> 148B 0.25967
145B -> 150B 0.19891

Excited State 13: 2.128-A 2.2161 eV 559.46 nm f=0.0001 <S**2>=0.882
139A -> 148A -0.16100
140A -> 148A 0.39630
140A -> 149A 0.11846
141A -> 148A 0.15780
144A -> 148A 0.16497
146A -> 148A 0.19448
139B -> 148B 0.22229
139B -> 150B 0.20510
140B -> 147B 0.14156
140B -> 148B 0.21340
140B -> 150B 0.16263
141B -> 147B 0.43798
141B -> 148B -0.10907
142B -> 147B -0.19956
144B -> 148B 0.13039
144B -> 150B 0.11231
146B -> 148B 0.30757
146B -> 150B 0.16222

Excited State 14: 2.122-A 2.2491 eV 551.26 nm f=0.0041 <S**2>=0.875
139A -> 148A -0.16072
140A -> 148A -0.11985
142A -> 148A -0.35809
143A -> 148A -0.20338
145A -> 148A -0.12210
147A -> 148A 0.15906
139B -> 147B 0.13056
140B -> 147B 0.56640
140B -> 148B -0.21262
140B -> 150B -0.16919
141B -> 147B -0.12042
141B -> 148B -0.25666
141B -> 150B -0.20503
142B -> 148B -0.19806
142B -> 150B -0.15588
143B -> 147B -0.13051
145B -> 148B 0.15017
145B -> 150B 0.10446

Excited State 15: 2.163-A 2.4862 eV 498.70 nm f=0.0035 <S**2>=0.920

142A -> 148A -0.12513
147A -> 148A -0.12819
123B -> 147B 0.12875
124B -> 147B -0.10386
128B -> 147B -0.14950
138B -> 147B -0.17626
139B -> 147B 0.81962
140B -> 147B -0.30054
141B -> 147B 0.19620

Excited State 16: 2.091-A 2.5556 eV 485.14 nm f=0.0143 <S**2>=0.843
105A -> 148A -0.19109
115A -> 148A -0.18386
121A -> 148A 0.12661
128A -> 148A 0.15482
129A -> 148A -0.29675
130A -> 148A -0.21079
135A -> 148A -0.18389
143A -> 148A 0.30353
105B -> 148B -0.14707
105B -> 150B -0.12398
117B -> 148B -0.16514
117B -> 150B -0.14143
129B -> 148B -0.16064
129B -> 150B -0.13158
130B -> 148B -0.27333
130B -> 150B -0.22448
135B -> 148B -0.17386
135B -> 150B -0.14216
142B -> 148B 0.16634
142B -> 150B 0.12734
143B -> 148B -0.17400
143B -> 150B -0.13469

Excited State 17: 3.025-A 2.6540 eV 467.15 nm f=0.0013 <S**2>=2.038
146A -> 149A -0.18207
146A -> 150A -0.17258
147A -> 149A 0.24915
147A -> 150A -0.12731
139B -> 148B -0.11600
139B -> 150B -0.10350
140B -> 148B -0.10666
144B -> 148B -0.16328
146B -> 148B 0.83621
146B -> 150B -0.10609

Excited State 18: 3.172-A 2.7747 eV 446.84 nm f=0.0043 <S**2>=2.266
146A -> 149A -0.28032
146A -> 150A 0.19123
147A -> 150A 0.48214
146B -> 149B 0.75918

Excited State 19: 2.973-A 2.9358 eV 422.32 nm f=0.0040 <S**2>=1.960
146A -> 148A -0.18589
146A -> 149A 0.21403
146A -> 150A 0.21128

147A -> 148A 0.11059
147A -> 149A -0.38388
147A -> 150A 0.14820
130B -> 147B 0.10985
144B -> 150B -0.12365
146B -> 148B 0.22952
146B -> 150B 0.71404

Excited State 20: 2.514-A 3.1085 eV 398.85 nm f=0.0007 <S**2>=1.331
144A -> 149A -0.18055
145A -> 149A 0.10430
145A -> 150A -0.12392
146A -> 148A 0.12570
105B -> 147B 0.10933
117B -> 147B 0.14682
129B -> 147B 0.18287
130B -> 147B 0.53571
133B -> 147B 0.14040
134B -> 147B 0.15868
135B -> 147B 0.53954
143B -> 147B -0.13389
144B -> 148B 0.20355
145B -> 149B 0.17931
146B -> 150B -0.15709

Excited State 21: 3.230-A 3.1784 eV 390.09 nm f=0.0379 <S**2>=2.359
144A -> 149A -0.34603
145A -> 150A 0.44358
127B -> 147B 0.13090
137B -> 147B 0.41511
138B -> 147B 0.12510
144B -> 149B 0.36555
145B -> 148B 0.24230
145B -> 149B -0.16092
145B -> 150B -0.26360
146B -> 153B 0.12155

Excited State 22: 3.175-A 3.2213 eV 384.89 nm f=0.0033 <S**2>=2.270
144A -> 148A 0.12733
144A -> 149A -0.32902
144A -> 150A -0.18934
145A -> 149A 0.19365
145A -> 150A -0.27977
146A -> 148A -0.11824
146A -> 151A 0.11820
147A -> 149A -0.14586
147A -> 152A -0.11020
117B -> 147B -0.14488
125B -> 147B 0.11509
129B -> 147B -0.13536
130B -> 147B -0.26640
133B -> 147B 0.10070
135B -> 147B -0.23715
144B -> 148B 0.25174
144B -> 150B -0.28627
145B -> 149B 0.35360

146B -> 151B -0.15765

Excited State 23: 2.187-A 3.2385 eV 382.84 nm f=0.0013 <S**2>=0.946
138B -> 147B 0.95574
139B -> 147B 0.18580

Excited State 24: 2.275-A 3.3622 eV 368.76 nm f=0.0226 <S**2>=1.044
146A -> 148A 0.10623
146A -> 149A -0.24169
147A -> 148A -0.13587
147A -> 149A 0.22123
147A -> 150A 0.43754
127B -> 147B 0.10785
137B -> 147B 0.51470
146B -> 149B -0.50467
146B -> 150B 0.11781

Excited State 25: 2.494-A 3.3980 eV 364.88 nm f=0.0510 <S**2>=1.305
144A -> 148A 0.15903
146A -> 148A -0.37956
146A -> 149A -0.19010
146A -> 150A -0.17747
147A -> 148A -0.34762
147A -> 149A 0.29192
147A -> 150A -0.26591
126B -> 147B 0.20482
132B -> 147B 0.15703
133B -> 147B 0.23900
134B -> 147B 0.13022
135B -> 147B 0.15498
136B -> 147B -0.10611
146B -> 148B -0.18814
146B -> 149B 0.12300
146B -> 150B 0.39729

Excited State 26: 2.464-A 3.4423 eV 360.18 nm f=0.0142 <S**2>=1.268
140A -> 148A -0.11555
144A -> 148A -0.16549
144A -> 149A -0.10682
146A -> 148A 0.70602
147A -> 149A 0.18386
126B -> 147B 0.12653
133B -> 147B 0.17773
136B -> 147B -0.33190
137B -> 147B -0.22368
146B -> 150B 0.29671

Excited State 27: 2.196-A 3.4639 eV 357.93 nm f=0.0068 <S**2>=0.955
146A -> 148A 0.22750
147A -> 149A 0.12421
130B -> 147B -0.15104
136B -> 147B 0.89869
146B -> 150B 0.17657

Excited State 28: 2.495-A 3.5011 eV 354.13 nm f=0.0278 <S**2>=1.306
144A -> 149A 0.10356

145A -> 150A -0.14705
146A -> 149A 0.22219
146A -> 150A -0.12132
146A -> 152A -0.12455
147A -> 148A 0.19634
147A -> 150A -0.39610
147A -> 151A 0.12992
137B -> 147B 0.61882
144B -> 149B -0.15827
145B -> 148B -0.14303
145B -> 150B 0.12513
146B -> 149B 0.30324
146B -> 153B -0.13428

Excited State 29: 2.381-A 3.5582 eV 348.44 nm f=0.0104 <S**2>=1.167
121A -> 148A -0.17148
131A -> 148A -0.11638
133A -> 148A -0.11887
139A -> 148A 0.17439
140A -> 148A 0.18806
142A -> 148A -0.16434
145A -> 148A 0.22543
146A -> 148A -0.21777
146A -> 149A -0.23203
147A -> 148A 0.56996
147A -> 149A 0.38264
133B -> 147B -0.15213
146B -> 150B 0.13928

Excited State 30: 2.326-A 3.5901 eV 345.35 nm f=0.0295 <S**2>=1.102
146A -> 148A -0.12101
146A -> 150A 0.10994
146A -> 151A -0.13051
147A -> 148A 0.26814
147A -> 149A -0.14356
147A -> 150A 0.15536
147A -> 152A 0.14052
125B -> 147B 0.14565
126B -> 147B 0.16606
129B -> 147B -0.12063
130B -> 147B -0.16295
133B -> 147B 0.65382
134B -> 147B 0.30257
135B -> 147B 0.10681
146B -> 150B -0.18050
146B -> 151B 0.12921

b) TD-DFT excitation energies and oscillator strengths for $[2]^{+}$.

Excitation energies and oscillator strengths:

Excited State 1: 2.015-A 0.5010 eV 2474.60 nm f=0.1976 <S**2>=0.765
146B -> 147B 0.99391
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.030-A 1.3766 eV 900.64 nm f=0.0008 <S**2>=0.780
143B -> 147B 0.96275
145B -> 147B -0.23342

Excited State 3: 2.033-A 1.5339 eV 808.27 nm f=0.0295 <S**2>=0.784
139B -> 147B 0.10621
140B -> 147B 0.14069
144B -> 147B 0.97567

Excited State 4: 2.030-A 1.5530 eV 798.37 nm f=0.0187 <S**2>=0.781
143B -> 147B 0.22960
145B -> 147B 0.95884

Excited State 5: 2.035-A 1.8590 eV 666.95 nm f=0.0002 <S**2>=0.785
137B -> 147B 0.10787
141B -> 147B 0.30808
142B -> 147B 0.92836

Excited State 6: 2.100-A 2.3615 eV 525.02 nm f=0.0183 <S**2>=0.853
139B -> 147B 0.53864
140B -> 147B 0.78083
143B -> 149B 0.11524
144B -> 147B -0.17752

Excited State 7: 2.037-A 2.3739 eV 522.28 nm f=0.0005 <S**2>=0.787
141B -> 147B 0.92399
142B -> 147B -0.29987

Excited State 8: 2.643-A 2.4909 eV 497.76 nm f=0.0007 <S**2>=1.496
142A -> 149A 0.12640
143A -> 149A 0.28800
143A -> 150A 0.25881
145A -> 149A -0.11923
147A -> 149A -0.17219
147A -> 150A -0.13553
128B -> 147B 0.12294
138B -> 147B -0.10288
139B -> 147B 0.65137
140B -> 147B -0.32104
142B -> 149B -0.13021
143B -> 149B -0.23459
143B -> 150B -0.25394

Excited State 9: 2.909-A 2.5114 eV 493.69 nm f=0.0007 <S**2>=1.866
142A -> 149A 0.12827
142A -> 150A 0.12979
143A -> 149A 0.38008
143A -> 150A 0.31067
147A -> 149A -0.14734
128B -> 147B -0.10070
139B -> 147B -0.42301
140B -> 147B 0.45192
142B -> 149B -0.10328
142B -> 150B -0.14806
143B -> 149B -0.34671
143B -> 150B -0.26123

Excited State 10: 2.638-A 2.6287 eV 471.66 nm f=0.0028 <S**2>=1.490
140A -> 149A 0.28176
140A -> 150A 0.23771
143A -> 149A 0.17592
143A -> 150A 0.15511
145A -> 149A 0.16622
145A -> 150A 0.12321
147A -> 149A 0.62458
147A -> 150A 0.41492
141B -> 149B -0.16930
141B -> 150B -0.15595
143B -> 149B -0.17543
143B -> 150B -0.15676
146B -> 148B 0.11108

Excited State 11: 3.196-A 2.6793 eV 462.76 nm f=0.0000 <S**2>=2.303
139A -> 149A 0.18980
139A -> 150A 0.15785
146A -> 149A -0.21332
147A -> 148A 0.14170
139B -> 149B -0.14521
139B -> 150B -0.13116
140B -> 149B -0.19564
140B -> 150B -0.17008
144B -> 150B -0.11718
146B -> 149B 0.75519
146B -> 150B 0.36532

Excited State 12: 3.091-A 2.7090 eV 457.68 nm f=0.0110 <S**2>=2.139
146A -> 148A -0.35173
147A -> 149A 0.18200
147A -> 150A -0.40212
139B -> 147B -0.12041
146B -> 148B 0.78422

Excited State 13: 3.004-A 2.7684 eV 447.86 nm f=0.0001 <S**2>=2.006
146A -> 149A 0.19464
146A -> 150A -0.29083
147A -> 148A -0.54365
146B -> 149B -0.27807
146B -> 150B 0.65993

Excited State 14: 2.228-A 3.0368 eV 408.28 nm f=0.0006 <S**2>=0.991
144A -> 149A -0.14091
145A -> 148A 0.14031
147A -> 148A 0.10957
129B -> 147B -0.13308
130B -> 147B 0.18607
132B -> 147B 0.30809
133B -> 147B -0.20282
135B -> 147B 0.13098
137B -> 147B 0.78736
142B -> 147B -0.12046
145B -> 148B -0.14690

Excited State 15: 2.967-A 3.0710 eV 403.73 nm f=0.0002 <S**2>=1.950
139A -> 149A -0.37138
139A -> 150A -0.32608
144A -> 149A -0.23468
144A -> 150A -0.21189
146A -> 149A 0.31864
146A -> 150A 0.22016
139B -> 149B 0.15335
139B -> 150B 0.13032
140B -> 149B 0.18880
140B -> 150B 0.16734
144B -> 149B 0.22685
144B -> 150B 0.17894
146B -> 149B 0.41476
146B -> 150B 0.29835

Excited State 16: 3.101-A 3.1486 eV 393.78 nm f=0.0223 <S**2>=2.154
143A -> 149A -0.14265
144A -> 148A 0.40274
145A -> 149A -0.23506
145A -> 150A 0.30670
146A -> 152A -0.10601
147A -> 149A -0.16863
147A -> 150A 0.24948
127B -> 147B -0.10705
136B -> 147B 0.32712
143B -> 150B -0.10442
144B -> 148B -0.38434
145B -> 149B 0.25694
145B -> 150B -0.24025
146B -> 148B 0.20426
146B -> 152B 0.12237

Excited State 17: 3.082-A 3.1698 eV 391.14 nm f=0.0175 <S**2>=2.124
144A -> 149A 0.21709
144A -> 150A -0.25146
145A -> 148A -0.36209
145A -> 152A -0.10009
146A -> 151A 0.13324
147A -> 148A -0.33619
147A -> 152A 0.12607
118B -> 147B 0.10058
130B -> 147B 0.10619
132B -> 147B 0.12222
137B -> 147B 0.27725
144B -> 149B -0.26917
144B -> 150B 0.23150
145B -> 148B 0.37875
146B -> 149B 0.18928
146B -> 150B -0.25818
146B -> 151B -0.15369

Excited State 18: 2.187-A 3.2571 eV 380.66 nm f=0.0152 <S**2>=0.946
142A -> 149A -0.12023
142A -> 150A -0.12775
143A -> 149A -0.18068

143A -> 150A -0.17020
145A -> 149A 0.10692
146A -> 148A 0.35121
147A -> 149A -0.32830
147A -> 150A 0.34812
127B -> 147B 0.11132
136B -> 147B -0.38334
143B -> 149B -0.25895
143B -> 150B -0.20204
146B -> 148B 0.44540

Excited State 19: 2.076-A 3.2713 eV 379.00 nm f=0.0008 <S**2>=0.827
134B -> 147B 0.12448
138B -> 147B 0.96080
139B -> 147B 0.12183
140B -> 147B -0.10534

Excited State 20: 3.374-A 3.2874 eV 377.15 nm f=0.0007 <S**2>=2.596
132A -> 149A -0.17098
132A -> 150A -0.15178
133A -> 149A -0.11763
136A -> 149A -0.20497
136A -> 150A -0.17677
137A -> 149A -0.12523
137A -> 150A -0.10773
142A -> 149A -0.33418
142A -> 150A -0.27990
143A -> 149A 0.19699
143A -> 150A 0.16456
147A -> 150A -0.13671
132B -> 149B 0.14499
132B -> 150B 0.13530
137B -> 149B 0.23007
137B -> 150B 0.20579
138B -> 147B 0.13627
142B -> 149B 0.38528
142B -> 150B 0.33193
145B -> 150B -0.11987

Excited State 21: 2.499-A 3.3992 eV 364.75 nm f=0.0807 <S**2>=1.311
144A -> 149A 0.11260
144A -> 150A -0.17488
145A -> 148A -0.22346
146A -> 149A -0.21601
146A -> 150A 0.18968
147A -> 148A 0.53290
122B -> 147B 0.10361
124B -> 147B 0.10581
126B -> 147B 0.11214
130B -> 147B 0.15518
133B -> 147B 0.12902
135B -> 147B -0.12982
144B -> 150B 0.17055
145B -> 148B 0.16651
146B -> 149B -0.30980
146B -> 150B 0.46855

Excited State 22: 2.391-A 3.4381 eV 360.62 nm f=0.0256 <S**2>=1.179
143A -> 149A -0.24298
143A -> 150A -0.20792
144A -> 148A -0.10127
146A -> 152A 0.13430
147A -> 151A 0.14048
127B -> 147B -0.11415
136B -> 147B 0.65939
143B -> 149B -0.31296
143B -> 150B -0.23496
144B -> 148B 0.19008
145B -> 150B 0.27713
146B -> 152B -0.14437

Excited State 23: 2.041-A 3.4598 eV 358.35 nm f=0.0025 <S**2>=0.791
147A -> 148A 0.10095
132B -> 147B 0.14929
133B -> 147B -0.13618
135B -> 147B 0.91504
137B -> 147B -0.27331

Excited State 24: 2.638-A 3.5272 eV 351.51 nm f=0.0170 <S**2>=1.490
142A -> 149A -0.14351
142A -> 150A -0.11132
143A -> 149A -0.17048
143A -> 150A -0.10597
146A -> 148A -0.19730
147A -> 149A 0.37343
147A -> 151A -0.10309
136B -> 147B -0.38954
141B -> 149B 0.22856
141B -> 150B 0.21118
143B -> 149B -0.18495
143B -> 150B -0.16546
145B -> 149B 0.41063
145B -> 150B 0.22429
146B -> 148B -0.22089

Excited State 25: 2.894-A 3.5755 eV 346.76 nm f=0.0005 <S**2>=1.844
146A -> 149A 0.63320
146A -> 150A 0.47840
133B -> 147B 0.13474
139B -> 149B -0.17204
139B -> 150B -0.14189
140B -> 149B -0.22569
140B -> 150B -0.19796
144B -> 149B -0.25284
144B -> 150B -0.25951

Excited State 26: 2.550-A 3.5884 eV 345.52 nm f=0.0039 <S**2>=1.376
143A -> 149A 0.28032
143A -> 150A 0.23842
145A -> 150A -0.10905
146A -> 148A 0.17491
147A -> 150A 0.39907

136B -> 147B 0.17081
141B -> 149B 0.38150
141B -> 150B 0.29201
143B -> 149B 0.26941
143B -> 150B 0.23667
145B -> 149B 0.27640
145B -> 150B 0.22446
146B -> 148B 0.17958

Excited State 27: 2.132-A 3.6606 eV 338.70 nm f=0.0094 <S**2>=0.887
146A -> 150A -0.14237
146A -> 151A -0.11106
147A -> 152A -0.12221
122B -> 147B 0.10573
124B -> 147B 0.16529
130B -> 147B 0.15459
132B -> 147B 0.26834
133B -> 147B 0.85757
135B -> 147B 0.10601
146B -> 151B 0.11710

Excited State 28: 2.032-A 3.6828 eV 336.66 nm f=0.0007 <S**2>=0.782
125B -> 147B 0.10803
134B -> 147B 0.96938
138B -> 147B -0.13932

Excited State 29: 2.050-A 3.7461 eV 330.97 nm f=0.0033 <S**2>=0.801
122B -> 147B 0.11114
130B -> 147B 0.37220
132B -> 147B 0.66795
133B -> 147B -0.28868
135B -> 147B -0.29826
137B -> 147B -0.41563

Excited State 30: 2.132-A 3.8084 eV 325.56 nm f=0.0069 <S**2>=0.887
146A -> 151A -0.12204
147A -> 148A -0.24025
147A -> 152A -0.13294
122B -> 147B 0.14684
124B -> 147B 0.14807
126B -> 147B 0.27839
129B -> 147B -0.37462
130B -> 147B 0.55155
132B -> 147B -0.50722
146B -> 151B 0.10768

c) TD-DFT excitation energies and oscillator strengths for [3]$^{+}$.

Excitation energies and oscillator strengths:

Excited State 1: 2.017-A 0.6759 eV 1834.31 nm f=0.2049 <S**2>=0.767
140B -> 147B -0.10448
144B -> 147B -0.14717
146B -> 147B 0.97842
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.028-A 1.2891 eV 961.78 nm f=0.0006 <S**2>=0.778
141B -> 147B 0.11575
142B -> 147B -0.10737
143B -> 147B 0.95499
145B -> 147B -0.23172

Excited State 3: 2.030-A 1.4655 eV 846.02 nm f=0.0940 <S**2>=0.780
140B -> 147B 0.28070
144B -> 147B 0.93783
146B -> 147B 0.16764

Excited State 4: 2.027-A 1.6019 eV 774.00 nm f=0.0209 <S**2>=0.777
143B -> 147B 0.22643
145B -> 147B 0.95777

Excited State 5: 2.031-A 1.7893 eV 692.91 nm f=0.0000 <S**2>=0.781
137B -> 147B 0.15110
141B -> 147B 0.49923
142B -> 147B 0.83853

Excited State 6: 2.064-A 2.3245 eV 533.38 nm f=0.0017 <S**2>=0.815
140B -> 147B 0.93266
144B -> 147B -0.29594
146B -> 148B 0.10494

Excited State 7: 2.033-A 2.3626 eV 524.79 nm f=0.0002 <S**2>=0.784
141B -> 147B 0.83634
142B -> 147B -0.47938
143B -> 147B -0.15662

Excited State 8: 3.055-A 2.7043 eV 458.48 nm f=0.0165 <S**2>=2.083
146A -> 148A 0.37773
147A -> 149A -0.47387
139B -> 147B -0.18611
140B -> 147B -0.13465
146B -> 148B 0.72552

Excited State 9: 2.101-A 2.7517 eV 450.57 nm f=0.0003 <S**2>=0.853
147A -> 149A -0.10145
123B -> 147B -0.11630
124B -> 147B -0.15071
128B -> 147B -0.15070
134B -> 147B 0.10468
138B -> 147B 0.17781
139B -> 147B 0.90925
146B -> 148B 0.15375

Excited State 10: 2.810-A 2.7561 eV 449.85 nm f=0.0040 <S**2>=1.724
145A -> 149A 0.10844
146A -> 149A -0.35550
147A -> 148A 0.70448
146B -> 149B 0.55902

Excited State 11: 2.479-A 3.0093 eV 412.00 nm f=0.0015 <S**2>=1.286
144A -> 148A 0.22015

145A -> 149A 0.17997
146A -> 149A 0.12348
147A -> 148A 0.15258
129B -> 147B -0.14555
132B -> 147B 0.20470
133B -> 147B -0.17484
137B -> 147B 0.74365
142B -> 147B -0.14230
144B -> 149B 0.18080
145B -> 148B -0.23203
146B -> 149B -0.24535

Excited State 12: 2.924-A 3.0802 eV 402.52 nm f=0.0137 <S**2>=1.888
144A -> 148A -0.31387
145A -> 149A -0.26641
146A -> 149A -0.17966
146A -> 151A 0.10786
147A -> 148A -0.29082
132B -> 147B 0.15601
137B -> 147B 0.48683
144B -> 149B -0.30956
145B -> 148B 0.33275
146B -> 149B 0.32769
146B -> 151B 0.11463

Excited State 13: 3.198-A 3.0831 eV 402.14 nm f=0.0059 <S**2>=2.307
144A -> 149A -0.38066
145A -> 148A -0.40822
146A -> 148A -0.14029
146A -> 152A 0.11787
147A -> 149A -0.36689
147A -> 151A -0.10476
135B -> 147B -0.14511
144B -> 148B 0.43951
145B -> 149B -0.35010
146B -> 148B -0.24025
146B -> 152B -0.12576

Excited State 14: 2.296-A 3.3140 eV 374.12 nm f=0.0023 <S**2>=1.068
144A -> 149A -0.13995
145A -> 148A -0.15682
146A -> 148A -0.40086
147A -> 149A 0.56476
135B -> 147B -0.24021
144B -> 148B 0.13617
146B -> 148B 0.56698

Excited State 15: 2.030-A 3.4072 eV 363.89 nm f=0.0008 <S**2>=0.780
134B -> 147B 0.12335
138B -> 147B 0.96245
139B -> 147B -0.21927

Excited State 16: 2.704-A 3.4225 eV 362.26 nm f=0.0735 <S**2>=1.578
144A -> 148A 0.24312
145A -> 149A 0.23091
146A -> 149A 0.19367

147A -> 148A -0.48035
144B -> 149B 0.22584
145B -> 148B -0.15241
146B -> 149B 0.65459

Excited State 17: 2.291-A 3.5848 eV 345.86 nm f=0.0091 <S**2>=1.062
140A -> 150A -0.19217
144A -> 150A -0.18769
146A -> 152A 0.13145
147A -> 149A 0.13750
147A -> 150A -0.57383
147A -> 151A -0.15556
127B -> 147B 0.14462
135B -> 147B 0.62099
144B -> 148B 0.11653
145B -> 149B -0.10079
145B -> 150B 0.11179
146B -> 152B -0.12366

Excited State 18: 2.239-A 3.5969 eV 344.70 nm f=0.0134 <S**2>=1.003
140A -> 150A 0.18713
143A -> 150A -0.12160
144A -> 150A 0.18352
146A -> 148A -0.19591
146A -> 152A 0.11597
147A -> 150A 0.60598
147A -> 151A -0.11504
127B -> 147B 0.12966
135B -> 147B 0.60620
146B -> 148B 0.10657
146B -> 152B -0.10745

Excited State 19: 2.034-A 3.6130 eV 343.17 nm f=0.0002 <S**2>=0.785
132B -> 147B -0.12912
133B -> 147B 0.16961
136B -> 147B 0.96602

Excited State 20: 2.597-A 3.7613 eV 329.64 nm f=0.1372 <S**2>=1.437
140A -> 149A 0.11519
143A -> 150A -0.15779
145A -> 148A -0.12730
146A -> 148A 0.73448
146A -> 152A 0.11391
147A -> 149A 0.45714
147A -> 150A 0.17087
135B -> 147B -0.12517
143B -> 150B 0.13867
144B -> 148B 0.14851
146B -> 148B -0.12811
146B -> 152B -0.10916

Excited State 21: 2.813-A 3.7860 eV 327.48 nm f=0.0012 <S**2>=1.728
141A -> 150A 0.19110
145A -> 150A 0.14255
146A -> 150A 0.20770
146A -> 151A -0.13034

147A -> 152A 0.14719
122B -> 147B 0.13247
125B -> 147B 0.13640
132B -> 147B 0.35110
133B -> 147B 0.50717
140B -> 150B -0.23795
144B -> 150B -0.18923
146B -> 150B 0.51895
146B -> 151B -0.13058

Excited State 22: 2.745-A 3.8081 eV 325.58 nm f=0.0058 <S**2>=1.633
141A -> 150A -0.21808
145A -> 150A -0.16333
146A -> 149A 0.16345
146A -> 150A -0.22121
125B -> 147B 0.12289
132B -> 147B 0.29150
133B -> 147B 0.60735
140B -> 150B 0.23319
144B -> 150B 0.17933
146B -> 150B -0.48022

Excited State 23: 3.406-A 3.8195 eV 324.61 nm f=0.0072 <S**2>=2.651
140A -> 150A 0.14128
142A -> 150A 0.12184
143A -> 149A -0.14822
143A -> 150A 0.64633
146A -> 148A 0.14022
147A -> 150A 0.18080
141B -> 150B -0.17787
143B -> 149B -0.15096
143B -> 150B -0.60904

Excited State 24: 2.036-A 3.8393 eV 322.93 nm f=0.0011 <S**2>=0.786
134B -> 147B 0.96819
138B -> 147B -0.14809
139B -> 147B -0.10228

Excited State 25: 2.540-A 3.8780 eV 319.71 nm f=0.0061 <S**2>=1.363
140A -> 148A 0.10010
145A -> 149A -0.14007
146A -> 149A 0.75311
146A -> 151A 0.12672
147A -> 148A 0.33209
118B -> 147B 0.10030
126B -> 147B -0.13301
129B -> 147B 0.13803
131B -> 147B 0.12745
132B -> 147B 0.16323
133B -> 147B -0.11145
144B -> 149B -0.10180
146B -> 149B 0.16906
146B -> 150B 0.13884
146B -> 151B 0.14187

Excited State 26: 2.104-A 3.8982 eV 318.06 nm f=0.0007 <S**2>=0.856

146A -> 149A -0.11260
131B -> 147B -0.10253
132B -> 147B 0.74262
133B -> 147B -0.44138
136B -> 147B 0.18697
137B -> 147B -0.34766
146B -> 150B -0.10766

Excited State 27: 2.223-A 3.9712 eV 312.21 nm f=0.0126 <S**2>=0.985
146A -> 149A -0.26192
146A -> 151A 0.12048
147A -> 152A -0.16377
122B -> 147B -0.18945
125B -> 147B -0.16772
126B -> 147B -0.24723
129B -> 147B 0.17796
131B -> 147B 0.71398
132B -> 147B 0.26620
133B -> 147B 0.13171
144B -> 149B 0.13191
146B -> 149B -0.12331
146B -> 151B 0.10479

Excited State 28: 2.106-A 3.9802 eV 311.50 nm f=0.0034 <S**2>=0.859
147A -> 151A -0.11187
127B -> 147B 0.26152
130B -> 147B 0.91736
146B -> 152B -0.10734

Excited State 29: 2.115-A 4.0341 eV 307.34 nm f=0.0002 <S**2>=0.868
123B -> 147B 0.29376
124B -> 147B 0.49717
127B -> 147B -0.10927
128B -> 147B 0.70720
138B -> 147B 0.10131
139B -> 147B 0.25307

Excited State 30: 2.470-A 4.0572 eV 305.59 nm f=0.0035 <S**2>=1.276
146A -> 151A -0.19059
147A -> 152A 0.18493
125B -> 147B 0.23185
129B -> 147B 0.73613
133B -> 147B -0.17503
137B -> 147B 0.13052
143B -> 148B -0.16294
145B -> 148B 0.28445
145B -> 152B -0.12811
146B -> 151B -0.24133

d) Optimized XYZ coordinates (Å) for 1. PBE0; SDDAll (Ni), 6-31G(d) all other atoms, in vacuum.

Ni	-0.00011900	1.15031000	-0.00006900
O	-1.26766700	-0.20738900	0.07146200
O	1.26747400	-0.20736800	-0.07173400
N	1.22802700	2.46112300	-0.54617500
N	-1.22828800	2.46096300	0.54626400

C	-2.55963500	-0.10969000	0.05064100
C	-3.37072300	-1.26720400	-0.22719400
C	-4.74406400	-1.11538100	-0.20073700
C	-5.43231400	0.08911000	0.08992800
C	-4.65193100	1.18788200	0.35278200
C	-3.23930200	1.11457500	0.32197300
C	-2.51099300	2.28791300	0.64630900
C	0.65358500	3.68741800	-1.08198200
C	-0.00063400	4.54563000	-0.00046300
C	-2.72257100	-2.61320700	-0.56198500
C	-1.84568300	-2.46543400	-1.81767000
C	-1.87053700	-3.09037700	0.62562000
C	-3.76092500	-3.70159800	-0.85387500
C	-6.96002700	0.10731000	0.09706300
C	-7.48433200	-0.89161600	1.14156400
C	-7.48819500	-0.28703200	-1.29183600
C	-7.51406200	1.49200700	0.44196100
H	-5.34975400	-1.98924600	-0.41799700
H	-5.10183600	2.14987300	0.58598400
H	-3.09606000	3.12654300	1.03954200
H	1.42005300	4.26498000	-1.61445200
H	-0.10230900	3.39698500	-1.82028000
H	-0.74396400	5.19584300	-0.47684900
H	-1.06613900	-1.71568900	-1.67028200
H	-1.36499900	-3.42315500	-2.05360800
H	-2.45628400	-2.17224200	-2.68050000
H	-2.49596700	-3.23395700	1.51517200
H	-1.39841600	-4.05141700	0.38526600
H	-1.08661500	-2.36927900	0.86106100
H	-4.39355600	-3.45041100	-1.71393200
H	-3.24001300	-4.63587800	-1.09195100
H	-4.40906500	-3.89864300	0.00879700
H	-8.58146300	-0.89568700	1.15012500
H	-7.15014400	-1.91344100	0.93177500
H	-7.13492100	-0.62562800	2.14559300
H	-8.58534000	-0.29120600	-1.29724200
H	-7.14488100	0.42064000	-2.05495100
H	-7.15061000	-1.28648200	-1.58711600
H	-7.19401100	1.82085800	1.43777700
H	-7.20079900	2.24753400	-0.28821300
H	-8.60968800	1.46427100	0.43946100
C	2.55944500	-0.10959300	-0.05057700
C	3.37065700	-1.26707200	0.22721400
C	4.74396300	-1.11511600	0.20096400
C	5.43213700	0.08947100	-0.08944200
C	4.65168500	1.18817400	-0.35237400
C	3.23905800	1.11475800	-0.32173400
C	2.51074200	2.28807800	-0.64610900
C	-0.65381100	3.68743200	1.08159800
C	2.72304600	-2.61336900	0.56174700
C	1.84707500	-2.46679200	1.81823600
C	1.87052500	-3.09043900	-0.62558200
C	3.76228400	-3.70122500	0.85232100
C	6.95984200	0.10772300	-0.09670500
C	7.48401100	-0.89428600	-1.13831900
C	7.48821100	-0.28250000	1.29328500

C	7.51373500	1.49144000	-0.44575000
H	5.34963700	-1.98903400	0.41809700
H	5.10155000	2.15022300	-0.58546100
H	3.09583500	3.12672300	-1.03928500
H	-1.42004300	4.26486400	1.61454400
H	0.10271100	3.39726800	1.81936300
H	0.74189500	5.19706200	0.47550900
H	1.06673600	-1.71770300	1.67177800
H	1.36742600	-3.42502200	2.05422200
H	2.45813800	-2.17339400	2.68067100
H	2.49552500	-3.23347900	-1.51552700
H	1.39889900	-4.05174200	-0.38533700
H	1.08618300	-2.36955800	-0.86029600
H	4.39538800	-3.45000700	1.71202800
H	3.24218400	-4.63599300	1.09029100
H	4.40995600	-3.89733700	-0.01092000
H	8.58113900	-0.89804400	-1.14735700
H	7.15022400	-1.91554400	-0.92512300
H	7.13405800	-0.63156500	-2.14302300
H	8.58535400	-0.28656800	1.29855700
H	7.14494400	0.42738000	2.05436800
H	7.15078500	-1.28112000	1.59153300
H	7.19394100	1.81715000	-1.44267700
H	7.20007300	2.24917300	0.28196400
H	8.60936700	1.46393100	-0.44284700

e) Optimized XYZ coordinates (Å) for 2. PBE0; SDDAll (Ni), 6-31G(d) all other atoms, in vacuum.

Pd	-0.00009200	-1.09984800	-0.00032200
O	-1.36966000	0.35544200	-0.21559800
O	1.36959000	0.35542500	0.21479700
N	1.35036100	-2.49884100	0.45345400
N	-1.35057700	-2.49888400	-0.45396900
C	-2.65511300	0.20786900	-0.13040500
C	-3.48150600	1.37238900	0.06928000
C	-4.85101100	1.19976200	0.11775700
C	-5.52495700	-0.03771000	-0.02844300
C	-4.73275700	-1.14080800	-0.22558200
C	-3.31862200	-1.05285900	-0.26298000
C	-2.62455000	-2.26720900	-0.53020000
C	0.81670300	-3.73836300	0.99697000
C	0.00024500	-4.56182900	-0.00088300
C	-2.84756400	2.75821600	0.22888800
C	-1.89439500	2.76214800	1.43677700
C	-2.08040300	3.13031700	-1.05151400
C	-3.89572400	3.84996900	0.46995500
C	-7.05113400	-0.08267700	0.02609400
C	-7.63132600	0.78721100	-1.10117200
C	-7.53740400	0.45394800	1.38231200
C	-7.58871000	-1.50572900	-0.14436000
H	-5.46397100	2.08132000	0.27573500
H	-5.17596600	-2.12509700	-0.35468700
H	-3.25005600	-3.10477100	-0.85758600
H	1.63319500	-4.35385800	1.39747000
H	0.17795200	-3.46269000	1.84418300
H	-0.66193400	-5.21613500	0.57854000

H	-1.09376200	2.03152300	1.31106900
H	-1.44243300	3.75529700	1.55236300
H	-2.44103900	2.53094800	2.35928400
H	-2.76337500	3.18224400	-1.90824300
H	-1.61110600	4.11526500	-0.93316400
H	-1.29938200	2.40046300	-1.27035800
H	-4.47409100	3.67377600	1.38511600
H	-3.38563900	4.81308500	0.58419700
H	-4.59412100	3.94737400	-0.37013400
H	-8.72801100	0.77689100	-1.06820500
H	-7.30583200	1.82985400	-1.01851800
H	-7.31463900	0.41564400	-2.08232500
H	-8.63339000	0.43583300	1.42967600
H	-7.14895100	-0.15586500	2.20588100
H	-7.21494400	1.48703400	1.55103000
H	-7.30387900	-1.93304900	-1.11301000
H	-7.22766500	-2.17282000	0.64729100
H	-8.68360900	-1.49700200	-0.09627900
C	2.65505500	0.20782200	0.12998700
C	3.48154900	1.37228500	-0.06958000
C	4.85107600	1.19966900	-0.11730400
C	5.52495800	-0.03777800	0.02934700
C	4.73266200	-1.14087200	0.22615200
C	3.31851600	-1.05290100	0.26296800
C	2.62432200	-2.26722600	0.53000100
C	-0.81710200	-3.73826700	-0.99799800
C	2.84779000	2.75813000	-0.22960600
C	1.89515300	2.76207400	-1.43791900
C	2.08013900	3.13045200	1.05043800
C	3.89621400	3.84970800	-0.47035200
C	7.05114200	-0.08276700	-0.02446000
C	7.63083800	0.78738900	1.10286600
C	7.53806200	0.45345300	-1.38061000
C	7.58853200	-1.50581000	0.14661600
H	5.46410400	2.08123300	-0.27498700
H	5.17581000	-2.12516700	0.35545300
H	3.24970900	-3.10482400	0.85752100
H	-1.63380600	-4.35380000	-1.39801400
H	-0.17903700	-3.46236500	-1.84565400
H	0.66313100	-5.21491800	-0.58086400
H	1.09443300	2.03147000	-1.31261600
H	1.44326800	3.75523100	-1.55369400
H	2.44220800	2.53086700	-2.36018200
H	2.76282600	3.18274900	1.90737700
H	1.61072800	4.11528200	0.93164200
H	1.29914800	2.40055300	1.26923900
H	4.47428100	3.67388800	-1.38577500
H	3.38637400	4.81303200	-0.58391800
H	4.59486800	3.94641900	0.36960400
H	8.72753900	0.77711700	1.07035700
H	7.30529000	1.82998500	1.01989700
H	7.31376000	0.41599200	2.08396400
H	8.63405100	0.43486800	-1.42761500
H	7.14960500	-0.15631300	-2.20421600
H	7.21613500	1.48666300	-1.54958400
H	7.30255700	-1.93315900	1.11491200

H	7.22842800	-2.17288700	-0.64548200
H	8.68349200	-1.49706800	0.09988900

f) Optimized XYZ coordinates (Å) for 3. PBE0; SDDAll (Ni), 6-31G(d) all other atoms, in vacuum.

Pt	-0.00005200	-1.03287200	-0.00031200
O	1.35796700	0.44369100	0.24646000
O	-1.35805200	0.44365400	-0.24725700
N	-1.36395800	-2.42456800	-0.41643800
N	1.36379500	-2.42447800	0.41612700
C	2.64879200	0.30485300	0.16544900
C	3.46717400	1.48592000	0.07004800
C	4.83543200	1.32396500	-0.03177400
C	5.51370000	0.08082900	-0.01878600
C	4.72935000	-1.03667000	0.12047400
C	3.31656700	-0.95846000	0.20521500
C	2.64123600	-2.18923400	0.44701800
C	-0.86271600	-3.67900500	-0.96392800
C	0.00019800	-4.49572600	-0.00060400
C	2.83111600	2.87993500	0.08638600
C	1.86041800	3.03480300	-1.09640300
C	2.08581700	3.08733600	1.41660200
C	3.87614800	3.99526500	-0.02912900
C	7.03624100	0.04333700	-0.14075000
C	7.66991000	0.82877000	1.01902100
C	7.45928600	0.67862700	-1.47532000
C	7.57925500	-1.38717000	-0.10058600
H	5.44234500	2.21885300	-0.12174000
H	5.17777900	-2.02587000	0.16679900
H	3.27954900	-3.03376600	0.72270600
H	-1.70362100	-4.29313400	-1.30998700
H	-0.27012900	-3.41723900	-1.84757000
H	0.63528200	-5.15012600	-0.60954900
H	1.06362000	2.29111500	-1.05419900
H	1.40556300	4.03321000	-1.07678200
H	2.39363400	2.92612100	-2.04878800
H	2.78331100	3.02825700	2.26100500
H	1.61859200	4.07999000	1.43315800
H	1.30556800	2.33737200	1.55591800
H	4.43551200	3.94351600	-0.97117700
H	3.36480000	4.96422900	-0.00563400
H	4.59154400	3.98237800	0.80208900
H	8.76383600	0.81868600	0.93532700
H	7.34755600	1.87550100	1.02640100
H	7.39649500	0.38820700	1.98446600
H	8.55195700	0.67008900	-1.57500100
H	7.03384700	0.12731400	-2.32147500
H	7.12624700	1.71916100	-1.55378700
H	7.33642900	-1.88715200	0.84447800
H	7.18441500	-1.99389700	-0.92393600
H	8.67095900	-1.37124900	-0.19484200
C	-2.64885100	0.30484200	-0.16571100
C	-3.46717400	1.48593600	-0.07011800
C	-4.83539700	1.32401300	0.03226500
C	-5.51366400	0.08086300	0.01973300
C	-4.72938900	-1.03665600	-0.11977300

C	-3.31664100	-0.95848300	-0.20505300
C	-2.64140400	-2.18928700	-0.44698200
C	0.86234800	-3.67896900	0.96330000
C	-2.83101800	2.87990600	-0.08693400
C	-1.85809300	3.03396400	1.09413600
C	-2.08807400	3.08789300	-1.41836900
C	-3.87566500	3.99533500	0.03106900
C	-7.03615300	0.04345500	0.14215500
C	-7.66999000	0.83138300	-1.01581300
C	-7.45858500	0.67617200	1.47814400
C	-7.57954000	-1.38683800	0.09931900
H	-5.44230700	2.21891700	0.12212400
H	-5.17784500	-2.02587000	-0.16577700
H	-3.27983600	-3.03381900	-0.72242200
H	1.70308300	-4.29302400	1.30987700
H	0.26914200	-3.41727700	1.84655400
H	-0.63431500	-5.15110100	0.60789500
H	-1.06162800	2.29002000	1.05013800
H	-1.40291100	4.03222200	1.07409000
H	-2.38961000	2.92507100	2.04744500
H	-2.78714400	3.02962300	-2.26152200
H	-1.62055200	4.08041000	-1.43512600
H	-1.30830600	2.33777400	-1.55955100
H	-4.43302100	3.94344700	0.97429700
H	-3.36427500	4.96426500	0.00671200
H	-4.59281100	3.98269700	-0.79863600
H	-8.76391000	0.82084200	-0.93213700
H	-7.34783200	1.87819400	-1.02078500
H	-7.39645200	0.39310500	-1.98226700
H	-8.55121200	0.66751900	1.57827000
H	-7.03281200	0.12318900	2.32303400
H	-7.12549400	1.71655100	1.55851100
H	-7.33746900	-1.88491400	-0.84694100
H	-7.18429700	-1.99537300	0.92113500
H	-8.67118700	-1.37085500	0.19427400

g) Optimized XYZ coordinates (Å) for [1]$^{+}$. PBE0; SDDAll (Ni), 6-31G(d) all other atoms, in vacuum.

Ni	0.00457100	1.17813500	-0.00394000
O	1.26634800	-0.17457900	-0.06329400
O	-1.26559800	-0.16836200	-0.01702900
N	-1.22061600	2.46753900	0.57173400
N	1.23337300	2.48264400	-0.54762700
C	2.55313000	-0.10235600	-0.03651400
C	3.34432000	-1.27001800	0.27517900
C	4.71831200	-1.12950000	0.22883300
C	5.40957500	0.06279000	-0.10064300
C	4.63745200	1.17688300	-0.39123400
C	3.23799900	1.12095200	-0.34654800
C	2.50982200	2.29933500	-0.67829200
C	-0.64200700	3.69980000	1.10235600
C	-0.00716900	4.55726400	0.00896600
C	2.68741500	-2.59891600	0.64380800
C	1.80664200	-2.41169700	1.89277600
C	1.84508800	-3.10482400	-0.54076000
C	3.72384300	-3.67947600	0.97099100

C	6.93306900	0.07253800	-0.11880600
C	7.43269800	-0.95806200	-1.14743500
C	7.45903700	-0.30207100	1.27840800
C	7.49695100	1.44482400	-0.49561900
H	5.32058800	-1.99967700	0.46205200
H	5.10772800	2.12098700	-0.64950300
H	3.09313100	3.12403700	-1.09716300
H	-1.40474400	4.27206800	1.64226000
H	0.11907100	3.40647000	1.83329900
H	0.73034300	5.21728600	0.47801900
H	1.01489900	-1.67835500	1.72777500
H	1.33770000	-3.36658700	2.15659800
H	2.41068700	-2.08824800	2.74851700
H	2.47444700	-3.26554500	-1.42368300
H	1.38440000	-4.06422400	-0.27854700
H	1.05115300	-2.40288100	-0.80039300
H	4.35539900	-3.40535000	1.82423200
H	3.19948300	-4.60247300	1.23897800
H	4.36922300	-3.91082500	0.11547100
H	8.52835700	-0.96413500	-1.16183500
H	7.10046800	-1.97411600	-0.90991800
H	7.08074300	-0.71338800	-2.15563700
H	8.55470900	-0.30761600	1.27150100
H	7.12781600	0.42031600	2.03254200
H	7.12655300	-1.29698300	1.59303800
H	7.18300800	1.75656000	-1.49880500
H	7.20226000	2.22005600	0.22146800
H	8.59080700	1.40175500	-0.49654600
C	-2.55245900	-0.10066400	0.00516900
C	-3.34852800	-1.27310000	-0.27648300
C	-4.72152200	-1.12874300	-0.22445900
C	-5.40823800	0.06831600	0.09895100
C	-4.63194400	1.18160900	0.37806200
C	-3.23230000	1.12383400	0.32209200
C	-2.50246500	2.29735000	0.66555200
C	0.64907100	3.71202500	-1.08089100
C	-2.69698400	-2.60768100	-0.63503400
C	-1.83533100	-2.44348100	-1.90081900
C	-1.83528200	-3.09106700	0.54473600
C	-3.73783700	-3.69397400	-0.92657100
C	-6.93152300	0.08099100	0.12843700
C	-7.42684000	-0.94232000	1.16621400
C	-7.46714100	-0.30071800	-1.26324600
C	-7.49011800	1.45676500	0.50039600
H	-5.32724900	-1.99984700	-0.44516800
H	-5.09815000	2.12635000	0.64135400
H	-3.08911800	3.12746300	1.06898600
H	1.41263300	4.29367200	-1.60957700
H	-0.09920800	3.41394600	-1.82329200
H	-0.76076200	5.19808300	-0.46114500
H	-1.03919000	-1.70989500	-1.75993000
H	-1.37397400	-3.40437600	-2.15631400
H	-2.45181900	-2.13199000	-2.75211700
H	-2.45063500	-3.23985900	1.43954200
H	-1.37384000	-4.05252900	0.29143400
H	-1.04064500	-2.38162500	0.78025300

H	-4.37919100	-3.43718100	-1.77784800
H	-3.21726100	-4.62279600	-1.18138700
H	-4.37317700	-3.90623000	-0.05865800
H	-8.52239900	-0.94605100	1.18764600
H	-7.09833900	-1.96053200	0.93276600
H	-7.06793600	-0.69238400	2.17067300
H	-8.56277100	-0.30451500	-1.24933500
H	-7.13955600	0.41685300	-2.02353400
H	-7.13797400	-1.29787700	-1.57421600
H	-7.16986900	1.77362800	1.49998300
H	-7.19744300	2.22707300	-0.22278800
H	-8.58406000	1.41634400	0.50766100

h) Optimized XYZ coordinates (Å) for [2]$^{+}$. PBE0; SDDAll (Ni), 6-31G(d) all other atoms, in vacuum.

Pd	-0.00000500	-1.12959800	-0.00031800
O	-1.36822400	0.31883500	-0.13754700
O	1.36807200	0.31877900	0.13683700
N	1.34980000	-2.50744600	0.46307100
N	-1.35005600	-2.50754000	-0.46339800
C	-2.64998300	0.19972800	-0.07742400
C	-3.45505600	1.37731300	0.15861100
C	-4.82640400	1.21723200	0.16052900
C	-5.50531000	-0.00714500	-0.05827500
C	-4.72253900	-1.12791300	-0.27729200
C	-3.31964300	-1.06080200	-0.27118700
C	-2.62269000	-2.27507300	-0.55135700
C	0.81095200	-3.75275600	1.00436200
C	0.00049800	-4.57134400	-0.00109200
C	-2.80748400	2.73983300	0.40933200
C	-1.90760800	2.66305100	1.65689500
C	-1.98388600	3.16518200	-0.81981200
C	-3.85415600	3.83000300	0.66446600
C	-7.02864100	-0.03833200	-0.04644300
C	-7.56077200	0.91061400	-1.13557200
C	-7.53372200	0.42817300	1.33065300
C	-7.57994500	-1.44083500	-0.31602100
H	-5.43652100	2.09477700	0.33986600
H	-5.18764100	-2.09296400	-0.45450000
H	-3.24524600	-3.10321100	-0.90048000
H	1.62624500	-4.36585300	1.40579900
H	0.17503300	-3.47149000	1.85108100
H	-0.66359400	-5.22562500	0.57390900
H	-1.10374400	1.93469100	1.53409300
H	-1.45424000	3.64370600	1.84177000
H	-2.49351400	2.39306900	2.54325100
H	-2.62292200	3.24952800	-1.70639400
H	-1.53608000	4.14870700	-0.63545100
H	-1.18056700	2.45849400	-1.03355400
H	-4.46743700	3.61887300	1.54835800
H	-3.33894300	4.77871300	0.84604700
H	-4.51651600	3.98027000	-0.19613400
H	-8.65645700	0.90069400	-1.13166200
H	-7.24012000	1.94533900	-0.97536500
H	-7.22134900	0.60093200	-2.13008600
H	-8.62930900	0.42027000	1.34465100

H	-7.17860900	-0.23440800	2.12758600
H	-7.20801300	1.44678700	1.56652500
H	-7.27857000	-1.81777000	-1.30055100
H	-7.26267700	-2.16065200	0.44773600
H	-8.67422200	-1.41211000	-0.30041900
C	2.64990400	0.19964200	0.07719400
C	3.45505200	1.37713000	-0.15886800
C	4.82640000	1.21703500	-0.16019700
C	5.50525300	-0.00726700	0.05920200
C	4.72241300	-1.12794000	0.27826100
C	3.31947900	-1.06080200	0.27158000
C	2.62241500	-2.27500900	0.55159000
C	-0.81157800	-3.75273600	-1.00537100
C	2.80768800	2.73966700	-0.41004700
C	1.90786100	2.66277500	-1.65763700
C	1.98416100	3.16551900	0.81896400
C	3.85460400	3.82952500	-0.66540700
C	7.02860400	-0.03839600	0.04786200
C	7.56037300	0.91119400	1.13658800
C	7.53406500	0.42735600	-1.32933900
C	7.57993900	-1.44071300	0.31837800
H	5.43657800	2.09454300	-0.33952000
H	5.18738800	-2.09296200	0.45592300
H	3.24476500	-3.10317600	0.90099400
H	-1.62725400	-4.36594000	-1.40586500
H	-0.17683800	-3.47122500	-1.85288900
H	0.66588100	-5.22350600	-0.57699600
H	1.10367600	1.93480800	-1.53458500
H	1.45491800	3.64354400	-1.84293500
H	2.49367800	2.39218900	-2.54386900
H	2.62310600	3.24966800	1.70563200
H	1.53675600	4.14920800	0.63448700
H	1.18055700	2.45915200	1.03267200
H	4.46791100	3.61796500	-1.54917700
H	3.33959600	4.77828100	-0.84731800
H	4.51692100	3.97989300	0.19520800
H	8.65606400	0.90172700	1.13265700
H	7.23929500	1.94572700	0.97598700
H	7.22108900	0.60176700	2.13122700
H	8.62965900	0.41959300	-1.34299200
H	7.17928400	-0.23576000	-2.12597800
H	7.20827900	1.44577900	-1.56593200
H	7.27824900	-1.81714500	1.30300600
H	7.26301100	-2.16097100	-0.44510500
H	8.67421900	-1.41191300	0.30314200

i) Optimized XYZ coordinates (Å) for [3]$^{+}$. PBE0; SDDAll (Ni), 6-31G(d) all other atoms, in vacuum.

Pt	0.00003400	-1.04431300	-0.00031100
O	-1.36318000	0.41327500	-0.15109400
O	1.36325300	0.41334600	0.15032200
N	1.35855900	-2.41509800	0.43564100
N	-1.35854100	-2.41530200	-0.43580100
C	-2.65270100	0.29872200	-0.08483400
C	-3.44779300	1.48527700	0.10871200
C	-4.81964300	1.32900600	0.12830600

C	-5.50581600	0.09940600	-0.03717100
C	-4.73067300	-1.02841200	-0.22177500
C	-3.32410100	-0.96431800	-0.23140400
C	-2.63873000	-2.18423000	-0.49228500
C	0.84317700	-3.67291200	0.98059500
C	0.00107100	-4.48708000	-0.00163200
C	-2.79771000	2.85643100	0.30492900
C	-1.89834600	2.82592100	1.55426500
C	-1.97720800	3.23208900	-0.94185800
C	-3.84189900	3.95802500	0.51781800
C	-7.02968400	0.07674200	-0.01264500
C	-7.56378200	0.97178900	-1.14525100
C	-7.52398100	0.61434300	1.34206300
C	-7.58835700	-1.33502500	-0.20698600
H	-5.42501800	2.21502400	0.27953500
H	-5.19759500	-1.99860900	-0.36172100
H	-3.26535600	-3.02262100	-0.80268500
H	1.67716000	-4.28342000	1.34326500
H	0.23954100	-3.40210300	1.85333600
H	-0.64348500	-5.14250900	0.59385500
H	-1.10014600	2.08701600	1.46261600
H	-1.43760200	3.80976700	1.69934200
H	-2.48652200	2.59647500	2.45045100
H	-2.61952000	3.28420600	-1.82855500
H	-1.52551600	4.22051400	-0.79758900
H	-1.17662100	2.51615000	-1.13261600
H	-4.45287200	3.78528500	1.41153900
H	-3.32394600	4.91219100	0.65860600
H	-4.50623900	4.07403700	-0.34651700
H	-8.65946000	0.97270100	-1.13196400
H	-7.23202500	2.01041400	-1.04267000
H	-7.23595700	0.60698400	-2.12489500
H	-8.61943200	0.60814900	1.36492300
H	-7.16318300	-0.00604800	2.16985200
H	-7.19688600	1.64365900	1.52288100
H	-7.29789600	-1.76067200	-1.17469800
H	-7.26482900	-2.01693800	0.58824500
H	-8.68230300	-1.30160900	-0.18191900
C	2.65278500	0.29879100	0.08477000
C	3.44787300	1.48532700	-0.10884900
C	4.81974400	1.32911900	-0.12783400
C	5.50591200	0.09961500	0.03847200
C	4.73076000	-1.02819200	0.22317300
C	3.32419100	-0.96417800	0.23211200
C	2.63871100	-2.18406700	0.49283300
C	-0.84363500	-3.67288200	-0.98183200
C	2.79749900	2.85623900	-0.30586000
C	1.89823000	2.82478400	-1.55521700
C	1.97661500	3.23204800	0.94062500
C	3.84123100	3.95820900	-0.51912200
C	7.02978300	0.07700300	0.01445200
C	7.56353400	0.97183700	1.14739300
C	7.52447700	0.61486500	-1.34000500
C	7.58842100	-1.33478900	0.20872100
H	5.42517100	2.21505400	-0.27927800
H	5.19767800	-1.99831100	0.36366500

H	3.26515000	-3.02244100	0.80365200
H	-1.67813700	-4.28361200	-1.34292700
H	-0.24199900	-3.40166400	-1.85582100
H	0.64772700	-5.13903200	-0.59864300
H	1.10047700	2.08542000	-1.46331400
H	1.43689200	3.80829600	-1.70065000
H	2.48655600	2.59536400	-2.45131100
H	2.61870300	3.28471500	1.82745500
H	1.52454800	4.22024100	0.79593900
H	1.17628800	2.51583000	1.13142600
H	4.45254500	3.78519300	-1.41255300
H	3.32285400	4.91203400	-0.66065800
H	4.50523800	4.07510300	0.34534700
H	8.65921600	0.97281400	1.13437700
H	7.23175400	2.01047200	1.04499300
H	7.23548000	0.60677400	2.12686200
H	8.61993500	0.60876800	-1.36249500
H	7.16399900	-0.00542400	-2.16801100
H	7.19734200	1.64418100	-1.52075500
H	7.29746400	-1.76070300	1.17617000
H	7.26535600	-2.01651700	-0.58685800
H	8.68237900	-1.30132700	0.18424900

References

(1) Gorelsky, S. I. *AOMix: Program for Molecular Orbital Analysis,* [*://www.sg-chem.net/*](://www.sg-chem.net/), University of Ottawa, 2007.