Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Radical cations and dications of bis[1]benzothieno[1,4]thiazine isomers

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1 Starting Materials

All starting materials were prepared according to previously published literature.[1-4]

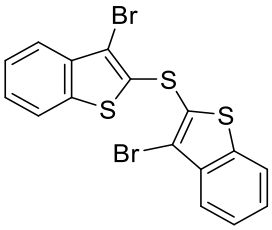


Figure S1: Bis(3-bromobenzo[*b*]thiophene-2-yl)sulfane (**1**).[1-4]

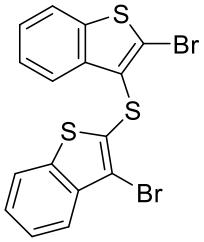


Figure S2: 2-Bromo-3-((3-bromobenzo[*b*]thiophen-2-yl)thio)benzo[*b*]thiophene (**2**).[1-4]

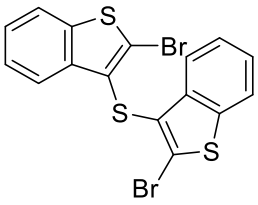


Figure S3: Bis(2-bromobenzo[*b*]thiophen-3-yl)sulfane (**3**).[1-4]

2 ^{1}H and ^{19}F NMR Spectra

2.1 *N*-(4-Fluorophenyl)bis[1]benzothieno[2,3-*b*:3′,2′-*e*][1,4]thiazine (**5**)

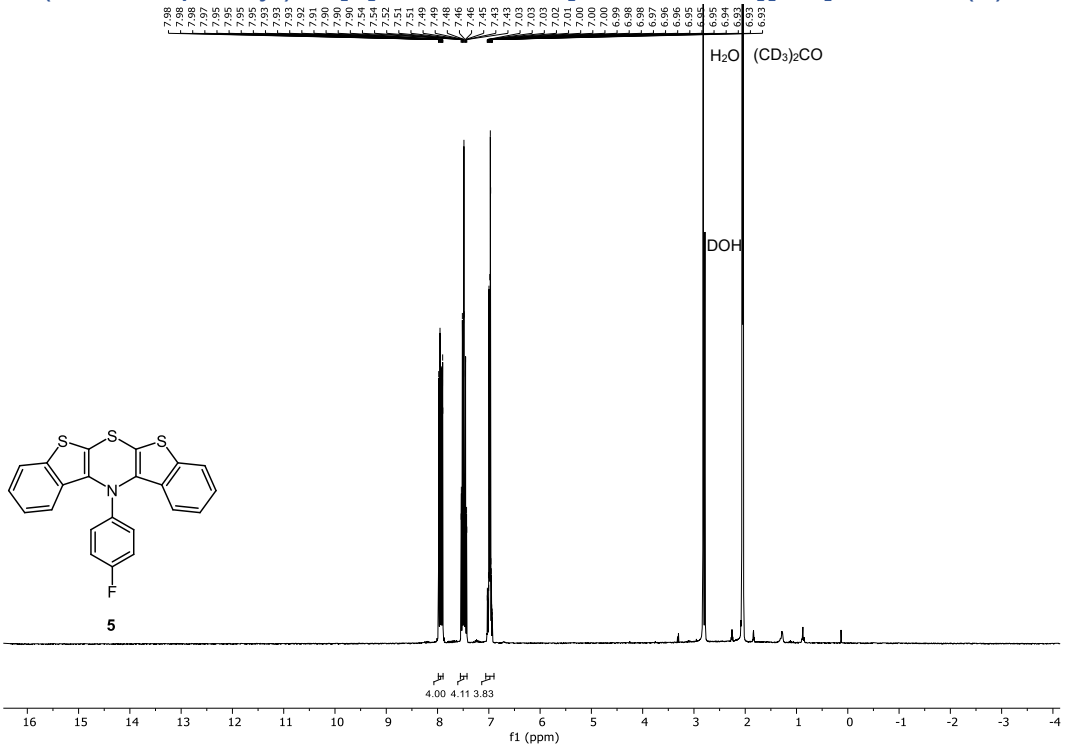


Figure S4: ^{1}H NMR spectrum of *N*-(4-fluorophenyl)bis[1]benzothieno[2,3-*b*:3′,2′-*e*][1,4]thiazine (**5**) (300 MHz, acetone-d_6, T = 298 K).

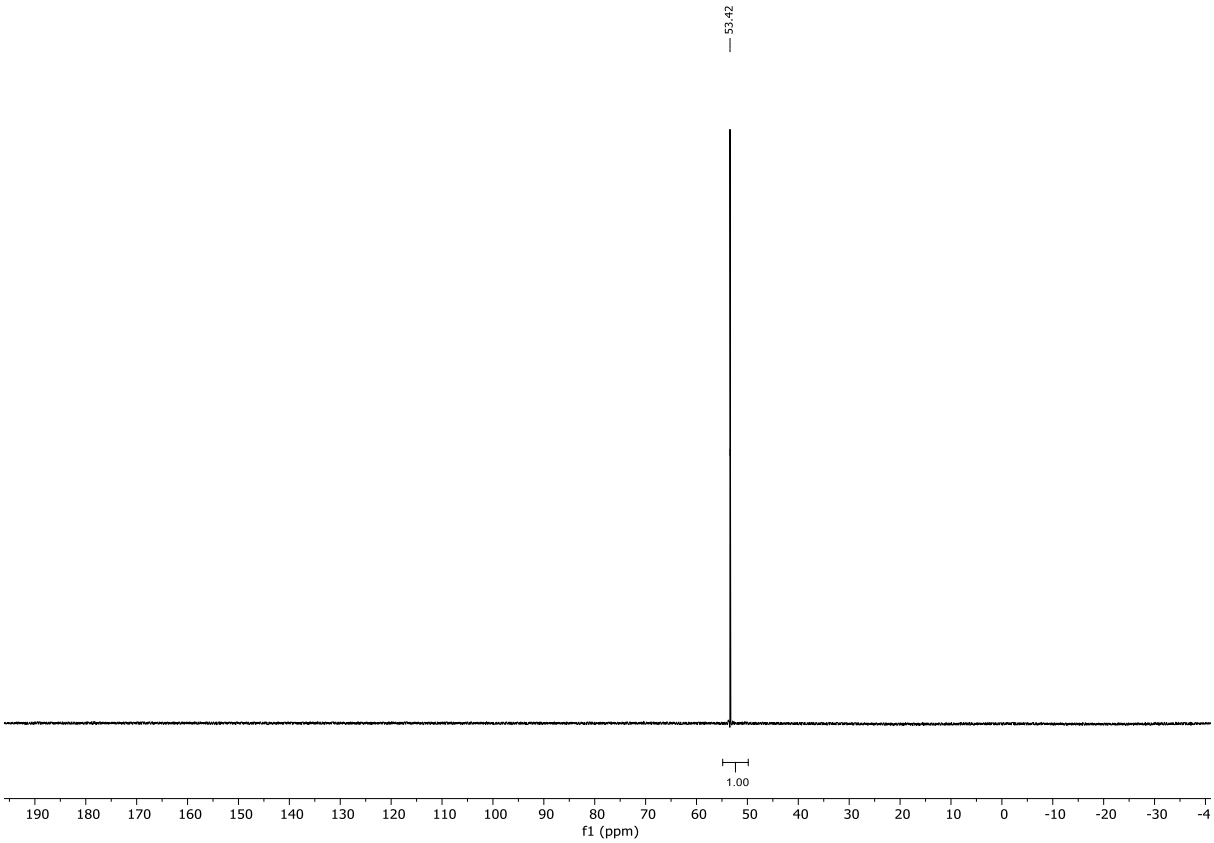


Figure S5: ^{19}F NMR spectrum of *N*-(4-fluorophenyl)bis[1]benzothieno[2,3-*b*:3′,2′-*e*][1,4]thiazine (**5**) (282 MHz, acetone-d_6,T = 298 K).

2.2 *N*-(4-Fluorophenyl)bis[1]benzothieno[2,3-*b*:2′,3′-*e*][1,4]-thiazine (**6**)

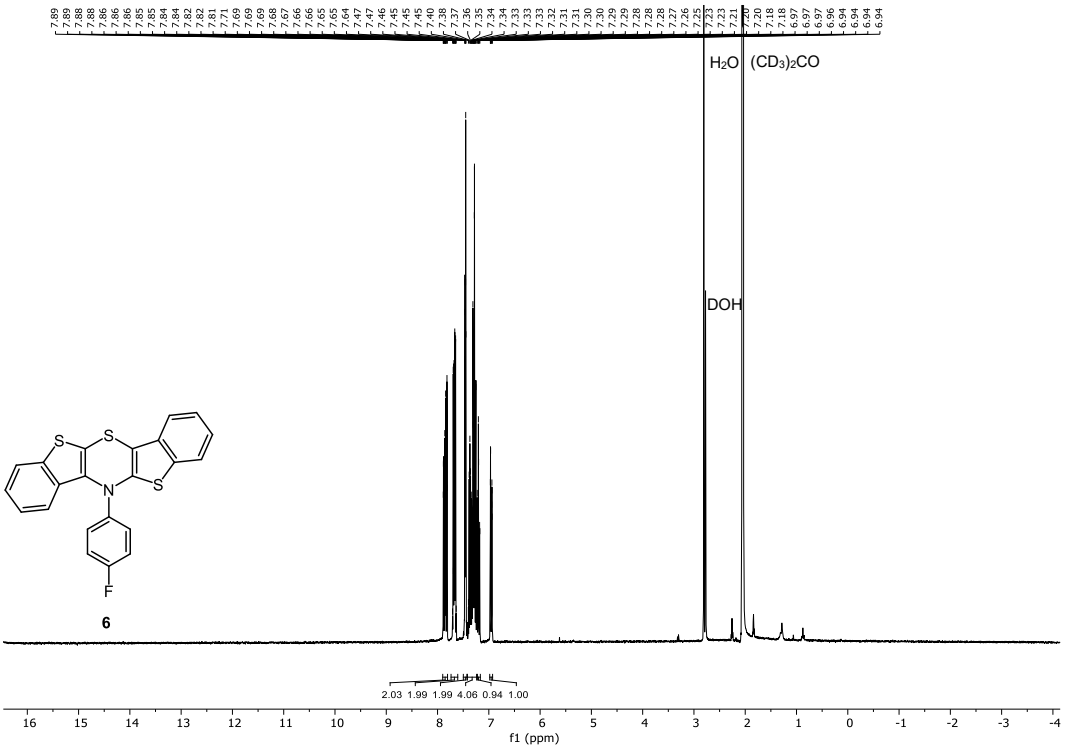


Figure S6: ^{1}H NMR spectrum of *N*-(4-fluorophenyl)bis[1]benzothieno[2,3-*b*:2′,3′-*e*][1,4]-thiazine (**6**) (300 MHz, acetone-d_6, T = 298 K).

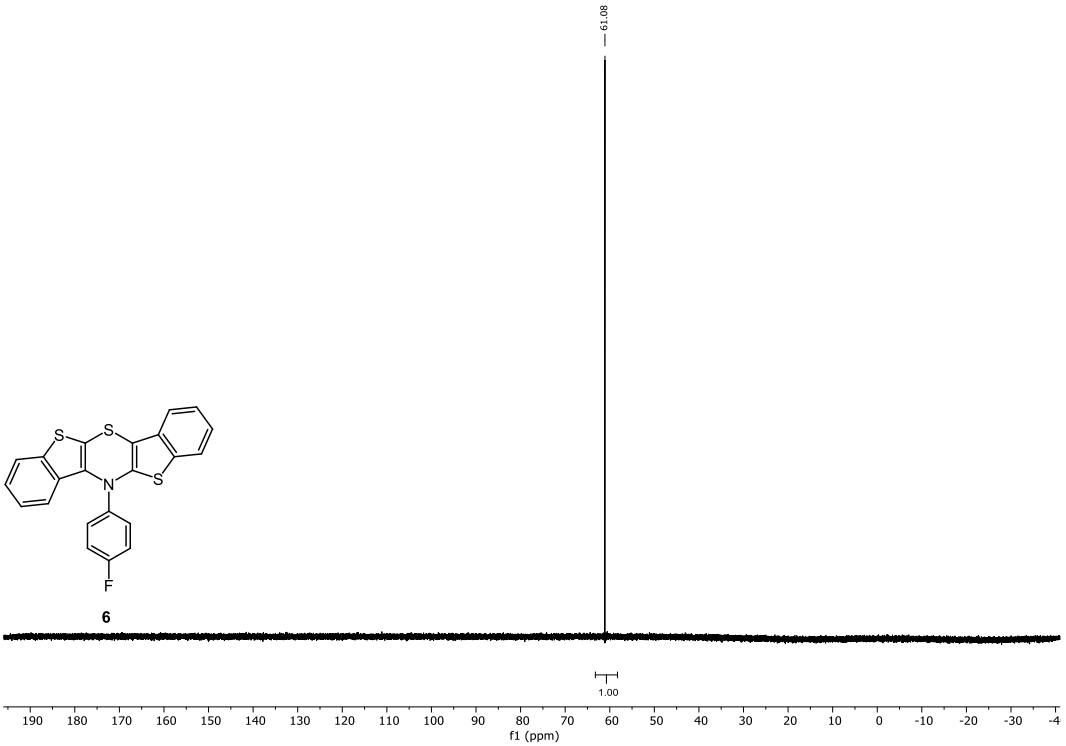


Figure S7: ^{19}F NMR spectrum of *N*-(4-fluorophenyl)bis[1]benzothieno[2,3-*b*:2′,3′-*e*][1,4]-thiazine (**6**) (282 MHz, acetone-d_6, T = 298 K).

2.3 *N*-(4-Fluorophenyl)bis[1]benzothieno[3,2-*b*:2',3'-*e*][1,4]thiazine (**7**)

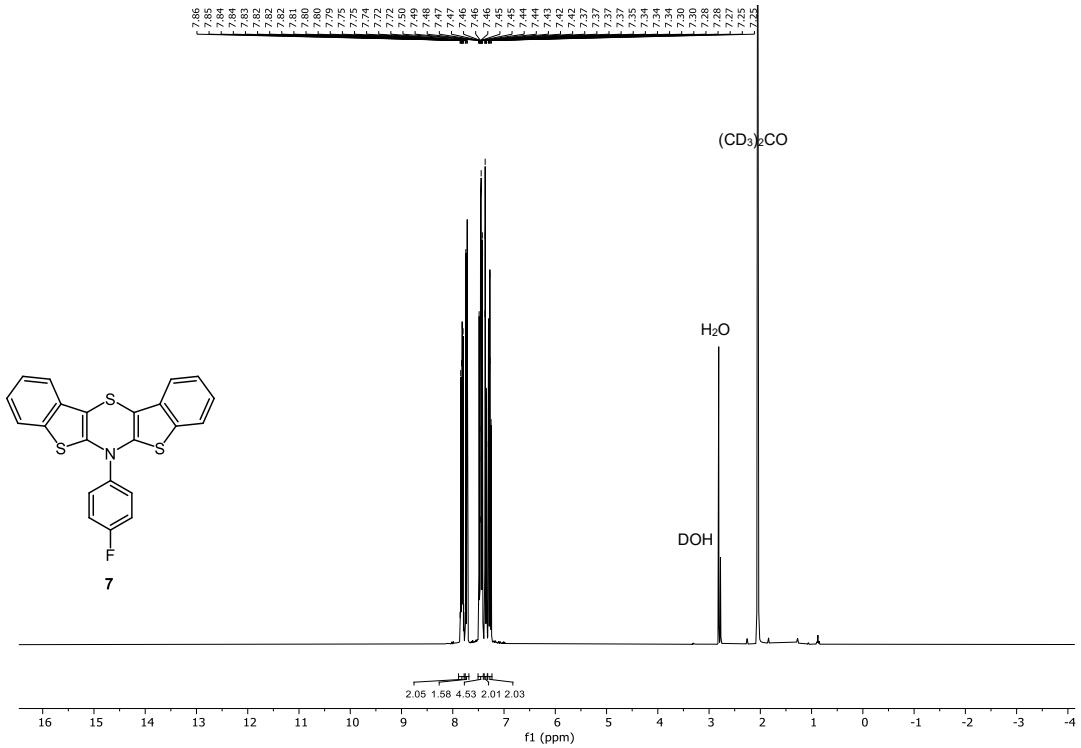


Figure S8: ^{1}H NMR spectrum of *N*-(4-fluorophenyl)bis[1]benzothieno[3,2-*b*:2',3'-*e*][1,4]thiazine (**7**) (300 MHz, acetone-d_6, T = 298 K).

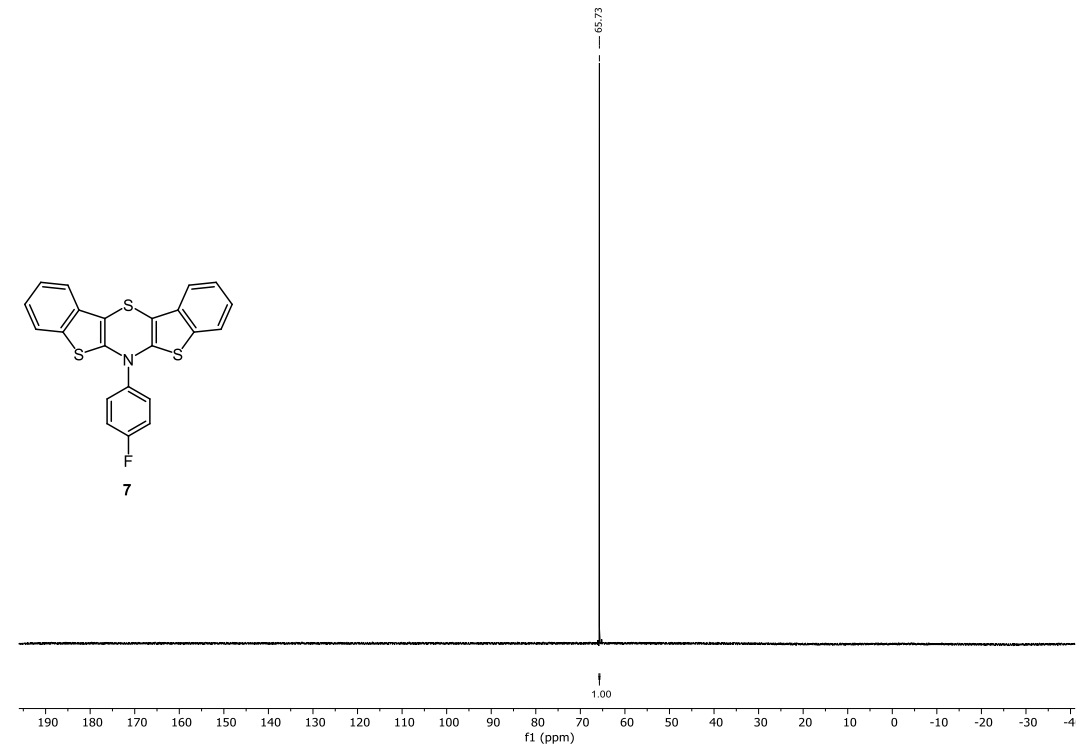


Figure S9: ^{19}F NMR spectrum of *N*-(4-fluorophenyl)bis[1]benzothieno[3,2-*b*:2',3'-*e*][1,4]thiazine (**7**) (282 MHz, acetone-d_6, T = 298 K).

2.4 Hexachloroantimonate salt of $\mathbf{5}^{2+}$

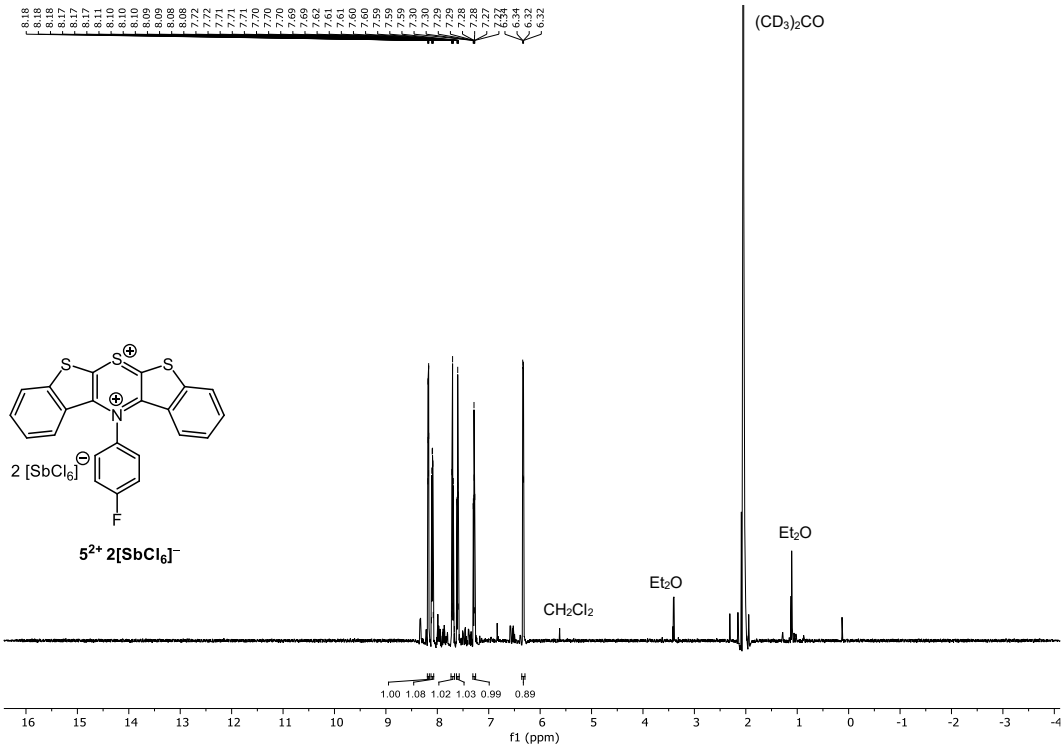


Figure S10: ^{1}H NMR spectrum of hexachloroantimonate(V) salt of $\mathbf{5}^{2+}$ (600 MHz, acetone-d_6, T = 298 K).

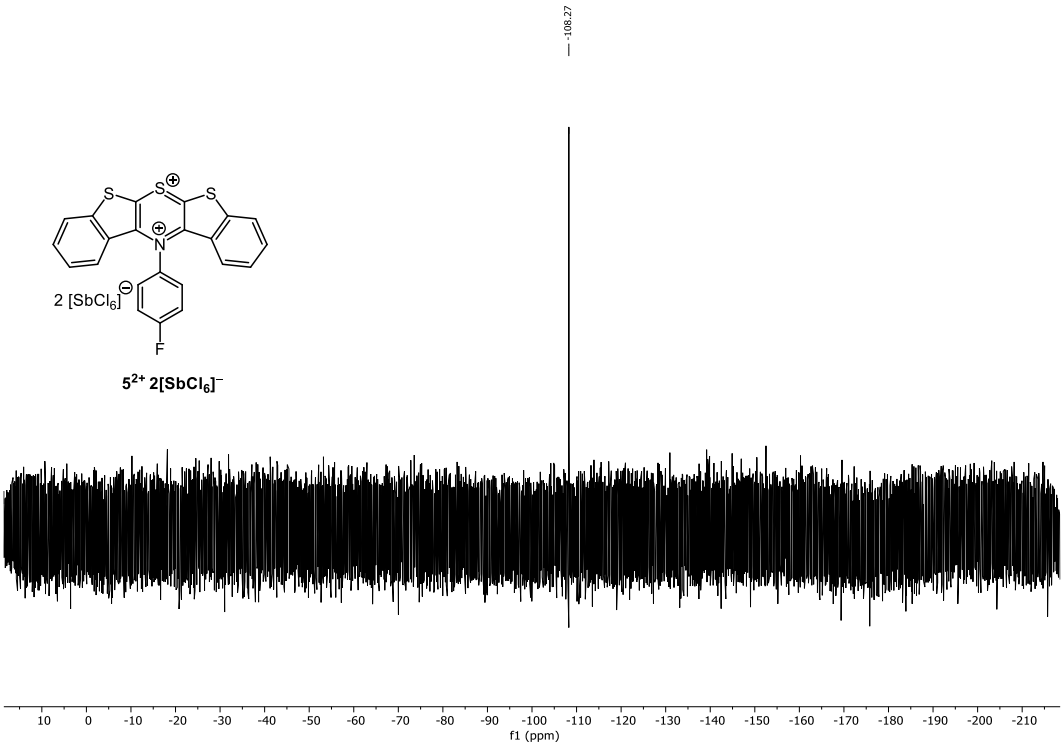


Figure S11: ^{19}F NMR spectrum of hexachloroantimonate(V) salt of $\mathbf{5}^{2+}$ (565 MHz, acetone-d_6, T = 298 K).

2.5 Hexachloroantimonate salt of $\mathbf{6}^{2+}$

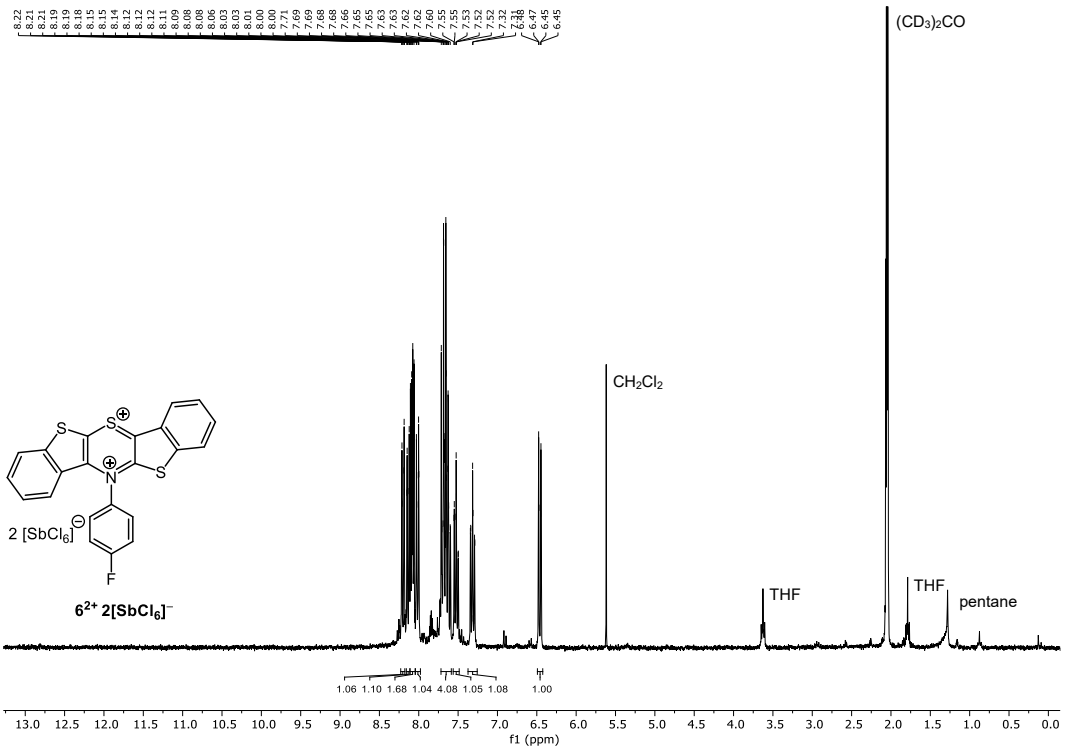


Figure S12: ^{1}H NMR spectrum of hexachloroantimonate(V) salt of $\mathbf{6}^{2+}$ (600 MHz, acetone-d_6, T = 298 K).

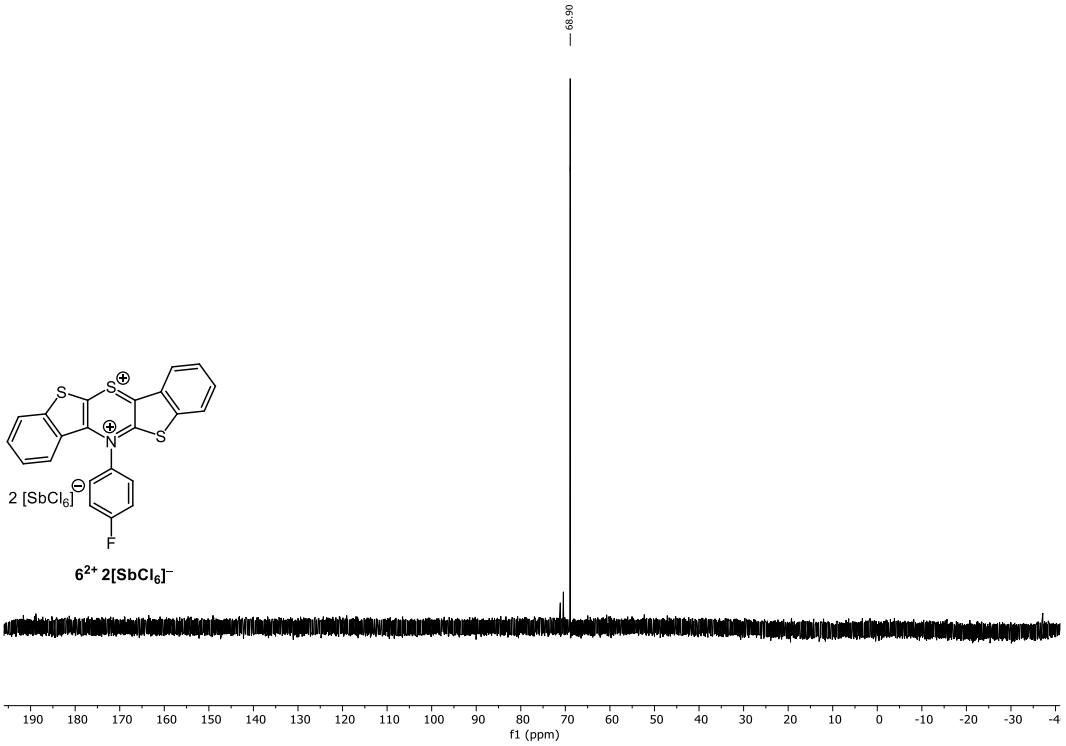


Figure S13: ^{19}F NMR spectrum of hexachloroantimonate(V) salt of $\mathbf{6}^{2+}$ (282 MHz, acetone-d_6, T = 298 K).

2.6 Hexachloroantimonate salt of $\mathbf{7}^{2+}$

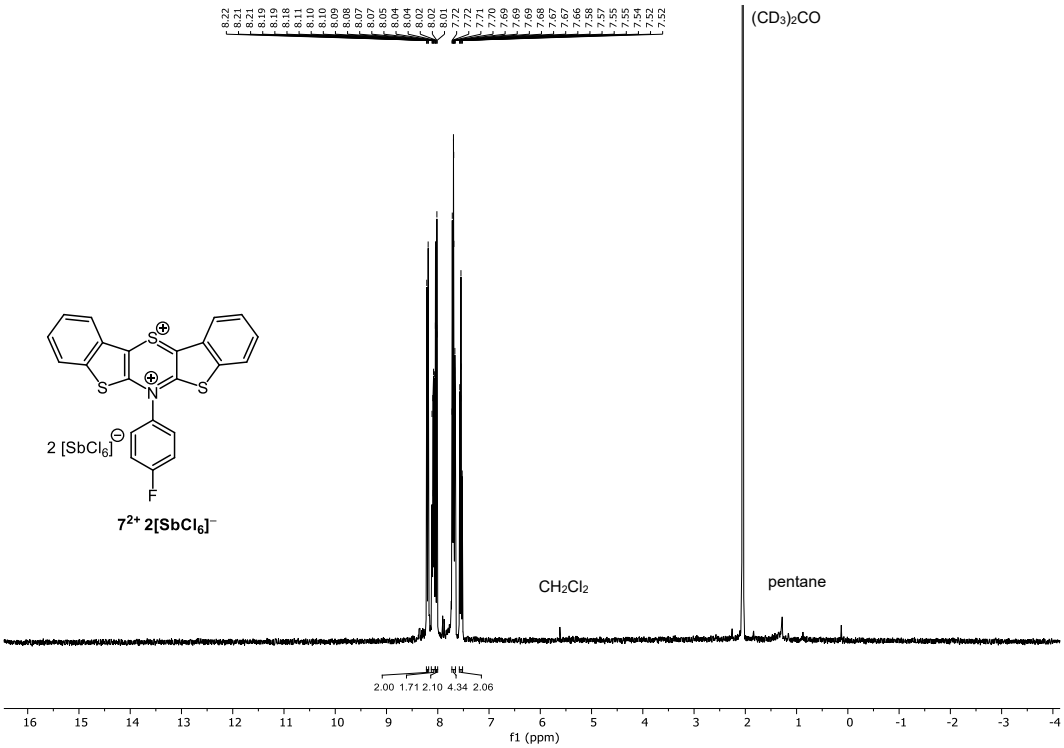


Figure S14: ^{1}H NMR spectrum of hexachloroantimonate(V) salt of $\mathbf{7}^{2+}$ (600 MHz, acetone-d_6, T = 298 K).

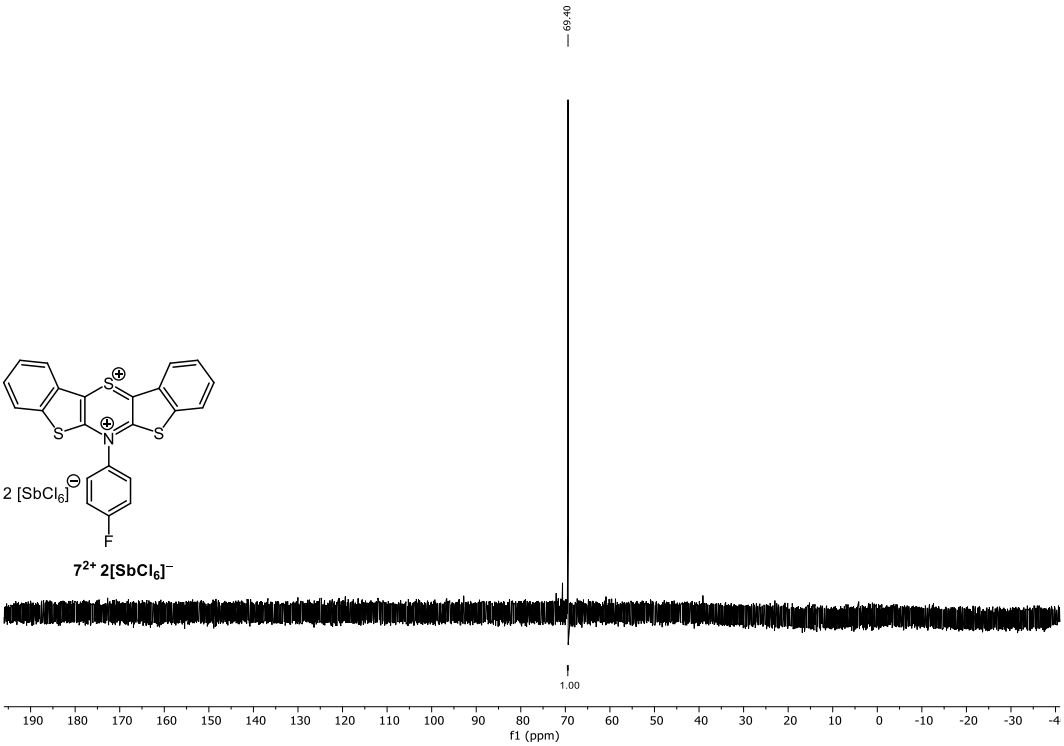


Figure S15: ^{19}F NMR spectrum of hexachloroantimonate(V) salt of $\mathbf{7}^{2+}$ (282 MHz, acetone-d_6, T = 298 K).

3 Simulated and experimental EPR-spectra of hexachloroantimonate radical cation salts of **5**$^{\bullet+}$, **6**$^{\bullet+}$ and **7**$^{\bullet+}$

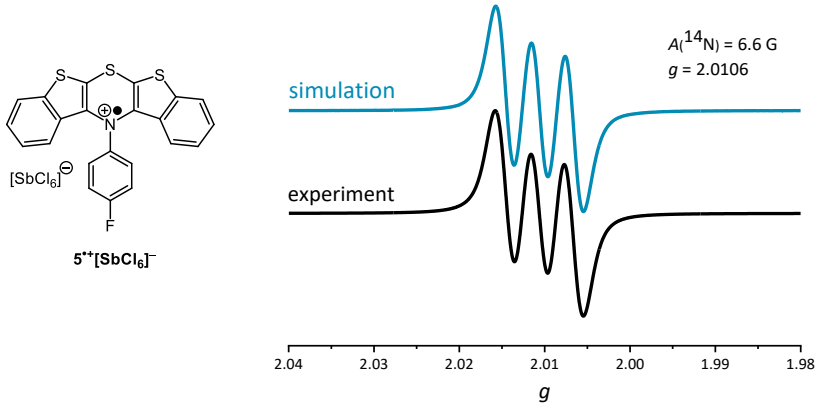


Figure S16: Simulated und experimental EPR spectrum of hexachloroantimonate salt of **5**$^{\bullet+}$ (THF, T = 298 K , g-factor referenced to external Mn^{2+} in ZnS).

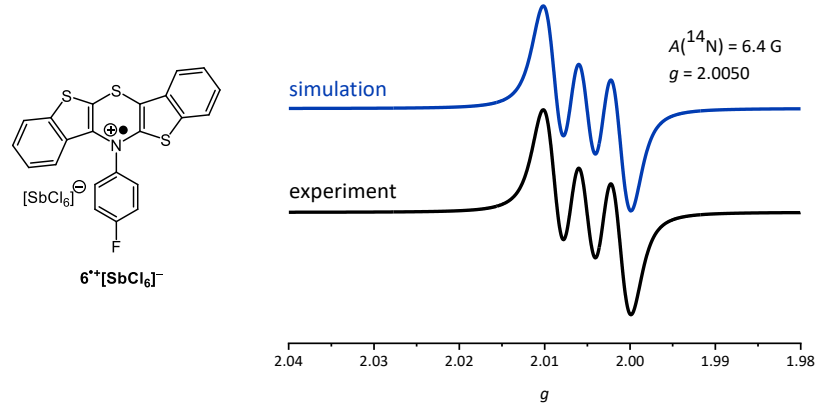


Figure S17: Simulated und experimental EPR spectrum of hexachloroantimonate salt of **6**$^{\bullet+}$ (THF, T = 298 K , g-factor referenced to external Mn^{2+} in ZnS).

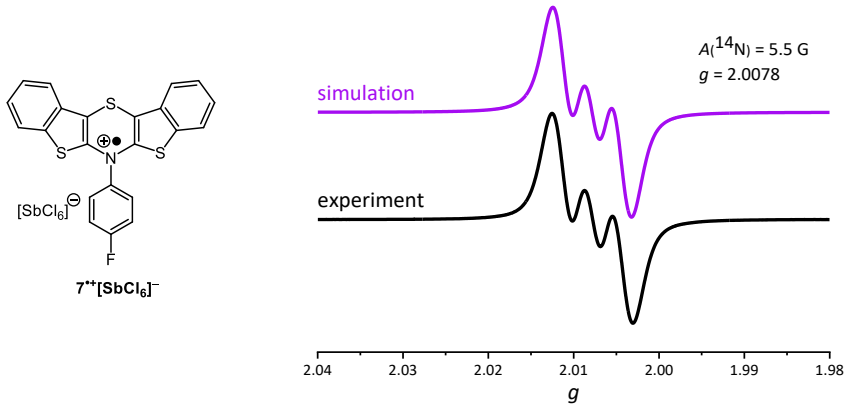


Figure S18: Simulated und experimental EPR spectrum of hexachloroantimonate salt of **7**$^{\bullet+}$ (THF, T = 298 K , g-factor referenced to external Mn^{2+} in ZnS).

4 Spectroelectrochemical data of *N*-*p*-fluorophenyl-BBTT regioisomers

The spectroelectrochemical experiments were performed with a Specac omni-cell liquid transmission cell and CaF_2 windows, equipped with Pt gauze as working and counter electrode and an Ag wire as pseudo-reference electrode, meltsealed in a polyethylene spacer (approximate path length 0.5 mm) in dichloromethane (20 ± 2 mM solutions in CH_2Cl_2, containing 0.1 M [^{n}Bu$_4$N][PF$_6$]).[5] UV/Vis spectra were recorded on a Varian Cary 5000 spectrometer using 1.0 cm cells (Hellma, Suprasil). The electrochemical part was carried out on a BioLogic SP-50 voltammetric analyzer. A UV/Vis spectrum was measured prior to application of voltage. Voltage was applied in the range from –500 mV to 1400 mV in steps of 100 mV. The exact range differed from system to system. The measurement started at low voltage rising to the maximum voltage and then decreased to lower voltages to reach the minimum voltage at the end of the measurement. A constant voltage was applied for six minutes. During this interval three UV/Vis spectra were recorded. The recording of the first UV/Vis spectrum at a certain voltage started when this voltage was applied and required ca. 90 s.

X-band CW EPR spectra were measured on a Miniscope MS 300 (Magnettech GmbH, Berlin, Germany) in solution (ca. 0.5 mM) at room temperature. *g*-factors were referenced to external Mn^{2+} in ZnS (*g* = 2.118, 2.066, 2.027, 1.986, 1.946, 1.906). The settings were as follows: *microwave frequency* = 9.48 GHz, *center field* = 3354.72 G; *sweep* = 499.77 G; *modulation amplitude* = 2000 mG; *receiver gain* = 10; *microwave attenuation* = 15 dB; *sweep time* = 90 s. Simulations of EPR spectra were performed with EasySpin (v 5.2.23) for Matlab R2016b.[6]

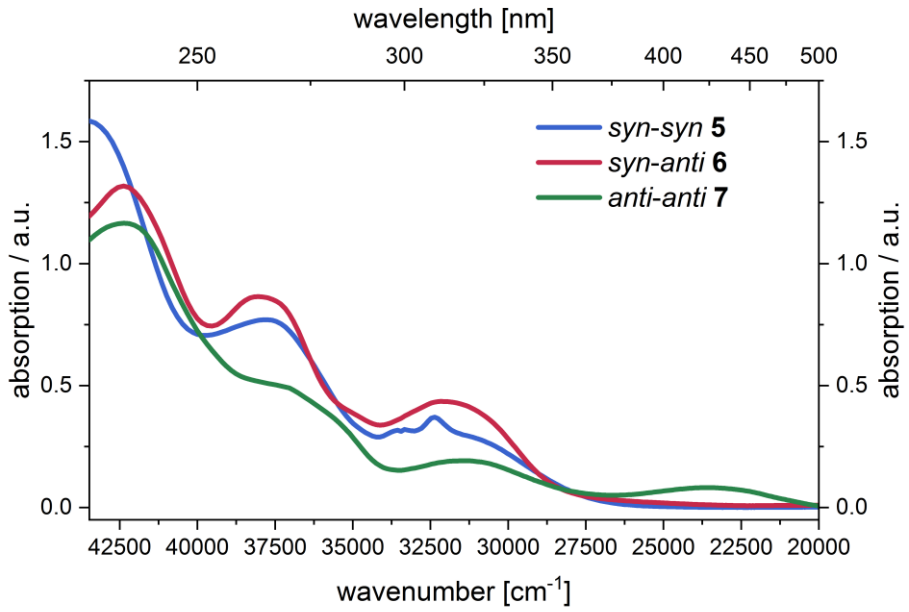


Figure S19: UV/Vis spectra of compounds **5**, **6**, and **7** in the spectroelectrochemical cell at zero potential (CH_2Cl_2, *T* = 293 K).

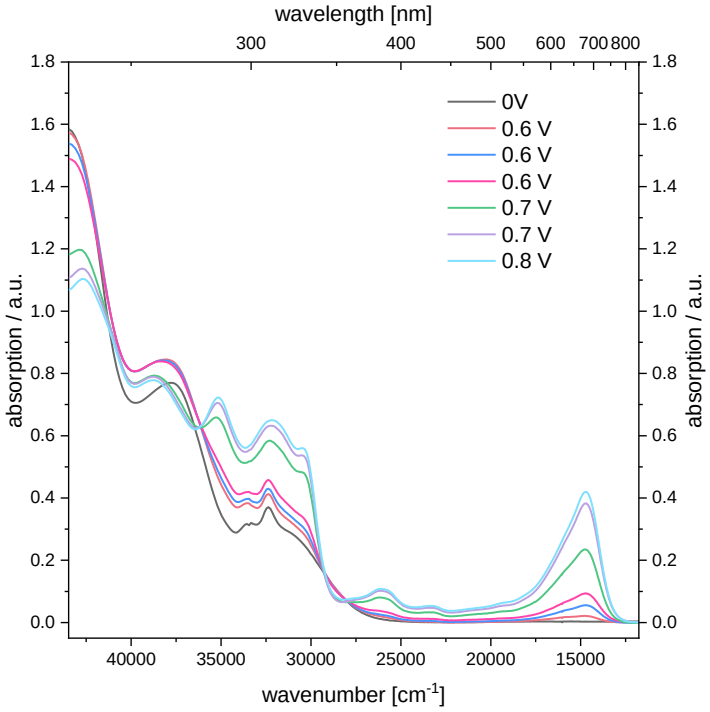


Figure S20: Spectroelectrochemical measurements of compound **5** forming the corresponding radical cation $\mathbf{5}^{\bullet+}$ (CH_2Cl_2, 293 K; electrolyte 0.1 M [^{n}Bu$_4$N][PF$_6$]; Pt working electrode, Pt counter electrode and Ag/AgCl pseudo reference electrode).

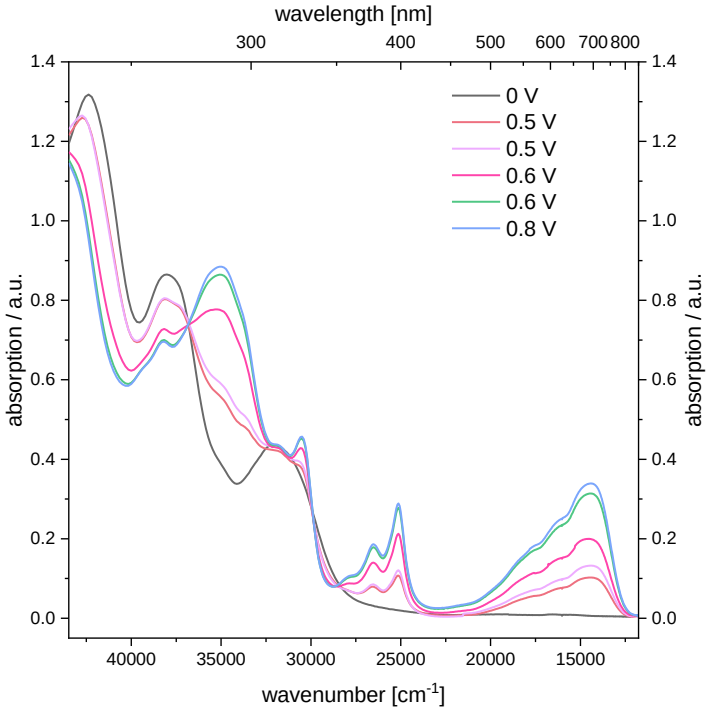


Figure S21: Spectroelectrochemical measurements of compounds **6** forming the corresponding radical cation **6**$^{\bullet+}$ (CH_2Cl_2, 293 K; electrolyte 0.1 M [*n*Bu_4N][PF_6]; Pt working electrode, Pt counter electrode and Ag/AgCl pseudo reference electrode).

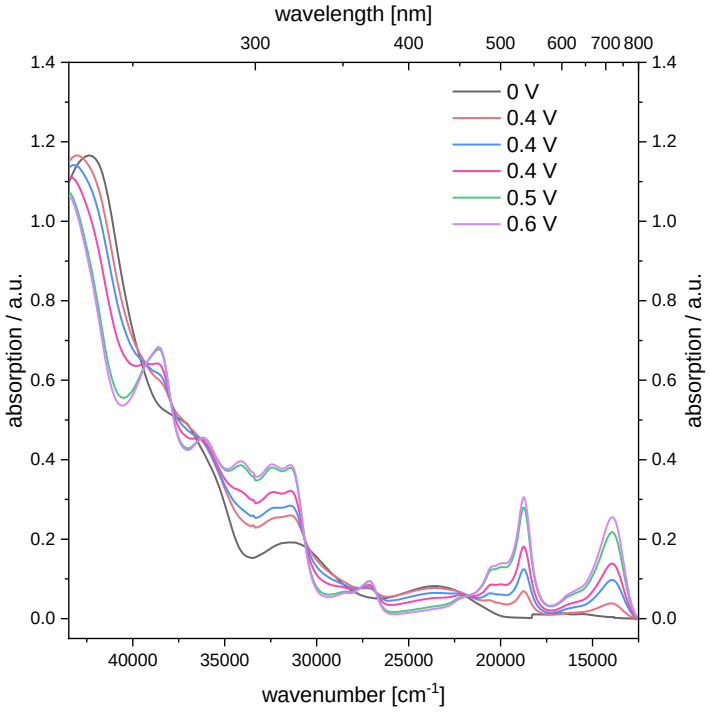


Figure S22: Spectroelectrochemical measurements of compounds **7** forming the corresponding radical cation **7**$^{\bullet+}$ (CH_2Cl_2, 293 K; electrolyte 0.1 M [*n*Bu_4N][PF_6]; Pt working electrode, Pt counter electrode and Ag/AgCl pseudo reference electrode).

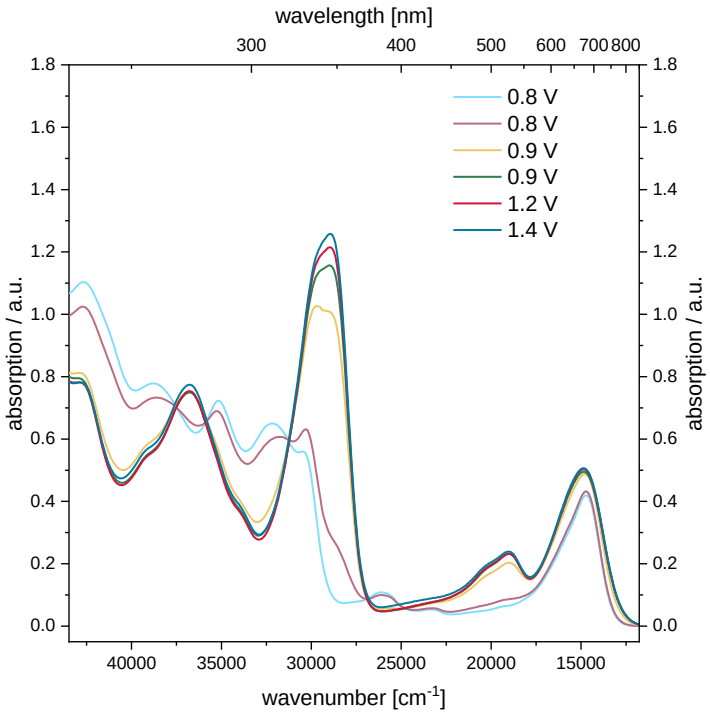


Figure S23: UV/Vis spectroelectrochemical measurements of radical cation **5**$^{\bullet+}$ forming the corresponding dications **5**$^{2+}$(CH_2Cl_2, 293 K; electrolyte 0.1 M [*n*Bu_4N][PF_6]; Pt working electrode, Pt counter electrode and Ag/AgCl pseudo reference electrode).

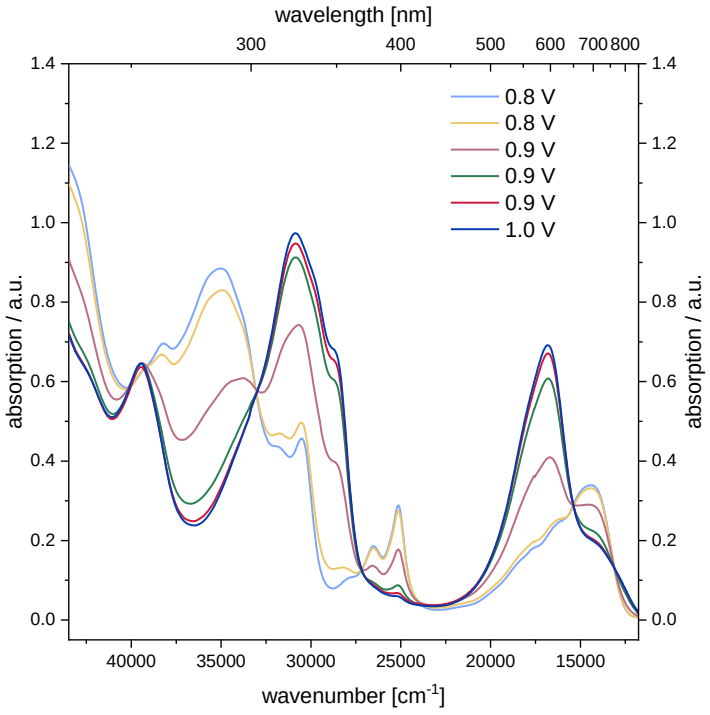


Figure S24: UV/Vis spectroelectrochemical measurements of radical cation **6**$^{\bullet+}$ forming the corresponding dications **6**$^{2+}$ (CH_2Cl_2, 293 K; electrolyte 0.1 M [*n*Bu_4N][PF_6]; Pt working electrode, Pt counter electrode and Ag/AgCl pseudo reference electrode).

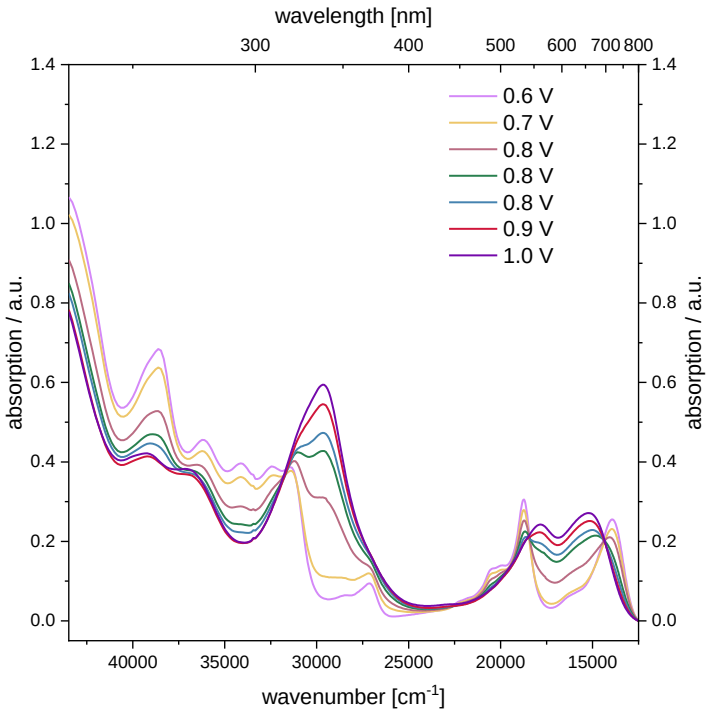


Figure S25: UV/Vis spectroelectrochemical measurements of radical cation **7**$^{\bullet+}$ forming the corresponding dications **7**$^{2+}$ (CH_2Cl_2, 293 K; electrolyte 0.1 M [*n*Bu_4N][PF_6]; Pt working electrode, Pt counter electrode and Ag/AgCl pseudo reference electrode).

In addition, a reduction of the obtained oxidized species back to the neutral state was achieved by lowering the applied potential. This was successfully performed for *syn-syn* derivate, while for *syn-anti* and *anti-anti* regioisomers irreversible side reactions of the dications were detected in addition to the proportional successful recovery of reduced compounds revealing the dications expected intrinsic instability.

Table S1: Spectroelectrochemical data of *N*-*p*-fluorophenyl-BBTTs **5**, **6**, and **7**, and corresponding radical cations $\mathbf{5}^{\bullet+}$, $\mathbf{6}^{\bullet+}$, and $\mathbf{7}^{\bullet+}$, and dications $\mathbf{5}^{2+}$, $\mathbf{6}^{2+}$, and $\mathbf{7}^{2+}$ (CH_2Cl_2, T = 293 K).

compound		**absorption maxima λ_{max} [nm]**	**isosbestic points [nm]**	
syn-syn	**5**	232, 263, 298, 309		
	$\mathbf{5}^{\bullet+}$	226, 234, 258, 284, 295 (sh), 311, 328, 382, 427, 494, 680	$\mathbf{5} \rightarrow \mathbf{5}^{\bullet+}$	243, 276, 342, 357
	$\mathbf{5}^{2+}$	227, 233, 272, 346, 494, 526, 672	$\mathbf{5}^{\bullet+} \rightarrow \mathbf{5}^{2+}$	266, 279, 320, 372, 401
syn-anti	**6**	235, 262, 311		
	$\mathbf{6}^{\bullet+}$	228, 262, 285, 315 (sh), 328, 360 (sh), 377, 398, 566 (sh), 617(sh), 694	$\mathbf{6} \rightarrow \mathbf{6}^{\bullet+}$	271, 317, 351
	$\mathbf{6}^{2+}$	224, 236 (sh), 253, 324, 349 (sh), 395, 595, 709 (sh)	$\mathbf{6}^{\bullet+} \rightarrow \mathbf{6}^{2+}$	249, 303, 368, 418, 649, 763
anti-anti	**7**	236, shoulder 268, 320, 423		
	$\mathbf{7}^{\bullet+}$	229, 259, 276, 293, 308, 318, 352, 369, 450 (sh), 490, 502, 534, 626 (sh), 717	$\mathbf{7} \rightarrow \mathbf{7}^{\bullet+}$	255, 264, 275, 326, 361, 374, 459
	$\mathbf{7}^{2+}$	223, 255, 271, 337, 561, 657	$\mathbf{7}^{\bullet+} \rightarrow \mathbf{7}^{2+}$	316, 444, 542, 697

Table S2: Experimental and TDDFT calculated (uB3LYP/6-311++G**, SCRF IEFPCM CH_2Cl_2) absorption spectra of radical cations (**5**$^{\bullet+}$, **6**$^{\bullet+}$, **7**$^{\bullet+}$) and dications (**5**$^{2+}$, **6**$^{2+}$, **7**$^{2+}$).

compound		calculated $\lambda_{max,cal}$ [nm] (oscillator strength f)	experimental $\lambda_{max,exp}$ [nm]	most dominant contribution (%)
syn-syn	**5**	339 (0.075)	309	HOMO → LUMO (94)
		292 (0.098)	298	HOMO-2 →LUMO+1 (68)
		278 (0.189)	263	HOMO-1 → LUMO+1 (56)
		245 (0.104)	232	HOMO → LUMO+10 (47)
		245 (0.269)	232	HOMO-1 → LUMO+3 (58)
		236 (0.080)	232	HOMO-1 →LUMO+4 (64)
	5$^{\bullet+}$	665 (0.191)	680	HOMO-1 → SOMO (100)
		398 (0.026)	382	HOMO-1 → LUMO (33)
		301 (0.412)	311	HOMO-2 → LUMO (60)
		300 (0.111)	311	HOMO-1 → LUMO (43)
	5^{2+}	736 (0.226)	672	HOMO → LUMO (92)
		563 (0.138)	526	HOMO-3 → LUMO (82)
		517 (0.078)	526	HOMO-4 → LUMO (91)
		470 (0.011)	494	HOMO-5 → LUMO (100)
		325 (0.578)	346	HOMO-1 → LUMO+1 (91)
syn-anti	**6**	382 (0.008)	-	HOMO → LUMO (97)
		331 (0.143)	311	HOMO → LUMO+1 (68)
		286 (0.103)	311	HOMO-1 → LUMO (77)
		269 (0.465)	262	HOMO-2 → LUMO (78)
		237 (0.150)	235	HOMO → LUMO+14 (32)
		231 (0.114)	235	HOMO-4 → LUMO+1 (46)
	6$^{\bullet+}$	714 (0.086)	694	HOMO-1 → SOMO (97)
		617 (0.156)	617	HOMO-2 → SOMO (95)
		577 (0.022)	566	HOMO-3 → SOMO (94)
		398 (0.022)	398	HOMO-6 → SOMO (57)
		391 (0.026)	377	HOMO-6 → SOMO (35)
		304 (0.102)	328	HOMO-1 → LUMO (26)
		286 (0.441)	285	HOMO-2 → LUMO (41)
	6^{2+}	817 (0.063)	broad 650-850	HOMO → LUMO (78)

		617 (0.354)	595	HOMO-1 → LUMO (64)
		387 (0.019)	395	HOMO-6 → LUMO (100)
		335 (0.135)	349	HOMO → LUMO+1 (100)
		311 (0.704)	324	HOMO-1 → LUMO+1 (100)
anti-anti	**7**	422 (0.144)	423	HOMO → LUMO (95)
		334 (0.081)	320	HOMO → LUMO+3 (84)
		279 (0.145)	268	HOMO-2 → LUMO (81)
		268 (0.178)	268	HOMO → LUMO+10 (71)
		243 (0.129)	236	HOMO → LUMO+15 (51)
		233 (0.147)	236	HOMO-2 → LUMO+6 (18)
	$7^{\bullet+}$	701 (0.154)	717	HOMO-1 → SOMO (98)
		538 (0.111)	534	HOMO-3 → SOMO (100)
		488 (0.077)	490	SOMO → LUMO (97)
		298 (0.156)	318	LUMO → LUMO+5 (50)
		292 (0.111)	308	HOMO-1 → LUMO (29)
		292 (0.215)	293	HOMO-2 → LUMO (38)
	7^{2+}	747 (0.163)	657	HOMO → LUMO (83)
		579 (0.363)	561	HOMO-2 → LUMO (84)
		328 (0.128)	337	HOMO → LUMO+1 (100)
		317 (0.490)	337	HOMO-1 → LUMO+1 (100)

5 Spectral data of hexachloroantimonate radical cation salts of **5**$^{\bullet+}$, **6**$^{\bullet+}$ and **6**$^{\bullet+}$

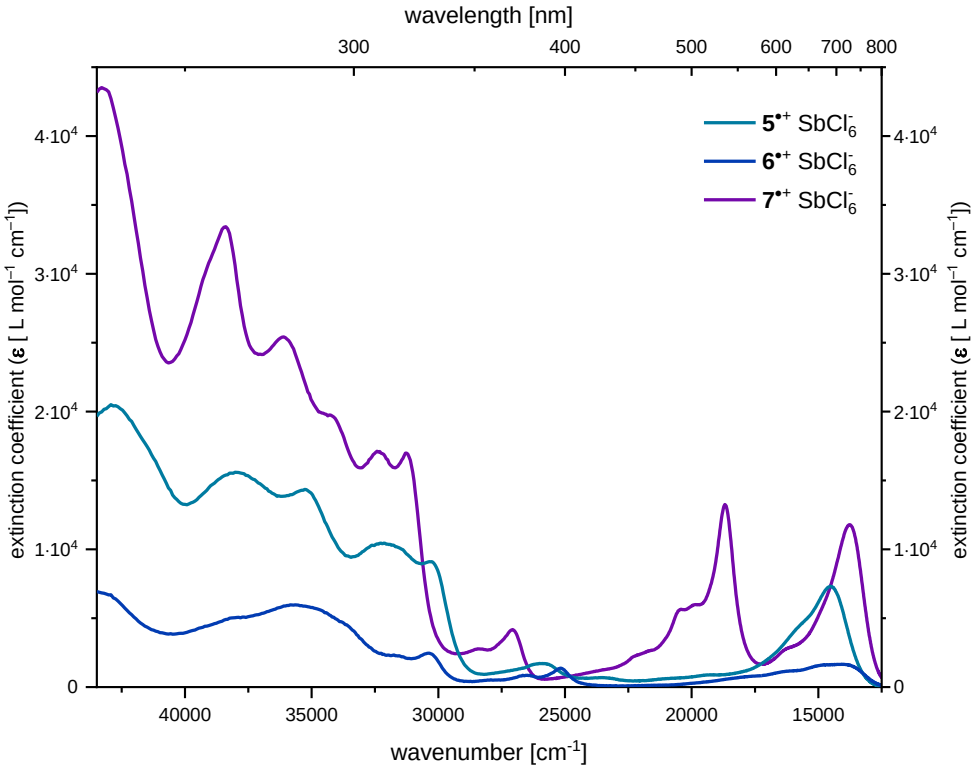


Figure S26: UV/Vis spectra from measurements of the hexachloroantimonate radical cation salts of **5**$^{\bullet+}$, **6**$^{\bullet+}$ and **7**$^{\bullet+}$ (CH_2Cl_2, T = 293 K).

Table S3: UV/Vis spectral data of hexachloroantimonate radical cations **5**$^{\bullet+}$, **6**$^{\bullet+}$, and **7**$^{\bullet+}$ (CH_2Cl_2, T = 293 K).

compound		**absorption maxima λ_{max} [nm] (ε [L mol^{-1}cm^{-1}])**
syn-syn	**5**$^{\bullet+}$	233 (20300), 263 (15700), 283 (14400), 311 (10500), 330 (9130), 386 (1740), shoulder 640 (4660), 688 (7350)
syn-anti	**6**$^{\bullet+}$	shoulder 264 (5060), 280 (5990), 329 (2450), shoulder 361 (500), 379 (840), 397 (1350), shoulder 569 (780), shoulder 628 (1180), 709 (1650)
anti-anti	**7**$^{\bullet+}$	261 (33200), 277 (25400), shoulder 292 (19700), 309 (17100), 320 (17000), shoulder 351 (2770), 370 (4170), shoulder 490 (5650), shoulder 503 (5980), 535 (13300), 726 (11800)

6 Data of Quantum Chemical Calculations

Quantum chemical calculations were performed on the DFT and TDDFT level of theory using the functionals and basis sets as implemented in the Gaussian 09 program package.[7]

6.1 Computed molecular orbital transitions of reduced compounds, radical cations and dications ((u)B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

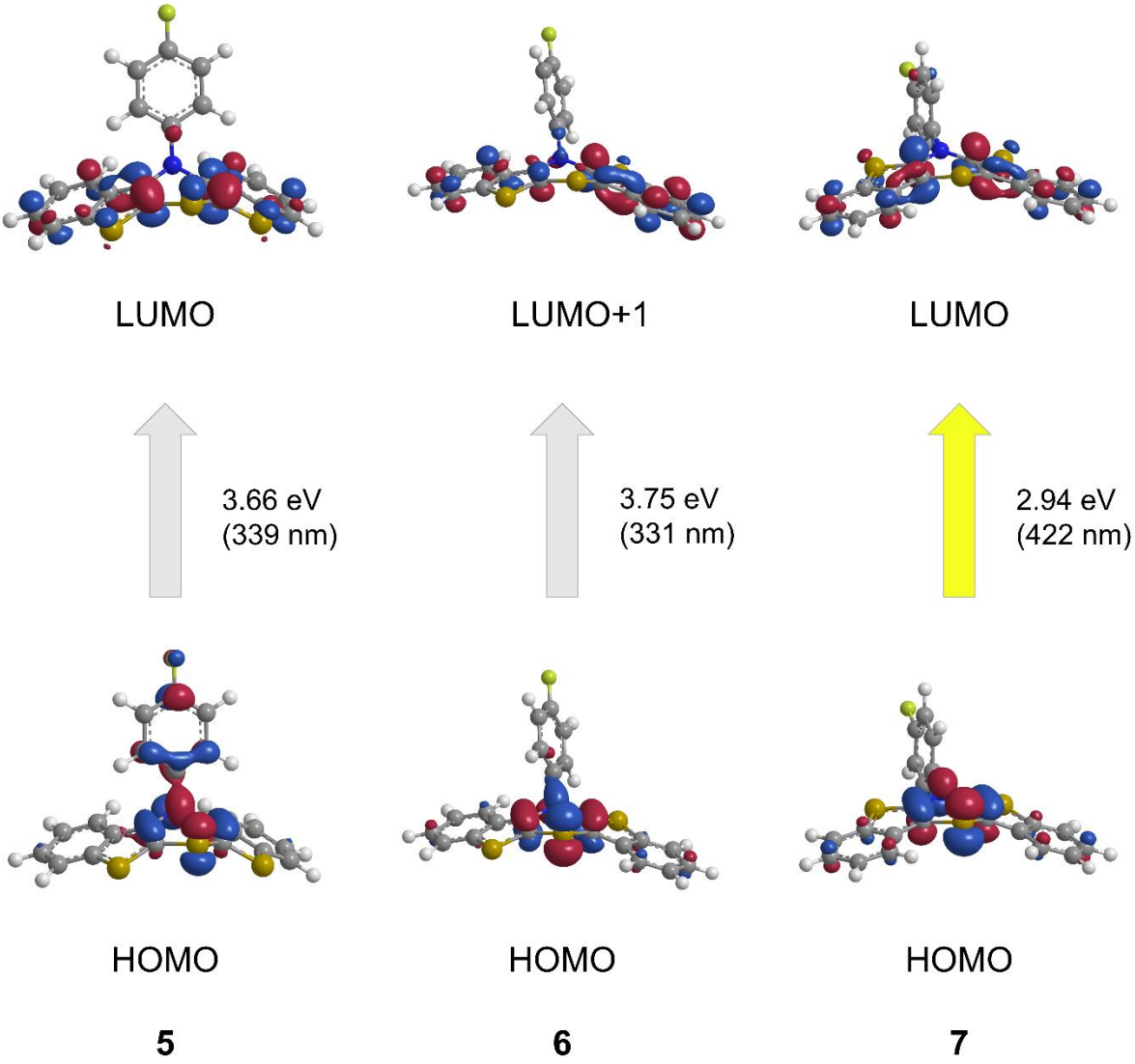


Figure S27: TDDFT calculated absorptions of neutral BBTTs **5**, **6**, and **7** illustrated by the relevant molecular orbital transitions (B3LYP/6-311++G**, IEFPCM CH_2Cl_2, isosurface value at 0.05 a.u.).

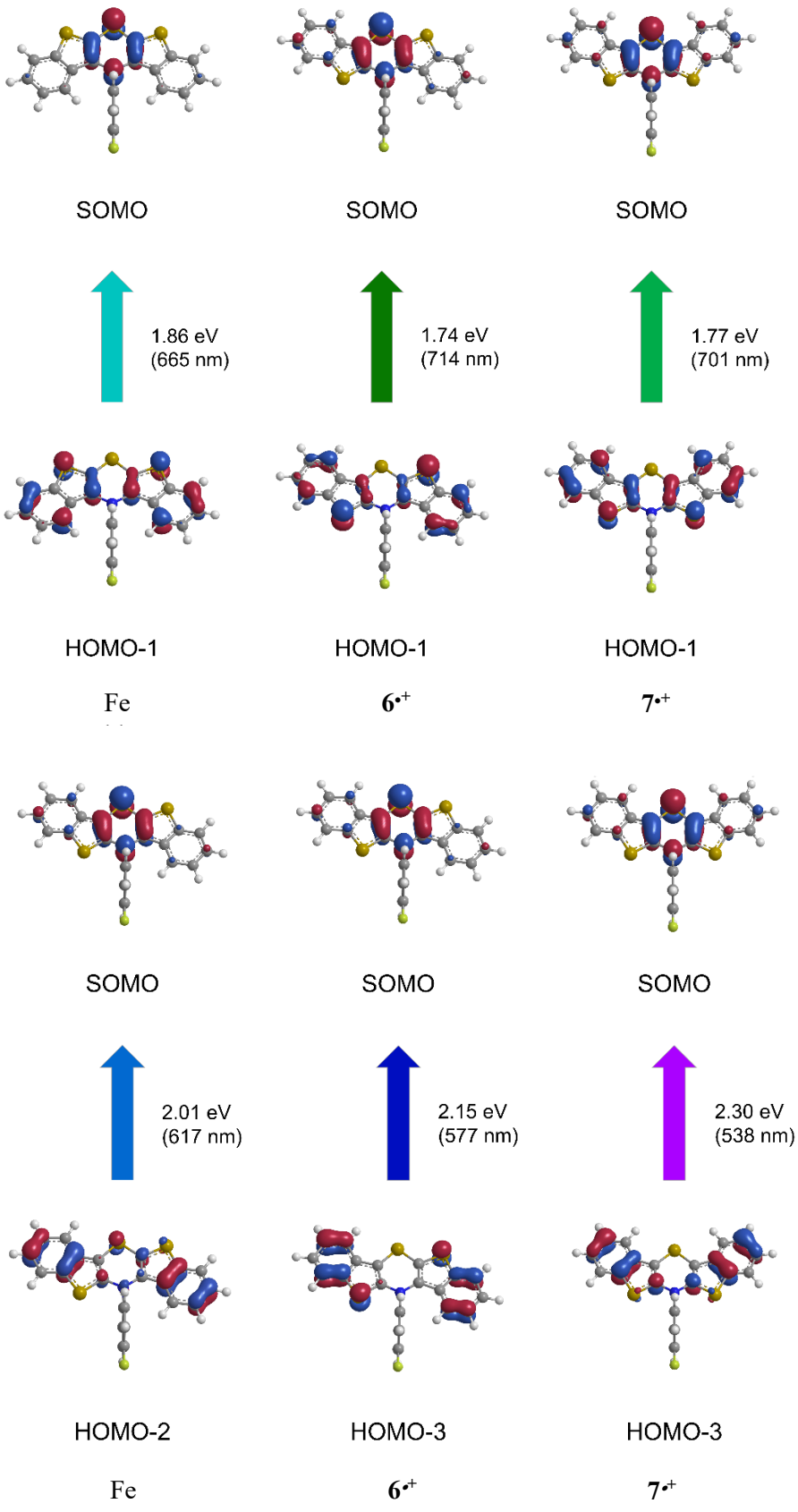


Figure S28: TDDFT calculated absorptions of radical cations **5**$^{\bullet+}$, **6**$^{\bullet+}$, and **7**$^{\bullet+}$ illustrated by the relevant molecular orbital transitions (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2, isosurface value at 0.05 a.u.).

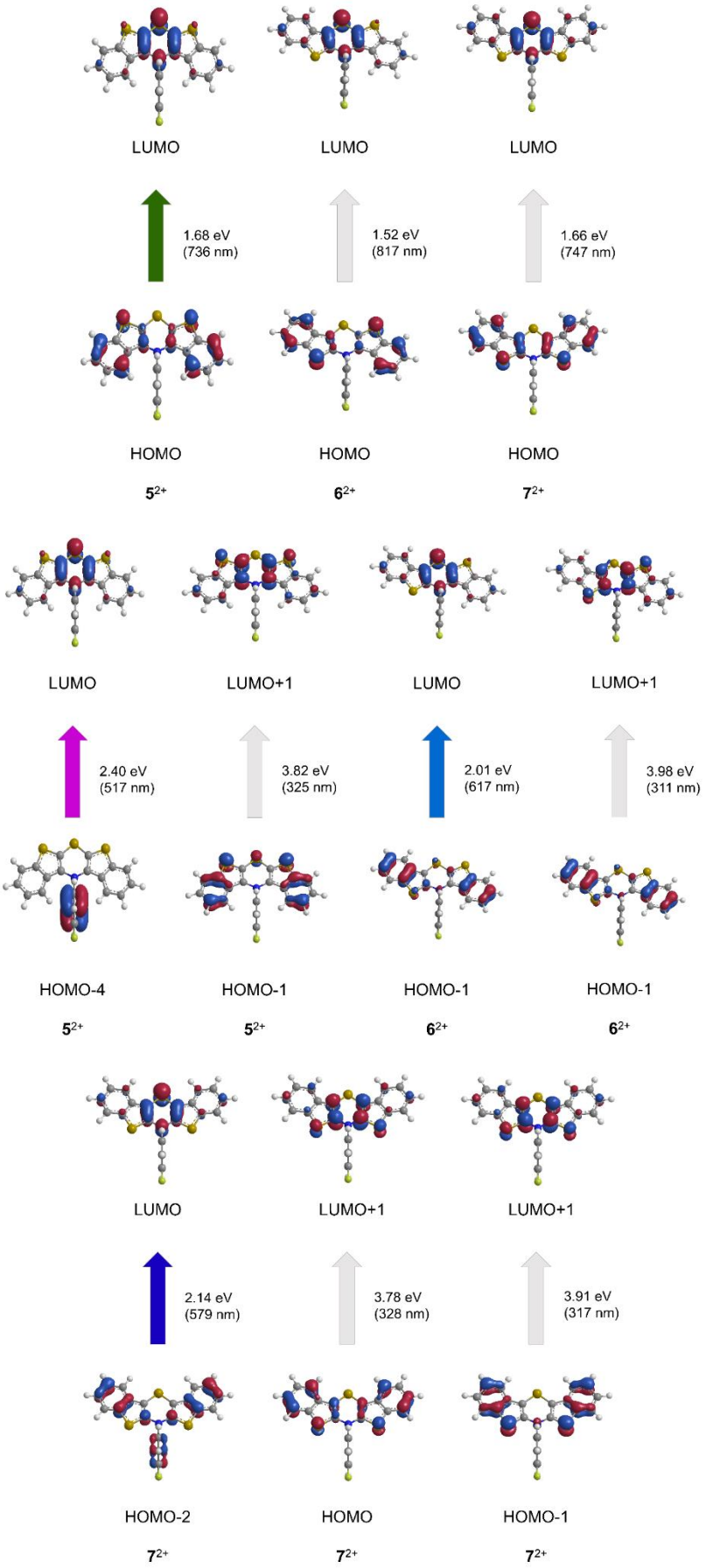


Figure S29: TDDFT calculated absorptions of dications **5**$^{2+}$, **6**$^{2+}$, and **7**$^{2+}$ illustrated by the relevant molecular orbital transitions (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2, isosurface value at 0.05 a.u.).

6.2 Computed zyx-coordinates of the S_0 state of compound **5** and excitation energies (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 0 Multiplicity = 1

C	1.30974	-1.29262	-1.23295
C	1.1888	-0.47915	-0.1461
N	0. 00000	0.27872	0.08332
C	-1.1888	-0.47915	-0.1461
C	-1.30974	-1.29262	-1.23295
S	0. 00000	-1.54576	-2.39995
C	-2.32392	-0.5562	0.74178
C	-3.31876	-1.42547	0.23897
S	-2.81414	-2.19705	-1.26463
S	2.81414	-2.19706	-1.26463
C	3.31876	-1.42547	0.23897
C	2.32392	-0.5562	0.74178
C	0. 00000	1.67543	-0.20443
C	4.52198	-1.63327	0.91523
C	4.71963	-0.97332	2.12257
C	3.73395	-0.11945	2.64649
C	2.54361	0.09447	1.96741
C	-2.54361	0.09447	1.96741
C	-3.73395	-0.11945	2.64649
C	-4.71963	-0.97331	2.12257
C	-4.52198	-1.63326	0.91523
C	-1.20606	2.38074	-0.34183
C	-1.20818	3.75149	-0.5889
C	0. 00000	4.41536	-0.70391
C	1.20818	3.75149	-0.5889
C	1.20606	2.38074	-0.34183
F	0. 00000	5.76	-0.94581
H	5.27823	-2.29904	0.51664
H	5.6439	-1.12533	2.66759

H 3.9081 0.37791 3.59359

H 1.78507 0.75482 2.37077

H -1.78507 0.75482 2.37077

H -3.9081 0.37791 3.59359

H -5.6439 -1.12532 2.66759

H -5.27823 -2.29904 0.51664

H -2.15361 1.86693 -0.26487

H -2.14024 4.29242 -0.69651

H 2.14024 4.29242 -0.69651

H 2.15361 1.86693 -0.26487

SCF Done: E(RB3LYP) = -2195.04828432 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.772350

Sum of electronic and thermal Energies= -2194.751487

Sum of electronic and thermal Enthalpies= -2194.750543

Sum of electronic and thermal Free Energies= -2194.822931

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.5750 eV 346.81 nm f=0.0449 <S**2>=0.000

104 ->106 0.69941

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

Total Energy, E(TD-HF/TD-KS) = -2194.91690685

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

Excited State 2: Singlet-A 3.6551 eV 339.21 nm f=0.0749 <S**2>=0.000

103 ->106 -0.10708

104 ->105 0.68703

Excited State 3: Singlet-A 4.1939 eV 295.63 nm f=0.0026 <S**2>=0.000

103 ->105 -0.11408

104 ->107 0.68182

Excited State 4: Singlet-A 4.2496 eV 291.75 nm f=0.0975 <S**2>=0.000

102 ->106 0.58517

103 ->105 -0.35194

Excited State 5: Singlet-A 4.2600 eV 291.04 nm f=0.0205 <S**2>=0.000

102 ->105 0.54044

103 ->106 -0.38250

104 ->108 -0.17060

Excited State 6: Singlet-A 4.3028 eV 288.15 nm f=0.0944 <S**2>=0.000

102 ->106 0.36355

103 ->105 0.57943

Excited State 7: Singlet-A 4.3389 eV 285.75 nm f=0.0106 <S**2>=0.000

100 ->106 -0.10254

101 ->105 -0.13727

102 ->105 0.21905

104 ->108 0.63698

Excited State 8: Singlet-A 4.4582 eV 278.10 nm f=0.1887 <S**2>=0.000

102 ->105 0.36503

102 ->108 0.11417

103 ->106 0.52861

104 ->105 0.11664

104 ->108 -0.12380

Excited State 9: Singlet-A 4.4964 eV 275.74 nm f=0.0012 <S**2>=0.000

100 ->105 0.13387

101 ->106 0.26071

103 ->108 -0.14165

104 ->109 0.59980

Excited State 10: Singlet-A 4.5956 eV 269.79 nm f=0.0005 <S**2>=0.000

100 ->106 0.11391

101 ->105 0.57540

102 ->108 -0.14537

103 ->106 0.14283

103 ->107 0.14694

104 ->108 0.19706

104 ->110 0.16512

Excited State 11: Singlet-A 4.6009 eV 269.48 nm f=0.0067 <S**2>=0.000

101 ->106 -0.22795

104 ->109 0.15617

104 ->111 0.59573

104 ->114 -0.12373

Excited State 12: Singlet-A 4.6140 eV 268.71 nm f=0.0781 <S**2>=0.000

101 ->105 -0.15246

103 ->111 -0.10807

104 ->110 0.64058

Excited State 13: Singlet-A 4.6424 eV 267.07 nm f=0.0362 <S**2>=0.000

100 ->105 0.12063

101 ->106 0.48851

102 ->107 0.11936

102 ->109 0.11936

104 ->109 -0.30546

104 ->111 0.27576

Excited State 14: Singlet-A 4.8314 eV 256.62 nm f=0.0145 <S**2>=0.000

100 ->106 0.29166

101 ->105 -0.26626

102 ->108 -0.11355

103 ->107 0.54209

Excited State 15: Singlet-A 4.8460 eV 255.85 nm f=0.0576 <S**2>=0.000

100 ->105 0.30262

101 ->106 -0.26890

102 ->107 0.51554

103 ->108 -0.16002

Excited State 16: Singlet-A 4.8847 eV 253.82 nm f=0.0287 <S**2>=0.000

100 ->105 0.42460

101 ->106 -0.15367

102 ->107 -0.40000

102 ->109 0.13794

103 ->108 -0.29529

Excited State 17: Singlet-A 4.9194 eV 252.03 nm f=0.0184 <S**2>=0.000

100 ->106 -0.17525

104 ->110 -0.11438

104 ->112 0.52060

104 ->113 -0.38763

Excited State 18: Singlet-A 4.9717 eV 249.38 nm f=0.0409 <S**2>=0.000

100 ->106 0.26938

101 ->105 -0.10716

103 ->107 -0.16202

103 ->109 0.14769

103 ->111 0.13837

104 ->112 0.41669

104 ->113 0.34795

104 ->115 0.12032

Excited State 19: Singlet-A 4.9930 eV 248.32 nm f=0.0668 <S**2>=0.000

100 ->106 -0.22155

101 ->108 -0.10334

102 ->108 0.27246

103 ->107 0.31510

103 ->109 -0.24796

104 ->112 0.11741

104 ->113 0.32556

104 ->115 0.22095

Excited State 20: Singlet-A 5.0020 eV 247.87 nm f=0.0230 <S**2>=0.000

101 ->111 0.18187

103 ->110 0.44571

103 ->113 -0.10291

104 ->114 -0.38078

104 ->118 0.19395

104 ->122 0.11041

Excited State 21: Singlet-A 5.0629 eV 244.89 nm f=0.1035 <S**2>=0.000

100 ->106 0.19734

102 ->108 0.14480

103 ->107 -0.14786

103 ->111 -0.27372

104 ->110 -0.12324

104 ->113 -0.21277

104 ->115 0.48377

Excited State 22: Singlet-A 5.0654 eV 244.77 nm f=0.2692 <S**2>=0.000

100 ->105 0.37764

103 ->108 0.53977

103 ->110 -0.11691

Excited State 23: Singlet-A 5.1244 eV 241.95 nm f=0.0504 <S**2>=0.000

100 ->106 0.21698

102 ->108 0.56014

102 ->110 -0.10031

103 ->109 0.16932

103 ->111 0.13288

104 ->115 -0.19530

Excited State 24: Singlet-A 5.1528 eV 240.62 nm f=0.0128 <S**2>=0.000

101 ->110 0.25717

102 ->110 0.16302

103 ->109 -0.12340

103 ->111 0.47005

104 ->113 -0.16564

104 ->115 0.27732

Excited State 25: Singlet-A 5.1682 eV 239.90 nm f=0.0413 <S**2>=0.000

101 ->111 0.15536

103 ->108 0.13568

103 ->110 0.36621

104 ->111 0.15609

104 ->114 0.47481

104 ->118 -0.10611

Excited State 26: Singlet-A 5.2277 eV 237.17 nm f=0.0124 <S**2>=0.000

99 ->105 0.11057

100 ->105 -0.11696

102 ->107 0.10299

102 ->109 0.58123

102 ->111 -0.23309

Excited State 27: Singlet-A 5.2601 eV 235.71 nm f=0.0803 <S**2>=0.000

100 ->106 -0.27259

102 ->110 0.14923

102 ->113 -0.11012

103 ->109 0.56391

104 ->115 0.11715

Excited State 28: Singlet-A 5.2606 eV 235.69 nm f=0.0663 <S**2>=0.000

101 ->107 0.46361

102 ->109 -0.21836

102 ->111 -0.37810

103 ->110 0.18490

Excited State 29: Singlet-A 5.2696 eV 235.28 nm f=0.0627 <S**2>=0.000

100 ->106 0.15808

102 ->110 0.59212

103 ->111 -0.19336

104 ->115 -0.14149

Excited State 30: Singlet-A 5.3058 eV 233.68 nm f=0.0011 <S**2>=0.000

101 ->107 0.46984

102 ->107 0.10977

102 ->109 0.12634

102 ->111 0.42687

Excited State 31: Singlet-A 5.4166 eV 228.90 nm f=0.0047 <S**2>=0.000

99 ->106 -0.16846

101 ->110 -0.10758

102 ->112 -0.19455

102 ->113 0.12169

103 ->114 -0.11384

104 ->116 0.13622

104 ->117 0.57113

Excited State 32: Singlet-A 5.4241 eV 228.58 nm f=0.0176 <S**2>=0.000

99 ->105 0.49673

103 ->110 -0.11580

103 ->112 0.21217

103 ->113 -0.15632

104 ->114 0.13042

104 ->118 0.32687

Excited State 33: Singlet-A 5.4279 eV 228.42 nm f=0.0004 <S**2>=0.000

99 ->105 0.46127

102 ->109 -0.11190

103 ->112 -0.19925

104 ->114 -0.15076

104 ->118 -0.37666

104 ->119 -0.12083

104 ->122 -0.10332

Excited State 34: Singlet-A 5.4334 eV 228.19 nm f=0.0118 <S**2>=0.000

99 ->106 0.55680

101 ->108 -0.19496

104 ->116 0.34083

Excited State 35: Singlet-A 5.4435 eV 227.77 nm f=0.0139 <S**2>=0.000

99 ->106 -0.31864

101 ->110 0.10146

102 ->112 -0.13798

102 ->113 -0.12412

104 ->116 0.52100

104 ->117 -0.19675

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 640.

Leave Link 914 at Tue Jan 5 20:00:31 2021, MaxMem= 1610612736 cpu: 45551.7

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

6.3 Computed zyx-coordinates of the S_0 state of compound **6** and excitation energies (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 0 Multiplicity = 1

C	-0.40793	-1.85991	0.77493
C	-0.94282	-0.87539	-0.0004
N	-0.2691	0.34458	-0.29153
C	1.13535	0.27366	-0.28737

C	1.89606	-0.61642	0.4059
S	1.17991	-1.78522	1.55195
S	-1.42276	-3.28986	0.88318
C	-2.64462	-2.51431	-0.12172
C	-2.23135	-1.23272	-0.55087
S	2.11588	1.29034	-1.35808
C	3.58792	0.51246	-0.78944
C	3.30801	-0.51951	0.13694
C	-0.90573	1.58239	0.09786
C	-0.93328	2.66179	-0.78768
C	-1.53209	3.86368	-0.41561
C	-2.11796	3.94973	0.83645
C	-2.12422	2.89104	1.73039
C	-1.50451	1.70191	1.35482
F	-2.71601	5.11673	1.20024
C	-3.86777	-3.0622	-0.50997
C	-4.68616	-2.31667	-1.35095
C	-4.28657	-1.04716	-1.79949
C	-3.0721	-0.50201	-1.40766
C	4.89409	0.82054	-1.16988
C	5.9344	0.07464	-0.62555
C	5.67434	-0.95887	0.28835
C	4.37472	-1.25876	0.67346
H	-0.50104	2.56438	-1.77577
H	-1.55986	4.7106	-1.08945
H	-2.59338	2.99998	2.70015
H	-1.48709	0.86467	2.04184
H	-4.16967	-4.04619	-0.17119
H	-5.63974	-2.72399	-1.66601
H	-4.93666	-0.48573	-2.46051
H	-2.77222	0.47783	-1.75715
H	5.09474	1.61617	-1.87755
H	6.95569	0.29432	-0.91391

H 6.49939 -1.52911 0.69913

H 4.18253 -2.05742 1.38093

SCF Done: E(RB3LYP) = -2195.04961264 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.773991

Sum of electronic and thermal Energies= -2194.752958

Sum of electronic and thermal Enthalpies= -2194.752013

Sum of electronic and thermal Free Energies= -2194.825650

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.2447 eV 382.12 nm f=0.0076 <S**2>=0.000

104 ->105 0.69517

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

Total Energy, E(TD-HF/TD-KS) = -2194.93037336

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

Excited State 2: Singlet-A 3.7115 eV 334.05 nm f=0.0373 <S**2>=0.000

104 ->106 -0.35516

104 ->107 0.59039

Excited State 3: Singlet-A 3.7498 eV 330.64 nm f=0.1427 <S**2>=0.000

104 ->106 0.58398

104 ->107 0.36770

Excited State 4: Singlet-A 3.9326 eV 315.27 nm f=0.0402 <S**2>=0.000

104 ->108 0.54708

104 ->109 0.36139

104 ->110 0.16544

104 ->111 -0.15952

Excited State 5: Singlet-A 3.9938 eV 310.44 nm f=0.0046 <S**2>=0.000

104 ->108 -0.43431

104 ->109 0.45990

104 ->110 0.13751

104 ->111 -0.21986

Excited State 6: Singlet-A 4.1263 eV 300.47 nm f=0.0044 <S**2>=0.000

104 ->109 -0.28212

104 ->110 0.60448

104 ->111 -0.14169

Excited State 7: Singlet-A 4.2011 eV 295.12 nm f=0.0076 <S**2>=0.000

104 ->109 0.21575

104 ->110 0.23705

104 ->111 0.60616

Excited State 8: Singlet-A 4.3336 eV 286.10 nm f=0.1027 <S**2>=0.000

102 ->105 -0.15061

103 ->105 0.62165

104 ->110 0.11622

104 ->112 -0.13712

Excited State 9: Singlet-A 4.4626 eV 277.83 nm f=0.0189 <S**2>=0.000

103 ->105 0.15157

104 ->112 0.60003

104 ->113 -0.16112

104 ->116 -0.12295

104 ->117 -0.11789

Excited State 10: Singlet-A 4.5810 eV 270.65 nm f=0.0104 <S**2>=0.000

101 ->105 -0.14204

102 ->105 -0.15715

103 ->106 -0.18434

104 ->113 0.59364

104 ->118 0.10016

Excited State 11: Singlet-A 4.5901 eV 270.11 nm f=0.0073 <S**2>=0.000

101 ->105 0.29429

102 ->105 0.10933

102 ->106 -0.13094

103 ->106 0.44537

104 ->112 0.15906

104 ->113 0.24053

104 ->115 0.18050

Excited State 12: Singlet-A 4.6089 eV 269.01 nm f=0.4647 <S**2>=0.000

101 ->105 -0.10942

102 ->105 0.62387

103 ->105 0.14846

104 ->113 0.10420

Excited State 13: Singlet-A 4.7304 eV 262.10 nm f=0.0223 <S**2>=0.000

101 ->105 0.32003

103 ->106 -0.31961

103 ->107 0.46156

103 ->109 -0.13120

104 ->115 0.12162

Excited State 14: Singlet-A 4.7478 eV 261.14 nm f=0.0174 <S**2>=0.000

101 ->105 -0.38493

103 ->106 0.30511

103 ->107 0.46481

Excited State 15: Singlet-A 4.8381 eV 256.27 nm f=0.0171 <S**2>=0.000

101 ->105 -0.17835

102 ->106 -0.12926

103 ->107 -0.16943

104 ->113 -0.10849

104 ->114 0.15716

104 ->115 0.49243

104 ->117 0.21954

Excited State 16: Singlet-A 4.8696 eV 254.61 nm f=0.0317 <S**2>=0.000

104 ->112 -0.14653

104 ->114 0.58566

104 ->115 -0.12264

104 ->117 -0.16896

104 ->119 0.15724

Excited State 17: Singlet-A 4.9030 eV 252.87 nm f=0.0268 <S**2>=0.000

100 ->105 0.27344

101 ->106 0.24818

102 ->106 0.25584

102 ->107 0.27406

102 ->108 -0.10681

103 ->109 0.32483

104 ->114 0.13891

104 ->115 0.14425

Excited State 18: Singlet-A 4.9288 eV 251.55 nm f=0.0224 <S**2>=0.000

100 ->105 -0.37045

101 ->105 0.19444

101 ->106 -0.12116

102 ->106 0.45812

102 ->107 -0.11043

103 ->108 0.15360

103 ->110 -0.11526

Excited State 19: Singlet-A 4.9619 eV 249.87 nm f=0.0050 <S**2>=0.000

100 ->105 0.18180

101 ->107 -0.14085

101 ->112 -0.10559

102 ->106 0.23411

102 ->107 -0.11922

103 ->107 -0.10617

103 ->108 -0.19561

103 ->109 -0.26854

103 ->110 -0.26115

103 ->111 0.33469

Excited State 20: Singlet-A 4.9937 eV 248.28 nm f=0.0287 <S**2>=0.000

100 ->105 0.31448

101 ->106 -0.16412

102 ->107 -0.11548

103 ->108 0.55739

Excited State 21: Singlet-A 5.0110 eV 247.42 nm f=0.0464 <S**2>=0.000

100 ->105 0.31315

101 ->106 -0.28815

102 ->106 0.10550

102 ->107 -0.27915

103 ->108 -0.28982

103 ->109 0.15400

103 ->111 -0.27120

Excited State 22: Singlet-A 5.0395 eV 246.02 nm f=0.0133 <S**2>=0.000

101 ->106 -0.32299

102 ->107 0.47456

102 ->108 0.11755

102 ->109 -0.17352

103 ->109 -0.12789

103 ->110 -0.12111

104 ->116 -0.15767

Excited State 23: Singlet-A 5.0796 eV 244.08 nm f=0.0029 <S**2>=0.000

102 ->107 0.14245

104 ->116 0.64210

Excited State 24: Singlet-A 5.1294 eV 241.71 nm f=0.0025 <S**2>=0.000

100 ->107 -0.11232

101 ->107 0.41182

101 ->109 -0.15714

101 ->111 0.17597

103 ->109 0.14518

103 ->110 -0.17103

103 ->111 0.19899

103 ->112 -0.24497

Excited State 25: Singlet-A 5.1571 eV 240.41 nm f=0.0084 <S**2>=0.000

100 ->107 0.10464

101 ->107 -0.21240

102 ->106 -0.10065

102 ->108 0.13947

102 ->109 0.12954

103 ->109 0.20859

103 ->110 -0.20363

104 ->117 0.20862

104 ->118 -0.18638

104 ->119 0.29528

104 ->120 0.21489

Excited State 26: Singlet-A 5.1910 eV 238.84 nm f=0.0760 <S**2>=0.000

100 ->107 -0.10008

101 ->106 0.12755

101 ->107 0.20097

103 ->109 -0.11646

103 ->110 -0.22556

103 ->111 -0.10501

104 ->114 0.14678

104 ->115 -0.28974

104 ->117 0.38913

Excited State 27: Singlet-A 5.1993 eV 238.46 nm f=0.0494 <S**2>=0.000

101 ->106 -0.12468

101 ->111 0.13030

102 ->106 0.12006

102 ->108 -0.15036

103 ->110 0.35764

103 ->111 0.13165

103 ->112 -0.15509

104 ->115 -0.10106

104 ->117 0.37897

104 ->119 0.11379

Excited State 28: Singlet-A 5.2228 eV 237.39 nm f=0.1503 <S**2>=0.000

100 ->106 0.16220

100 ->107 -0.20955

101 ->107 0.13760

103 ->109 -0.22818

103 ->111 -0.15922

104 ->114 -0.10164

104 ->118 -0.18229

104 ->119 0.40062

Excited State 29: Singlet-A 5.2450 eV 236.39 nm f=0.0030 <S**2>=0.000

98 ->105 -0.10151

100 ->107 0.27580

101 ->107 0.32402

102 ->108 0.33569

102 ->109 0.26157

102 ->110 0.12050

102 ->111 -0.13371

Excited State 30: Singlet-A 5.2594 eV 235.74 nm f=0.0413 <S**2>=0.000

99 ->105 0.10982

99 ->108 -0.12486

100 ->107 0.39000

102 ->107 -0.11367

102 ->108 -0.33288

102 ->109 -0.12850

102 ->110 -0.17293

103 ->110 -0.14393

104 ->118 -0.10125

104 ->119 0.14390

Excited State 31: Singlet-A 5.2874 eV 234.49 nm f=0.0609 <S**2>=0.000

101 ->106 -0.22682

101 ->107 0.15515

101 ->109 0.14937

101 ->111 -0.16104

102 ->108 -0.16235

103 ->109 0.21234

103 ->111 0.28920

103 ->112 0.27267

104 ->119 0.10348

104 ->120 -0.22214

104 ->121 0.10143

Excited State 32: Singlet-A 5.2907 eV 234.35 nm f=0.0319 <S**2>=0.000

101 ->107 -0.13509

102 ->110 0.11525

103 ->110 -0.15976

103 ->112 -0.11183

104 ->118 0.45936

104 ->119 0.28754

104 ->120 -0.19292

104 ->121 0.14344

Excited State 33: Singlet-A 5.3141 eV 233.31 nm f=0.0110 <S**2>=0.000

102 ->108 -0.13408

102 ->110 -0.14083

103 ->110 0.10037

103 ->112 0.15400

104 ->118 0.38660

104 ->120 0.40178

104 ->123 0.16235

Excited State 34: Singlet-A 5.3476 eV 231.85 nm f=0.0604 <S**2>=0.000

100 ->106 0.31389

101 ->106 -0.11249

102 ->108 -0.26473

102 ->109 0.22711

102 ->110 0.15594

102 ->111 -0.28699

103 ->110 -0.16212

103 ->111 -0.18416

104 ->119 -0.18869

Excited State 35: Singlet-A 5.3712 eV 230.83 nm f=0.1143 <S**2>=0.000

100 ->106 0.47850

100 ->107 0.13121

101 ->108 0.18088

102 ->108 0.17205

102 ->109 -0.21509

102 ->111 0.18825

103 ->109 0.11767

103 ->111 0.11886

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 640.

Leave Link 914 at Tue Jan 5 21:06:48 2021, MaxMem= 1610612736 cpu: 44432.5

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

6.4 Computed zyx-coordinates of the S_0 state of compound **7** and excitation energies (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 0 Multiplicity = 1

C	1.33373	-1.33761	0.35053
C	1.19211	-0.01004	0.07969
N	0. 00000	0.71339	0.1536
C	-1.19211	-0.01004	0.07969
C	-1.33374	-1.3376	0.35053
S	0. 00000	-2.31908	1.02644
C	0. 00000	2.15245	0.17192
C	0.00001	2.82364	1.39636
C	0.00001	4.21472	1.42833
C	0.00001	4.90028	0.2226
C	0.00001	4.26139	-1.00678
C	0. 00000	2.86831	-1.02705
C	-3.52269	-0.81153	-0.36511
C	-2.65821	-1.83511	0.09102
S	-2.68054	0.72961	-0.52259
C	-4.86622	-1.05332	-0.64484
C	-5.35436	-2.3464	-0.47689
C	-4.51108	-3.37643	-0.03257
C	-3.17445	-3.13157	0.25456
C	2.6582	-1.83512	0.09102
C	3.52269	-0.81154	-0.36511
S	2.68054	0.7296	-0.52259
C	3.17444	-3.13158	0.25456
C	4.51107	-3.37645	-0.03257
C	5.35435	-2.34641	-0.47689
C	4.86621	-1.05333	-0.64484

H	0.00001	2.25538	2.31834
H	0.00001	4.7595	2.36377
H	0.00001	4.84002	-1.92157
H	0.00000	2.34002	-1.97258
H	-5.51541	-0.25731	-0.99033
H	-6.39507	-2.55639	-0.694
H	-4.90921	-4.37717	0.08984
H	-2.53033	-3.93305	0.59821
H	2.53031	-3.93306	0.59821
H	4.90919	-4.37718	0.08984
H	6.39506	-2.55641	-0.694
H	5.51541	-0.25732	-0.99033
F	0.00001	6.25744	0.24894

SCF Done: E(RB3LYP) = -2195.05316484 A.U. after 1 cycles

Sum of electronic and zero-point Energies= -2194.777705

Sum of electronic and thermal Energies= -2194.756501

Sum of electronic and thermal Enthalpies= -2194.755557

Sum of electronic and thermal Free Energies= -2194.830146

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9408 eV 421.59 nm f=0.1437 <S**2>=0.000

104 ->105 0.68850

104 ->106 0.10629

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

Total Energy, E(TD-HF/TD-KS) = -2194.94509074

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

Excited State 2: Singlet-A 3.2481 eV 381.71 nm f=0.0007 <S**2>=0.000

104 ->105 -0.11542

104 ->106 0.68901

Excited State 3: Singlet-A 3.3948 eV 365.22 nm f=0.0049 <S**2>=0.000

104 ->107 0.70149

Excited State 4: Singlet-A 3.7116 eV 334.05 nm f=0.0814 <S**2>=0.000

103 ->105 -0.10463

104 ->108 0.64714

104 ->109 0.12474

104 ->111 -0.18964

Excited State 5: Singlet-A 3.7338 eV 332.06 nm f=0.0204 <S**2>=0.000

104 ->110 0.64076

104 ->112 -0.24139

Excited State 6: Singlet-A 3.7621 eV 329.56 nm f=0.0011 <S**2>=0.000

104 ->108 -0.13832

104 ->109 0.68456

Excited State 7: Singlet-A 3.9459 eV 314.21 nm f=0.0040 <S**2>=0.000

104 ->110 0.26467

104 ->112 0.62743

104 ->115 0.14040

Excited State 8: Singlet-A 4.0145 eV 308.84 nm f=0.0266 <S**2>=0.000

104 ->108 0.18808

104 ->111 0.60595

104 ->113 0.26504

Excited State 9: Singlet-A 4.2041 eV 294.91 nm f=0.0079 <S**2>=0.000

104 ->111 -0.26463

104 ->113 0.62810

104 ->116 -0.13686

Excited State 10: Singlet-A 4.4370 eV 279.43 nm f=0.1142 <S**2>=0.000

102 ->109 0.10484

103 ->105 0.64759

104 ->114 -0.12536

Excited State 11: Singlet-A 4.4495 eV 278.65 nm f=0.1445 <S**2>=0.000

102 ->105 0.63647

104 ->115 -0.12654

104 ->118 0.17238

Excited State 12: Singlet-A 4.5373 eV 273.25 nm f=0.0101 <S**2>=0.000

103 ->105 0.13448

104 ->114 0.66924

Excited State 13: Singlet-A 4.5825 eV 270.56 nm f=0.0066 <S**2>=0.000

103 ->106 0.68410

Excited State 14: Singlet-A 4.6303 eV 267.77 nm f=0.1777 <S**2>=0.000

102 ->105 0.18146

104 ->112 -0.15027

104 ->115 0.59534

104 ->118 -0.23198

Excited State 15: Singlet-A 4.6826 eV 264.78 nm f=0.0016 <S**2>=0.000

102 ->106 0.67324

Excited State 16: Singlet-A 4.7383 eV 261.66 nm f=0.0020 <S**2>=0.000

101 ->105 -0.19767

102 ->108 0.15077

103 ->107 0.64157

Excited State 17: Singlet-A 4.7968 eV 258.47 nm f=0.1173 <S**2>=0.000

102 ->105 -0.11029

104 ->115 0.27192

104 ->118 0.57058

104 ->120 0.21532

Excited State 18: Singlet-A 4.8588 eV 255.18 nm f=0.0100 <S**2>=0.000

104 ->113 0.11149

104 ->116 0.66745

104 ->117 0.10313

Excited State 19: Singlet-A 4.8655 eV 254.82 nm f=0.0080 <S**2>=0.000

102 ->107 0.67402

103 ->109 0.11590

Excited State 20: Singlet-A 4.9049 eV 252.77 nm f=0.0497 <S**2>=0.000

101 ->105 0.48170

102 ->108 -0.18835

102 ->109 -0.10638

103 ->107 0.26804

103 ->110 0.24810

103 ->112 0.13688

104 ->117 -0.13956

Excited State 21: Singlet-A 4.9274 eV 251.62 nm f=0.0680 <S**2>=0.000

102 ->106 -0.10511

102 ->107 -0.14329

102 ->110 0.20033

103 ->108 0.56959

103 ->109 0.19603

103 ->111 -0.10894

Excited State 22: Singlet-A 4.9395 eV 251.01 nm f=0.0010 <S**2>=0.000

101 ->105 0.12129

104 ->117 0.65845

Excited State 23: Singlet-A 5.0120 eV 247.37 nm f=0.0019 <S**2>=0.000

101 ->105 0.24451

101 ->106 0.24808

102 ->108 0.45390

102 ->111 -0.24094

103 ->110 0.10348

103 ->112 -0.19230

Excited State 24: Singlet-A 5.0377 eV 246.11 nm f=0.0067 <S**2>=0.000

104 ->119 0.67407

Excited State 25: Singlet-A 5.0559 eV 245.23 nm f=0.0562 <S**2>=0.000

100 ->105 -0.15478

101 ->108 0.14229

102 ->112 -0.10460

103 ->108 -0.15957

103 ->109 0.40496

104 ->118 -0.13203

104 ->120 0.39851

104 ->122 0.10490

104 ->127 -0.16085

Excited State 26: Singlet-A 5.1004 eV 243.09 nm f=0.1292 <S**2>=0.000

101 ->108 -0.11327

103 ->108 0.22497

103 ->109 -0.34687

104 ->118 -0.13751

104 ->120 0.50316

Excited State 27: Singlet-A 5.1064 eV 242.80 nm f=0.0171 <S**2>=0.000

101 ->105 -0.27522

101 ->106 0.34981

102 ->108 -0.25766

102 ->111 -0.13501

103 ->110 0.39949

103 ->112 -0.12143

Excited State 28: Singlet-A 5.1530 eV 240.61 nm f=0.0048 <S**2>=0.000

101 ->106 0.48800

103 ->110 -0.36250

103 ->112 0.27465

Excited State 29: Singlet-A 5.1615 eV 240.21 nm f=0.0015 <S**2>=0.000

100 ->105 -0.29517

100 ->106 -0.11598

101 ->109 -0.11082

102 ->110 0.16420

102 ->112 0.17462

103 ->109 -0.13609

103 ->111 0.40852

103 ->113 0.15060

104 ->118 0.16059

104 ->122 0.19276

104 ->127 -0.12643

Excited State 30: Singlet-A 5.2198 eV 237.53 nm f=0.0428 <S**2>=0.000

100 ->105 0.32953

102 ->110 -0.11235

103 ->108 0.12250

104 ->122 0.51269

104 ->127 -0.24263

Excited State 31: Singlet-A 5.2392 eV 236.64 nm f=0.0363 <S**2>=0.000

98 ->107 0.22808

99 ->105 0.17471

99 ->106 -0.31169

101 ->107 0.43819

102 ->108 -0.20327

102 ->109 0.13778

102 ->111 -0.16481

Excited State 32: Singlet-A 5.2545 eV 235.96 nm f=0.0037 <S**2>=0.000

102 ->109 -0.28007

103 ->112 -0.11160

104 ->123 0.55737

104 ->124 0.16250

Excited State 33: Singlet-A 5.2594 eV 235.74 nm f=0.0484 <S**2>=0.000

100 ->105 0.32048

101 ->111 0.11054

102 ->110 -0.20746

102 ->112 0.26905

103 ->108 0.11578

103 ->109 0.23902

103 ->111 0.33544

104 ->122 -0.17953

Excited State 34: Singlet-A 5.3001 eV 233.93 nm f=0.0089 <S**2>=0.000

104 ->121 0.66455

104 ->124 -0.11171

Excited State 35: Singlet-A 5.3179 eV 233.15 nm f=0.1466 <S**2>=0.000

99 ->106 -0.15798

101 ->106 0.17702

101 ->107 0.16192

102 ->108 0.17678

102 ->109 -0.27584

102 ->111 0.29711

103 ->110 0.16876

103 ->112 0.15812

104 ->121 0.15088

104 ->123 -0.25291

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 640.

Leave Link 914 at Tue Jan 5 21:40:11 2021, MaxMem= 1610612736 cpu: 41077.6

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

6.5 Computed zyx-coordinates of the D_0 state of compound **5**$^{\bullet+}$ and excitation energies (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 1 Multiplicity = 2

C	1.30999	-2.14913	-0.0002
C	1.22699	-0.75866	0.00001
N	0.00000	-0.09237	0.00000
C	-1.22698	-0.75867	-0.00001
C	-1.30997	-2.14914	0.0002
S	0.00002	-3.27944	0.00000
C	-2.56174	-0.15273	-0.00009
C	-3.56759	-1.15062	0.00013
S	-2.92461	-2.78068	0.00043
S	2.92464	-2.78066	-0.00043
C	3.56761	-1.15059	-0.00013
C	2.56174	-0.15271	0.00009
C	-0.00001	1.35639	0.00000
C	4.93072	-0.86321	-0.0001
C	5.32242	0.46709	0.00017
C	4.35688	1.48131	0.00041
C	3.00169	1.18967	0.00038
C	-3.0017	1.18964	-0.00038
C	-4.35689	1.48127	-0.00042
C	-5.32242	0.46705	-0.00017
C	-4.9307	-0.86325	0.0001
C	0.00006	2.03558	-1.2155
C	0.00004	3.42742	-1.21921
C	-0.00003	4.09076	0.00000

C	-0.00009	3.42742	1.21921
C	-0.00008	2.03558	1.2155
F	-0.00004	5.44186	0.00000
H	5.66287	-1.66139	-0.00026
H	6.37612	0.71797	0.00022
H	4.66877	2.51854	0.00062
H	2.307	2.01023	0.00061
H	-2.30701	2.01021	-0.00062
H	-4.66878	2.51851	-0.00064
H	-6.37612	0.71792	-0.00022
H	-5.66285	-1.66144	0.00026
H	0.0001	1.48547	-2.14809
H	0.00009	3.9891	-2.14418
H	-0.00015	3.98909	2.14419
H	-0.00012	1.48547	2.1481

SCF Done: E(UB3LYP) = -2194.84500198 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.568632

Sum of electronic and thermal Energies= -2194.547872

Sum of electronic and thermal Enthalpies= -2194.546928

Sum of electronic and thermal Free Energies= -2194.619648

Excitation energies and oscillator strengths:

Excited State 1: 2.012-A 1.8542 eV 668.67 nm f=0.0024 <S**2>=0.762

102B ->104B 0.99311

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

Total Energy, E(TD-HF/TD-KS) = -2194.79068908

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

Excited State 2: 2.019-A 1.8633 eV 665.40 nm f=0.1905 <S**2>=0.769

103B ->104B 0.99374

Excited State 3: 2.035-A 2.3146 eV 535.65 nm f=0.0416 <S**2>=0.785

104A ->105A 0.62578

101B ->104B 0.76066

Excited State 4: 2.094-A 2.5007 eV 495.80 nm f=0.0070 <S**2>=0.847

104A ->105A 0.74332

101B ->104B -0.63448

Excited State 5: 2.013-A 2.7494 eV 450.95 nm f=0.0000 <S**2>=0.763

100B ->104B 0.99706

Excited State 6: 2.223-A 2.8270 eV 438.57 nm f=0.0000 <S**2>=0.986

103A ->105A 0.15707

104A ->106A 0.14857

99B ->104B 0.93087

103B ->105B -0.18626

Excited State 7: 2.019-A 3.1024 eV 399.64 nm f=0.0083 <S**2>=0.770

98B ->104B 0.99166

Excited State 8: 2.983-A 3.1174 eV 397.71 nm f=0.0260 <S**2>=1.975

101A ->105A -0.12355

102A ->110A 0.10208

103A ->105A -0.42220

104A ->106A -0.52065

99B ->104B 0.32132

99B ->108B -0.11048

101B ->105B 0.15754

103B ->105B 0.55240

Excited State 9: 3.261-A 3.5415 eV 350.09 nm f=0.0006 <S**2>=2.408

102A ->105A 0.67671

103A ->106A -0.22624

104A ->107A 0.12258

97B ->104B -0.34335

101B ->108B -0.12023

102B ->105B -0.49253

103B ->108B 0.16701

Excited State 10: 2.623-A 3.5941 eV 344.96 nm f=0.0014 <S**2>=1.470

101A ->105A 0.16802

102A ->106A 0.23539

103A ->105A -0.42805

104A ->106A 0.45448

96B ->104B 0.62476

101B ->105B -0.17060

102B ->108B -0.17354

103B ->105B 0.21234

Excited State 11: 2.958-A 3.6319 eV 341.37 nm f=0.0093 <S**2>=1.938

99A ->105A 0.20425

101A ->106A -0.18727

102A ->105A -0.29142

102A ->107A -0.10700

102A ->112A 0.14971

103A ->106A -0.14852

103A ->110A -0.20667

104A ->105A 0.10290

104A ->107A 0.51596

104A ->114A -0.11608

97B ->104B -0.35328

99B ->105B -0.19520

101B ->108B 0.12218

101B ->109B -0.13595

102B ->105B 0.25574

102B ->106B 0.12059

102B ->112B -0.17570

103B ->108B 0.18053

103B ->109B 0.17338

Excited State 12: 2.035-A 3.6730 eV 337.55 nm f=0.0000 <S**2>=0.786

104A ->108A 0.74403

104A ->109A -0.64132

Excited State 13: 2.142-A 3.7261 eV 332.75 nm f=0.0031 <S**2>=0.897

104A ->107A 0.62149

97B ->104B 0.72904

102B ->105B -0.19530

Excited State 14: 3.461-A 3.7662 eV 329.20 nm f=0.0001 <S**2>=2.745

98A ->107A -0.40470

98A ->112A -0.16322

100A ->108A -0.48480

100A ->109A -0.17895

103A ->107A 0.13312

98B ->106B -0.40636

98B ->112B -0.15802

100B ->107B 0.49598

100B ->110B 0.14290

103B ->106B -0.12787

Excited State 15: 2.772-A 3.8328 eV 323.48 nm f=0.0000 <S**2>=1.671

99A ->105A -0.17410

101A ->110A -0.15102

102A ->107A 0.15591

102A ->112A -0.20601

103A ->106A 0.20892

103A ->110A 0.19055

104A ->107A 0.56321

97B ->104B -0.42122

99B ->105B 0.17638

101B ->109B 0.16271

102B ->106B -0.15309

102B ->112B 0.18821

103B ->108B -0.22231

103B ->109B -0.17431

Excited State 16: 2.757-A 3.8479 eV 322.22 nm f=0.0243 <S**2>=1.651

99A ->106A 0.14239

101A ->105A -0.27245

102A ->106A -0.16466

102A ->110A 0.21100

103A ->105A -0.17338

103A ->107A 0.13549

103A ->112A -0.16908

104A ->106A 0.57196

104A ->110A -0.23005

96B ->104B -0.36428

99B ->108B -0.12265

101B ->112B -0.13095

102B ->109B -0.23800

103B ->106B -0.14331

103B ->112B 0.14308

Excited State 17: 2.030-A 3.9360 eV 315.00 nm f=0.0000 <S**2>=0.781

104A ->108A 0.66127

104A ->109A 0.73079

104A ->115A -0.11154

Excited State 18: 2.776-A 3.9386 eV 314.79 nm f=0.0009 <S**2>=1.676

101A ->105A -0.21278

102A ->106A -0.13299

102A ->110A 0.14437

103A ->105A 0.43402

103A ->107A 0.12337

103A ->112A -0.13766

104A ->106A -0.13929

104A ->110A -0.22864

96B ->104B 0.63838

101B ->105B 0.27721

101B ->112B -0.10225

102B ->108B 0.14340

102B ->109B -0.17444

Excited State 19: 3.179-A 3.9642 eV 312.76 nm f=0.0067 <S**2>=2.276

101A ->105A 0.42806

102A ->106A 0.21222

102A ->110A 0.17920

103A ->107A 0.17491

103A ->112A -0.17024

104A ->106A -0.28583

104A ->110A -0.34979

92B ->104B 0.11232

99B ->109B -0.11651

101B ->105B -0.36834

102B ->108B -0.18960

102B ->109B -0.14736

103B ->105B -0.27270

103B ->106B -0.17993

103B ->112B 0.16266

103B ->114B 0.11265

Excited State 20: 2.115-A 4.1149 eV 301.30 nm f=0.0002 <S**2>=0.868

103A ->109A 0.12028

104A ->111A 0.96844

Excited State 21: 2.040-A 4.1169 eV 301.16 nm f=0.4119 <S**2>=0.790

102A ->105A 0.59581

104A ->112A 0.14140

102B ->105B 0.75141

Excited State 22: 2.168-A 4.1272 eV 300.41 nm f=0.1105 <S**2>=0.925

101A ->112A -0.10542

102A ->110A -0.13451

103A ->105A 0.52978

104A ->106A 0.11219

104A ->110A -0.35134

96B ->104B -0.15107

101B ->105B -0.24221

102B ->108B -0.12607

103B ->105B 0.63957

Excited State 23: 2.520-A 4.2469 eV 291.94 nm f=0.0196 <S**2>=1.338

101A ->105A 0.19814

101A ->107A -0.11900

101A ->112A 0.14044

102A ->106A 0.11297

102A ->110A 0.22385

103A ->105A 0.25428

104A ->110A 0.73710

101B ->105B -0.13444

101B ->106B 0.14568

101B ->112B -0.17963

102B ->109B -0.29005

103B ->105B 0.20348

Excited State 24: 2.807-A 4.3073 eV 287.85 nm f=0.0330 <S**2>=1.720

99A ->105A 0.15185

101A ->106A -0.13737

102A ->107A 0.10013

102A ->112A -0.10395

103A ->106A -0.31798

103A ->110A 0.24216

104A ->112A 0.68534

104A ->114A -0.13993

94B ->104B -0.13096

99B ->105B -0.13991

101B ->108B 0.12925

102B ->106B -0.15213

102B ->112B 0.11054

103B ->108B 0.27869

103B ->109B -0.22656

Excited State 25: 3.004-A 4.3975 eV 281.94 nm f=0.0065 <S**2>=2.006

99A ->105A -0.19366

101A ->110A 0.23617

102A ->107A -0.27932

102A ->112A 0.22509

103A ->106A 0.22872

104A ->112A 0.57742

104A ->114A 0.11261

99B ->105B 0.19352

101B ->109B -0.25978

102B ->106B 0.30690

102B ->112B -0.24541

103B ->108B -0.23828

Excited State 26: 3.444-A 4.5255 eV 273.97 nm f=0.0000 <S**2>=2.716

98A ->108A 0.18353

100A ->105A 0.38041

100A ->107A 0.56886

100A ->112A 0.18700

98B ->107B 0.19819

100B ->105B -0.19779

100B ->106B -0.56243

100B ->112B -0.17579

103B ->107B 0.11469

Excited State 27: 3.365-A 4.5806 eV 270.67 nm f=0.0006 <S**2>=2.580

98A ->105A 0.11036

98A ->107A 0.33314

98A ->112A 0.12221

100A ->108A -0.36998

100A ->109A -0.12909

102A ->106A -0.12832

102A ->110A 0.13148

103A ->107A -0.16186

98B ->106B 0.33183

98B ->112B 0.11462

100B ->107B 0.36990

100B ->110B 0.10071

101B ->105B -0.13220

102B ->109B -0.12542

103B ->106B 0.51699

Excited State 28: 3.055-A 4.6363 eV 267.42 nm f=0.0000 <S**2>=2.083

102A ->108A 0.27163

102A ->109A -0.35847

103A ->111A 0.35185

104A ->109A 0.12969

104A ->115A 0.50289

104A ->118A -0.25289

102B ->107B -0.27258

102B ->110B 0.34528

103B ->111B -0.26164

Excited State 29: 3.283-A 4.6605 eV 266.03 nm f=0.0010 <S**2>=2.444

97A ->105A 0.15599

98A ->105A 0.18246

98A ->107A 0.21094

99A ->106A 0.16425

100A ->108A -0.18346

101A ->105A -0.30520

101A ->112A -0.11289

102A ->106A 0.43449

102A ->110A -0.15919

103A ->114A -0.17474

104A ->110A 0.13916

97B ->105B -0.13558

98B ->105B 0.14710

98B ->106B 0.20907

99B ->108B -0.15119

100B ->107B 0.18098

101B ->105B 0.11216

101B ->106B -0.12113

101B ->112B 0.12825

102B ->108B -0.18160

102B ->109B 0.17410

103B ->106B -0.32906

103B ->114B 0.17400

Excited State 30: 2.438-A 4.6729 eV 265.33 nm f=0.0121 <S**2>=1.236

98A ->107A 0.14830

100A ->108A -0.10307

101A ->105A 0.55365

103A ->107A -0.26168

98B ->106B 0.16497

100B ->107B 0.14144

101B ->105B 0.38925

102B ->108B 0.28395

103B ->106B -0.42946

103B ->112B 0.13915

103B ->114B -0.14355

Excited State 31: 3.056-A 4.7053 eV 263.50 nm f=0.0001 <S**2>=2.085

98A ->108A -0.10562

100A ->105A 0.63078

102A ->111A 0.13516

103A ->108A 0.19272

102B ->111B -0.23089

103B ->107B -0.58842

103B ->110B 0.24517

Excited State 32: 2.975-A 4.7218 eV 262.58 nm f=0.0003 <S**2>=1.962

100A ->105A 0.66884

100A ->107A -0.21961

102A ->111A -0.13863

103A ->109A 0.11880

100B ->106B 0.24238

102B ->111B 0.23695

103B ->107B 0.46479

103B ->110B -0.26613

Excited State 33: 3.025-A 4.7363 eV 261.78 nm f=0.0029 <S**2>=2.037

96A ->105A 0.14750

101A ->106A -0.41895

102A ->105A 0.22371

102A ->107A 0.14879

102A ->114A -0.20158

103A ->106A 0.47087

104A ->112A -0.16926

104A ->114A -0.15129

94B ->104B -0.42592

96B ->105B -0.10060

101B ->108B 0.27645

101B ->109B -0.11346

102B ->105B -0.14205

102B ->114B 0.14721

103B ->109B -0.19098

Excited State 34: 3.372-A 4.7567 eV 260.65 nm f=0.0190 <S**2>=2.593

97A ->105A -0.19045

98A ->105A -0.15345

99A ->106A -0.27828

101A ->105A -0.22191

101A ->107A -0.15457

101A ->114A 0.14906

102A ->106A 0.40348

102A ->110A 0.20065

103A ->114A 0.15540

104A ->123A 0.11271

92B ->104B -0.11155

97B ->105B 0.21886

98B ->105B -0.15169

99B ->108B 0.29171

101B ->105B 0.18169

101B ->106B 0.13651

101B ->114B -0.14141

102B ->108B -0.31077

102B ->109B -0.15090

103B ->105B -0.14717

103B ->114B -0.22587

Excited State 35: 2.654-A 4.7916 eV 258.75 nm f=0.1334 <S**2>=1.511

99A ->105A	-0.25474
102A ->107A	0.17596
103A ->110A	0.11320
104A ->105A	0.11373
104A ->112A	-0.11721
104A ->114A	0.49545
102B ->105B	0.13378
102B ->106B	0.42325
103B ->108B	0.54067
103B ->109B	-0.21544

Excited State 36: 2.663-A 4.8069 eV 257.93 nm f=0.0005 <S**2>=1.523

97A ->105A	0.12070
98A ->107A	-0.13223
99A ->106A	0.13004
101A ->105A	0.25992
102A ->106A	0.34664
103A ->112A	0.10587
103A ->114A	-0.15368
104A ->123A	-0.10865
92B ->104B	-0.16469
96B ->104B	-0.10086
97B ->105B	-0.11206
98B ->106B	-0.14393
99B ->108B	-0.10951
101B ->105B	0.50986
103B ->106B	0.53433
103B ->112B	0.12746

Excited State 37: 2.387-A 4.8185 eV 257.31 nm f=0.0000 <S**2>=1.175

103A ->111A	0.13279
104A ->115A	0.44571
104A ->118A	-0.19786
95B ->104B	-0.39892

101B ->111B -0.12365

102B ->107B 0.53062

102B ->110B -0.42304

103B ->111B 0.24907

Excited State 38: 2.084-A 4.8303 eV 256.68 nm f=0.0000 <S**2>=0.835

104A ->115A 0.20115

95B ->104B 0.90888

102B ->107B 0.23282

102B ->110B -0.18166

103B ->111B 0.10603

Excited State 39: 2.518-A 4.8530 eV 255.48 nm f=0.0223 <S**2>=1.335

101A ->106A -0.21295

102A ->107A -0.11391

103A ->106A -0.15669

104A ->114A 0.61535

99B ->105B 0.15529

101B ->108B 0.19514

102B ->106B -0.58976

102B ->112B -0.11036

102B ->114B 0.11104

103B ->109B 0.15319

Excited State 40: 2.672-A 4.8549 eV 255.38 nm f=0.0003 <S**2>=1.535

102A ->111A 0.32236

103A ->108A 0.35018

103A ->109A -0.28985

104A ->113A -0.40700

104A ->116A -0.19025

100B ->105B 0.13323

102B ->111B -0.22903

103B ->107B 0.53715

103B ->110B 0.24076

Excited State 41: 2.880-A 4.8631 eV 254.95 nm f=0.0019 <S**2>=1.824

99A ->105A 0.47208

101A ->110A -0.13058

102A ->107A 0.35048

103A ->106A 0.47485

103A ->110A -0.12363

104A ->112A 0.24557

104A ->114A 0.30708

94B ->104B 0.21195

99B ->105B -0.29892

103B ->109B 0.18755

Excited State 42: 2.111-A 4.8763 eV 254.26 nm f=0.0008 <S**2>=0.864

102A ->111A 0.10678

103A ->108A 0.21118

104A ->113A 0.82987

104A ->116A -0.12996

104A ->117A 0.34259

104A ->122A 0.10814

102B ->111B -0.10696

103B ->107B 0.21364

Excited State 43: 2.783-A 4.8901 eV 253.54 nm f=0.0005 <S**2>=1.687

98A ->107A 0.15947

101A ->105A 0.13867

101A ->107A 0.10127

101A ->112A -0.11980

102A ->106A -0.20855

102A ->110A -0.12889

103A ->107A 0.80795

104A ->110A 0.14805

98B ->106B 0.14084

101B ->105B 0.12772

102B ->108B -0.10234

102B ->109B 0.12607

103B ->112B 0.15925

Excited State 44: 2.267-A 4.9175 eV 252.13 nm f=0.0423 <S**2>=1.034

99A ->105A -0.22303

103A ->106A 0.26005

104A ->114A -0.28171

94B ->104B 0.68038

101B ->109B -0.12939

102B ->106B -0.36949

102B ->112B -0.13557

103B ->108B 0.26745

103B ->109B -0.19475

Excited State 45: 2.783-A 4.9209 eV 251.95 nm f=0.0001 <S**2>=1.687

98A ->108A -0.20115

103A ->108A 0.60308

104A ->116A 0.15701

104A ->117A -0.13258

98B ->107B -0.24466

100B ->105B -0.56434

102B ->111B 0.17387

103B ->110B -0.31411

Excited State 46: 2.199-A 4.9291 eV 251.54 nm f=0.0011 <S**2>=0.959

104A ->113A 0.22164

104A ->116A 0.65208

104A ->117A -0.41648

88B ->104B -0.14615

90B ->104B 0.17115

93B ->104B -0.34276

100B ->105B 0.21109

102B ->111B -0.17504

103B ->110B 0.11387

Excited State 47: 3.139-A 4.9410 eV 250.93 nm f=0.0002 <S**2>=2.213

99A ->105A 0.51500

99A ->107A 0.12354

99A ->112A -0.12362

101A ->110A 0.11941

102A ->107A -0.47120

103A ->110A 0.25333

104A ->112A -0.17597

104A ->114A 0.15536

94B ->104B 0.18534

99B ->105B -0.12567

99B ->106B -0.12204

99B ->112B 0.11532

102B ->106B 0.11955

103B ->108B -0.15857

103B ->109B -0.45064

Excited State 48: 2.158-A 4.9417 eV 250.89 nm f=0.1140 <S**2>=0.914

102A ->106A -0.11647

104A ->106A 0.12515

104A ->119A 0.10926

104A ->123A 0.13855

89B ->104B -0.27374

92B ->104B 0.73590

101B ->105B 0.31008

101B ->106B 0.10621

102B ->108B -0.35273

102B ->109B -0.12993

Excited State 49: 2.994-A 4.9495 eV 250.50 nm f=0.0003 <S**2>=1.991

98A ->108A -0.13286

100A ->107A 0.22591

103A ->108A 0.36964

104A ->116A -0.10365

100B ->105B 0.72157

100B ->106B -0.18200

102B ->111B 0.23934

103B ->107B -0.14474

103B ->110B -0.32579

Excited State 50: 2.339-A 4.9513 eV 250.41 nm f=0.0000 <S**2>=1.118

101A ->111A -0.16307

102A ->108A 0.68737

102A ->109A -0.39953

103A ->111A 0.11108

104A ->115A -0.44586

104A ->118A 0.17605

102B ->107B 0.25717

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 910.

Leave Link 914 at Sat Sep 15 18:43:44 2018, MaxMem= 1610612736 cpu: 150344.1

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

6.6 Computed zyx-coordinates of the D_0 state of compound **6**$^{\bullet+}$ and excitation energies (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 1 Multiplicity = 2

C	-0.32961	-2.23046	0.01609
C	-0.94834	-0.98232	-0.00713
N	-0.20278	0.19598	-0.01416
C	1.171	0.17544	-0.01442
C	1.98438	-0.94781	0.00015
S	1.37131	-2.57454	0.03003
S	-1.43742	-3.56781	0.03038
C	-2.79593	-2.45689	0.00088
C	-2.40012	-1.09749	-0.02134
S	2.08991	1.66961	-0.02952
C	3.60053	0.75919	-0.01719
C	3.38624	-0.63671	-0.00155
C	-0.83291	1.50539	0.00122
C	-1.08546	2.15374	-1.20632
C	-1.66566	3.41826	-1.19135
C	-1.96958	3.99094	0.03525
C	-1.71675	3.36146	1.24575

C	-1.13584	2.09759	1.22606
F	-2.53532	5.21778	0.05188
C	-4.1308	-2.8551	-0.00603
C	-5.10976	-1.87226	-0.03899
C	-4.75104	-0.51781	-0.06594
C	-3.42213	-0.12491	-0.05747
C	4.88145	1.30394	-0.02225
C	5.96355	0.42934	-0.01064
C	5.77035	-0.96139	0.00555
C	4.49439	-1.50195	0.01018
H	-0.83936	1.67665	-2.14669
H	-1.87996	3.95039	-2.10892
H	-1.96918	3.85101	2.17723
H	-0.92684	1.57684	2.15225
H	-4.39514	-3.90491	0.01267
H	-6.15493	-2.15668	-0.04503
H	-5.52372	0.24059	-0.09388
H	-3.19387	0.92723	-0.08034
H	5.03415	2.37591	-0.03455
H	6.96975	0.83052	-0.01412
H	6.63018	-1.61985	0.01436
H	4.35769	-2.57704	0.0221

SCF Done: E(UB3LYP) = -2194.86954093 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.592824

Sum of electronic and thermal Energies= -2194.571951

Sum of electronic and thermal Enthalpies= -2194.571007

Sum of electronic and thermal Free Energies= -2194.645049

Excitation energies and oscillator strengths:

Excited State 1: 2.015-A 1.7371 eV 713.74 nm f=0.0858 <S**2>=0.765

102B ->104B -0.17349

103B ->104B 0.97636

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

Total Energy, E(TD-HF/TD-KS) = -2194.80570348

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

Excited State 2: 2.031-A 2.0103 eV 616.75 nm f=0.1564 <S**2>=0.781

104A ->105A 0.15310

102B ->104B 0.96261

103B ->104B 0.15530

Excited State 3: 2.029-A 2.1472 eV 577.43 nm f=0.0219 <S**2>=0.779

104A ->105A -0.21402

101B ->104B 0.95712

102B ->104B 0.11781

Excited State 4: 2.111-A 2.4978 eV 496.37 nm f=0.0103 <S**2>=0.864

104A ->105A 0.92893

101B ->104B 0.23625

102B ->104B -0.11396

Excited State 5: 2.014-A 2.7615 eV 448.98 nm f=0.0002 <S**2>=0.764

100B ->104B 0.99649

Excited State 6: 2.083-A 2.9164 eV 425.12 nm f=0.0004 <S**2>=0.835

98B ->104B -0.31076

99B ->104B 0.91565

Excited State 7: 2.455-A 3.1121 eV 398.39 nm f=0.0221 <S**2>=1.257

102A ->105A 0.14903

103A ->105A -0.26116

104A ->108A 0.20334

97B ->104B 0.24981

98B ->104B 0.73158

99B ->104B 0.31230

102B ->105B 0.15595

103B ->105B 0.30245

Excited State 8: 2.827-A 3.1702 eV 391.09 nm f=0.0259 <S**2>=1.748

101A ->105A -0.10352

102A ->105A -0.21448

103A ->105A 0.33526

104A ->106A -0.14599

104A ->108A -0.32825

97B ->104B -0.13336

98B ->104B 0.56231

99B ->104B 0.14587

102B ->105B -0.22436

103B ->105B -0.44090

Excited State 9: 2.132-A 3.3400 eV 371.21 nm f=0.0018 <S**2>=0.886

102A ->105A -0.11834

104A ->108A -0.23438

97B ->104B 0.91208

98B ->104B -0.12181

102B ->105B -0.13729

Excited State 10: 3.259-A 3.6091 eV 343.53 nm f=0.0265 <S**2>=2.406

101A ->105A 0.35275

101A ->108A 0.10699

102A ->105A 0.15886

103A ->105A 0.55179

104A ->106A 0.12488

104A ->108A 0.23037

95B ->104B 0.11562

96B ->104B -0.12837

97B ->104B 0.19796

101B ->105B -0.14558

102B ->105B 0.41501

103B ->105B -0.29669

Excited State 11: 2.058-A 3.6348 eV 341.11 nm f=0.0003 <S**2>=0.809

104A ->106A 0.21992

104A ->107A 0.81128

104A ->108A -0.13213

104A ->109A -0.46584

104A ->110A 0.10899

104A ->115A 0.10165

Excited State 12: 3.179-A 3.7195 eV 333.34 nm f=0.0009 <S**2>=2.276

98A ->105A 0.10213

99A ->106A -0.10339

100A ->107A -0.11422

101A ->105A -0.23287

101A ->108A 0.11945

101A ->110A -0.15491

102A ->105A 0.21718

102A ->110A 0.13258

103A ->105A 0.15592

103A ->106A -0.24592

103A ->108A -0.17760

103A ->111A -0.18510

104A ->106A 0.39165

104A ->107A -0.10676

104A ->110A 0.13268

96B ->104B 0.10953

99B ->104B -0.10203

100B ->107B 0.11381

101B ->105B 0.23660

101B ->110B -0.20882

103B ->105B -0.10434

103B ->106B -0.20330

103B ->108B -0.23318

103B ->111B -0.15220

Excited State 13: 3.447-A 3.7807 eV 327.94 nm f=0.0005 <S**2>=2.720

98A ->106A -0.15831

99A ->106A -0.33249

99A ->108A 0.11423

99A ->111A 0.13251

100A ->107A -0.43417

100A ->109A -0.21236

103A ->108A 0.10416

98B ->106B 0.27531

98B ->111B -0.10660

99B ->106B 0.26669

100B ->107B 0.45191

100B ->109B 0.18791

103B ->108B 0.10088

Excited State 14: 2.521-A 3.8121 eV 325.23 nm f=0.0012 <S**2>=1.339

101A ->105A 0.24196

102A ->105A -0.22644

103A ->108A 0.13547

104A ->106A 0.70891

104A ->107A -0.22891

104A ->108A -0.26792

104A ->110A -0.11553

96B ->104B -0.21111

101B ->105B -0.24035

102B ->105B -0.12247

103B ->108B 0.10900

Excited State 15: 2.963-A 3.8670 eV 320.62 nm f=0.0209 <S**2>=1.945

98A ->105A -0.13226

101A ->105A -0.40936

101A ->108A -0.11446

101A ->110A 0.14901

102A ->108A -0.16941

103A ->105A 0.12033

103A ->111A 0.18684

104A ->105A 0.10143

104A ->106A 0.42032

104A ->108A 0.32075

96B ->104B 0.22563

99B ->105B 0.12664

101B ->105B 0.21976

101B ->110B 0.17127

102B ->105B -0.11308

102B ->108B 0.21642

102B ->111B -0.13015

103B ->105B -0.10176

103B ->106B 0.10408

103B ->111B 0.14535

Excited State 16: 2.760-A 3.9575 eV 313.29 nm f=0.0297 <S**2>=1.654

101A ->110A -0.11274

102A ->105A -0.41415

102A ->108A 0.11535

102A ->110A 0.13339

103A ->110A 0.13786

104A ->107A 0.15307

104A ->108A 0.62280

104A ->109A 0.13607

95B ->104B 0.11325

96B ->104B -0.20696

101B ->105B -0.14299

101B ->110B -0.15943

101B ->111B 0.11086

102B ->105B -0.19427

102B ->108B -0.10709

103B ->110B 0.12728

Excited State 17: 2.064-A 3.9799 eV 311.53 nm f=0.0011 <S**2>=0.815

104A ->107A 0.47182

104A ->108A -0.17940

104A ->109A 0.81131

104A ->110A -0.14845

104A ->115A -0.11323

Excited State 18: 3.133-A 3.9927 eV 310.53 nm f=0.0095 <S**2>=2.203

97A ->105A 0.15282

97A ->110A 0.10367

101A ->106A 0.16735

101A ->111A 0.21533

102A ->105A 0.18028

102A ->106A -0.11830

102A ->110A 0.10717

102A ->111A -0.11839

103A ->105A 0.23742

103A ->110A 0.31556

104A ->106A 0.11954

104A ->108A -0.14144

104A ->110A -0.15607

104A ->111A -0.16213

96B ->104B 0.12934

97B ->105B 0.14520

97B ->110B -0.12647

101B ->106B 0.17257

101B ->108B 0.13049

101B ->111B 0.23000

102B ->105B 0.16664

103B ->105B 0.36532

103B ->110B 0.30270

103B ->114B 0.10150

Excited State 19: 2.287-A 4.0846 eV 303.54 nm f=0.1016 <S**2>=1.057

101A ->105A -0.13870

103A ->105A 0.47694

103A ->110A -0.15427

104A ->106A -0.16808

104A ->110A -0.38490

104A ->111A 0.26530

96B ->104B -0.23118

102B ->105B -0.27780

103B ->105B 0.46746

103B ->110B -0.12258

Excited State 20: 2.300-A 4.1117 eV 301.54 nm f=0.0445 <S**2>=1.072

101A ->105A	0.14175
102A ->105A	-0.28159
102A ->111A	0.11606
103A ->105A	0.33457
104A ->109A	0.12732
104A ->110A	0.63984
96B ->104B	0.35946
102B ->105B	-0.18216
103B ->105B	0.32671

Excited State 21: 2.304-A 4.1662 eV 297.60 nm f=0.0086 <S**2>=1.077

102A ->105A	-0.11527
104A ->110A	-0.42400
104A ->111A	0.15946
96B ->104B	0.75771
101B ->105B	-0.29151
102B ->111B	0.10467

Excited State 22: 2.435-A 4.2892 eV 289.06 nm f=0.0120 <S**2>=1.232

101A ->105A	0.20903
101A ->111A	0.13555
102A ->105A	0.18932
102A ->108A	-0.12193
102A ->110A	0.16680
103A ->105A	-0.12855
104A ->111A	0.78120
95B ->104B	0.13424
101B ->111B	0.13817
102B ->108B	0.13823
102B ->110B	-0.18770
103B ->105B	-0.10142

Excited State 23: 2.113-A 4.3407 eV 285.63 nm f=0.4406 <S**2>=0.866

101A ->105A	-0.31360
102A ->105A	-0.46212

104A ->111A 0.27173

95B ->104B -0.38217

96B ->104B -0.12242

101B ->105B 0.10492

102B ->105B 0.61804

Excited State 24: 2.567-A 4.4131 eV 280.94 nm f=0.0003 <S**2>=1.397

103A ->107A -0.28274

103A ->109A 0.23972

104A ->109A -0.11602

104A ->112A 0.78020

104A ->115A -0.17863

104A ->116A 0.13416

103B ->107B -0.25178

103B ->109B 0.18535

Excited State 25: 3.088-A 4.4336 eV 279.64 nm f=0.0108 <S**2>=2.134

98A ->105A -0.21374

99A ->105A 0.14821

101A ->105A 0.11333

101A ->106A -0.10104

101A ->110A -0.20512

102A ->105A -0.17994

102A ->106A -0.12061

102A ->108A -0.23920

103A ->106A -0.15819

103A ->108A 0.17198

103A ->111A -0.18947

104A ->110A -0.11183

104A ->111A -0.18606

104A ->113A 0.14294

104A ->114A 0.25146

95B ->104B 0.17585

98B ->105B -0.14153

99B ->105B 0.19685

101B ->105B 0.25778

101B ->110B -0.20239

102B ->106B 0.21876

102B ->108B 0.25014

102B ->111B 0.16008

103B ->106B -0.15736

103B ->108B 0.15296

103B ->111B -0.16639

Excited State 26: 2.369-A 4.4528 eV 278.44 nm f=0.0031 <S**2>=1.153

101A ->105A 0.47249

102A ->105A -0.26925

103A ->108A -0.11667

104A ->110A -0.15115

99B ->105B -0.10073

101B ->105B 0.64530

103B ->106B 0.14629

103B ->108B -0.25309

103B ->111B 0.17733

Excited State 27: 3.166-A 4.5560 eV 272.13 nm f=0.0001 <S**2>=2.256

99A ->107A 0.16158

100A ->105A -0.14235

100A ->106A 0.32345

100A ->107A -0.11151

100A ->108A -0.10436

100A ->111A -0.11088

103A ->107A 0.17025

104A ->112A 0.31451

104A ->115A -0.16295

98B ->107B -0.12028

99B ->107B -0.13834

100B ->106B -0.32512

101B ->112B 0.10267

103B ->106B 0.15593

103B ->107B 0.56229

103B ->109B -0.21432

Excited State 28: 2.351-A 4.5759 eV 270.95 nm f=0.2616 <S**2>=1.132

101A ->105A -0.13921

102A ->105A -0.22499

104A ->108A -0.21277

95B ->104B 0.72712

97B ->105B -0.16545

102B ->105B 0.25426

103B ->105B 0.19752

Excited State 29: 3.326-A 4.5958 eV 269.78 nm f=0.0011 <S**2>=2.515

99A ->106A 0.19101

99A ->107A -0.16552

100A ->105A 0.21515

100A ->106A -0.40157

100A ->107A -0.13869

100A ->108A 0.13318

100A ->109A -0.10010

100A ->111A 0.11929

104A ->112A 0.14241

104A ->115A -0.11257

98B ->106B -0.12296

98B ->107B 0.12865

99B ->106B -0.17890

99B ->107B 0.11975

100B ->105B 0.10746

100B ->106B 0.41758

100B ->107B 0.16848

100B ->111B -0.10867

103B ->106B 0.25797

103B ->107B 0.29909

103B ->109B -0.20830

Excited State 30: 3.347-A 4.6044 eV 269.28 nm f=0.0046 <S**2>=2.550

98A ->106A	0.10965
99A ->106A	0.30816
100A ->105A	-0.13762
100A ->106A	0.15984
100A ->107A	-0.36085
100A ->109A	-0.13532
103A ->106A	0.11820
103A ->111A	-0.10841
104A ->112A	-0.13045
98B ->106B	-0.22524
99B ->106B	-0.25439
100B ->106B	-0.19421
100B ->107B	0.36389
100B ->109B	0.12639
103B ->106B	0.13859
103B ->107B	-0.35081
103B ->109B	0.18615

Excited State 31: 2.142-A 4.6687 eV 265.57 nm f=0.0001 <S**2>=0.897

104A ->109A	0.12735
104A ->112A	0.28457
104A ->115A	0.86745
104A ->121A	0.10723

Excited State 32: 3.130-A 4.7133 eV 263.05 nm f=0.0067 <S**2>=2.200

97A ->105A	0.16944
99A ->106A	-0.10345
101A ->105A	-0.16511
101A ->108A	0.27119
101A ->111A	-0.14893
103A ->108A	0.27550
103A ->114A	-0.11039
104A ->111A	0.16602
104A ->114A	-0.12904

95B ->104B 0.22425

97B ->105B 0.12914

98B ->106B 0.13732

100B ->107B -0.10681

101B ->105B 0.11615

101B ->108B 0.13626

101B ->111B -0.10691

102B ->106B 0.16224

102B ->108B -0.16958

102B ->110B 0.11197

102B ->111B 0.14461

103B ->106B 0.50412

103B ->107B -0.10670

103B ->108B 0.13112

103B ->114B 0.12429

Excited State 33: 2.452-A 4.7300 eV 262.12 nm f=0.0001 <S**2>=1.253

100A ->105A 0.33448

101A ->112A 0.12261

102A ->107A 0.13348

103A ->106A 0.24431

103A ->107A 0.67802

103A ->109A -0.26399

104A ->112A 0.22758

103B ->106B -0.14534

103B ->107B -0.34316

Excited State 34: 2.862-A 4.7467 eV 261.20 nm f=0.0005 <S**2>=1.798

100A ->105A 0.84853

100A ->106A 0.15730

103A ->107A -0.23556

103A ->109A 0.13355

104A ->112A -0.10498

100B ->106B -0.15018

103B ->106B -0.10735

103B ->107B 0.15863

Excited State 35: 3.030-A 4.7564 eV 260.67 nm f=0.0044 <S**2>=2.045

97A ->105A -0.22164

100A ->105A 0.24236

101A ->108A -0.27321

102A ->105A 0.12339

102A ->108A 0.16772

102A ->110A 0.20443

103A ->106A -0.16856

103A ->108A 0.18694

103A ->114A 0.15083

104A ->110A 0.11066

104A ->111A -0.14735

104A ->114A -0.12477

95B ->104B -0.15659

97B ->105B -0.20721

101B ->108B -0.19238

102B ->106B 0.13501

102B ->110B -0.23482

102B ->111B 0.10129

103B ->106B 0.42154

103B ->114B -0.14706

Excited State 36: 3.057-A 4.7909 eV 258.79 nm f=0.0010 <S**2>=2.086

101A ->105A -0.18786

102A ->108A 0.18890

103A ->106A 0.36870

103A ->107A -0.10933

103A ->108A 0.48765

104A ->113A 0.10332

104A ->114A 0.20609

101B ->105B 0.25054

101B ->114B 0.10240

102B ->108B -0.23039

103B ->106B -0.34180

103B ->107B 0.14303

103B ->108B 0.23808

Excited State 37: 2.426-A 4.8295 eV 256.72 nm f=0.0043 <S**2>=1.222

98A ->105A 0.14110

99A ->105A -0.14377

101A ->105A -0.12420

102A ->108A 0.10854

104A ->113A 0.38354

104A ->114A 0.58977

92B ->104B 0.13231

95B ->104B -0.13773

101B ->105B -0.17035

102B ->110B 0.12039

103B ->106B 0.27594

103B ->108B -0.30551

103B ->110B 0.13067

Excited State 38: 2.033-A 4.8454 eV 255.88 nm f=0.0001 <S**2>=0.783

88B ->104B -0.13979

91B ->104B 0.23056

93B ->104B 0.25146

94B ->104B 0.91003

Excited State 39: 2.932-A 4.8605 eV 255.08 nm f=0.0005 <S**2>=1.899

99A ->107A -0.12642

100A ->106A 0.10784

101A ->107A 0.18046

101A ->109A -0.13240

103A ->107A -0.13905

103A ->109A -0.16803

103A ->112A 0.19930

104A ->112A 0.11395

104A ->113A 0.48491

104A ->114A -0.29846

104A ->115A -0.12256

98B ->107B 0.10737

99B ->107B 0.11250

100B ->105B -0.12380

100B ->106B -0.12311

101B ->107B 0.21544

101B ->109B -0.17713

103B ->107B -0.16636

103B ->109B -0.35214

103B ->112B 0.22826

Excited State 40: 2.860-A 4.8900 eV 253.54 nm f=0.0101 <S**2>=1.796

99A ->105A 0.13599

102A ->106A -0.15248

102A ->111A -0.10868

103A ->106A 0.44701

103A ->107A -0.15504

103A ->108A -0.14464

104A ->110A 0.16571

104A ->113A -0.13545

99B ->110B -0.11461

101B ->105B -0.14539

102B ->106B 0.51355

102B ->111B 0.21437

103B ->106B -0.16336

103B ->108B -0.34617

103B ->111B 0.22831

Excited State 41: 2.536-A 4.8952 eV 253.28 nm f=0.0014 <S**2>=1.358

99A ->107A 0.10270

104A ->113A 0.60845

104A ->114A -0.39352

104A ->117A -0.10165

104A ->118A 0.11699

99B ->107B -0.10013

101B ->107B -0.12688

101B ->109B 0.11129

102B ->106B 0.12889

102B ->107B 0.15362

102B ->109B -0.13282

103B ->107B 0.19796

103B ->109B 0.38334

103B ->112B -0.13052

Excited State 42: 2.782-A 4.9121 eV 252.41 nm f=0.0009 <S**2>=1.684

101A ->107A -0.13728

101A ->109A 0.12980

102A ->107A 0.10719

103A ->107A -0.20439

103A ->112A -0.16069

104A ->116A -0.10117

88B ->104B -0.24117

91B ->104B 0.46044

93B ->104B 0.27512

94B ->104B -0.30270

101B ->107B -0.26387

101B ->109B 0.20428

102B ->112B 0.10177

103B ->107B -0.17663

103B ->109B -0.27278

103B ->112B -0.24765

Excited State 43: 2.688-A 4.9254 eV 251.72 nm f=0.0007 <S**2>=1.556

101A ->107A 0.15167

101A ->109A -0.12861

102A ->107A -0.13511

103A ->107A 0.17888

103A ->112A 0.19370

104A ->113A -0.11887

104A ->116A -0.10571

88B ->104B -0.25560

91B ->104B 0.48038

93B ->104B 0.32736

94B ->104B -0.21832

101B ->107B 0.23276

101B ->109B -0.15149

102B ->107B 0.26599

103B ->107B 0.16009

103B ->109B 0.20552

103B ->112B 0.20629

Excited State 44: 2.806-A 4.9531 eV 250.32 nm f=0.0003 <S**2>=1.719

99A ->107A -0.13768

92B ->104B 0.10912

93B ->104B -0.40873

98B ->107B 0.13498

99B ->107B 0.13583

100B ->105B -0.45180

102B ->107B 0.56063

102B ->109B -0.18056

103B ->108B 0.10809

Excited State 45: 2.273-A 4.9631 eV 249.81 nm f=0.0004 <S**2>=1.041

88B ->104B 0.15732

91B ->104B -0.38071

93B ->104B 0.72554

100B ->105B -0.43792

Excited State 46: 2.811-A 4.9692 eV 249.51 nm f=0.0016 <S**2>=1.726

98A ->108A 0.15712

99A ->105A -0.16726

102A ->106A -0.13572

102A ->108A -0.20212

102A ->111A -0.11257

102A ->114A -0.13024

103A ->106A 0.25521

103A ->107A -0.12126

103A ->108A -0.27746

104A ->114A -0.14963

104A ->122A -0.18796

90B ->104B 0.13532

92B ->104B 0.35104

99B ->105B -0.11190

99B ->108B 0.10990

100B ->105B 0.35449

102B ->107B -0.11827

102B ->114B -0.15607

103B ->108B 0.26962

103B ->110B 0.14150

Excited State 47: 2.942-A 4.9766 eV 249.13 nm f=0.0048 <S**2>=1.914

99A ->107A -0.10210

103A ->106A -0.30621

103A ->107A 0.11028

103A ->108A 0.21786

91B ->104B -0.19017

93B ->104B 0.18662

100B ->105B 0.50275

100B ->106B -0.12087

102B ->106B 0.21455

102B ->107B 0.34860

102B ->110B 0.12098

103B ->106B -0.14369

103B ->109B -0.20620

103B ->110B 0.17389

103B ->111B 0.18076

Excited State 48: 3.071-A 4.9780 eV 249.06 nm f=0.0121 <S**2>=2.108

99A ->106A -0.11800

102A ->110A 0.15341

103A ->106A 0.35212

103A ->108A -0.11549

103A ->111A -0.12456

104A ->111A -0.12924

104A ->114A 0.15874

91B ->104B -0.10292

92B ->104B -0.15873

99B ->106B 0.13752

100B ->105B 0.36520

101B ->108B 0.10020

102B ->106B -0.11362

102B ->107B 0.37614

102B ->109B -0.16837

102B ->110B -0.20626

103B ->106B 0.15146

103B ->109B -0.15853

103B ->110B -0.25854

103B ->111B -0.24107

Excited State 49: 2.928-A 5.0008 eV 247.93 nm f=0.0224 <S**2>=1.893

98A ->105A -0.13798

99A ->105A 0.38122

101A ->110A -0.10525

102A ->108A 0.22012

102A ->110A -0.11825

103A ->108A -0.23131

104A ->111A 0.11754

90B ->104B -0.15298

92B ->104B -0.34258

97B ->105B -0.13045

100B ->105B 0.11968

101B ->108B -0.19847

102B ->106B -0.12965

102B ->108B -0.30789

102B ->110B 0.27187

103B ->108B 0.17339

103B ->110B 0.31921

Excited State 50: 2.792-A 5.0117 eV 247.39 nm f=0.0258 <S**2>=1.698

98A ->110A -0.11292

99A ->105A 0.38396

102A ->106A -0.12992

102A ->108A 0.17244

102A ->110A 0.12059

102A ->111A -0.16516

103A ->106A -0.25346

103A ->108A -0.30523

103A ->111A 0.14088

104A ->110A 0.13616

104A ->114A 0.18671

90B ->104B 0.12325

92B ->104B 0.28944

97B ->105B 0.12468

98B ->106B -0.10117

102B ->108B -0.13150

102B ->110B -0.22139

103B ->108B 0.28351

103B ->110B -0.18320

103B ->111B 0.13392

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 910.

Leave Link 914 at Sat Sep 15 19:37:39 2018, MaxMem= 1610612736 cpu: 172610.9

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

6.7 Computed zyx-coordinates of the D_0 state of compound **7**$^{\bullet+}$ and excitation energies (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 1 Multiplicity = 2

C -1.33555 -1.42298 0.00004

C	-1.19255	-0.04302	-0.0005
N	0.00000	0.64047	-0.00063
C	1.19255	-0.04302	-0.0005
C	1.33555	-1.42298	0.00004
S	0.00000	-2.54345	0.00044
C	0.00000	2.09373	-0.0002
C	0.00000	2.77253	-1.21785
C	0.00000	4.16328	-1.219
C	0.00000	4.82442	0.00076
C	0.00000	4.16245	1.22004
C	0.00000	2.77169	1.21791
C	3.58612	-0.73075	-0.0004
C	2.71084	-1.83995	0.00008
S	2.72041	0.80792	-0.00087
C	4.96918	-0.88828	-0.00041
C	5.47964	-2.18265	0.00008
C	4.62615	-3.29735	0.00057
C	3.24955	-3.13836	0.00059
C	-2.71084	-1.83995	0.00008
C	-3.58612	-0.73075	-0.0004
S	-2.72041	0.80792	-0.00087
C	-3.24955	-3.13836	0.00059
C	-4.62615	-3.29735	0.00057
C	-5.47964	-2.18265	0.00008
C	-4.96918	-0.88829	-0.00041
H	0.00000	2.2224	-2.15044
H	0.00000	4.72576	-2.14337
H	0.00000	4.72425	2.14483
H	0.00000	2.22094	2.15014
H	5.63135	-0.03152	-0.00077
H	6.55293	-2.32912	0.00009
H	5.0494	-4.29422	0.00097
H	2.60018	-4.00591	0.00099

H	-2.60018	-4.00591	0.00099
H	-5.0494	-4.29422	0.00097
H	-6.55293	-2.32912	0.00009
H	-5.63135	-0.03152	-0.00077
F	0.00000	6.17535	0.00121

SCF Done: E(UB3LYP) = -2194.87671877 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.600413

Sum of electronic and thermal Energies= -2194.579338

Sum of electronic and thermal Enthalpies= -2194.578394

Sum of electronic and thermal Free Energies= -2194.652956

Excitation energies and oscillator strengths:

Excited State 1: 2.025-A 1.7675 eV 701.48 nm f=0.1540 <S**2>=0.775

104A ->105A 0.15280

103B ->104B 0.98017

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

Total Energy, E(TD-HF/TD-KS) = -2194.81176560

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

Excited State 2: 2.016-A 1.8698 eV 663.07 nm f=0.0020 <S**2>=0.766

102B ->104B 0.99510

Excited State 3: 2.028-A 2.3048 eV 537.94 nm f=0.1112 <S**2>=0.778

101B ->104B 0.98793

Excited State 4: 2.077-A 2.5402 eV 488.10 nm f=0.0771 <S**2>=0.828

104A ->105A 0.96349

103B ->104B -0.15585

Excited State 5: 2.131-A 2.6367 eV 470.23 nm f=0.0008 <S**2>=0.886

103A ->105A -0.10749

104A ->108A 0.11629

100B ->104B 0.96069

103B ->105B 0.14212

Excited State 6: 2.012-A 2.7954 eV 443.52 nm f=0.0000 <S**2>=0.762

99B ->104B 0.99707

Excited State 7: 2.018-A 3.1059 eV 399.19 nm f=0.0011 <S**2>=0.768

98B ->104B 0.99637

Excited State 8: 3.211-A 3.2277 eV 384.12 nm f=0.0095 <S**2>=2.327

101A ->105A -0.18011

102A ->109A -0.11197

103A ->105A -0.46947

104A ->108A 0.36423

100B ->104B -0.23662

100B ->108B -0.11600

101B ->105B -0.17056

103B ->105B 0.63299

Excited State 9: 2.333-A 3.5120 eV 353.03 nm f=0.0058 <S**2>=1.111

99A ->105A 0.14096

102A ->105A 0.15221

103A ->108A 0.17634

104A ->110A -0.11547

104A ->114A 0.13308

97B ->104B 0.88645

100B ->105B -0.15442

103B ->108B 0.14447

Excited State 10: 3.415-A 3.7037 eV 334.76 nm f=0.0071 <S**2>=2.665

101A ->108A -0.14630

102A ->105A 0.72051

97B ->104B -0.12341

101B ->109B -0.14753

102B ->105B -0.60333

Excited State 11: 2.032-A 3.7100 eV 334.19 nm f=0.0000 <S**2>=0.783

104A ->106A 0.89806

104A ->112A -0.40752

Excited State 12: 2.602-A 3.7123 eV 333.98 nm f=0.0000 <S**2>=1.443

101A ->105A -0.24455

102A ->108A 0.17800

103A ->105A 0.32954

104A ->108A 0.35363

104A ->109A -0.19311

96B ->104B 0.69294

101B ->105B -0.23005

102B ->109B -0.14910

103B ->105B -0.19621

Excited State 13: 3.469-A 3.7960 eV 326.62 nm f=0.0000 <S**2>=2.758

98A ->107A -0.42462

98A ->110A 0.13365

100A ->106A -0.48696

100A ->112A -0.17395

101A ->107A 0.12390

98B ->107B 0.42944

98B ->110B -0.12335

99B ->106B 0.49301

99B ->112B 0.15703

101B ->107B 0.12588

Excited State 14: 3.203-A 3.8452 eV 322.44 nm f=0.0000 <S**2>=2.315

99A ->105A -0.22640

99A ->110A -0.13186

101A ->109A 0.20375

102A ->107A -0.14890

102A ->110A -0.29526

103A ->108A -0.27642

103A ->109A -0.22658

104A ->105A -0.10557

104A ->110A 0.14196

104A ->114A -0.13531

97B ->104B 0.39602

97B ->108B 0.12870

100B ->105B 0.24989

100B ->110B 0.16612

101B ->108B -0.13699

101B ->109B -0.17952

102B ->107B 0.13276

102B ->110B 0.26390

103B ->108B -0.33816

Excited State 15: 2.072-A 3.8961 eV 318.23 nm f=0.0008 <S**2>=0.824

102A ->105A 0.12556

104A ->107A 0.96082

104A ->110A 0.17994

Excited State 16: 3.181-A 4.0030 eV 309.73 nm f=0.0045 <S**2>=2.280

97A ->105A -0.12354

99A ->108A 0.12814

99A ->109A 0.10630

101A ->110A -0.10877

102A ->109A 0.32634

103A ->105A -0.19560

103A ->107A 0.14869

103A ->110A 0.34090

104A ->108A -0.25438

104A ->109A -0.31760

96B ->104B 0.25524

97B ->105B 0.15185

100B ->108B 0.19501

101B ->110B -0.16599

102B ->108B 0.24200

102B ->109B 0.17395

103B ->105B 0.23939

103B ->107B -0.11560

103B ->110B -0.29753

Excited State 17: 2.807-A 4.0557 eV 305.71 nm f=0.0072 <S**2>=1.720

101A ->105A -0.39262

102A ->108A 0.16253

102A ->109A 0.10289

103A ->105A 0.50878

104A ->109A 0.23584

96B ->104B -0.42185

101B ->105B -0.35993

102B ->108B 0.12228

103B ->105B 0.27444

103B ->110B -0.10292

Excited State 18: 2.068-A 4.0696 eV 304.66 nm f=0.0000 <S**2>=0.820

104A ->111A 0.97880

Excited State 19: 2.038-A 4.0761 eV 304.17 nm f=0.0000 <S**2>=0.788

104A ->106A 0.42942

104A ->112A 0.87868

104A ->116A -0.11531

Excited State 20: 2.668-A 4.0792 eV 303.94 nm f=0.0007 <S**2>=1.529

101A ->105A 0.31562

101A ->110A -0.16448

102A ->109A 0.21634

103A ->105A 0.11702

104A ->108A 0.51087

104A ->109A 0.49625

96B ->104B 0.17186

101B ->105B 0.31065

101B ->110B -0.15146

102B ->108B 0.11409

102B ->109B 0.22180

103B ->105B 0.16070

Excited State 21: 2.217-A 4.1365 eV 299.73 nm f=0.0230 <S**2>=0.979

101A ->105A -0.28631

104A ->108A -0.51754

104A ->109A 0.59437

93B ->104B 0.14433

96B ->104B 0.43400

103B ->105B 0.14290

103B ->110B 0.10437

Excited State 22: 2.126-A 4.1661 eV 297.60 nm f=0.1555 <S**2>=0.880

101A ->109A -0.14288

102A ->105A 0.41538

103A ->109A -0.11154

104A ->107A -0.24146

104A ->110A 0.69272

102B ->105B 0.45889

Excited State 23: 2.410-A 4.2415 eV 292.31 nm f=0.1110 <S**2>=1.202

101A ->105A 0.24593

102A ->108A -0.11844

103A ->105A 0.54114

104A ->108A -0.17899

104A ->109A -0.27952

93B ->104B 0.13650

96B ->104B 0.12845

101B ->105B 0.32085

101B ->110B 0.15698

102B ->108B -0.22506

103B ->105B 0.51279

Excited State 24: 2.220-A 4.2436 eV 292.17 nm f=0.2149 <S**2>=0.983

101A ->109A 0.10079

102A ->105A 0.44061

104A ->110A -0.57194

101B ->108B -0.15532

102B ->105B 0.59356

102B ->110B 0.15649

Excited State 25: 3.187-A 4.4406 eV 279.21 nm f=0.0216 <S**2>=2.290

99A ->105A -0.29973

101A ->108A -0.18699

101A ->109A -0.10748

102A ->107A 0.14471

102A ->110A 0.25423

103A ->108A -0.21430

103A ->109A 0.28384

104A ->114A -0.31006

95B ->104B 0.31806

97B ->104B 0.12430

100B ->105B 0.33335

101B ->108B 0.20278

102B ->107B -0.14491

102B ->110B -0.25117

103B ->109B 0.34973

Excited State 26: 3.434-A 4.6131 eV 268.76 nm f=0.0000 <S**2>=2.699

98A ->106A 0.29459

100A ->105A 0.17350

100A ->107A 0.48217

100A ->110A -0.13512

101A ->106A -0.12463

102A ->111A -0.11322

103A ->106A 0.18381

98B ->106B -0.30783

99B ->105B -0.11440

99B ->107B -0.47403

99B ->110B 0.11876

101B ->106B -0.14003

102B ->111B 0.15361

103B ->106B -0.36718

103B ->112B 0.10920

Excited State 27: 2.619-A 4.6162 eV 268.59 nm f=0.0242 <S**2>=1.464

98A ->107A -0.21925

100A ->106A 0.23140

101A ->105A 0.35986

101A ->107A 0.10399

93B ->104B 0.59844

97B ->105B 0.10851

98B ->107B 0.23166

99B ->106B -0.23671

100B ->109B -0.10052

101B ->105B -0.31742

103B ->107B 0.20791

103B ->114B 0.12241

Excited State 28: 3.143-A 4.6271 eV 267.96 nm f=0.0088 <S**2>=2.220

98A ->107A 0.38667

98A ->110A -0.10557

100A ->106A -0.38446

100A ->112A -0.11963

101A ->105A 0.20571

101A ->107A -0.11606

103A ->107A 0.12740

93B ->104B 0.40406

98B ->107B -0.38552

99B ->106B 0.38550

99B ->112B 0.10658

101B ->105B -0.20919

101B ->107B -0.14248

Excited State 29: 3.260-A 4.6687 eV 265.57 nm f=0.0001 <S**2>=2.406

100A ->105A 0.17976

100A ->107A 0.28686

102A ->111A 0.21519

103A ->106A -0.14828

103A ->112A 0.13301

99B ->107B -0.30374

102B ->111B -0.32654

103B ->106B 0.65434

103B ->112B -0.27740

Excited State 30: 3.399-A 4.7197 eV 262.70 nm f=0.0000 <S**2>=2.639

101A ->111A -0.11141

102A ->106A -0.35971

102A ->112A 0.21158

103A ->111A 0.28912

101B ->111B -0.16496

102B ->106B 0.55386

102B ->112B -0.28911

103B ->111B -0.48807

Excited State 31: 2.427-A 4.7341 eV 261.90 nm f=0.0901 <S**2>=1.223

97A ->105A -0.11766

101A ->105A -0.33244

101A ->110A 0.11935

102A ->109A -0.21274

103A ->114A -0.12327

104A ->108A 0.20659

93B ->104B 0.41192

97B ->105B 0.10678

100B ->108B 0.12801

101B ->105B 0.47331

101B ->110B 0.10132

103B ->105B -0.16997

103B ->107B -0.40978

103B ->110B -0.24676

Excited State 32: 2.822-A 4.7449 eV 261.30 nm f=0.0199 <S**2>=1.740

99A ->105A 0.33123

101A ->108A -0.12528

101A ->109A 0.19370

102A ->107A -0.15462

102A ->114A -0.13134

103A ->108A 0.13289

104A ->110A 0.20568

104A ->114A -0.46421

95B ->104B 0.47591

100B ->105B -0.28852

101B ->109B -0.17436

102B ->107B 0.14950

102B ->110B 0.10593

103B ->108B 0.21921

Excited State 33: 2.039-A 4.7846 eV 259.13 nm f=0.0020 <S**2>=0.789

84B ->104B 0.11299

88B ->104B 0.18704

91B ->104B 0.91283

92B ->104B -0.27497

103B ->106B -0.12901

Excited State 34: 2.876-A 4.8026 eV 258.16 nm f=0.0002 <S**2>=1.818

98A ->106A -0.14648

100A ->105A 0.95120

98B ->106B 0.11344

99B ->107B 0.10939

Excited State 35: 2.985-A 4.8200 eV 257.23 nm f=0.0155 <S**2>=1.977

97A ->105A 0.15237

98A ->105A 0.10222

99A ->108A -0.19122

101A ->105A -0.28617

101A ->110A -0.17189

102A ->108A -0.20685

102A ->109A 0.23005

103A ->110A -0.15552

103A ->114A 0.18063

104A ->109A -0.22869

104A ->121A -0.23100

93B ->104B 0.38981

97B ->105B -0.18123

100B ->108B -0.18977

101B ->105B 0.11790

101B ->107B -0.10680

101B ->110B -0.21369

102B ->108B 0.19050

102B ->109B 0.22952

103B ->110B 0.22369

103B ->114B -0.20603

Excited State 36: 2.637-A 4.8383 eV 256.25 nm f=0.0002 <S**2>=1.489

100A ->105A 0.10587

100A ->107A -0.10848

101A ->106A -0.12004

102A ->111A -0.45181

103A ->106A 0.54850

103A ->112A -0.23836

104A ->113A 0.11518

102B ->111B 0.21011

103B ->106B 0.52898

Excited State 37: 2.059-A 4.8618 eV 255.02 nm f=0.0010 <S**2>=0.809

104A ->113A 0.95439

104A ->117A -0.17220

Excited State 38: 3.015-A 4.8651 eV 254.85 nm f=0.0367 <S**2>=2.023

97A ->105A -0.13164

99A ->108A 0.16342

101A ->105A -0.27063

101A ->114A -0.11526

102A ->108A -0.13255

103A ->107A -0.14043

103A ->114A -0.16911

104A ->109A -0.10724

104A ->121A 0.18495

97B ->105B 0.17606

100B ->109B -0.19537

101B ->105B 0.19267

103B ->107B 0.71891

103B ->114B 0.18629

Excited State 39: 2.459-A 4.8688 eV 254.65 nm f=0.0142 <S**2>=1.262

99A ->105A -0.18123

103A ->109A -0.10786

104A ->114A 0.30782

95B ->104B 0.66179

100B ->105B -0.34191

100B ->110B 0.15702

101B ->108B 0.10664

103B ->108B -0.35044

103B ->109B -0.26381

Excited State 40: 2.024-A 4.8697 eV 254.60 nm f=0.0000 <S**2>=0.774

94B ->104B 0.99173

Excited State 41: 2.094-A 4.8954 eV 253.27 nm f=0.0000 <S**2>=0.846

101A ->111A 0.12472

102A ->106A 0.70854

102A ->112A -0.21555

103A ->111A -0.29707

102B ->106B 0.52627

103B ->111B -0.18987

Excited State 42: 2.304-A 4.9284 eV 251.57 nm f=0.2607 <S**2>=1.078

99A ->105A 0.28182

101A ->108A -0.12246

103A ->108A 0.13275

104A ->114A 0.55177

95B ->104B 0.29074

100B ->105B 0.53219

101B ->109B -0.10508

102B ->107B 0.32272

103B ->109B 0.11293

Excited State 43: 2.936-A 4.9419 eV 250.88 nm f=0.0001 <S**2>=1.905

98A ->106A -0.33847

100A ->107A 0.21925

101A ->106A 0.10657

102A ->111A -0.12487

103A ->106A -0.19604

91B ->104B 0.18159

92B ->104B 0.51795

98B ->106B 0.36107

99B ->105B -0.35431

99B ->107B -0.21507

101B ->106B 0.10520

102B ->111B 0.23939

103B ->112B 0.15935

Excited State 44: 2.565-A 4.9489 eV 250.53 nm f=0.0000 <S**2>=1.395

98A ->106A 0.26015

100A ->107A -0.19087

103A ->106A 0.13191

91B ->104B 0.19509

92B ->104B 0.78773

98B ->106B -0.26838

99B ->107B 0.18210

102B ->111B -0.15103

103B ->112B -0.12980

Excited State 45: 2.684-A 4.9552 eV 250.21 nm f=0.0090 <S**2>=1.551

99A ->105A 0.68067

99A ->110A -0.12891

101A ->109A -0.16566

102A ->107A 0.23624

102A ->114A 0.10682

103A ->108A -0.18035

103A ->109A -0.14485

104A ->110A -0.14922

104A ->114A -0.29534

100B ->105B 0.26336

102B ->107B -0.13767

103B ->108B -0.28094

103B ->109B -0.15635

Excited State 46: 3.211-A 4.9804 eV 248.95 nm f=0.0028 <S**2>=2.327

98A ->105A -0.11930

99A ->108A -0.12070

101A ->114A 0.19497

102A ->108A 0.52125

104A ->121A -0.16495

93B ->104B 0.11879

97B ->105B -0.10308

100B ->109B 0.18112

101B ->105B 0.27582

101B ->114B 0.18509

102B ->108B 0.25191

102B ->109B -0.31566

103B ->107B 0.37941

103B ->110B -0.20706

103B ->114B -0.12833

Excited State 47: 2.895-A 4.9991 eV 248.01 nm f=0.0003 <S**2>=1.846

100A ->107A 0.16245

103A ->106A -0.30253

92B ->104B 0.12382

99B ->105B 0.83732

101B ->106B -0.11365

102B ->111B 0.29265

103B ->106B 0.14163

103B ->112B 0.11101

Excited State 48: 3.188-A 5.0071 eV 247.62 nm f=0.0000 <S**2>=2.291

102A ->106A -0.28480

103A ->111A -0.16114

104A ->116A 0.12339

104A ->118A -0.16509

102B ->106B 0.56456

103B ->111B 0.68820

Excited State 49: 3.309-A 5.0143 eV 247.26 nm f=0.0116 <S**2>=2.488

99A ->105A 0.30705

101A ->108A -0.18922

103A ->108A -0.37205

103A ->109A 0.13725

104A ->105A -0.11239

104A ->114A 0.23335

95B ->104B -0.20124

100B ->105B -0.43748

100B ->114B -0.10122

101B ->109B -0.11433

103B ->108B -0.24243

103B ->109B 0.51166

Excited State 50: 3.091-A 5.0261 eV 246.68 nm f=0.0000 <S**2>=2.138

98A ->106A -0.25118

100A ->107A 0.15011

101A ->106A 0.14937

103A ->106A 0.47760

103A ->112A -0.11923

98B ->106B 0.26302

99B ->105B 0.36726

99B ->107B -0.21357

101B ->106B 0.30533

102B ->111B -0.43777

103B ->106B -0.20706

103B ->112B -0.12320

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 910.

Leave Link 914 at Sat Sep 15 18:09:14 2018, MaxMem= 1610612736 cpu: 134397.4

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

6.8 Computed zyx-coordinates of the S_0 state of compound **5**$^{2+}$ and excitation energies (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 2 Multiplicity = 1

C -1.31222 -2.16806 0.00008

C	-1.22095	-0.74156	-0.00002
N	0.00002	-0.1142	0.00000
C	1.22103	-0.74148	0.00002
C	1.31239	-2.16798	-0.00008
S	0.00012	-3.24341	0.00000
C	2.54542	-0.13881	0.00009
C	3.54865	-1.14093	-0.00006
S	2.91116	-2.78037	-0.00021
S	-2.91097	-2.78055	0.00021
C	-3.54855	-1.14114	0.00006
C	-2.54537	-0.13897	-0.00009
C	-0.00005	1.34835	0.00000
C	-4.90767	-0.86524	0.00006
C	-5.30128	0.4692	-0.00013
C	-4.34354	1.4884	-0.00032
C	-2.98754	1.20448	-0.00029
C	2.98753	1.20466	0.00029
C	4.34351	1.48865	0.00032
C	5.30131	0.4695	0.00012
C	4.90776	-0.86496	-0.00006
C	-0.00028	2.01526	1.22084
C	-0.00035	3.40642	1.22055
C	-0.00021	4.0698	0.00000
C	0.00001	3.40642	-1.22055
C	0.00009	2.01526	-1.22084
F	-0.00028	5.41493	0.00000
H	-5.63966	-1.66314	0.00019
H	-6.35593	0.71464	-0.00014
H	-4.66135	2.52309	-0.00049
H	-2.29657	2.0274	-0.00045
H	2.29652	2.02755	0.00045
H	4.66127	2.52335	0.00048
H	6.35594	0.71499	0.00013

H	5.63979	-1.66282	-0.0002
H	-0.00038	1.46488	2.15326
H	-0.00052	3.96793	2.14536
H	0.00011	3.96793	-2.14536
H	0.00024	1.46488	-2.15326

SCF Done: E(UB3LYP) = -2194.63413811 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.356249

Sum of electronic and thermal Energies= -2194.335685

Sum of electronic and thermal Enthalpies= -2194.334741

Sum of electronic and thermal Free Energies= -2194.406370

Excitation energies and oscillator strengths:

Excited State 1: 3.000-A 0.9692 eV 1279.29 nm f=0.0000 <S**2>=2.000

100A ->104A 0.11244

103A ->104A 0.69939

100B ->104B -0.11244

103B ->104B -0.69939

103A <-104A 0.11375

103B <-104B -0.11375

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

Total Energy, E(TD-HF/TD-KS) = -2194.59852194

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

Excited State 2: 3.000-A 1.2533 eV 989.30 nm f=0.0000 <S**2>=2.000

102A ->104A 0.70066

102B ->104B -0.70066

Excited State 3: 1.000-A 1.6231 eV 763.86 nm f=0.0035 <S**2>=0.000

102A ->104A 0.70574

102B ->104B 0.70574

Excited State 4: 1.000-A 1.6845 eV 736.01 nm f=0.2255 <S**2>=0.000

100A ->104A -0.20492

103A ->104A 0.67708

100B ->104B -0.20492

103B ->104B 0.67708

Excited State 5: 3.000-A 1.8116 eV 684.40 nm f=0.0000 <S**2>=2.000

100A ->104A 0.69309

103A ->104A -0.10891

100B ->104B -0.69309

103B ->104B 0.10891

Excited State 6: 3.000-A 2.0109 eV 616.55 nm f=0.0000 <S**2>=2.000

101A ->104A 0.70516

101B ->104B -0.70516

Excited State 7: 1.000-A 2.0256 eV 612.08 nm f=0.0000 <S**2>=0.000

101A ->104A 0.70547

101B ->104B 0.70547

Excited State 8: 3.000-A 2.1109 eV 587.36 nm f=0.0000 <S**2>=2.000

98A ->104A -0.69001

103A ->105A 0.10906

98B ->104B 0.69001

103B ->105B -0.10906

Excited State 9: 1.000-A 2.2029 eV 562.83 nm f=0.1378 <S**2>=0.000

99A ->104A 0.23303

100A ->104A 0.63910

103A ->104A 0.18174

99B ->104B 0.23303

100B ->104B 0.63910

103B ->104B 0.18174

Excited State 10: 3.000-A 2.3169 eV 535.14 nm f=0.0000 <S**2>=2.000

99A ->104A 0.69833

99B ->104B -0.69833

Excited State 11: 1.000-A 2.3963 eV 517.40 nm f=0.0778 <S**2>=0.000

99A ->104A 0.66571

100A ->104A -0.21105

99B ->104B 0.66571

100B ->104B -0.21105

Excited State 12: 1.000-A 2.6377 eV 470.05 nm f=0.0111 <S**2>=0.000

98A ->104A 0.69899

98B ->104B 0.69899

Excited State 13: 3.000-A 2.8480 eV 435.33 nm f=0.0000 <S**2>=2.000

96A ->104A -0.23772

98A ->104A -0.11822

103A ->105A -0.62208

96B ->104B 0.23772

98B ->104B 0.11822

103B ->105B 0.62208

Excited State 14: 3.000-A 3.0562 eV 405.69 nm f=0.0000 <S**2>=2.000

97A ->104A 0.61554

102A ->105A 0.29449

103A ->106A -0.11123

97B ->104B -0.61554

102B ->105B -0.29449

103B ->106B 0.11123

Excited State 15: 3.000-A 3.1829 eV 389.53 nm f=0.0000 <S**2>=2.000

96A ->104A -0.61431

100A ->105A 0.18347

102A ->106A 0.12742

103A ->105A 0.21997

96B ->104B 0.61431

100B ->105B -0.18347

102B ->106B -0.12742

103B ->105B -0.21997

Excited State 16: 3.000-A 3.2287 eV 384.01 nm f=0.0000 <S**2>=2.000

92A ->104A -0.12240

97A ->104A -0.29801

100A ->106A 0.12848

102A ->105A 0.60338

92B ->104B 0.12240

97B ->104B 0.29801

100B ->106B -0.12848

102B ->105B -0.60338

Excited State 17: 1.000-A 3.4860 eV 355.67 nm f=0.0001 <S**2>=0.000

97A ->104A 0.66572

102A ->105A -0.21397

97B ->104B 0.66572

102B ->105B -0.21397

Excited State 18: 1.000-A 3.6260 eV 341.93 nm f=0.0907 <S**2>=0.000

96A ->104A -0.28608

100A ->105A -0.10671

103A ->105A 0.63112

96B ->104B -0.28608

100B ->105B -0.10671

103B ->105B 0.63112

Excited State 19: 3.000-A 3.6615 eV 338.61 nm f=0.0000 <S**2>=2.000

86A ->104A -0.10313

96A ->104A -0.18045

100A ->105A -0.60982

102A ->106A -0.21776

103A ->105A 0.12383

86B ->104B 0.10313

96B ->104B 0.18045

100B ->105B 0.60982

102B ->106B 0.21776

103B ->105B -0.12383

Excited State 20: 3.000-A 3.7017 eV 334.94 nm f=0.0000 <S**2>=2.000

97A ->104A 0.10596

98A ->105A -0.35258

98A ->113A 0.14552

100A ->106A 0.13751

100A ->110A -0.15802

102A ->107A 0.16954

102A ->112A -0.19247

103A ->106A 0.37862

103A ->110A 0.23201

97B ->104B -0.10596

98B ->105B 0.35258

98B ->113B -0.14552

100B ->106B -0.13751

100B ->110B 0.15802

102B ->107B -0.16954

102B ->112B 0.19247

103B ->106B -0.37862

103B ->110B -0.23201

Excited State 21: 1.000-A 3.7348 eV 331.97 nm f=0.0206 <S**2>=0.000

96A ->104A 0.62121

100A ->105A 0.11508

103A ->105A 0.29707

96B ->104B 0.62121

100B ->105B 0.11508

103B ->105B 0.29707

Excited State 22: 3.000-A 3.7912 eV 327.03 nm f=0.0000 <S**2>=2.000

99A ->107A 0.39302

99A ->112A 0.20277

101A ->108A 0.36536

101A ->109A -0.36421

103A ->107A 0.13048

99B ->107B -0.39302

99B ->112B -0.20277

101B ->108B -0.36536

101B ->109B 0.36421

103B ->107B -0.13048

Excited State 23: 1.000-A 3.8198 eV 324.58 nm f=0.5783 <S**2>=0.000

97A ->104A 0.20942

102A ->105A 0.66186

97B ->104B 0.20942

102B ->105B 0.66186

Excited State 24: 3.000-A 4.0020 eV 309.81 nm f=0.0000 <S**2>=2.000

97A ->105A	0.17530
98A ->106A	0.19095
98A ->110A	0.13334
99A ->105A	-0.12027
100A ->107A	-0.13895
100A ->112A	0.18102
102A ->110A	0.37540
103A ->107A	0.27822
103A ->112A	-0.22068
103A ->113A	0.17128
97B ->105B	-0.17530
98B ->106B	-0.19095
98B ->110B	-0.13334
99B ->105B	0.12027
100B ->107B	0.13895
100B ->112B	-0.18102
102B ->110B	-0.37540
103B ->107B	-0.27822
103B ->112B	0.22068
103B ->113B	-0.17128

Excited State 25: 3.000-A 4.1207 eV 300.88 nm f=0.0000 <S**2>=2.000

101A ->105A	-0.70021
101B ->105B	0.70021

Excited State 26: 1.000-A 4.1448 eV 299.13 nm f=0.0004 <S**2>=0.000

101A ->105A	0.70582
101B ->105B	0.70582

Excited State 27: 3.000-A 4.2178 eV 293.96 nm f=0.0000 <S**2>=2.000

92A ->104A	-0.56501
100A ->106A	0.14434
100A ->110A	0.10123
102A ->105A	-0.12383
102A ->107A	-0.14753

102A ->112A 0.12792

103A ->106A 0.12371

103A ->110A -0.19654

92B ->104B 0.56501

100B ->106B -0.14434

100B ->110B -0.10123

102B ->105B 0.12383

102B ->107B 0.14753

102B ->112B -0.12792

103B ->106B -0.12371

103B ->110B 0.19654

Excited State 28: 3.000-A 4.2185 eV 293.90 nm f=0.0000 <S**2>=2.000

95A ->104A -0.70208

95B ->104B 0.70208

Excited State 29: 1.000-A 4.2588 eV 291.13 nm f=0.0000 <S**2>=0.000

95A ->104A 0.70411

95B ->104B 0.70411

Excited State 30: 3.000-A 4.3648 eV 284.05 nm f=0.0000 <S**2>=2.000

92A ->104A 0.27100

98A ->105A -0.44647

100A ->110A 0.21105

102A ->107A -0.23353

102A ->112A 0.23286

103A ->110A -0.17875

92B ->104B -0.27100

98B ->105B 0.44647

100B ->110B -0.21105

102B ->107B 0.23353

102B ->112B -0.23286

103B ->110B 0.17875

Excited State 31: 3.000-A 4.3911 eV 282.35 nm f=0.0000 <S**2>=2.000

97A ->105A 0.13398

99A ->105A -0.61924

101A ->108A 0.12821

101A ->109A -0.12231

102A ->110A -0.11488

97B ->105B -0.13398

99B ->105B 0.61924

101B ->108B -0.12821

101B ->109B 0.12231

102B ->110B 0.11488

Excited State 32: 1.000-A 4.4077 eV 281.29 nm f=0.0275 <S**2>=0.000

96A ->104A -0.14048

100A ->105A 0.66458

96B ->104B -0.14048

100B ->105B 0.66458

Excited State 33: 3.000-A 4.4366 eV 279.46 nm f=0.0000 <S**2>=2.000

88A ->104A -0.11034

94A ->104A -0.69455

88B ->104B 0.11034

94B ->104B 0.69455

Excited State 34: 3.000-A 4.4723 eV 277.23 nm f=0.0000 <S**2>=2.000

92A ->104A 0.14604

98A ->105A 0.36845

102A ->105A 0.11287

103A ->106A 0.51989

103A ->110A -0.12146

92B ->104B -0.14604

98B ->105B -0.36845

102B ->105B -0.11287

103B ->106B -0.51989

103B ->110B 0.12146

Excited State 35: 1.000-A 4.4774 eV 276.91 nm f=0.0143 <S**2>=0.000

99A ->105A 0.70362

99B ->105B 0.70362

Excited State 36: 1.000-A 4.4918 eV 276.02 nm f=0.0006 <S**2>=0.000

94A ->104A 0.70242

94B ->104B 0.70242

Excited State 37: 1.000-A 4.5195 eV 274.33 nm f=0.3150 <S**2>=0.000

98A ->105A 0.69835

98B ->105B 0.69835

Excited State 38: 3.000-A 4.5346 eV 273.42 nm f=0.0000 <S**2>=2.000

83A ->104A 0.14524

86A ->104A 0.20702

87A ->104A 0.23937

93A ->104A -0.51236

97A ->105A 0.10460

99A ->105A 0.16408

100A ->105A -0.12381

102A ->106A 0.10006

103A ->113A 0.10014

83B ->104B -0.14524

86B ->104B -0.20702

87B ->104B -0.23937

93B ->104B 0.51236

97B ->105B -0.10460

99B ->105B -0.16408

100B ->105B 0.12381

102B ->106B -0.10006

103B ->113B -0.10014

Excited State 39: 3.000-A 4.6052 eV 269.23 nm f=0.0000 <S**2>=2.000

93A ->104A 0.21102

97A ->105A 0.11584

99A ->107A 0.19881

100A ->105A -0.16293

100A ->112A -0.11182

101A ->108A -0.16288

101A ->109A 0.15031

102A ->106A 0.45339

102A ->110A -0.12693

103A ->107A 0.17766

93B ->104B -0.21102

97B ->105B -0.11584

99B ->107B -0.19881

100B ->105B 0.16293

100B ->112B 0.11182

101B ->108B 0.16288

101B ->109B -0.15031

102B ->106B -0.45339

102B ->110B 0.12693

103B ->107B -0.17766

Excited State 40: 3.000-A 4.6067 eV 269.14 nm f=0.0000 <S**2>=2.000

99A ->108A 0.19075

99A ->109A -0.18423

101A ->107A 0.58279

101A ->112A 0.22879

103A ->108A 0.14352

99B ->108B -0.19075

99B ->109B 0.18423

101B ->107B -0.58279

101B ->112B -0.22879

103B ->108B -0.14352

Excited State 41: 3.000-A 4.6511 eV 266.57 nm f=0.0000 <S**2>=2.000

99A ->105A -0.14925

99A ->107A 0.37958

99A ->112A 0.16476

100A ->105A 0.12953

101A ->108A -0.26433

101A ->109A 0.24307

102A ->106A -0.34018

99B ->105B 0.14925

99B ->107B -0.37958

99B ->112B -0.16476

100B ->105B -0.12953

101B ->108B 0.26433

101B ->109B -0.24307

102B ->106B 0.34018

Excited State 42: 1.000-A 4.6899 eV 264.36 nm f=0.0270 <S**2>=0.000

93A ->104A 0.70176

93B ->104B 0.70176

Excited State 43: 1.000-A 4.7261 eV 262.34 nm f=0.0024 <S**2>=0.000

92A ->104A 0.67893

103A ->106A 0.12029

92B ->104B 0.67893

103B ->106B 0.12029

Excited State 44: 3.000-A 4.7328 eV 261.97 nm f=0.0000 <S**2>=2.000

91A ->104A 0.69914

91B ->104B -0.69914

Excited State 45: 3.000-A 4.7419 eV 261.47 nm f=0.0000 <S**2>=2.000

88A ->104A -0.17713

90A ->104A -0.20931

101A ->107A 0.12512

102A ->111A 0.23501

103A ->108A -0.53975

103A ->109A -0.16673

88B ->104B 0.17713

90B ->104B 0.20931

101B ->107B -0.12512

102B ->111B -0.23501

103B ->108B 0.53975

103B ->109B 0.16673

Excited State 46: 3.000-A 4.7552 eV 260.74 nm f=0.0000 <S**2>=2.000

82A ->104A -0.12993

84A ->104A 0.10355

88A ->104A -0.38010

90A ->104A -0.47640

102A ->111A -0.13004

103A ->108A 0.23480

82B ->104B 0.12993

84B ->104B -0.10355

88B ->104B 0.38010

90B ->104B 0.47640

102B ->111B 0.13004

103B ->108B -0.23480

Excited State 47: 3.000-A 4.7606 eV 260.44 nm f=0.0000 <S**2>=2.000

93A ->104A 0.28186

97A ->105A 0.29539

98A ->106A 0.30649

99A ->105A 0.17196

100A ->107A 0.11617

100A ->113A 0.10824

102A ->106A -0.19725

102A ->110A -0.17802

103A ->113A 0.21650

93B ->104B -0.28186

97B ->105B -0.29539

98B ->106B -0.30649

99B ->105B -0.17196

100B ->107B -0.11617

100B ->113B -0.10824

102B ->106B 0.19725

102B ->110B 0.17802

103B ->113B -0.21650

Excited State 48: 1.000-A 4.7864 eV 259.03 nm f=0.0000 <S**2>=0.000

91A ->104A 0.70215

91B ->104B 0.70215

Excited State 49: 3.000-A 4.7892 eV 258.88 nm f=0.0000 <S**2>=2.000

100A ->111A -0.10800

102A ->108A -0.51176

102A ->109A -0.25028

102A ->115A -0.10179

103A ->111A 0.35222

100B ->111B 0.10800

102B ->108B 0.51176

102B ->109B 0.25028

102B ->115B 0.10179

103B ->111B -0.35222

Excited State 50: 3.000-A 4.8155 eV 257.47 nm f=0.0000 <S**2>=2.000

92A ->104A 0.20406

96A ->105A -0.25600

100A ->106A 0.44610

100A ->110A -0.12183

102A ->112A -0.10398

102A ->113A -0.24030

103A ->106A -0.12648

103A ->110A -0.23238

92B ->104B -0.20406

96B ->105B 0.25600

100B ->106B -0.44610

100B ->110B 0.12183

102B ->112B 0.10398

102B ->113B 0.24030

103B ->106B 0.12648

103B ->110B 0.23238

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 910.

Leave Link 914 at Wed Oct 10 00:39:56 2018, MaxMem= 1879048192 cpu: 163090.9

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

6.9 Computed zyx-coordinates of the S_0 state of compound **6**$^{2+}$ and excitation energies (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 2 Multiplicity = 1

C	-0.31494	-2.24811	0.02175
C	-0.94876	-0.96624	-0.01296
N	-0.19463	0.1761	-0.02041
C	1.16158	0.1907	-0.02376
C	1.99421	-0.95851	-0.00646
S	1.36112	-2.5388	0.03232
S	-1.41285	-3.56537	0.05296
C	-2.77598	-2.44779	0.00806
C	-2.38914	-1.08501	-0.03123
S	2.06428	1.6738	-0.03642
C	3.57927	0.76184	-0.02155
C	3.38206	-0.64056	-0.00558
C	-0.83505	1.49705	-0.00011
C	-1.06669	2.15148	-1.20758
C	-1.65016	3.41338	-1.17886
C	-1.97295	3.96831	0.05209
C	-1.73668	3.32215	1.25832
C	-1.15429	2.06022	1.2335
F	-2.53915	5.18844	0.07757
C	-4.10094	-2.85681	-0.00071
C	-5.0856	-1.8742	-0.05725
C	-4.73965	-0.51858	-0.10523
C	-3.41517	-0.11514	-0.09201
C	4.85005	1.3178	-0.02444
C	5.93815	0.44681	-0.00959
C	5.7644	-0.94853	0.0077
C	4.49906	-1.50177	0.01004
H	-0.80854	1.68979	-2.15233
H	-1.85247	3.9576	-2.09184

H -2.00257 3.79825 2.19282

H -0.95891 1.52798 2.15606

H -4.36306 -3.90614 0.03183

H -6.12825 -2.16655 -0.06631

H -5.5182 0.23174 -0.15341

H -3.19253 0.9372 -0.1323

H 4.99773 2.38977 -0.0368

H 6.94008 0.85795 -0.01094

H 6.63299 -1.59399 0.01907

H 4.37101 -2.57737 0.02241

SCF Done: E(UB3LYP) = -2194.64452845 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.366512

Sum of electronic and thermal Energies= -2194.345977

Sum of electronic and thermal Enthalpies= -2194.345032

Sum of electronic and thermal Free Energies= -2194.416284

Excitation energies and oscillator strengths:

Excited State 1: 3.000-A 0.9369 eV 1323.33 nm f=0.0000 <S**2>=2.000

102A ->104A 0.18721

103A ->104A -0.68360

102B ->104B -0.18721

103B ->104B 0.68360

103A <-104A -0.11107

103B <-104B 0.11107

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

Total Energy, E(TD-HF/TD-KS) = -2194.61009760

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

Excited State 2: 3.000-A 1.3264 eV 934.71 nm f=0.0000 <S**2>=2.000

102A ->104A 0.67296

103A ->104A 0.18096

102B ->104B -0.67296

103B ->104B -0.18096

Excited State 3: 1.000-A 1.5177 eV 816.92 nm f=0.0626 <S**2>=0.000

102A ->104A 0.32832

103A ->104A 0.62510

102B ->104B 0.32832

103B ->104B 0.62510

Excited State 4: 3.000-A 1.5968 eV 776.46 nm f=0.0000 <S**2>=2.000

101A ->104A 0.69704

101B ->104B -0.69704

Excited State 5: 1.000-A 1.8647 eV 664.90 nm f=0.0139 <S**2>=0.000

101A ->104A 0.69159

101B ->104B 0.69159

Excited State 6: 3.000-A 2.0063 eV 617.99 nm f=0.0000 <S**2>=2.000

100A ->104A 0.70422

100B ->104B -0.70422

Excited State 7: 1.000-A 2.0079 eV 617.49 nm f=0.3537 <S**2>=0.000

100A ->104A 0.30428

102A ->104A 0.55896

103A ->104A -0.28593

100B ->104B 0.30428

102B ->104B 0.55896

103B ->104B -0.28593

Excited State 8: 1.000-A 2.0272 eV 611.60 nm f=0.0967 <S**2>=0.000

100A ->104A 0.63639

102A ->104A -0.26171

103A ->104A 0.14339

100B ->104B 0.63639

102B ->104B -0.26171

103B ->104B 0.14339

Excited State 9: 3.000-A 2.2213 eV 558.15 nm f=0.0000 <S**2>=2.000

98A ->104A 0.38040

99A ->104A 0.58954

98B ->104B -0.38040

99B ->104B -0.58954

Excited State 10: 1.000-A 2.3256 eV 533.12 nm f=0.0118 <S**2>=0.000

99A ->104A 0.70198

99B ->104B 0.70198

Excited State 11: 3.000-A 2.3821 eV 520.48 nm f=0.0000 <S**2>=2.000

97A ->104A 0.12845

98A ->104A 0.57430

99A ->104A -0.37367

97B ->104B -0.12845

98B ->104B -0.57430

99B ->104B 0.37367

Excited State 12: 3.000-A 2.6456 eV 468.64 nm f=0.0000 <S**2>=2.000

97A ->104A 0.59661

98A ->104A -0.10869

103A ->105A -0.31118

97B ->104B -0.59661

98B ->104B 0.10869

103B ->105B 0.31118

Excited State 13: 1.000-A 2.8897 eV 429.05 nm f=0.0058 <S**2>=0.000

98A ->104A 0.68828

98B ->104B 0.68828

Excited State 14: 3.000-A 2.9860 eV 415.22 nm f=0.0000 <S**2>=2.000

97A ->104A -0.32976

102A ->105A 0.15332

103A ->105A -0.57649

97B ->104B 0.32976

102B ->105B -0.15332

103B ->105B 0.57649

Excited State 15: 1.000-A 3.2014 eV 387.28 nm f=0.0187 <S**2>=0.000

97A ->104A 0.69400

97B ->104B 0.69400

Excited State 16: 3.000-A 3.3208 eV 373.36 nm f=0.0000 <S**2>=2.000

94A ->104A 0.12029

96A ->104A -0.26529

101A ->105A 0.33701

102A ->105A 0.49653

94B ->104B -0.12029

96B ->104B 0.26529

101B ->105B -0.33701

102B ->105B -0.49653

Excited State 17: 3.000-A 3.4170 eV 362.85 nm f=0.0000 <S**2>=2.000

96A ->104A 0.36909

101A ->105A -0.34843

102A ->105A 0.40432

103A ->105A 0.14517

103A ->106A -0.13475

96B ->104B -0.36909

101B ->105B 0.34843

102B ->105B -0.40432

103B ->105B -0.14517

103B ->106B 0.13475

Excited State 18: 3.000-A 3.6965 eV 335.41 nm f=0.0000 <S**2>=2.000

96A ->104A 0.47843

101A ->105A 0.37309

101A ->110A 0.11984

103A ->106A 0.19967

96B ->104B -0.47843

101B ->105B -0.37309

101B ->110B -0.11984

103B ->106B -0.19967

Excited State 19: 1.000-A 3.7020 eV 334.91 nm f=0.1347 <S**2>=0.000

103A ->105A 0.68477

103B ->105B 0.68477

Excited State 20: 3.000-A 3.7996 eV 326.31 nm f=0.0000 <S**2>=2.000

99A ->108A -0.37806

99A ->111A 0.20363

100A ->106A -0.14739

100A ->107A 0.33348

100A ->109A -0.33884

100A ->110A 0.13721

99B ->108B 0.37806

99B ->111B -0.20363

100B ->106B 0.14739

100B ->107B -0.33348

100B ->109B 0.33884

100B ->110B -0.13721

Excited State 21: 3.000-A 3.8564 eV 321.50 nm f=0.0000 <S**2>=2.000

96A ->104A -0.19288

98A ->105A 0.25524

99A ->105A 0.12394

101A ->105A -0.24915

101A ->110A 0.23358

102A ->106A -0.22335

102A ->108A -0.10596

103A ->106A 0.22514

103A ->108A -0.13484

103A ->111A -0.18839

96B ->104B 0.19288

98B ->105B -0.25524

99B ->105B -0.12394

101B ->105B 0.24915

101B ->110B -0.23358

102B ->106B 0.22335

102B ->108B 0.10596

103B ->106B -0.22514

103B ->108B 0.13484

103B ->111B 0.18839

Excited State 22: 1.000-A 3.8867 eV 319.00 nm f=0.0059 <S**2>=0.000

96A ->104A 0.62674

101A ->105A 0.30119

96B ->104B 0.62674

101B ->105B 0.30119

Excited State 23: 3.000-A 3.9493 eV 313.94 nm f=0.0000 <S**2>=2.000

87A ->104A -0.11343

92A ->104A 0.11143

94A ->104A 0.58277

101A ->111A -0.12130

103A ->105A -0.11306

103A ->110A 0.17074

87B ->104B 0.11343

92B ->104B -0.11143

94B ->104B -0.58277

101B ->111B 0.12130

103B ->105B 0.11306

103B ->110B -0.17074

Excited State 24: 1.000-A 3.9824 eV 311.33 nm f=0.7041 <S**2>=0.000

102A ->105A 0.69321

102B ->105B 0.69321

Excited State 25: 3.000-A 4.0407 eV 306.84 nm f=0.0000 <S**2>=2.000

87A ->104A -0.10792

94A ->104A 0.19765

97A ->105A 0.21944

97A ->110A 0.11777

98A ->106A -0.11490

101A ->106A -0.16090

101A ->108A 0.18005

101A ->111A 0.24431

102A ->105A -0.10695

102A ->110A -0.15236

102A ->113A -0.11924

103A ->109A -0.12531

103A ->110A -0.30530

103A ->113A 0.15099

87B ->104B 0.10792

94B ->104B -0.19765

97B ->105B -0.21944

97B ->110B -0.11777

98B ->106B 0.11490

101B ->106B 0.16090

101B ->108B -0.18005

101B ->111B -0.24431

102B ->105B 0.10695

102B ->110B 0.15236

102B ->113B 0.11924

103B ->109B 0.12531

103B ->110B 0.30530

103B ->113B -0.15099

Excited State 26: 1.000-A 4.1324 eV 300.03 nm f=0.0199 <S**2>=0.000

96A ->104A -0.28534

101A ->105A 0.61671

96B ->104B -0.28534

101B ->105B 0.61671

Excited State 27: 3.000-A 4.1485 eV 298.87 nm f=0.0000 <S**2>=2.000

100A ->105A 0.69941

100B ->105B -0.69941

Excited State 28: 1.000-A 4.1690 eV 297.39 nm f=0.0004 <S**2>=0.000

100A ->105A 0.70087

100B ->105B 0.70087

Excited State 29: 3.000-A 4.3032 eV 288.12 nm f=0.0000 <S**2>=2.000

95A ->104A 0.69116

95B ->104B -0.69116

Excited State 30: 1.000-A 4.3459 eV 285.29 nm f=0.0000 <S**2>=0.000

95A ->104A 0.69586

95B ->104B 0.69586

Excited State 31: 3.000-A 4.3559 eV 284.63 nm f=0.0000 <S**2>=2.000

87A ->104A -0.10159

98A ->105A 0.29088

99A ->105A 0.39326

101A ->110A -0.22288

102A ->106A -0.12284

102A ->111A 0.10283

103A ->106A 0.10391

103A ->108A 0.22466

103A ->111A 0.19521

87B ->104B 0.10159

98B ->105B -0.29088

99B ->105B -0.39326

101B ->110B 0.22288

102B ->106B 0.12284

102B ->111B -0.10283

103B ->106B -0.10391

103B ->108B -0.22466

103B ->111B -0.19521

Excited State 32: 3.000-A 4.4236 eV 280.28 nm f=0.0000 <S**2>=2.000

93A ->104A 0.69354

93B ->104B -0.69354

Excited State 33: 3.000-A 4.4489 eV 278.69 nm f=0.0000 <S**2>=2.000

98A ->105A -0.21699

99A ->105A 0.53220

101A ->110A 0.12074

102A ->106A 0.16637

103A ->106A -0.18455

103A ->108A -0.11838

103A ->111A -0.11519

98B ->105B 0.21699

99B ->105B -0.53220

101B ->110B -0.12074

102B ->106B -0.16637

103B ->106B 0.18455

103B ->108B 0.11838

103B ->111B 0.11519

Excited State 34: 1.000-A 4.4530 eV 278.43 nm f=0.0167 <S**2>=0.000

99A ->105A 0.70382

99B ->105B 0.70382

Excited State 35: 1.000-A 4.4741 eV 277.11 nm f=0.0005 <S**2>=0.000

93A ->104A 0.69777

93B ->104B 0.69777

Excited State 36: 3.000-A 4.5579 eV 272.02 nm f=0.0000 <S**2>=2.000

83A ->104A -0.11617

86A ->104A -0.14292

87A ->104A 0.24137

92A ->104A 0.32684

97A ->105A -0.26687

98A ->105A -0.12958

101A ->105A -0.11347

101A ->106A 0.16790

101A ->108A 0.12540

101A ->111A 0.11787

102A ->105A -0.12995

102A ->110A -0.14216

103A ->106A 0.19009

83B ->104B 0.11617

86B ->104B 0.14292

87B ->104B -0.24137

92B ->104B -0.32684

97B ->105B 0.26687

98B ->105B 0.12958

101B ->105B 0.11347

101B ->106B -0.16790

101B ->108B -0.12540

101B ->111B -0.11787

102B ->105B 0.12995

102B ->110B 0.14216

103B ->106B -0.19009

Excited State 37: 3.000-A 4.5766 eV 270.91 nm f=0.0000 <S**2>=2.000

88A ->104A -0.14037

89A ->104A 0.25374

90A ->104A 0.22344

99A ->107A -0.10413

99A ->109A 0.11671

100A ->108A 0.17710

103A ->106A 0.21276

103A ->107A -0.43290

103A ->109A -0.11271

88B ->104B 0.14037

89B ->104B -0.25374

90B ->104B -0.22344

99B ->107B 0.10413

99B ->109B -0.11671

100B ->108B -0.17710

103B ->106B -0.21276

103B ->107B 0.43290

103B ->109B 0.11271

Excited State 38: 3.000-A 4.5922 eV 269.99 nm f=0.0000 <S**2>=2.000

82A ->104A -0.10991

88A ->104A -0.20663

89A ->104A 0.38426

90A ->104A 0.36018

100A ->108A -0.18558

103A ->107A 0.24326

82B ->104B 0.10991

88B ->104B 0.20663

89B ->104B -0.38426

90B ->104B -0.36018

100B ->108B 0.18558

103B ->107B -0.24326

Excited State 39: 1.000-A 4.5974 eV 269.68 nm f=0.0206 <S**2>=0.000

94A ->104A 0.68367

94B ->104B 0.68367

Excited State 40: 3.000-A 4.6132 eV 268.76 nm f=0.0000 <S**2>=2.000

98A ->105A 0.11891

99A ->108A -0.40110

99A ->111A 0.19025

100A ->106A 0.13843

100A ->107A -0.29278

100A ->109A 0.26250

100A ->110A -0.10360

103A ->106A -0.12590

103A ->108A -0.16326

98B ->105B -0.11891

99B ->108B 0.40110

99B ->111B -0.19025

100B ->106B -0.13843

100B ->107B 0.29278

100B ->109B -0.26250

100B ->110B 0.10360

103B ->106B 0.12590

103B ->108B 0.16326

Excited State 41: 3.000-A 4.6371 eV 267.38 nm f=0.0000 <S**2>=2.000

92A ->104A 0.42281

98A ->105A 0.20782

100A ->108A 0.18848

101A ->105A 0.13092

102A ->106A -0.10020

103A ->106A -0.34565

92B ->104B -0.42281

98B ->105B -0.20782

100B ->108B -0.18848

101B ->105B -0.13092

102B ->106B 0.10020

103B ->106B 0.34565

Excited State 42: 3.000-A 4.6437 eV 267.00 nm f=0.0000 <S**2>=2.000

92A ->104A 0.21778

99A ->107A 0.16199

99A ->109A -0.12587

100A ->108A -0.43517

100A ->111A 0.19206

103A ->107A -0.28813

103A ->109A -0.15661

92B ->104B -0.21778

99B ->107B -0.16199

99B ->109B 0.12587

100B ->108B 0.43517

100B ->111B -0.19206

103B ->107B 0.28813

103B ->109B 0.15661

Excited State 43: 3.000-A 4.6709 eV 265.44 nm f=0.0000 <S**2>=2.000

92A ->104A 0.27731

97A ->105A 0.26016

98A ->105A -0.23541

99A ->105A 0.11986

99A ->108A -0.13311

101A ->106A -0.15537

102A ->110A 0.15216

103A ->106A 0.22810

103A ->107A 0.19981

103A ->113A 0.11695

92B ->104B -0.27731

97B ->105B -0.26016

98B ->105B 0.23541

99B ->105B -0.11986

99B ->108B 0.13311

101B ->106B 0.15537

102B ->110B -0.15216

103B ->106B -0.22810

103B ->107B -0.19981

103B ->113B -0.11695

Excited State 44: 1.000-A 4.6942 eV 264.12 nm f=0.0090 <S**2>=0.000

92A ->104A 0.70057

92B ->104B 0.70057

Excited State 45: 1.000-A 4.7551 eV 260.74 nm f=0.0001 <S**2>=0.000

103A ->106A -0.29155

103A ->107A 0.60220

103A ->109A 0.15509

103B ->106B -0.29155

103B ->107B 0.60220

103B ->109B 0.15509

Excited State 46: 3.000-A 4.8080 eV 257.87 nm f=0.0000 <S**2>=2.000

89A ->104A -0.18868

90A ->104A 0.24852

91A ->104A 0.59713

89B ->104B 0.18868

90B ->104B -0.24852

91B ->104B -0.59713

Excited State 47: 3.000-A 4.8103 eV 257.75 nm f=0.0000 <S**2>=2.000

91A ->104A -0.14628

92A ->104A -0.10447

96A ->105A 0.10094

98A ->105A -0.28720

101A ->113A 0.11264

102A ->106A -0.37551

102A ->107A -0.14171

102A ->108A -0.21205

102A ->111A -0.13168

103A ->108A 0.16860

103A ->111A 0.12123

91B ->104B 0.14628

92B ->104B 0.10447

96B ->105B -0.10094

98B ->105B 0.28720

101B ->113B -0.11264

102B ->106B 0.37551

102B ->107B 0.14171

102B ->108B 0.21205

102B ->111B 0.13168

103B ->108B -0.16860

103B ->111B -0.12123

Excited State 48: 1.000-A 4.8214 eV 257.16 nm f=0.0008 <S**2>=0.000

88A ->104A -0.10754

89A ->104A 0.23592

90A ->104A 0.62956

91A ->104A 0.17190

88B ->104B -0.10754

89B ->104B 0.23592

90B ->104B 0.62956

91B ->104B 0.17190

Excited State 49: 3.000-A 4.8469 eV 255.80 nm f=0.0000 <S**2>=2.000

83A ->104A -0.19378

86A ->104A -0.17442

87A ->104A 0.45187

92A ->104A -0.19801

94A ->104A 0.14854

97A ->105A 0.12424

98A ->105A 0.14389

101A ->106A -0.14908

102A ->110A 0.13707

83B ->104B 0.19378

86B ->104B 0.17442

87B ->104B -0.45187

92B ->104B 0.19801

94B ->104B -0.14854

97B ->105B -0.12424

98B ->105B -0.14389

101B ->106B 0.14908

102B ->110B -0.13707

Excited State 50: 3.000-A 4.8544 eV 255.40 nm f=0.0000 <S**2>=2.000

88A ->104A 0.10027

89A ->104A -0.36048

90A ->104A 0.47730

91A ->104A -0.31727

88B ->104B -0.10027

89B ->104B 0.36048

90B ->104B -0.47730

91B ->104B 0.31727

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 910.

Leave Link 914 at Wed Oct 10 01:35:48 2018, MaxMem= 1879048192 cpu: 199672.8

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

6.10 Computed zyx-coordinates of the S_0 state of compound **7**$^{2+}$ and excitation energies (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Charge = 2 Multiplicity = 1

C -1.33375 -1.44213 -0.00006

C -1.18959 -0.02803 -0.00005

N 0.00000 0.61855 -0.00004

C 1.18959 -0.02803 -0.00005

C 1.33375 -1.44213 -0.00006

S 0. 00000 -2.5084 -0.00011

C	0. 00000	2.08538	0.00002
C	0. 00000	2.75205	-1.22347
C	0. 00000	4.14167	-1.2208
C	0. 00000	4.80285	0.00013
C	0. 00000	4.14156	1.221
C	0. 00000	2.75195	1.22357
C	3.56578	-0.72656	-0.00003
C	2.69951	-1.84816	-0.00004
S	2.69964	0.81796	-0.00006
C	4.94475	-0.87216	0.00000
C	5.46011	-2.16779	0.00004
C	4.61917	-3.29387	0.00005
C	3.24558	-3.14786	0.00001
C	-2.69951	-1.84816	-0.00004
C	-3.56578	-0.72656	-0.00003
S	-2.69964	0.81796	-0.00006
C	-3.24558	-3.14786	0.00001
C	-4.61917	-3.29387	0.00005
C	-5.46011	-2.16779	0.00004
C	-4.94475	-0.87216	0. 00000
F	0. 00000	6.14827	0.00019
H	0. 00000	2.20044	-2.15515
H	0.00000	4.70407	-2.14496
H	0. 00000	4.7039	2.14521
H	0. 00000	2.20026	2.1552
H	5.60478	-0.01459	0.00000
H	6.5343	-2.3055	0.00006
H	5.05405	-4.28484	0.00008
H	2.60198	-4.01865	0.00003
H	-2.60198	-4.01865	0.00003
H	-5.05405	-4.28484	0.00008
H	-6.5343	-2.3055	0.00006
H	-5.60478	-0.01459	0.00000

SCF Done: E(UB3LYP) = -2194.65117442 A.U. after 2 cycles

Sum of electronic and zero-point Energies= -2194.373813

Sum of electronic and thermal Energies= -2194.353774

Sum of electronic and thermal Enthalpies= -2194.352830

Sum of electronic and thermal Free Energies= -2194.423366

Excitation energies and oscillator strengths:

Excited State 1: 3.000-A" 0.9252 eV 1340.12 nm f=0.0000 <S**2>=2.000

101A ->104A -0.11218

103A ->104A -0.70396

101B ->104B 0.11218

103B ->104B 0.70396

103A <-104A -0.12948

103B <-104B 0.12948

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

Total Energy, E(TD-HF/TD-KS) = -2194.61712387

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

Excited State 2: 3.000-A' 1.2988 eV 954.62 nm f=0.0000 <S**2>=2.000

102A ->104A 0.69834

102B ->104B -0.69834

Excited State 3: 1.000-A' 1.5858 eV 781.86 nm f=0.0030 <S**2>=0.000

102A ->104A 0.70629

102B ->104B 0.70629

Excited State 4: 1.000-A" 1.6606 eV 746.64 nm f=0.1629 <S**2>=0.000

101A ->104A -0.28867

103A ->104A 0.64432

101B ->104B -0.28867

103B ->104B 0.64432

Excited State 5: 3.000-A" 1.7057 eV 726.90 nm f=0.0000 <S**2>=2.000

99A ->104A 0.16822

101A ->104A 0.67492

103A ->104A -0.10816

99B ->104B -0.16822

101B ->104B -0.67492

103B ->104B 0.10816

Excited State 6: 3.000-A' 1.9575 eV 633.39 nm f=0.0000 <S**2>=2.000

98A ->104A -0.68804

102A ->104A -0.10030

98B ->104B 0.68804

102B ->104B 0.10030

Excited State 7: 3.000-A" 2.0194 eV 613.95 nm f=0.0000 <S**2>=2.000

100A ->104A 0.70528

100B ->104B -0.70528

Excited State 8: 1.000-A" 2.0315 eV 610.30 nm f=0.0000 <S**2>=0.000

100A ->104A 0.70551

100B ->104B 0.70551

Excited State 9: 1.000-A" 2.1396 eV 579.48 nm f=0.3625 <S**2>=0.000

101A ->104A 0.64144

103A ->104A 0.28417

101B ->104B 0.64144

103B ->104B 0.28417

Excited State 10: 3.000-A" 2.2996 eV 539.16 nm f=0.0000 <S**2>=2.000

99A ->104A 0.68467

101A ->104A -0.17076

99B ->104B -0.68467

101B ->104B 0.17076

Excited State 11: 1.000-A" 2.3497 eV 527.65 nm f=0.0600 <S**2>=0.000

99A ->104A 0.69924

99B ->104B 0.69924

Excited State 12: 1.000-A' 2.6536 eV 467.24 nm f=0.0143 <S**2>=0.000

98A ->104A 0.69890

98B ->104B 0.69890

Excited State 13: 3.000-A' 2.9666 eV 417.93 nm f=0.0000 <S**2>=2.000

96A ->104A 0.14882

98A ->104A 0.10898

103A ->105A -0.64891

96B ->104B -0.14882

98B ->104B -0.10898

103B ->105B 0.64891

Excited State 14: 3.000-A" 3.0093 eV 412.00 nm f=0.0000 <S**2>=2.000

97A ->104A 0.68133

97B ->104B -0.68133

Excited State 15: 3.000-A' 3.2638 eV 379.87 nm f=0.0000 <S**2>=2.000

96A ->104A -0.63828

101A ->105A -0.21946

102A ->107A 0.11531

103A ->105A -0.11786

96B ->104B 0.63828

101B ->105B 0.21946

102B ->107B -0.11531

103B ->105B 0.11786

Excited State 16: 3.000-A" 3.3466 eV 370.47 nm f=0.0000 <S**2>=2.000

92A ->104A 0.11492

101A ->107A -0.10501

102A ->105A 0.67248

92B ->104B -0.11492

101B ->107B 0.10501

102B ->105B -0.67248

Excited State 17: 1.000-A" 3.4919 eV 355.06 nm f=0.0003 <S**2>=0.000

97A ->104A 0.69012

102A ->105A 0.10479

97B ->104B 0.69012

102B ->105B 0.10479

Excited State 18: 1.000-A' 3.7032 eV 334.80 nm f=0.0077 <S**2>=0.000

96A ->104A 0.68031

101A ->105A -0.15046

96B ->104B 0.68031

101B ->105B -0.15046

Excited State 19: 3.000-A' 3.7438 eV 331.17 nm f=0.0000 <S**2>=2.000

96A ->104A -0.22021

99A ->105A 0.14685

101A ->105A 0.59770

102A ->107A -0.13610

103A ->105A -0.14139

96B ->104B 0.22021

99B ->105B -0.14685

101B ->105B -0.59770

102B ->107B 0.13610

103B ->105B 0.14139

Excited State 20: 1.000-A' 3.7790 eV 328.09 nm f=0.1276 <S**2>=0.000

103A ->105A 0.69289

103B ->105B 0.69289

Excited State 21: 3.000-A' 3.8175 eV 324.78 nm f=0.0000 <S**2>=2.000

99A ->108A -0.33393

99A ->111A 0.19456

100A ->106A -0.43165

100A ->112A -0.27860

101A ->108A 0.20970

101A ->111A -0.10542

99B ->108B 0.33393

99B ->111B -0.19456

100B ->106B 0.43165

100B ->112B 0.27860

101B ->108B -0.20970

101B ->111B 0.10542

Excited State 22: 3.000-A" 3.8456 eV 322.41 nm f=0.0000 <S**2>=2.000

97A ->104A -0.10278

98A ->105A -0.35320

98A ->111A 0.13661

98A ->113A -0.11272

99A ->110A 0.11400

101A ->110A 0.19094

102A ->108A 0.19024

102A ->111A 0.23802

103A ->107A -0.30622

103A ->110A -0.23171

97B ->104B 0.10278

98B ->105B 0.35320

98B ->111B -0.13661

98B ->113B 0.11272

99B ->110B -0.11400

101B ->110B -0.19094

102B ->108B -0.19024

102B ->111B -0.23802

103B ->107B 0.30622

103B ->110B 0.23171

Excited State 23: 1.000-A" 3.9130 eV 316.85 nm f=0.4904 <S**2>=0.000

102A ->105A 0.68891

102B ->105B 0.68891

Excited State 24: 3.000-A' 4.0507 eV 306.08 nm f=0.0000 <S**2>=2.000

97A ->105A -0.14354

98A ->107A 0.16037

98A ->110A 0.13546

99A ->111A 0.10374

101A ->108A 0.14319

101A ->111A 0.17739

102A ->110A 0.41147

103A ->108A -0.18497

103A ->111A -0.29947

103A ->113A 0.11064

97B ->105B 0.14354

98B ->107B -0.16037

98B ->110B -0.13546

99B ->111B -0.10374

101B ->108B -0.14319

101B ->111B -0.17739

102B ->110B -0.41147

103B ->108B 0.18497

103B ->111B 0.29947

103B ->113B -0.11064

Excited State 25: 3.000-A" 4.1333 eV 299.96 nm f=0.0000 <S**2>=2.000

92A ->104A 0.59698

98A ->105A -0.13636

101A ->107A -0.11217

102A ->105A -0.11222

102A ->111A -0.12622

103A ->107A -0.13126

103A ->110A 0.13848

92B ->104B -0.59698

98B ->105B 0.13636

101B ->107B 0.11217

102B ->105B 0.11222

102B ->111B 0.12622

103B ->107B 0.13126

103B ->110B -0.13848

Excited State 26: 3.000-A' 4.1700 eV 297.32 nm f=0.0000 <S**2>=2.000

100A ->105A 0.70402

100B ->105B -0.70402

Excited State 27: 1.000-A' 4.1896 eV 295.93 nm f=0.0001 <S**2>=0.000

100A ->105A 0.70539

100B ->105B 0.70539

Excited State 28: 3.000-A' 4.3287 eV 286.43 nm f=0.0000 <S**2>=2.000

83A ->104A -0.16518

88A ->104A -0.59110

94A ->104A 0.18256

97A ->105A -0.13856

103A ->113A 0.11201

83B ->104B 0.16518

88B ->104B 0.59110

94B ->104B -0.18256

97B ->105B 0.13856

103B ->113B -0.11201

Excited State 29: 1.000-A' 4.3292 eV 286.39 nm f=0.0311 <S**2>=0.000

96A ->104A 0.11679

99A ->105A -0.20257

101A ->105A 0.65133

96B ->104B 0.11679

99B ->105B -0.20257

101B ->105B 0.65133

Excited State 30: 3.000-A" 4.3395 eV 285.71 nm f=0.0000 <S**2>=2.000

95A ->104A 0.70138

95B ->104B -0.70138

Excited State 31: 1.000-A" 4.3838 eV 282.82 nm f=0.0000 <S**2>=0.000

95A ->104A 0.70372

95B ->104B 0.70372

Excited State 32: 3.000-A' 4.4308 eV 279.82 nm f=0.0000 <S**2>=2.000

89A ->104A -0.10792

93A ->104A 0.69391

89B ->104B 0.10792

93B ->104B -0.69391

Excited State 33: 3.000-A" 4.4385 eV 279.34 nm f=0.0000 <S**2>=2.000

92A ->104A -0.23936

98A ->105A -0.52211

101A ->110A -0.18925

102A ->108A -0.19231

102A ->111A -0.19555

103A ->110A 0.13487

92B ->104B 0.23936

98B ->105B 0.52211

101B ->110B 0.18925

102B ->108B 0.19231

102B ->111B 0.19555

103B ->110B -0.13487

Excited State 34: 3.000-A' 4.4471 eV 278.80 nm f=0.0000 <S**2>=2.000

99A ->105A 0.65467

101A ->105A -0.19679

99B ->105B -0.65467

101B ->105B 0.19679

Excited State 35: 1.000-A' 4.4791 eV 276.81 nm f=0.0003 <S**2>=0.000

93A ->104A 0.70330

93B ->104B 0.70330

Excited State 36: 3.000-A' 4.4976 eV 275.67 nm f=0.0000 <S**2>=2.000

82A ->104A 0.14030

89A ->104A 0.56482

90A ->104A -0.36796

93A ->104A 0.11416

82B ->104B -0.14030

89B ->104B -0.56482

90B ->104B 0.36796

93B ->104B -0.11416

Excited State 37: 1.000-A' 4.5242 eV 274.05 nm f=0.0072 <S**2>=0.000

99A ->105A 0.66848

101A ->105A 0.16664

99B ->105B 0.66848

101B ->105B 0.16664

Excited State 38: 1.000-A" 4.5545 eV 272.22 nm f=0.2687 <S**2>=0.000

92A ->104A 0.11691

98A ->105A 0.69159

92B ->104B 0.11691

98B ->105B 0.69159

Excited State 39: 3.000-A' 4.6244 eV 268.11 nm f=0.0000 <S**2>=2.000

99A ->105A 0.10763

99A ->108A 0.38145

99A ->111A -0.19558

100A ->106A -0.40069

100A ->112A -0.22050

101A ->108A -0.23632

101A ->111A 0.12982

99B ->105B -0.10763

99B ->108B -0.38145

99B ->111B 0.19558

100B ->106B 0.40069

100B ->112B 0.22050

101B ->108B 0.23632

101B ->111B -0.12982

Excited State 40: 3.000-A' 4.6382 eV 267.31 nm f=0.0000 <S**2>=2.000

99A ->106A -0.32609

99A ->112A -0.18584

100A ->108A -0.42832

100A ->111A 0.21642

101A ->106A 0.23949

103A ->106A -0.20708

99B ->106B 0.32609

99B ->112B 0.18584

100B ->108B 0.42832

100B ->111B -0.21642

101B ->106B -0.23949

103B ->106B 0.20708

Excited State 41: 1.000-A" 4.6542 eV 266.39 nm f=0.0013 <S**2>=0.000

92A ->104A 0.67728

98A ->105A -0.11791

92B ->104B 0.67728

98B ->105B -0.11791

Excited State 42: 3.000-A' 4.6595 eV 266.09 nm f=0.0000 <S**2>=2.000

88A ->104A 0.14780

94A ->104A 0.66571

88B ->104B -0.14780

94B ->104B -0.66571

Excited State 43: 1.000-A' 4.6783 eV 265.02 nm f=0.0132 <S**2>=0.000

94A ->104A 0.70098

94B ->104B 0.70098

Excited State 44: 3.000-A" 4.7305 eV 262.10 nm f=0.0000 <S**2>=2.000

91A ->104A 0.69604

91B ->104B -0.69604

Excited State 45: 3.000-A' 4.7422 eV 261.45 nm f=0.0000 <S**2>=2.000

100A ->108A 0.23536

100A ->111A -0.11752

102A ->109A 0.34686

103A ->106A -0.47508

103A ->112A 0.21740

100B ->108B -0.23536

100B ->111B 0.11752

102B ->109B -0.34686

103B ->106B 0.47508

103B ->112B -0.21740

Excited State 46: 3.000-A" 4.7545 eV 260.77 nm f=0.0000 <S**2>=2.000

92A ->104A -0.19500

96A ->105A -0.12069

98A ->105A 0.22692

98A ->113A -0.12814

101A ->107A -0.12475

102A ->111A -0.12344

103A ->107A -0.53242

103A ->110A 0.18184

92B ->104B 0.19500

96B ->105B 0.12069

98B ->105B -0.22692

98B ->113B 0.12814

101B ->107B 0.12475

102B ->111B 0.12344

103B ->107B 0.53242

103B ->110B -0.18184

Excited State 47: 3.000-A" 4.7943 eV 258.61 nm f=0.0000 <S**2>=2.000

101A ->109A -0.13548

102A ->106A -0.44021

102A ->112A 0.20229

102A ->116A -0.10481

103A ->109A 0.45498

101B ->109B 0.13548

102B ->106B 0.44021

102B ->112B -0.20229

102B ->116B 0.10481

103B ->109B -0.45498

Excited State 48: 1.000-A" 4.8071 eV 257.92 nm f=0.0000 <S**2>=0.000

91A ->104A 0.70236

91B ->104B 0.70236

Excited State 49: 1.000-A' 4.8093 eV 257.80 nm f=0.0019 <S**2>=0.000

89A ->104A 0.50528

90A ->104A -0.48202

89B ->104B 0.50528

90B ->104B -0.48202

Excited State 50: 3.000-A' 4.8339 eV 256.49 nm f=0.0000 <S**2>=2.000

88A ->104A 0.13762

97A ->105A -0.19124

98A ->107A 0.10010

98A ->110A 0.16423

99A ->105A 0.11063

101A ->108A -0.17100

101A ->111A -0.14901

101A ->113A -0.13778

102A ->107A 0.32011

102A ->110A -0.24696

103A ->108A	-0.19378
103A ->111A	-0.26029
103A ->113A	0.12197
88B ->104B	-0.13762
97B ->105B	0.19124
98B ->107B	-0.10010
98B ->110B	-0.16423
99B ->105B	-0.11063
101B ->108B	0.17100
101B ->111B	0.14901
101B ->113B	0.13778
102B ->107B	-0.32011
102B ->110B	0.24696
103B ->108B	0.19378
103B ->111B	0.26029
103B ->113B	-0.12197

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 LETran= 910.

Leave Link 914 at Wed Oct 10 00:19:30 2018, MaxMem= 1879048192 cpu: 174266.1

(Enter /software/gaussian/g09/ivybridge_xe2015/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

6.11 Computed xyz-coordinates of the T_0 state of compound $\mathbf{5}^{2+}$ (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

C	1.30653	-2.16447	0.00003
C	1.22223	-0.75299	0.00005
N	-0.00012	-0.08181	-0.00000
C	-1.22288	-0.75230	-0.00005
C	-1.30790	-2.16375	-0.00003
S	-0.00099	-3.30401	0.00001
C	-2.54429	-0.15649	-0.00007
C	-3.55134	-1.15309	-0.00008
S	-2.90394	-2.78153	-0.00006

S	2.90227	-2.78302	0.00006
C	3.55047	-1.15490	0.00008
C	2.54389	-0.15782	0.00007
C	0.00046	1.36975	-0.00000
C	4.90429	-0.87374	0.00009
C	5.30400	0.47456	0.00011
C	4.35060	1.48437	0.00011
C	2.98705	1.19008	0.00008
C	-2.98690	1.19161	-0.00009
C	-4.35032	1.48650	-0.00011
C	-5.30417	0.47712	-0.00012
C	-4.90503	-0.87135	-0.00010
C	0.00104	2.04636	-1.21742
C	0.00167	3.43834	-1.21989
C	0.00173	4.10232	0.00000
C	0.00123	3.43833	1.21989
C	0.00061	2.04635	1.21742
F	0.00234	5.44893	0.00000
H	5.64106	-1.66753	0.00010
H	6.35945	0.71506	0.00012
H	4.66048	2.52113	0.00012
H	2.29303	2.01090	0.00008
H	-2.29258	2.01216	-0.00008
H	-4.65975	2.52340	-0.00012
H	-6.35952	0.71808	-0.00013
H	-5.64214	-1.66482	-0.00010
H	0.00098	1.49609	-2.15002
H	0.00210	3.99999	-2.14474
H	0.00133	3.99999	2.14474
H	0.00022	1.49609	2.15002

SCF Done: E(UB3LYP) = -2194.59906514 A.U. after 15 cycles

6.12 Computed xyz-coordinates of the T_0 state of compound $\mathbf{6}^{2+}$ (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

C	-0.31111	-2.23726	0.02703
C	-0.94303	-0.97787	-0.01541
N	-0.21331	0.19763	-0.02709
C	1.16535	0.17677	-0.02603
C	1.99365	-0.95688	-0.00254
S	1.39960	-2.58597	0.04407
S	-1.40026	-3.55739	0.06098
C	-2.77171	-2.46684	0.00839
C	-2.38696	-1.10738	-0.03749
S	2.05674	1.65418	-0.04797
C	3.58157	0.77061	-0.02877
C	3.38618	-0.62619	-0.00493
C	-0.84779	1.50884	0.00101
C	-1.08533	2.17462	-1.20078
C	-1.66926	3.43691	-1.17016
C	-1.99278	3.98711	0.06245
C	-1.75607	3.33625	1.26579
C	-1.17077	2.07509	1.23385
F	-2.56107	5.20786	0.09250
C	-4.09539	-2.88064	-0.00242
C	-5.09580	-1.89783	-0.06808
C	-4.75306	-0.55341	-0.12246
C	-3.41468	-0.14571	-0.10743
C	4.84406	1.33984	-0.03480
C	5.95526	0.47587	-0.01585
C	5.78735	-0.90507	0.00862
C	4.50935	-1.47125	0.01454
H	-0.82808	1.71539	-2.14714
H	-1.87215	3.98451	-2.08108
H	-2.02321	3.80865	2.20192

H	-0.97402	1.53969	2.15451
H	-4.35485	-3.93072	0.03565
H	-6.13540	-2.19910	-0.07805
H	-5.52776	0.20025	-0.17740
H	-3.19639	0.90787	-0.15463
H	4.98118	2.41334	-0.05292
H	6.95073	0.90098	-0.02024
H	6.65412	-1.55288	0.02321
H	4.39721	-2.54873	0.03286

SCF Done: E(UB3LYP) = -2194.61073704 A.U. after 15 cycles

6.13 Computed xyz-coordinates of the T_0 state of compound **7**$^{2+}$ (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

C	1.43782	0.00001	1.33218
C	0.03412	-0.00002	1.18912
N	-0.64953	-0.00001	0.00000
C	0.03412	-0.00002	-1.18912
C	1.43782	0.00001	-1.33218
S	2.56963	0.00004	0.00000
C	-2.10671	0.00003	0.00000
C	-2.78142	-1.22041	0.00000
C	-4.17143	-1.22041	0.00000
C	-4.83286	0.00012	0.00000
C	-4.17135	1.22061	0.00000
C	-2.78133	1.22051	0.00000
C	0.72853	-0.00006	-3.56848
C	1.84102	-0.00002	-2.69482
S	-0.80898	0.00003	-2.69101
C	0.87659	-0.00011	-4.94008
C	2.18845	-0.00012	-5.46351
C	3.30101	-0.00009	-4.62449

C	3.14468	-0.00003	-3.24148
C	1.84102	-0.00002	2.69482
C	0.72853	-0.00006	3.56848
S	-0.80898	0.00003	2.69101
C	3.14468	-0.00003	3.24148
C	3.30101	-0.00009	4.62449
C	2.18845	-0.00012	5.46351
C	0.87659	-0.00011	4.94008
F	-6.17994	0.00017	0.00000
H	-2.23002	-2.15228	0.00000
H	-4.73414	-2.14448	0.00000
H	-4.73400	2.14472	0.00000
H	-2.22987	2.15234	0.00000
H	0.02306	-0.00012	-5.60577
H	2.32125	-0.00015	-6.53791
H	4.29608	-0.00010	-5.04945
H	4.01525	-0.00001	-2.59698
H	4.01525	-0.00001	2.59698
H	4.29608	-0.00010	5.04945
H	2.32125	-0.00015	6.53791
H	0.02306	-0.00012	5.60577

SCF Done: E(UB3LYP) = -2194.61705627 A.U. after 15 cycles

6.14 Mulliken atomic spin densities of **5**$^{\bullet+}$ (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Mulliken atomic spin densities:

1	C	0.034116
2	C	0.069562
3	N	0.283662
4	C	0.069567
5	C	0.034114

6	S	0.156276
7	C	-0.012690
8	C	0.005288
9	S	0.025008
10	S	0.025005
11	C	0.005295
12	C	-0.012690
13	C	-0.003245
14	C	0.002103
15	C	0.037536
16	C	-0.015198
17	C	0.039591
18	C	0.039593
19	C	-0.015197
20	C	0.037531
21	C	0.002101
22	C	0.086726
23	C	-0.047243
24	C	0.121236
25	C	-0.047240
26	C	0.086729
27	F	0.010815
28	H	0.001198
29	H	-0.002070
30	H	0.000915
31	H	-0.002527
32	H	-0.002526
33	H	0.000915
34	H	-0.002070
35	H	0.001198
36	H	-0.008826
37	H	0.002134
38	H	0.002134

39 H -0.008827

Sum of Mulliken atomic spin densities = 1.00000

6.15 Mulliken atomic spin densities of **6**$^{\bullet+}$ (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Mulliken atomic spin densities:

1 C 0.150921
2 C 0.082427
3 N 0.247827
4 C 0.030543
5 C 0.157349
6 S 0.228764
7 S 0.008137
8 C 0.025136
9 C -0.020341
10 S -0.010633
11 C 0.060423
12 C -0.033954
13 C -0.018894
14 C 0.000641
15 C 0.001570
16 C 0.000326
17 C 0.001783
18 C -0.002262
19 F 0.000042
20 C -0.013849
21 C 0.039604
22 C -0.017896
23 C 0.034924
24 C -0.037096
25 C 0.077545
26 C -0.035109

27	C	0.054926
28	H	-0.000349
29	H	0.000492
30	H	0.000559
31	H	-0.000609
32	H	0.000786
33	H	-0.002343
34	H	0.000880
35	H	-0.001884
36	H	0.001864
37	H	-0.004725
38	H	0.001871
39	H	-0.009395

Sum of Mulliken atomic spin densities = 1.00000

6.16 Mulliken atomic spin densities of **7**$^{\bullet+}$ (uB3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Mulliken atomic spin densities:

1	C	0.165965
2	C	0.037944
3	N	0.228154
4	C	0.037944
5	C	0.165965
6	S	0.253630
7	C	-0.023247
8	C	0.005209
9	C	0.003908
10	C	-0.002387
11	C	0.003889
12	C	0.004982
13	C	0.053097
14	C	-0.035946

15	S	-0.009930
16	C	-0.034757
17	C	0.071139
18	C	-0.031985
19	C	0.056118
20	C	-0.035946
21	C	0.053097
22	S	-0.009930
23	C	0.056118
24	C	-0.031985
25	C	0.071139
26	C	-0.034757
27	H	-0.000340
28	H	0.000606
29	H	0.000609
30	H	-0.000346
31	H	0.001721
32	H	-0.004442
33	H	0.001770
34	H	-0.008048
35	H	-0.008048
36	H	0.001770
37	H	-0.004442
38	H	0.001721
39	F	0.000038

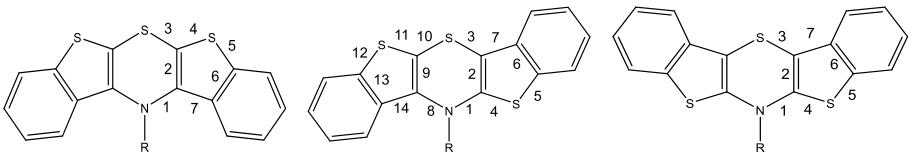
Sum of Mulliken atomic spin densities = 1.00000

6.17 Wiberg bond orders - overview

The calculated Wiberg bond orders (BO) were employed to estimate the delocalization of the spin density of the radical cations using the extracting by multiwfn.[8]

Table 4: Wiberg bond orders (BO) from parent BBTTs **5**, **6**, and **7**, and radical cations **5**$^{\bullet+}$, **6**$^{\bullet+}$, and **7**$^{\bullet+}$ as well as the relative change of BO given as Δ ($BO_X^{\bullet+}$-BO_X^{2+}) in the BBTT-core ((u)B3LYP/6-311G**).[8]

compound



		1 (8)	**2 (9)**	**3 (10)**	**4 (11)**	**5 (12)**	**6 (13)**	**7 (14)**
syn-syn	**BO_5**	1.099	1.581	1.256	1.304	1.271	1.295	1.132
	$BO_5^{\bullet+}$	1.232	1.42	1.353	1.349	1.259	1.296	1.111
	$\Delta(BO_5 - BO_5^{\bullet+})$ [%]	12.14	-10.18	7.65	3.52	-0.94	0.07	-1.80
syn-anti	**BO_6**	1.186 (1.112)	1.582 (1.583)	1.186 (1.255)	1.232 (1.296)	1.267 (1.270)	1.293 (1.298)	1.172 (1.124)
	$BO_6^{\bullet+}$	1.294 (1.218)	1.407 (1.420)	1.301 (1.353)	1.263 (1.346)	1.233 (1.260)	1.287 (1.294)	1.187 (1.123)
	$\Delta(BO_6 - BO_6^{\bullet+})$ [%]	9.08 (9.61)	-11.02 (-10.26)	9.72 (7.75)	2.56 (3.91)	-2.67 (-0.83)	-0.42 (-0.36)	1.28 (-0.09)
anti-anti	**BO_7**	1.193	1.564	1.184	1.231	1.253	1.289	1.179
	$BO_7^{\bullet+}$	1.265	1.438	1.285	1.275	1.209	1.293	1.193
	$\Delta(BO_7 - BO_7^{\bullet+})$ [%]	6.03	-8.09	8.52	3.57	-3.52	0.37	1.17

6.18 Wiberg bond orders extracted of **5** extracted by multiwfn (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Bond orders with absolute value >= 0.050000

#	1:	1(C)	2(C)	1.58094889
#	2:	1(C)	3(N)	0.12303733
#	3:	1(C)	4(C)	0.05645994
#	4:	1(C)	5(C)	0.09415285
#	5:	1(C)	6(S)	1.25647173

6: 1(C) 10(S) 1.30358701
7: 1(C) 11(C) 0.14495509
8: 1(C) 12(C) 0.14335953
9: 2(C) 3(N) 1.09873732
10: 2(C) 4(C) 0.10627940
11: 2(C) 5(C) 0.05645992
12: 2(C) 6(S) 0.15554023
13: 2(C) 10(S) 0.20351658
14: 2(C) 11(C) 0.13225960
15: 2(C) 12(C) 1.13169165
16: 2(C) 13(C) 0.09484785
17: 2(C) 17(C) 0.10417185
18: 3(N) 4(C) 1.09873717
19: 3(N) 5(C) 0.12303740
20: 3(N) 7(C) 0.09683911
21: 3(N) 12(C) 0.09683913
22: 3(N) 13(C) 1.14616064
23: 3(N) 22(C) 0.12939237
24: 3(N) 26(C) 0.12939250
25: 4(C) 5(C) 1.58094951
26: 4(C) 6(S) 0.15554031
27: 4(C) 7(C) 1.13169145
28: 4(C) 8(C) 0.13225966
29: 4(C) 9(S) 0.20351644
30: 4(C) 13(C) 0.09484782
31: 4(C) 18(C) 0.10417178
32: 5(C) 6(S) 1.25647192
33: 5(C) 7(C) 0.14335957
34: 5(C) 8(C) 0.14495509
35: 5(C) 9(S) 1.30358564
36: 6(S) 9(S) 0.13477448
37: 6(S) 10(S) 0.13477453
38: 7(C) 8(C) 1.29541743

39: 7(C) 9(S) 0.15838788
40: 7(C) 18(C) 1.32185935
41: 7(C) 19(C) 0.13143948
42: 7(C) 20(C) 0.10968708
43: 7(C) 21(C) 0.11958582
44: 7(C) 32(H) 0.07673876
45: 8(C) 9(S) 1.27127252
46: 8(C) 18(C) 0.11632330
47: 8(C) 19(C) 0.11816576
48: 8(C) 20(C) 0.13533442
49: 8(C) 21(C) 1.41367486
50: 8(C) 35(H) 0.08033328
51: 9(S) 21(C) 0.13793566
52: 10(S) 11(C) 1.27127191
53: 10(S) 12(C) 0.15838769
54: 10(S) 14(C) 0.13793567
55: 11(C) 12(C) 1.29541612
56: 11(C) 14(C) 1.41367633
57: 11(C) 15(C) 0.13533443
58: 11(C) 16(C) 0.11816575
59: 11(C) 17(C) 0.11632327
60: 11(C) 28(H) 0.08033340
61: 12(C) 14(C) 0.11958582
62: 12(C) 15(C) 0.10968718
63: 12(C) 16(C) 0.13143952
64: 12(C) 17(C) 1.32186022
65: 12(C) 31(H) 0.07673878
66: 13(C) 22(C) 1.34787579
67: 13(C) 23(C) 0.12793651
68: 13(C) 24(C) 0.11674106
69: 13(C) 25(C) 0.12793665
70: 13(C) 26(C) 1.34787717
71: 13(C) 36(H) 0.07369752

# 72:	13(C)	39(H)	0.07369757
# 73:	14(C)	15(C)	1.50060472
# 74:	14(C)	16(C)	0.12746508
# 75:	14(C)	17(C)	0.13332599
# 76:	14(C)	28(H)	0.86876751
# 77:	14(C)	29(H)	0.08376729
# 78:	15(C)	16(C)	1.41765967
# 79:	15(C)	17(C)	0.12876544
# 80:	15(C)	28(H)	0.08206142
# 81:	15(C)	29(H)	0.87780288
# 82:	15(C)	30(H)	0.08130335
# 83:	16(C)	17(C)	1.51736902
# 84:	16(C)	29(H)	0.08109739
# 85:	16(C)	30(H)	0.87668267
# 86:	16(C)	31(H)	0.08057308
# 87:	17(C)	30(H)	0.08488065
# 88:	17(C)	31(H)	0.85280005
# 89:	18(C)	19(C)	1.51736952
# 90:	18(C)	20(C)	0.12876543
# 91:	18(C)	21(C)	0.13332608
# 92:	18(C)	32(H)	0.85280022
# 93:	18(C)	33(H)	0.08488067
# 94:	19(C)	20(C)	1.41765905
# 95:	19(C)	21(C)	0.12746517
# 96:	19(C)	32(H)	0.08057314
# 97:	19(C)	33(H)	0.87668277
# 98:	19(C)	34(H)	0.08109733
# 99:	20(C)	21(C)	1.50060617
# 100:	20(C)	33(H)	0.08130339
# 101:	20(C)	34(H)	0.87780261
# 102:	20(C)	35(H)	0.08206145
# 103:	21(C)	34(H)	0.08376731
# 104:	21(C)	35(H)	0.86876739

#	105:	22(C)	23(C)	1.46176560
#	106:	22(C)	24(C)	0.14206353
#	107:	22(C)	25(C)	0.13220943
#	108:	22(C)	26(C)	0.12354869
#	109:	22(C)	36(H)	0.83592996
#	110:	22(C)	37(H)	0.08211446
#	111:	23(C)	24(C)	1.40919217
#	112:	23(C)	25(C)	0.13028951
#	113:	23(C)	26(C)	0.13220920
#	114:	23(C)	27(F)	0.13726138
#	115:	23(C)	36(H)	0.07924998
#	116:	23(C)	37(H)	0.86447953
#	117:	24(C)	25(C)	1.40919257
#	118:	24(C)	26(C)	0.14206350
#	119:	24(C)	27(F)	1.32330443
#	120:	24(C)	37(H)	0.08251531
#	121:	24(C)	38(H)	0.08251526
#	122:	25(C)	26(C)	1.46176496
#	123:	25(C)	27(F)	0.13726145
#	124:	25(C)	38(H)	0.86447932
#	125:	25(C)	39(H)	0.07924999
#	126:	26(C)	38(H)	0.08211437
#	127:	26(C)	39(H)	0.83592971

6.19 Wiberg bond orders of **6** extracted by multiwfn (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Bond orders with absolute value >= 0.050000

#	1:	1(C)	2(C)	1.58265147
#	2:	1(C)	3(N)	0.13133045
#	3:	1(C)	4(C)	0.05279380
#	4:	1(C)	5(C)	0.09121155
#	5:	1(C)	6(S)	1.25537428

6: 1(C) 7(S) 1.29574321
7: 1(C) 8(C) 0.14271290
8: 1(C) 9(C) 0.14203531
9: 2(C) 3(N) 1.11155942
10: 2(C) 4(C) 0.10418824
11: 2(C) 5(C) 0.05059049
12: 2(C) 6(S) 0.15519409
13: 2(C) 7(S) 0.20091394
14: 2(C) 8(C) 0.13119802
15: 2(C) 9(C) 1.12380065
16: 2(C) 13(C) 0.09608415
17: 2(C) 23(C) 0.10322991
18: 3(N) 4(C) 1.18632617
19: 3(N) 5(C) 0.13746102
20: 3(N) 9(C) 0.09625664
21: 3(N) 10(S) 0.12000341
22: 3(N) 13(C) 1.08294799
23: 3(N) 14(C) 0.12315430
24: 3(N) 18(C) 0.11557614
25: 4(C) 5(C) 1.58182934
26: 4(C) 6(S) 0.14882954
27: 4(C) 10(S) 1.23188881
28: 4(C) 11(C) 0.13700409
29: 4(C) 12(C) 0.14569560
30: 4(C) 13(C) 0.10022033
31: 5(C) 6(S) 1.18608255
32: 5(C) 10(S) 0.19448428
33: 5(C) 11(C) 0.13213400
34: 5(C) 12(C) 1.17181593
35: 5(C) 27(C) 0.11100924
36: 6(S) 7(S) 0.13887327
37: 6(S) 12(C) 0.11663240
38: 7(S) 8(C) 1.27025932

# 39:	7(S)	9(C)	0.16032844
# 40:	7(S)	20(C)	0.13856999
# 41:	8(C)	9(C)	1.29826777
# 42:	8(C)	20(C)	1.41647440
# 43:	8(C)	21(C)	0.13509177
# 44:	8(C)	22(C)	0.11872859
# 45:	8(C)	23(C)	0.11668869
# 46:	8(C)	32(H)	0.08047290
# 47:	9(C)	20(C)	0.11932530
# 48:	9(C)	21(C)	0.10984086
# 49:	9(C)	22(C)	0.13118632
# 50:	9(C)	23(C)	1.32462544
# 51:	9(C)	35(H)	0.07571539
# 52:	10(S)	11(C)	1.26711500
# 53:	10(S)	12(C)	0.15835153
# 54:	10(S)	14(C)	0.05619502
# 55:	10(S)	24(C)	0.13970275
# 56:	11(C)	12(C)	1.29280056
# 57:	11(C)	24(C)	1.41972531
# 58:	11(C)	25(C)	0.13505828
# 59:	11(C)	26(C)	0.11876808
# 60:	11(C)	27(C)	0.11681103
# 61:	11(C)	36(H)	0.08040125
# 62:	12(C)	24(C)	0.11869901
# 63:	12(C)	25(C)	0.11002887
# 64:	12(C)	26(C)	0.13109754
# 65:	12(C)	27(C)	1.34121337
# 66:	12(C)	39(H)	0.07737945
# 67:	13(C)	14(C)	1.38172985
# 68:	13(C)	15(C)	0.13096716
# 69:	13(C)	16(C)	0.12481410
# 70:	13(C)	17(C)	0.13056579
# 71:	13(C)	18(C)	1.37393427

72: 13(C) 28(H) 0.07622623
73: 13(C) 31(H) 0.07558172
74: 14(C) 15(C) 1.45655999
75: 14(C) 16(C) 0.14188231
76: 14(C) 17(C) 0.13334741
77: 14(C) 18(C) 0.12441079
78: 14(C) 28(H) 0.84799924
79: 14(C) 29(H) 0.08198645
80: 15(C) 16(C) 1.40956806
81: 15(C) 17(C) 0.12846817
82: 15(C) 18(C) 0.13400791
83: 15(C) 19(F) 0.13881619
84: 15(C) 28(H) 0.07957183
85: 15(C) 29(H) 0.86450149
86: 16(C) 17(C) 1.40569831
87: 16(C) 18(C) 0.14232975
88: 16(C) 19(F) 1.33806632
89: 16(C) 29(H) 0.08258740
90: 16(C) 30(H) 0.08247811
91: 17(C) 18(C) 1.46106927
92: 17(C) 19(F) 0.13844472
93: 17(C) 30(H) 0.86435622
94: 17(C) 31(H) 0.07860108
95: 18(C) 30(H) 0.08220839
96: 18(C) 31(H) 0.84215115
97: 20(C) 21(C) 1.49813995
98: 20(C) 22(C) 0.12776457
99: 20(C) 23(C) 0.13303123
100: 20(C) 32(H) 0.86880460
101: 20(C) 33(H) 0.08371429
102: 21(C) 22(C) 1.42098307
103: 21(C) 23(C) 0.12875825
104: 21(C) 32(H) 0.08194076

# 105:	21(C)	33(H)	0.87791433
# 106:	21(C)	34(H)	0.08134919
# 107:	22(C)	23(C)	1.51411783
# 108:	22(C)	33(H)	0.08129348
# 109:	22(C)	34(H)	0.87665688
# 110:	22(C)	35(H)	0.08069918
# 111:	23(C)	34(H)	0.08485478
# 112:	23(C)	35(H)	0.84876687
# 113:	24(C)	25(C)	1.49484044
# 114:	24(C)	26(C)	0.12776030
# 115:	24(C)	27(C)	0.13295024
# 116:	24(C)	36(H)	0.86877309
# 117:	24(C)	37(H)	0.08364923
# 118:	25(C)	26(C)	1.42572925
# 119:	25(C)	27(C)	0.12789345
# 120:	25(C)	36(H)	0.08185787
# 121:	25(C)	37(H)	0.87809683
# 122:	25(C)	38(H)	0.08151749
# 123:	26(C)	27(C)	1.51274709
# 124:	26(C)	37(H)	0.08143638
# 125:	26(C)	38(H)	0.87735167
# 126:	26(C)	39(H)	0.08171155
# 127:	27(C)	38(H)	0.08462383
# 128:	27(C)	39(H)	0.86207859

6.20 Wiberg bond orders of **7** extracted by multiwfn (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Bond orders with absolute value >= 0.050000

# 1:	1(C)	2(C)	1.56397627
# 2:	1(C)	3(N)	0.14673314
# 3:	1(C)	4(C)	0.05162217
# 4:	1(C)	5(C)	0.09316786

5: 1(C) 6(S) 1.18378244
6: 1(C) 20(C) 1.17910164
7: 1(C) 21(C) 0.13243288
8: 1(C) 22(S) 0.18586661
9: 1(C) 23(C) 0.11253513
10: 2(C) 3(N) 1.19343718
11: 2(C) 4(C) 0.10530640
12: 2(C) 5(C) 0.05162217
13: 2(C) 6(S) 0.14585284
14: 2(C) 7(C) 0.10142515
15: 2(C) 20(C) 0.14757593
16: 2(C) 21(C) 0.13667312
17: 2(C) 22(S) 1.23067429
18: 3(N) 4(C) 1.19343774
19: 3(N) 5(C) 0.14673323
20: 3(N) 7(C) 1.07105270
21: 3(N) 8(C) 0.11627229
22: 3(N) 12(C) 0.11520951
23: 3(N) 15(S) 0.11508799
24: 3(N) 22(S) 0.11508795
25: 4(C) 5(C) 1.56397631
26: 4(C) 6(S) 0.14585277
27: 4(C) 7(C) 0.10142514
28: 4(C) 13(C) 0.13667308
29: 4(C) 14(C) 0.14757590
30: 4(C) 15(S) 1.23067401
31: 5(C) 6(S) 1.18378208
32: 5(C) 13(C) 0.13243291
33: 5(C) 14(C) 1.17910172
34: 5(C) 15(S) 0.18586655
35: 5(C) 19(C) 0.11253515
36: 6(S) 14(C) 0.11880477
37: 6(S) 19(C) 0.05006291

38: 6(S) 20(C) 0.11880480
39: 6(S) 23(C) 0.05006291
40: 7(C) 8(C) 1.38091932
41: 7(C) 9(C) 0.13214407
42: 7(C) 10(C) 0.12615634
43: 7(C) 11(C) 0.13128055
44: 7(C) 12(C) 1.38297652
45: 7(C) 15(S) 0.06879937
46: 7(C) 22(S) 0.06879942
47: 7(C) 27(H) 0.07702682
48: 7(C) 30(H) 0.07636708
49: 8(C) 9(C) 1.46746363
50: 8(C) 10(C) 0.14275753
51: 8(C) 11(C) 0.13460384
52: 8(C) 12(C) 0.12414021
53: 8(C) 27(H) 0.85290105
54: 8(C) 28(H) 0.08258567
55: 9(C) 10(C) 1.40139084
56: 9(C) 11(C) 0.12754380
57: 9(C) 12(C) 0.13206415
58: 9(C) 27(H) 0.07965918
59: 9(C) 28(H) 0.86411323
60: 9(C) 39(F) 0.13896823
61: 10(C) 11(C) 1.41081672
62: 10(C) 12(C) 0.14254223
63: 10(C) 28(H) 0.08227461
64: 10(C) 29(H) 0.08256978
65: 10(C) 39(F) 1.34770754
66: 11(C) 12(C) 1.45369916
67: 11(C) 29(H) 0.86379673
68: 11(C) 30(H) 0.07872176
69: 11(C) 39(F) 0.13974707
70: 12(C) 29(H) 0.08201226

# 71:	12(C)	30(H)	0.84806139
# 72:	13(C)	14(C)	1.28872433
# 73:	13(C)	15(S)	1.25319016
# 74:	13(C)	16(C)	1.42779088
# 75:	13(C)	17(C)	0.13541266
# 76:	13(C)	18(C)	0.11923142
# 77:	13(C)	19(C)	0.11713617
# 78:	13(C)	31(H)	0.08072406
# 79:	14(C)	15(S)	0.15664438
# 80:	14(C)	16(C)	0.11835267
# 81:	14(C)	17(C)	0.10879922
# 82:	14(C)	18(C)	0.13061721
# 83:	14(C)	19(C)	1.33839920
# 84:	14(C)	34(H)	0.07736447
# 85:	15(S)	16(C)	0.13920266
# 86:	16(C)	17(C)	1.48772073
# 87:	16(C)	18(C)	0.12768948
# 88:	16(C)	19(C)	0.13130437
# 89:	16(C)	31(H)	0.86879615
# 90:	16(C)	32(H)	0.08345981
# 91:	17(C)	18(C)	1.42933648
# 92:	17(C)	19(C)	0.12776553
# 93:	17(C)	31(H)	0.08155001
# 94:	17(C)	32(H)	0.87852748
# 95:	17(C)	33(H)	0.08162953
# 96:	18(C)	19(C)	1.51079503
# 97:	18(C)	32(H)	0.08157520
# 98:	18(C)	33(H)	0.87748154
# 99:	18(C)	34(H)	0.08164534
# 100:	19(C)	33(H)	0.08458109
# 101:	19(C)	34(H)	0.86244127
# 102:	20(C)	21(C)	1.28872440
# 103:	20(C)	22(S)	0.15664438

# 104:	20(C)	23(C)	1.33839916
# 105:	20(C)	24(C)	0.13061720
# 106:	20(C)	25(C)	0.10879922
# 107:	20(C)	26(C)	0.11835266
# 108:	20(C)	35(H)	0.07736446
# 109:	21(C)	22(S)	1.25319003
# 110:	21(C)	23(C)	0.11713619
# 111:	21(C)	24(C)	0.11923141
# 112:	21(C)	25(C)	0.13541267
# 113:	21(C)	26(C)	1.42779088
# 114:	21(C)	38(H)	0.08072406
# 115:	22(S)	26(C)	0.13920265
# 116:	23(C)	24(C)	1.51079506
# 117:	23(C)	25(C)	0.12776553
# 118:	23(C)	26(C)	0.13130439
# 119:	23(C)	35(H)	0.86244127
# 120:	23(C)	36(H)	0.08458109
# 121:	24(C)	25(C)	1.42933650
# 122:	24(C)	26(C)	0.12768949
# 123:	24(C)	35(H)	0.08164535
# 124:	24(C)	36(H)	0.87748153
# 125:	24(C)	37(H)	0.08157520
# 126:	25(C)	26(C)	1.48772073
# 127:	25(C)	36(H)	0.08162953
# 128:	25(C)	37(H)	0.87852747
# 129:	25(C)	38(H)	0.08155000
# 130:	26(C)	37(H)	0.08345981
# 131:	26(C)	38(H)	0.86879615

6.21 Wiberg bond orders of **5**$^{\bullet+}$ extracted by multiwfn (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Bond orders with absolute value >= 0.050000

1: 1(C) 2(C) Alpha: 0.770246 Beta: 0.649691 Total: 1.419937
2: 1(C) 3(N) Alpha: 0.074106 Beta: 0.051404 Total: 0.125511
3: 1(C) 4(C) Alpha: 0.021443 Beta: 0.046052 Total: 0.067495
4: 1(C) 5(C) Alpha: 0.047142 Beta: 0.060720 Total: 0.107862
5: 1(C) 6(S) Alpha: 0.625563 Beta: 0.727037 Total: 1.352600
6: 1(C) 10(S) Alpha: 0.657494 Beta: 0.691985 Total: 1.349479
7: 1(C) 11(C) Alpha: 0.075737 Beta: 0.062092 Total: 0.137830
8: 1(C) 12(C) Alpha: 0.069503 Beta: 0.065362 Total: 0.134865
9: 2(C) 3(N) Alpha: 0.576599 Beta: 0.655518 Total: 1.232117
10: 2(C) 4(C) Alpha: 0.047878 Beta: 0.063502 Total: 0.111380
11: 2(C) 5(C) Alpha: 0.021443 Beta: 0.046052 Total: 0.067495
12: 2(C) 6(S) Alpha: 0.072325 Beta: 0.055262 Total: 0.127587
13: 2(C) 10(S) Alpha: 0.105491 Beta: 0.082681 Total: 0.188172
14: 2(C) 11(C) Alpha: 0.064834 Beta: 0.064612 Total: 0.129447
15: 2(C) 12(C) Alpha: 0.559782 Beta: 0.551558 Total: 1.111340
16: 2(C) 13(C) Alpha: 0.046724 Beta: 0.050129 Total: 0.096853
17: 2(C) 17(C) Alpha: 0.048151 Beta: 0.048014 Total: 0.096165
18: 3(N) 4(C) Alpha: 0.576599 Beta: 0.655518 Total: 1.232117
19: 3(N) 5(C) Alpha: 0.074106 Beta: 0.051404 Total: 0.125511
20: 3(N) 6(S) Alpha: 0.023848 Beta: 0.049637 Total: 0.073486
21: 3(N) 7(C) Alpha: 0.045415 Beta: 0.046327 Total: 0.091742
22: 3(N) 12(C) Alpha: 0.045415 Beta: 0.046327 Total: 0.091742
23: 3(N) 13(C) Alpha: 0.527979 Beta: 0.511015 Total: 1.038995
24: 3(N) 22(C) Alpha: 0.057823 Beta: 0.053670 Total: 0.111493
25: 3(N) 26(C) Alpha: 0.057823 Beta: 0.053670 Total: 0.111493
26: 4(C) 5(C) Alpha: 0.770246 Beta: 0.649691 Total: 1.419937
27: 4(C) 6(S) Alpha: 0.072325 Beta: 0.055262 Total: 0.127587
28: 4(C) 7(C) Alpha: 0.559783 Beta: 0.551559 Total: 1.111341
29: 4(C) 8(C) Alpha: 0.064835 Beta: 0.064612 Total: 0.129447
30: 4(C) 9(S) Alpha: 0.105491 Beta: 0.082681 Total: 0.188172
31: 4(C) 13(C) Alpha: 0.046724 Beta: 0.050129 Total: 0.096853
32: 4(C) 18(C) Alpha: 0.048151 Beta: 0.048014 Total: 0.096165
33: 5(C) 6(S) Alpha: 0.625563 Beta: 0.727037 Total: 1.352600

34: 5(C) 7(C) Alpha: 0.069503 Beta: 0.065362 Total: 0.134865
35: 5(C) 8(C) Alpha: 0.075737 Beta: 0.062092 Total: 0.137830
36: 5(C) 9(S) Alpha: 0.657494 Beta: 0.691984 Total: 1.349478
37: 6(S) 9(S) Alpha: 0.073854 Beta: 0.098879 Total: 0.172733
38: 6(S) 10(S) Alpha: 0.073854 Beta: 0.098879 Total: 0.172734
39: 7(C) 8(C) Alpha: 0.647111 Beta: 0.649160 Total: 1.296271
40: 7(C) 9(S) Alpha: 0.076063 Beta: 0.074745 Total: 0.150808
41: 7(C) 18(C) Alpha: 0.654607 Beta: 0.657935 Total: 1.312542
42: 7(C) 19(C) Alpha: 0.064353 Beta: 0.064277 Total: 0.128630
43: 7(C) 20(C) Alpha: 0.053725 Beta: 0.055254 Total: 0.108979
44: 7(C) 21(C) Alpha: 0.058194 Beta: 0.058348 Total: 0.116542
45: 7(C) 32(H) Alpha: 0.035304 Beta: 0.035338 Total: 0.070642
46: 8(C) 9(S) Alpha: 0.637515 Beta: 0.621869 Total: 1.259384
47: 8(C) 18(C) Alpha: 0.059249 Beta: 0.060135 Total: 0.119384
48: 8(C) 19(C) Alpha: 0.058159 Beta: 0.059869 Total: 0.118028
49: 8(C) 20(C) Alpha: 0.067611 Beta: 0.068086 Total: 0.135697
50: 8(C) 21(C) Alpha: 0.705486 Beta: 0.713784 Total: 1.419270
51: 8(C) 35(H) Alpha: 0.040277 Beta: 0.040447 Total: 0.080725
52: 9(S) 21(C) Alpha: 0.070796 Beta: 0.069573 Total: 0.140369
53: 10(S) 11(C) Alpha: 0.637515 Beta: 0.621869 Total: 1.259384
54: 10(S) 12(C) Alpha: 0.076062 Beta: 0.074745 Total: 0.150807
55: 10(S) 14(C) Alpha: 0.070796 Beta: 0.069573 Total: 0.140369
56: 11(C) 12(C) Alpha: 0.647111 Beta: 0.649160 Total: 1.296271
57: 11(C) 14(C) Alpha: 0.705487 Beta: 0.713785 Total: 1.419271
58: 11(C) 15(C) Alpha: 0.067611 Beta: 0.068086 Total: 0.135697
59: 11(C) 16(C) Alpha: 0.058159 Beta: 0.059869 Total: 0.118028
60: 11(C) 17(C) Alpha: 0.059249 Beta: 0.060135 Total: 0.119384
61: 11(C) 28(H) Alpha: 0.040277 Beta: 0.040447 Total: 0.080725
62: 12(C) 14(C) Alpha: 0.058194 Beta: 0.058348 Total: 0.116542
63: 12(C) 15(C) Alpha: 0.053725 Beta: 0.055254 Total: 0.108979
64: 12(C) 16(C) Alpha: 0.064353 Beta: 0.064277 Total: 0.128630
65: 12(C) 17(C) Alpha: 0.654608 Beta: 0.657936 Total: 1.312543
66: 12(C) 31(H) Alpha: 0.035304 Beta: 0.035339 Total: 0.070642

67: 13(C) 22(C) Alpha: 0.686886 Beta: 0.684011 Total: 1.370897
68: 13(C) 23(C) Alpha: 0.067119 Beta: 0.067158 Total: 0.134277
69: 13(C) 24(C) Alpha: 0.064212 Beta: 0.064206 Total: 0.128418
70: 13(C) 25(C) Alpha: 0.067119 Beta: 0.067158 Total: 0.134277
71: 13(C) 26(C) Alpha: 0.686885 Beta: 0.684010 Total: 1.370895
72: 13(C) 36(H) Alpha: 0.038525 Beta: 0.038578 Total: 0.077104
73: 13(C) 39(H) Alpha: 0.038525 Beta: 0.038578 Total: 0.077103
74: 14(C) 15(C) Alpha: 0.751433 Beta: 0.739956 Total: 1.491389
75: 14(C) 16(C) Alpha: 0.065066 Beta: 0.064809 Total: 0.129875
76: 14(C) 17(C) Alpha: 0.067359 Beta: 0.063636 Total: 0.130995
77: 14(C) 28(H) Alpha: 0.432104 Beta: 0.432417 Total: 0.864521
78: 14(C) 29(H) Alpha: 0.041859 Beta: 0.041633 Total: 0.083492
79: 15(C) 16(C) Alpha: 0.707025 Beta: 0.711821 Total: 1.418847
80: 15(C) 17(C) Alpha: 0.064786 Beta: 0.065939 Total: 0.130725
81: 15(C) 28(H) Alpha: 0.040665 Beta: 0.040501 Total: 0.081165
82: 15(C) 29(H) Alpha: 0.437767 Beta: 0.436960 Total: 0.874727
83: 15(C) 30(H) Alpha: 0.040300 Beta: 0.040429 Total: 0.080730
84: 16(C) 17(C) Alpha: 0.757221 Beta: 0.750714 Total: 1.507935
85: 16(C) 29(H) Alpha: 0.040555 Beta: 0.040639 Total: 0.081194
86: 16(C) 30(H) Alpha: 0.436098 Beta: 0.436464 Total: 0.872562
87: 16(C) 31(H) Alpha: 0.040559 Beta: 0.040419 Total: 0.080978
88: 17(C) 30(H) Alpha: 0.042557 Beta: 0.042477 Total: 0.085034
89: 17(C) 31(H) Alpha: 0.416577 Beta: 0.415754 Total: 0.832331
90: 18(C) 19(C) Alpha: 0.757221 Beta: 0.750715 Total: 1.507936
91: 18(C) 20(C) Alpha: 0.064786 Beta: 0.065939 Total: 0.130725
92: 18(C) 21(C) Alpha: 0.067359 Beta: 0.063636 Total: 0.130995
93: 18(C) 32(H) Alpha: 0.416577 Beta: 0.415754 Total: 0.832330
94: 18(C) 33(H) Alpha: 0.042557 Beta: 0.042477 Total: 0.085034
95: 19(C) 20(C) Alpha: 0.707025 Beta: 0.711821 Total: 1.418846
96: 19(C) 21(C) Alpha: 0.065066 Beta: 0.064809 Total: 0.129875
97: 19(C) 32(H) Alpha: 0.040559 Beta: 0.040419 Total: 0.080978
98: 19(C) 33(H) Alpha: 0.436098 Beta: 0.436464 Total: 0.872561
99: 19(C) 34(H) Alpha: 0.040555 Beta: 0.040639 Total: 0.081194

100: 20(C) 21(C) Alpha: 0.751434 Beta: 0.739956 Total: 1.491390
101: 20(C) 33(H) Alpha: 0.040300 Beta: 0.040429 Total: 0.080730
102: 20(C) 34(H) Alpha: 0.437767 Beta: 0.436960 Total: 0.874727
103: 20(C) 35(H) Alpha: 0.040665 Beta: 0.040501 Total: 0.081165
104: 21(C) 34(H) Alpha: 0.041859 Beta: 0.041633 Total: 0.083492
105: 21(C) 35(H) Alpha: 0.432104 Beta: 0.432417 Total: 0.864521
106: 22(C) 23(C) Alpha: 0.724507 Beta: 0.723932 Total: 1.448438
107: 22(C) 24(C) Alpha: 0.071503 Beta: 0.071537 Total: 0.143040
108: 22(C) 25(C) Alpha: 0.067188 Beta: 0.067262 Total: 0.134450
109: 22(C) 26(C) Alpha: 0.062951 Beta: 0.062374 Total: 0.125325
110: 22(C) 36(H) Alpha: 0.420632 Beta: 0.420706 Total: 0.841338
111: 22(C) 37(H) Alpha: 0.041119 Beta: 0.041007 Total: 0.082126
112: 23(C) 24(C) Alpha: 0.696870 Beta: 0.696817 Total: 1.393687
113: 23(C) 25(C) Alpha: 0.064366 Beta: 0.064305 Total: 0.128671
114: 23(C) 26(C) Alpha: 0.067188 Beta: 0.067262 Total: 0.134450
115: 23(C) 27(F) Alpha: 0.069770 Beta: 0.069764 Total: 0.139534
116: 23(C) 36(H) Alpha: 0.038890 Beta: 0.038893 Total: 0.077784
117: 23(C) 37(H) Alpha: 0.430309 Beta: 0.430074 Total: 0.860383
118: 24(C) 25(C) Alpha: 0.696870 Beta: 0.696816 Total: 1.393686
119: 24(C) 26(C) Alpha: 0.071503 Beta: 0.071537 Total: 0.143040
120: 24(C) 27(F) Alpha: 0.681652 Beta: 0.681730 Total: 1.363382
121: 24(C) 37(H) Alpha: 0.040872 Beta: 0.040867 Total: 0.081739
122: 24(C) 38(H) Alpha: 0.040872 Beta: 0.040867 Total: 0.081739
123: 25(C) 26(C) Alpha: 0.724508 Beta: 0.723932 Total: 1.448440
124: 25(C) 27(F) Alpha: 0.069770 Beta: 0.069764 Total: 0.139534
125: 25(C) 38(H) Alpha: 0.430309 Beta: 0.430075 Total: 0.860383
126: 25(C) 39(H) Alpha: 0.038890 Beta: 0.038893 Total: 0.077784
127: 26(C) 38(H) Alpha: 0.041119 Beta: 0.041007 Total: 0.082126
128: 26(C) 39(H) Alpha: 0.420632 Beta: 0.420706 Total: 0.841338

6.22 Wiberg bond orders of **6**$^{\bullet+}$ extracted by multiwfn (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Bond orders with absolute value >= 0.050000

#	1:	1(C)	2(C)	Alpha:	0.768835	Beta: 0.651485	Total: 1.420321
#	2:	1(C)	3(N)	Alpha:	0.071769	Beta: 0.051292	Total: 0.123061
#	3:	1(C)	4(C)	Alpha:	0.023205	Beta: 0.047867	Total: 0.071073
#	4:	1(C)	5(C)	Alpha:	0.046020	Beta: 0.059096	Total: 0.105115
#	5:	1(C)	6(S)	Alpha:	0.625409	Beta: 0.727196	Total: 1.352605
#	6:	1(C)	7(S)	Alpha:	0.658725	Beta: 0.687697	Total: 1.346422
#	7:	1(C)	8(C)	Alpha:	0.075529	Beta: 0.061788	Total: 0.137318
#	8:	1(C)	9(C)	Alpha:	0.069392	Beta: 0.065214	Total: 0.134605
#	9:	2(C)	3(N)	Alpha:	0.572036	Beta: 0.646350	Total: 1.218386
#	10:	2(C)	4(C)	Alpha:	0.050076	Beta: 0.066569	Total: 0.116645
#	11:	2(C)	5(C)	Alpha:	0.020451	Beta: 0.045257	Total: 0.065708
#	12:	2(C)	6(S)	Alpha:	0.072470	Beta: 0.054981	Total: 0.127452
#	13:	2(C)	7(S)	Alpha:	0.105682	Beta: 0.083914	Total: 0.189595
#	14:	2(C)	8(C)	Alpha:	0.065820	Beta: 0.065615	Total: 0.131435
#	15:	2(C)	9(C)	Alpha:	0.564836	Beta: 0.557962	Total: 1.122798
#	16:	2(C)	13(C)	Alpha:	0.044417	Beta: 0.047211	Total: 0.091629
#	17:	2(C)	23(C)	Alpha:	0.049279	Beta: 0.049119	Total: 0.098398
#	18:	3(N)	4(C)	Alpha:	0.608709	Beta: 0.685301	Total: 1.294010
#	19:	3(N)	5(C)	Alpha:	0.074298	Beta: 0.051837	Total: 0.126135
#	20:	3(N)	6(S)	Alpha:	0.022664	Beta: 0.049061	Total: 0.071725
#	21:	3(N)	9(C)	Alpha:	0.045638	Beta: 0.046901	Total: 0.092539
#	22:	3(N)	10(S)	Alpha:	0.060385	Beta: 0.071731	Total: 0.132116
#	23:	3(N)	13(C)	Alpha:	0.523673	Beta: 0.508871	Total: 1.032544
#	24:	3(N)	14(C)	Alpha:	0.056913	Beta: 0.053234	Total: 0.110148
#	25:	3(N)	18(C)	Alpha:	0.056880	Beta: 0.053202	Total: 0.110082
#	26:	4(C)	5(C)	Alpha:	0.761281	Beta: 0.646108	Total: 1.407389
#	27:	4(C)	6(S)	Alpha:	0.070788	Beta: 0.057318	Total: 0.128106
#	28:	4(C)	10(S)	Alpha:	0.632424	Beta: 0.631053	Total: 1.263478
#	29:	4(C)	11(C)	Alpha:	0.069666	Beta: 0.058303	Total: 0.127968
#	30:	4(C)	12(C)	Alpha:	0.072076	Beta: 0.068384	Total: 0.140460
#	31:	4(C)	13(C)	Alpha:	0.054645	Beta: 0.058135	Total: 0.112780
#	32:	5(C)	6(S)	Alpha:	0.599472	Beta: 0.701838	Total: 1.301310

33: 5(C) 10(S) Alpha: 0.097889 Beta: 0.081166 Total: 0.179056
34: 5(C) 11(C) Alpha: 0.067315 Beta: 0.065259 Total: 0.132574
35: 5(C) 12(C) Alpha: 0.593770 Beta: 0.593068 Total: 1.186838
36: 5(C) 27(C) Alpha: 0.056842 Beta: 0.055241 Total: 0.112083
37: 6(S) 7(S) Alpha: 0.074075 Beta: 0.098122 Total: 0.172197
38: 6(S) 12(C) Alpha: 0.059648 Beta: 0.063406 Total: 0.123053
39: 6(S) 27(C) Alpha: 0.025256 Beta: 0.032529 Total: 0.057785
40: 7(S) 8(C) Alpha: 0.637229 Beta: 0.622451 Total: 1.259681
41: 7(S) 9(C) Alpha: 0.075985 Beta: 0.074894 Total: 0.150879
42: 7(S) 20(C) Alpha: 0.070049 Beta: 0.069150 Total: 0.139198
43: 8(C) 9(C) Alpha: 0.646141 Beta: 0.647406 Total: 1.293547
44: 8(C) 20(C) Alpha: 0.705671 Beta: 0.713571 Total: 1.419242
45: 8(C) 21(C) Alpha: 0.067651 Beta: 0.068151 Total: 0.135801
46: 8(C) 22(C) Alpha: 0.058061 Beta: 0.059401 Total: 0.117462
47: 8(C) 23(C) Alpha: 0.058751 Beta: 0.059650 Total: 0.118401
48: 8(C) 32(H) Alpha: 0.040267 Beta: 0.040434 Total: 0.080701
49: 9(C) 20(C) Alpha: 0.058566 Beta: 0.058678 Total: 0.117244
50: 9(C) 21(C) Alpha: 0.053693 Beta: 0.054789 Total: 0.108483
51: 9(C) 22(C) Alpha: 0.064861 Beta: 0.064785 Total: 0.129645
52: 9(C) 23(C) Alpha: 0.655309 Beta: 0.657327 Total: 1.312636
53: 9(C) 35(H) Alpha: 0.035960 Beta: 0.035971 Total: 0.071930
54: 10(S) 11(C) Alpha: 0.620419 Beta: 0.612860 Total: 1.233280
55: 10(S) 12(C) Alpha: 0.074798 Beta: 0.074157 Total: 0.148955
56: 10(S) 13(C) Alpha: 0.046540 Beta: 0.046774 Total: 0.093314
57: 10(S) 24(C) Alpha: 0.067621 Beta: 0.068249 Total: 0.135870
58: 11(C) 12(C) Alpha: 0.645654 Beta: 0.641776 Total: 1.287430
59: 11(C) 24(C) Alpha: 0.710508 Beta: 0.714926 Total: 1.425435
60: 11(C) 25(C) Alpha: 0.068147 Beta: 0.068784 Total: 0.136931
61: 11(C) 26(C) Alpha: 0.059264 Beta: 0.057183 Total: 0.116447
62: 11(C) 27(C) Alpha: 0.058019 Beta: 0.058976 Total: 0.116995
63: 11(C) 36(H) Alpha: 0.040203 Beta: 0.040363 Total: 0.080566
64: 12(C) 24(C) Alpha: 0.059465 Beta: 0.059345 Total: 0.118810
65: 12(C) 25(C) Alpha: 0.054651 Beta: 0.053386 Total: 0.108037

66: 12(C) 26(C) Alpha: 0.065933 Beta: 0.065947 Total: 0.131880
67: 12(C) 27(C) Alpha: 0.666880 Beta: 0.660337 Total: 1.327218
68: 12(C) 39(H) Alpha: 0.038541 Beta: 0.038363 Total: 0.076904
69: 13(C) 14(C) Alpha: 0.688215 Beta: 0.685786 Total: 1.374001
70: 13(C) 15(C) Alpha: 0.067181 Beta: 0.067237 Total: 0.134418
71: 13(C) 16(C) Alpha: 0.063374 Beta: 0.063367 Total: 0.126741
72: 13(C) 17(C) Alpha: 0.067147 Beta: 0.067201 Total: 0.134348
73: 13(C) 18(C) Alpha: 0.687819 Beta: 0.685246 Total: 1.373066
74: 13(C) 28(H) Alpha: 0.038389 Beta: 0.038419 Total: 0.076808
75: 13(C) 31(H) Alpha: 0.038398 Beta: 0.038432 Total: 0.076831
76: 14(C) 15(C) Alpha: 0.727856 Beta: 0.727311 Total: 1.455167
77: 14(C) 16(C) Alpha: 0.071601 Beta: 0.071630 Total: 0.143232
78: 14(C) 17(C) Alpha: 0.066310 Beta: 0.066369 Total: 0.132679
79: 14(C) 18(C) Alpha: 0.062565 Beta: 0.062074 Total: 0.124639
80: 14(C) 28(H) Alpha: 0.422636 Beta: 0.422702 Total: 0.845338
81: 14(C) 29(H) Alpha: 0.041163 Beta: 0.041053 Total: 0.082216
82: 15(C) 16(C) Alpha: 0.699109 Beta: 0.699085 Total: 1.398194
83: 15(C) 17(C) Alpha: 0.064193 Beta: 0.064134 Total: 0.128327
84: 15(C) 18(C) Alpha: 0.066427 Beta: 0.066516 Total: 0.132943
85: 15(C) 19(F) Alpha: 0.070037 Beta: 0.070035 Total: 0.140072
86: 15(C) 28(H) Alpha: 0.039169 Beta: 0.039166 Total: 0.078335
87: 15(C) 29(H) Alpha: 0.430770 Beta: 0.430586 Total: 0.861356
88: 16(C) 17(C) Alpha: 0.698553 Beta: 0.698458 Total: 1.397011
89: 16(C) 18(C) Alpha: 0.071626 Beta: 0.071668 Total: 0.143294
90: 16(C) 19(F) Alpha: 0.681884 Beta: 0.681960 Total: 1.363844
91: 16(C) 29(H) Alpha: 0.040926 Beta: 0.040915 Total: 0.081841
92: 16(C) 30(H) Alpha: 0.040913 Beta: 0.040899 Total: 0.081811
93: 17(C) 18(C) Alpha: 0.728686 Beta: 0.728161 Total: 1.456846
94: 17(C) 19(F) Alpha: 0.069971 Beta: 0.069960 Total: 0.139931
95: 17(C) 30(H) Alpha: 0.430787 Beta: 0.430578 Total: 0.861366
96: 17(C) 31(H) Alpha: 0.039163 Beta: 0.039162 Total: 0.078324
97: 18(C) 30(H) Alpha: 0.041192 Beta: 0.041085 Total: 0.082277
98: 18(C) 31(H) Alpha: 0.422516 Beta: 0.422581 Total: 0.845097

99: 20(C) 21(C) Alpha: 0.751261 Beta: 0.740265 Total: 1.491525
100: 20(C) 22(C) Alpha: 0.064678 Beta: 0.064388 Total: 0.129067
101: 20(C) 23(C) Alpha: 0.067288 Beta: 0.063740 Total: 0.131027
102: 20(C) 32(H) Alpha: 0.432326 Beta: 0.432681 Total: 0.865007
103: 20(C) 33(H) Alpha: 0.041821 Beta: 0.041602 Total: 0.083423
104: 21(C) 22(C) Alpha: 0.706793 Beta: 0.710381 Total: 1.417174
105: 21(C) 23(C) Alpha: 0.064758 Beta: 0.065954 Total: 0.130712
106: 21(C) 32(H) Alpha: 0.040703 Beta: 0.040550 Total: 0.081253
107: 21(C) 33(H) Alpha: 0.437875 Beta: 0.436999 Total: 0.874874
108: 21(C) 34(H) Alpha: 0.040305 Beta: 0.040413 Total: 0.080718
109: 22(C) 23(C) Alpha: 0.758172 Beta: 0.752959 Total: 1.511132
110: 22(C) 33(H) Alpha: 0.040500 Beta: 0.040560 Total: 0.081060
111: 22(C) 34(H) Alpha: 0.436293 Beta: 0.436691 Total: 0.872984
112: 22(C) 35(H) Alpha: 0.040497 Beta: 0.040379 Total: 0.080877
113: 23(C) 34(H) Alpha: 0.042517 Beta: 0.042465 Total: 0.084982
114: 23(C) 35(H) Alpha: 0.418083 Beta: 0.417223 Total: 0.835307
115: 24(C) 25(C) Alpha: 0.746471 Beta: 0.738308 Total: 1.484779
116: 24(C) 26(C) Alpha: 0.063737 Beta: 0.063113 Total: 0.126851
117: 24(C) 27(C) Alpha: 0.066325 Beta: 0.063606 Total: 0.129931
118: 24(C) 36(H) Alpha: 0.432739 Beta: 0.433549 Total: 0.866288
119: 24(C) 37(H) Alpha: 0.041598 Beta: 0.041411 Total: 0.083009
120: 25(C) 26(C) Alpha: 0.712171 Beta: 0.705387 Total: 1.417558
121: 25(C) 27(C) Alpha: 0.064066 Beta: 0.066116 Total: 0.130182
122: 25(C) 36(H) Alpha: 0.040580 Beta: 0.040512 Total: 0.081092
123: 25(C) 37(H) Alpha: 0.438759 Beta: 0.437000 Total: 0.875759
124: 25(C) 38(H) Alpha: 0.040500 Beta: 0.040449 Total: 0.080949
125: 26(C) 27(C) Alpha: 0.756857 Beta: 0.761491 Total: 1.518348
126: 26(C) 37(H) Alpha: 0.040508 Beta: 0.040362 Total: 0.080869
127: 26(C) 38(H) Alpha: 0.437088 Beta: 0.437813 Total: 0.874901
128: 26(C) 39(H) Alpha: 0.040745 Beta: 0.040805 Total: 0.081550
129: 27(C) 38(H) Alpha: 0.042237 Beta: 0.042416 Total: 0.084653
130: 27(C) 39(H) Alpha: 0.430744 Beta: 0.429148 Total: 0.859892

6.23 Wiberg bond orders of **7**$^{\bullet+}$ extracted by multiwfn (B3LYP/6-311++G**, IEFPCM CH_2Cl_2)

Bond orders with absolute value >= 0.050000

1: 1(C) 2(C) Alpha: 0.776553 Beta: 0.660965 Total: 1.437518
2: 1(C) 3(N) Alpha: 0.055308 Beta: 0.036663 Total: 0.091971
3: 1(C) 5(C) Alpha: 0.032086 Beta: 0.043031 Total: 0.075117
4: 1(C) 6(S) Alpha: 0.588399 Beta: 0.696199 Total: 1.284597
5: 1(C) 20(C) Alpha: 0.597833 Beta: 0.595101 Total: 1.192934
6: 1(C) 21(C) Alpha: 0.052308 Beta: 0.051204 Total: 0.103512
7: 1(C) 22(S) Alpha: 0.080631 Beta: 0.063423 Total: 0.144054
8: 1(C) 23(C) Alpha: 0.042535 Beta: 0.041379 Total: 0.083914
9: 2(C) 3(N) Alpha: 0.594297 Beta: 0.671079 Total: 1.265376
10: 2(C) 4(C) Alpha: 0.040619 Beta: 0.057223 Total: 0.097842
11: 2(C) 6(S) Alpha: 0.055780 Beta: 0.042424 Total: 0.098204
12: 2(C) 7(C) Alpha: 0.039806 Beta: 0.042858 Total: 0.082664
13: 2(C) 20(C) Alpha: 0.060729 Beta: 0.056731 Total: 0.117460
14: 2(C) 21(C) Alpha: 0.056377 Beta: 0.045020 Total: 0.101397
15: 2(C) 22(S) Alpha: 0.636526 Beta: 0.638090 Total: 1.274616
16: 3(N) 4(C) Alpha: 0.594297 Beta: 0.671079 Total: 1.265376
17: 3(N) 5(C) Alpha: 0.055308 Beta: 0.036663 Total: 0.091971
18: 3(N) 6(S) Alpha: 0.014616 Beta: 0.039351 Total: 0.053967
19: 3(N) 7(C) Alpha: 0.508361 Beta: 0.494804 Total: 1.003165
20: 3(N) 8(C) Alpha: 0.036418 Beta: 0.033349 Total: 0.069767
21: 3(N) 12(C) Alpha: 0.036418 Beta: 0.033349 Total: 0.069767
22: 3(N) 15(S) Alpha: 0.035287 Beta: 0.046544 Total: 0.081831
23: 3(N) 22(S) Alpha: 0.035287 Beta: 0.046544 Total: 0.081831
24: 4(C) 5(C) Alpha: 0.776553 Beta: 0.660965 Total: 1.437518
25: 4(C) 6(S) Alpha: 0.055780 Beta: 0.042424 Total: 0.098204
26: 4(C) 7(C) Alpha: 0.039806 Beta: 0.042858 Total: 0.082664
27: 4(C) 13(C) Alpha: 0.056377 Beta: 0.045020 Total: 0.101397
28: 4(C) 14(C) Alpha: 0.060729 Beta: 0.056731 Total: 0.117460
29: 4(C) 15(S) Alpha: 0.636526 Beta: 0.638090 Total: 1.274616

30: 5(C) 6(S) Alpha: 0.588399 Beta: 0.696199 Total: 1.284598
31: 5(C) 13(C) Alpha: 0.052308 Beta: 0.051204 Total: 0.103512
32: 5(C) 14(C) Alpha: 0.597833 Beta: 0.595101 Total: 1.192934
33: 5(C) 15(S) Alpha: 0.080631 Beta: 0.063423 Total: 0.144054
34: 5(C) 19(C) Alpha: 0.042535 Beta: 0.041379 Total: 0.083914
35: 6(S) 14(C) Alpha: 0.038041 Beta: 0.042043 Total: 0.080084
36: 6(S) 20(C) Alpha: 0.038041 Beta: 0.042043 Total: 0.080084
37: 7(C) 8(C) Alpha: 0.699754 Beta: 0.697407 Total: 1.397161
38: 7(C) 9(C) Alpha: 0.053977 Beta: 0.054057 Total: 0.108034
39: 7(C) 10(C) Alpha: 0.048674 Beta: 0.048663 Total: 0.097337
40: 7(C) 11(C) Alpha: 0.053975 Beta: 0.054055 Total: 0.108029
41: 7(C) 12(C) Alpha: 0.699751 Beta: 0.697400 Total: 1.397151
42: 7(C) 27(H) Alpha: 0.034000 Beta: 0.034018 Total: 0.068018
43: 7(C) 30(H) Alpha: 0.033999 Beta: 0.034016 Total: 0.068015
44: 8(C) 9(C) Alpha: 0.725329 Beta: 0.724794 Total: 1.450123
45: 8(C) 10(C) Alpha: 0.057267 Beta: 0.057306 Total: 0.114572
46: 8(C) 11(C) Alpha: 0.052993 Beta: 0.053076 Total: 0.106069
47: 8(C) 12(C) Alpha: 0.050761 Beta: 0.050496 Total: 0.101258
48: 8(C) 27(H) Alpha: 0.457652 Beta: 0.457659 Total: 0.915311
49: 8(C) 28(H) Alpha: 0.034640 Beta: 0.034510 Total: 0.069150
50: 9(C) 10(C) Alpha: 0.711270 Beta: 0.711226 Total: 1.422496
51: 9(C) 11(C) Alpha: 0.052529 Beta: 0.052451 Total: 0.104980
52: 9(C) 12(C) Alpha: 0.052999 Beta: 0.053082 Total: 0.106081
53: 9(C) 27(H) Alpha: 0.034298 Beta: 0.034287 Total: 0.068585
54: 9(C) 28(H) Alpha: 0.457822 Beta: 0.457659 Total: 0.915481
55: 9(C) 39(F) Alpha: 0.045351 Beta: 0.045351 Total: 0.090702
56: 10(C) 11(C) Alpha: 0.711281 Beta: 0.711237 Total: 1.422518
57: 10(C) 12(C) Alpha: 0.057269 Beta: 0.057308 Total: 0.114578
58: 10(C) 28(H) Alpha: 0.035929 Beta: 0.035917 Total: 0.071847
59: 10(C) 29(H) Alpha: 0.035929 Beta: 0.035917 Total: 0.071847
60: 10(C) 39(F) Alpha: 0.680732 Beta: 0.680816 Total: 1.361548
61: 11(C) 12(C) Alpha: 0.725329 Beta: 0.724792 Total: 1.450121
62: 11(C) 29(H) Alpha: 0.457821 Beta: 0.457658 Total: 0.915478

63: 11(C) 30(H) Alpha: 0.034298 Beta: 0.034287 Total: 0.068586
64: 11(C) 39(F) Alpha: 0.045352 Beta: 0.045351 Total: 0.090702
65: 12(C) 29(H) Alpha: 0.034641 Beta: 0.034510 Total: 0.069151
66: 12(C) 30(H) Alpha: 0.457653 Beta: 0.457660 Total: 0.915313
67: 13(C) 14(C) Alpha: 0.647980 Beta: 0.645468 Total: 1.293448
68: 13(C) 15(S) Alpha: 0.608922 Beta: 0.600106 Total: 1.209028
69: 13(C) 16(C) Alpha: 0.708814 Beta: 0.713930 Total: 1.422745
70: 13(C) 17(C) Alpha: 0.053808 Beta: 0.054718 Total: 0.108526
71: 13(C) 18(C) Alpha: 0.045351 Beta: 0.043849 Total: 0.089201
72: 13(C) 19(C) Alpha: 0.045545 Beta: 0.046447 Total: 0.091992
73: 13(C) 31(H) Alpha: 0.033899 Beta: 0.034076 Total: 0.067975
74: 14(C) 15(S) Alpha: 0.055643 Beta: 0.055060 Total: 0.110704
75: 14(C) 16(C) Alpha: 0.047988 Beta: 0.047838 Total: 0.095826
76: 14(C) 17(C) Alpha: 0.041425 Beta: 0.040559 Total: 0.081984
77: 14(C) 18(C) Alpha: 0.052873 Beta: 0.052765 Total: 0.105638
78: 14(C) 19(C) Alpha: 0.667611 Beta: 0.662857 Total: 1.330468
79: 14(C) 34(H) Alpha: 0.032935 Beta: 0.032766 Total: 0.065701
80: 15(S) 16(C) Alpha: 0.045696 Beta: 0.046004 Total: 0.091700
81: 16(C) 17(C) Alpha: 0.738884 Beta: 0.730137 Total: 1.469022
82: 16(C) 18(C) Alpha: 0.049629 Beta: 0.048963 Total: 0.098592
83: 16(C) 19(C) Alpha: 0.053647 Beta: 0.050757 Total: 0.104404
84: 16(C) 31(H) Alpha: 0.457006 Beta: 0.457802 Total: 0.914808
85: 16(C) 32(H) Alpha: 0.034814 Beta: 0.034590 Total: 0.069404
86: 17(C) 18(C) Alpha: 0.703199 Beta: 0.698034 Total: 1.401234
87: 17(C) 19(C) Alpha: 0.050017 Beta: 0.052124 Total: 0.102141
88: 17(C) 31(H) Alpha: 0.034036 Beta: 0.033962 Total: 0.067998
89: 17(C) 32(H) Alpha: 0.462064 Beta: 0.460333 Total: 0.922396
90: 17(C) 33(H) Alpha: 0.033361 Beta: 0.033343 Total: 0.066704
91: 18(C) 19(C) Alpha: 0.750329 Beta: 0.753513 Total: 1.503842
92: 18(C) 32(H) Alpha: 0.033369 Beta: 0.033230 Total: 0.066599
93: 18(C) 33(H) Alpha: 0.460531 Beta: 0.461263 Total: 0.921793
94: 18(C) 34(H) Alpha: 0.034901 Beta: 0.034918 Total: 0.069820
95: 19(C) 33(H) Alpha: 0.035422 Beta: 0.035583 Total: 0.071005

96: 19(C) 34(H) Alpha: 0.457362 Beta: 0.455731 Total: 0.913094
97: 20(C) 21(C) Alpha: 0.647980 Beta: 0.645468 Total: 1.293448
98: 20(C) 22(S) Alpha: 0.055643 Beta: 0.055060 Total: 0.110704
99: 20(C) 23(C) Alpha: 0.667611 Beta: 0.662857 Total: 1.330468
100: 20(C) 24(C) Alpha: 0.052873 Beta: 0.052765 Total: 0.105638
101: 20(C) 25(C) Alpha: 0.041425 Beta: 0.040559 Total: 0.081984
102: 20(C) 26(C) Alpha: 0.047988 Beta: 0.047838 Total: 0.095826
103: 20(C) 35(H) Alpha: 0.032935 Beta: 0.032766 Total: 0.065701
104: 21(C) 22(S) Alpha: 0.608922 Beta: 0.600106 Total: 1.209028
105: 21(C) 23(C) Alpha: 0.045545 Beta: 0.046447 Total: 0.091992
106: 21(C) 24(C) Alpha: 0.045351 Beta: 0.043849 Total: 0.089201
107: 21(C) 25(C) Alpha: 0.053808 Beta: 0.054718 Total: 0.108527
108: 21(C) 26(C) Alpha: 0.708814 Beta: 0.713930 Total: 1.422744
109: 21(C) 38(H) Alpha: 0.033899 Beta: 0.034076 Total: 0.067975
110: 22(S) 26(C) Alpha: 0.045695 Beta: 0.046004 Total: 0.091700
111: 23(C) 24(C) Alpha: 0.750329 Beta: 0.753513 Total: 1.503842
112: 23(C) 25(C) Alpha: 0.050017 Beta: 0.052124 Total: 0.102141
113: 23(C) 26(C) Alpha: 0.053647 Beta: 0.050757 Total: 0.104404
114: 23(C) 35(H) Alpha: 0.457362 Beta: 0.455731 Total: 0.913094
115: 23(C) 36(H) Alpha: 0.035422 Beta: 0.035583 Total: 0.071005
116: 24(C) 25(C) Alpha: 0.703199 Beta: 0.698034 Total: 1.401233
117: 24(C) 26(C) Alpha: 0.049629 Beta: 0.048963 Total: 0.098592
118: 24(C) 35(H) Alpha: 0.034901 Beta: 0.034918 Total: 0.069820
119: 24(C) 36(H) Alpha: 0.460531 Beta: 0.461263 Total: 0.921793
120: 24(C) 37(H) Alpha: 0.033369 Beta: 0.033230 Total: 0.066599
121: 25(C) 26(C) Alpha: 0.738885 Beta: 0.730138 Total: 1.469023
122: 25(C) 36(H) Alpha: 0.033361 Beta: 0.033343 Total: 0.066704
123: 25(C) 37(H) Alpha: 0.462063 Beta: 0.460333 Total: 0.922396
124: 25(C) 38(H) Alpha: 0.034036 Beta: 0.033962 Total: 0.067998
125: 26(C) 37(H) Alpha: 0.034814 Beta: 0.034591 Total: 0.069404
126: 26(C) 38(H) Alpha: 0.457006 Beta: 0.457802 Total: 0.914808

6.24 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(0) calculation of compound **5**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	1.31222	2.16806	0.00008
C	0	1.22095	0.74156	-0.00002
N	0	-0.00002	0.1142	0.00000
C	0	-1.22103	0.74148	0.00002
C	0	-1.31239	2.16798	-0.00008
S	0	-0.00012	3.24341	0.00000
C	0	-2.54542	0.13881	0.00009
C	0	-3.54865	1.14093	-0.00006
S	0	-2.91116	2.78037	-0.00021
S	0	2.91097	2.78055	0.00021
C	0	3.54855	1.14114	0.00006
C	0	2.54537	0.13897	-0.00009
C	0	0.00005	-1.34835	0.00000
C	0	4.90767	0.86524	0.00006
C	0	5.30128	-0.4692	-0.00013
C	0	4.34354	-1.4884	-0.00032
C	0	2.98754	-1.20448	-0.00029
C	0	-2.98753	-1.20466	0.00029
C	0	-4.34351	-1.48865	0.00032
C	0	-5.30131	-0.4695	0.00012
C	0	-4.90776	0.86496	-0.00006
C	0	0.00028	-2.01526	1.22084
C	0	0.00035	-3.40642	1.22055
C	0	0.00021	-4.0698	0.00000
C	0	-0.00001	-3.40642	-1.22055
C	0	-0.00009	-2.01526	-1.22084
F	0	0.00028	-5.41493	0.00000
H	0	5.63966	1.66314	0.00019

H	0	6.35593	-0.71464	-0.00014
H	0	4.66135	-2.52309	-0.00049
H	0	2.29657	-2.0274	-0.00045
H	0	-2.29652	-2.02755	0.00045
H	0	-4.66127	-2.52335	0.00048
H	0	-6.35594	-0.71499	0.00013
H	0	-5.63979	1.66282	-0.0002
H	0	0.00038	-1.46488	2.15326
H	0	0.00052	-3.96792	2.14536
H	0	-0.00011	-3.96792	-2.14536
H	0	-0.00024	-1.46488	-2.15326
Bq	0	-0.00006	1.52945	0.00000
Bq	0	-2.30773	1.39392	-0.00005
Bq	0	2.30761	1.39406	0.00005
Bq	0	-3.93903	-0.16969	0.00012
Bq	0	3.93899	-0.16945	-0.00012

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 8.6242 Anisotropy = 187.2544

XX= -33.1425 YX= 2.0694 ZX= -0.0141

XY= 0.4810 YY= -74.4453 ZY= -0.0077

XZ= 0.0001 YZ= -0.0095 ZZ= 133.4605

Eigenvalues: -74.4847 -33.1032 133.4605

2 C Isotropic = 34.1300 Anisotropy = 124.7825

XX= -10.3885 YX= 8.4820 ZX= 0.0071

XY= 6.4837 YY= -4.5398 ZY= -0.0065

XZ= -0.0001 YZ= -0.0059 ZZ= 117.3183

Eigenvalues: -15.4981 0.5698 117.3183

3 N Isotropic = 28.5597 Anisotropy = 226.1142

XX= -40.6105 YX= 0.0004 ZX= 0.0064

XY= 0.0022 YY= -53.0129 ZY= -0.0000

XZ= 0.0056 YZ= -0.0001 ZZ= 179.3025

Eigenvalues: -53.0129 -40.6105 179.3025

4 C Isotropic = 34.1301 Anisotropy = 124.7822

XX= -10.3872 YX= -8.4813 ZX= 0.0070

XY= -6.4834 YY= -4.5406 ZY= 0.0064

XZ= -0.0001 YZ= 0.0057 ZZ= 117.3183

Eigenvalues: -15.4971 0.5692 117.3183

5 C Isotropic = 8.6239 Anisotropy = 187.2538

XX= -33.1436 YX= -2.0672 ZX= -0.0140

XY= -0.4778 YY= -74.4445 ZY= 0.0075

XZ= 0.0001 YZ= 0.0092 ZZ= 133.4597

Eigenvalues: -74.4837 -33.1044 133.4597

6 S Isotropic = 169.5480 Anisotropy = 506.6246

XX= 65.0317 YX= 0.0035 ZX= -0.0314

XY= 0.0089 YY= -63.6854 ZY= -0.0001

XZ= -0.0504 YZ= 0.0001 ZZ= 507.2977

Eigenvalues: -63.6854 65.0316 507.2977

7 C Isotropic = 53.0795 Anisotropy = 140.4270

XX= -23.4751 YX= -5.4889 ZX= 0.0007

XY= -6.4631 YY= 36.0161 ZY= 0.0172

XZ= -0.0099 YZ= 0.0128 ZZ= 146.6975

Eigenvalues: -24.0695 36.6105 146.6975

8 C Isotropic = 33.4447 Anisotropy = 133.2856

XX= 19.8152 YX= -14.7625 ZX= -0.0040

XY= -13.9488 YY= -41.7829 ZY= 0.0172

XZ= 0.0137 YZ= 0.0150 ZZ= 122.3018

Eigenvalues: -44.9642 22.9966 122.3018

9 S Isotropic = 216.3211 Anisotropy = 247.2318

XX= 270.1146 YX= 33.8050 ZX= -0.0060

XY= 22.5303 YY= -2.2937 ZY= 0.0345

XZ= 0.0009 YZ= 0.0107 ZZ= 381.1422

Eigenvalues: -5.1758 272.9967 381.1422

10 S Isotropic = 216.3197 Anisotropy = 247.2272

XX= 270.1166 YX= -33.7865 ZX= -0.0060

XY= -22.5124 YY= -2.2953 ZY= -0.0349

XZ= 0.0011 YZ= -0.0110 ZZ= 381.1378

Eigenvalues: -5.1737 272.9950 381.1378

11 C Isotropic = 33.4448 Anisotropy = 133.2842

XX= 19.8148 YX= 14.7654 ZX= -0.0040

XY= 13.9535 YY= -41.7813 ZY= -0.0175

XZ= 0.0139 YZ= -0.0153 ZZ= 122.3010

Eigenvalues: -44.9644 22.9979 122.3010

12 C Isotropic = 53.0799 Anisotropy = 140.4251

XX= -23.4755 YX= 5.4874 ZX= 0.0007

XY= 6.4590 YY= 36.0186 ZY= -0.0173

XZ= -0.0098 YZ= -0.0129 ZZ= 146.6966

Eigenvalues: -24.0693 36.6124 146.6966

13 C Isotropic = 42.0407 Anisotropy = 109.2846

XX= 114.8971 YX= 0.0097 ZX= -0.0061

XY= 0.0092 YY= -56.2555 ZY= 0.0001

XZ= -0.0092 YZ= -0.0000 ZZ= 67.4805

Eigenvalues: -56.2555 67.4805 114.8971

14 C Isotropic = 50.8192 Anisotropy = 181.0659

XX= -10.8204 YX= -38.8240 ZX= -0.0108

XY= -37.6150 YY= -8.2518 ZY= -0.0264

XZ= -0.0082 YZ= -0.0237 ZZ= 171.5298

Eigenvalues: -47.7771 28.7050 171.5298

15 C Isotropic = 32.5389 Anisotropy = 215.2410

XX= -72.0932 YX= 17.8435 ZX= -0.0043

XY= 11.8839 YY= -6.3231 ZY= -0.0280

XZ= -0.0036 YZ= -0.0316 ZZ= 176.0328

Eigenvalues: -75.2963 -3.1199 176.0328

16 C Isotropic = 44.7228 Anisotropy = 198.8607

XX= 17.8056 YX= 22.7231 ZX= 0.0002

XY= 22.3566 YY= -60.9338 ZY= -0.0391

XZ= 0.0018 YZ= -0.0359 ZZ= 177.2966

Eigenvalues: -66.9295 23.8013 177.2966

17 C Isotropic = 45.2898 Anisotropy = 187.3520

XX= 4.4418 YX= -32.4804 ZX= -0.0110

XY= -24.0553 YY= -38.7636 ZY= -0.0353

XZ= -0.0156 YZ= -0.0307 ZZ= 170.1911

Eigenvalues: -52.7382 18.4165 170.1911

18 C Isotropic = 45.2912 Anisotropy = 187.3534

XX= 4.4393 YX= 32.4834 ZX= -0.0111

XY= 24.0578 YY= -38.7591 ZY= 0.0352

XZ= -0.0158 YZ= 0.0305 ZZ= 170.1935

Eigenvalues: -52.7373 18.4175 170.1935

19 C Isotropic = 44.7224 Anisotropy = 198.8607

XX= 17.8080 YX= -22.7195 ZX= 0.0001

XY= -22.3525 YY= -60.9370 ZY= 0.0389

XZ= 0.0016 YZ= 0.0357 ZZ= 177.2961

Eigenvalues: -66.9304 23.8014 177.2962

20 C Isotropic = 32.5391 Anisotropy = 215.2415

XX= -72.0918 YX= -17.8465 ZX= -0.0045

XY= -11.8868 YY= -6.3243 ZY= 0.0279

XZ= -0.0037 YZ= 0.0315 ZZ= 176.0334

Eigenvalues: -75.2962 -3.1198 176.0334

21 C Isotropic = 50.8193 Anisotropy = 181.0662

XX= -10.8249 YX= 38.8249 ZX= -0.0109

XY= 37.6153 YY= -8.2472 ZY= 0.0262

XZ= -0.0083 YZ= 0.0236 ZZ= 171.5301

Eigenvalues: -47.7779 28.7057 171.5301

22 C Isotropic = 55.5242 Anisotropy = 168.0419

XX= 167.5521 YX= 0.0035 ZX= -0.0260

XY= 0.0059 YY= 17.3872 ZY= -30.0529

XZ= -0.0264 YZ= -14.9487 ZZ= -18.3668

Eigenvalues: -29.2278 28.2482 167.5521

23 C Isotropic = 51.0896 Anisotropy = 174.9540

XX= 167.7256 YX= 0.0131 ZX= -0.0278

XY= 0.0120 YY= 11.6454 ZY= 27.2136

XZ= -0.0295 YZ= 20.2064 ZZ= -26.1022

Eigenvalues: -37.5333 23.0765 167.7256

24 C Isotropic = 4.8956 Anisotropy = 119.4877

XX= 84.5540 YX= 0.0080 ZX= -0.0100

XY= 0.0091 YY= -81.0886 ZY= -0.0000

XZ= -0.0106 YZ= -0.0000 ZZ= 11.2213

Eigenvalues: -81.0886 11.2213 84.5540

25 C Isotropic = 51.0897 Anisotropy = 174.9539

XX= 167.7257 YX= 0.0047 ZX= -0.0247

XY= 0.0054 YY= 11.6454 ZY= -27.2137

XZ= -0.0264 YZ= -20.2064 ZZ= -26.1018

Eigenvalues: -37.5330 23.0765 167.7257

26 C Isotropic = 55.5243 Anisotropy = 168.0420

XX= 167.5523 YX= 0.0136 ZX= -0.0296

XY= 0.0111 YY= 17.3873 ZY= 30.0528

XZ= -0.0259 YZ= 14.9488 ZZ= -18.3666

Eigenvalues: -29.2276 28.2483 167.5523

27 F Isotropic = 249.6607 Anisotropy = 151.1915

XX= 350.4551 YX= 0.0049 ZX= -0.0302

XY= 0.0052 YY= 254.7321 ZY= 0.0000

XZ= -0.0307 YZ= -0.0001 ZZ= 143.7951

Eigenvalues: 143.7951 254.7321 350.4551

28 H Isotropic = 23.4031 Anisotropy = 8.1994

XX= 27.7961 YX= -2.1996 ZX= -0.0001

XY= -2.2052 YY= 24.3500 ZY= 0.0004

XZ= -0.0000 YZ= 0.0008 ZZ= 18.0632

Eigenvalues: 18.0632 23.2767 28.8693

29 H Isotropic = 23.1534 Anisotropy = 5.3074

XX= 23.8742 YX= 0.8495 ZX= 0.0003

XY= 0.6131 YY= 26.5019 ZY= 0.0011

XZ= 0.0001 YZ= 0.0009 ZZ= 19.0842

Eigenvalues: 19.0842 23.6844 26.6917

30 H Isotropic = 23.8128 Anisotropy = 8.8338

XX= 29.6233 YX= 0.8638 ZX= 0.0001

XY= 0.5840 YY= 23.0437 ZY= 0.0002

XZ= -0.0006 YZ= 0.0010 ZZ= 18.7714

Eigenvalues: 18.7714 22.9650 29.7020

31 H Isotropic = 25.3600 Anisotropy = 18.1124

XX= 37.4239 YX= 1.2592 ZX= -0.0026

XY= -2.0452 YY= 23.4164 ZY= 0.0004

XZ= -0.0023 YZ= 0.0006 ZZ= 15.2397

Eigenvalues: 15.2397 23.4054 37.4350

32 H Isotropic = 25.3596 Anisotropy = 18.1112

XX= 37.4226 YX= -1.2578 ZX= -0.0026

XY= 2.0463 YY= 23.4163 ZY= -0.0004

XZ= -0.0022 YZ= -0.0006 ZZ= 15.2397

Eigenvalues: 15.2397 23.4052 37.4337

33 H Isotropic = 23.8127 Anisotropy = 8.8335

XX= 29.6231 YX= -0.8635 ZX= 0.0001

XY= -0.5835 YY= 23.0437 ZY= -0.0002

XZ= -0.0006 YZ= -0.0010 ZZ= 18.7713

Eigenvalues: 18.7713 22.9651 29.7017

34 H Isotropic = 23.1534 Anisotropy = 5.3074

XX= 23.8743 YX= -0.8496 ZX= 0.0003

XY= -0.6131 YY= 26.5019 ZY= -0.0011

XZ= 0.0001 YZ= -0.0009 ZZ= 19.0842

Eigenvalues: 19.0842 23.6844 26.6917

35 H Isotropic = 23.4031 Anisotropy = 8.1995

XX= 27.7959 YX= 2.1999 ZX= -0.0001

XY= 2.2054 YY= 24.3502 ZY= -0.0004

XZ= -0.0000 YZ= -0.0008 ZZ= 18.0633

Eigenvalues: 18.0633 23.2767 28.8694

36 H Isotropic = 24.2921 Anisotropy = 8.6556

XX= 21.8309 YX= -0.0006 ZX= 0.0004

XY= 0.0002 YY= 26.6324 ZY= -2.4213

XZ= 0.0002 YZ= -6.3828 ZZ= 24.4130

Eigenvalues: 20.9830 21.8309 30.0625

37 H Isotropic = 23.4843 Anisotropy = 4.4620

XX= 21.0119 YX= -0.0001 ZX= 0.0004

XY= 0.0001 YY= 26.4563 ZY= 1.1252

XZ= 0.0001 YZ= -0.9303 ZZ= 22.9848

Eigenvalues: 21.0119 22.9820 26.4590

38 H Isotropic = 23.4843 Anisotropy = 4.4620

XX= 21.0120 YX= -0.0004 ZX= 0.0006

XY= -0.0008 YY= 26.4563 ZY= -1.1252

XZ= 0.0004 YZ= 0.9303 ZZ= 22.9848

Eigenvalues: 21.0120 22.9821 26.4590

39 H Isotropic = 24.2921 Anisotropy = 8.6556

XX= 21.8309 YX= -0.0002 ZX= 0.0002

XY= -0.0009 YY= 26.6324 ZY= 2.4213

XZ= 0.0002 YZ= 6.3828 ZZ= 24.4130

Eigenvalues: 20.9830 21.8309 30.0625

40 Bq Isotropic = 6.9440 Anisotropy = 11.8768

XX= 4.7986 YX= -0.0003 ZX= 0.0004

XY= -0.0002 YY= 14.8619 ZY= 0.0000

XZ= 0.0003 YZ= 0.0000 ZZ= 1.1716

Eigenvalues: 1.1716 4.7986 14.8619

41 Bq Isotropic = 7.2871 Anisotropy = 25.7166

XX= 11.2883 YX= -5.0502 ZX= 0.0013

XY= -4.4695 YY= 22.7077 ZY= -0.0041

XZ= 0.0019 YZ= -0.0027 ZZ= -12.1347

Eigenvalues: -12.1347 9.5645 24.4315

42 Bq Isotropic = 7.2870 Anisotropy = 25.7168

XX= 11.2878 YX= 5.0495 ZX= 0.0013

XY= 4.4691 YY= 22.7082 ZY= 0.0042

XZ= 0.0019 YZ= 0.0028 ZZ= -12.1349

Eigenvalues: -12.1350 9.5645 24.4316

43 Bq Isotropic = 8.1576 Anisotropy = 1.9350

XX= 7.7336 YX= -1.2716 ZX= 0.0000

XY= 0.4783 YY= 7.2917 ZY= -0.0003

XZ= -0.0010 YZ= 0.0005 ZZ= 9.4476

Eigenvalues: 7.0586 7.9667 9.4476

44 Bq Isotropic = 8.1576 Anisotropy = 1.9348

XX= 7.7337 YX= 1.2717 ZX= 0.0000

XY= -0.4782 YY= 7.2917 ZY= 0.0003

XZ= -0.0010 YZ= -0.0005 ZZ= 9.4474

Eigenvalues: 7.0585 7.9668 9.4474

6.25 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(1) calculation of compound **6**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	1.31222	2.16806	0.00008
C	0	1.22095	0.74156	-0.00002
N	0	-0.00002	0.1142	0.
C	0	-1.22103	0.74148	0.00002
C	0	-1.31239	2.16798	-0.00008
S	0	-0.00012	3.24341	0.
C	0	-2.54542	0.13881	0.00009
C	0	-3.54865	1.14093	-0.00006
S	0	-2.91116	2.78037	-0.00021
S	0	2.91097	2.78055	0.00021
C	0	3.54855	1.14114	0.00006
C	0	2.54537	0.13897	-0.00009
C	0	0.00005	-1.34835	0.
C	0	4.90767	0.86524	0.00006
C	0	5.30128	-0.4692	-0.00013
C	0	4.34354	-1.4884	-0.00032
C	0	2.98754	-1.20448	-0.00029
C	0	-2.98753	-1.20466	0.00029
C	0	-4.34351	-1.48865	0.00032
C	0	-5.30131	-0.4695	0.00012

C	0	-4.90776	0.86496	-0.00006
C	0	0.00028	-2.01526	1.22084
C	0	0.00035	-3.40642	1.22055
C	0	0.00021	-4.0698	0.
C	0	-0.00001	-3.40642	-1.22055
C	0	-0.00009	-2.01526	-1.22084
F	0	0.00028	-5.41493	0.
H	0	5.63966	1.66314	0.00019
H	0	6.35593	-0.71464	-0.00014
H	0	4.66135	-2.52309	-0.00049
H	0	2.29657	-2.0274	-0.00045
H	0	-2.29652	-2.02755	0.00045
H	0	-4.66127	-2.52335	0.00048
H	0	-6.35594	-0.71499	0.00013
H	0	-5.63979	1.66282	-0.0002
H	0	0.00038	-1.46488	2.15326
H	0	0.00052	-3.96792	2.14536
H	0	-0.00011	-3.96792	-2.14536
H	0	-0.00024	-1.46488	-2.15326
Bq	0	-0.00005	1.52945	1.
Bq	0	-2.30776	1.39403	0.99995
Bq	0	2.30758	1.39394	1.00005
Bq	0	-3.93904	-0.16955	1.00012
Bq	0	3.93898	-0.16959	0.99988

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 8.6242 Anisotropy = 187.2544

XX= -33.1425 YX= 2.0694 ZX= -0.0141

XY= 0.4810 YY= -74.4453 ZY= -0.0077

XZ= 0.0001 YZ= -0.0095 ZZ= 133.4605

Eigenvalues: -74.4847 -33.1032 133.4605

2 C Isotropic = 34.1300 Anisotropy = 124.7825

XX= -10.3885 YX= 8.4820 ZX= 0.0071

XY= 6.4837 YY= -4.5398 ZY= -0.0065

XZ= -0.0001 YZ= -0.0059 ZZ= 117.3183

Eigenvalues: -15.4981 0.5698 117.3183

3 N Isotropic = 28.5597 Anisotropy = 226.1142

XX= -40.6105 YX= 0.0004 ZX= 0.0064

XY= 0.0022 YY= -53.0129 ZY= -0.0000

XZ= 0.0056 YZ= -0.0001 ZZ= 179.3025

Eigenvalues: -53.0129 -40.6105 179.3025

4 C Isotropic = 34.1301 Anisotropy = 124.7822

XX= -10.3872 YX= -8.4813 ZX= 0.0070

XY= -6.4834 YY= -4.5406 ZY= 0.0064

XZ= -0.0001 YZ= 0.0057 ZZ= 117.3183

Eigenvalues: -15.4971 0.5692 117.3183

5 C Isotropic = 8.6239 Anisotropy = 187.2538

XX= -33.1436 YX= -2.0672 ZX= -0.0140

XY= -0.4778 YY= -74.4445 ZY= 0.0075

XZ= 0.0001 YZ= 0.0092 ZZ= 133.4597

Eigenvalues: -74.4837 -33.1044 133.4597

6 S Isotropic = 169.5480 Anisotropy = 506.6246

XX= 65.0317 YX= 0.0035 ZX= -0.0314

XY= 0.0089 YY= -63.6854 ZY= -0.0001

XZ= -0.0504 YZ= 0.0001 ZZ= 507.2977

Eigenvalues: -63.6854 65.0316 507.2977

7 C Isotropic = 53.0795 Anisotropy = 140.4270

XX= -23.4751 YX= -5.4889 ZX= 0.0007

XY= -6.4631 YY= 36.0161 ZY= 0.0172

XZ= -0.0099 YZ= 0.0128 ZZ= 146.6975

Eigenvalues: -24.0695 36.6105 146.6975

8 C Isotropic = 33.4447 Anisotropy = 133.2856

XX= 19.8152 YX= -14.7625 ZX= -0.0040

XY= -13.9488 YY= -41.7829 ZY= 0.0172

XZ= 0.0137 YZ= 0.0150 ZZ= 122.3018

Eigenvalues: -44.9642 22.9966 122.3018

9 S Isotropic = 216.3211 Anisotropy = 247.2318

XX= 270.1146 YX= 33.8050 ZX= -0.0060

XY= 22.5303 YY= -2.2937 ZY= 0.0345

XZ= 0.0009 YZ= 0.0107 ZZ= 381.1422

Eigenvalues: -5.1758 272.9967 381.1422

10 S Isotropic = 216.3197 Anisotropy = 247.2272

XX= 270.1166 YX= -33.7865 ZX= -0.0060

XY= -22.5124 YY= -2.2953 ZY= -0.0349

XZ= 0.0011 YZ= -0.0110 ZZ= 381.1378

Eigenvalues: -5.1737 272.9950 381.1378

11 C Isotropic = 33.4448 Anisotropy = 133.2842

XX= 19.8148 YX= 14.7654 ZX= -0.0040

XY= 13.9535 YY= -41.7813 ZY= -0.0175

XZ= 0.0139 YZ= -0.0153 ZZ= 122.3010

Eigenvalues: -44.9644 22.9979 122.3010

12 C Isotropic = 53.0799 Anisotropy = 140.4251

XX= -23.4755 YX= 5.4874 ZX= 0.0007

XY= 6.4590 YY= 36.0186 ZY= -0.0173

XZ= -0.0098 YZ= -0.0129 ZZ= 146.6966

Eigenvalues: -24.0693 36.6124 146.6966

13 C Isotropic = 42.0407 Anisotropy = 109.2846

XX= 114.8971 YX= 0.0097 ZX= -0.0061

XY= 0.0092 YY= -56.2555 ZY= 0.0001

XZ= -0.0092 YZ= -0.0000 ZZ= 67.4805

Eigenvalues: -56.2555 67.4805 114.8971

14 C Isotropic = 50.8192 Anisotropy = 181.0659

XX= -10.8204 YX= -38.8240 ZX= -0.0108

XY= -37.6150 YY= -8.2518 ZY= -0.0264

XZ= -0.0082 YZ= -0.0237 ZZ= 171.5298

Eigenvalues: -47.7771 28.7050 171.5298

15 C Isotropic = 32.5389 Anisotropy = 215.2410

XX= -72.0932 YX= 17.8435 ZX= -0.0043

XY= 11.8839 YY= -6.3231 ZY= -0.0280

XZ= -0.0036 YZ= -0.0316 ZZ= 176.0328

Eigenvalues: -75.2963 -3.1199 176.0328

16 C Isotropic = 44.7228 Anisotropy = 198.8607

XX= 17.8056 YX= 22.7231 ZX= 0.0002

XY= 22.3566 YY= -60.9338 ZY= -0.0391

XZ= 0.0018 YZ= -0.0359 ZZ= 177.2966

Eigenvalues: -66.9295 23.8013 177.2966

17 C Isotropic = 45.2898 Anisotropy = 187.3520

XX= 4.4418 YX= -32.4804 ZX= -0.0110

XY= -24.0553 YY= -38.7636 ZY= -0.0353

XZ= -0.0156 YZ= -0.0307 ZZ= 170.1911

Eigenvalues: -52.7382 18.4165 170.1911

18 C Isotropic = 45.2912 Anisotropy = 187.3534

XX= 4.4393 YX= 32.4834 ZX= -0.0111

XY= 24.0578 YY= -38.7591 ZY= 0.0352

XZ= -0.0158 YZ= 0.0305 ZZ= 170.1935

Eigenvalues: -52.7373 18.4175 170.1935

19 C Isotropic = 44.7224 Anisotropy = 198.8607

XX= 17.8080 YX= -22.7195 ZX= 0.0001

XY= -22.3525 YY= -60.9370 ZY= 0.0389

XZ= 0.0016 YZ= 0.0357 ZZ= 177.2961

Eigenvalues: -66.9304 23.8014 177.2962

20 C Isotropic = 32.5391 Anisotropy = 215.2415

XX= -72.0918 YX= -17.8465 ZX= -0.0045

XY= -11.8868 YY= -6.3243 ZY= 0.0279

XZ= -0.0037 YZ= 0.0315 ZZ= 176.0334

Eigenvalues: -75.2962 -3.1198 176.0334

21 C Isotropic = 50.8193 Anisotropy = 181.0662

XX= -10.8249 YX= 38.8249 ZX= -0.0109

XY= 37.6153 YY= -8.2472 ZY= 0.0262

XZ= -0.0083 YZ= 0.0236 ZZ= 171.5301

Eigenvalues: -47.7779 28.7057 171.5301

22 C Isotropic = 55.5242 Anisotropy = 168.0419

XX= 167.5521 YX= 0.0035 ZX= -0.0260

XY= 0.0059 YY= 17.3872 ZY= -30.0529

XZ= -0.0264 YZ= -14.9487 ZZ= -18.3668

Eigenvalues: -29.2278 28.2482 167.5521

23 C Isotropic = 51.0896 Anisotropy = 174.9540

XX= 167.7256 YX= 0.0131 ZX= -0.0278

XY= 0.0120 YY= 11.6454 ZY= 27.2136

XZ= -0.0295 YZ= 20.2064 ZZ= -26.1022

Eigenvalues: -37.5333 23.0765 167.7256

24 C Isotropic = 4.8956 Anisotropy = 119.4877

XX= 84.5540 YX= 0.0080 ZX= -0.0100

XY= 0.0091 YY= -81.0886 ZY= -0.0000

XZ= -0.0106 YZ= -0.0000 ZZ= 11.2213

Eigenvalues: -81.0886 11.2213 84.5540

25 C Isotropic = 51.0897 Anisotropy = 174.9539

XX= 167.7257 YX= 0.0047 ZX= -0.0247

XY= 0.0054 YY= 11.6454 ZY= -27.2137

XZ= -0.0264 YZ= -20.2064 ZZ= -26.1018

Eigenvalues: -37.5330 23.0765 167.7257

26 C Isotropic = 55.5243 Anisotropy = 168.0420

XX= 167.5523 YX= 0.0136 ZX= -0.0296

XY= 0.0111 YY= 17.3873 ZY= 30.0528

XZ= -0.0259 YZ= 14.9488 ZZ= -18.3666

Eigenvalues: -29.2276 28.2483 167.5523

27 F Isotropic = 249.6607 Anisotropy = 151.1915

XX= 350.4551 YX= 0.0049 ZX= -0.0302

XY= 0.0052 YY= 254.7321 ZY= 0.0000

XZ= -0.0307 YZ= -0.0001 ZZ= 143.7951

Eigenvalues: 143.7951 254.7321 350.4551

28 H Isotropic = 23.4031 Anisotropy = 8.1994

XX= 27.7961 YX= -2.1996 ZX= -0.0001

XY= -2.2052 YY= 24.3500 ZY= 0.0004

XZ= -0.0000 YZ= 0.0008 ZZ= 18.0632

Eigenvalues: 18.0632 23.2767 28.8693

29 H Isotropic = 23.1534 Anisotropy = 5.3074

XX= 23.8742 YX= 0.8495 ZX= 0.0003

XY= 0.6131 YY= 26.5019 ZY= 0.0011

XZ= 0.0001 YZ= 0.0009 ZZ= 19.0842

Eigenvalues: 19.0842 23.6844 26.6917

30 H Isotropic = 23.8128 Anisotropy = 8.8338

XX= 29.6233 YX= 0.8638 ZX= 0.0001

XY= 0.5840 YY= 23.0437 ZY= 0.0002

XZ= -0.0006 YZ= 0.0010 ZZ= 18.7714

Eigenvalues: 18.7714 22.9650 29.7020

31 H Isotropic = 25.3600 Anisotropy = 18.1124

XX= 37.4239 YX= 1.2592 ZX= -0.0026

XY= -2.0452 YY= 23.4164 ZY= 0.0004

XZ= -0.0023 YZ= 0.0006 ZZ= 15.2397

Eigenvalues: 15.2397 23.4054 37.4350

32 H Isotropic = 25.3596 Anisotropy = 18.1112

XX= 37.4226 YX= -1.2578 ZX= -0.0026

XY= 2.0463 YY= 23.4163 ZY= -0.0004

XZ= -0.0022 YZ= -0.0006 ZZ= 15.2397

Eigenvalues: 15.2397 23.4052 37.4337

33 H Isotropic = 23.8127 Anisotropy = 8.8335

XX= 29.6231 YX= -0.8635 ZX= 0.0001

XY= -0.5835 YY= 23.0437 ZY= -0.0002

XZ= -0.0006 YZ= -0.0010 ZZ= 18.7713

Eigenvalues: 18.7713 22.9651 29.7017

34 H Isotropic = 23.1534 Anisotropy = 5.3074

XX= 23.8743 YX= -0.8496 ZX= 0.0003

XY= -0.6131 YY= 26.5019 ZY= -0.0011

XZ= 0.0001 YZ= -0.0009 ZZ= 19.0842

Eigenvalues: 19.0842 23.6844 26.6917

35 H Isotropic = 23.4031 Anisotropy = 8.1995

XX= 27.7959 YX= 2.1999 ZX= -0.0001

XY= 2.2054 YY= 24.3502 ZY= -0.0004

XZ= -0.0000 YZ= -0.0008 ZZ= 18.0633

Eigenvalues: 18.0633 23.2767 28.8694

36 H Isotropic = 24.2921 Anisotropy = 8.6556

XX= 21.8309 YX= -0.0006 ZX= 0.0004

XY= 0.0002 YY= 26.6324 ZY= -2.4213

XZ= 0.0002 YZ= -6.3828 ZZ= 24.4130

Eigenvalues: 20.9830 21.8309 30.0625

37 H Isotropic = 23.4843 Anisotropy = 4.4620

XX= 21.0119 YX= -0.0001 ZX= 0.0004

XY= 0.0001 YY= 26.4563 ZY= 1.1252

XZ= 0.0001 YZ= -0.9303 ZZ= 22.9848

Eigenvalues: 21.0119 22.9820 26.4590

38 H Isotropic = 23.4843 Anisotropy = 4.4620

XX= 21.0120 YX= -0.0004 ZX= 0.0006

XY= -0.0008 YY= 26.4563 ZY= -1.1252

XZ= 0.0004 YZ= 0.9303 ZZ= 22.9848

Eigenvalues: 21.0120 22.9821 26.4590

39 H Isotropic = 24.2921 Anisotropy = 8.6556

XX= 21.8309 YX= -0.0002 ZX= 0.0002

XY= -0.0009 YY= 26.6324 ZY= 2.4213

XZ= 0.0002 YZ= 6.3828 ZZ= 24.4130

Eigenvalues: 20.9830 21.8309 30.0625

40 Bq Isotropic = 7.2166 Anisotropy = 15.4777

XX= 0.7318 YX= 0.0006 ZX= -0.0002

XY= 0.0011 YY= 3.5505 ZY= -1.2924

XZ= -0.0001 YZ= -1.7696 ZZ= 17.3675

Eigenvalues: 0.7318 3.3829 17.5351

41 Bq Isotropic = 6.1710 Anisotropy = 6.7376

XX= 1.7273 YX= -1.6421 ZX= 1.0045

XY= -1.6259 YY= 6.2817 ZY= -2.1257

XZ= -0.1879 YZ= 0.7628 ZZ= 10.5041

Eigenvalues: 1.1982 6.6521 10.6628

42 Bq Isotropic = 6.1708 Anisotropy = 6.7365

XX= 1.7277 YX= 1.6436 ZX= -1.0047

XY= 1.6276 YY= 6.2819 ZY= -2.1243

XZ= 0.1884 YZ= 0.7605 ZZ= 10.5029

Eigenvalues: 1.1976 6.6530 10.6618

43 Bq Isotropic = 9.8285 Anisotropy = 23.1347

XX= 2.8560 YX= -0.7003 ZX= -1.8109

XY= 0.5249 YY= 1.6180 ZY= -1.1567

XZ= -2.3484 YZ= -0.9664 ZZ= 25.0116

Eigenvalues: 1.5408 2.6931 25.2517

44 Bq Isotropic = 9.8284 Anisotropy = 23.1328

XX= 2.8568 YX= 0.7004 ZX= 1.8100

XY= -0.5243 YY= 1.6184 ZY= -1.1623

XZ= 2.3456 YZ= -0.9739 ZZ= 25.0099

Eigenvalues: 1.5403 2.6945 25.2502

6.26 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(-1) calculation of compound **7**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	1.31222	2.16806	0.00008
C	0	1.22095	0.74156	-0.00002
N	0	-0.00002	0.1142	0.00000
C	0	-1.22103	0.74148	0.00002
C	0	-1.31239	2.16798	-0.00008
S	0	-0.00012	3.24341	0.00000
C	0	-2.54542	0.13881	0.00009
C	0	-3.54865	1.14093	-0.00006
S	0	-2.91116	2.78037	-0.00021
S	0	2.91097	2.78055	0.00021
C	0	3.54855	1.14114	0.00006
C	0	2.54537	0.13897	-0.00009

C	0	0.00005	-1.34835	0.00000
C	0	4.90767	0.86524	0.00006
C	0	5.30128	-0.4692	-0.00013
C	0	4.34354	-1.4884	-0.00032
C	0	2.98754	-1.20448	-0.00029
C	0	-2.98753	-1.20466	0.00029
C	0	-4.34351	-1.48865	0.00032
C	0	-5.30131	-0.4695	0.00012
C	0	-4.90776	0.86496	-0.00006
C	0	0.00028	-2.01526	1.22084
C	0	0.00035	-3.40642	1.22055
C	0	0.00021	-4.0698	0.00000
C	0	-0.00001	-3.40642	-1.22055
C	0	-0.00009	-2.01526	-1.22084
F	0	0.00028	-5.41493	0.00000
H	0	5.63966	1.66314	0.00019
H	0	6.35593	-0.71464	-0.00014
H	0	4.66135	-2.52309	-0.00049
H	0	2.29657	-2.0274	-0.00045
H	0	-2.29652	-2.02755	0.00045
H	0	-4.66127	-2.52335	0.00048
H	0	-6.35594	-0.71499	0.00013
H	0	-5.63979	1.66282	-0.0002
H	0	0.00038	-1.46488	2.15326
H	0	0.00052	-3.96792	2.14536
H	0	-0.00011	-3.96792	-2.14536
H	0	-0.00024	-1.46488	-2.15326
Bq	0	-0.00008	1.52945	-1.00000
Bq	0	-2.30769	1.3938	-1.00005
Bq	0	2.30764	1.39417	-0.99995
Bq	0	-3.93902	-0.16982	-0.99988
Bq	0	3.939	-0.16932	-1.00012

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 8.6242 Anisotropy = 187.2544

XX= -33.1425 YX= 2.0694 ZX= -0.0141

XY= 0.4810 YY= -74.4453 ZY= -0.0077

XZ= 0.0001 YZ= -0.0095 ZZ= 133.4605

Eigenvalues: -74.4847 -33.1032 133.4605

2 C Isotropic = 34.1300 Anisotropy = 124.7825

XX= -10.3885 YX= 8.4820 ZX= 0.0071

XY= 6.4837 YY= -4.5398 ZY= -0.0065

XZ= -0.0001 YZ= -0.0059 ZZ= 117.3183

Eigenvalues: -15.4981 0.5698 117.3183

3 N Isotropic = 28.5597 Anisotropy = 226.1142

XX= -40.6105 YX= 0.0004 ZX= 0.0064

XY= 0.0022 YY= -53.0129 ZY= -0.0000

XZ= 0.0056 YZ= -0.0001 ZZ= 179.3025

Eigenvalues: -53.0129 -40.6105 179.3025

4 C Isotropic = 34.1301 Anisotropy = 124.7822

XX= -10.3872 YX= -8.4813 ZX= 0.0070

XY= -6.4834 YY= -4.5406 ZY= 0.0064

XZ= -0.0001 YZ= 0.0057 ZZ= 117.3183

Eigenvalues: -15.4971 0.5692 117.3183

5 C Isotropic = 8.6239 Anisotropy = 187.2538

XX= -33.1436 YX= -2.0672 ZX= -0.0140

XY= -0.4778 YY= -74.4445 ZY= 0.0075

XZ= 0.0001 YZ= 0.0092 ZZ= 133.4597

Eigenvalues: -74.4837 -33.1044 133.4597

6 S Isotropic = 169.5480 Anisotropy = 506.6246

XX= 65.0317 YX= 0.0035 ZX= -0.0314

XY= 0.0089 YY= -63.6854 ZY= -0.0001

XZ= -0.0504 YZ= 0.0001 ZZ= 507.2977

Eigenvalues: -63.6854 65.0316 507.2977

7 C Isotropic = 53.0795 Anisotropy = 140.4270

XX= -23.4751 YX= -5.4889 ZX= 0.0007

XY= -6.4631 YY= 36.0161 ZY= 0.0172

XZ= -0.0099 YZ= 0.0128 ZZ= 146.6975

Eigenvalues: -24.0695 36.6105 146.6975

8 C Isotropic = 33.4447 Anisotropy = 133.2856

XX= 19.8152 YX= -14.7625 ZX= -0.0040

XY= -13.9488 YY= -41.7829 ZY= 0.0172

XZ= 0.0137 YZ= 0.0150 ZZ= 122.3018

Eigenvalues: -44.9642 22.9966 122.3018

9 S Isotropic = 216.3211 Anisotropy = 247.2318

XX= 270.1146 YX= 33.8050 ZX= -0.0060

XY= 22.5303 YY= -2.2937 ZY= 0.0345

XZ= 0.0009 YZ= 0.0107 ZZ= 381.1422

Eigenvalues: -5.1758 272.9967 381.1422

10 S Isotropic = 216.3197 Anisotropy = 247.2272

XX= 270.1166 YX= -33.7865 ZX= -0.0060

XY= -22.5124 YY= -2.2953 ZY= -0.0349

XZ= 0.0011 YZ= -0.0110 ZZ= 381.1378

Eigenvalues: -5.1737 272.9950 381.1378

11 C Isotropic = 33.4448 Anisotropy = 133.2842

XX= 19.8148 YX= 14.7654 ZX= -0.0040

XY= 13.9535 YY= -41.7813 ZY= -0.0175

XZ= 0.0139 YZ= -0.0153 ZZ= 122.3010

Eigenvalues: -44.9644 22.9979 122.3010

12 C Isotropic = 53.0799 Anisotropy = 140.4251

XX= -23.4755 YX= 5.4874 ZX= 0.0007

XY= 6.4590 YY= 36.0186 ZY= -0.0173

XZ= -0.0098 YZ= -0.0129 ZZ= 146.6966

Eigenvalues: -24.0693 36.6124 146.6966

13 C Isotropic = 42.0407 Anisotropy = 109.2846

XX= 114.8971 YX= 0.0097 ZX= -0.0061

XY= 0.0092 YY= -56.2555 ZY= 0.0001

XZ= -0.0092 YZ= -0.0000 ZZ= 67.4805

Eigenvalues: -56.2555 67.4805 114.8971

14 C Isotropic = 50.8192 Anisotropy = 181.0659

XX= -10.8204 YX= -38.8240 ZX= -0.0108

XY= -37.6150 YY= -8.2518 ZY= -0.0264

XZ= -0.0082 YZ= -0.0237 ZZ= 171.5298

Eigenvalues: -47.7771 28.7050 171.5298

15 C Isotropic = 32.5389 Anisotropy = 215.2410

XX= -72.0932 YX= 17.8435 ZX= -0.0043

XY= 11.8839 YY= -6.3231 ZY= -0.0280

XZ= -0.0036 YZ= -0.0316 ZZ= 176.0328

Eigenvalues: -75.2963 -3.1199 176.0328

16 C Isotropic = 44.7228 Anisotropy = 198.8607

XX= 17.8056 YX= 22.7231 ZX= 0.0002

XY= 22.3566 YY= -60.9338 ZY= -0.0391

XZ= 0.0018 YZ= -0.0359 ZZ= 177.2966

Eigenvalues: -66.9295 23.8013 177.2966

17 C Isotropic = 45.2898 Anisotropy = 187.3520

XX= 4.4418 YX= -32.4804 ZX= -0.0110

XY= -24.0553 YY= -38.7636 ZY= -0.0353

XZ= -0.0156 YZ= -0.0307 ZZ= 170.1911

Eigenvalues: -52.7382 18.4165 170.1911

18 C Isotropic = 45.2912 Anisotropy = 187.3534

XX= 4.4393 YX= 32.4834 ZX= -0.0111

XY= 24.0578 YY= -38.7591 ZY= 0.0352

XZ= -0.0158 YZ= 0.0305 ZZ= 170.1935

Eigenvalues: -52.7373 18.4175 170.1935

19 C Isotropic = 44.7224 Anisotropy = 198.8607

XX= 17.8080 YX= -22.7195 ZX= 0.0001

XY= -22.3525 YY= -60.9370 ZY= 0.0389

XZ= 0.0016 YZ= 0.0357 ZZ= 177.2961

Eigenvalues: -66.9304 23.8014 177.2962

20 C Isotropic = 32.5391 Anisotropy = 215.2415

XX= -72.0918 YX= -17.8465 ZX= -0.0045

XY= -11.8868 YY= -6.3243 ZY= 0.0279

XZ= -0.0037 YZ= 0.0315 ZZ= 176.0334

Eigenvalues: -75.2962 -3.1198 176.0334

21 C Isotropic = 50.8193 Anisotropy = 181.0662

XX= -10.8249 YX= 38.8249 ZX= -0.0109

XY= 37.6153 YY= -8.2472 ZY= 0.0262

XZ= -0.0083 YZ= 0.0236 ZZ= 171.5301

Eigenvalues: -47.7779 28.7057 171.5301

22 C Isotropic = 55.5242 Anisotropy = 168.0419

XX= 167.5521 YX= 0.0035 ZX= -0.0260

XY= 0.0059 YY= 17.3872 ZY= -30.0529

XZ= -0.0264 YZ= -14.9487 ZZ= -18.3668

Eigenvalues: -29.2278 28.2482 167.5521

23 C Isotropic = 51.0896 Anisotropy = 174.9540

XX= 167.7256 YX= 0.0131 ZX= -0.0278

XY= 0.0120 YY= 11.6454 ZY= 27.2136

XZ= -0.0295 YZ= 20.2064 ZZ= -26.1022

Eigenvalues: -37.5333 23.0765 167.7256

24 C Isotropic = 4.8956 Anisotropy = 119.4877

XX= 84.5540 YX= 0.0080 ZX= -0.0100

XY= 0.0091 YY= -81.0886 ZY= -0.0000

XZ= -0.0106 YZ= -0.0000 ZZ= 11.2213

Eigenvalues: -81.0886 11.2213 84.5540

25 C Isotropic = 51.0897 Anisotropy = 174.9539

XX= 167.7257 YX= 0.0047 ZX= -0.0247

XY= 0.0054 YY= 11.6454 ZY= -27.2137

XZ= -0.0264 YZ= -20.2064 ZZ= -26.1018

Eigenvalues: -37.5330 23.0765 167.7257

26 C Isotropic = 55.5243 Anisotropy = 168.0420

XX= 167.5523 YX= 0.0136 ZX= -0.0296

XY= 0.0111 YY= 17.3873 ZY= 30.0528

XZ= -0.0259 YZ= 14.9488 ZZ= -18.3666

Eigenvalues: -29.2276 28.2483 167.5523

27 F Isotropic = 249.6607 Anisotropy = 151.1915

XX= 350.4551 YX= 0.0049 ZX= -0.0302

XY= 0.0052 YY= 254.7321 ZY= 0.0000

XZ= -0.0307 YZ= -0.0001 ZZ= 143.7951

Eigenvalues: 143.7951 254.7321 350.4551

28 H Isotropic = 23.4031 Anisotropy = 8.1994

XX= 27.7961 YX= -2.1996 ZX= -0.0001

XY= -2.2052 YY= 24.3500 ZY= 0.0004

XZ= -0.0000 YZ= 0.0008 ZZ= 18.0632

Eigenvalues: 18.0632 23.2767 28.8693

29 H Isotropic = 23.1534 Anisotropy = 5.3074

XX= 23.8742 YX= 0.8495 ZX= 0.0003

XY= 0.6131 YY= 26.5019 ZY= 0.0011

XZ= 0.0001 YZ= 0.0009 ZZ= 19.0842

Eigenvalues: 19.0842 23.6844 26.6917

30 H Isotropic = 23.8128 Anisotropy = 8.8338

XX= 29.6233 YX= 0.8638 ZX= 0.0001

XY= 0.5840 YY= 23.0437 ZY= 0.0002

XZ= -0.0006 YZ= 0.0010 ZZ= 18.7714

Eigenvalues: 18.7714 22.9650 29.7020

31 H Isotropic = 25.3600 Anisotropy = 18.1124

XX= 37.4239 YX= 1.2592 ZX= -0.0026

XY= -2.0452 YY= 23.4164 ZY= 0.0004

XZ= -0.0023 YZ= 0.0006 ZZ= 15.2397

Eigenvalues: 15.2397 23.4054 37.4350

32 H Isotropic = 25.3596 Anisotropy = 18.1112

XX= 37.4226 YX= -1.2578 ZX= -0.0026

XY= 2.0463 YY= 23.4163 ZY= -0.0004

XZ= -0.0022 YZ= -0.0006 ZZ= 15.2397

Eigenvalues: 15.2397 23.4052 37.4337

33 H Isotropic = 23.8127 Anisotropy = 8.8335

XX= 29.6231 YX= -0.8635 ZX= 0.0001

XY= -0.5835 YY= 23.0437 ZY= -0.0002

XZ= -0.0006 YZ= -0.0010 ZZ= 18.7713

Eigenvalues: 18.7713 22.9651 29.7017

34 H Isotropic = 23.1534 Anisotropy = 5.3074

XX= 23.8743 YX= -0.8496 ZX= 0.0003

XY= -0.6131 YY= 26.5019 ZY= -0.0011

XZ= 0.0001 YZ= -0.0009 ZZ= 19.0842

Eigenvalues: 19.0842 23.6844 26.6917

35 H Isotropic = 23.4031 Anisotropy = 8.1995

XX= 27.7959 YX= 2.1999 ZX= -0.0001

XY= 2.2054 YY= 24.3502 ZY= -0.0004

XZ= -0.0000 YZ= -0.0008 ZZ= 18.0633

Eigenvalues: 18.0633 23.2767 28.8694

36 H Isotropic = 24.2921 Anisotropy = 8.6556

XX= 21.8309 YX= -0.0006 ZX= 0.0004

XY= 0.0002 YY= 26.6324 ZY= -2.4213

XZ= 0.0002 YZ= -6.3828 ZZ= 24.4130

Eigenvalues: 20.9830 21.8309 30.0625

37 H Isotropic = 23.4843 Anisotropy = 4.4620

XX= 21.0119 YX= -0.0001 ZX= 0.0004

XY= 0.0001 YY= 26.4563 ZY= 1.1252

XZ= 0.0001 YZ= -0.9303 ZZ= 22.9848

Eigenvalues: 21.0119 22.9820 26.4590

38 H Isotropic = 23.4843 Anisotropy = 4.4620

XX= 21.0120 YX= -0.0004 ZX= 0.0006

XY= -0.0008 YY= 26.4563 ZY= -1.1252

XZ= 0.0004 YZ= 0.9303 ZZ= 22.9848

Eigenvalues: 21.0120 22.9821 26.4590

39 H Isotropic = 24.2921 Anisotropy = 8.6556

XX= 21.8309 YX= -0.0002 ZX= 0.0002

XY= -0.0009 YY= 26.6324 ZY= 2.4213

XZ= 0.0002 YZ= 6.3828 ZZ= 24.4130

Eigenvalues: 20.9830 21.8309 30.0625

40 Bq Isotropic = 7.2166 Anisotropy = 15.4777

XX= 0.7318 YX= -0.0006 ZX= -0.0004

XY= -0.0013 YY= 3.5505 ZY= 1.2924

XZ= -0.0003 YZ= 1.7696 ZZ= 17.3675

Eigenvalues: 0.7318 3.3829 17.5351

41 Bq Isotropic = 6.1708 Anisotropy = 6.7369

XX= 1.7279 YX= -1.6439 ZX= -1.0048

XY= -1.6277 YY= 6.2815 ZY= 2.1243

XZ= 0.1885 YZ= -0.7604 ZZ= 10.5032

Eigenvalues: 1.1976 6.6527 10.6621

42 Bq Isotropic = 6.1710 Anisotropy = 6.7372

XX= 1.7271 YX= 1.6418 ZX= 1.0043

XY= 1.6257 YY= 6.2821 ZY= 2.1256

XZ= -0.1878 YZ= -0.7629 ZZ= 10.5038

Eigenvalues: 1.1982 6.6524 10.6625

43 Bq Isotropic = 9.8283 Anisotropy = 23.1330

XX= 2.8567 YX= -0.7002 ZX= 1.8099

XY= 0.5245 YY= 1.6183 ZY= 1.1624

XZ= 2.3456 YZ= 0.9740 ZZ= 25.0100

Eigenvalues: 1.5403 2.6944 25.2503

44 Bq Isotropic = 9.8286 Anisotropy = 23.1345

XX= 2.8561 YX= 0.7005 ZX= -1.8109

XY= -0.5247 YY= 1.6181 ZY= 1.1566

XZ= -2.3484 YZ= 0.9663 ZZ= 25.0115

Eigenvalues: 1.5408 2.6933 25.2516

6.27 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(0) calculation of compound **6**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	-0.31494	-2.24811	0.02175
C	0	-0.94876	-0.96624	-0.01296
N	0	-0.19463	0.1761	-0.02041
C	0	1.16158	0.1907	-0.02376

C	0	1.99421	-0.95851	-0.00646
S	0	1.36112	-2.5388	0.03232
S	0	-1.41285	-3.56537	0.05296
C	0	-2.77598	-2.44779	0.00806
C	0	-2.38914	-1.08501	-0.03123
S	0	2.06428	1.6738	-0.03642
C	0	3.57927	0.76184	-0.02155
C	0	3.38206	-0.64056	-0.00558
C	0	-0.83505	1.49705	-0.00011
C	0	-1.06669	2.15148	-1.20758
C	0	-1.65016	3.41338	-1.17886
C	0	-1.97295	3.96831	0.05209
C	0	-1.73668	3.32215	1.25832
C	0	-1.15429	2.06022	1.2335
F	0	-2.53915	5.18844	0.07757
C	0	-4.10094	-2.85681	-0.00071
C	0	-5.0856	-1.8742	-0.05725
C	0	-4.73965	-0.51858	-0.10523
C	0	-3.41517	-0.11514	-0.09201
C	0	4.85004	1.3178	-0.02444
C	0	5.93815	0.44681	-0.00959
C	0	5.7644	-0.94853	0.0077
C	0	4.49906	-1.50177	0.01004
H	0	-0.80854	1.68979	-2.15233
H	0	-1.85247	3.9576	-2.09184
H	0	-2.00257	3.79825	2.19282
H	0	-0.95891	1.52798	2.15606
H	0	-4.36306	-3.90614	0.03183
H	0	-6.12825	-2.16655	-0.06631
H	0	-5.5182	0.23174	-0.15341
H	0	-3.19253	0.9372	-0.1323
H	0	4.99772	2.38977	-0.0368
H	0	6.94008	0.85795	-0.01094

H	0	6.63299	-1.59399	0.01907
H	0	4.37101	-2.57737	0.02241
Bq	0	0.50976	-1.05748	-0.00159
Bq	0	-1.56833	-2.0625	0.00772
Bq	0	2.43628	0.20546	-0.01875
Bq	0	-3.75108	-1.48292	-0.04639
Bq	0	4.66883	-0.09407	-0.00724

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 9.3917 Anisotropy = 185.0070

XX= -44.5881 YX= 17.9852 ZX= -0.5833

XY= 15.5494 YY= -59.7709 ZY= 5.2661

XZ= -2.1844 YZ= 6.8789 ZZ= 132.5339

Eigenvalues: -70.7539 -33.8008 132.7297

2 C Isotropic = 35.1802 Anisotropy = 125.9955

XX= -14.0536 YX= -1.4983 ZX= -2.2998

XY= 5.2924 YY= 0.5323 ZY= 2.0009

XZ= -2.5824 YZ= 3.8565 ZZ= 119.0619

Eigenvalues: -14.3549 0.7184 119.1772

3 N Isotropic = 26.0242 Anisotropy = 236.2315

XX= -36.3797 YX= 15.9117 ZX= 0.1228

XY= 7.3499 YY= -69.0467 ZY= 0.1076

XZ= -1.2875 YZ= 3.3445 ZZ= 183.4989

Eigenvalues: -72.7775 -32.6618 183.5119

4 C Isotropic = 13.6598 Anisotropy = 133.0554

XX= -43.9186 YX= 11.7932 ZX= -0.4822

XY= 9.4077 YY= -17.4294 ZY= 1.1537

XZ= -3.3524 YZ= 1.4052 ZZ= 102.3273

Eigenvalues: -47.6715 -13.7125 102.3634

5 C Isotropic = 31.0434 Anisotropy = 156.3685

XX= -40.9515 YX= 7.6994 ZX= -0.8405

XY= 17.6868 YY= -1.1241 ZY= 3.2698

XZ= -1.0651 YZ= 3.3700 ZZ= 135.2059

Eigenvalues: -44.6718 2.5130 135.2891

6 S Isotropic = 194.1439 Anisotropy = 473.7719

XX= 84.6794 YX= 43.6961 ZX= -1.3440

XY= 10.7764 YY= -11.7520 ZY= 12.6652

XZ= -0.1119 YZ= 19.2297 ZZ= 509.5044

Eigenvalues: -19.3736 91.8135 509.9918

7 S Isotropic = 219.2011 Anisotropy = 233.2354

XX= 226.7348 YX= 94.9439 ZX= -4.4324

XY= 94.4477 YY= 56.5925 ZY= 9.5964

XZ= -8.6800 YZ= 10.1367 ZZ= 374.2759

Eigenvalues: 13.9884 268.9235 374.6913

8 C Isotropic = 32.7577 Anisotropy = 134.9467

XX= -6.4846 YX= 33.4805 ZX= -2.2183

XY= 31.4800 YY= -17.8123 ZY= 4.8437

XZ= -4.6176 YZ= 2.5935 ZZ= 122.5700

Eigenvalues: -45.2705 20.8215 122.7222

9 C Isotropic = 54.5208 Anisotropy = 141.2346

XX= -13.2968 YX= -23.2660 ZX= -2.5821

XY= -24.1273 YY= 28.3820 ZY= 4.1411

XZ= -0.9577 YZ= 4.5284 ZZ= 148.4772

Eigenvalues: -24.0141 38.8993 148.6772

10 S Isotropic = 252.0373 Anisotropy = 125.8992

XX= 267.4735 YX= 106.9415 ZX= -0.9441

XY= 52.0039 YY= 152.9017 ZY= 3.1669

XZ= 5.9823 YZ= -1.8631 ZZ= 335.7368

Eigenvalues: 112.2189 307.9230 335.9701

11 C Isotropic = 31.8257 Anisotropy = 134.3918

XX= -10.2324 YX= 24.8792 ZX= -0.7532

XY= 24.6674 YY= -15.6930 ZY= 1.4455

XZ= -2.2041 YZ= -1.6830 ZZ= 121.4024

Eigenvalues: -37.8911 11.9479 121.4202

12 C Isotropic = 46.2773 Anisotropy = 142.4032

XX= -6.8970 YX= -19.3520 ZX= -0.4860

XY= -19.8033 YY= 4.5528 ZY= 1.7054

XZ= -1.1647 YZ= 2.2171 ZZ= 141.1762

Eigenvalues: -21.5712 19.1905 141.2128

13 C Isotropic = 40.7437 Anisotropy = 107.5639

XX= 84.1067 YX= 63.5094 ZX= 2.3794

XY= 58.9771 YY= -20.3417 ZY= -0.0412

XZ= 2.4021 YZ= -0.1657 ZZ= 58.4662

Eigenvalues: -48.6154 58.3936 112.4530

14 C Isotropic = 54.2899 Anisotropy = 169.6460

XX= 142.0806 YX= 53.8978 ZX= 19.8671

XY= 55.1215 YY= 47.2820 ZY= -17.9841

XZ= 16.9547 YZ= -17.2365 ZZ= -26.4930

Eigenvalues: -36.4382 31.9206 167.3872

15 C Isotropic = 53.3227 Anisotropy = 169.9585

XX= 140.6460 YX= 56.8743 ZX= -3.5783

XY= 58.1432 YY= 37.2847 ZY= 27.0587

XZ= -2.7645 YZ= 25.8942 ZZ= -17.9626

Eigenvalues: -32.8559 26.1956 166.6283

16 C Isotropic = 4.9342 Anisotropy = 119.9130

XX= 54.6781 YX= 64.5811 ZX= 3.6318

XY= 64.0988 YY= -53.0771 ZY= -0.1626

XZ= 3.9229 YZ= -0.1802 ZZ= 13.2017

Eigenvalues: -83.1506 13.0770 84.8762

17 C Isotropic = 52.8651 Anisotropy = 170.9648

XX= 139.0903 YX= 58.3090 ZX= 17.6168

XY= 59.0030 YY= 40.9164 ZY= -20.5195

XZ= 17.7331 YZ= -17.0584 ZZ= -21.4115

Eigenvalues: -34.2936 26.0471 166.8416

18 C Isotropic = 54.0869 Anisotropy = 168.7305

XX= 143.4469 YX= 51.7763 ZX= -3.8559

XY= 54.2502 YY= 42.7555 ZY= 28.6402

XZ= -1.3904 YZ= 25.2017 ZZ= -23.9416

Eigenvalues: -36.1133 31.8001 166.5739

19 F Isotropic = 247.8245 Anisotropy = 153.6208

XX= 332.9888 YX= 36.1123 ZX= 7.6468

XY= 37.2136 YY= 269.7441 ZY= 6.0211

XZ= 8.2078 YZ= 6.2753 ZZ= 140.7406

Eigenvalues: 140.2388 252.9963 350.2384

20 C Isotropic = 50.8989 Anisotropy = 181.2179

XX= 21.7213 YX= -20.4639 ZX= -1.8609

XY= -21.1653 YY= -40.4904 ZY= 7.2934

XZ= -2.3507 YZ= 5.5539 ZZ= 171.4658

Eigenvalues: -46.9525 27.9384 171.7108

21 C Isotropic = 32.4878 Anisotropy = 214.6349

XX= -69.5556 YX= -17.2774 ZX= -4.2225

XY= -21.9605 YY= -8.1147 ZY= 6.9322

XZ= -5.6789 YZ= 8.1087 ZZ= 175.1336

Eigenvalues: -75.3138 -2.8006 175.5777

22 C Isotropic = 44.5519 Anisotropy = 200.6143

XX= -19.2848 YX= 44.0666 ZX= -6.0195

XY= 44.9889 YY= -24.8459 ZY= 9.3583

XZ= -6.2848 YZ= 9.0554 ZZ= 177.7866

Eigenvalues: -67.1669 22.5279 178.2948

23 C Isotropic = 45.8670 Anisotropy = 188.2135

XX= 18.8449 YX= -0.5711 ZX= -2.7312

XY= 5.3216 YY= -52.2415 ZY= 9.6448

XZ= 1.6345 YZ= 7.8896 ZZ= 170.9975

Eigenvalues: -52.6654 18.9237 171.3426

24 C Isotropic = 51.5170 Anisotropy = 180.8279

XX= 28.0406 YX= -10.9109 ZX= -0.3452

XY= -13.4140 YY= -45.5311 ZY= 2.6456

XZ= -0.1188 YZ= 2.1575 ZZ= 172.0415

Eigenvalues: -47.5145 29.9965 172.0690

25 C Isotropic = 28.1932 Anisotropy = 217.8594

XX= -68.4119 YX= -25.4405 ZX= -0.6466

XY= -26.7352 YY= -20.3923 ZY= 2.4430

XZ= -0.2281 YZ= 3.5311 ZZ= 173.3838

Eigenvalues: -79.8595 -8.9937 173.4328

26 C Isotropic = 43.0264 Anisotropy = 202.8673

XX= -26.4773 YX= 37.9896 ZX= -1.2692

XY= 43.4247 YY= -22.6767 ZY= 2.7408

XZ= -1.3153 YZ= 2.5749 ZZ= 178.2332

Eigenvalues: -65.3600 16.1679 178.2712

27 C Isotropic = 49.7786 Anisotropy = 182.9519

XX= 31.0980 YX= 4.0080 ZX= -0.5871

XY= 5.1584 YY= -53.4673 ZY= 2.8298

XZ= 0.1997 YZ= 3.2688 ZZ= 171.7051

Eigenvalues: -53.7564 31.3457 171.7465

28 H Isotropic = 24.3326 Anisotropy = 9.0557

XX= 23.0265 YX= -1.7367 ZX= 1.1617

XY= -2.2204 YY= 25.4708 ZY= -2.2990

XZ= 2.3199 YZ= -6.5245 ZZ= 24.5006

Eigenvalues: 20.5470 22.0812 30.3698

29 H Isotropic = 23.5276 Anisotropy = 4.7148

XX= 21.6982 YX= -2.3614 ZX= -0.7232

XY= -2.3253 YY= 25.5593 ZY= 0.8772

XZ= -0.1848 YZ= -0.9964 ZZ= 23.3253

Eigenvalues: 20.5246 23.3874 26.6708

30 H Isotropic = 23.5939 Anisotropy = 4.8468

XX= 21.6211 YX= -2.4809 ZX= 0.2976

XY= -2.2530 YY= 25.7466 ZY= -1.0909

XZ= -0.1748 YZ= 0.9829 ZZ= 23.4141

Eigenvalues: 20.5438 23.4128 26.8252

31 H Isotropic = 24.4800 Anisotropy = 9.2311

XX= 22.9971 YX= -1.9446 ZX= -1.3457

XY= -2.1884 YY= 25.4883 ZY= 2.2409

XZ= -2.4285 YZ= 6.5175 ZZ= 24.9545

Eigenvalues: 20.8327 21.9731 30.6340

32 H Isotropic = 23.3666 Anisotropy = 8.2351

XX= 28.8471 YX= 0.2902 ZX= 0.1672

XY= 0.0968 YY= 23.2610 ZY= -0.1537

XZ= 0.2008 YZ= -0.1734 ZZ= 17.9917

Eigenvalues: 17.9833 23.2598 28.8567

33 H Isotropic = 23.1811 Anisotropy = 5.4621

XX= 23.8525 YX= -0.6663 ZX= 0.1173

XY= -0.9042 YY= 26.6037 ZY= -0.3057

XZ= 0.0758 YZ= -0.2341 ZZ= 19.0872

Eigenvalues: 19.0766 23.6443 26.8226

34 H Isotropic = 23.8311 Anisotropy = 8.4721

XX= 27.4417 YX= 3.1407 ZX= 0.0819

XY= 2.8508 YY= 25.0716 ZY= -0.0922

XZ= 0.2659 YZ= -0.0878 ZZ= 18.9799

Eigenvalues: 18.9718 23.0423 29.4791

35 H Isotropic = 24.9400 Anisotropy = 16.6166

XX= 33.7486 YX= 6.8203 ZX= 0.7985

XY= 2.9295 YY= 25.4281 ZY= 0.1239

XZ= 0.4132 YZ= 0.3409 ZZ= 15.6433

Eigenvalues: 15.6225 23.1799 36.0177

36 H Isotropic = 23.5995 Anisotropy = 9.0377

XX= 29.5824 YX= 0.3838 ZX= -0.0020

XY= 0.7026 YY= 22.6328 ZY= -0.0556

XZ= -0.0047 YZ= -0.0869 ZZ= 18.5833

Eigenvalues: 18.5820 22.5918 29.6246

37 H Isotropic = 23.1361 Anisotropy = 5.6810

XX= 24.0118 YX= -1.9194 ZX= 0.0171

XY= -1.6615 YY= 25.8210 ZY= -0.0977

XZ= 0.0739 YZ= -0.0548 ZZ= 19.5754

Eigenvalues: 19.5744 22.9104 26.9234

38 H Isotropic = 23.4391 Anisotropy = 5.7149

XX= 25.9638 YX= 1.5805 ZX= -0.0202

XY= 1.9512 YY= 24.8220 ZY= -0.0761

XZ= -0.0095 YZ= -0.0535 ZZ= 19.5315

Eigenvalues: 19.5307 23.5375 27.2491

39 H Isotropic = 22.9831 Anisotropy = 9.9099

XX= 29.4656 YX= -1.0989 ZX= 0.0250

XY= -0.8043 YY= 22.2821 ZY= -0.1125

XZ= 0.0282 YZ= -0.0619 ZZ= 17.2014

Eigenvalues: 17.1999 22.1596 29.5897

40 Bq Isotropic = 7.1943 Anisotropy = 11.9540

XX= 6.6920 YX= -3.9178 ZX= -0.1070

XY= -3.1631 YY= 13.6804 ZY= -0.1819

XZ= -0.0988 YZ= -0.3510 ZZ= 1.2104

Eigenvalues: 1.1977 5.2216 15.1636

41 Bq Isotropic = 7.3753 Anisotropy = 25.7071

XX= 10.2018 YX= -2.1329 ZX= 0.3979

XY= -3.0157 YY= 24.0191 ZY= -1.1072

XZ= 0.0532 YZ= -0.9498 ZZ= -12.0949

Eigenvalues: -12.1252 9.7379 24.5134

42 Bq Isotropic = 6.3947 Anisotropy = 27.4239

XX= 10.9946 YX= -5.5740 ZX= 0.0152

XY= -4.1616 YY= 22.9395 ZY= -0.4309

XZ= -0.0796 YZ= -0.5614 ZZ= -14.7500

Eigenvalues: -14.7569 9.2637 24.6773

43 Bq Isotropic = 8.2569 Anisotropy = 2.5844

XX= 7.5083 YX= 1.2663 ZX= -0.0334

XY= -0.3012 YY= 7.2860 ZY= 0.0232

XZ= -0.0115 YZ= 0.1723 ZZ= 9.9763

Eigenvalues: 6.8993 7.8915 9.9798

44 Bq Isotropic = 5.9903 Anisotropy = 3.6506

XX= 7.7910 YX= -1.2591 ZX= -0.0128

XY= -0.8073 YY= 6.7373 ZY= 0.0483

XZ= 0.0405 YZ= -0.0861 ZZ= 3.4426

Eigenvalues: 3.4424 6.1044 8.4240

6.28 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(1) calculation of compound **6**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	-0.31494	-2.24811	0.02175
C	0	-0.94876	-0.96624	-0.01296
N	0	-0.19463	0.1761	-0.02041
C	0	1.16158	0.1907	-0.02376
C	0	1.99421	-0.95851	-0.00646
S	0	1.36112	-2.5388	0.03232
S	0	-1.41285	-3.56537	0.05296
C	0	-2.77598	-2.44779	0.00806
C	0	-2.38914	-1.08501	-0.03123
S	0	2.06428	1.6738	-0.03642
C	0	3.57927	0.76184	-0.02155
C	0	3.38206	-0.64056	-0.00558
C	0	-0.83505	1.49705	-0.00011
C	0	-1.06669	2.15148	-1.20758
C	0	-1.65016	3.41338	-1.17886
C	0	-1.97295	3.96831	0.05209
C	0	-1.73668	3.32215	1.25832
C	0	-1.15429	2.06022	1.2335
F	0	-2.53915	5.18844	0.07757
C	0	-4.10094	-2.85681	-0.00071
C	0	-5.0856	-1.8742	-0.05725
C	0	-4.73965	-0.51858	-0.10523
C	0	-3.41517	-0.11514	-0.09201
C	0	4.85004	1.3178	-0.02444
C	0	5.93815	0.44681	-0.00959
C	0	5.7644	-0.94853	0.0077
C	0	4.49906	-1.50177	0.01004
H	0	-0.80854	1.68979	-2.15233

H	0	-1.85247	3.9576	-2.09184
H	0	-2.00257	3.79825	2.19282
H	0	-0.95891	1.52798	2.15606
H	0	-4.36306	-3.90614	0.03183
H	0	-6.12825	-2.16655	-0.06631
H	0	-5.5182	0.23174	-0.15341
H	0	-3.19253	0.9372	-0.1323
H	0	4.99772	2.38977	-0.0368
H	0	6.94008	0.85795	-0.01094
H	0	6.63299	-1.59399	0.01907
H	0	4.37101	-2.57737	0.02241
Bq	0	0.50509	-1.03728	0.9982
Bq	0	-1.57813	-2.03091	1.00717
Bq	0	2.43295	0.21731	0.98117
Bq	0	-3.77107	-1.44247	0.95259
Bq	0	4.66512	-0.08135	0.99268

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 9.3917 Anisotropy = 185.0070

XX= -44.5881 YX= 17.9852 ZX= -0.5833

XY= 15.5493 YY= -59.7709 ZY= 5.2661

XZ= -2.1844 YZ= 6.8789 ZZ= 132.5339

Eigenvalues: -70.7538 -33.8008 132.7296

2 C Isotropic = 35.1802 Anisotropy = 125.9955

XX= -14.0536 YX= -1.4983 ZX= -2.2998

XY= 5.2923 YY= 0.5323 ZY= 2.0009

XZ= -2.5824 YZ= 3.8565 ZZ= 119.0619

Eigenvalues: -14.3549 0.7184 119.1772

3 N Isotropic = 26.0242 Anisotropy = 236.2315

XX= -36.3797 YX= 15.9117 ZX= 0.1228

XY= 7.3499 YY= -69.0467 ZY= 0.1076

XZ= -1.2875 YZ= 3.3445 ZZ= 183.4989

Eigenvalues: -72.7776 -32.6618 183.5119

4 C Isotropic = 13.6598 Anisotropy = 133.0554

XX= -43.9185 YX= 11.7931 ZX= -0.4822

XY= 9.4077 YY= -17.4294 ZY= 1.1537

XZ= -3.3524 YZ= 1.4052 ZZ= 102.3273

Eigenvalues: -47.6715 -13.7125 102.3634

5 C Isotropic = 31.0434 Anisotropy = 156.3685

XX= -40.9515 YX= 7.6994 ZX= -0.8405

XY= 17.6868 YY= -1.1241 ZY= 3.2698

XZ= -1.0651 YZ= 3.3700 ZZ= 135.2060

Eigenvalues: -44.6718 2.5130 135.2891

6 S Isotropic = 194.1439 Anisotropy = 473.7719

XX= 84.6794 YX= 43.6961 ZX= -1.3440

XY= 10.7765 YY= -11.7520 ZY= 12.6652

XZ= -0.1119 YZ= 19.2297 ZZ= 509.5043

Eigenvalues: -19.3736 91.8135 509.9918

7 S Isotropic = 219.2010 Anisotropy = 233.2354

XX= 226.7348 YX= 94.9439 ZX= -4.4324

XY= 94.4477 YY= 56.5924 ZY= 9.5964

XZ= -8.6800 YZ= 10.1367 ZZ= 374.2759

Eigenvalues: 13.9884 268.9235 374.6913

8 C Isotropic = 32.7577 Anisotropy = 134.9467

XX= -6.4846 YX= 33.4805 ZX= -2.2183

XY= 31.4800 YY= -17.8123 ZY= 4.8437

XZ= -4.6176 YZ= 2.5935 ZZ= 122.5700

Eigenvalues: -45.2705 20.8215 122.7222

9 C Isotropic = 54.5208 Anisotropy = 141.2346

XX= -13.2968 YX= -23.2660 ZX= -2.5821

XY= -24.1273 YY= 28.3820 ZY= 4.1411

XZ= -0.9577 YZ= 4.5284 ZZ= 148.4772

Eigenvalues: -24.0141 38.8993 148.6772

10 S Isotropic = 252.0373 Anisotropy = 125.8992

XX= 267.4735 YX= 106.9415 ZX= -0.9441

XY= 52.0039 YY= 152.9016 ZY= 3.1669

XZ= 5.9823 YZ= -1.8631 ZZ= 335.7368

Eigenvalues: 112.2188 307.9230 335.9701

11 C Isotropic = 31.8257 Anisotropy = 134.3918

XX= -10.2324 YX= 24.8792 ZX= -0.7532

XY= 24.6674 YY= -15.6930 ZY= 1.4455

XZ= -2.2041 YZ= -1.6830 ZZ= 121.4024

Eigenvalues: -37.8911 11.9479 121.4202

12 C Isotropic = 46.2773 Anisotropy = 142.4032

XX= -6.8970 YX= -19.3520 ZX= -0.4860

XY= -19.8032 YY= 4.5528 ZY= 1.7054

XZ= -1.1647 YZ= 2.2171 ZZ= 141.1762

Eigenvalues: -21.5712 19.1905 141.2128

13 C Isotropic = 40.7437 Anisotropy = 107.5639

XX= 84.1067 YX= 63.5094 ZX= 2.3794

XY= 58.9771 YY= -20.3417 ZY= -0.0412

XZ= 2.4021 YZ= -0.1657 ZZ= 58.4662

Eigenvalues: -48.6154 58.3936 112.4530

14 C Isotropic = 54.2899 Anisotropy = 169.6459

XX= 142.0805 YX= 53.8978 ZX= 19.8671

XY= 55.1215 YY= 47.2820 ZY= -17.9841

XZ= 16.9547 YZ= -17.2365 ZZ= -26.4930

Eigenvalues: -36.4382 31.9206 167.3871

15 C Isotropic = 53.3227 Anisotropy = 169.9585

XX= 140.6460 YX= 56.8743 ZX= -3.5783

XY= 58.1432 YY= 37.2847 ZY= 27.0587

XZ= -2.7645 YZ= 25.8942 ZZ= -17.9626

Eigenvalues: -32.8559 26.1956 166.6283

16 C Isotropic = 4.9342 Anisotropy = 119.9130

XX= 54.6781 YX= 64.5811 ZX= 3.6318

XY= 64.0988 YY= -53.0771 ZY= -0.1626

XZ= 3.9229 YZ= -0.1802 ZZ= 13.2017

Eigenvalues: -83.1506 13.0770 84.8762

17 C Isotropic = 52.8651 Anisotropy = 170.9648

XX= 139.0903 YX= 58.3090 ZX= 17.6168

XY= 59.0030 YY= 40.9164 ZY= -20.5195

XZ= 17.7331 YZ= -17.0584 ZZ= -21.4115

Eigenvalues: -34.2936 26.0471 166.8416

18 C Isotropic = 54.0869 Anisotropy = 168.7305

XX= 143.4469 YX= 51.7763 ZX= -3.8559

XY= 54.2502 YY= 42.7555 ZY= 28.6402

XZ= -1.3904 YZ= 25.2017 ZZ= -23.9416

Eigenvalues: -36.1133 31.8001 166.5739

19 F Isotropic = 247.8245 Anisotropy = 153.6208

XX= 332.9888 YX= 36.1123 ZX= 7.6468

XY= 37.2136 YY= 269.7441 ZY= 6.0211

XZ= 8.2078 YZ= 6.2753 ZZ= 140.7406

Eigenvalues: 140.2388 252.9963 350.2384

20 C Isotropic = 50.8989 Anisotropy = 181.2179

XX= 21.7213 YX= -20.4639 ZX= -1.8609

XY= -21.1653 YY= -40.4904 ZY= 7.2934

XZ= -2.3507 YZ= 5.5539 ZZ= 171.4658

Eigenvalues: -46.9525 27.9384 171.7108

21 C Isotropic = 32.4878 Anisotropy = 214.6349

XX= -69.5556 YX= -17.2774 ZX= -4.2225

XY= -21.9605 YY= -8.1147 ZY= 6.9322

XZ= -5.6789 YZ= 8.1087 ZZ= 175.1336

Eigenvalues: -75.3138 -2.8006 175.5777

22 C Isotropic = 44.5519 Anisotropy = 200.6143

XX= -19.2848 YX= 44.0666 ZX= -6.0195

XY= 44.9889 YY= -24.8459 ZY= 9.3583

XZ= -6.2848 YZ= 9.0554 ZZ= 177.7866

Eigenvalues: -67.1669 22.5279 178.2948

23 C Isotropic = 45.8670 Anisotropy = 188.2135

XX= 18.8449 YX= -0.5711 ZX= -2.7312

XY= 5.3216 YY= -52.2414 ZY= 9.6448

XZ= 1.6345 YZ= 7.8896 ZZ= 170.9975

Eigenvalues: -52.6654 18.9237 171.3426

24 C Isotropic = 51.5170 Anisotropy = 180.8280

XX= 28.0406 YX= -10.9110 ZX= -0.3452

XY= -13.4140 YY= -45.5312 ZY= 2.6456

XZ= -0.1188 YZ= 2.1575 ZZ= 172.0415

Eigenvalues: -47.5145 29.9965 172.0689

25 C Isotropic = 28.1932 Anisotropy = 217.8594

XX= -68.4119 YX= -25.4405 ZX= -0.6466

XY= -26.7353 YY= -20.3923 ZY= 2.4430

XZ= -0.2281 YZ= 3.5311 ZZ= 173.3838

Eigenvalues: -79.8595 -8.9937 173.4328

26 C Isotropic = 43.0264 Anisotropy = 202.8673

XX= -26.4773 YX= 37.9896 ZX= -1.2692

XY= 43.4247 YY= -22.6767 ZY= 2.7408

XZ= -1.3153 YZ= 2.5749 ZZ= 178.2332

Eigenvalues: -65.3600 16.1679 178.2712

27 C Isotropic = 49.7786 Anisotropy = 182.9519

XX= 31.0980 YX= 4.0080 ZX= -0.5871

XY= 5.1584 YY= -53.4673 ZY= 2.8298

XZ= 0.1997 YZ= 3.2688 ZZ= 171.7051

Eigenvalues: -53.7564 31.3457 171.7465

28 H Isotropic = 24.3326 Anisotropy = 9.0557

XX= 23.0265 YX= -1.7367 ZX= 1.1617

XY= -2.2204 YY= 25.4708 ZY= -2.2990

XZ= 2.3199 YZ= -6.5245 ZZ= 24.5006

Eigenvalues: 20.5470 22.0812 30.3698

29 H Isotropic = 23.5276 Anisotropy = 4.7148

XX= 21.6982 YX= -2.3614 ZX= -0.7232

XY= -2.3253 YY= 25.5593 ZY= 0.8772

XZ= -0.1848 YZ= -0.9964 ZZ= 23.3253

Eigenvalues: 20.5246 23.3874 26.6708

30 H Isotropic = 23.5939 Anisotropy = 4.8468

XX= 21.6211 YX= -2.4809 ZX= 0.2976

XY= -2.2530 YY= 25.7466 ZY= -1.0909

XZ= -0.1748 YZ= 0.9829 ZZ= 23.4141

Eigenvalues: 20.5438 23.4128 26.8252

31 H Isotropic = 24.4800 Anisotropy = 9.2311

XX= 22.9971 YX= -1.9446 ZX= -1.3457

XY= -2.1884 YY= 25.4883 ZY= 2.2409

XZ= -2.4285 YZ= 6.5175 ZZ= 24.9545

Eigenvalues: 20.8327 21.9731 30.6340

32 H Isotropic = 23.3666 Anisotropy = 8.2351

XX= 28.8471 YX= 0.2902 ZX= 0.1672

XY= 0.0968 YY= 23.2610 ZY= -0.1537

XZ= 0.2008 YZ= -0.1734 ZZ= 17.9917

Eigenvalues: 17.9833 23.2598 28.8567

33 H Isotropic = 23.1811 Anisotropy = 5.4621

XX= 23.8525 YX= -0.6663 ZX= 0.1173

XY= -0.9042 YY= 26.6037 ZY= -0.3057

XZ= 0.0758 YZ= -0.2341 ZZ= 19.0872

Eigenvalues: 19.0766 23.6443 26.8226

34 H Isotropic = 23.8311 Anisotropy = 8.4721

XX= 27.4417 YX= 3.1407 ZX= 0.0819

XY= 2.8508 YY= 25.0716 ZY= -0.0922

XZ= 0.2659 YZ= -0.0878 ZZ= 18.9799

Eigenvalues: 18.9718 23.0423 29.4791

35 H Isotropic = 24.9400 Anisotropy = 16.6166

XX= 33.7486 YX= 6.8203 ZX= 0.7985

XY= 2.9295 YY= 25.4281 ZY= 0.1239

XZ= 0.4132 YZ= 0.3409 ZZ= 15.6433

Eigenvalues: 15.6225 23.1799 36.0177

36 H Isotropic = 23.5995 Anisotropy = 9.0377

XX= 29.5824 YX= 0.3838 ZX= -0.0020

XY= 0.7027 YY= 22.6328 ZY= -0.0556

XZ= -0.0047 YZ= -0.0869 ZZ= 18.5833

Eigenvalues: 18.5820 22.5918 29.6246

37 H Isotropic = 23.1361 Anisotropy = 5.6810

XX= 24.0118 YX= -1.9194 ZX= 0.0171

XY= -1.6615 YY= 25.8210 ZY= -0.0977

XZ= 0.0739 YZ= -0.0548 ZZ= 19.5754

Eigenvalues: 19.5744 22.9104 26.9234

38 H Isotropic = 23.4391 Anisotropy = 5.7149

XX= 25.9638 YX= 1.5805 ZX= -0.0202

XY= 1.9512 YY= 24.8220 ZY= -0.0761

XZ= -0.0095 YZ= -0.0535 ZZ= 19.5315

Eigenvalues: 19.5307 23.5375 27.2491

39 H Isotropic = 22.9831 Anisotropy = 9.9099

XX= 29.4656 YX= -1.0989 ZX= 0.0250

XY= -0.8043 YY= 22.2821 ZY= -0.1125

XZ= 0.0282 YZ= -0.0619 ZZ= 17.2014

Eigenvalues: 17.1999 22.1596 29.5897

40 Bq Isotropic = 7.5401 Anisotropy = 15.3715

XX= 1.2676 YX= -1.0918 ZX= -0.6575

XY= -0.6962 YY= 3.7670 ZY= 1.1541

XZ= -0.5433 YZ= 1.9553 ZZ= 17.5856

Eigenvalues: 0.9802 3.8523 17.7877

41 Bq Isotropic = 6.3463 Anisotropy = 6.8605

XX= 1.8348 YX= -0.5982 ZX= -0.1916

XY= -1.6448 YY= 6.5253 ZY= 2.5152

XZ= -0.1307 YZ= -0.5407 ZZ= 10.6788

Eigenvalues: 1.5800 6.5389 10.9200

42 Bq Isotropic = 5.7176 Anisotropy = 5.7874

XX= 3.0758 YX= -3.1401 ZX= 1.3260

XY= -1.7643 YY= 5.3145 ZY= -2.8177

XZ= 0.0570 YZ= 0.1973 ZZ= 8.7625

Eigenvalues: 1.4972 6.0797 9.5759

43 Bq Isotropic = 10.1373 Anisotropy = 23.0502

XX= 2.7356 YX= 0.9860 ZX= -2.6259

XY= -0.2345 YY= 2.5387 ZY= 0.9933

XZ= -2.8584 YZ= 0.9240 ZZ= 25.1375

Eigenvalues: 1.9639 2.9438 25.5041

44 Bq Isotropic = 8.3519 Anisotropy = 17.7772

XX= 3.0868 YX= -1.1859 ZX= 1.8755

XY= -0.7628 YY= 1.9976 ZY= 0.1491

XZ= 2.0852 YZ= 0.5487 ZZ= 19.9712

Eigenvalues: 1.3297 3.5225 20.2034

6.29 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(-1) calculation of compound **6**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	-0.31494	-2.24811	0.02175
C	0	-0.94876	-0.96624	-0.01296
N	0	-0.19463	0.1761	-0.02041
C	0	1.16158	0.1907	-0.02376
C	0	1.99421	-0.95851	-0.00646
S	0	1.36112	-2.5388	0.03232
S	0	-1.41285	-3.56537	0.05296
C	0	-2.77598	-2.44779	0.00806
C	0	-2.38914	-1.08501	-0.03123
S	0	2.06428	1.6738	-0.03642
C	0	3.57927	0.76184	-0.02155
C	0	3.38206	-0.64056	-0.00558
C	0	-0.83505	1.49705	-0.00011
C	0	-1.06669	2.15148	-1.20758
C	0	-1.65016	3.41338	-1.17886
C	0	-1.97295	3.96831	0.05209
C	0	-1.73668	3.32215	1.25832
C	0	-1.15429	2.06022	1.2335
F	0	-2.53915	5.18844	0.07757
C	0	-4.10094	-2.85681	-0.00071
C	0	-5.0856	-1.8742	-0.05725

C	0	-4.73965	-0.51858	-0.10523
C	0	-3.41517	-0.11514	-0.09201
C	0	4.85004	1.3178	-0.02444
C	0	5.93815	0.44681	-0.00959
C	0	5.7644	-0.94853	0.0077
C	0	4.49906	-1.50177	0.01004
H	0	-0.80854	1.68979	-2.15233
H	0	-1.85247	3.9576	-2.09184
H	0	-2.00257	3.79825	2.19282
H	0	-0.95891	1.52798	2.15606
H	0	-4.36306	-3.90614	0.03183
H	0	-6.12825	-2.16655	-0.06631
H	0	-5.5182	0.23174	-0.15341
H	0	-3.19253	0.9372	-0.1323
H	0	4.99772	2.38977	-0.0368
H	0	6.94008	0.85795	-0.01094
H	0	6.63299	-1.59399	0.01907
H	0	4.37101	-2.57737	0.02241
Bq	0	0.51443	-1.07768	-1.00137
Bq	0	-1.55854	-2.0941	-0.99174
Bq	0	2.43961	0.1936	-1.01868
Bq	0	-3.73109	-1.52338	-1.04538
Bq	0	4.67254	-0.10678	-1.00715

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 9.3917 Anisotropy = 185.0070

XX= -44.5881 YX= 17.9852 ZX= -0.5833

XY= 15.5494 YY= -59.7709 ZY= 5.2661

XZ= -2.1844 YZ= 6.8789 ZZ= 132.5339

Eigenvalues: -70.7539 -33.8008 132.7297

2 C Isotropic = 35.1802 Anisotropy = 125.9955

XX= -14.0536 YX= -1.4983 ZX= -2.2998

XY= 5.2924 YY= 0.5323 ZY= 2.0009

XZ= -2.5824 YZ= 3.8565 ZZ= 119.0619

Eigenvalues: -14.3549 0.7184 119.1772

3 N Isotropic = 26.0242 Anisotropy = 236.2315

XX= -36.3797 YX= 15.9117 ZX= 0.1228

XY= 7.3499 YY= -69.0467 ZY= 0.1076

XZ= -1.2875 YZ= 3.3445 ZZ= 183.4989

Eigenvalues: -72.7775 -32.6618 183.5119

4 C Isotropic = 13.6598 Anisotropy = 133.0554

XX= -43.9186 YX= 11.7932 ZX= -0.4822

XY= 9.4077 YY= -17.4294 ZY= 1.1537

XZ= -3.3524 YZ= 1.4052 ZZ= 102.3273

Eigenvalues: -47.6715 -13.7125 102.3634

5 C Isotropic = 31.0434 Anisotropy = 156.3685

XX= -40.9515 YX= 7.6994 ZX= -0.8405

XY= 17.6868 YY= -1.1241 ZY= 3.2698

XZ= -1.0651 YZ= 3.3700 ZZ= 135.2059

Eigenvalues: -44.6718 2.5130 135.2891

6 S Isotropic = 194.1439 Anisotropy = 473.7719

XX= 84.6794 YX= 43.6961 ZX= -1.3440

XY= 10.7764 YY= -11.7520 ZY= 12.6652

XZ= -0.1119 YZ= 19.2297 ZZ= 509.5044

Eigenvalues: -19.3736 91.8135 509.9918

7 S Isotropic = 219.2011 Anisotropy = 233.2354

XX= 226.7348 YX= 94.9439 ZX= -4.4324

XY= 94.4477 YY= 56.5925 ZY= 9.5964

XZ= -8.6800 YZ= 10.1367 ZZ= 374.2759

Eigenvalues: 13.9884 268.9235 374.6913

8 C Isotropic = 32.7577 Anisotropy = 134.9467

XX= -6.4846 YX= 33.4805 ZX= -2.2183

XY= 31.4800 YY= -17.8123 ZY= 4.8437

XZ= -4.6176 YZ= 2.5935 ZZ= 122.5700

Eigenvalues: -45.2705 20.8215 122.7222

9 C Isotropic = 54.5208 Anisotropy = 141.2346

XX= -13.2968 YX= -23.2660 ZX= -2.5821

XY= -24.1273 YY= 28.3820 ZY= 4.1411

XZ= -0.9577 YZ= 4.5284 ZZ= 148.4772

Eigenvalues: -24.0141 38.8993 148.6772

10 S Isotropic = 252.0373 Anisotropy = 125.8992

XX= 267.4735 YX= 106.9415 ZX= -0.9441

XY= 52.0039 YY= 152.9017 ZY= 3.1669

XZ= 5.9823 YZ= -1.8631 ZZ= 335.7368

Eigenvalues: 112.2189 307.9230 335.9701

11 C Isotropic = 31.8257 Anisotropy = 134.3918

XX= -10.2324 YX= 24.8792 ZX= -0.7532

XY= 24.6674 YY= -15.6930 ZY= 1.4455

XZ= -2.2041 YZ= -1.6830 ZZ= 121.4024

Eigenvalues: -37.8911 11.9479 121.4202

12 C Isotropic = 46.2773 Anisotropy = 142.4032

XX= -6.8970 YX= -19.3520 ZX= -0.4860

XY= -19.8033 YY= 4.5528 ZY= 1.7054

XZ= -1.1647 YZ= 2.2171 ZZ= 141.1762

Eigenvalues: -21.5712 19.1905 141.2128

13 C Isotropic = 40.7437 Anisotropy = 107.5639

XX= 84.1067 YX= 63.5094 ZX= 2.3794

XY= 58.9771 YY= -20.3417 ZY= -0.0412

XZ= 2.4021 YZ= -0.1657 ZZ= 58.4662

Eigenvalues: -48.6154 58.3936 112.4530

14 C Isotropic = 54.2899 Anisotropy = 169.6460

XX= 142.0806 YX= 53.8978 ZX= 19.8671

XY= 55.1215 YY= 47.2820 ZY= -17.9841

XZ= 16.9547 YZ= -17.2365 ZZ= -26.4930

Eigenvalues: -36.4382 31.9206 167.3872

15 C Isotropic = 53.3227 Anisotropy = 169.9585

XX= 140.6460 YX= 56.8743 ZX= -3.5783

XY= 58.1432 YY= 37.2847 ZY= 27.0587

XZ= -2.7645 YZ= 25.8942 ZZ= -17.9626

Eigenvalues: -32.8559 26.1956 166.6283

16 C Isotropic = 4.9342 Anisotropy = 119.9130

XX= 54.6781 YX= 64.5811 ZX= 3.6318

XY= 64.0988 YY= -53.0771 ZY= -0.1626

XZ= 3.9229 YZ= -0.1802 ZZ= 13.2017

Eigenvalues: -83.1506 13.0770 84.8762

17 C Isotropic = 52.8651 Anisotropy = 170.9648

XX= 139.0903 YX= 58.3090 ZX= 17.6168

XY= 59.0030 YY= 40.9164 ZY= -20.5195

XZ= 17.7331 YZ= -17.0584 ZZ= -21.4115

Eigenvalues: -34.2936 26.0471 166.8416

18 C Isotropic = 54.0869 Anisotropy = 168.7305

XX= 143.4469 YX= 51.7763 ZX= -3.8559

XY= 54.2502 YY= 42.7555 ZY= 28.6402

XZ= -1.3904 YZ= 25.2017 ZZ= -23.9416

Eigenvalues: -36.1133 31.8001 166.5739

19 F Isotropic = 247.8245 Anisotropy = 153.6208

XX= 332.9888 YX= 36.1123 ZX= 7.6468

XY= 37.2136 YY= 269.7441 ZY= 6.0211

XZ= 8.2078 YZ= 6.2753 ZZ= 140.7406

Eigenvalues: 140.2388 252.9963 350.2384

20 C Isotropic = 50.8989 Anisotropy = 181.2179

XX= 21.7213 YX= -20.4639 ZX= -1.8609

XY= -21.1653 YY= -40.4904 ZY= 7.2934

XZ= -2.3507 YZ= 5.5539 ZZ= 171.4658

Eigenvalues: -46.9525 27.9384 171.7108

21 C Isotropic = 32.4878 Anisotropy = 214.6349

XX= -69.5556 YX= -17.2774 ZX= -4.2225

XY= -21.9605 YY= -8.1147 ZY= 6.9322

XZ= -5.6789 YZ= 8.1087 ZZ= 175.1336

Eigenvalues: -75.3138 -2.8006 175.5777

22 C Isotropic = 44.5519 Anisotropy = 200.6143

XX= -19.2848 YX= 44.0666 ZX= -6.0195

XY= 44.9889 YY= -24.8459 ZY= 9.3583

XZ= -6.2848 YZ= 9.0554 ZZ= 177.7866

Eigenvalues: -67.1669 22.5279 178.2948

23 C Isotropic = 45.8670 Anisotropy = 188.2135

XX= 18.8449 YX= -0.5711 ZX= -2.7312

XY= 5.3216 YY= -52.2415 ZY= 9.6448

XZ= 1.6345 YZ= 7.8896 ZZ= 170.9975

Eigenvalues: -52.6654 18.9237 171.3426

24 C Isotropic = 51.5170 Anisotropy = 180.8279

XX= 28.0406 YX= -10.9109 ZX= -0.3452

XY= -13.4140 YY= -45.5311 ZY= 2.6456

XZ= -0.1188 YZ= 2.1575 ZZ= 172.0415

Eigenvalues: -47.5145 29.9965 172.0690

25 C Isotropic = 28.1932 Anisotropy = 217.8594

XX= -68.4119 YX= -25.4405 ZX= -0.6466

XY= -26.7352 YY= -20.3923 ZY= 2.4430

XZ= -0.2281 YZ= 3.5311 ZZ= 173.3838

Eigenvalues: -79.8595 -8.9937 173.4328

26 C Isotropic = 43.0264 Anisotropy = 202.8673

XX= -26.4773 YX= 37.9896 ZX= -1.2692

XY= 43.4247 YY= -22.6767 ZY= 2.7408

XZ= -1.3153 YZ= 2.5749 ZZ= 178.2332

Eigenvalues: -65.3600 16.1679 178.2712

27 C Isotropic = 49.7786 Anisotropy = 182.9519

XX= 31.0980 YX= 4.0080 ZX= -0.5871

XY= 5.1584 YY= -53.4673 ZY= 2.8298

XZ= 0.1997 YZ= 3.2688 ZZ= 171.7051

Eigenvalues: -53.7564 31.3457 171.7465

28 H Isotropic = 24.3326 Anisotropy = 9.0557

XX= 23.0265 YX= -1.7367 ZX= 1.1617

XY= -2.2204 YY= 25.4708 ZY= -2.2990

XZ= 2.3199 YZ= -6.5245 ZZ= 24.5006

Eigenvalues: 20.5470 22.0812 30.3698

29 H Isotropic = 23.5276 Anisotropy = 4.7148

XX= 21.6982 YX= -2.3614 ZX= -0.7232

XY= -2.3253 YY= 25.5593 ZY= 0.8772

XZ= -0.1848 YZ= -0.9964 ZZ= 23.3253

Eigenvalues: 20.5246 23.3874 26.6708

30 H Isotropic = 23.5939 Anisotropy = 4.8468

XX= 21.6211 YX= -2.4809 ZX= 0.2976

XY= -2.2530 YY= 25.7466 ZY= -1.0909

XZ= -0.1748 YZ= 0.9829 ZZ= 23.4141

Eigenvalues: 20.5438 23.4128 26.8252

31 H Isotropic = 24.4800 Anisotropy = 9.2311

XX= 22.9971 YX= -1.9446 ZX= -1.3457

XY= -2.1884 YY= 25.4883 ZY= 2.2409

XZ= -2.4285 YZ= 6.5175 ZZ= 24.9545

Eigenvalues: 20.8327 21.9731 30.6340

32 H Isotropic = 23.3666 Anisotropy = 8.2351

XX= 28.8471 YX= 0.2902 ZX= 0.1672

XY= 0.0968 YY= 23.2610 ZY= -0.1537

XZ= 0.2008 YZ= -0.1734 ZZ= 17.9917

Eigenvalues: 17.9833 23.2598 28.8567

33 H Isotropic = 23.1811 Anisotropy = 5.4621

XX= 23.8525 YX= -0.6663 ZX= 0.1173

XY= -0.9042 YY= 26.6037 ZY= -0.3057

XZ= 0.0758 YZ= -0.2341 ZZ= 19.0872

Eigenvalues: 19.0766 23.6443 26.8226

34 H Isotropic = 23.8311 Anisotropy = 8.4721

XX= 27.4417 YX= 3.1407 ZX= 0.0819

XY= 2.8508 YY= 25.0716 ZY= -0.0922

XZ= 0.2659 YZ= -0.0878 ZZ= 18.9799

Eigenvalues: 18.9718 23.0423 29.4791

35 H Isotropic = 24.9400 Anisotropy = 16.6166

XX= 33.7486 YX= 6.8203 ZX= 0.7985

XY= 2.9295 YY= 25.4281 ZY= 0.1239

XZ= 0.4132 YZ= 0.3409 ZZ= 15.6433

Eigenvalues: 15.6225 23.1799 36.0177

36 H Isotropic = 23.5995 Anisotropy = 9.0377

XX= 29.5824 YX= 0.3838 ZX= -0.0020

XY= 0.7026 YY= 22.6328 ZY= -0.0556

XZ= -0.0047 YZ= -0.0869 ZZ= 18.5833

Eigenvalues: 18.5820 22.5918 29.6246

37 H Isotropic = 23.1361 Anisotropy = 5.6810

XX= 24.0118 YX= -1.9194 ZX= 0.0171

XY= -1.6615 YY= 25.8210 ZY= -0.0977

XZ= 0.0739 YZ= -0.0548 ZZ= 19.5754

Eigenvalues: 19.5744 22.9104 26.9234

38 H Isotropic = 23.4391 Anisotropy = 5.7149

XX= 25.9638 YX= 1.5805 ZX= -0.0202

XY= 1.9512 YY= 24.8220 ZY= -0.0761

XZ= -0.0095 YZ= -0.0535 ZZ= 19.5315

Eigenvalues: 19.5307 23.5375 27.2491

39 H Isotropic = 22.9831 Anisotropy = 9.9099

XX= 29.4656 YX= -1.0989 ZX= 0.0250

XY= -0.8043 YY= 22.2821 ZY= -0.1125

XZ= 0.0282 YZ= -0.0619 ZZ= 17.2014

Eigenvalues: 17.1999 22.1596 29.5897

40 Bq Isotropic = 7.4304 Anisotropy = 15.1734

XX= 1.3829 YX= -0.7547 ZX= 0.3334

XY= -0.6280 YY= 3.4521 ZY= -0.6029

XZ= 0.2826 YZ= -1.5431 ZZ= 17.4562

Eigenvalues: 1.1731 3.5721 17.5460

41 Bq Isotropic = 6.4577 Anisotropy = 7.0086

XX= 2.1056 YX= -0.9430 ZX= 0.2913

XY= -1.9558 YY= 6.2747 ZY= -2.5074

XZ= -0.4163 YZ= 0.8967 ZZ= 10.9928

Eigenvalues: 1.6415 6.6016 11.1301

42 Bq Isotropic = 5.6636 Anisotropy = 5.9474

XX= 3.0317 YX= -3.1155 ZX= -1.4947

XY= -1.8758 YY= 5.2743 ZY= 3.0078

XZ= -0.1861 YZ= -0.2654 ZZ= 8.6849

Eigenvalues: 1.4168 5.9455 9.6286

43 Bq Isotropic = 10.2275 Anisotropy = 23.4260

XX= 2.6074 YX= 0.9351 ZX= 1.8044

XY= -0.4152 YY= 2.4420 ZY= 0.5773

XZ= 2.2247 YZ= 1.2383 ZZ= 25.6332

Eigenvalues: 2.2381 2.5997 25.8449

44 Bq Isotropic = 8.3271 Anisotropy = 17.8155

XX= 3.0724 YX= -1.2120 ZX= -2.0637

XY= -0.8360 YY= 1.9798 ZY= 0.4374

XZ= -2.2410 YZ= -0.1191 ZZ= 19.9292

Eigenvalues: 1.3103 3.4670 20.2042

6.30 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(0) calculation of compound **7**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	-0.00006	-1.44213	1.33375
C	0	-0.00005	-0.02803	1.18959
N	0	-0.00004	0.61855	0.00000
C	0	-0.00005	-0.02803	-1.18959
C	0	-0.00006	-1.44213	-1.33375
S	0	-0.00011	-2.5084	0.00000
C	0	0.00002	2.08538	0.00000
C	0	-1.22347	2.75205	0.00000
C	0	-1.22080	4.14167	0.00000
C	0	0.00013	4.80285	0.00000
C	0	1.22100	4.14156	0.00000
C	0	1.22357	2.75195	0.00000
C	0	-0.00003	-0.72656	-3.56578

C	0	-0.00004	-1.84816	-2.69951
S	0	-0.00006	0.81796	-2.69964
C	0	0.00000	-0.87216	-4.94475
C	0	0.00004	-2.16779	-5.46011
C	0	0.00005	-3.29387	-4.61916
C	0	0.00001	-3.14786	-3.24558
C	0	-0.00004	-1.84816	2.69951
C	0	-0.00003	-0.72656	3.56578
S	0	-0.00006	0.81796	2.69964
C	0	0.00001	-3.14786	3.24558
C	0	0.00005	-3.29387	4.61916
C	0	0.00004	-2.16779	5.46011
C	0	0.00000	-0.87216	4.94475
F	0	0.00019	6.14827	0.00000
H	0	-2.15515	2.20044	0.00000
H	0	-2.14496	4.70407	0.00000
H	0	2.14521	4.7039	0.00000
H	0	2.1552	2.20026	0.00000
H	0	0.00000	-0.01459	-5.60478
H	0	0.00006	-2.3055	-6.5343
H	0	0.00008	-4.28484	-5.05405
H	0	0.00003	-4.01865	-2.60198
H	0	0.00003	-4.01865	2.60198
H	0	0.00008	-4.28484	5.05405
H	0	0.00006	-2.3055	6.5343
H	0	0.00000	-0.01459	5.60478
Bq	0	-0.00006	-0.80503	0.00000
Bq	0	-0.00005	-0.64539	2.29766
Bq	0	-0.00005	-0.64539	-2.29766
Bq	0	0.00001	-2.0094	4.08915
Bq	0	0.00001	-2.0094	-4.08915

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 31.6297 Anisotropy = 155.5934

XX= 135.3586 YX= 0.0030 ZX= 0.0000

XY= -0.0008 YY= -20.8366 ZY= 28.4124

XZ= -0.0034 YZ= 17.3730 ZZ= -19.6329

Eigenvalues: -43.1353 2.6659 135.3586

2 C Isotropic = 14.9744 Anisotropy = 135.9760

XX= 105.6251 YX= 0.0011 ZX= -0.0017

XY= -0.0011 YY= -34.3519 ZY= 13.6703

XZ= 0.0017 YZ= 19.5442 ZZ= -26.3500

Eigenvalues: -47.4334 -13.2686 105.6251

3 N Isotropic = 18.1822 Anisotropy = 252.4910

XX= 186.5096 YX= 0.0012 ZX= -0.0000

XY= -0.0076 YY= -91.3892 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= -40.5738

Eigenvalues: -91.3892 -40.5738 186.5096

4 C Isotropic = 14.9744 Anisotropy = 135.9760

XX= 105.6251 YX= 0.0011 ZX= 0.0017

XY= -0.0011 YY= -34.3520 ZY= -13.6703

XZ= -0.0017 YZ= -19.5442 ZZ= -26.3500

Eigenvalues: -47.4334 -13.2686 105.6251

5 C Isotropic = 31.6297 Anisotropy = 155.5934

XX= 135.3586 YX= 0.0030 ZX= -0.0000

XY= -0.0008 YY= -20.8366 ZY= -28.4124

XZ= 0.0034 YZ= -17.3730 ZZ= -19.6329

Eigenvalues: -43.1353 2.6659 135.3586

6 S Isotropic = 227.0636 Anisotropy = 454.4424

XX= 530.0252 YX= 0.0039 ZX= -0.0000

XY= -0.0147 YY= 49.7176 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 101.4480

Eigenvalues: 49.7176 101.4480 530.0252

7 C Isotropic = 40.2839 Anisotropy = 104.8051

XX= 51.6604 YX= -0.0035 ZX= 0.0000

XY= -0.0038 YY= -40.9627 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 110.1540

Eigenvalues: -40.9627 51.6604 110.1540

8 C Isotropic = 52.0766 Anisotropy = 168.1106

XX= -31.6214 YX= -28.4703 ZX= -0.0000

XY= -27.5246 YY= 23.7009 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= 164.1504

Eigenvalues: -43.3175 35.3970 164.1504

9 C Isotropic = 55.5472 Anisotropy = 168.9673

XX= -14.4124 YX= 25.6475 ZX= -0.0000

XY= 26.7314 YY= 12.8619 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 168.1921

Eigenvalues: -30.3025 28.7520 168.1921

10 C Isotropic = 3.9431 Anisotropy = 120.0812

XX= 13.2753 YX= -0.0035 ZX= -0.0000

XY= -0.0046 YY= -85.4432 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 83.9973

Eigenvalues: -85.4432 13.2753 83.9973

11 C Isotropic = 55.5461 Anisotropy = 168.9674

XX= -14.4189 YX= -25.6461 ZX= 0.0000

XY= -26.7294 YY= 12.8661 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 168.1910

Eigenvalues: -30.3046 28.7518 168.1910

12 C Isotropic = 52.0753 Anisotropy = 168.1082

XX= -31.6187 YX= 28.4747 ZX= 0.0000

XY= 27.5295 YY= 23.6971 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 164.1474

Eigenvalues: -43.3191 35.3975 164.1474

13 C Isotropic = 31.8833 Anisotropy = 133.8335

XX= 121.1056 YX= -0.0013 ZX= 0.0082

XY= 0.0021 YY= -35.9409 ZY= -12.8727

XZ= 0.0020 YZ= -10.9252 ZZ= 10.4853

Eigenvalues: -38.8129 13.3573 121.1056

14 C Isotropic = 45.6633 Anisotropy = 144.0725

XX= 141.7116 YX= 0.0033 ZX= 0.0012

XY= 0.0027 YY= 16.9661 ZY= 4.5776

XZ= 0.0043 YZ= 5.1366 ZZ= -21.6879

Eigenvalues: -22.2888 17.5671 141.7116

15 S Isotropic = 257.0829 Anisotropy = 136.3820

XX= 348.0043 YX= 0.0057 ZX= 0.0050

XY= 0.0060 YY= 118.4180 ZY= 32.9938

XZ= 0.0042 YZ= -16.8338 ZZ= 304.8266

Eigenvalues: 118.0684 305.1762 348.0043

16 C Isotropic = 50.4658 Anisotropy = 180.1892

XX= 170.5919 YX= 0.0013 ZX= 0.0040

XY= 0.0028 YY= -18.3012 ZY= 38.8605

XZ= 0.0030 YZ= 37.0287 ZZ= -0.8934

Eigenvalues: -48.5274 29.3327 170.5919

17 C Isotropic = 28.3720 Anisotropy = 217.3149

XX= 173.2486 YX= 0.0036 ZX= 0.0017

XY= 0.0041 YY= -9.5437 ZY= -6.2660

XZ= 0.0054 YZ= -8.0777 ZZ= -78.5888

Eigenvalues: -79.3259 -8.8066 173.2486

18 C Isotropic = 42.9484 Anisotropy = 201.7566

XX= 177.4527 YX= 0.0062 ZX= 0.0048

XY= 0.0065 YY= -58.4002 ZY= -25.2555

XZ= 0.0041 YZ= -20.3289 ZZ= 9.7926

Eigenvalues: -65.3166 16.7090 177.4527

19 C Isotropic = 49.3494 Anisotropy = 182.3722

XX= 170.9308 YX= 0.0107 ZX= 0.0059

XY= 0.0057 YY= -36.8562 ZY= 35.2301

XZ= 0.0024 YZ= 34.5112 ZZ= 13.9734

Eigenvalues: -54.5908 31.7081 170.9308

20 C Isotropic = 45.6633 Anisotropy = 144.0725

XX= 141.7116 YX= 0.0033 ZX= -0.0012

XY= 0.0027 YY= 16.9661 ZY= -4.5776

XZ= -0.0043 YZ= -5.1366 ZZ= -21.6879

Eigenvalues: -22.2888 17.5671 141.7116

21 C Isotropic = 31.8833 Anisotropy = 133.8335

XX= 121.1056 YX= -0.0013 ZX= -0.0082

XY= 0.0021 YY= -35.9409 ZY= 12.8727

XZ= -0.0020 YZ= 10.9252 ZZ= 10.4853

Eigenvalues: -38.8129 13.3573 121.1056

22 S Isotropic = 257.0829 Anisotropy = 136.3820

XX= 348.0043 YX= 0.0057 ZX= -0.0050

XY= 0.0060 YY= 118.4180 ZY= -32.9938

XZ= -0.0042 YZ= 16.8338 ZZ= 304.8266

Eigenvalues: 118.0684 305.1762 348.0043

23 C Isotropic = 49.3494 Anisotropy = 182.3722

XX= 170.9308 YX= 0.0107 ZX= -0.0059

XY= 0.0057 YY= -36.8562 ZY= -35.2301

XZ= -0.0024 YZ= -34.5112 ZZ= 13.9734

Eigenvalues: -54.5908 31.7081 170.9308

24 C Isotropic = 42.9484 Anisotropy = 201.7566

XX= 177.4527 YX= 0.0062 ZX= -0.0048

XY= 0.0065 YY= -58.4002 ZY= 25.2555

XZ= -0.0041 YZ= 20.3289 ZZ= 9.7926

Eigenvalues: -65.3166 16.7090 177.4527

25 C Isotropic = 28.3720 Anisotropy = 217.3149

XX= 173.2486 YX= 0.0036 ZX= -0.0017

XY= 0.0041 YY= -9.5437 ZY= 6.2660

XZ= -0.0054 YZ= 8.0777 ZZ= -78.5888

Eigenvalues: -79.3259 -8.8066 173.2486

26 C Isotropic = 50.4658 Anisotropy = 180.1892

XX= 170.5919 YX= 0.0013 ZX= -0.0040

XY= 0.0028 YY= -18.3012 ZY= -38.8605

XZ= -0.0030 YZ= -37.0287 ZZ= -0.8934

Eigenvalues: -48.5274 29.3327 170.5919

27 F Isotropic = 247.4593 Anisotropy = 158.1882

XX= 138.1475 YX= 0.0057 ZX= 0.0000

XY= 0.0050 YY= 251.3123 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 352.9181

Eigenvalues: 138.1475 251.3123 352.9181

28 H Isotropic = 24.3206 Anisotropy = 9.4554

XX= 24.6129 YX= -6.8356 ZX= -0.0000

XY= -2.9307 YY= 26.6575 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 21.6913

Eigenvalues: 20.6462 21.6913 30.6241

29 H Isotropic = 23.8604 Anisotropy = 4.7176

XX= 24.0033 YX= -0.3332 ZX= -0.0000

XY= 1.1054 YY= 26.9558 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 20.6220

Eigenvalues: 20.6220 23.9536 27.0054

30 H Isotropic = 23.8604 Anisotropy = 4.7178

XX= 24.0032 YX= 0.3334 ZX= 0.0000

XY= -1.1053 YY= 26.9560 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= 20.6221

Eigenvalues: 20.6221 23.9536 27.0056

31 H Isotropic = 24.3207 Anisotropy = 9.4556

XX= 24.6136 YX= 6.8359 ZX= 0.0000

XY= 2.9307 YY= 26.6572 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 21.6912

Eigenvalues: 20.6464 21.6912 30.6244

32 H Isotropic = 23.5691 Anisotropy = 8.8041

XX= 18.5420 YX= -0.0002 ZX= -0.0002

XY= -0.0001 YY= 23.9457 ZY= 2.3645

XZ= -0.0001 YZ= 2.8105 ZZ= 28.2196

Eigenvalues: 18.5420 22.7268 29.4385

33 H Isotropic = 23.0893 Anisotropy = 5.6620

XX= 19.5159 YX= -0.0002 ZX= -0.0003

XY= -0.0001 YY= 26.8635 ZY= -0.0912

XZ= -0.0000 YZ= 0.1802 ZZ= 22.8885

Eigenvalues: 19.5159 22.8880 26.8640

34 H Isotropic = 23.4109 Anisotropy = 5.7935

XX= 19.5273 YX= -0.0001 ZX= -0.0001

XY= -0.0000 YY= 23.4864 ZY= -0.5831

XZ= -0.0001 YZ= -0.3228 ZZ= 27.2191

Eigenvalues: 19.5273 23.4322 27.2733

35 H Isotropic = 22.9697 Anisotropy = 10.0549

XX= 17.1347 YX= -0.0006 ZX= -0.0006

XY= -0.0002 YY= 24.7282 ZY= 3.5123

XZ= -0.0002 YZ= 3.6956 ZZ= 27.0462

Eigenvalues: 17.1347 22.1015 29.6729

36 H Isotropic = 22.9697 Anisotropy = 10.0549

XX= 17.1347 YX= -0.0006 ZX= 0.0006

XY= -0.0002 YY= 24.7282 ZY= -3.5123

XZ= 0.0002 YZ= -3.6956 ZZ= 27.0462

Eigenvalues: 17.1347 22.1015 29.6729

37 H Isotropic = 23.4109 Anisotropy = 5.7935

XX= 19.5273 YX= -0.0001 ZX= 0.0001

XY= -0.0000 YY= 23.4864 ZY= 0.5831

XZ= 0.0001 YZ= 0.3228 ZZ= 27.2191

Eigenvalues: 19.5273 23.4322 27.2733

38 H Isotropic = 23.0893 Anisotropy = 5.6620

XX= 19.5159 YX= -0.0002 ZX= 0.0003

XY= -0.0001 YY= 26.8635 ZY= 0.0912

XZ= 0.0000 YZ= -0.1802 ZZ= 22.8885

Eigenvalues: 19.5159 22.8880 26.8640

39 H Isotropic = 23.5691 Anisotropy = 8.8041

XX= 18.5420 YX= -0.0002 ZX= 0.0002

XY= -0.0001 YY= 23.9457 ZY= -2.3645

XZ= 0.0001 YZ= -2.8105 ZZ= 28.2196

Eigenvalues: 18.5420 22.7268 29.4385

40 Bq Isotropic = 6.6419 Anisotropy = 11.4192

XX= 0.8545 YX= -0.0004 ZX= -0.0000

XY= 0.0006 YY= 14.2546 ZY= -0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 4.8164

Eigenvalues: 0.8545 4.8164 14.2546

41 Bq Isotropic = 6.4954 Anisotropy = 27.0951

XX= -14.1318 YX= 0.0004 ZX= 0.0002

XY= -0.0004 YY= 23.8866 ZY= 4.1438

XZ= 0.0001 YZ= 2.1705 ZZ= 9.7315

Eigenvalues: -14.1318 9.0592 24.5588

42 Bq Isotropic = 6.4954 Anisotropy = 27.0951

XX= -14.1318 YX= 0.0004 ZX= -0.0002

XY= -0.0004 YY= 23.8866 ZY= -4.1438

XZ= -0.0001 YZ= -2.1705 ZZ= 9.7315

Eigenvalues: -14.1318 9.0592 24.5588

43 Bq Isotropic = 6.0240 Anisotropy = 3.2078

XX= 3.7370 YX= -0.0001 ZX= 0.0005

XY= -0.0002 YY= 7.7566 ZY= -0.5926

XZ= 0.0001 YZ= -1.0112 ZZ= 6.5786

Eigenvalues: 3.7370 6.1726 8.1626

44 Bq Isotropic = 6.0240 Anisotropy = 3.2078

XX= 3.7370 YX= -0.0001 ZX= -0.0005

XY= -0.0002 YY= 7.7566 ZY= 0.5926

XZ= -0.0001 YZ= 1.0112 ZZ= 6.5786

Eigenvalues: 3.7370 6.1726 8.1626

6.31 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(1) calculation of compound **7**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	-0.00006	-1.44213	1.33375
C	0	-0.00005	-0.02803	1.18959
N	0	-0.00004	0.61855	0.00000
C	0	-0.00005	-0.02803	-1.18959
C	0	-0.00006	-1.44213	-1.33375

S	0	-0.00011	-2.5084	0.00000
C	0	0.00002	2.08538	0.00000
C	0	-1.22347	2.75205	0.00000
C	0	-1.2208	4.14167	0.00000
C	0	0.00013	4.80285	0.00000
C	0	1.221	4.14156	0.00000
C	0	1.22357	2.75195	0.00000
C	0	-0.00003	-0.72656	-3.56578
C	0	-0.00004	-1.84816	-2.69951
S	0	-0.00006	0.81796	-2.69964
C	0	0.00000	-0.87216	-4.94475
C	0	0.00004	-2.16779	-5.46011
C	0	0.00005	-3.29387	-4.61916
C	0	0.00001	-3.14786	-3.24558
C	0	-0.00004	-1.84816	2.69951
C	0	-0.00003	-0.72656	3.56578
S	0	-0.00006	0.81796	2.69964
C	0	0.00001	-3.14786	3.24558
C	0	0.00005	-3.29387	4.61916
C	0	0.00004	-2.16779	5.46011
C	0	0.00000	-0.87216	4.94475
F	0	0.00019	6.14827	0.00000
H	0	-2.15515	2.20044	0.00000
H	0	-2.14496	4.70407	0.00000
H	0	2.14521	4.7039	0.00000
H	0	2.1552	2.20026	0.00000
H	0	0.00000	-0.01459	-5.60478
H	0	0.00006	-2.3055	-6.5343
H	0	0.00008	-4.28484	-5.05405
H	0	0.00003	-4.01865	-2.60198
H	0	0.00003	-4.01865	2.60198
H	0	0.00008	-4.28484	5.05405
H	0	0.00006	-2.3055	6.5343

H 0 0.00000 -0.01459 5.60478

Bq 0 0.99994 -0.80504 0.00000

Bq 0 0.99995 -0.64538 2.29764

Bq 0 0.99995 -0.64538 -2.29764

Bq 0 1.00001 -2.00938 4.08913

Bq 0 1.00001 -2.00938 -4.08913

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 31.6297 Anisotropy = 155.5934

XX= 135.3586 YX= 0.0030 ZX= 0.0000

XY= -0.0008 YY= -20.8366 ZY= 28.4124

XZ= -0.0034 YZ= 17.3730 ZZ= -19.6329

Eigenvalues: -43.1353 2.6659 135.3586

2 C Isotropic = 14.9744 Anisotropy = 135.9760

XX= 105.6251 YX= 0.0011 ZX= -0.0017

XY= -0.0011 YY= -34.3519 ZY= 13.6703

XZ= 0.0017 YZ= 19.5442 ZZ= -26.3500

Eigenvalues: -47.4334 -13.2686 105.6251

3 N Isotropic = 18.1822 Anisotropy = 252.4910

XX= 186.5096 YX= 0.0012 ZX= -0.0000

XY= -0.0076 YY= -91.3892 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= -40.5738

Eigenvalues: -91.3892 -40.5738 186.5096

4 C Isotropic = 14.9744 Anisotropy = 135.9760

XX= 105.6251 YX= 0.0011 ZX= 0.0017

XY= -0.0011 YY= -34.3519 ZY= -13.6703

XZ= -0.0017 YZ= -19.5442 ZZ= -26.3500

Eigenvalues: -47.4334 -13.2686 105.6251

5 C Isotropic = 31.6297 Anisotropy = 155.5934

XX= 135.3586 YX= 0.0030 ZX= -0.0000

XY= -0.0008 YY= -20.8366 ZY= -28.4124

XZ= 0.0034 YZ= -17.3730 ZZ= -19.6329

Eigenvalues: -43.1353 2.6659 135.3586

6 S Isotropic = 227.0636 Anisotropy = 454.4424

XX= 530.0252 YX= 0.0039 ZX= -0.0000

XY= -0.0147 YY= 49.7176 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 101.4480

Eigenvalues: 49.7176 101.4480 530.0252

7 C Isotropic = 40.2839 Anisotropy = 104.8051

XX= 51.6604 YX= -0.0035 ZX= 0.0000

XY= -0.0038 YY= -40.9627 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 110.1540

Eigenvalues: -40.9627 51.6604 110.1540

8 C Isotropic = 52.0766 Anisotropy = 168.1106

XX= -31.6214 YX= -28.4703 ZX= -0.0000

XY= -27.5246 YY= 23.7009 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= 164.1504

Eigenvalues: -43.3175 35.3970 164.1504

9 C Isotropic = 55.5472 Anisotropy = 168.9673

XX= -14.4124 YX= 25.6475 ZX= -0.0000

XY= 26.7314 YY= 12.8619 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 168.1921

Eigenvalues: -30.3025 28.7520 168.1921

10 C Isotropic = 3.9431 Anisotropy = 120.0812

XX= 13.2753 YX= -0.0035 ZX= -0.0000

XY= -0.0046 YY= -85.4432 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 83.9973

Eigenvalues: -85.4432 13.2753 83.9973

11 C Isotropic = 55.5461 Anisotropy = 168.9674

XX= -14.4189 YX= -25.6461 ZX= 0.0000

XY= -26.7294 YY= 12.8661 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 168.1910

Eigenvalues: -30.3046 28.7518 168.1910

12 C Isotropic = 52.0753 Anisotropy = 168.1082

XX= -31.6187 YX= 28.4747 ZX= 0.0000

XY= 27.5295 YY= 23.6971 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 164.1474

Eigenvalues: -43.3191 35.3975 164.1474

13 C Isotropic = 31.8833 Anisotropy = 133.8335

XX= 121.1056 YX= -0.0013 ZX= 0.0082

XY= 0.0021 YY= -35.9409 ZY= -12.8727

XZ= 0.0020 YZ= -10.9252 ZZ= 10.4853

Eigenvalues: -38.8129 13.3573 121.1056

14 C Isotropic = 45.6633 Anisotropy = 144.0725

XX= 141.7116 YX= 0.0033 ZX= 0.0012

XY= 0.0027 YY= 16.9661 ZY= 4.5776

XZ= 0.0043 YZ= 5.1366 ZZ= -21.6879

Eigenvalues: -22.2888 17.5671 141.7116

15 S Isotropic = 257.0829 Anisotropy = 136.3820

XX= 348.0043 YX= 0.0057 ZX= 0.0050

XY= 0.0060 YY= 118.4180 ZY= 32.9938

XZ= 0.0042 YZ= -16.8338 ZZ= 304.8266

Eigenvalues: 118.0684 305.1762 348.0043

16 C Isotropic = 50.4658 Anisotropy = 180.1892

XX= 170.5919 YX= 0.0013 ZX= 0.0040

XY= 0.0028 YY= -18.3012 ZY= 38.8605

XZ= 0.0030 YZ= 37.0287 ZZ= -0.8934

Eigenvalues: -48.5274 29.3327 170.5919

17 C Isotropic = 28.3720 Anisotropy = 217.3149

XX= 173.2486 YX= 0.0036 ZX= 0.0017

XY= 0.0041 YY= -9.5437 ZY= -6.2660

XZ= 0.0054 YZ= -8.0777 ZZ= -78.5888

Eigenvalues: -79.3259 -8.8066 173.2486

18 C Isotropic = 42.9484 Anisotropy = 201.7566

XX= 177.4527 YX= 0.0062 ZX= 0.0048

XY= 0.0065 YY= -58.4002 ZY= -25.2555

XZ= 0.0041 YZ= -20.3289 ZZ= 9.7926

Eigenvalues: -65.3166 16.7090 177.4527

19 C Isotropic = 49.3494 Anisotropy = 182.3722

XX= 170.9308 YX= 0.0107 ZX= 0.0059

XY= 0.0057 YY= -36.8562 ZY= 35.2301

XZ= 0.0024 YZ= 34.5112 ZZ= 13.9734

Eigenvalues: -54.5908 31.7081 170.9308

20 C Isotropic = 45.6633 Anisotropy = 144.0725

XX= 141.7116 YX= 0.0033 ZX= -0.0012

XY= 0.0027 YY= 16.9661 ZY= -4.5776

XZ= -0.0043 YZ= -5.1366 ZZ= -21.6879

Eigenvalues: -22.2888 17.5671 141.7116

21 C Isotropic = 31.8833 Anisotropy = 133.8335

XX= 121.1056 YX= -0.0013 ZX= -0.0082

XY= 0.0021 YY= -35.9409 ZY= 12.8727

XZ= -0.0020 YZ= 10.9252 ZZ= 10.4853

Eigenvalues: -38.8129 13.3573 121.1056

22 S Isotropic = 257.0829 Anisotropy = 136.3820

XX= 348.0043 YX= 0.0057 ZX= -0.0050

XY= 0.0060 YY= 118.4180 ZY= -32.9938

XZ= -0.0042 YZ= 16.8338 ZZ= 304.8266

Eigenvalues: 118.0684 305.1762 348.0043

23 C Isotropic = 49.3494 Anisotropy = 182.3722

XX= 170.9308 YX= 0.0107 ZX= -0.0059

XY= 0.0057 YY= -36.8562 ZY= -35.2301

XZ= -0.0024 YZ= -34.5112 ZZ= 13.9734

Eigenvalues: -54.5908 31.7081 170.9308

24 C Isotropic = 42.9484 Anisotropy = 201.7566

XX= 177.4527 YX= 0.0062 ZX= -0.0048

XY= 0.0065 YY= -58.4002 ZY= 25.2555

XZ= -0.0041 YZ= 20.3289 ZZ= 9.7926

Eigenvalues: -65.3166 16.7090 177.4527

25 C Isotropic = 28.3720 Anisotropy = 217.3149

XX= 173.2486 YX= 0.0036 ZX= -0.0017

XY= 0.0041 YY= -9.5437 ZY= 6.2660

XZ= -0.0054 YZ= 8.0777 ZZ= -78.5888

Eigenvalues: -79.3259 -8.8066 173.2486

26 C Isotropic = 50.4658 Anisotropy = 180.1892

XX= 170.5919 YX= 0.0013 ZX= -0.0040

XY= 0.0028 YY= -18.3012 ZY= -38.8605

XZ= -0.0030 YZ= -37.0287 ZZ= -0.8934

Eigenvalues: -48.5274 29.3327 170.5919

27 F Isotropic = 247.4593 Anisotropy = 158.1882

XX= 138.1475 YX= 0.0057 ZX= -0.0000

XY= 0.0050 YY= 251.3123 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 352.9181

Eigenvalues: 138.1475 251.3123 352.9181

28 H Isotropic = 24.3206 Anisotropy = 9.4554

XX= 24.6129 YX= -6.8356 ZX= -0.0000

XY= -2.9307 YY= 26.6575 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 21.6913

Eigenvalues: 20.6462 21.6913 30.6241

29 H Isotropic = 23.8604 Anisotropy = 4.7176

XX= 24.0033 YX= -0.3332 ZX= -0.0000

XY= 1.1054 YY= 26.9558 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 20.6220

Eigenvalues: 20.6220 23.9536 27.0054

30 H Isotropic = 23.8604 Anisotropy = 4.7178

XX= 24.0032 YX= 0.3334 ZX= 0.0000

XY= -1.1053 YY= 26.9560 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= 20.6221

Eigenvalues: 20.6221 23.9536 27.0056

31 H Isotropic = 24.3207 Anisotropy = 9.4556

XX= 24.6136 YX= 6.8359 ZX= 0.0000

XY= 2.9307 YY= 26.6572 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 21.6912

Eigenvalues: 20.6464 21.6912 30.6244

32 H Isotropic = 23.5691 Anisotropy = 8.8041

XX= 18.5420 YX= -0.0002 ZX= -0.0002

XY= -0.0001 YY= 23.9457 ZY= 2.3645

XZ= -0.0001 YZ= 2.8105 ZZ= 28.2196

Eigenvalues: 18.5420 22.7268 29.4385

33 H Isotropic = 23.0893 Anisotropy = 5.6620

XX= 19.5159 YX= -0.0002 ZX= -0.0003

XY= -0.0001 YY= 26.8635 ZY= -0.0912

XZ= -0.0000 YZ= 0.1802 ZZ= 22.8885

Eigenvalues: 19.5159 22.8880 26.8640

34 H Isotropic = 23.4109 Anisotropy = 5.7935

XX= 19.5273 YX= -0.0001 ZX= -0.0001

XY= -0.0000 YY= 23.4864 ZY= -0.5831

XZ= -0.0001 YZ= -0.3228 ZZ= 27.2191

Eigenvalues: 19.5273 23.4322 27.2733

35 H Isotropic = 22.9697 Anisotropy = 10.0549

XX= 17.1347 YX= -0.0006 ZX= -0.0006

XY= -0.0002 YY= 24.7282 ZY= 3.5123

XZ= -0.0002 YZ= 3.6956 ZZ= 27.0462

Eigenvalues: 17.1347 22.1015 29.6729

36 H Isotropic = 22.9697 Anisotropy = 10.0549

XX= 17.1347 YX= -0.0006 ZX= 0.0006

XY= -0.0002 YY= 24.7282 ZY= -3.5123

XZ= 0.0002 YZ= -3.6956 ZZ= 27.0462

Eigenvalues: 17.1347 22.1015 29.6729

37 H Isotropic = 23.4109 Anisotropy = 5.7935

XX= 19.5273 YX= -0.0001 ZX= 0.0001

XY= -0.0000 YY= 23.4864 ZY= 0.5831

XZ= 0.0001 YZ= 0.3228 ZZ= 27.2191

Eigenvalues: 19.5273 23.4322 27.2733

38 H Isotropic = 23.0893 Anisotropy = 5.6620

XX= 19.5159 YX= -0.0002 ZX= 0.0003

XY= -0.0001 YY= 26.8635 ZY= 0.0912

XZ= 0.0000 YZ= -0.1802 ZZ= 22.8885

Eigenvalues: 19.5159 22.8880 26.8640

39 H Isotropic = 23.5691 Anisotropy = 8.8041

XX= 18.5420 YX= -0.0002 ZX= 0.0002

XY= -0.0001 YY= 23.9457 ZY= -2.3645

XZ= 0.0001 YZ= -2.8105 ZZ= 28.2196

Eigenvalues: 18.5420 22.7268 29.4385

40 Bq Isotropic = 7.1225 Anisotropy = 16.0328

XX= 17.6569 YX= 2.1039 ZX= -0.0000

XY= 0.8979 YY= 3.1956 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 0.5149

Eigenvalues: 0.5149 3.0415 17.8111

41 Bq Isotropic = 5.9647 Anisotropy = 5.6131

XX= 9.1378 YX= 0.7961 ZX= 0.4886

XY= -3.0952 YY= 7.3796 ZY= 0.7770

XZ= -0.3077 YZ= -0.7920 ZZ= 1.3766

Eigenvalues: 1.3756 6.8117 9.7067

42 Bq Isotropic = 5.9647 Anisotropy = 5.6131

XX= 9.1378 YX= 0.7961 ZX= -0.4886

XY= -3.0952 YY= 7.3796 ZY= -0.7770

XZ= 0.3077 YZ= 0.7920 ZZ= 1.3766

Eigenvalues: 1.3756 6.8117 9.7067

43 Bq Isotropic = 8.2012 Anisotropy = 18.1615

XX= 20.0676 YX= -0.7496 ZX= 2.1198

XY= -1.0324 YY= 2.7736 ZY= -0.6816

XZ= 1.6043 YZ= -1.0014 ZZ= 1.7625

Eigenvalues: 1.2064 3.0884 20.3089

44 Bq Isotropic = 8.2012 Anisotropy = 18.1615

XX= 20.0676 YX= -0.7496 ZX= -2.1198

XY= -1.0324 YY= 2.7736 ZY= 0.6816

XZ= -1.6043 YZ= 1.0014 ZZ= 1.7625

Eigenvalues: 1.2064 3.0884 20.3089

6.32 Computed xyz-coordinates and GIAO nuclear magnetic shielding tensors of NICS(-1) calculation of compound **7**$^{2+}$ (Bq = ghost atom, B3LYP/6-311+G**)

Charge = 2 Multiplicity = 1

C	0	-0.00006	-1.44213	1.33375
C	0	-0.00005	-0.02803	1.18959
N	0	-0.00004	0.61855	0.00000
C	0	-0.00005	-0.02803	-1.18959
C	0	-0.00006	-1.44213	-1.33375
S	0	-0.00011	-2.5084	0.00000
C	0	0.00002	2.08538	0.00000
C	0	-1.22347	2.75205	0.00000
C	0	-1.2208	4.14167	0.00000
C	0	0.00013	4.80285	0.00000
C	0	1.221	4.14156	0.00000
C	0	1.22357	2.75195	0.00000
C	0	-0.00003	-0.72656	-3.56578
C	0	-0.00004	-1.84816	-2.69951
S	0	-0.00006	0.81796	-2.69964
C	0	0.00000	-0.87216	-4.94475
C	0	0.00004	-2.16779	-5.46011
C	0	0.00005	-3.29387	-4.61916
C	0	0.00001	-3.14786	-3.24558
C	0	-0.00004	-1.84816	2.69951
C	0	-0.00003	-0.72656	3.56578
S	0	-0.00006	0.81796	2.69964
C	0	0.00001	-3.14786	3.24558
C	0	0.00005	-3.29387	4.61916
C	0	0.00004	-2.16779	5.46011
C	0	0.00000	-0.87216	4.94475
F	0	0.00019	6.14827	0.00000
H	0	-2.15515	2.20044	0.00000

H	0	-2.14496	4.70407	0.00000
H	0	2.14521	4.7039	0.00000
H	0	2.1552	2.20026	0.00000
H	0	0.00000	-0.01459	-5.60478
H	0	0.00006	-2.3055	-6.5343
H	0	0.00008	-4.28484	-5.05405
H	0	0.00003	-4.01865	-2.60198
H	0	0.00003	-4.01865	2.60198
H	0	0.00008	-4.28484	5.05405
H	0	0.00006	-2.3055	6.5343
H	0	0.00000	-0.01459	5.60478
Bq	0	-1.00006	-0.80502	0.00000
Bq	0	-1.00005	-0.64539	2.29767
Bq	0	-1.00005	-0.64539	-2.29767
Bq	0	-1.00000	-2.00942	4.08917
Bq	0	-1.00000	-2.00942	-4.08917

Calculating GIAO nuclear magnetic shielding tensors.

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 31.6297 Anisotropy = 155.5934

XX= 135.3586 YX= 0.0030 ZX= 0.0000

XY= -0.0008 YY= -20.8366 ZY= 28.4124

XZ= -0.0034 YZ= 17.3730 ZZ= -19.6329

Eigenvalues: -43.1353 2.6659 135.3586

2 C Isotropic = 14.9744 Anisotropy = 135.9760

XX= 105.6251 YX= 0.0011 ZX= -0.0017

XY= -0.0011 YY= -34.3519 ZY= 13.6703

XZ= 0.0017 YZ= 19.5442 ZZ= -26.3500

Eigenvalues: -47.4334 -13.2686 105.6251

3 N Isotropic = 18.1822 Anisotropy = 252.4910

XX= 186.5096 YX= 0.0012 ZX= 0.0000

XY= -0.0076 YY= -91.3892 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= -40.5738

Eigenvalues: -91.3892 -40.5738 186.5096

4 C Isotropic = 14.9744 Anisotropy = 135.9760

XX= 105.6251 YX= 0.0011 ZX= 0.0017

XY= -0.0011 YY= -34.3520 ZY= -13.6703

XZ= -0.0017 YZ= -19.5442 ZZ= -26.3500

Eigenvalues: -47.4334 -13.2686 105.6251

5 C Isotropic = 31.6297 Anisotropy = 155.5934

XX= 135.3586 YX= 0.0030 ZX= -0.0000

XY= -0.0008 YY= -20.8366 ZY= -28.4124

XZ= 0.0034 YZ= -17.3730 ZZ= -19.6329

Eigenvalues: -43.1353 2.6659 135.3586

6 S Isotropic = 227.0636 Anisotropy = 454.4424

XX= 530.0252 YX= 0.0039 ZX= -0.0000

XY= -0.0147 YY= 49.7176 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 101.4480

Eigenvalues: 49.7176 101.4480 530.0252

7 C Isotropic = 40.2839 Anisotropy = 104.8051

XX= 51.6604 YX= -0.0035 ZX= 0.0000

XY= -0.0038 YY= -40.9627 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 110.1540

Eigenvalues: -40.9627 51.6604 110.1540

8 C Isotropic = 52.0766 Anisotropy = 168.1106

XX= -31.6214 YX= -28.4703 ZX= -0.0000

XY= -27.5246 YY= 23.7009 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= 164.1504

Eigenvalues: -43.3175 35.3970 164.1504

9 C Isotropic = 55.5472 Anisotropy = 168.9673

XX= -14.4124 YX= 25.6475 ZX= -0.0000

XY= 26.7314 YY= 12.8619 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 168.1921

Eigenvalues: -30.3025 28.7520 168.1921

10 C Isotropic = 3.9431 Anisotropy = 120.0812

XX= 13.2753 YX= -0.0035 ZX= -0.0000

XY= -0.0046 YY= -85.4432 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 83.9973

Eigenvalues: -85.4432 13.2753 83.9973

11 C Isotropic = 55.5461 Anisotropy = 168.9674

XX= -14.4189 YX= -25.6461 ZX= 0.0000

XY= -26.7294 YY= 12.8661 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 168.1910

Eigenvalues: -30.3046 28.7518 168.1910

12 C Isotropic = 52.0753 Anisotropy = 168.1082

XX= -31.6187 YX= 28.4747 ZX= 0.0000

XY= 27.5295 YY= 23.6971 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 164.1474

Eigenvalues: -43.3191 35.3975 164.1474

13 C Isotropic = 31.8833 Anisotropy = 133.8335

XX= 121.1056 YX= -0.0013 ZX= 0.0082

XY= 0.0021 YY= -35.9409 ZY= -12.8727

XZ= 0.0020 YZ= -10.9252 ZZ= 10.4853

Eigenvalues: -38.8129 13.3573 121.1056

14 C Isotropic = 45.6633 Anisotropy = 144.0725

XX= 141.7116 YX= 0.0033 ZX= 0.0012

XY= 0.0027 YY= 16.9661 ZY= 4.5776

XZ= 0.0043 YZ= 5.1366 ZZ= -21.6879

Eigenvalues: -22.2888 17.5671 141.7116

15 S Isotropic = 257.0829 Anisotropy = 136.3820

XX= 348.0043 YX= 0.0057 ZX= 0.0050

XY= 0.0060 YY= 118.4180 ZY= 32.9938

XZ= 0.0042 YZ= -16.8338 ZZ= 304.8266

Eigenvalues: 118.0684 305.1762 348.0043

16 C Isotropic = 50.4658 Anisotropy = 180.1892

XX= 170.5919 YX= 0.0013 ZX= 0.0040

XY= 0.0028 YY= -18.3012 ZY= 38.8605

XZ= 0.0030 YZ= 37.0287 ZZ= -0.8934

Eigenvalues: -48.5274 29.3327 170.5919

17 C Isotropic = 28.3720 Anisotropy = 217.3149

XX= 173.2486 YX= 0.0036 ZX= 0.0017

XY= 0.0041 YY= -9.5437 ZY= -6.2660

XZ= 0.0054 YZ= -8.0777 ZZ= -78.5888

Eigenvalues: -79.3259 -8.8066 173.2486

18 C Isotropic = 42.9484 Anisotropy = 201.7566

XX= 177.4527 YX= 0.0062 ZX= 0.0048

XY= 0.0065 YY= -58.4002 ZY= -25.2555

XZ= 0.0041 YZ= -20.3289 ZZ= 9.7926

Eigenvalues: -65.3166 16.7090 177.4527

19 C Isotropic = 49.3494 Anisotropy = 182.3722

XX= 170.9308 YX= 0.0107 ZX= 0.0059

XY= 0.0057 YY= -36.8562 ZY= 35.2301

XZ= 0.0024 YZ= 34.5112 ZZ= 13.9734

Eigenvalues: -54.5908 31.7081 170.9308

20 C Isotropic = 45.6633 Anisotropy = 144.0725

XX= 141.7116 YX= 0.0033 ZX= -0.0012

XY= 0.0027 YY= 16.9661 ZY= -4.5776

XZ= -0.0043 YZ= -5.1366 ZZ= -21.6879

Eigenvalues: -22.2888 17.5671 141.7116

21 C Isotropic = 31.8833 Anisotropy = 133.8335

XX= 121.1056 YX= -0.0013 ZX= -0.0082

XY= 0.0021 YY= -35.9409 ZY= 12.8727

XZ= -0.0020 YZ= 10.9252 ZZ= 10.4853

Eigenvalues: -38.8129 13.3573 121.1056

22 S Isotropic = 257.0829 Anisotropy = 136.3820

XX= 348.0043 YX= 0.0057 ZX= -0.0050

XY= 0.0060 YY= 118.4180 ZY= -32.9938

XZ= -0.0042 YZ= 16.8338 ZZ= 304.8266

Eigenvalues: 118.0684 305.1762 348.0043

23 C Isotropic = 49.3494 Anisotropy = 182.3722

XX= 170.9308 YX= 0.0107 ZX= -0.0059

XY= 0.0057 YY= -36.8562 ZY= -35.2301

XZ= -0.0024 YZ= -34.5112 ZZ= 13.9734

Eigenvalues: -54.5908 31.7081 170.9308

24 C Isotropic = 42.9484 Anisotropy = 201.7566

XX= 177.4527 YX= 0.0062 ZX= -0.0048

XY= 0.0065 YY= -58.4002 ZY= 25.2555

XZ= -0.0041 YZ= 20.3289 ZZ= 9.7926

Eigenvalues: -65.3166 16.7090 177.4527

25 C Isotropic = 28.3720 Anisotropy = 217.3149

XX= 173.2486 YX= 0.0036 ZX= -0.0017

XY= 0.0041 YY= -9.5437 ZY= 6.2660

XZ= -0.0054 YZ= 8.0777 ZZ= -78.5888

Eigenvalues: -79.3259 -8.8066 173.2486

26 C Isotropic = 50.4658 Anisotropy = 180.1892

XX= 170.5919 YX= 0.0013 ZX= -0.0040

XY= 0.0028 YY= -18.3012 ZY= -38.8605

XZ= -0.0030 YZ= -37.0287 ZZ= -0.8934

Eigenvalues: -48.5274 29.3327 170.5919

27 F Isotropic = 247.4593 Anisotropy = 158.1882

XX= 138.1475 YX= 0.0057 ZX= -0.0000

XY= 0.0050 YY= 251.3123 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 352.9181

Eigenvalues: 138.1475 251.3123 352.9181

28 H Isotropic = 24.3206 Anisotropy = 9.4554

XX= 24.6129 YX= -6.8356 ZX= -0.0000

XY= -2.9307 YY= 26.6575 ZY= 0.0000

XZ= -0.0000 YZ= -0.0000 ZZ= 21.6913

Eigenvalues: 20.6462 21.6913 30.6241

29 H Isotropic = 23.8604 Anisotropy = 4.7176

XX= 24.0033 YX= -0.3332 ZX= -0.0000

XY= 1.1054 YY= 26.9558 ZY= 0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 20.6220

Eigenvalues: 20.6220 23.9536 27.0054

30 H Isotropic = 23.8604 Anisotropy = 4.7178

XX= 24.0032 YX= 0.3334 ZX= 0.0000

XY= -1.1053 YY= 26.9560 ZY= 0.0000

XZ= 0.0000 YZ= 0.0000 ZZ= 20.6221

Eigenvalues: 20.6221 23.9536 27.0056

31 H Isotropic = 24.3207 Anisotropy = 9.4556

XX= 24.6136 YX= 6.8359 ZX= 0.0000

XY= 2.9307 YY= 26.6572 ZY= 0.0000

XZ= 0.0000 YZ= -0.0000 ZZ= 21.6912

Eigenvalues: 20.6464 21.6912 30.6244

32 H Isotropic = 23.5691 Anisotropy = 8.8041

XX= 18.5420 YX= -0.0002 ZX= -0.0002

XY= -0.0001 YY= 23.9457 ZY= 2.3645

XZ= -0.0001 YZ= 2.8105 ZZ= 28.2196

Eigenvalues: 18.5420 22.7268 29.4385

33 H Isotropic = 23.0893 Anisotropy = 5.6620

XX= 19.5159 YX= -0.0002 ZX= -0.0003

XY= -0.0001 YY= 26.8635 ZY= -0.0912

XZ= -0.0000 YZ= 0.1802 ZZ= 22.8885

Eigenvalues: 19.5159 22.8880 26.8640

34 H Isotropic = 23.4109 Anisotropy = 5.7935

XX= 19.5273 YX= -0.0001 ZX= -0.0001

XY= -0.0000 YY= 23.4864 ZY= -0.5831

XZ= -0.0001 YZ= -0.3228 ZZ= 27.2191

Eigenvalues: 19.5273 23.4322 27.2733

35 H Isotropic = 22.9697 Anisotropy = 10.0549

XX= 17.1347 YX= -0.0006 ZX= -0.0006

XY= -0.0002 YY= 24.7282 ZY= 3.5123

XZ= -0.0002 YZ= 3.6956 ZZ= 27.0462

Eigenvalues: 17.1347 22.1015 29.6729

36 H Isotropic = 22.9697 Anisotropy = 10.0549

XX= 17.1347 YX= -0.0006 ZX= 0.0006

XY= -0.0002 YY= 24.7282 ZY= -3.5123

XZ= 0.0002 YZ= -3.6956 ZZ= 27.0462

Eigenvalues: 17.1347 22.1015 29.6729

37 H Isotropic = 23.4109 Anisotropy = 5.7935

XX= 19.5273 YX= -0.0001 ZX= 0.0001

XY= -0.0000 YY= 23.4864 ZY= 0.5831

XZ= 0.0001 YZ= 0.3228 ZZ= 27.2191

Eigenvalues: 19.5273 23.4322 27.2733

38 H Isotropic = 23.0893 Anisotropy = 5.6620

XX= 19.5159 YX= -0.0002 ZX= 0.0003

XY= -0.0001 YY= 26.8635 ZY= 0.0912

XZ= 0.0000 YZ= -0.1802 ZZ= 22.8885

Eigenvalues: 19.5159 22.8880 26.8640

39 H Isotropic = 23.5691 Anisotropy = 8.8041

XX= 18.5420 YX= -0.0002 ZX= 0.0002

XY= -0.0001 YY= 23.9457 ZY= -2.3645

XZ= 0.0001 YZ= -2.8105 ZZ= 28.2196

Eigenvalues: 18.5420 22.7268 29.4385

40 Bq Isotropic = 7.1226 Anisotropy = 16.0334

XX= 17.6573 YX= -2.1050 ZX= -0.0000

XY= -0.8978 YY= 3.1959 ZY= -0.0000

XZ= -0.0000 YZ= 0.0000 ZZ= 0.5146

Eigenvalues: 0.5146 3.0417 17.8115

41 Bq Isotropic = 5.9644 Anisotropy = 5.6131

XX= 9.1375 YX= -0.7957 ZX= -0.4891

XY= 3.0948 YY= 7.3795 ZY= 0.7776

XZ= 0.3075 YZ= -0.7912 ZZ= 1.3762

Eigenvalues: 1.3751 6.8116 9.7065

42 Bq Isotropic = 5.9644 Anisotropy = 5.6131

XX= 9.1375 YX= -0.7957 ZX= 0.4891

XY= 3.0948 YY= 7.3795 ZY= -0.7776

XZ= -0.3075 YZ= 0.7912 ZZ= 1.3762

Eigenvalues: 1.3751 6.8116 9.7065

43 Bq Isotropic = 8.2010 Anisotropy = 18.1611

XX= 20.0669 YX= 0.7504 ZX= -2.1200

XY= 1.0329 YY= 2.7734 ZY= -0.6818

XZ= -1.6050 YZ= -1.0014 ZZ= 1.7627

Eigenvalues: 1.2064 3.0881 20.3084

44 Bq Isotropic = 8.2010 Anisotropy = 18.1611

XX= 20.0669 YX= 0.7504 ZX= 2.1201

XY= 1.0329 YY= 2.7734 ZY= 0.6818

XZ= 1.6050 YZ= 1.0014 ZZ= 1.7627

Eigenvalues: 1.2064 3.0881 20.3084

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