# Electronic Supplementary Information

## Dinuclear Ruthenium Acetylide Complexes with Diethynylated Anthrahydroquinone and Anthraquinone Frameworks: A Multi-Stimuli-Responsive Organometallic Switch

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**Table of Contents**

**Table S6.** Cartesian coordinates of optimized geometry of **2'$^{C4}$**.
**Table S7.** Cartesian coordinates of optimized geometry of **3'$^{C4}$**.
**Table S8.** Cartesian coordinates of optimized geometry of [**1'$^{Cl}$**]$^{+}$.
**Table S9.** Cartesian coordinates of optimized geometry of [**2'$^{Cl}$**]$^{+}$.
**Table S10.** Cartesian coordinates of optimized geometry of [**3'$^{Cl}$**]$^{+}$.
**Table S11.** Cartesian coordinates of optimized geometry of [**1'$^{C4}$**]$^{+}$.
**Table S12.** Cartesian coordinates of optimized geometry of [**2'$^{C4}$**]$^{+}$.
**Table S13.** Cartesian coordinates of optimized geometry of [**3'$^{C4}$**]$^{+}$.

## I. NMR and MS spectroscopic data

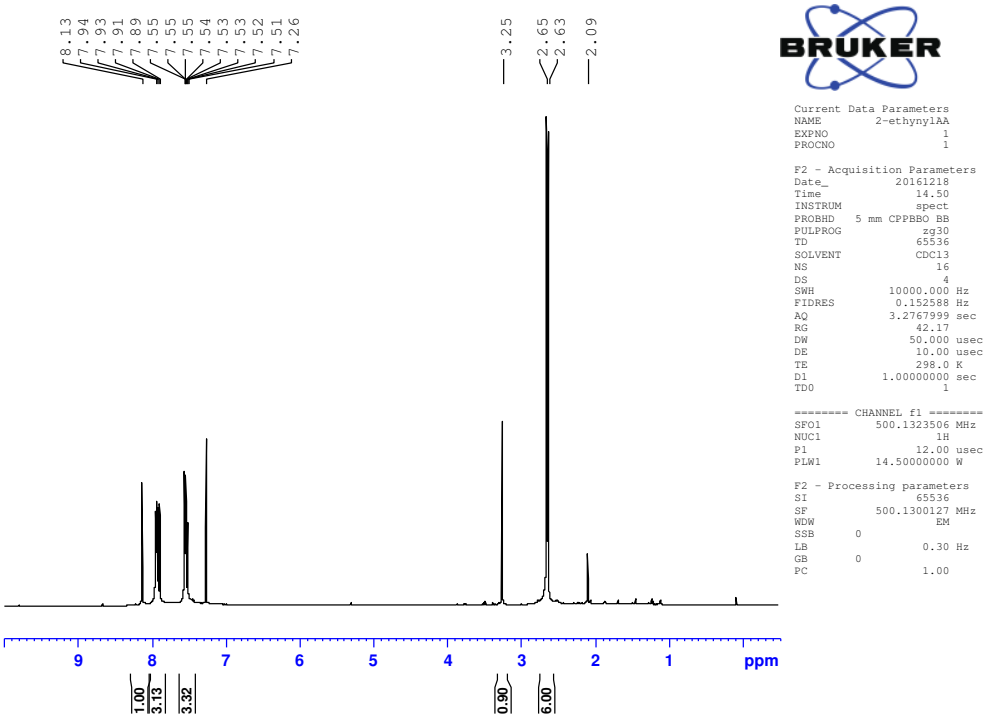


**Figure S1a.** A $^{1}$H NMR spectrum of **6** (500 MHz, $CDCl_3$, r.t.).

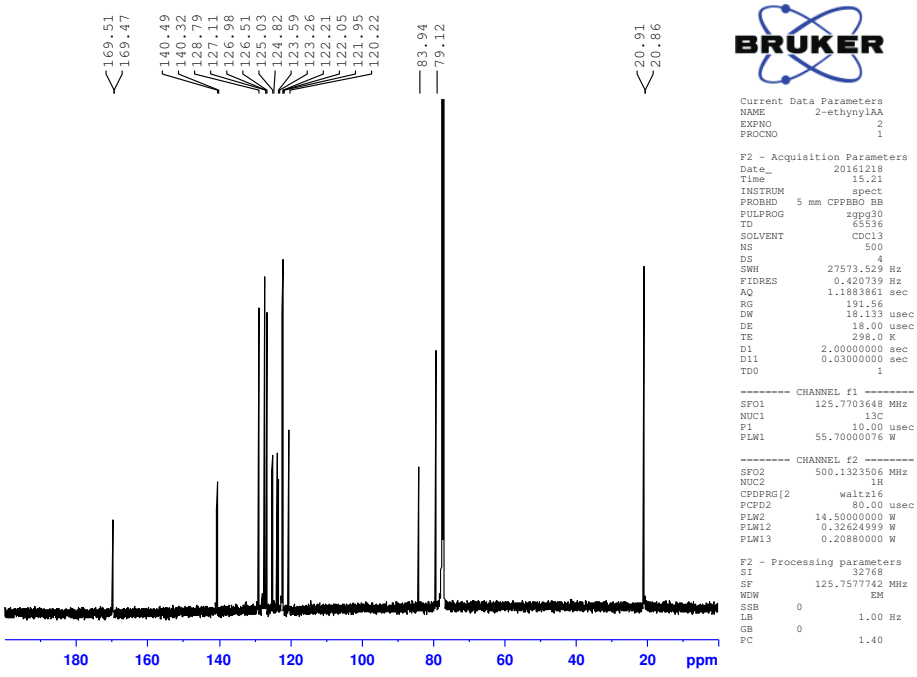


**Figure S1b.** A $^{13}$C{$^{1}$H} NMR spectrum of **6** (126 MHz, $CDCl_3$, r.t.).

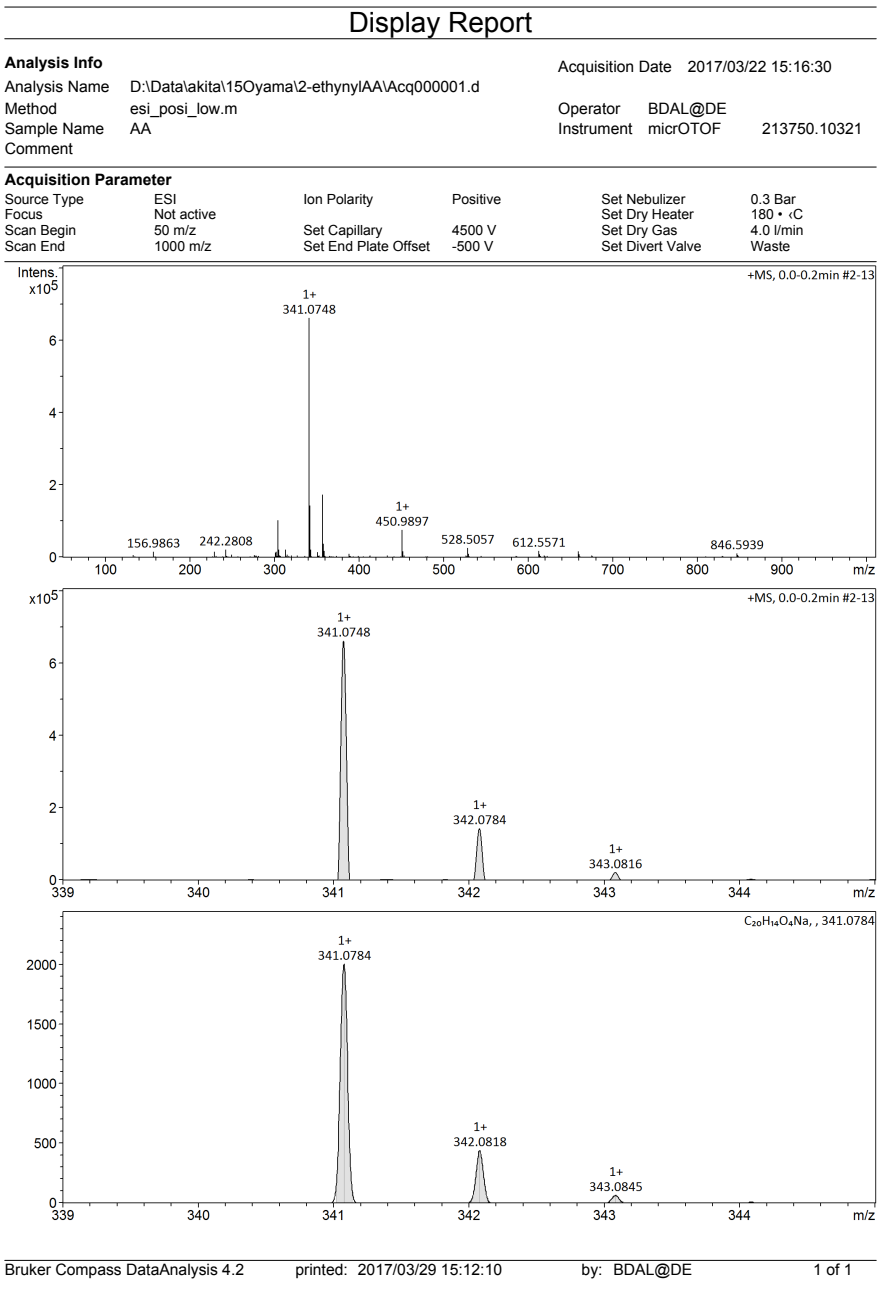


**Figure S1c.** ESI-TOF MS spectra of **6**.

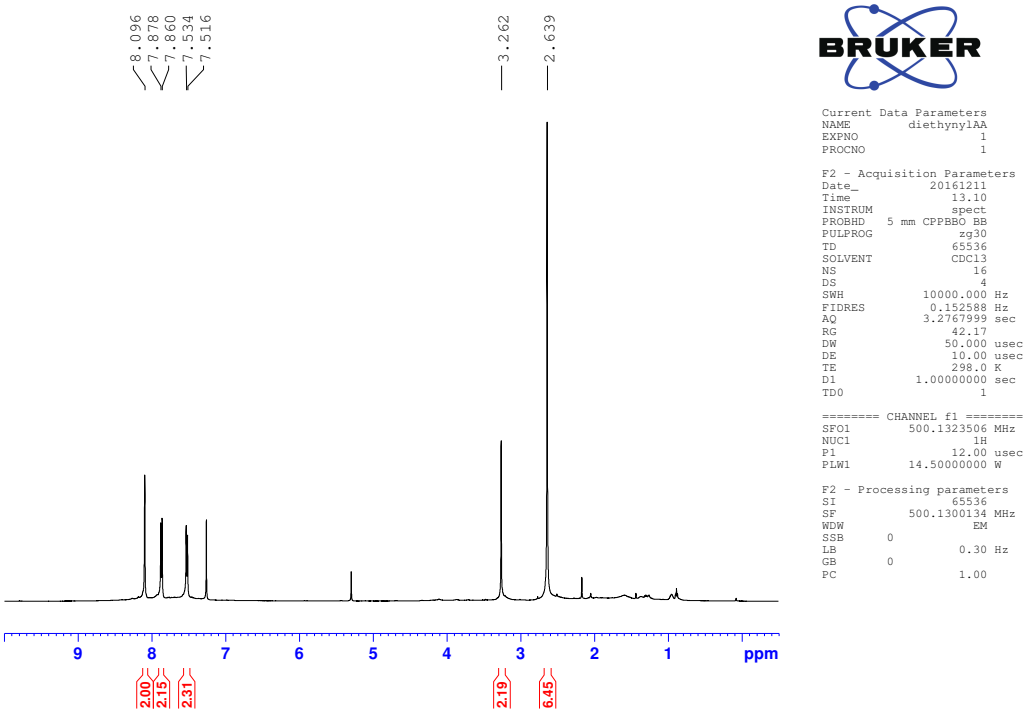


**Figure S2a.** A $^{1}$H NMR spectrum of **7** (500 MHz, $CDCl_3$, r.t.).

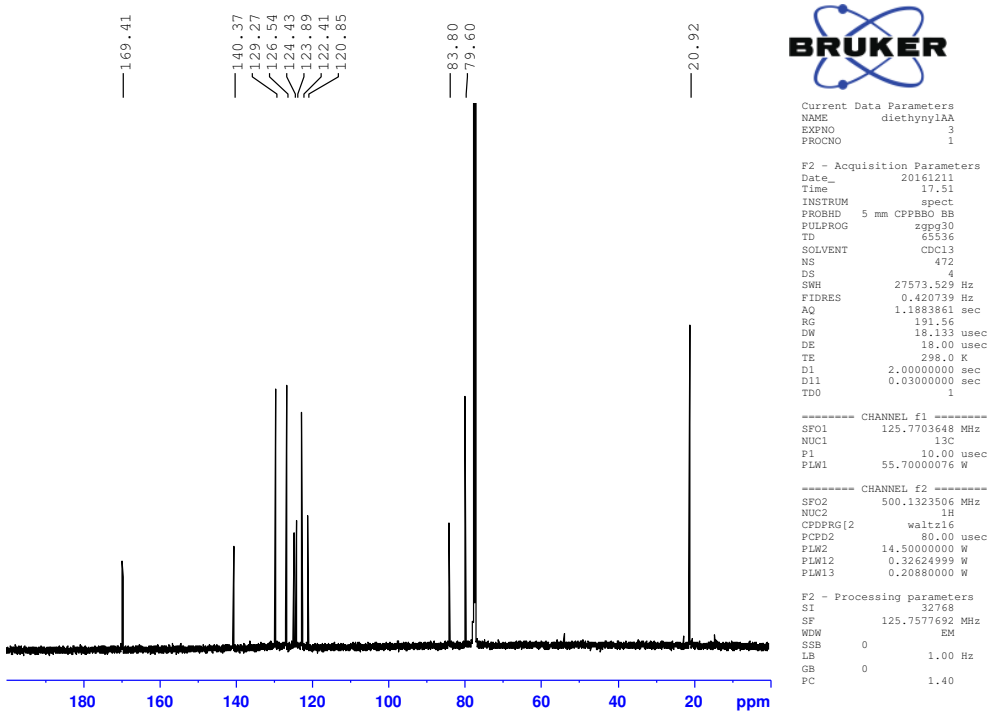


**Figure S2b.** A $^{13}$C{$^{1}$H} NMR spectrum of **7** (126 MHz, $CDCl_3$, r.t.).

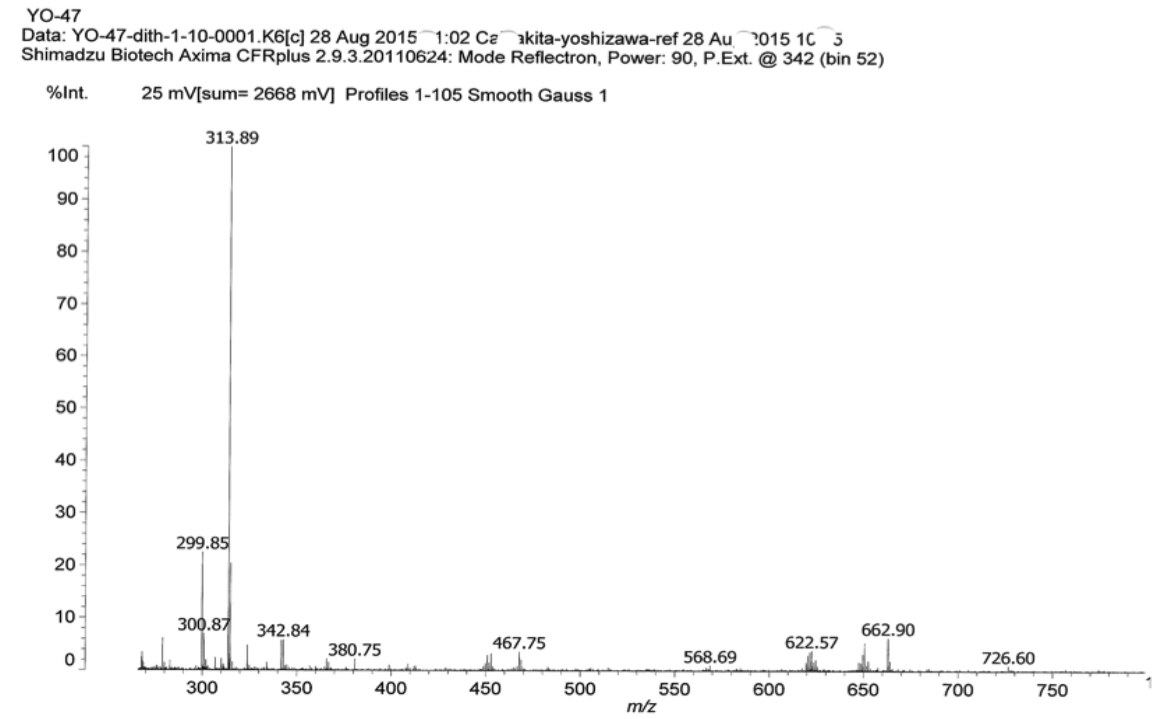


**Figure S2c.** A MALDI-TOF MS spectrum of **7**.

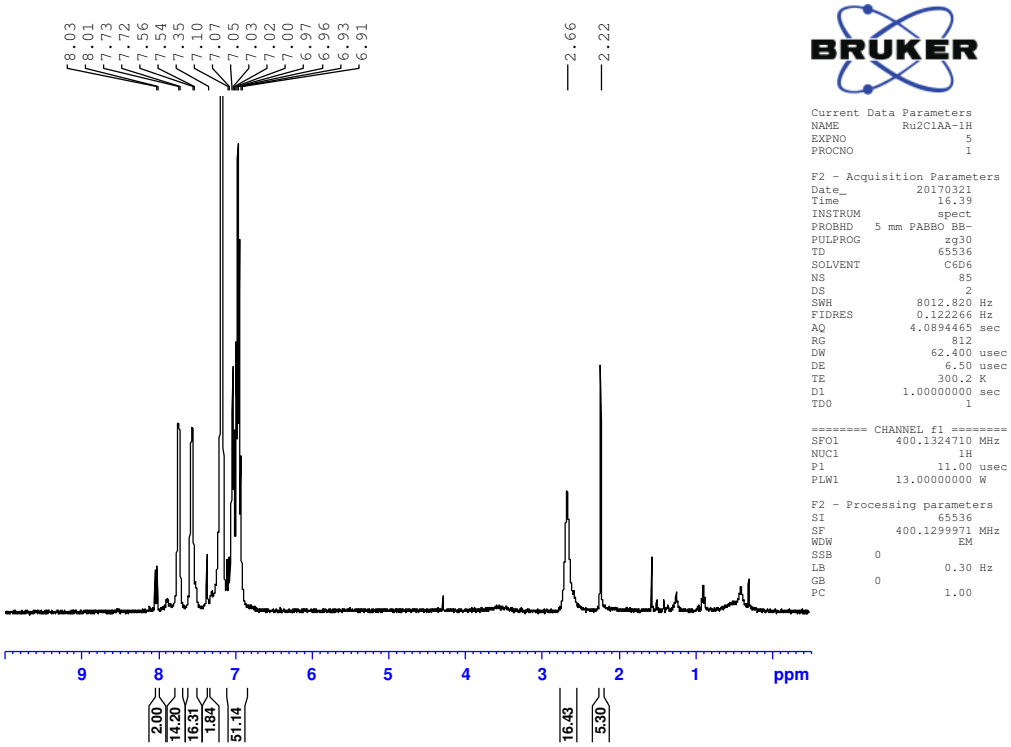


**Figure S3a.** A $^{1}$H NMR spectrum of $\mathbf{1^{Cl}}$ (400 MHz, $C_6D_6$, r.t.).

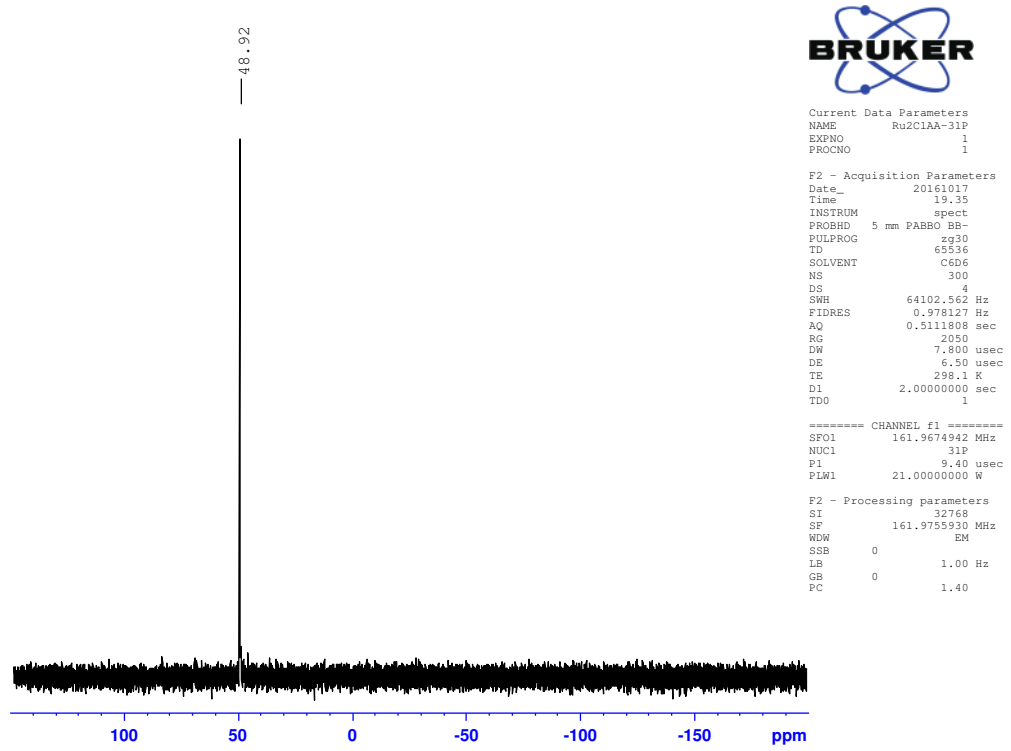


**Figure S3b.** A $^{31}$P {$^{1}$H} NMR spectrum of $\mathbf{1^{Cl}}$ (162 MHz, $C_6D_6$, r.t.).

# Display Report

**Analysis Info**

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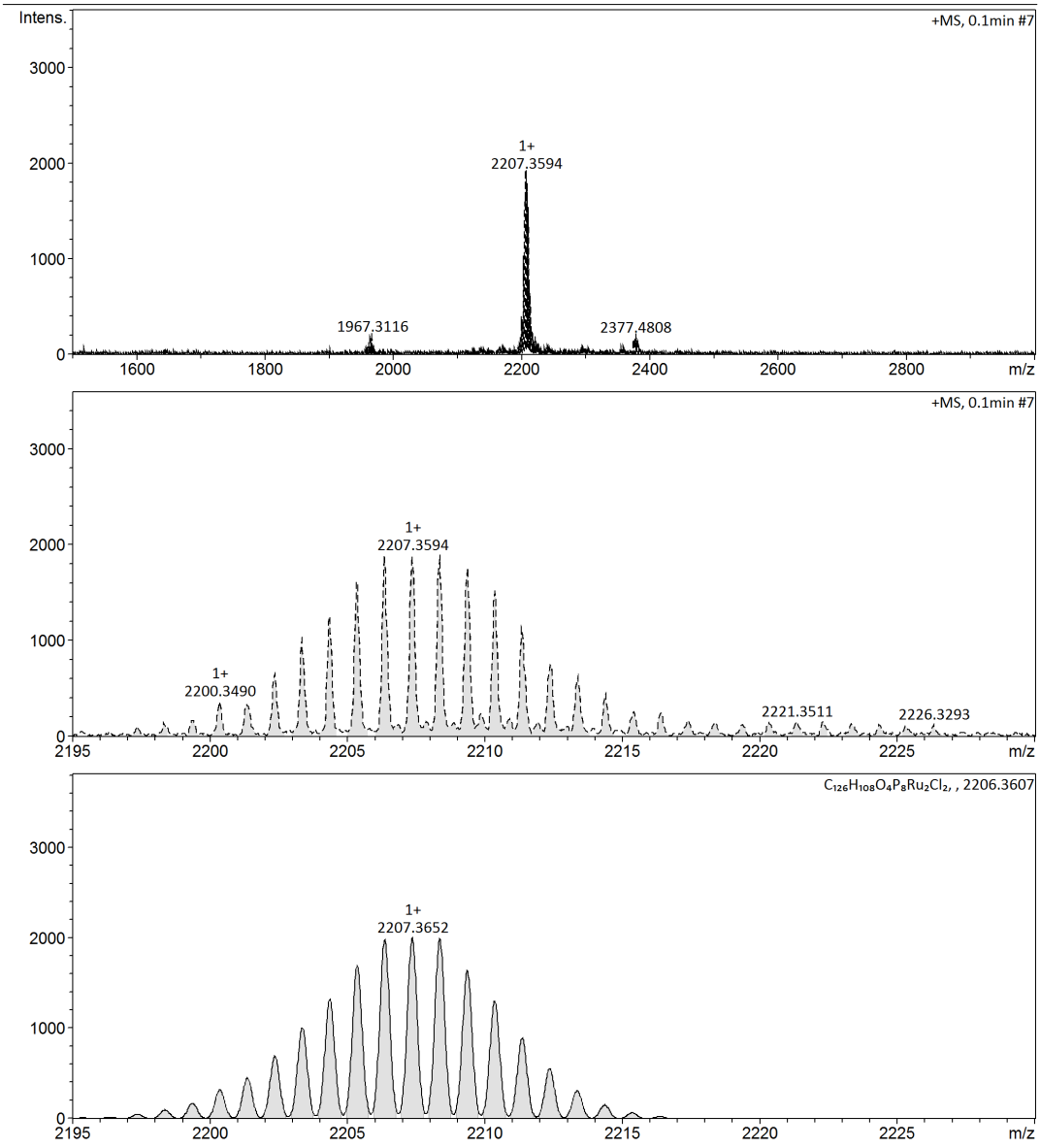


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**Figure S3c.** ESI-TOF MS spectra of $\mathbf{1^{Cl}}$.

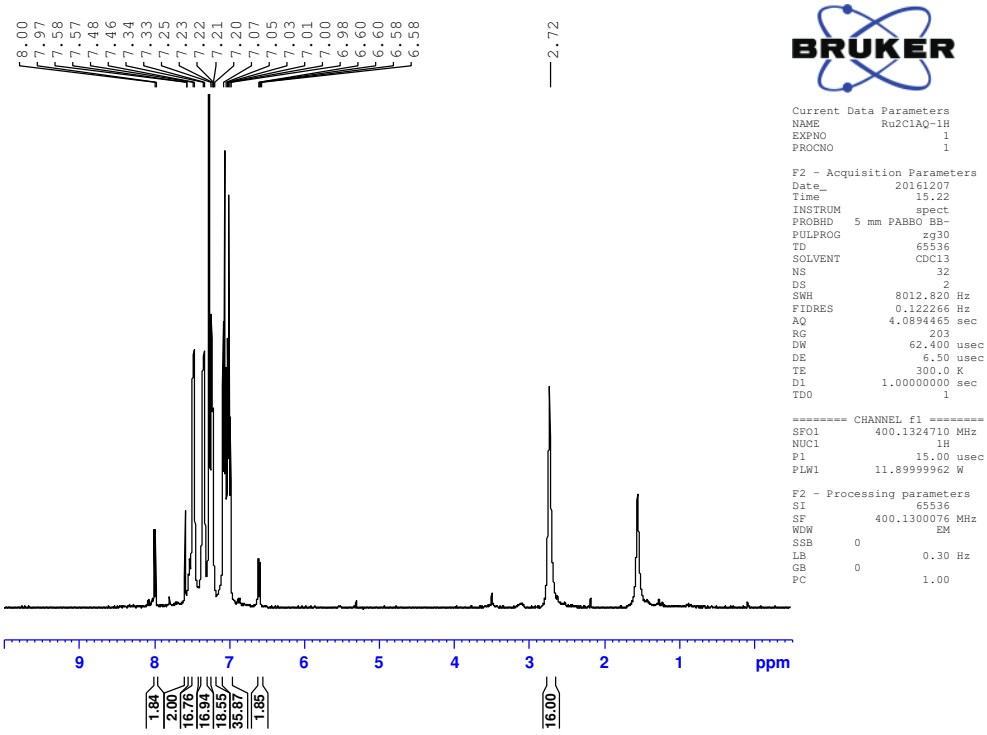



**Figure S4a.** A $^{1}$H NMR spectrum of **2$^{Cl}$** (400 MHz, $CDCl_3$, r.t.).

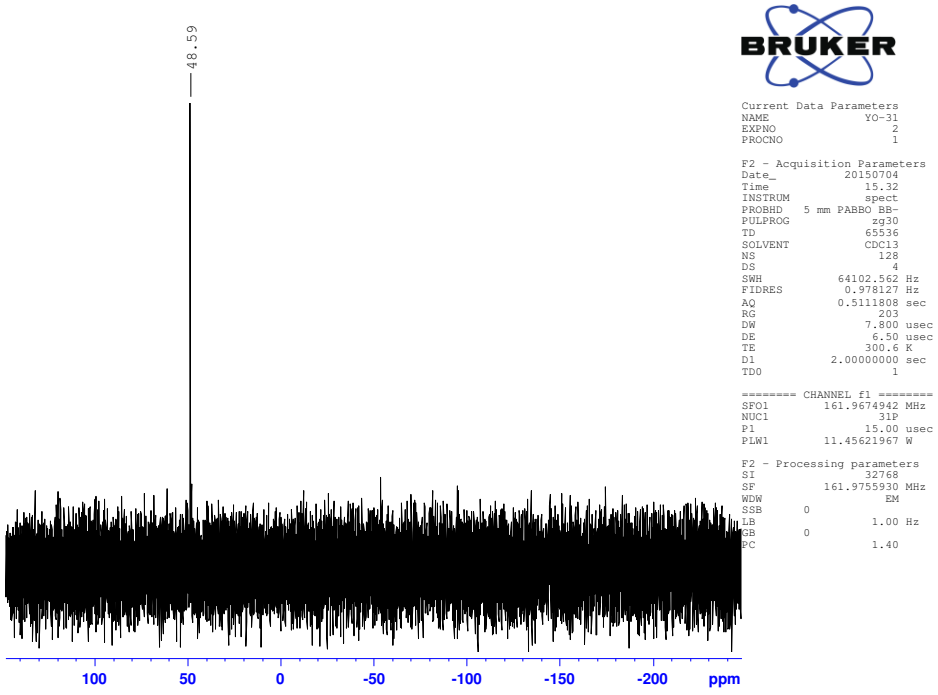



**Figure S4b.** A $^{31}$P $\{^{1}H\}$ NMR spectrum of **2$^{Cl}$** (162 MHz, $CDCl_3$, r.t.).

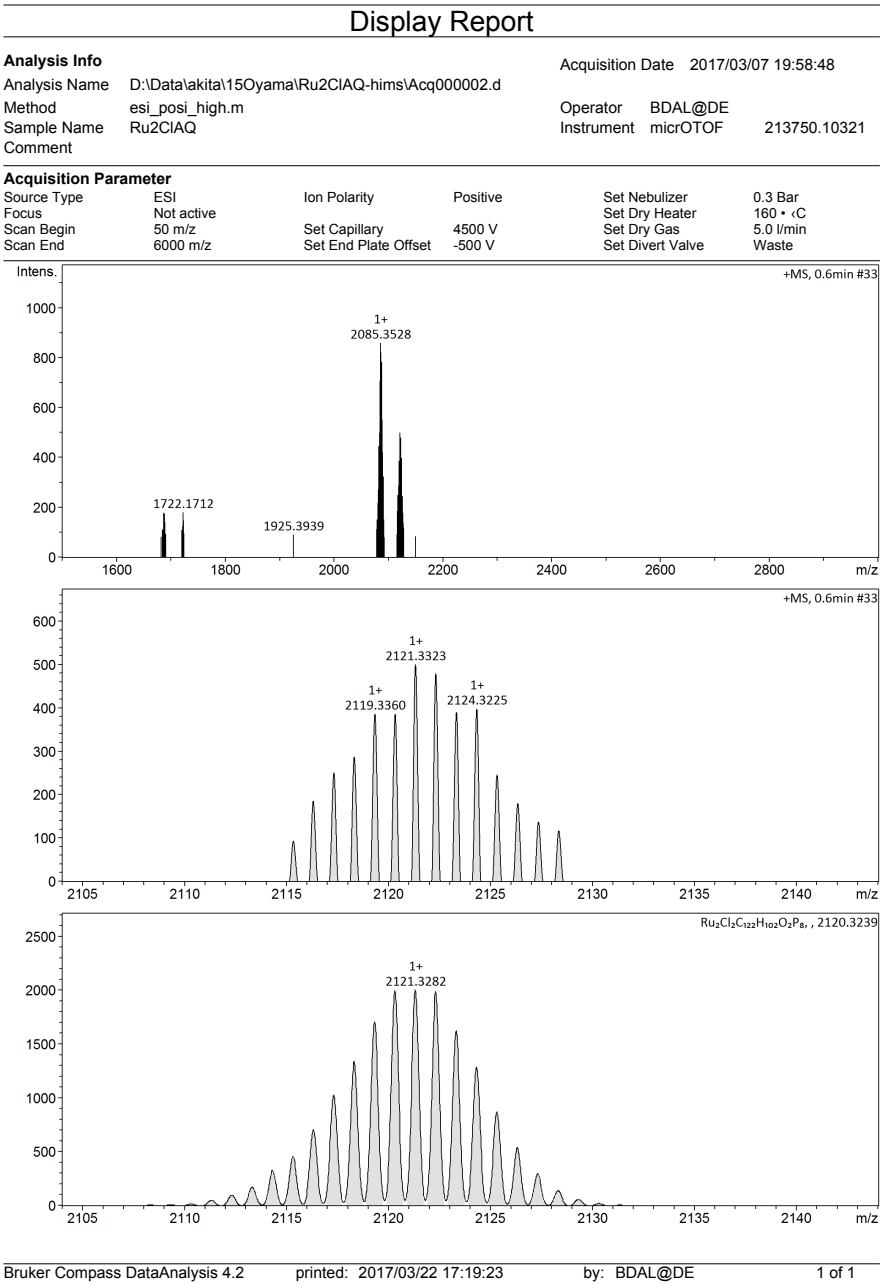



**Figure S4c.** ESI-TOF MS spectra of $\mathbf{2}^{\mathbf{Cl}}$.

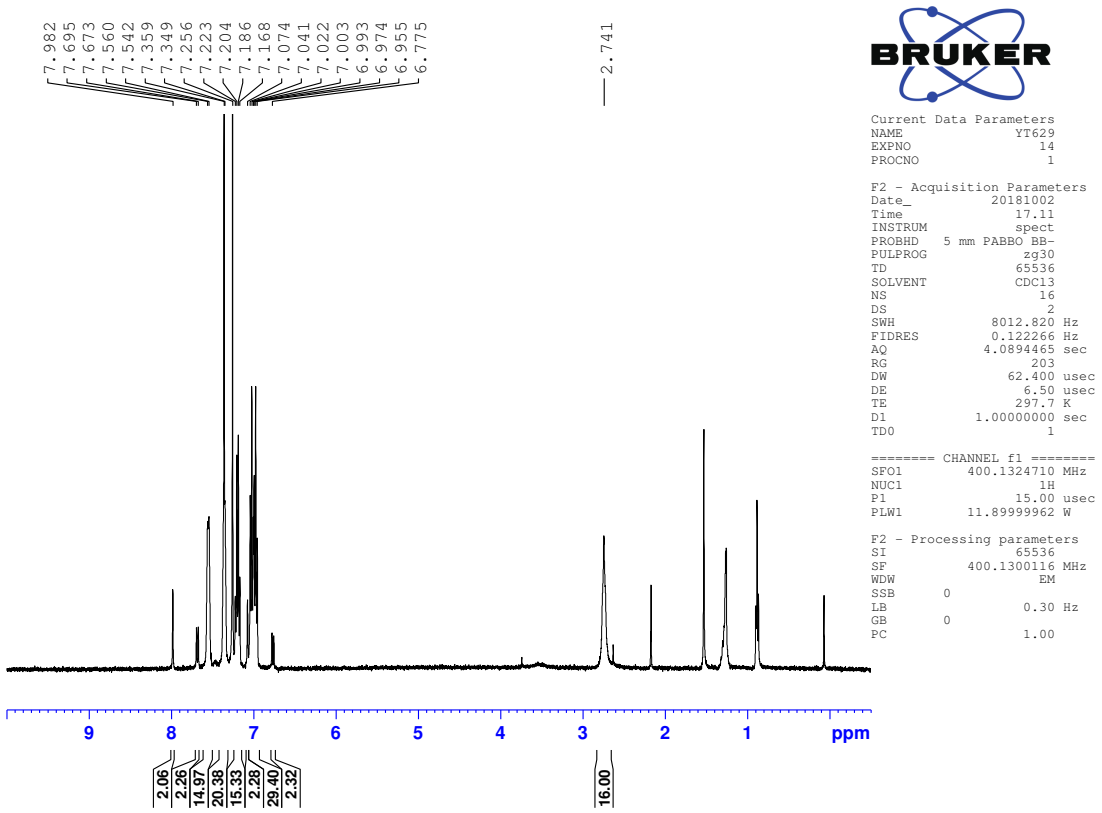



**Figure S5a.** A $^{1}$H NMR spectrum of **3$^{Cl}$** (400 MHz, $CDCl_3$, r.t.).

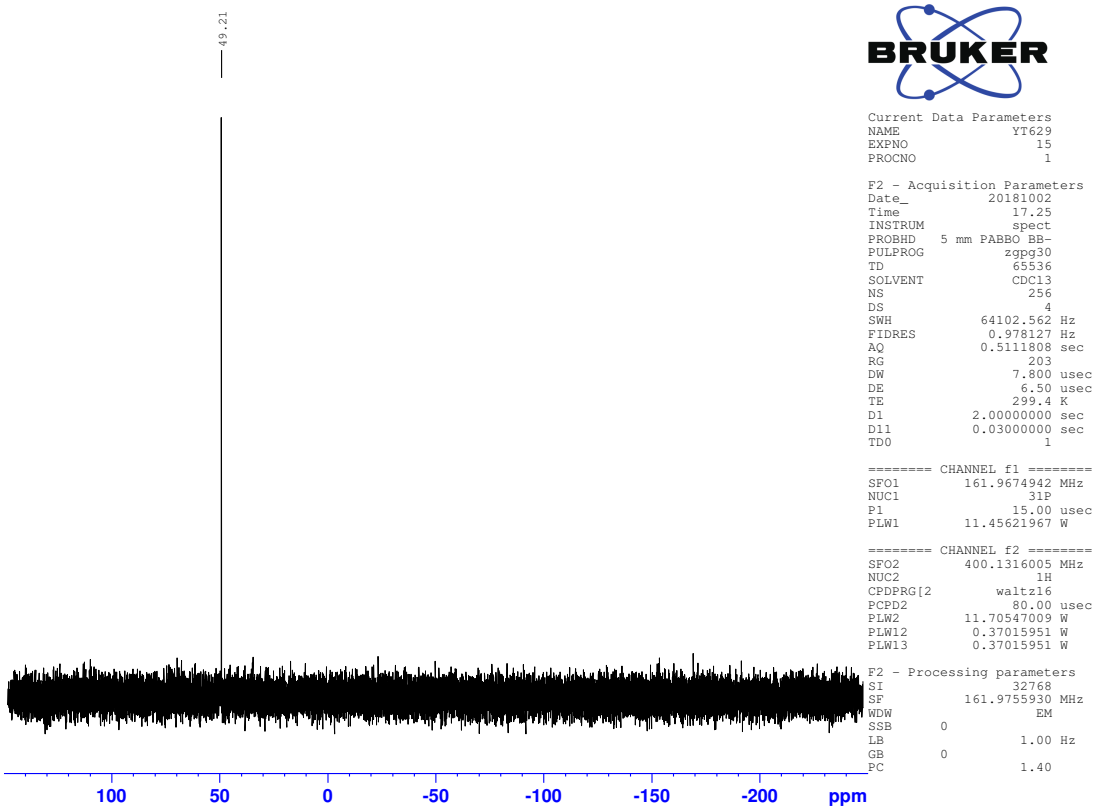



**Figure S5b.** A $^{31}P$ $\{^{1}H\}$ NMR spectrum of $\mathbf{3^{Cl}}$ (162 MHz, $CDCl_3$, r.t.).

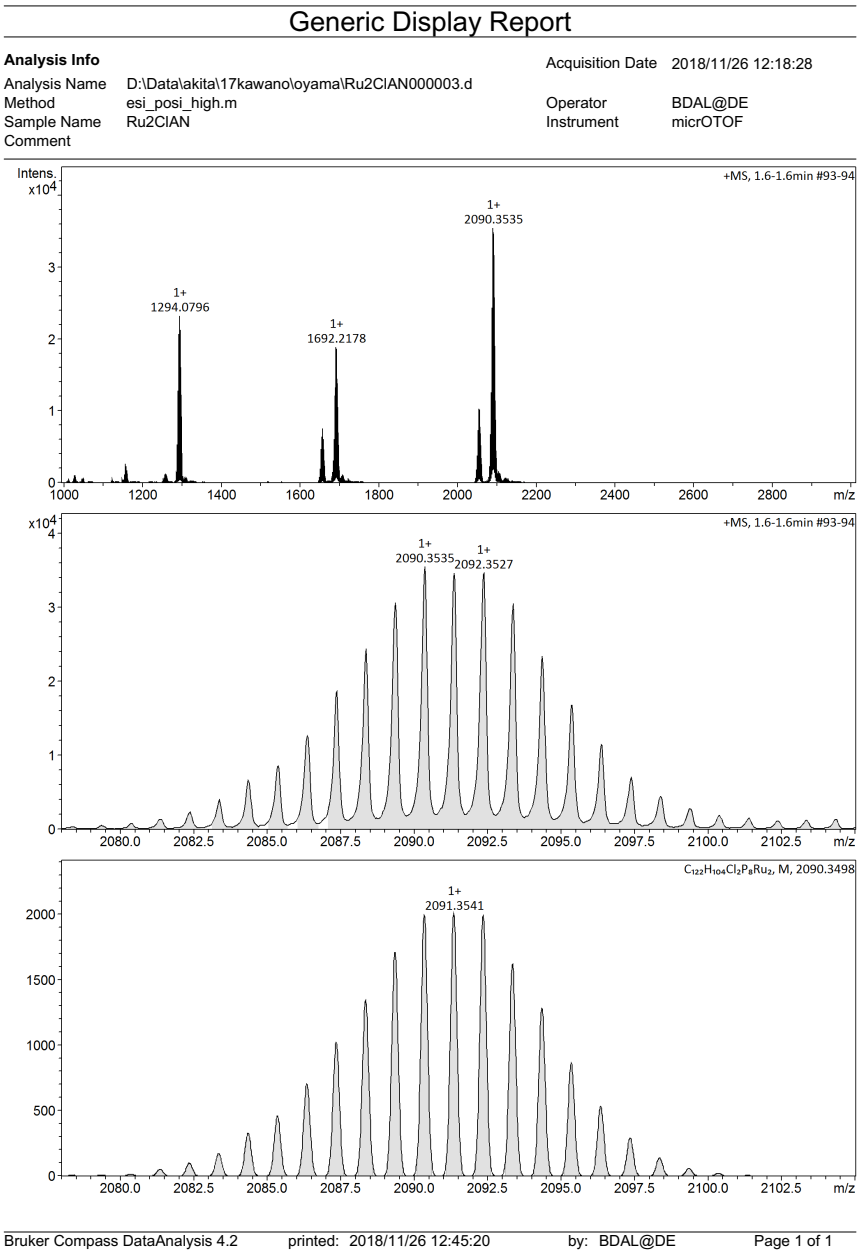
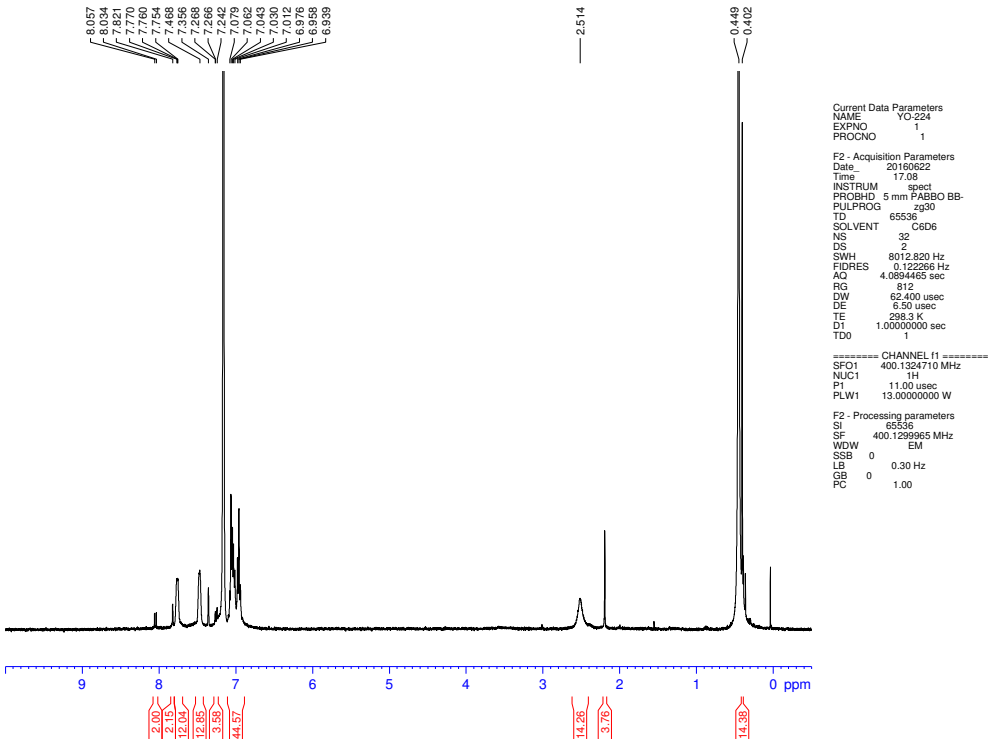



**Figure S5c.** ESI-TOF-MS spectra of $\mathbf{3^{Cl}}$.

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PLW1 13.00000000 W

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**Figure S6a.** A $^{1}$H NMR spectrum of $\mathbf{1}^{\mathbf{C4TMS}}$ (400 MHz, $C_6D_6$, r.t.).

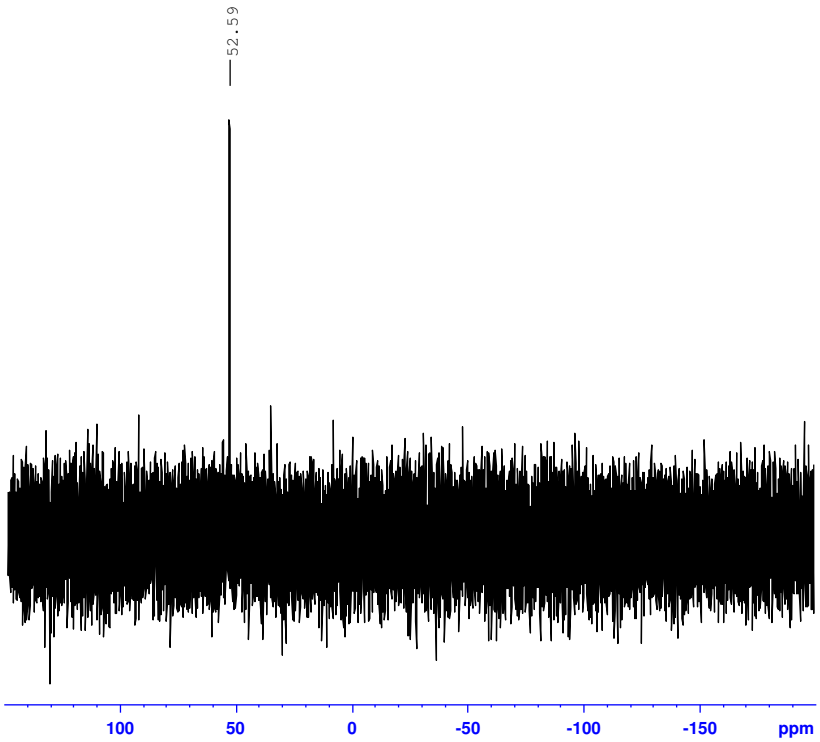


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**Figure S6b.** A $^{31}$P NMR spectrum of $\mathbf{1}^{\mathbf{C4TMS}}$ (162 MHz, $C_6D_6$, r.t.).

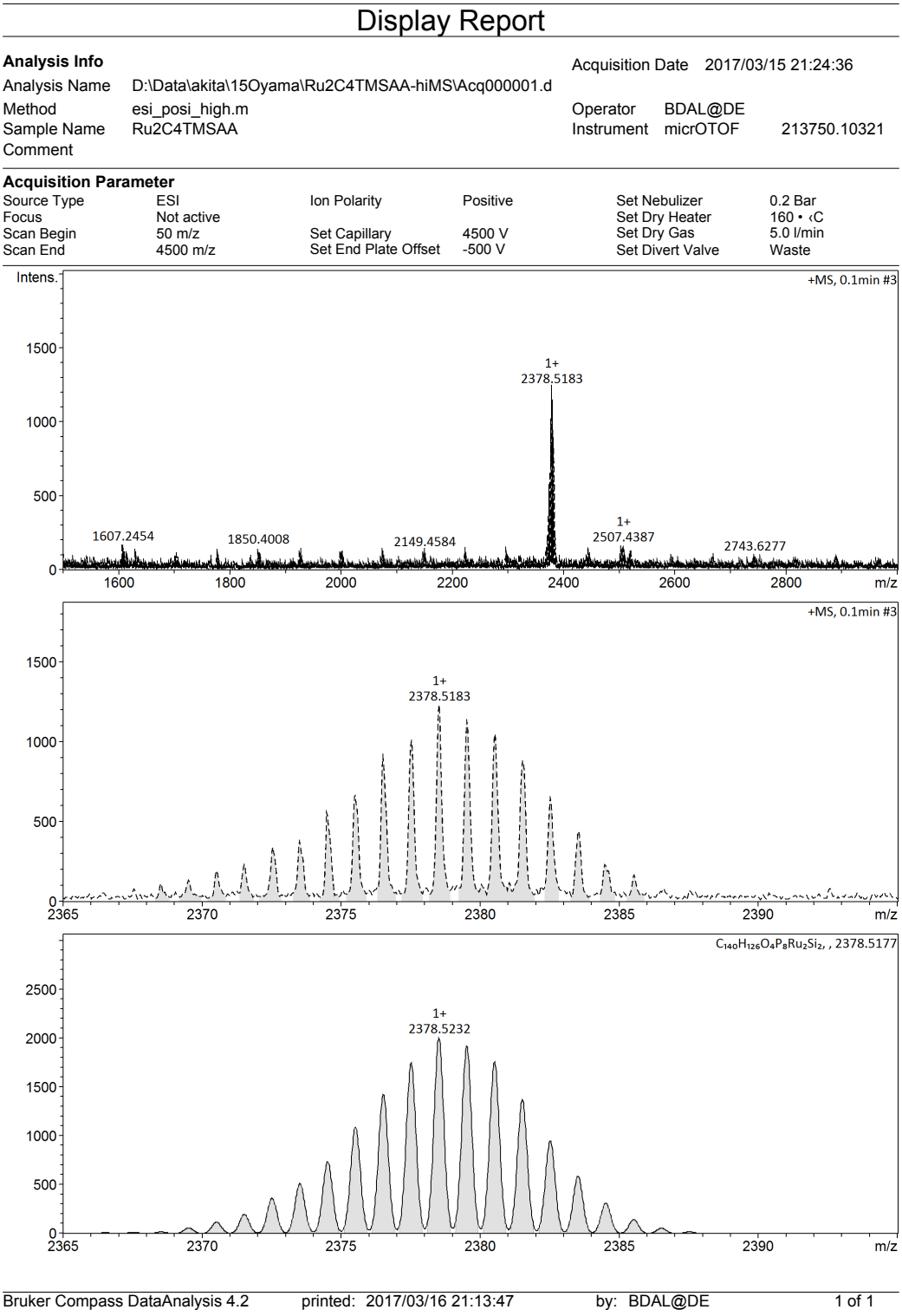


**Figure S6c.** ESI-TOF MS spectra of $\mathbf{1}^{\mathbf{C4TMS}}$.

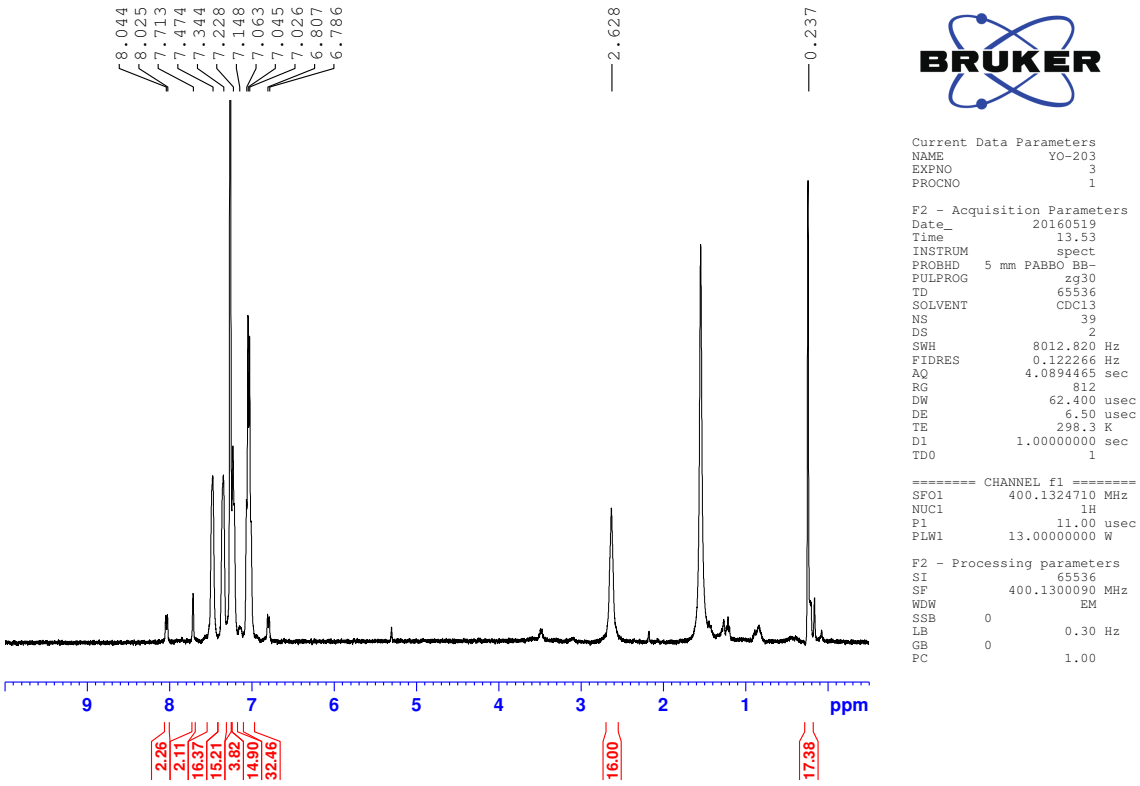


**Figure S7a.** A $^{1}$H NMR spectrum of **2**$^{\mathbf{C4TMS}}$ (400 MHz, $CDCl_3$, r.t.).

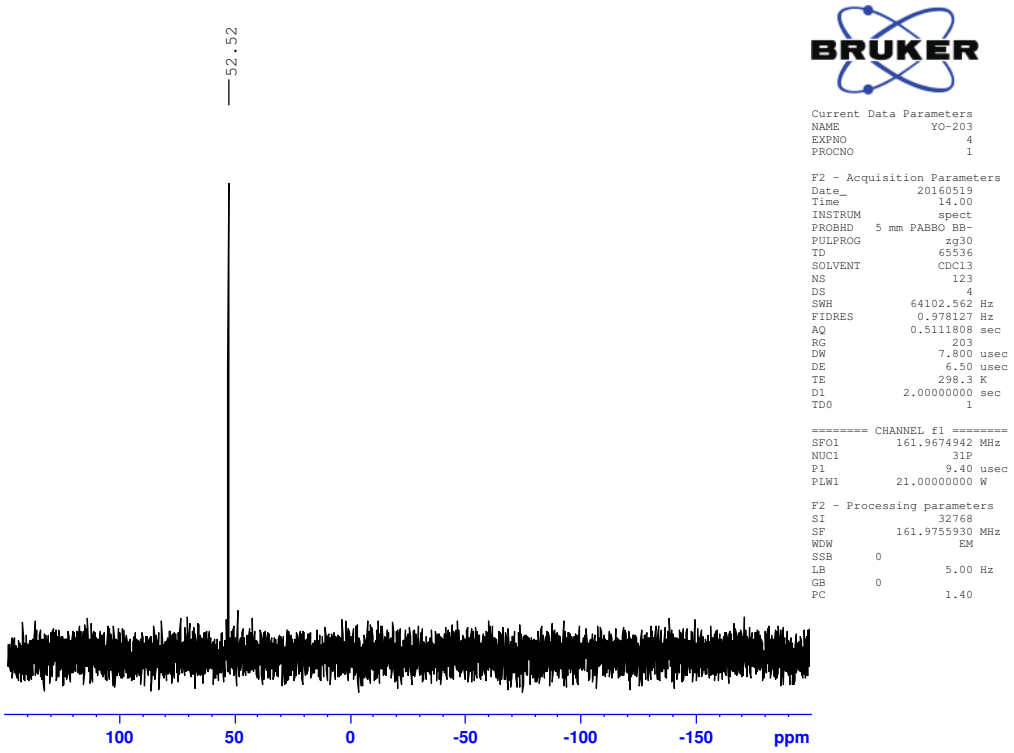


**Figure S7b.** A $^{31}$P $\{^{1}H\}$NMR spectrum of **2**$^{\mathbf{C4TMS}}$ (162 MHz, $CDCl_3$, r.t.)

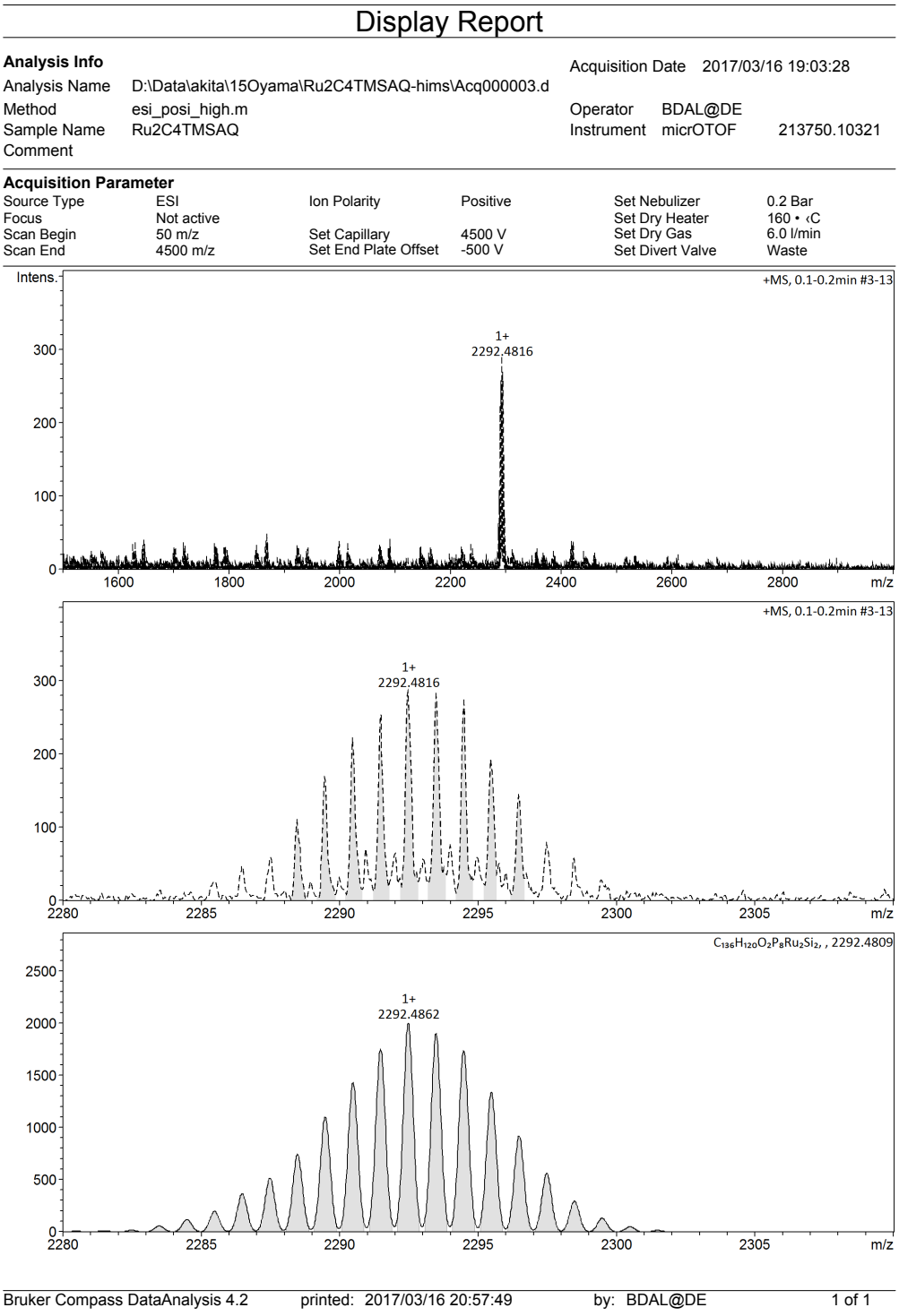


**Figure S7c.** ESI-TOF MS spectra of **2**$^{\mathbf{C4TMS}}$.

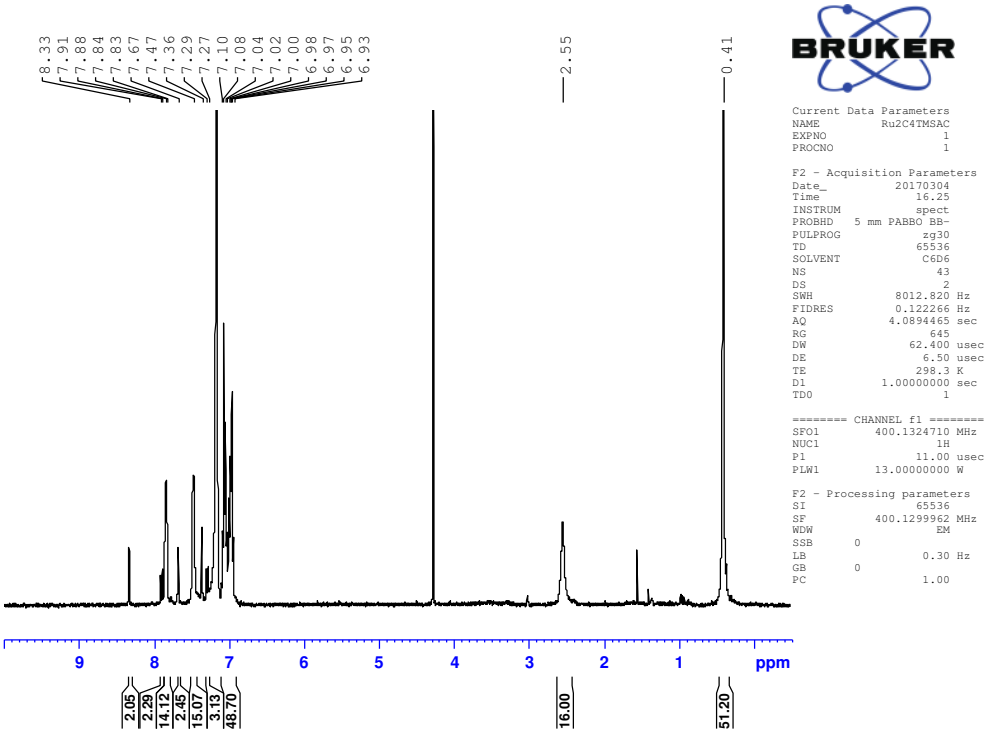


**Figure S8a.** A $^{1}$H NMR spectrum of **3**$^{\mathbf{C4TMS}}$ (400 MHz, $CDCl_3$, r.t.).

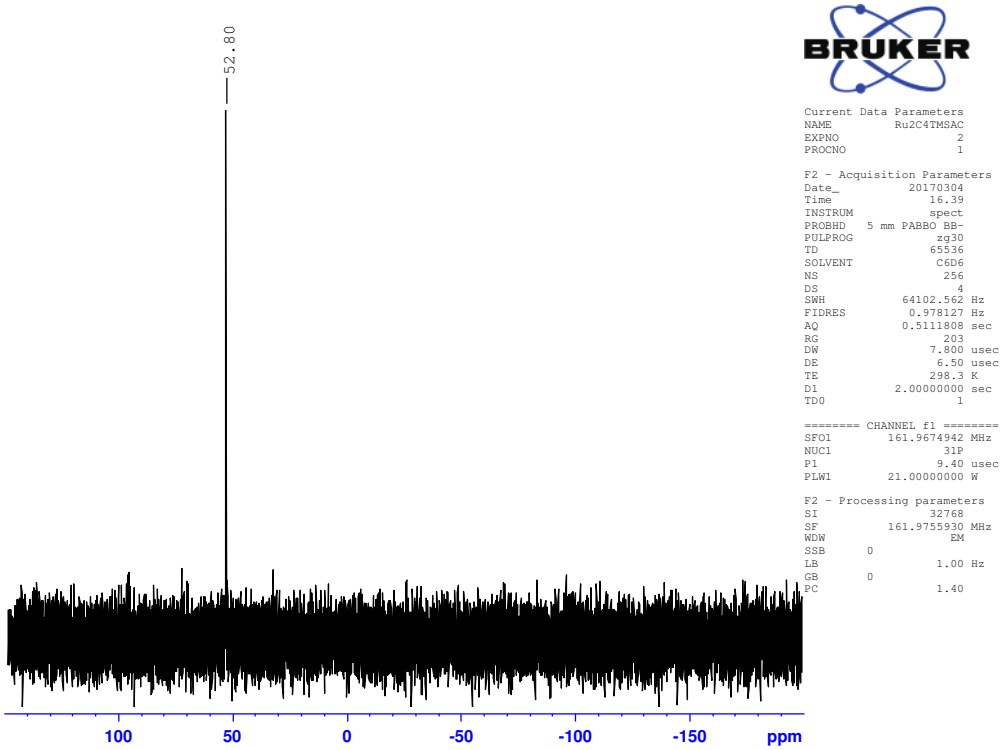


**Figure S8b.** A $^{31}$P NMR spectrum of **3**$^{\mathbf{C4TMS}}$ (162 MHz, $CDCl_3$, r.t.).

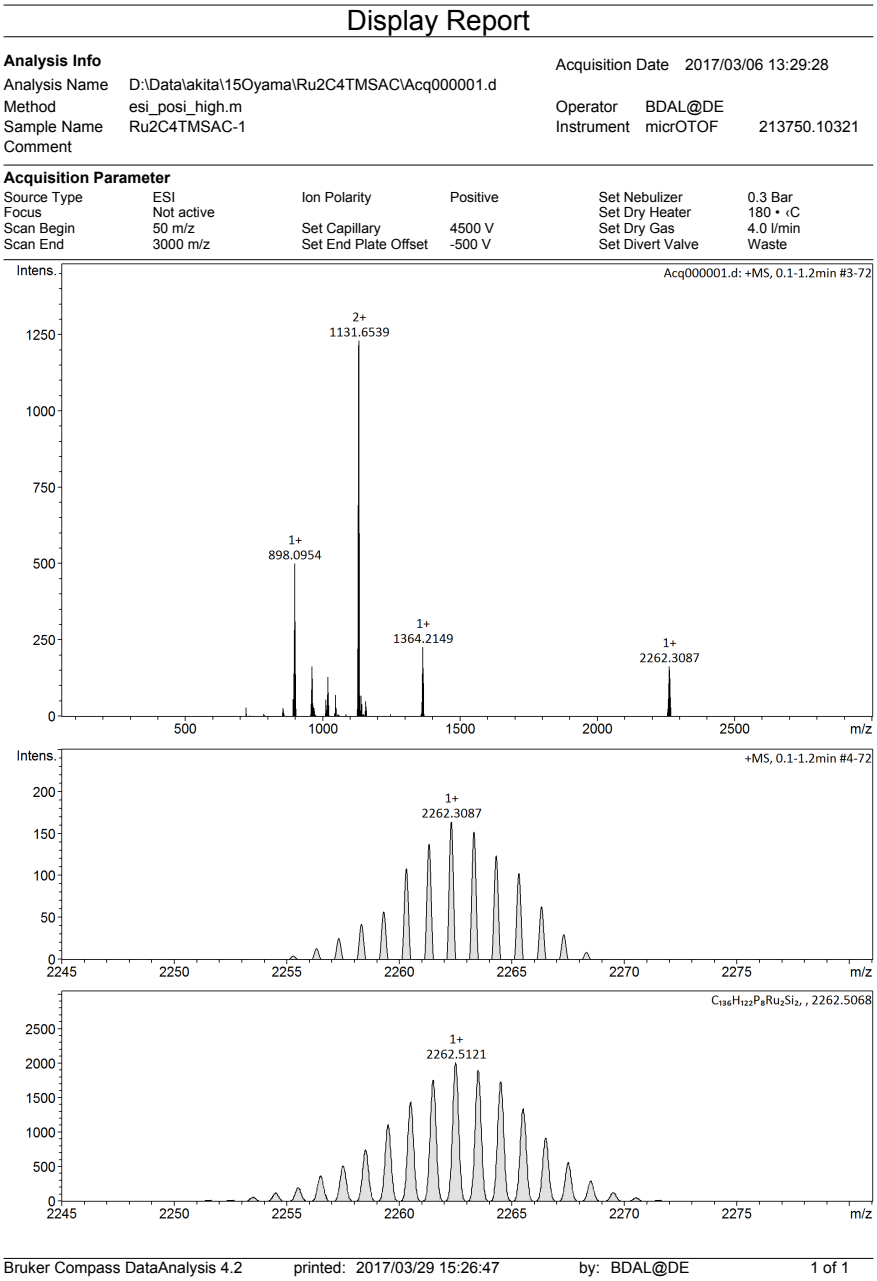


**Figure S8c.** ESI-TOF MS spectra of $\mathbf{3^{C4TMS}}$.

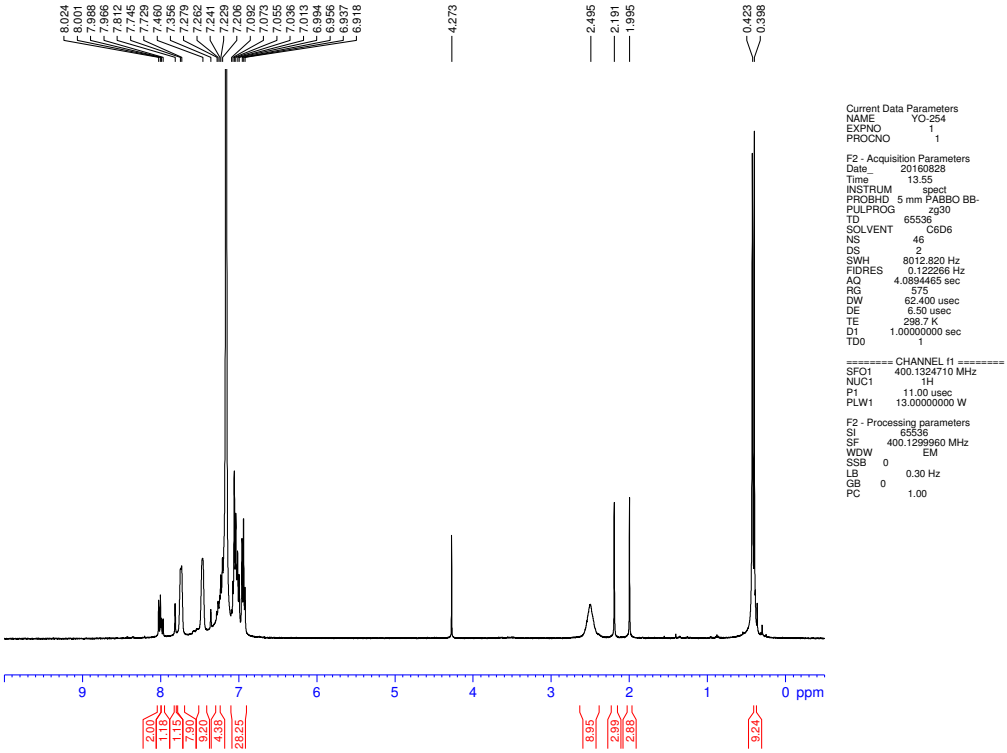


**Figure S9a.** A $^{1}$H NMR spectrum of **4** (400 MHz, $C_6D_6$, r.t.).

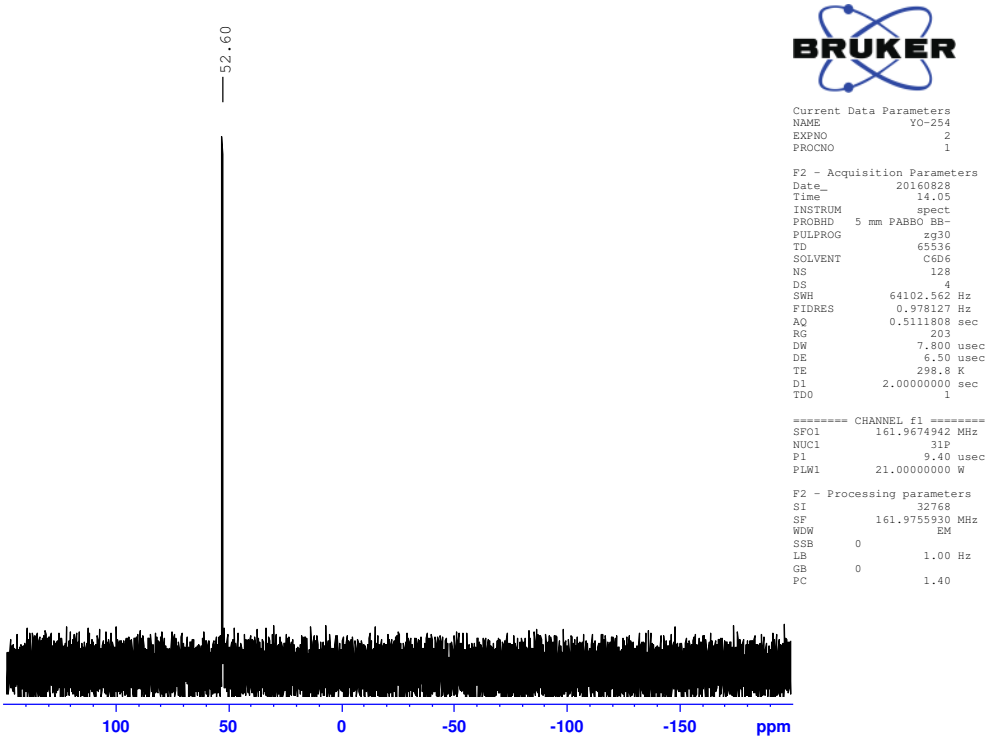


**Figure S9b.** A $^{31}$P NMR spectrum of **4** (162 MHz, $C_6D_6$, r.t.).

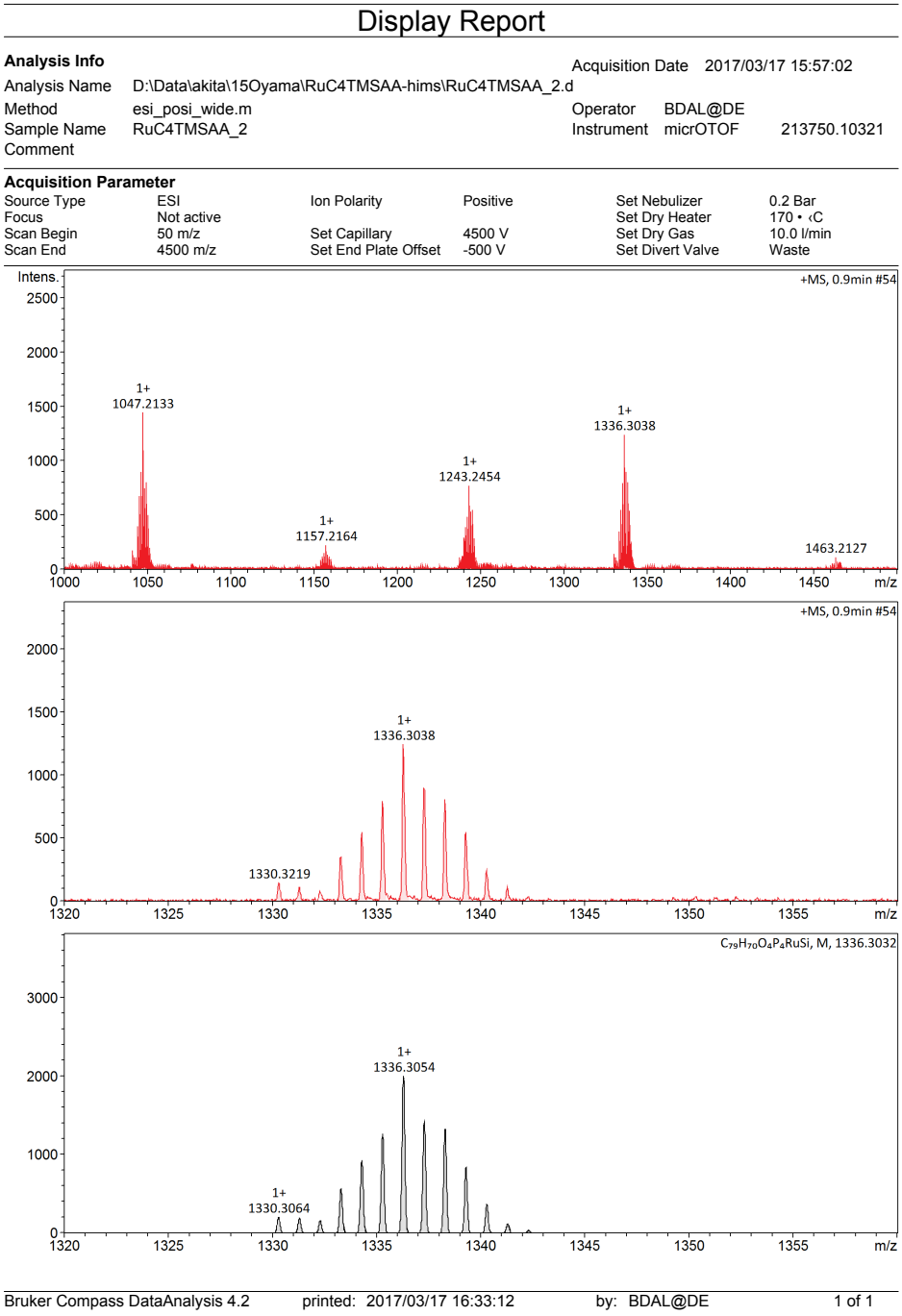


**Figure S9c.** ESI-TOF MS spectra of **4**.

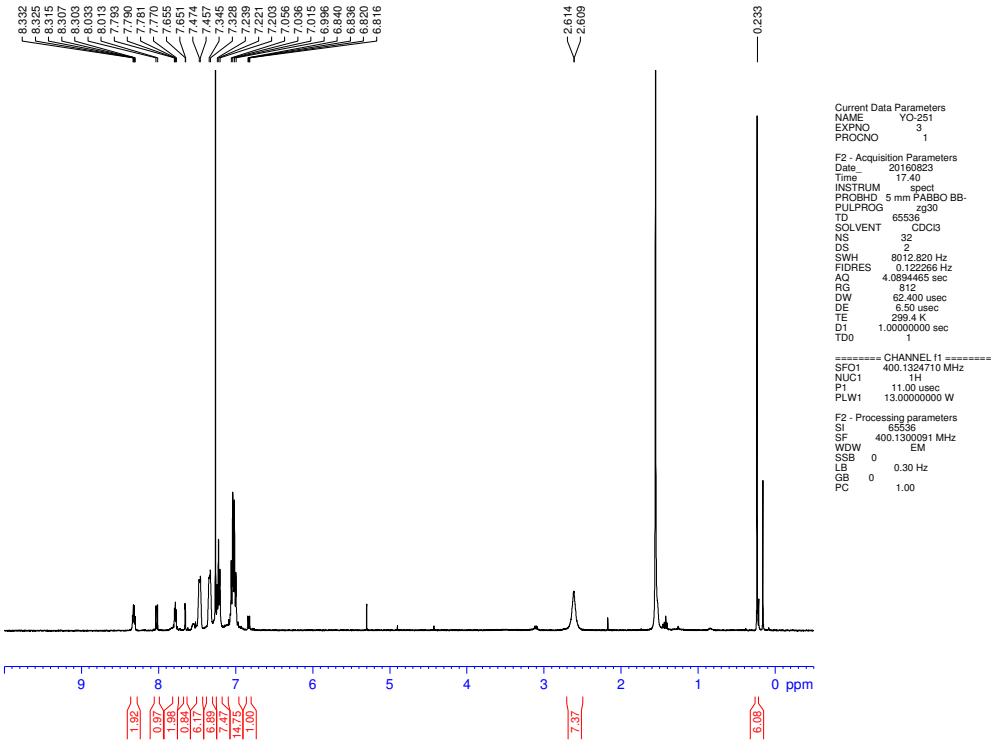


**Figure S10a.** $^{1}$H NMR spectrum of **5** (400 MHz, $CDCl_3$, r.t.)

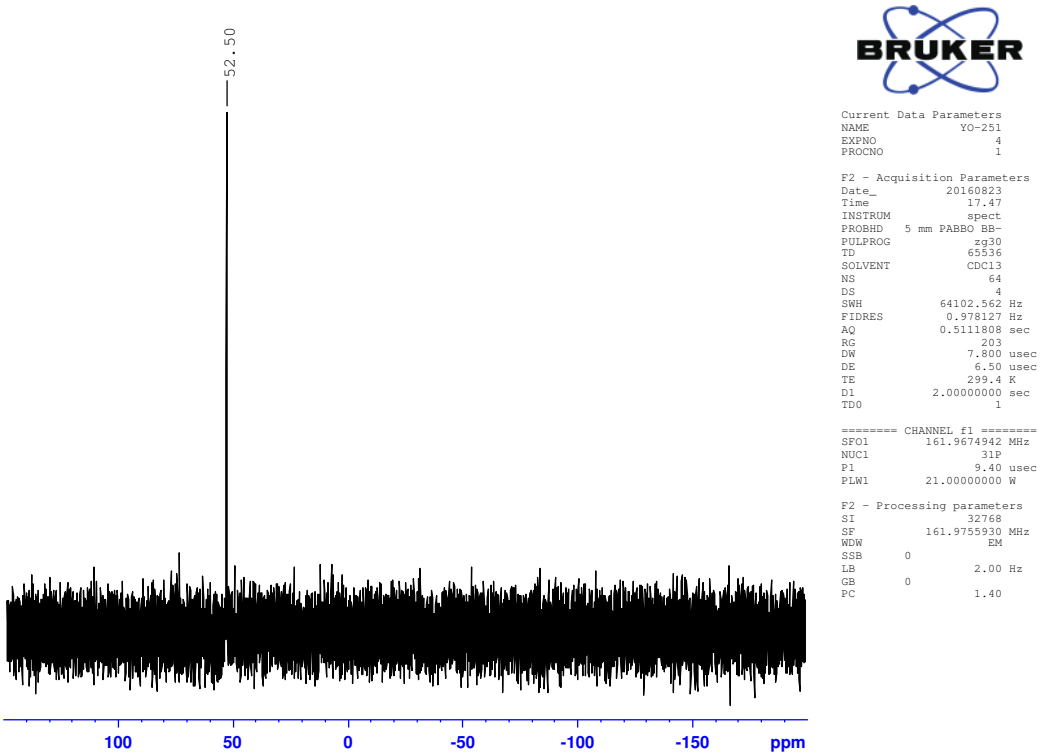


**Figure S10b.** A $^{31}$P NMR spectrum of **5** (162 MHz, $CDCl_3$, r.t.).

Display Report

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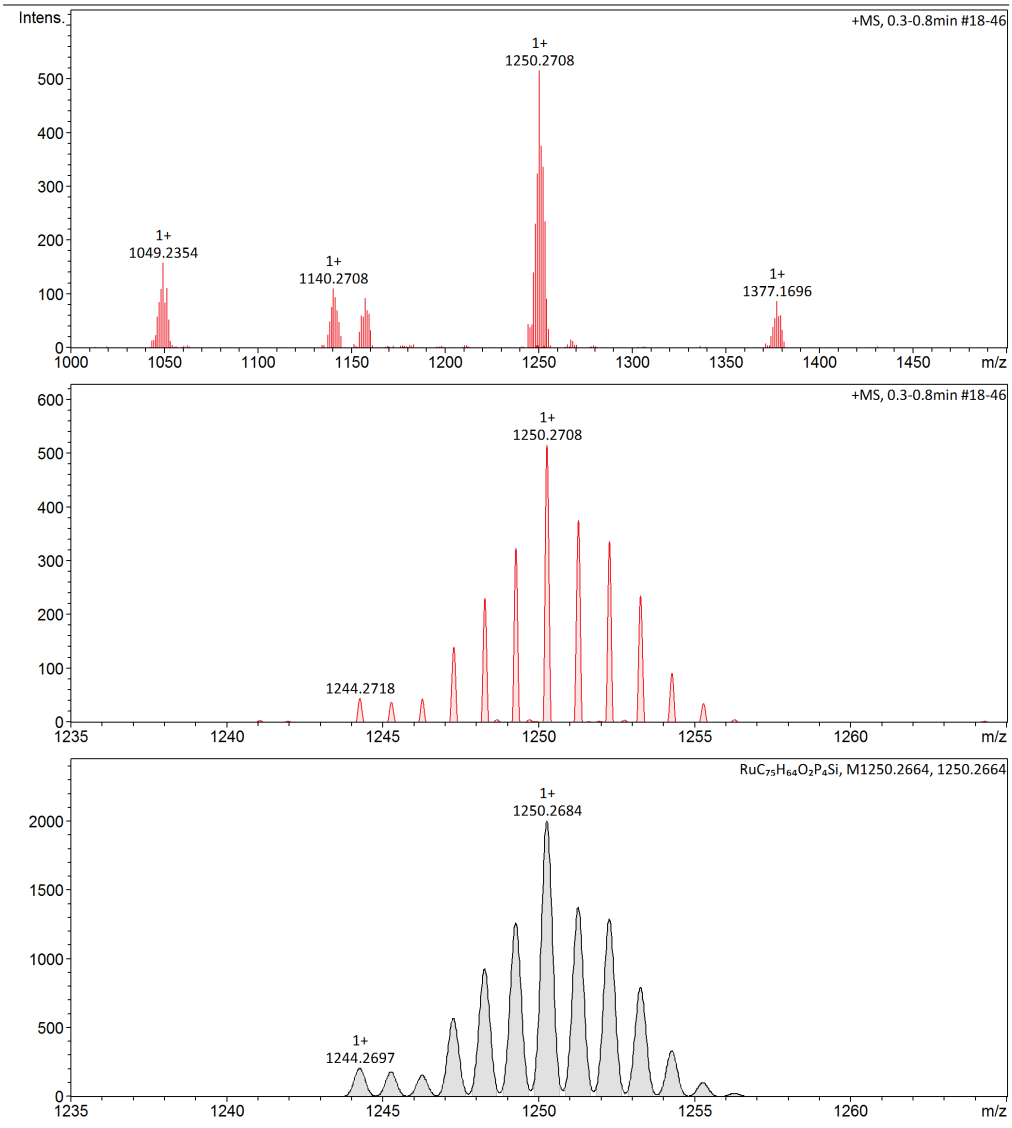


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**Figure S10c.** ESI-TOF MS spectra of **5**.

## II. Single-crystal X-ray crystallography

**$3^{C4}$**: Single crystals of **$3^{C4}$** were obtained by slow diffusion of hexane into a dichloromethane solution of **$3^{C4}$**. A suitable crystal was selected and data was collected on a Bruker model APEX2 platform-CCD X-ray diffractometer system. The crystal was kept at 90(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program and refined with the ShelXL [3] refinement package using Least Squares minimisation. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed at calculated positions and refined by applying riding models. The TMS group was solved as an orientational disorder model. As a satisfactory disorder model for the solvent was not found, the OLEX2 Solvent Mask routine (the PLATON/SQUEEZE analogue) was used to mask out the disordered density of a half of hexane molecule.

**Crystal Data** for $C_{136}H_{122}P_8Ru_2Si_2$ ($M$ =2262.41 g/mol): monoclinic, space group $P2_1/c$ (no. 14), $a$ = 28.758(5) Å, $b$ = 12.1471(19) Å, $c$ = 18.658(3) Å, $\beta$ = 96.383(2)°, $V$ = 6477.5(18) Å$^3$, $Z$ = 2, $T$ = 87(2) K, μ(MoKα) = 0.396 mm$^{-1}$, *Dcalc* = 1.160 g/cm$^3$, 30233 reflections measured (2.85° ≤ 2Θ ≤ 50.054°), 11447 unique ($R_{int}$ = 0.0659, $R_{sigma}$ = 0.0908) which were used in all calculations. The final $R_1$ was 0.0454 (I > 2σ(I)) and $wR_2$ was 0.1189 (all data).

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann. (2009), J. Appl. Cryst. 42, 339-341.
2. G. M. Sheldrick, (2015) Acta Cryst. A71, 3-8.
3. G. M. Sheldrick, (2015). Acta Cryst. C71, 3-8.

## III. Electrochemical, spectroscopic and theoretical data

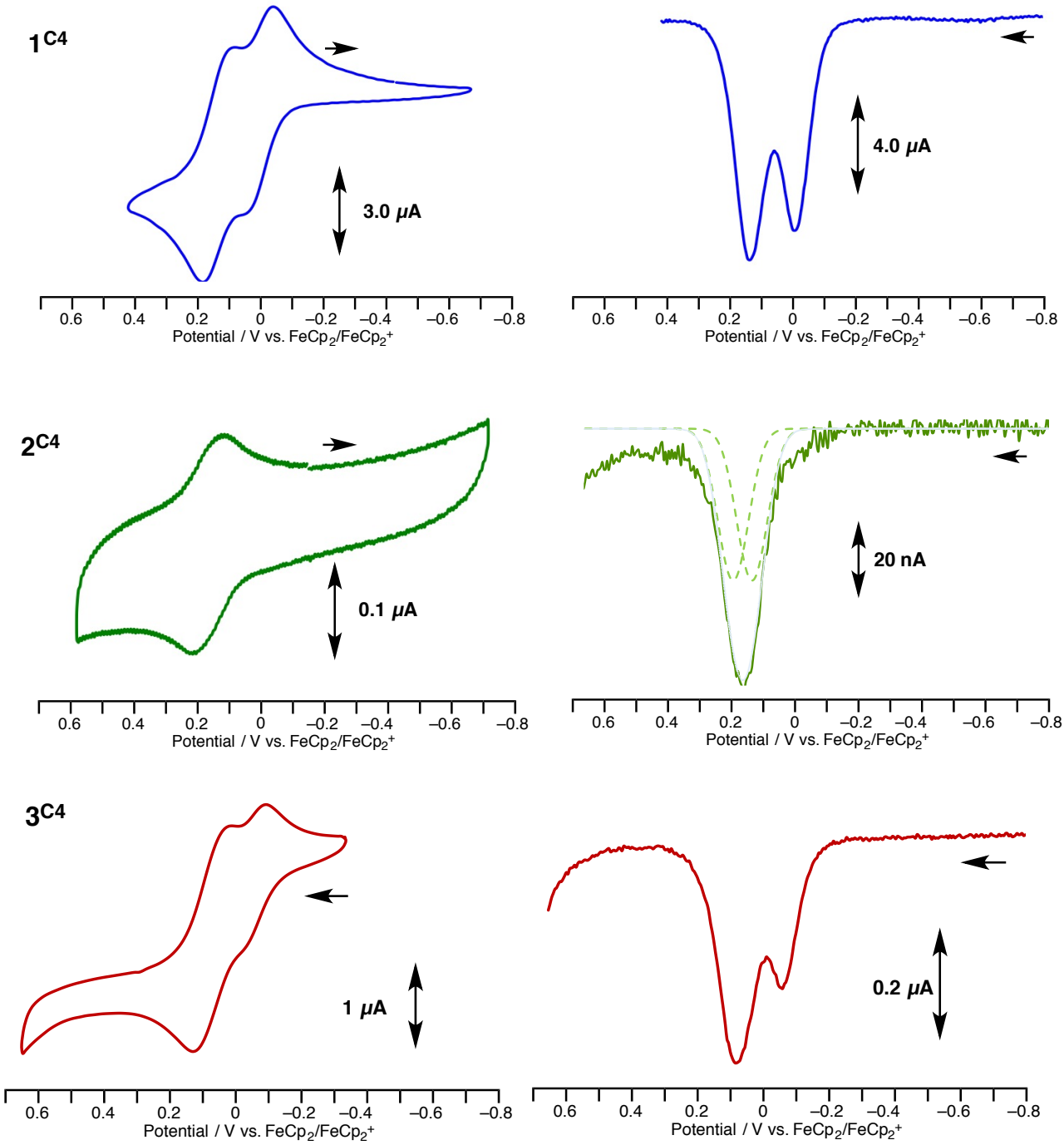


**Figure S11a.** CV and DPV charts for $\mathbf{1}^{C4}$-$\mathbf{3}^{C4}$.

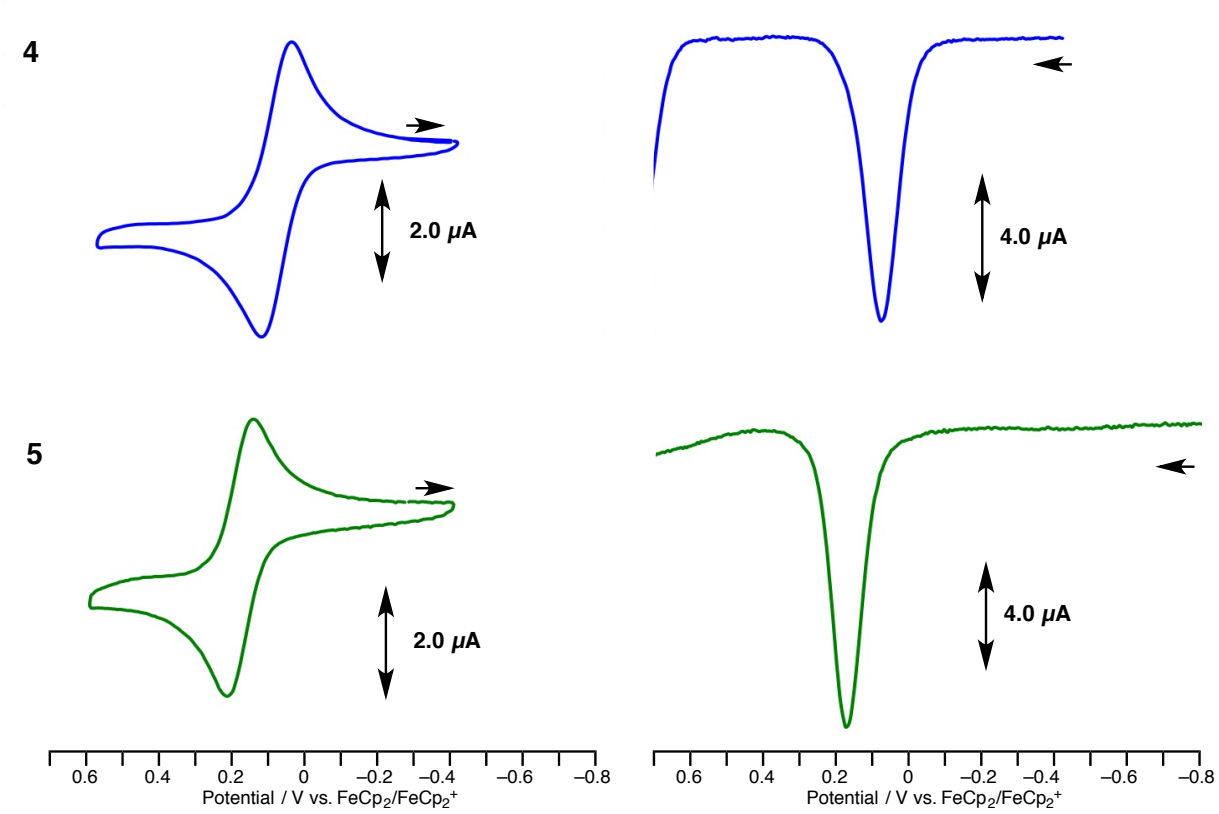


**Figure S11b.** CV and DPV charts for **4** and **5**.

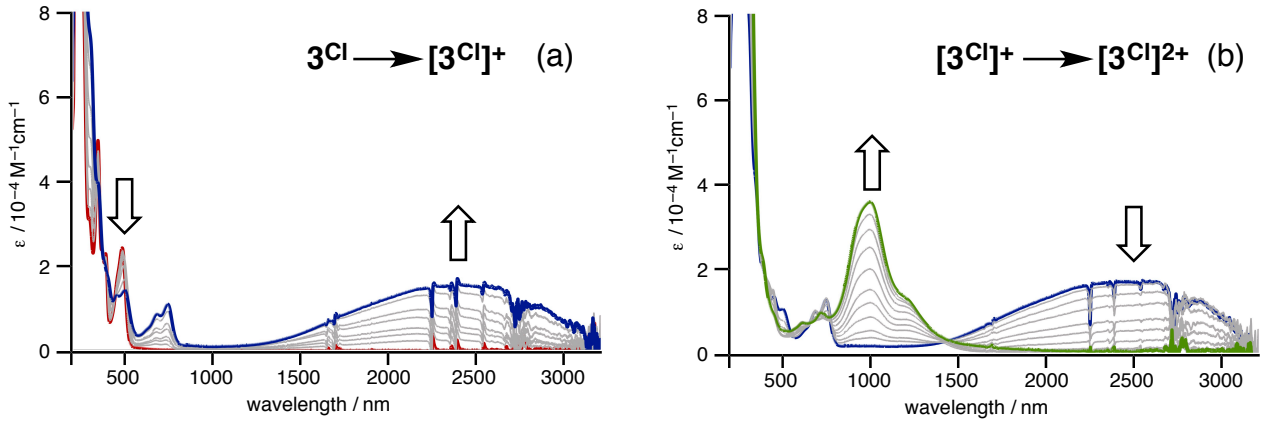


**Figure S12.** UV-Vis-NIR spectral changes of $\mathbf{3^{Cl}}$ upon addition of magic blue as observed in $CH_2Cl_2$. Spectral changes for (a) $\mathbf{3^{Cl}}$ to $[\mathbf{3^{Cl}}]^+$ and (b) $[\mathbf{3^{Cl}}]^+$ to $[\mathbf{3^{Cl}}]^{2+}$.

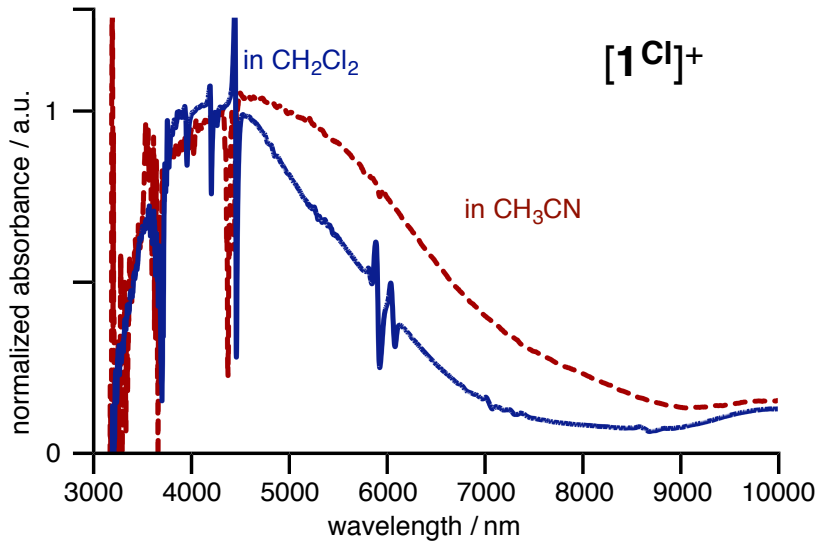


**Figure S13.** Normalized NIR spectra of $[\mathbf{1}^{\mathbf{Cl}}]^+$ (blue solid; in $CH_2Cl_2$, red dashed; in $CH_3CN$).

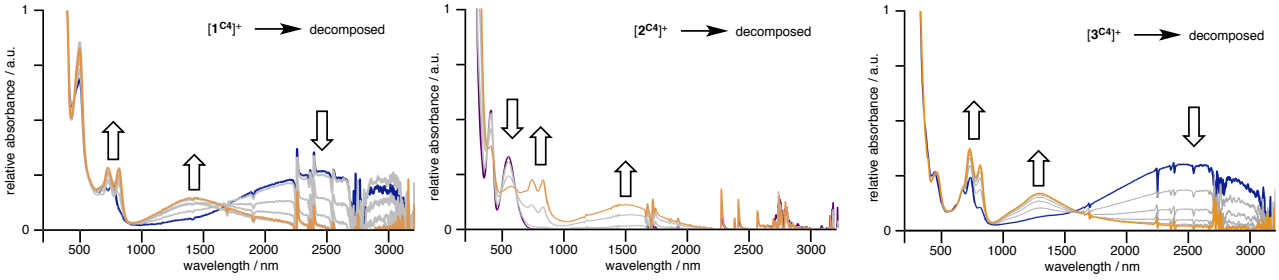


**Figure S14.** UV-Vis-NIR spectral changes of $[\mathbf{1}^{\mathbf{C4}}]^+$ - $[\mathbf{3}^{\mathbf{C4}}]^+$ observed in $CH_2Cl_2$. The spectral changes were completed within 10 min at room temperature.

**Table S1.** UV-Vis-NIR spectral data of $[\mathbf{3}^{\mathbf{R}}]^{n+}$ (R = Cl, $C_4$, $n$ = 0-2) observed in $CH_2Cl_2$.

| complex | λ / nm (ε x $10^3$ / $M^{-1}cm^{-1}$) | | |
|---|---|---|---|
| | $n = 0$ | $n = 1$ | $n = 2$ |
| $\mathbf{3}^{\mathbf{Cl}}$ | 257 (90.0) 347 (49.5) 484 (24.1) | 262 (101) 452 (13.0) 497 (14.1) 683 (8.6) 742 (10.8) | 298 (176) 992 (35.7) |
| $\mathbf{3}^{\mathbf{C4}}$ | 245 (96.3) 310 (46.8) 349 (35.8) 473 (19.8) | – | – |

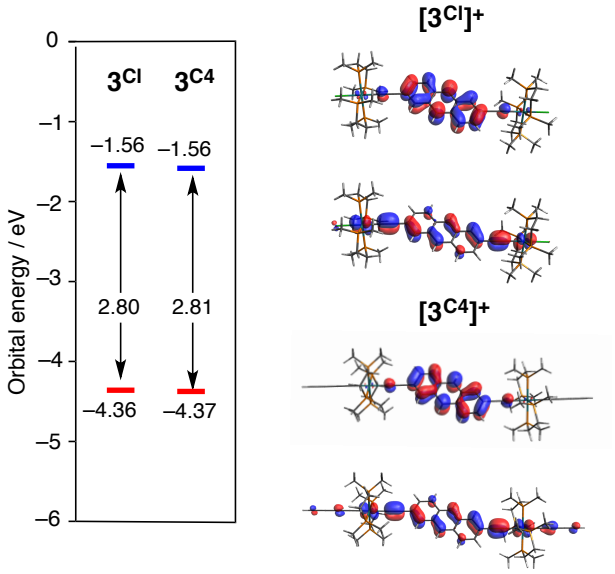


**Figure S15.** (left) HOMO and LUMO Energy levels of Kohn-Sham frontier orbitals of **3'** obtained at the B3LYP/LanL2DZ(Ru), 6-31G(d) levels of theory combined with the CPCM continuum solvent method ($CH_2Cl_2$). (right) Orbital distributions of LUMOs and HOMOs.

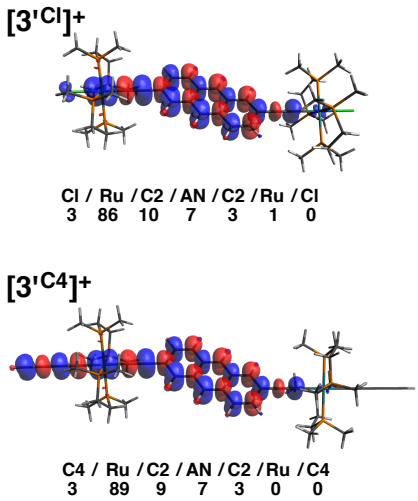


**Figure S16.** (a) Spin density distributions of the models of $[\mathbf{3'^{R}}]^{+}$ (R =Cl, $C_4$) at the BLYP35/Def2SVP levels of theory combined with the CPCM continuum solvent methods ($CH_2Cl_2$).

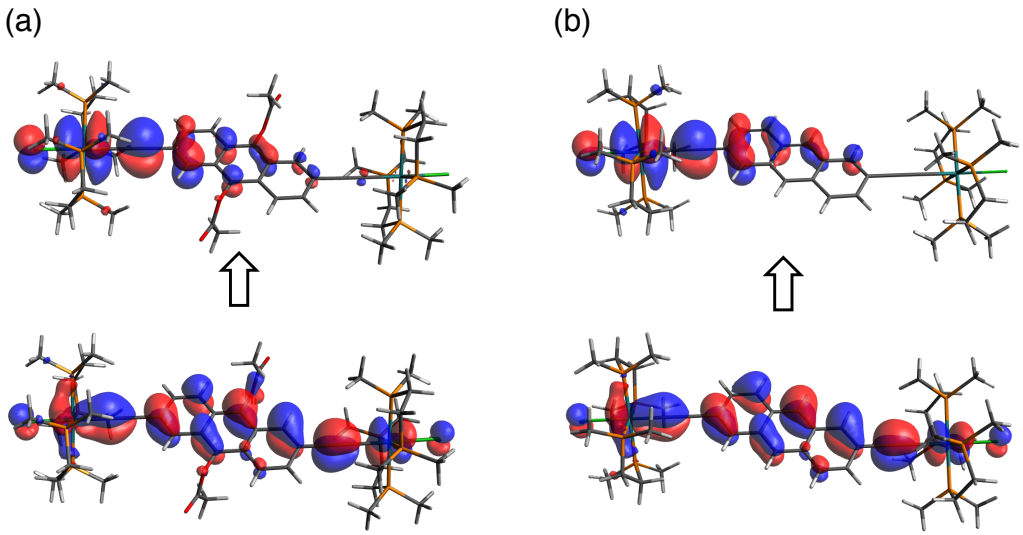


**Figure S17.** Natural transition orbitals (NTO) of the lowest-energy transitions for (a) $[\mathbf{1'^{Cl}}]^{+}$ and (b) $[\mathbf{3'^{Cl}}]^{+}$ obtained by the TDDFT at the BLYP35/Def2SVP levels of theory with CPCM ($CH_2Cl_2$).

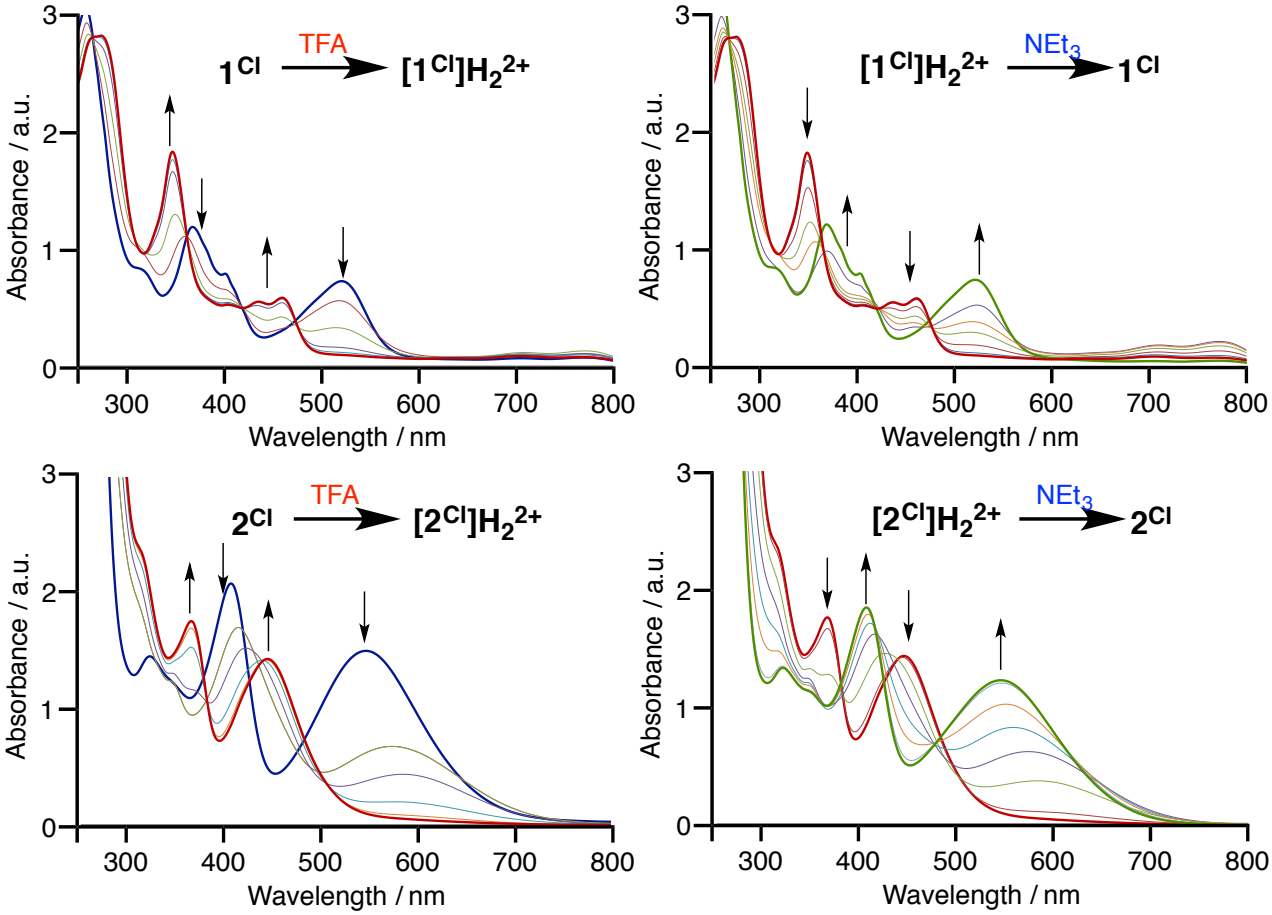


**Figure S18.** Protonation and deprotonation reactions with TFA and $NEt_3$ of $\mathbf{1}^{Cl}$ and $\mathbf{2}^{Cl}$ recorded in $CH_2Cl_2$.

**Table S2.** Cartesian coordinates of optimized geometry of **1'$^{Cl}$**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.82857800 | -0.36093400 | -0.17013800 | H | 6.65344600 | 3.66530700 | -2.12239100 |
| C | -3.71473300 | 0.62227100 | 0.25840800 | H | 5.82578800 | 2.15296900 | -1.63455200 |
| C | -3.15575300 | 1.84069700 | 0.79294200 | H | 9.14397700 | 3.91055400 | -0.06669200 |
| C | -1.80635300 | 2.04541000 | 0.86562800 | H | 10.41866900 | 2.96985600 | -0.86760100 |
| C | -1.41870400 | -0.19052400 | -0.09723400 | H | 9.38279600 | 4.07768800 | -1.82142300 |
| C | -0.88161100 | 1.04906000 | 0.41628800 | H | 10.14955200 | -1.94770100 | -3.75232700 |
| H | -3.83921100 | 2.60819400 | 1.14412600 | H | 10.90382900 | -0.81706000 | -2.58484700 |
| H | -3.22421600 | -1.28133400 | -0.58468600 | H | 10.53344400 | -2.47298400 | -2.09182800 |
| H | -1.41910000 | 2.96990900 | 1.28073700 | H | 7.83876700 | -3.44167600 | -2.10247400 |
| C | -0.50825900 | -1.18348800 | -0.50681400 | H | 6.44296500 | -2.35035200 | -2.24963800 |
| C | 0.88040700 | -1.00785700 | -0.46551700 | H | 7.47831100 | -2.68460600 | -3.66967400 |
| C | 1.41759100 | 0.23178200 | 0.04783900 | H | 6.23163600 | -3.03734900 | 0.83973900 |
| C | 0.50709000 | 1.22514800 | 0.45644400 | H | 7.53213500 | -3.99444500 | 0.10127500 |
| C | 1.80503500 | -2.00586700 | -0.91127800 | H | 7.21937300 | -4.14082500 | 1.84532800 |
| C | 3.15443600 | -1.80339600 | -0.83364600 | H | 9.95136100 | -3.74557800 | 2.22244700 |
| C | 3.71353500 | -0.58509400 | -0.29887000 | H | 10.29074700 | -3.37984600 | 0.51060700 |
| C | 2.82755700 | 0.40083400 | 0.12368300 | H | 10.79950900 | -2.23494200 | 1.75836200 |
| H | 1.41778800 | -2.93045000 | -1.32620000 | H | 10.20062200 | 2.25365500 | 2.36983100 |
| H | 3.83784600 | -2.57372500 | -1.17864400 | H | 8.82483900 | 3.36006900 | 2.15847400 |
| H | 3.22324600 | 1.32127200 | 0.53812600 | H | 9.11119200 | 2.61023700 | 3.74480700 |
| C | 5.12289100 | -0.42290000 | -0.21328300 | H | 5.71212700 | 0.77622500 | 2.55328200 |
| C | -5.12393200 | 0.45452300 | 0.18217000 | H | 6.44109500 | 1.89759400 | 3.74405600 |
| C | 6.34706300 | -0.26947800 | -0.12475300 | H | 6.12127700 | 2.42632700 | 2.07238700 |
| C | -6.34722500 | 0.28748800 | 0.10776100 | H | -10.32224900 | -1.42729300 | -2.87195200 |
| H | 8.33495900 | -0.15727700 | -4.39695700 | H | -9.21898100 | -1.55660500 | -4.27764300 |
| H | 6.92173500 | 0.20213800 | -3.39550800 | H | -9.06807700 | -2.68248300 | -2.90835200 |
| C | 8.01815300 | 0.17002100 | -3.39931900 | H | -6.49679800 | -1.11107400 | -4.07475700 |
| H | 8.20542600 | 2.32654000 | -3.71273400 | H | -5.71661700 | -0.38909900 | -2.63240000 |
| C | 8.59499200 | 1.54516800 | -3.04928600 | H | -6.29015600 | -2.06169600 | -2.58149100 |
| H | 9.68644600 | 1.53952900 | -3.15927000 | H | -8.73752900 | -3.89097300 | -0.93877300 |
| C | 7.46719500 | -2.53309000 | -2.58476700 | H | -9.15869100 | -4.47681900 | 0.68630700 |
| C | 10.18778700 | -1.63367500 | -2.70336100 | H | -10.18353900 | -3.25249000 | -0.12340300 |
| P | 8.52091800 | -1.08971300 | -2.11508700 | H | -6.09407200 | -3.16707800 | -0.13892200 |
| C | 6.61421700 | 2.86416000 | -1.37643900 | H | -5.79892100 | -2.33209000 | 1.38983100 |
| P | 8.23316700 | 1.97748100 | -1.26496800 | H | -6.52797800 | -3.96737100 | 1.39325500 |
| C | 9.40989300 | 3.37419900 | -0.98190000 | H | -7.35122400 | 1.59740700 | 4.22220900 |
| Ru | 8.32995300 | -0.04173800 | 0.02256900 | H | -6.29935000 | 1.48274200 | 2.77778800 |

| | | | |
|---|---|---|---|
| C | 7.23301100 | -3.44583300 | 0.99862800 |
| P | 8.40639900 | -2.05354300 | 1.31571200 |
| C | 10.01825400 | -2.94494100 | 1.47758600 |
| P | 8.11346400 | 1.01724100 | 2.16106500 |
| C | 6.43554700 | 1.58269300 | 2.69489100 |
| C | 9.16637000 | 2.45110800 | 2.66219200 |
| C | 7.98371000 | -1.61943800 | 3.08585000 |
| H | 6.88886000 | -1.60584300 | 3.15503100 |
| C | 8.55724600 | -0.24937600 | 3.46056500 |
| H | 8.34234500 | -2.40498100 | 3.76170900 |
| H | 9.65245500 | -0.28980600 | 3.49973200 |
| H | 8.20403900 | 0.07842800 | 4.44577400 |
| H | -8.16521600 | 3.24203600 | -3.04317100 |
| H | -6.78644700 | 2.26469500 | -2.51932600 |
| C | -7.88204100 | 2.30101300 | -2.55624400 |
| H | -7.99083200 | 1.00350900 | -4.31361000 |
| C | -8.43249400 | 1.08851700 | -3.31353900 |
| H | -9.51761700 | 1.18228300 | -3.44448100 |
| C | -7.45475100 | 3.62961100 | -0.03904400 |
| C | -10.13647600 | 3.08996600 | -0.89908100 |
| P | -8.47615400 | 2.28299900 | -0.78568900 |
| C | -6.50190200 | -1.06442700 | -2.98035900 |
| P | -8.13976600 | -0.48657200 | -2.34605400 |
| C | -9.30084400 | -1.65157500 | -3.18923300 |
| Ru | -8.32838300 | 0.02953400 | -0.01188300 |
| C | -7.30976900 | 1.70187800 | 3.13251200 |
| P | -8.49688800 | 0.54132200 | 2.32001500 |
| C | -10.11634500 | 1.12895000 | 2.99207600 |
| P | -8.16100800 | -2.23095700 | 0.76454600 |
| C | -6.48492000 | -3.00567000 | 0.87055300 |
| C | -9.15898100 | -3.60079000 | 0.02827900 |
| C | -8.18539700 | -1.03056400 | 3.28771100 |
| H | -7.09844900 | -1.11833800 | 3.40820500 |
| C | -8.73688300 | -2.24911200 | 2.54083100 |
| H | -8.61680000 | -0.94402500 | 4.29208300 |
| H | -9.83275200 | -2.22101300 | 2.51607200 |
| H | -8.44029100 | -3.18650700 | 3.02696100 |
| H | 6.36994200 | 3.29896400 | -0.40191000 |
| H | -7.55386400 | 2.73502100 | 2.87070400 |
| H | -10.91170500 | 0.45495300 | 2.66604400 |
| H | -10.09116800 | 1.17853500 | 4.08628700 |
| H | -10.33414100 | 2.12578900 | 2.59545300 |
| H | -10.82772000 | 2.43702000 | -1.43703800 |
| H | -10.53633700 | 3.24262500 | 0.10815500 |
| H | -10.06719600 | 4.05827500 | -1.40697800 |
| H | -6.43916200 | 3.25850000 | 0.12110700 |
| H | -7.42752200 | 4.50589500 | -0.69594200 |
| H | -7.87684500 | 3.92976300 | 0.92446500 |
| O | 1.01271600 | 2.40544900 | 1.01202700 |
| O | -1.01396800 | -2.36378200 | -1.06233700 |
| C | 1.32289900 | 3.50132800 | 0.23874600 |
| C | -1.32396700 | -3.45980000 | -0.28916500 |
| C | 1.07408000 | 3.40449900 | -1.24667600 |
| H | 1.66754700 | 2.59637800 | -1.68530300 |
| H | 0.02100200 | 3.18962800 | -1.45209700 |
| H | 1.35207600 | 4.35395000 | -1.70462500 |
| C | -1.07421800 | -3.36351400 | 1.19614300 |
| H | -0.02084200 | -3.14954100 | 1.40098400 |
| H | -1.66679600 | -2.55506400 | 1.63535200 |
| H | -1.35263600 | -4.31288700 | 1.65399600 |
| O | 1.77305900 | 4.47024200 | 0.80337100 |
| O | -1.77463000 | -4.42846600 | -0.85381800 |
| Cl | 10.92831200 | 0.27713100 | 0.24841800 |
| Cl | -10.92416900 | -0.35651900 | -0.17108900 |

**Table S3.** Cartesian coordinates of optimized geometry of **2'$^{Cl}$**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.82471200 | 0.36174900 | 0.06321800 | O | 0.99650500 | 2.49030100 | 0.02491700 |
| C | 3.74078200 | -0.71803700 | 0.07892400 | H | -6.72951300 | 0.75113900 | -3.45765600 |
| C | 3.19641500 | -2.03057500 | 0.10912200 | H | -7.30558800 | 2.41401700 | -3.73895500 |
| C | 1.82669700 | -2.23925800 | 0.12192900 | H | -6.28969300 | 2.02714500 | -2.31580900 |
| C | 1.44838900 | 0.15530000 | 0.07254300 | H | -9.45049500 | 0.01890400 | -3.88113000 |
| C | 0.92803500 | -1.15970400 | 0.10285700 | H | -10.75770400 | 0.55741100 | -2.80365100 |
| H | 3.87535200 | -2.87820100 | 0.12087000 | H | -9.99088900 | 1.71198300 | -3.93833600 |
| H | 3.19571200 | 1.38062200 | 0.04030700 | H | -10.17540400 | 3.44315300 | 2.34988400 |
| H | 1.42152100 | -3.24597100 | 0.14531400 | H | -10.98393400 | 2.19072900 | 1.35397300 |
| C | 0.54068700 | 1.34271500 | 0.04634200 | H | -10.23152900 | 1.74477500 | 2.89027600 |
| C | -0.91269700 | 1.08535500 | 0.04380000 | H | -6.30093100 | 2.41028200 | 1.98033500 |
| C | -1.43328900 | -0.22945600 | 0.07654500 | H | -7.41349800 | 3.68650400 | 2.55941800 |
| C | -0.52547800 | -1.41673600 | 0.11238900 | H | -7.42747800 | 2.07637700 | 3.31226600 |
| C | -1.81087900 | 2.16484900 | 0.00667400 | H | -5.86068600 | -0.64172900 | 2.78072500 |
| C | -3.18038600 | 1.95587700 | -0.00050800 | H | -7.16119600 | -0.11606100 | 3.87198800 |
| C | -3.72530400 | 0.64338800 | 0.03180800 | H | -6.59864800 | -1.80110200 | 3.92584100 |
| C | -2.80982300 | -0.43605600 | 0.07260300 | H | -9.27396700 | -2.54919400 | 3.75732400 |
| H | -1.40536200 | 3.17138800 | -0.01776300 | H | -9.87547400 | -0.89174800 | 3.49207300 |
| H | -3.85961800 | 2.80275600 | -0.03194300 | H | -10.31857000 | -2.16708500 | 2.35154100 |
| H | -3.18059400 | -1.45496000 | 0.09948900 | H | -9.16810800 | -3.81955000 | -2.56368100 |
| C | -5.12395800 | 0.42338300 | 0.02118500 | H | -10.31365100 | -2.58011800 | -1.96306500 |
| C | 5.13866100 | -0.49342000 | 0.06089900 | H | -9.20744600 | -2.20106600 | -3.30005800 |
| C | -6.34774500 | 0.23446900 | 0.00041900 | H | -5.63627300 | -2.25426600 | -1.35239400 |
| C | 6.35945200 | -0.28585200 | 0.04298000 | H | -6.41600000 | -3.52099900 | -2.34982000 |
| H | -8.88683400 | 4.32381900 | 0.26250800 | H | -6.40140400 | -1.82146800 | -2.88664900 |
| H | -7.40093000 | 3.57754300 | -0.33513100 | H | 10.51416600 | 1.65381200 | 2.60275400 |
| C | -8.46547800 | 3.39585900 | -0.14218600 | H | 9.43278300 | 2.46568000 | 3.77725800 |
| H | -9.01816500 | 3.69681200 | -2.23650200 | H | 9.56692300 | 0.69255100 | 3.75785800 |
| C | -9.17573500 | 2.96987600 | -1.43061800 | H | 6.67892000 | 2.13794600 | 3.73235300 |
| H | -10.25717600 | 2.89321800 | -1.26484600 | H | 5.79921700 | 1.36405500 | 2.37783400 |
| C | -7.30247200 | 2.61362400 | 2.36813500 | H | 6.73407500 | 0.37152100 | 3.50389200 |
| C | -10.14192400 | 2.39967300 | 2.01773700 | H | 11.06839800 | -1.54481700 | 1.97535600 |
| P | -8.55617500 | 2.03745900 | 1.13881500 | H | 9.90207600 | -1.54375200 | 3.31624900 |
| C | -7.08559700 | 1.66463500 | -2.97092600 | H | 10.42724700 | -3.09050100 | 2.61361600 |
| P | -8.58977100 | 1.27863900 | -1.96710800 | H | 7.14116100 | -2.15807000 | 2.93181600 |
| C | -9.81947100 | 0.85407100 | -3.27887300 | H | 6.56359100 | -2.87087500 | 1.42080400 |
| Ru | -8.31784900 | -0.05783300 | 0.00633800 | H | 7.73870400 | -3.76231900 | 2.43649200 |

| | | | |
|---|---|---|---|
| C | -6.79093600 | -0.94785900 | 3.26628700 |
| P | -8.03252300 | -1.39281400 | 1.97225000 |
| C | -9.51706600 | -1.79945000 | 2.99639400 |
| P | -8.06700300 | -2.15276900 | -1.13334900 |
| C | -6.47532400 | -2.47974400 | -2.01509200 |
| C | -9.31067000 | -2.75231900 | -2.36119400 |
| C | -7.41709400 | -3.07219600 | 1.43210600 |
| H | -6.33818200 | -2.97219000 | 1.26078000 |
| C | -8.12360300 | -3.51367200 | 0.14705800 |
| H | -7.55442600 | -3.80214000 | 2.23888300 |
| H | -9.18294400 | -3.71882600 | 0.34431200 |
| H | -7.68314500 | -4.43183500 | -0.25967600 |
| H | 7.27506700 | 4.35894300 | -0.40184500 |
| H | 6.19050200 | 3.12879100 | 0.25828000 |
| C | 7.24052900 | 3.35323700 | 0.03389000 |
| H | 7.69513700 | 3.90212000 | 2.10157800 |
| C | 8.09034700 | 3.26072900 | 1.30470300 |
| H | 9.11797700 | 3.58663900 | 1.10232700 |
| C | 6.42874800 | 2.16030400 | -2.45314400 |
| C | 9.16041600 | 2.96893500 | -2.11540300 |
| P | 7.80345500 | 2.08855700 | -1.22062300 |
| C | 6.70604800 | 1.33588500 | 2.98687000 |
| P | 8.19061700 | 1.49031700 | 1.89581100 |
| C | 9.56025200 | 1.58945700 | 3.13205600 |
| Ru | 8.31703700 | 0.07323500 | -0.03609200 |
| C | 7.05718200 | -1.41364700 | -3.19026400 |
| P | 8.43116000 | -1.35106100 | -1.95636100 |
| C | 9.91957300 | -1.25612400 | -3.04836000 |
| P | 8.80969100 | -1.94414400 | 1.16198700 |
| C | 7.43307800 | -2.77433700 | 2.07556700 |
| C | 10.18874600 | -2.04534400 | 2.38751000 |
| C | 8.46624100 | -3.12005100 | -1.35405700 |
| H | 7.42732000 | -3.40349800 | -1.14490700 |
| C | 9.31760000 | -3.23881500 | -0.08630100 |
| H | 8.83191400 | -3.78149900 | -2.14861900 |
| H | 10.37478600 | -3.05982300 | -0.31703100 |
| H | 9.24364100 | -4.23941200 | 0.35637400 |
| O | -0.98138000 | -2.56398000 | 0.14575900 |
| H | 7.14617300 | -2.30391400 | -3.82232000 |
| H | 6.10099700 | -1.43190800 | -2.66087700 |
| H | 7.08582200 | -0.52761400 | -3.83042200 |
| H | 10.82390300 | -1.31873400 | -2.43880100 |
| H | 9.91082600 | -2.06120800 | -3.79136900 |
| H | 9.93009100 | -0.29213300 | -3.56657100 |
| H | 10.01634600 | 3.09668500 | -1.44886700 |
| H | 9.48633300 | 2.36412200 | -2.96735500 |
| H | 8.81964800 | 3.94462800 | -2.47893600 |
| H | 6.15822000 | 3.19970900 | -2.66873200 |
| H | 6.73488500 | 1.67931900 | -3.38633200 |
| H | 5.56065300 | 1.63016200 | -2.05297800 |
| Cl | 10.89502700 | 0.54834900 | -0.13317200 |
| Cl | -10.91429900 | -0.44023100 | -0.01984100 |

**Table S4.** Cartesian coordinates of optimized geometry of **3'$^{Cl}$**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.81899500 | 0.44347200 | 0.14557700 | H | -6.44943000 | -2.93010400 | -3.06398700 |
| C | 3.72619600 | -0.60864100 | 0.11582500 | H | -5.68981700 | -1.63241200 | -2.08872500 |
| C | 3.19521800 | -1.95301300 | 0.09703600 | H | -9.03406900 | -3.80998200 | -1.32281700 |
| C | 1.84963300 | -2.19436000 | 0.10132100 | H | -10.29341300 | -2.68968600 | -1.88254200 |
| C | 1.41052200 | 0.23195300 | 0.15085100 | H | -9.17534400 | -3.44839700 | -3.05845000 |
| C | 0.90062100 | -1.12148700 | 0.12525400 | H | -9.86921800 | 2.94597500 | -3.16460200 |
| H | 3.89905800 | -2.78052800 | 0.07656000 | H | -10.72063200 | 1.56087400 | -2.40913900 |
| H | 3.18917400 | 1.46580300 | 0.16064100 | H | -10.33939800 | 2.99154600 | -1.44498300 |
| H | 1.47711400 | -3.21637900 | 0.08445600 | H | -6.25825300 | 2.75246600 | -1.39796500 |
| C | 0.49120700 | 1.29507900 | 0.17562700 | H | -7.19393100 | 3.53276900 | -2.70850700 |
| C | -0.89088200 | 1.07719100 | 0.17006200 | H | -7.63638900 | 3.80528900 | -1.00864200 |
| C | -1.40100300 | -0.27599100 | 0.13937600 | H | -6.36921700 | 2.59973300 | 1.76199200 |
| C | -0.48156200 | -1.33936100 | 0.12077400 | H | -7.65906000 | 3.71751200 | 1.27008300 |
| C | -1.83913100 | 2.15050500 | 0.19015300 | H | -7.43827200 | 3.33856400 | 2.99282200 |
| C | -3.18472200 | 1.90988800 | 0.17460700 | H | -10.16557500 | 2.83004500 | 3.07402000 |
| C | -3.71646500 | 0.56632400 | 0.13673800 | H | -10.41665700 | 2.97379600 | 1.31445500 |
| C | -2.80990100 | -0.48651100 | 0.12413500 | H | -10.95372200 | 1.51132800 | 2.14957300 |
| H | -1.46609900 | 3.17214900 | 0.21623900 | H | -9.41626400 | -3.64540900 | 2.70271900 |
| H | -3.88752600 | 2.73831700 | 0.18889100 | H | -10.41257000 | -2.85600800 | 1.44209400 |
| H | -3.18048700 | -1.50832000 | 0.09732900 | H | -9.05125100 | -3.90103400 | 0.98135800 |
| C | -5.12645700 | 0.36115100 | 0.10638000 | H | -5.91383200 | -1.66737200 | 2.28471100 |
| C | 5.13508300 | -0.40063600 | 0.09658200 | H | -6.73948900 | -3.04553800 | 3.07762300 |
| C | -6.35007700 | 0.19076400 | 0.06649200 | H | -6.33352700 | -3.10322900 | 1.34356200 |
| C | 6.35953700 | -0.23201500 | 0.07191300 | H | 10.50667700 | 2.25268500 | 2.15438700 |
| H | -8.06436800 | 1.36119000 | -4.20297600 | H | 9.41127000 | 3.33191100 | 3.07251700 |
| H | -6.70504000 | 0.70129200 | -3.28415000 | H | 9.53977100 | 1.60968200 | 3.49760900 |
| C | -7.79988100 | 0.75090100 | -3.33099700 | H | 6.65779500 | 3.02648400 | 3.05106800 |
| H | -7.97090300 | -1.21551200 | -4.27258000 | H | 5.79597200 | 1.92548900 | 1.92993900 |
| C | -8.39375500 | -0.65743600 | -3.42852600 | H | 6.70570200 | 1.26164900 | 3.29326100 |
| H | -9.47851600 | -0.60443400 | -3.58272900 | H | 10.97745000 | -1.02411600 | 2.44460300 |
| C | -7.25468100 | 3.06654000 | -1.71901300 | H | 9.75059600 | -0.68437400 | 3.68522300 |
| C | -9.97891600 | 2.34757000 | -2.25335700 | H | 10.28064600 | -2.35951600 | 3.41293200 |
| P | -8.36533700 | 1.59018900 | -1.75984800 | H | 7.01116400 | -1.36953600 | 3.34477000 |
| C | -6.47306200 | -2.39391700 | -2.10902400 | H | 6.47665200 | -2.41042000 | 2.02045900 |
| P | -8.11887500 | -1.59618600 | -1.83412500 | H | 7.59268300 | -3.05218300 | 3.26678800 |
| C | -9.26797900 | -3.02807700 | -2.05086200 | H | 7.19009900 | -3.19633100 | -3.10299800 |
| Ru | -8.34211900 | -0.04742000 | -0.01989100 | H | 6.14166000 | -2.04916600 | -2.21434900 |

| | | | |
|---|---|---|---|
| C | -7.38879500 | 2.92908900 | 1.97791600 |
| P | -8.53707300 | 1.49203600 | 1.79763700 |
| C | -10.17767900 | 2.27979700 | 2.12662200 |
| P | -8.29112700 | -1.69269600 | 1.72014100 |
| C | -6.66320700 | -2.45259700 | 2.15967100 |
| C | -9.40219400 | -3.17012300 | 1.71559400 |
| C | -8.19954600 | 0.55682600 | 3.38148900 |
| H | -7.10926600 | 0.50422700 | 3.49136700 |
| C | -8.79616700 | -0.85201000 | 3.31127500 |
| H | -8.58813700 | 1.11690400 | 4.24053800 |
| H | -9.89194100 | -0.80375400 | 3.30980000 |
| H | -8.49557600 | -1.46031400 | 4.17292100 |
| H | 7.37077900 | 4.11892600 | -1.49944100 |
| H | 6.25557200 | 3.09683200 | -0.58317300 |
| C | 7.31353200 | 3.25568000 | -0.82545900 |
| H | 7.71365400 | 4.30579700 | 1.05084900 |
| C | 8.12529300 | 3.48388900 | 0.45278500 |
| H | 9.16107800 | 3.74718000 | 0.20531000 |
| C | 6.56263000 | 1.48129100 | -2.95709800 |
| C | 9.29373000 | 2.33286100 | -2.74480500 |
| P | 7.89838800 | 1.71230000 | -1.70138200 |
| C | 6.69180500 | 2.05734700 | 2.54154700 |
| P | 8.19435200 | 1.91733600 | 1.47255500 |
| C | 9.54472100 | 2.32239400 | 2.66812400 |
| Ru | 8.34136300 | 0.05985600 | -0.03326900 |
| C | 7.10193700 | -2.17322700 | -2.72147500 |
| P | 8.46426700 | -1.80206800 | -1.52864900 |
| C | 9.96154800 | -1.98867500 | -2.59765200 |
| P | 8.75005300 | -1.59736100 | 1.64590600 |
| C | 7.32237300 | -2.17384200 | 2.67060300 |
| C | 10.07081200 | -1.40169800 | 2.92400800 |
| C | 8.48300800 | -3.36650600 | -0.50321800 |
| H | 7.43823000 | -3.59704700 | -0.26053300 |
| C | 9.29402300 | -3.16119400 | 0.77959300 |
| H | 8.87186800 | -4.20217800 | -1.09738200 |
| H | 10.35840000 | -3.03928000 | 0.54477000 |
| H | 9.20276000 | -4.01997100 | 1.45564200 |
| H | -6.27327500 | -3.10325400 | -1.29954500 |
| H | 7.14236400 | -1.48102200 | -3.56700900 |
| H | 10.86114600 | -1.88290400 | -1.98699400 |
| H | 9.96336700 | -2.95936000 | -3.10575900 |
| H | 9.97107000 | -1.19289000 | -3.34925200 |
| H | 10.13340100 | 2.61387900 | -2.10490900 |
| H | 9.63329300 | 1.53313900 | -3.41056800 |
| H | 8.98012500 | 3.19131100 | -3.34908700 |
| H | 6.31191900 | 2.43460500 | -3.43513200 |
| H | 6.89001400 | 0.77984300 | -3.72965500 |
| H | 5.67783500 | 1.07235600 | -2.46243900 |
| H | -0.85576800 | -2.36133000 | 0.09907900 |
| H | 0.86537100 | 2.31707900 | 0.19645400 |
| Cl | 10.94072200 | 0.44202700 | -0.16178400 |
| Cl | -10.94861200 | -0.37090500 | -0.14477700 |

**Table S5.** Cartesian coordinates of optimized geometry of **1'$^{C4}$**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.82746500 | 0.40788300 | 0.09445900 | H | -8.70784900 | 1.98777200 | -3.89086200 |
| C | -3.71398800 | -0.59015400 | -0.29525700 | C | -11.69707000 | 0.26356800 | 0.24385300 |
| C | -3.15657800 | -1.82533200 | -0.79135400 | C | -13.05143400 | 0.41894300 | 0.34104900 |
| C | -1.80747000 | -2.03160400 | -0.86359800 | C | 11.69775100 | -0.32051200 | -0.12333300 |
| C | -1.41745800 | 0.23533300 | 0.02256300 | C | 13.05189500 | -0.49592300 | -0.18178700 |
| C | -0.88179900 | -1.02064300 | -0.45079600 | C | 14.26174300 | -0.65220300 | -0.23318300 |
| H | -3.84114600 | -2.60537700 | -1.11120000 | C | -14.26144900 | 0.55747700 | 0.42744600 |
| H | -3.22168800 | 1.34181400 | 0.47911100 | H | -15.31792500 | 0.67845100 | 0.50300100 |
| H | -1.42148700 | -2.96924800 | -1.24934000 | H | 15.31805000 | -0.78880000 | -0.27840100 |
| C | -0.50620100 | 1.24090000 | 0.39761600 | H | 6.38063800 | -3.24564200 | -0.00098700 |
| C | 0.88242000 | 1.06242100 | 0.36202400 | H | 6.68927300 | -3.87196800 | 1.63906300 |
| C | 1.41804800 | -0.19386700 | -0.11057900 | H | 5.87356800 | -2.29489300 | 1.40074400 |
| C | 0.50680100 | -1.19882800 | -0.48725900 | H | 9.15032400 | -3.86958400 | -0.42543700 |
| C | 1.80799200 | 2.07242100 | 0.77742200 | H | 10.44617500 | -3.04882300 | 0.47005300 |
| C | 3.15709900 | 1.86375300 | 0.71153400 | H | 9.40913500 | -4.25533900 | 1.29032600 |
| C | 3.71445300 | 0.62720600 | 0.21896400 | H | 10.09330800 | 1.54188100 | 4.03909500 |
| C | 2.82803600 | -0.36831500 | -0.17735500 | H | 10.91035000 | 0.62429100 | 2.73542900 |
| H | 1.42183500 | 3.01067300 | 1.16150100 | H | 10.45527000 | 2.31243400 | 2.47326700 |
| H | 3.84176900 | 2.64192200 | 1.03570700 | H | 6.38410500 | 1.97313700 | 2.53391000 |
| H | 3.22259700 | -1.30264000 | -0.56067600 | H | 7.38331100 | 2.15869800 | 4.00750600 |
| C | 5.12473400 | 0.45698800 | 0.15252900 | H | 7.72720800 | 3.13660100 | 2.56389000 |
| C | -5.12431100 | -0.42615500 | -0.21464700 | H | 6.38589200 | 3.19733200 | -0.43464400 |
| C | 6.35168200 | 0.30653300 | 0.09673900 | H | 7.68618400 | 4.02002200 | 0.45311200 |
| C | -6.35168100 | -0.28712900 | -0.14048700 | H | 7.41858100 | 4.40342600 | -1.26206300 |
| H | 8.39029600 | -0.40474800 | 4.40723900 | H | 10.13873200 | 4.01607900 | -1.62243200 |
| H | 6.96755300 | -0.65303600 | 3.38762800 | H | 10.45290500 | 3.38981700 | 0.01672700 |
| C | 8.06318300 | -0.59975000 | 3.37882700 | H | 10.95228500 | 2.43800400 | -1.38719800 |
| H | 8.28800900 | -2.77486200 | 3.39095500 | H | 9.44540800 | -2.00978600 | -3.98067700 |
| C | 8.65654800 | -1.90316500 | 2.83695000 | H | 10.44858200 | -1.81774600 | -2.51111000 |
| H | 9.74942200 | -1.89388300 | 2.93201200 | H | 9.11025100 | -2.98648600 | -2.53441500 |
| C | 7.39336000 | 2.15504700 | 2.91198500 | H | 5.91466500 | -0.48996600 | -2.70040300 |
| C | 10.15162900 | 1.37871200 | 2.95740100 | H | 6.73304500 | -1.40262600 | -4.00735400 |
| P | 8.52065600 | 0.83647100 | 2.27421500 | H | 6.37866400 | -2.17601300 | -2.44133200 |
| C | 6.64802300 | -2.96690100 | 1.02324900 | H | -10.39721700 | 2.17367700 | 2.25633500 |
| P | 8.27609900 | -2.09013700 | 1.01603200 | H | -9.30048300 | 2.74881200 | 3.54913100 |
| C | 9.43318500 | -3.45262800 | 0.54514000 | H | -9.16265300 | 3.39906900 | 1.90045100 |
| C | 10.46828700 | -0.15866900 | -0.06795600 | H | -6.55950100 | 2.31901600 | 3.46597400 |

| | | | |
|---|---|---|---|
| Ru | 8.41726200 | 0.07415800 | 0.01351500 |
| C | 7.39807400 | 3.60193300 | -0.51544500 |
| P | 8.55068100 | 2.23732000 | -0.99049600 |
| C | 10.18043700 | 3.11127800 | -1.00627700 |
| P | 8.30617100 | -0.68992300 | -2.24677000 |
| C | 6.67630300 | -1.24039900 | -2.92542800 |
| C | 9.43854500 | -2.00402200 | -2.88515700 |
| C | 8.16125800 | 2.04946200 | -2.80933300 |
| H | 7.06792400 | 2.03762800 | -2.89864300 |
| C | 8.75484900 | 0.74725000 | -3.35382000 |
| H | 8.52520200 | 2.92184500 | -3.36531200 |
| H | 9.85030300 | 0.80311700 | -3.36814300 |
| H | 8.42333900 | 0.55132400 | -4.38062900 |
| H | -8.09961600 | -2.15116800 | 3.89715200 |
| H | -6.74931300 | -1.33959300 | 3.09368700 |
| C | -7.84346900 | -1.40518000 | 3.13516800 |
| H | -8.02660100 | 0.38206100 | 4.38230300 |
| C | -8.44936400 | -0.03706900 | 3.46140900 |
| H | -9.53258100 | -0.12566100 | 3.61091200 |
| C | -7.28860200 | -3.42123600 | 1.15953100 |
| C | -10.01235600 | -2.82780600 | 1.82568100 |
| P | -8.41059000 | -1.98193200 | 1.45129300 |
| C | -6.57051100 | 1.93395200 | 2.44045700 |
| P | -8.19737400 | 1.15125700 | 2.03954500 |
| C | -9.37959600 | 2.50068400 | 2.48501400 |
| C | -10.46733600 | 0.12012900 | 0.15430300 |
| Ru | -8.41699900 | -0.08202900 | 0.00417100 |
| C | -7.45902000 | -2.67212600 | -2.47466400 |
| P | -8.63105100 | -1.31351300 | -2.03119800 |
| C | -10.26359400 | -2.08297900 | -2.43573700 |
| P | -8.41442800 | 1.81847200 | -1.44263500 |
| C | -6.81142700 | 2.66610600 | -1.80697200 |
| C | -9.53990600 | 3.25649400 | -1.15717600 |
| C | -8.36640800 | -0.12717700 | -3.45225300 |
| H | -7.28194600 | -0.04152800 | -3.59436800 |
| C | -8.97098500 | 1.24257700 | -3.13050700 |
| H | -8.78421600 | -0.54575000 | -4.37568400 |
| H | -10.06560400 | 1.17980400 | -3.09707100 |
| H | -5.77152000 | 1.20040400 | 2.30859800 |
| H | -6.38473500 | 2.76202300 | 1.74885800 |
| H | -10.53268800 | 2.88485500 | -0.89057700 |
| H | -9.16266600 | 3.87125500 | -0.33486600 |
| H | -9.60756100 | 3.87986700 | -2.05558600 |
| H | -6.44594300 | 3.15818700 | -0.90020300 |
| H | -6.06669900 | 1.92583100 | -2.10939800 |
| H | -6.93170800 | 3.41678000 | -2.59576100 |
| H | -7.53369000 | -2.91578600 | -3.54013400 |
| H | -6.44071100 | -2.35307300 | -2.23822100 |
| H | -7.68681800 | -3.57055800 | -1.89433900 |
| H | -11.05689500 | -1.34220400 | -2.30902000 |
| H | -10.27539600 | -2.47109300 | -3.46009500 |
| H | -10.45871000 | -2.90688800 | -1.74171400 |
| H | -10.75577900 | -2.08718700 | 2.13066700 |
| H | -10.38244700 | -3.32151700 | 0.92156100 |
| H | -9.88890400 | -3.57709200 | 2.61528300 |
| H | -7.21159700 | -4.04129400 | 2.05950000 |
| H | -7.67446100 | -4.03890900 | 0.34341000 |
| H | -6.29941200 | -3.04898000 | 0.88105100 |
| O | 1.01108900 | -2.39675600 | -1.00462000 |
| O | -1.01042500 | 2.43884800 | 0.91498300 |
| C | 1.31600300 | -3.46967900 | -0.19751100 |
| C | -1.31763800 | 3.51082500 | 0.10747800 |
| C | 1.06658800 | -3.32576800 | 1.28395400 |
| H | 1.65949000 | -2.50403000 | 1.69724900 |
| H | 0.01325000 | -3.10489500 | 1.48166600 |
| H | 1.34426000 | -4.26020700 | 1.77196100 |
| C | -1.06961100 | 3.36619100 | -1.37413100 |
| H | -0.01641800 | 3.14542700 | -1.57273800 |
| H | -1.66271000 | 2.54407600 | -1.78639200 |
| H | -1.34803800 | 4.30026500 | -1.86240700 |
| O | 1.76218000 | -4.45745700 | -0.73167800 |
| O | -1.76447100 | 4.49839300 | 0.64148500 |

**Table S6.** Cartesian coordinates of optimized geometry of **2'$^{C4}$**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.83042800 | -0.31380500 | -0.04759200 | H | -9.34699800 | 4.31561400 | 0.08584200 |
| C | -3.73540600 | 0.77460800 | -0.04128100 | O | 1.00372800 | 2.57605600 | -0.04511100 |
| C | -3.17899500 | 2.08172300 | -0.04283500 | O | -1.02185700 | -2.45962700 | -0.06955100 |
| C | -1.80704600 | 2.27790200 | -0.04615100 | C | -11.65227800 | -0.59460500 | 0.02621100 |
| C | -1.45193400 | -0.12039300 | -0.05304500 | C | -12.99718800 | -0.83699800 | 0.05195600 |
| C | -0.91927200 | 1.18968300 | -0.05023100 | C | 11.67782900 | 0.42016200 | 0.10035600 |
| H | -3.84968900 | 2.93591800 | -0.03992900 | C | 13.03290700 | 0.59759200 | 0.12173900 |
| H | -3.21115100 | -1.32933400 | -0.04813000 | C | 14.24327000 | 0.75585700 | 0.14230800 |
| H | -1.39238100 | 3.28098500 | -0.04516600 | C | -14.19840600 | -1.05380900 | 0.07341400 |
| C | -0.55567200 | -1.31638600 | -0.06258500 | H | -15.24710400 | -1.24447500 | 0.09424800 |
| C | 0.90088300 | -1.07313100 | -0.06549400 | H | 15.30046000 | 0.89218300 | 0.16033400 |
| C | 1.43386800 | 0.23669200 | -0.05581000 | H | 6.88590600 | -0.37216100 | -3.54448700 |
| C | 0.53744500 | 1.43287100 | -0.04996000 | H | 7.44161600 | -1.99897200 | -4.01648200 |
| C | 1.78804800 | -2.16182000 | -0.07655500 | H | 6.38792300 | -1.77214800 | -2.58579100 |
| C | 3.15974100 | -1.96591500 | -0.07608400 | H | 9.64762100 | 0.32027800 | -3.80726800 |
| C | 3.71701000 | -0.65888900 | -0.06131500 | H | 10.89815600 | -0.36415400 | -2.74703400 |
| C | 2.81268600 | 0.42983400 | -0.05241900 | H | 10.15582100 | -1.36845000 | -4.02970600 |
| H | 1.37289400 | -3.16465300 | -0.08501400 | H | 10.17696800 | -3.76727200 | 1.99219900 |
| H | 3.83067700 | -2.81985300 | -0.08535100 | H | 11.01212400 | -2.44190200 | 1.12399300 |
| H | 3.19305600 | 1.44549500 | -0.04315400 | H | 10.26581900 | -2.13245100 | 2.69684500 |
| C | 5.11941500 | -0.45374900 | -0.05340400 | H | 6.32596100 | -2.64532000 | 1.71208400 |
| C | -5.13674300 | 0.56269300 | -0.03109400 | H | 7.42136900 | -3.98717900 | 2.16239800 |
| C | 6.34593400 | -0.28054100 | -0.04380600 | H | 7.44749500 | -2.46372100 | 3.07787000 |
| C | -6.35939300 | 0.36462000 | -0.01073900 | H | 5.90060400 | 0.34464700 | 2.78976900 |
| H | 8.88050800 | -4.39915800 | -0.18978000 | H | 7.15382900 | -0.34089000 | 3.84616600 |
| H | 7.41842600 | -3.55812900 | -0.71797800 | H | 6.64501100 | 1.34709800 | 4.07249200 |
| C | 8.48409200 | -3.42347400 | -0.49556700 | H | 9.35230600 | 1.98657800 | 4.05498600 |
| H | 9.05815600 | -3.50519600 | -2.60443800 | H | 9.91383300 | 0.36170100 | 3.58306400 |
| C | 9.22007700 | -2.87539100 | -1.72144400 | H | 10.40756700 | 1.76347800 | 2.62516900 |
| H | 10.30075400 | -2.84347600 | -1.53551000 | H | 9.37760100 | 3.96904800 | -2.12005500 |
| C | 7.32241500 | -2.89908200 | 2.08241700 | H | 10.47211900 | 2.62932000 | -1.66151400 |
| C | 10.16350700 | -2.69594300 | 1.76386000 | H | 9.35844500 | 2.44399800 | -3.03303600 |
| P | 8.58826900 | -2.21260900 | 0.92406000 | H | 5.78303500 | 2.42288200 | -1.09699300 |
| C | 7.20997900 | -1.34724300 | -3.16701200 | H | 6.62138600 | 3.75017500 | -1.95882600 |
| P | 8.68482300 | -1.12050500 | -2.07553000 | H | 6.53698200 | 2.11674100 | -2.66702100 |
| C | 9.97340300 | -0.58448200 | -3.28655600 | H | -10.53155500 | -1.33857100 | 2.77658400 |
| C | 10.44769600 | 0.25735200 | 0.08521700 | H | -9.44334100 | -2.09611200 | 3.97908300 |

| | | | |
|---|---|---|---|
| Ru | 8.39828700 | -0.00848400 | 0.01950900 |
| C | 6.82644900 | 0.56451000 | 3.32763400 |
| P | 8.11199200 | 1.10396300 | 2.11473000 |
| C | 9.58647500 | 1.33570800 | 3.20558200 |
| P | 8.20555000 | 2.19529600 | -0.88529400 |
| C | 6.63442600 | 2.67843800 | -1.73244800 |
| C | 9.47727600 | 2.88121100 | -2.03763000 |
| C | 7.56977800 | 2.85634300 | 1.75992300 |
| H | 6.48940700 | 2.81948100 | 1.57339900 |
| C | 8.30398400 | 3.40700900 | 0.53418300 |
| H | 7.72858200 | 3.48724400 | 2.64270200 |
| H | 9.36891100 | 3.54692000 | 0.75708000 |
| H | 7.90327100 | 4.38069800 | 0.22774900 |
| H | -7.42272600 | -4.31250600 | -0.09521200 |
| H | -6.29566800 | -3.06008200 | 0.44057100 |
| C | -7.35606200 | -3.27898700 | 0.26529300 |
| H | -7.75213100 | -3.66580200 | 2.38107100 |
| C | -8.16274600 | -3.07820100 | 1.55127600 |
| H | -9.20121700 | -3.40024400 | 1.40525300 |
| C | -6.59850600 | -2.27718200 | -2.32154600 |
| C | -9.32908900 | -3.01454500 | -1.85438200 |
| P | -7.93549100 | -2.09578600 | -1.05904400 |
| C | -6.71263100 | -1.05968800 | 3.06328900 |
| P | -8.22057900 | -1.26813300 | 2.01361900 |
| C | -9.56530300 | -1.26027600 | 3.28149300 |
| C | -10.43103500 | -0.37566500 | 0.00008700 |
| Ru | -8.39772700 | -0.00100200 | -0.00602400 |
| C | -7.23383300 | 1.25002200 | -3.29688100 |
| P | -8.57436700 | 1.26575800 | -2.02444700 |
| C | -10.08641000 | 1.06698400 | -3.07007500 |
| P | -8.85348300 | 2.09343800 | 1.04802200 |
| C | -7.46078400 | 3.00508900 | 1.85309300 |
| C | -10.19617400 | 2.27635000 | 2.30451000 |
| C | -8.61868300 | 3.07629100 | -1.56208700 |
| H | -7.57762300 | 3.39002400 | -1.41645900 |
| C | -9.42288900 | 3.28304100 | -0.27555900 |
| H | -9.02519800 | 3.66723300 | -2.39154200 |
| H | -10.48535500 | 3.07419300 | -0.45103200 |
| H | -9.54290600 | -0.32614000 | 3.84963700 |
| H | -6.68107100 | -1.80781700 | 3.86285400 |
| H | -5.81954500 | -1.14356200 | 2.43922200 |
| H | -6.71772500 | -0.06090700 | 3.51143700 |
| H | -11.08314400 | 1.73777900 | 1.96105100 |
| H | -9.87694300 | 1.85196800 | 3.26060500 |
| H | -10.44136200 | 3.33323000 | 2.45648300 |
| H | -7.12839800 | 2.45212000 | 2.73732600 |
| H | -6.61725600 | 3.06771400 | 1.16127700 |
| H | -7.76906800 | 4.01137100 | 2.15702400 |
| H | -7.35348400 | 2.08610100 | -3.99461200 |
| H | -6.26553100 | 1.32351300 | -2.79513300 |
| H | -7.26285800 | 0.31578800 | -3.86447900 |
| H | -10.97791500 | 1.15738700 | -2.44468800 |
| H | -10.11453500 | 1.81454100 | -3.87029100 |
| H | -10.08937500 | 0.06769100 | -3.51706000 |
| H | -10.16734400 | -3.08325100 | -1.15672400 |
| H | -9.67118100 | -2.46280600 | -2.73566300 |
| H | -9.01706200 | -4.01871800 | -2.16142000 |
| H | -6.34958600 | -3.33357600 | -2.47068900 |
| H | -6.92444100 | -1.85786800 | -3.27760400 |
| H | -5.71219200 | -1.73393600 | -1.98393300 |

**Table S7.** Cartesian coordinates of optimized geometry of **3'$^{C4}$**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.82217900 | -0.42463400 | 0.06740800 | H | -9.12300000 | 4.21998200 | 1.10535000 |
| C | -3.72014500 | 0.60517300 | -0.18318800 | C | -11.70211200 | -0.42325400 | 0.11132900 |
| C | -3.17800200 | 1.90604900 | -0.50393800 | C | -13.05658800 | -0.59564700 | 0.16907300 |
| C | -1.83043500 | 2.12922100 | -0.55983700 | C | 11.70507200 | 0.39237400 | -0.06394400 |
| C | -1.41172800 | -0.23078300 | 0.02068700 | C | 13.05993500 | 0.56836100 | -0.09557000 |
| C | -0.89058600 | 1.07962800 | -0.30094800 | C | 14.27066900 | 0.72497800 | -0.12342800 |
| H | -3.87469100 | 2.71587600 | -0.70219200 | C | -14.26687700 | -0.75001200 | 0.21958700 |
| H | -3.20095100 | -1.41458200 | 0.31034500 | H | -15.32343500 | -0.88441500 | 0.26489100 |
| H | -1.44942900 | 3.11868200 | -0.80347100 | H | 15.32754400 | 0.86216800 | -0.14846900 |
| C | -0.50174100 | -1.27027300 | 0.27962400 | H | 6.55280400 | 2.12947100 | -2.66316900 |
| C | 0.88222200 | -1.06892500 | 0.23533700 | H | 6.79852400 | 1.15384300 | -4.13433600 |
| C | 1.40358000 | 0.24114300 | -0.08712300 | H | 5.93329600 | 0.47327500 | -2.71903100 |
| C | 0.49345100 | 1.28044600 | -0.34733000 | H | 9.35165100 | 2.66877900 | -2.85811600 |
| C | 1.82141400 | -2.11722500 | 0.50053600 | H | 10.57038000 | 1.38411300 | -2.74053900 |
| C | 3.16896000 | -1.89240800 | 0.45252400 | H | 9.54900200 | 1.52403300 | -4.20439800 |
| C | 3.71186900 | -0.59216500 | 0.13141700 | H | 10.14154700 | -4.06996700 | -1.28764100 |
| C | 2.81431000 | 0.43553500 | -0.12933000 | H | 10.93003900 | -2.46263200 | -1.28361000 |
| H | 1.44000100 | -3.10642100 | 0.74464000 | H | 10.55193300 | -3.26118300 | 0.24700500 |
| H | 3.86443300 | -2.70107500 | 0.65940000 | H | 6.46621800 | -3.19534800 | 0.08451700 |
| H | 3.19359900 | 1.42469800 | -0.37410300 | H | 7.46457400 | -4.46612200 | -0.68529400 |
| C | 5.12428300 | -0.40074400 | 0.09173900 | H | 7.85530200 | -3.89060000 | 0.95053500 |
| C | -5.13179100 | 0.41689400 | -0.12910300 | H | 6.26715700 | -1.42773500 | 2.72626700 |
| C | 6.35038200 | -0.24192000 | 0.05895700 | H | 7.50826400 | -2.68719800 | 2.88451400 |
| C | -6.35830400 | 0.26699000 | -0.07290200 | H | 7.26037500 | -1.53238000 | 4.21369100 |
| H | 8.32599100 | -3.23020500 | -3.00274700 | H | 10.01445800 | -1.14035300 | 4.17484300 |
| H | 6.94177700 | -2.22746600 | -2.54377300 | H | 10.29744900 | -2.10243800 | 2.70127600 |
| C | 8.03708700 | -2.28179600 | -2.53376200 | H | 10.88710600 | -0.43636200 | 2.77716800 |
| H | 8.23949100 | -0.99266200 | -4.28909500 | H | 9.37675500 | 4.45901800 | 0.71863700 |
| C | 8.63947100 | -1.08297900 | -3.27211500 | H | 10.38628000 | 3.18415400 | -0.02853000 |
| H | 9.72696700 | -1.19810800 | -3.36029500 | H | 9.01497700 | 3.87845400 | -0.92173600 |
| C | 7.47979700 | -3.58740900 | -0.03116400 | H | 5.89415300 | 2.47167500 | 1.26103400 |
| C | 10.20219100 | -3.10210800 | -0.77795500 | H | 6.69195200 | 4.07505700 | 1.27974700 |
| P | 8.55448100 | -2.26161800 | -0.73961800 | H | 6.30275200 | 3.26952600 | -0.26205700 |
| C | 6.75238200 | 1.12117200 | -3.04026300 | H | -10.47083300 | -1.88948200 | 2.51098900 |
| P | 8.33988700 | 0.50150300 | -2.32200200 | H | -9.35031900 | -2.91001900 | 3.46357100 |
| C | 9.57267500 | 1.62891900 | -3.11411600 | H | -9.40989600 | -1.15338900 | 3.72913700 |
| C | 10.47438000 | 0.23088000 | -0.03323700 | H | -6.58940200 | -2.65671400 | 3.27192300 |

| | | | |
|---|---|---|---|
| Ru | 8.42300200 | -0.00231800 | 0.01149100 |
| C | 7.26063800 | -1.64949900 | 3.12438700 |
| P | 8.48544100 | -0.50524400 | 2.34502600 |
| C | 10.07433200 | -1.10032800 | 3.08168700 |
| P | 8.27689500 | 2.25827200 | 0.75996200 |
| C | 6.63370100 | 3.10776500 | 0.76866200 |
| C | 9.37108700 | 3.57764200 | 0.06794400 |
| C | 8.15430700 | 1.07586000 | 3.28963100 |
| H | 7.06443000 | 1.18247700 | 3.35608400 |
| C | 8.76239000 | 2.27920000 | 2.56333400 |
| H | 8.53519400 | 0.98812000 | 4.31417000 |
| H | 9.85780000 | 2.23193000 | 2.59361100 |
| H | 8.45978100 | 3.22533800 | 3.02819100 |
| H | -7.61739200 | -4.20295400 | -1.10836100 |
| H | -6.42382200 | -3.10862100 | -0.39584200 |
| C | -7.49886300 | -3.27490300 | -0.53608000 |
| H | -7.75536800 | -4.11252800 | 1.46804300 |
| C | -8.20872100 | -3.35422400 | 0.81846700 |
| H | -9.26157300 | -3.63054100 | 0.68130900 |
| C | -6.91944900 | -1.75400700 | -2.90737200 |
| C | -9.62750700 | -2.51980100 | -2.36677800 |
| P | -8.13851400 | -1.82185000 | -1.51993500 |
| C | -6.63788100 | -1.74579600 | 2.66528600 |
| P | -8.19443100 | -1.68780400 | 1.66830500 |
| C | -9.48111100 | -1.93958700 | 2.97223000 |
| C | -10.47174600 | -0.26644200 | 0.05513300 |
| Ru | -8.42478000 | -0.00031800 | -0.00632000 |
| C | -7.35849000 | 1.91418300 | -3.00029500 |
| P | -8.62993400 | 1.69369200 | -1.67649200 |
| C | -10.20065000 | 1.79950000 | -2.64785400 |
| P | -8.68794000 | 1.82081500 | 1.51270300 |
| C | -7.19748800 | 2.47425900 | 2.39140500 |
| C | -9.93273300 | 1.77169500 | 2.87835700 |
| C | -8.55624000 | 3.35569600 | -0.82202000 |
| H | -7.49403800 | 3.59097200 | -0.68093100 |
| C | -9.27284700 | 3.29833300 | 0.53013100 |
| H | -8.97921600 | 4.13231900 | -1.47052500 |
| H | -10.35305600 | 3.17317900 | 0.38572100 |
| H | -5.77632800 | -1.69591100 | 1.99518700 |
| H | -6.59939400 | -0.87545900 | 3.32832400 |
| H | -10.86685000 | 1.35267800 | 2.49546600 |
| H | -9.57098900 | 1.13561200 | 3.69128800 |
| H | -10.11336900 | 2.77644400 | 3.27595200 |
| H | -6.84759000 | 1.73033100 | 3.11422400 |
| H | -6.39413300 | 2.64314500 | 1.67035200 |
| H | -7.42637000 | 3.40513300 | 2.92177700 |
| H | -7.46192800 | 2.89550100 | -3.47631700 |
| H | -6.36436800 | 1.82056500 | -2.55585100 |
| H | -7.47325900 | 1.14181500 | -3.76592900 |
| H | -11.05371100 | 1.78144900 | -1.96516200 |
| H | -10.22977300 | 2.70937700 | -3.25730700 |
| H | -10.27878600 | 0.92846300 | -3.30652500 |
| H | -10.40992200 | -2.71663900 | -1.62969200 |
| H | -10.01629000 | -1.78488200 | -3.07884200 |
| H | -9.38277200 | -3.44217000 | -2.90488000 |
| H | -6.72085300 | -2.75801800 | -3.29830300 |
| H | -7.31058900 | -1.13520600 | -3.71991000 |
| H | -5.99024200 | -1.30877300 | -2.54285000 |
| H | 0.87649400 | 2.26989900 | -0.59058400 |
| H | -0.88477100 | -2.25965800 | 0.52317400 |

**Table S8.** Cartesian coordinates of optimized geometry of $[\mathbf{1'^{Cl}}]^+$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.82983300 | -0.38230600 | -0.13301100 | H | 7.58596000 | -1.99734300 | -4.13495600 |
| C | -3.73063200 | 0.65789600 | 0.18094900 | H | 6.45055200 | -1.81722800 | -2.72198500 |
| C | -3.16489800 | 1.94421200 | 0.57491000 | H | 9.91232700 | 0.20918300 | -3.74340900 |
| C | -1.79850600 | 2.15804100 | 0.62121800 | H | 11.08560500 | -0.56741200 | -2.60346200 |
| C | -1.40515400 | -0.20306600 | -0.07824200 | H | 10.35340500 | -1.53288100 | -3.96745200 |
| C | -0.86312400 | 1.10447300 | 0.28303100 | H | 10.17569600 | -3.84362800 | 2.08266900 |
| H | -3.85757100 | 2.76281600 | 0.84124800 | H | 11.02733800 | -2.54066600 | 1.13008900 |
| H | -3.23340700 | -1.36125600 | -0.44007700 | H | 10.30956300 | -2.15349000 | 2.73574000 |
| H | -1.40779200 | 3.14240300 | 0.93199100 | H | 7.45626500 | -2.44234700 | 3.20137800 |
| C | -0.48698800 | -1.26340600 | -0.36857300 | H | 6.27311400 | -2.65741400 | 1.84470300 |
| C | 0.91799000 | -1.07667700 | -0.35677500 | H | 7.37912400 | -4.02147400 | 2.32165500 |
| C | 1.45796000 | 0.23291600 | 0.00438800 | H | 5.69715900 | 0.69397600 | 2.68562100 |
| C | 0.54476800 | 1.29345000 | 0.29239800 | H | 6.80844200 | -0.24376200 | 3.76299200 |
| C | 1.85322300 | -2.13541500 | -0.69329000 | H | 6.51917800 | 1.51431800 | 4.08730700 |
| C | 3.22012900 | -1.92972100 | -0.64213400 | H | 9.28126600 | 1.92098000 | 4.20987100 |
| C | 3.77548800 | -0.64213000 | -0.24330300 | H | 9.70450500 | 0.21846300 | 3.74179900 |
| C | 2.88300700 | 0.40857900 | 0.06794500 | H | 10.41579400 | 1.59434500 | 2.81727100 |
| H | 1.45774800 | -3.11736700 | -1.00448500 | H | 10.53982600 | 2.49773300 | -1.82717700 |
| H | 3.91445100 | -2.74803700 | -0.90385100 | H | 9.29941200 | 2.39984400 | -3.14878200 |
| H | 3.29115800 | 1.38450100 | 0.37880500 | H | 9.50530700 | 3.94395300 | -2.22760500 |
| C | 5.19615400 | -0.45128500 | -0.16706800 | H | 5.81859300 | 2.62506700 | -0.95121200 |
| C | -5.15803400 | 0.47653600 | 0.12190200 | H | 6.69054200 | 3.84819100 | -1.98118900 |
| C | 6.43749600 | -0.28379900 | -0.09934600 | H | 6.44852000 | 2.14628300 | -2.57069100 |
| C | -6.39454900 | 0.29987800 | 0.06937700 | H | -10.38688100 | -2.16184800 | -2.41500900 |
| H | 8.74616400 | -4.52721700 | -0.10654900 | H | -9.31458900 | -2.55536700 | -3.84020700 |
| H | 7.31638500 | -3.59288600 | -0.66648600 | H | -9.05122800 | -3.36983200 | -2.24426000 |
| C | 8.40533200 | -3.51684100 | -0.43469000 | H | -6.57848300 | -2.05966900 | -3.80235700 |
| H | 9.01200200 | -3.66969600 | -2.55961400 | H | -5.77110800 | -0.90117300 | -2.65041200 |
| C | 9.20013200 | -3.02472200 | -1.66918000 | H | -6.24667600 | -2.54328600 | -2.08314800 |
| H | 10.29755200 | -3.05229400 | -1.46939500 | H | -8.84853600 | -4.06960000 | -0.01741100 |
| C | 7.29172100 | -2.91619600 | 2.20821800 | H | -9.33234900 | -4.24374900 | 1.71832000 |
| C | 10.17919600 | -2.76234500 | 1.81286700 | H | -10.32201300 | -3.20656800 | 0.58936800 |
| P | 8.56754800 | -2.30294700 | 0.99652400 | H | -6.15604500 | -3.15706000 | 0.63671600 |
| C | 7.31928800 | -1.37047900 | -3.25311600 | H | -5.90087200 | -2.03673900 | 2.02207500 |
| P | 8.77112600 | -1.23652000 | -2.09149600 | H | -6.67190700 | -3.66359100 | 2.30339800 |
| C | 10.17107300 | -0.73328000 | -3.21278300 | H | -7.59491700 | 2.59453000 | 3.82660200 |
| Ru | 8.39103200 | -0.02522000 | 0.04141500 | H | -6.42541800 | 2.10534200 | 2.51862000 |

| | | | |
|---|---|---|---|
| C | 6.63068200 | 0.74592000 | 3.28771000 |
| P | 8.06151800 | 1.19109200 | 2.18007500 |
| C | 9.50850300 | 1.24394100 | 3.35443300 |
| P | 8.26637000 | 2.26076500 | -0.90687300 |
| C | 6.64854100 | 2.77738900 | -1.67545300 |
| C | 9.53034500 | 2.83240800 | -2.15009600 |
| C | 7.71611600 | 3.00124000 | 1.77226200 |
| H | 6.61753800 | 3.08420400 | 1.59574200 |
| C | 8.50803100 | 3.46174500 | 0.52384500 |
| H | 7.95324800 | 3.63163400 | 2.66126500 |
| H | 9.60312500 | 3.48973300 | 0.73398800 |
| H | 8.20294300 | 4.48616800 | 0.20402200 |
| H | -8.37637500 | 2.47200400 | -3.77680300 |
| H | -6.92802700 | 1.66892900 | -3.07544500 |
| C | -8.04464800 | 1.66431800 | -3.08133300 |
| H | -8.15922700 | -0.03453700 | -4.50341500 |
| C | -8.58143500 | 0.27850700 | -3.51864100 |
| H | -9.69177700 | 0.30798500 | -3.63147000 |
| C | -7.54411700 | 3.56937900 | -0.93580600 |
| C | -10.27883000 | 2.83011000 | -1.55037300 |
| P | -8.58774400 | 2.06376000 | -1.31300400 |
| C | -6.54009600 | -1.69876200 | -2.74812000 |
| P | -8.20547300 | -1.03808600 | -2.20772200 |
| C | -9.35315400 | -2.41741000 | -2.73434800 |
| Ru | -8.39887600 | 0.01738100 | -0.02059900 |
| C | -7.47255600 | 2.41339300 | 2.73309200 |
| P | -8.64096200 | 1.07045300 | 2.15780000 |
| C | -10.30295000 | 1.79266000 | 2.62455500 |
| P | -8.26638500 | -2.03718000 | 1.27816400 |
| C | -6.58883400 | -2.80233100 | 1.60012300 |
| C | -9.29506000 | -3.54001400 | 0.85403900 |
| C | -8.35376600 | -0.25420500 | 3.48336000 |
| H | -7.25070300 | -0.29904100 | 3.65126600 |
| C | -8.88672200 | -1.63289700 | 3.01974200 |
| H | -8.81891900 | 0.06443400 | 4.44658700 |
| H | -10.00115300 | -1.62417400 | 2.96221800 |
| H | -8.59494100 | -2.44499800 | 3.72807000 |
| H | 7.03170300 | -0.35202800 | -3.59970500 |
| H | -7.68370100 | 3.36050400 | 2.18834300 |
| H | -11.10417300 | 1.05824100 | 2.39268800 |
| H | -10.32802000 | 2.06771000 | 3.70478500 |
| H | -10.48579800 | 2.70637700 | 2.01321800 |
| H | -11.00568800 | 2.04742200 | -1.85768300 |
| H | -10.62572800 | 3.25445100 | -0.58033100 |
| H | -10.24203600 | 3.64416500 | -2.31149300 |
| H | -6.49360500 | 3.25268100 | -0.75242800 |
| H | -7.57598300 | 4.29046000 | -1.78582100 |
| H | -7.93103500 | 4.07769100 | -0.02413400 |
| O | 1.06373900 | 2.53330400 | 0.68209900 |
| O | -0.99829400 | -2.50573700 | -0.76406100 |
| C | 1.34167100 | 3.56909900 | -0.20367000 |
| C | -1.31364400 | -3.52800100 | 0.12298300 |
| C | 1.00961300 | 3.34870900 | -1.67791500 |
| H | 1.54744900 | 2.46043800 | -2.07950500 |
| H | -0.08141300 | 3.17017600 | -1.81195400 |
| H | 1.31111800 | 4.25649100 | -2.24021000 |
| C | -1.05289500 | -3.28337100 | 1.60795700 |
| H | 0.02435200 | -3.06799400 | 1.79022300 |
| H | -1.63795000 | -2.40907800 | 1.97269100 |
| H | -1.35253800 | -4.19400500 | 2.16666700 |
| O | 1.82270300 | 4.57475800 | 0.25567000 |
| O | -1.76862700 | -4.54358300 | -0.34171900 |
| Cl | 10.87060700 | 0.32623300 | 0.19559400 |
| Cl | -10.96078600 | -0.40887800 | -0.13833000 |

**Table S9.** Cartesian coordinates of optimized geometry of $[\mathbf{2'^{Cl}}]^+$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.83583300 | 0.39265600 | -0.04478400 | O | 0.96478500 | 2.53324600 | -0.12786900 |
| C | 3.76253400 | -0.69824400 | -0.00622400 | H | -6.82282500 | 1.20257000 | -3.32187900 |
| C | 3.20915300 | -2.02362900 | 0.04001700 | H | -7.63674300 | 2.80318600 | -3.60316000 |
| C | 1.82351100 | -2.23530100 | 0.05231600 | H | -6.61375600 | 2.52887400 | -2.12093100 |
| C | 1.44276300 | 0.18303500 | -0.03569600 | H | -9.49556300 | 0.18719600 | -3.92368000 |
| C | 0.91472900 | -1.14438900 | 0.01582000 | H | -10.90123800 | 0.47157300 | -2.81073000 |
| H | 3.89690800 | -2.88804300 | 0.06732800 | H | -10.27983500 | 1.81789900 | -3.86942500 |
| H | 3.21323400 | 1.42843500 | -0.08333000 | H | -10.34197200 | 3.15624500 | 2.81920300 |
| H | 1.41433000 | -3.26029600 | 0.09078800 | H | -11.14594100 | 1.87022200 | 1.80315700 |
| C | 0.52599100 | 1.38777200 | -0.08286400 | H | -10.14592500 | 1.39839200 | 3.22948800 |
| C | -0.96488700 | 1.12458900 | -0.07310800 | H | -6.40083400 | 2.62771000 | 1.88113600 |
| C | -1.48263800 | -0.20177600 | -0.01362200 | H | -7.59411100 | 3.66980000 | 2.77817900 |
| C | -0.56027800 | -1.40934200 | 0.03348900 | H | -7.27729000 | 1.97049000 | 3.32052600 |
| C | -1.86291800 | 2.22144600 | -0.12280400 | H | -5.91136200 | -0.69604300 | 2.85101000 |
| C | -3.25105300 | 2.01119000 | -0.11429000 | H | -7.31041400 | -0.32300700 | 3.94369300 |
| C | -3.78832700 | 0.68512600 | -0.04988000 | H | -6.60543600 | -1.98954700 | 3.92592900 |
| C | -2.87793500 | -0.41100400 | 0.00087400 | H | -9.24300400 | -2.92383600 | 3.64124400 |
| H | -1.44786100 | 3.24310600 | -0.16932200 | H | -10.00393900 | -1.29164200 | 3.39756200 |
| H | -3.94215600 | 2.87194500 | -0.15610600 | H | -10.28218800 | -2.58857500 | 2.17991300 |
| H | -3.25675400 | -1.44558800 | 0.05112700 | H | -9.30909700 | -3.80014700 | -2.71429000 |
| C | -5.21592600 | 0.46026000 | -0.03528500 | H | -10.46596800 | -2.65044300 | -1.89635500 |
| C | 5.18290600 | -0.47314800 | -0.01221100 | H | -9.50447400 | -2.10729400 | -3.32984100 |
| C | -6.44833500 | 0.26102700 | -0.02482300 | H | -5.69416000 | -2.14936900 | -1.69054900 |
| C | 6.41722500 | -0.27343300 | -0.00293700 | H | -6.54399000 | -3.33055800 | -2.78554100 |
| H | -9.46332400 | 4.29114000 | 0.58110800 | H | -6.61911600 | -1.54661900 | -3.11866300 |
| H | -7.88665600 | 3.82126500 | -0.13318200 | H | 10.56802100 | 1.62394800 | 2.70553400 |
| C | -8.91625100 | 3.45319400 | 0.08886900 | H | 9.46739700 | 2.52202200 | 3.85310100 |
| H | -9.61144200 | 3.80214900 | -1.98375400 | H | 9.54101700 | 0.71309800 | 3.88446500 |
| C | -9.62758400 | 2.99893500 | -1.20965900 | H | 6.70186500 | 2.20147300 | 3.79471200 |
| H | -10.69562500 | 2.74538400 | -1.01250600 | H | 5.78918200 | 1.51872600 | 2.37306700 |
| C | -7.36601100 | 2.63480100 | 2.43314900 | H | 6.65940600 | 0.41050900 | 3.49530900 |
| C | -10.24281100 | 2.13036200 | 2.39569300 | H | 11.08066100 | -1.48708200 | 2.20065500 |
| P | -8.72761500 | 2.02956600 | 1.31477400 | H | 9.80732800 | -1.57822100 | 3.48662600 |
| C | -7.33195500 | 2.06140100 | -2.82944500 | H | 10.46277400 | -3.10669900 | 2.77136300 |
| P | -8.82663700 | 1.44361300 | -1.90394800 | H | 7.03159400 | -2.25641900 | 2.85176900 |
| C | -9.99378400 | 0.92920900 | -3.26076200 | H | 6.65269100 | -3.07644400 | 1.29469700 |
| Ru | -8.41884100 | -0.06998100 | 0.02060900 | H | 7.80250000 | -3.85713400 | 2.47225100 |

| | | | |
|---|---|---|---|
| C | -6.84575100 | -1.10092300 | 3.29772700 |
| P | -8.03140900 | -1.58625100 | 1.94590900 |
| C | -9.53595200 | -2.16097100 | 2.88355100 |
| P | -8.13142000 | -2.17388200 | -1.27274500 |
| C | -6.59562300 | -2.32035500 | -2.31824000 |
| C | -9.48794400 | -2.74110100 | -2.41632200 |
| C | -7.27472100 | -3.16443400 | 1.25407200 |
| H | -6.19970600 | -2.94218400 | 1.05456000 |
| C | -8.00008000 | -3.59985700 | -0.04303100 |
| H | -7.31091200 | -3.96578600 | 2.02930100 |
| H | -9.04253000 | -3.92998800 | 0.17864600 |
| H | -7.48149100 | -4.45835000 | -0.53090900 |
| H | 7.48298100 | 4.43967500 | -0.45324200 |
| H | 6.31638500 | 3.21654900 | 0.15959800 |
| C | 7.40153700 | 3.41939100 | -0.00791900 |
| H | 7.75599400 | 3.97561900 | 2.11022500 |
| C | 8.18727900 | 3.31244400 | 1.32265000 |
| H | 9.24936800 | 3.62362400 | 1.17588800 |
| C | 6.67937300 | 2.22823900 | -2.56523800 |
| C | 9.44196300 | 2.96642600 | -2.08850300 |
| P | 8.00107800 | 2.11996300 | -1.24619900 |
| C | 6.69632100 | 1.41173000 | 3.00767500 |
| P | 8.22947000 | 1.52158800 | 1.94015400 |
| C | 9.58523700 | 1.60831800 | 3.22487300 |
| Ru | 8.40868100 | 0.07005400 | -0.00925300 |
| C | 7.28013800 | -1.50079200 | -3.23970300 |
| P | 8.63722500 | -1.36510300 | -1.95941900 |
| C | 10.15565600 | -1.17894800 | -3.03689900 |
| P | 8.87380700 | -1.97800500 | 1.22391400 |
| C | 7.45725200 | -2.88927700 | 2.03962400 |
| C | 10.18781600 | -2.04847100 | 2.55219700 |
| C | 8.74796700 | -3.15702000 | -1.35390500 |
| H | 7.69699000 | -3.50791600 | -1.21524900 |
| C | 9.52913400 | -3.24571100 | -0.01946000 |
| H | 9.20648500 | -3.79865400 | -2.14377400 |
| H | 10.60711700 | -3.00428500 | -0.17839300 |
| H | 9.47883300 | -4.27119500 | 0.41880200 |
| O | -1.02194000 | -2.54881000 | 0.08287800 |
| H | 7.46082100 | -2.37540800 | -3.90745900 |
| H | 6.30031200 | -1.61768500 | -2.72604400 |
| H | 7.24887900 | -0.57821000 | -3.86111100 |
| H | 11.06428500 | -1.15012600 | -2.39768500 |
| H | 10.22491900 | -2.01302800 | -3.77356500 |
| H | 10.09264400 | -0.21244300 | -3.58808400 |
| H | 10.29481900 | 3.04832900 | -1.38061800 |
| H | 9.77440000 | 2.34588300 | -2.95208400 |
| H | 9.14713900 | 3.97629000 | -2.45801900 |
| H | 6.45670500 | 3.29355300 | -2.80809600 |
| H | 7.02789600 | 1.71840900 | -3.49135600 |
| H | 5.75526000 | 1.72530000 | -2.20406600 |
| Cl | 10.96836900 | 0.50422400 | 0.02996000 |
| Cl | -10.87825400 | -0.47798100 | 0.04855600 |

**Table S10.** Cartesian coordinates of optimized geometry of $[\mathbf{3'^{Cl}}]^+$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.81225400 | 0.48770300 | -0.00609000 | H | 6.55484000 | -3.32781500 | -2.82619200 |
| C | -3.73219800 | -0.57941500 | 0.04031000 | H | 5.69716600 | -2.17186700 | -1.71000800 |
| C | -3.19180800 | -1.93680500 | 0.10058300 | H | 9.48200200 | -2.05448400 | -3.39223300 |
| C | -1.82943500 | -2.17857800 | 0.11491600 | H | 10.47310800 | -2.58350400 | -1.97383400 |
| C | -1.38920300 | 0.27521000 | 0.00168500 | H | 9.32987300 | -3.75367700 | -2.78247500 |
| C | -0.87215700 | -1.09102800 | 0.06664900 | H | 9.30344600 | -2.96104200 | 3.57634500 |
| H | -3.90385100 | -2.78153800 | 0.13536900 | H | 10.33132900 | -2.57660400 | 2.11861600 |
| H | -3.18953300 | 1.52612000 | -0.05112100 | H | 10.03129100 | -1.31007800 | 3.36210300 |
| H | -1.44981000 | -3.21715600 | 0.16261200 | H | 5.92781100 | -0.78493200 | 2.84294500 |
| C | -0.45956100 | 1.35828600 | -0.05464200 | H | 6.66291100 | -2.07087800 | 3.90010100 |
| C | 0.93786700 | 1.14310600 | -0.04855400 | H | 7.32689100 | -0.38767900 | 3.92592200 |
| C | 1.45357000 | -0.22508000 | 0.02299200 | H | 6.37693200 | 2.58182000 | 1.91084200 |
| C | 0.52851500 | -1.30784100 | 0.07852400 | H | 7.26600000 | 1.91207300 | 3.33617500 |
| C | 1.89514000 | 2.23487900 | -0.11309100 | H | 7.56908500 | 3.62003800 | 2.81370000 |
| C | 3.25752000 | 2.00093600 | -0.10840800 | H | 10.32115300 | 3.13065600 | 2.82366600 |
| C | 3.78927200 | 0.64161000 | -0.03258200 | H | 10.13556000 | 1.37030200 | 3.22656700 |
| C | 2.87587900 | -0.43582000 | 0.03330200 | H | 11.12424600 | 1.85236700 | 1.79637600 |
| H | 1.51062900 | 3.27092400 | -0.16854300 | H | 10.23303000 | 1.87691100 | -3.86861800 |
| H | 3.97010800 | 2.84378100 | -0.16097500 | H | 10.86533400 | 0.51675600 | -2.83351300 |
| H | 3.26130500 | -1.47030400 | 0.09245100 | H | 9.45775500 | 0.24285300 | -3.94653800 |
| C | 5.20553400 | 0.41490900 | -0.02651700 | H | 6.56855100 | 2.53470300 | -2.10031600 |
| C | -5.16008300 | -0.36965300 | 0.02918400 | H | 7.58562900 | 2.83940600 | -3.58069000 |
| C | 6.44790300 | 0.23123200 | -0.02641000 | H | 6.78506100 | 1.22845800 | -3.32155300 |
| C | -6.39852500 | -0.20477200 | 0.00756800 | H | -10.48127800 | 2.55330900 | -1.98205200 |
| H | 7.38514500 | -4.00994600 | 1.96941700 | H | -9.36576200 | 3.87480500 | -2.56961300 |
| H | 6.24558800 | -2.99393500 | 1.01936100 | H | -9.34048900 | 2.24165900 | -3.35146900 |
| C | 7.32653500 | -3.19901300 | 1.20551400 | H | -6.59136500 | 3.62786200 | -2.43275800 |
| H | 7.53901800 | -4.46517000 | -0.59925800 | H | -5.73266600 | 2.42587200 | -1.36458500 |
| C | 8.04596300 | -3.60320400 | -0.10508500 | H | -6.47770500 | 1.87896200 | -2.91010500 |
| H | 9.09674200 | -3.91619200 | 0.10200800 | H | -10.85404300 | -0.52395900 | -2.85150900 |
| C | 6.87590400 | -1.17145700 | 3.27725300 | H | -9.51433200 | -0.01519100 | -3.95960500 |
| C | 9.57865100 | -2.17821700 | 2.83242100 | H | -10.10061300 | -1.72757400 | -3.99892300 |
| P | 8.06062500 | -1.61395500 | 1.90898200 | H | -6.74489000 | -0.76818000 | -3.47099200 |
| C | 6.59517500 | -2.32201200 | -2.34820600 | H | -6.36862800 | -2.13855000 | -2.36620700 |
| P | 8.13895000 | -2.15654600 | -1.31575600 | H | -7.40307100 | -2.42042000 | -3.83995000 |
| C | 9.49046700 | -2.69250000 | -2.48146100 | H | -7.55870100 | -3.75289400 | 2.59814600 |
| Ru | 8.39414900 | -0.07261900 | 0.00190200 | H | -6.38882300 | -2.49411900 | 1.99342100 |

| | | | |
|---|---|---|---|
| C | 7.34580000 | 2.58800900 | 2.45661200 |
| P | 8.70304600 | 2.00195900 | 1.32143400 |
| C | 10.22375700 | 2.10649400 | 2.39546000 |
| P | 8.78926500 | 1.46068200 | -1.90275300 |
| C | 7.28901800 | 2.08364800 | -2.81730500 |
| C | 9.95417800 | 0.97685600 | -3.27335700 |
| C | 8.87540800 | 3.44552100 | 0.11495000 |
| H | 7.84180400 | 3.80835500 | -0.09741400 |
| C | 9.58305300 | 3.01389700 | -1.19345300 |
| H | 9.41837900 | 4.28139100 | 0.61535100 |
| H | 10.65360400 | 2.76467400 | -1.00454900 |
| H | 9.55772000 | 3.82728300 | -1.95668400 |
| H | -7.74769900 | 3.86998400 | 2.28259500 |
| H | -6.48171900 | 3.04151900 | 1.31114700 |
| C | -7.58445500 | 3.13042800 | 1.46251100 |
| H | -7.83819100 | 4.51009500 | -0.25612900 |
| C | -8.28042000 | 3.56910700 | 0.15014500 |
| H | -9.36461100 | 3.76587900 | 0.32978200 |
| C | -6.95181500 | 0.99954400 | 3.34155300 |
| C | -9.71517100 | 1.80319100 | 3.01119900 |
| P | -8.18717000 | 1.41853200 | 2.00072900 |
| C | -6.59337900 | 2.57999000 | -2.05175700 |
| P | -8.19004300 | 2.19682400 | -1.15394800 |
| C | -9.47061200 | 2.77989100 | -2.38606700 |
| Ru | -8.41178800 | 0.06424800 | -0.00199800 |
| C | -7.41249800 | -2.66660600 | 2.39288200 |
| P | -8.67154500 | -2.05958800 | 1.14923800 |
| C | -10.27827900 | -2.40757700 | 2.04380200 |
| P | -8.67032500 | -1.28984700 | -2.00802000 |
| C | -7.15322800 | -1.70329800 | -3.02353500 |
| C | -9.90909200 | -0.85004900 | -3.33802800 |
| C | -8.59527300 | -3.43500200 | -0.15126400 |
| H | -7.51213000 | -3.63863500 | -0.33093900 |
| C | -9.28934200 | -2.99470000 | -1.46418400 |
| H | -9.04303300 | -4.37223500 | 0.25736300 |
| H | -10.39099900 | -2.89839700 | -1.31232700 |
| H | -9.13118900 | -3.73744600 | -2.28250000 |
| H | 6.59701800 | -1.53931500 | -3.14038500 |
| H | -7.52230100 | -2.10606200 | 3.34796300 |
| H | -11.13514500 | -2.16007900 | 1.38072000 |
| H | -10.33177900 | -3.47387000 | 2.36552500 |
| H | -10.34128900 | -1.75284900 | 2.94346000 |
| H | -10.52804200 | 2.15935700 | 2.34213500 |
| H | -10.06656300 | 0.86966800 | 3.50794100 |
| H | -9.49348100 | 2.56915300 | 3.79061600 |
| H | -6.80663400 | 1.86976000 | 4.02362000 |
| H | -7.32241400 | 0.13737200 | 3.94001400 |
| H | -5.98056100 | 0.72251700 | 2.87539500 |
| H | 0.91452700 | -2.34399000 | 0.13004600 |
| H | -0.84543700 | 2.39439000 | -0.10668700 |
| Cl | -10.98934300 | 0.41149700 | -0.06480200 |
| Cl | 10.88077300 | -0.45349600 | 0.00462200 |

**Table S11.** Cartesian coordinates of optimized geometry of $[\mathbf{1'^{C4}}]^+$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.87861900 | 0.43625700 | 0.06049600 | H | -9.45141500 | -3.73691300 | -2.44631400 |
| C | -3.75995600 | -0.62146400 | -0.25042100 | C | -11.76063000 | 0.28511600 | 0.22373600 |
| C | -3.19220800 | -1.90410900 | -0.64683500 | C | -13.13814500 | 0.43900400 | 0.30721300 |
| C | -1.82361200 | -2.09814800 | -0.69672700 | C | 11.76693900 | -0.49307100 | -0.13468600 |
| C | -1.45069700 | 0.27317300 | 0.00064300 | C | 13.13774400 | -0.72083700 | -0.19098900 |
| C | -0.89874700 | -1.03134100 | -0.35948600 | C | 14.35253700 | -0.92259300 | -0.24069900 |
| H | -3.87862500 | -2.72890600 | -0.90910300 | C | -14.35898900 | 0.57561700 | 0.38103500 |
| H | -3.29577700 | 1.40895200 | 0.36963300 | H | -15.43714400 | 0.69623900 | 0.44631600 |
| H | -1.41935600 | -3.07674900 | -1.00721000 | H | 15.42283100 | -1.10034400 | -0.28458200 |
| C | -0.54728700 | 1.34089400 | 0.29098200 | H | 6.24801900 | -3.15948100 | 0.47786400 |
| C | 0.86255900 | 1.16394600 | 0.28404000 | H | 6.59492100 | -3.62607000 | 2.19775900 |
| C | 1.41560100 | -0.13872500 | -0.07671400 | H | 5.81517300 | -2.02510100 | 1.80765300 |
| C | 0.50823700 | -1.20618400 | -0.36922200 | H | 9.02914000 | -3.99611400 | 0.12651400 |
| C | 1.78871100 | 2.22489600 | 0.62476200 | H | 10.39800300 | -3.12415600 | 0.92485700 |
| C | 3.15713400 | 2.02208600 | 0.58191900 | H | 9.27180100 | -4.16071800 | 1.91205300 |
| C | 3.73237200 | 0.74035100 | 0.18953200 | H | 10.30856700 | 2.06181000 | 3.81111200 |
| C | 2.84278700 | -0.30618200 | -0.12802000 | H | 11.07020400 | 0.82770200 | 2.70836200 |
| H | 1.38940900 | 3.20600700 | 0.93480700 | H | 10.74484000 | 2.49065600 | 2.10135100 |
| H | 3.84275100 | 2.84608900 | 0.84988400 | H | 6.57356800 | 2.44302100 | 2.31000200 |
| H | 3.25512400 | -1.28150100 | -0.43484500 | H | 7.65440700 | 2.78467100 | 3.73555500 |
| C | 5.16325700 | 0.56502400 | 0.13539300 | H | 8.00842800 | 3.53144200 | 2.12623500 |
| C | -5.18588800 | -0.44766200 | -0.17772800 | H | 6.55031500 | 3.23442200 | -0.93608500 |
| C | 6.39800900 | 0.38054900 | 0.08347300 | H | 7.91190700 | 4.10601000 | -0.12456600 |
| C | -6.42993300 | -0.31023300 | -0.12076300 | H | 7.68411200 | 4.27416200 | -1.91180400 |
| H | 8.50649300 | 0.20832200 | 4.48613700 | H | 10.36123400 | 3.73818900 | -2.18397900 |
| H | 7.03048800 | -0.10162000 | 3.50825900 | H | 10.69878500 | 3.27016100 | -0.46258900 |
| C | 8.14653700 | -0.11745400 | 3.48100900 | H | 11.13832600 | 2.13725700 | -1.79141000 |
| H | 8.24805000 | -2.30875700 | 3.80850000 | H | 9.30532700 | -2.67208800 | -3.72743200 |
| C | 8.66324700 | -1.53287400 | 3.12195400 | H | 10.37785600 | -2.33673400 | -2.29460800 |
| H | 9.77537200 | -1.57736300 | 3.20965400 | H | 8.93849900 | -3.42058000 | -2.12190800 |
| C | 7.62312400 | 2.61859500 | 2.63332600 | H | 5.88383600 | -0.71538300 | -2.71313000 |
| C | 10.36031400 | 1.68199700 | 2.76409300 | H | 6.65085200 | -1.94658200 | -3.81610600 |
| P | 8.67076700 | 1.14067300 | 2.16736700 | H | 6.20862300 | -2.37978200 | -2.10909700 |
| C | 6.56393400 | -2.77718600 | 1.47551400 | H | -10.68228300 | 2.66763600 | -1.49104400 |
| P | 8.24643800 | -1.97031700 | 1.32665200 | H | -9.57596800 | 3.91287100 | -2.22618500 |
| C | 9.34464100 | -3.45887000 | 1.04857200 | H | -9.76984600 | 2.29074100 | -3.00718400 |
| C | 10.53459900 | -0.27710700 | -0.07955900 | H | -6.82656100 | 3.59203500 | -2.39349000 |

| | | | |
|---|---|---|---|
| Ru | 8.47470400 | 0.05678800 | 0.00208700 |
| C | 7.60431100 | 3.57054300 | -1.05036200 |
| P | 8.70453200 | 2.08217200 | -1.32216600 |
| C | 10.38772200 | 2.88882800 | -1.46213900 |
| P | 8.28170800 | -1.02848700 | -2.16427000 |
| C | 6.59448500 | -1.56901600 | -2.76850100 |
| C | 9.32968500 | -2.50791000 | -2.62475200 |
| C | 8.29660900 | 1.64495700 | -3.11969700 |
| H | 7.18501300 | 1.69105300 | -3.21390300 |
| C | 8.81349800 | 0.22880900 | -3.47547200 |
| H | 8.71705500 | 2.42002400 | -3.80396300 |
| H | 9.92959700 | 0.21172900 | -3.49667800 |
| H | 8.45875600 | -0.09696600 | -4.48244300 |
| H | -7.48309800 | 3.57343000 | 2.47692500 |
| H | -6.34799800 | 2.73870900 | 1.35996500 |
| C | -7.42720700 | 2.87963200 | 1.60516300 |
| H | -7.73502400 | 4.37369500 | -0.00044500 |
| C | -8.20421600 | 3.43954600 | 0.38856400 |
| H | -9.25247000 | 3.69423700 | 0.67339600 |
| C | -6.84931200 | 0.60463600 | 3.36147200 |
| C | -9.58791800 | 1.57913100 | 3.14672100 |
| P | -8.09264000 | 1.19000400 | 2.10307200 |
| C | -6.82058200 | 2.52683500 | -2.06593000 |
| P | -8.31302900 | 2.17137900 | -1.00585700 |
| C | -9.72437100 | 2.82523200 | -2.03306700 |
| C | -10.51959800 | 0.14788400 | 0.15527400 |
| Ru | -8.45727500 | -0.08237800 | 0.01370500 |
| C | -7.21652200 | -2.98848300 | 2.07020900 |
| P | -8.62191700 | -2.33351000 | 1.03569200 |
| C | -10.11953900 | -2.68881100 | 2.08871200 |
| P | -8.84523100 | -1.35227200 | -2.07463400 |
| C | -7.35651000 | -1.73797300 | -3.12880300 |
| C | -10.09711800 | -0.76708600 | -3.32470200 |
| C | -8.72719400 | -3.60151500 | -0.35897300 |
| H | -7.67824600 | -3.85220100 | -0.64485600 |
| C | -9.50692800 | -3.04299900 | -1.57459400 |
| H | -9.19300900 | -4.53760100 | 0.02950100 |
| H | -10.58613900 | -2.90397600 | -1.32802000 |
| H | -5.89267000 | 2.31339600 | -1.49193600 |
| H | -6.83822200 | 1.86801200 | -2.96333400 |
| H | -11.03114700 | -0.45785500 | -2.80675300 |
| H | -9.68751600 | 0.09880400 | -3.89102000 |
| H | -10.32173800 | -1.58819700 | -4.04410800 |
| H | -6.92671300 | -0.78960400 | -3.52268100 |
| H | -6.57844000 | -2.24280300 | -2.51572400 |
| H | -7.64889200 | -2.39195700 | -3.98242000 |
| H | -7.36615200 | -4.07602000 | 2.26295400 |
| H | -6.25590500 | -2.83060900 | 1.53311700 |
| H | -7.17624400 | -2.45372300 | 3.04440600 |
| H | -11.04568000 | -2.48036100 | 1.51011000 |
| H | -10.11198400 | -3.75301900 | 2.41945700 |
| H | -10.10881400 | -2.02730700 | 2.98421500 |
| H | -10.35927600 | 2.08984400 | 2.52999100 |
| H | -10.02551200 | 0.63204400 | 3.53498500 |
| H | -9.29828500 | 2.22953400 | 4.00400000 |
| H | -6.63044800 | 1.42521700 | 4.08325300 |
| H | -7.26188900 | -0.26220600 | 3.92415700 |
| H | -5.91151400 | 0.29691600 | 2.84943300 |
| O | 1.03103500 | -2.44385400 | -0.76424500 |
| O | -1.07661900 | 2.57620700 | 0.68169900 |
| C | 1.34980700 | -3.46548100 | 0.12232800 |
| C | -1.36042300 | 3.61143000 | -0.20252900 |
| C | 1.08028500 | -3.22566200 | 1.60652000 |
| H | 1.65555600 | -2.34668300 | 1.97551200 |
| H | 0.00029200 | -3.02040200 | 1.78415700 |
| H | 1.38557300 | -4.13451400 | 2.16506700 |
| C | -1.02865700 | 3.39435300 | -1.67735700 |
| H | 0.06315400 | 3.22168500 | -1.81273600 |
| H | -1.56224900 | 2.50366400 | -2.07926100 |
| H | -1.33544900 | 4.30115000 | -2.23838900 |
| O | 1.81451500 | -4.47672800 | -0.34218400 |
| O | -1.84619900 | 4.61421100 | 0.25823000 |

**Table S12.** Cartesian coordinates of optimized geometry of $[\mathbf{2'^{C4}}]^+$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.84281300 | 0.37880600 | 0.01590900 | H | -9.14656800 | -4.25239200 | -1.28427100 |
| C | -3.75728400 | -0.72116200 | 0.02645300 | O | 1.04037800 | -2.53039300 | 0.02174600 |
| C | -3.19403900 | -2.04186900 | 0.03531800 | O | -0.99178200 | 2.53727100 | -0.00474900 |
| C | -1.80600100 | -2.24161200 | 0.03183200 | C | -11.79393200 | 0.50270100 | -0.00480200 |
| C | -1.44738500 | 0.18157600 | 0.01279600 | C | -13.16858800 | 0.71401500 | -0.00784700 |
| C | -0.90844500 | -1.14162100 | 0.02040200 | C | 11.76449100 | -0.51427600 | -0.02761600 |
| H | -3.87463600 | -2.91235700 | 0.04499800 | C | 13.13428500 | -0.73261800 | -0.03183900 |
| H | -3.22963400 | 1.41179800 | 0.00965100 | C | 14.35004200 | -0.92663100 | -0.03577900 |
| H | -1.38720700 | -3.26335600 | 0.03806600 | C | -14.38661600 | 0.90147200 | -0.00991700 |
| C | -0.54091200 | 1.39549400 | 0.00170000 | H | -15.45984000 | 1.06657000 | -0.01202100 |
| C | 0.95116600 | 1.14530800 | -0.00082500 | H | 15.42344000 | -1.09787900 | -0.03924300 |
| C | 1.48186800 | -0.17723100 | 0.00600400 | H | 7.06840500 | 1.29392000 | 3.39829500 |
| C | 0.57084000 | -1.39358200 | 0.01653800 | H | 7.58225800 | 3.03506300 | 3.44784100 |
| C | 1.83992400 | 2.25043400 | -0.01000100 | H | 6.46703600 | 2.43545600 | 2.13709400 |
| C | 3.22992400 | 2.05214700 | -0.01166700 | H | 9.96869100 | 0.80959200 | 3.68065900 |
| C | 3.78013400 | 0.73033500 | -0.00507800 | H | 11.14069600 | 1.36054500 | 2.41631800 |
| C | 2.87907400 | -0.37418800 | 0.00292600 | H | 10.31601900 | 2.57634400 | 3.49199800 |
| H | 1.41628600 | 3.26967800 | -0.01535500 | H | 10.31451900 | 3.12109000 | -2.99627800 |
| H | 3.91279700 | 2.92048800 | -0.01844600 | H | 11.14469500 | 2.21713200 | -1.65044500 |
| H | 3.26731300 | -1.40651000 | 0.00805300 | H | 10.52550500 | 1.31851100 | -3.08492600 |
| C | 5.21112900 | 0.51780000 | -0.00564200 | H | 6.42943800 | 1.99421500 | -2.55646100 |
| C | -5.18234300 | -0.50959400 | 0.02645200 | H | 7.54547400 | 3.19900800 | -3.34205100 |
| C | 6.44326500 | 0.32359700 | 0.00169800 | H | 7.67296000 | 1.44251700 | -3.75573900 |
| C | -6.41767800 | -0.32191600 | 0.01047300 | H | 5.83697600 | -1.32504700 | -2.45114200 |
| H | 8.80941900 | 4.37385000 | -1.10823800 | H | 7.02199800 | -0.79934400 | -3.71464800 |
| H | 7.36655000 | 3.60944300 | -0.35676800 | H | 6.65046900 | -2.55971900 | -3.51453000 |
| C | 8.46332600 | 3.48982900 | -0.52234400 | H | 9.38164200 | -3.03257600 | -3.46758500 |
| H | 8.98618600 | 4.23346600 | 1.49714500 | H | 9.91885100 | -1.29863600 | -3.40419700 |
| C | 9.21874300 | 3.37493600 | 0.82430100 | H | 10.49544600 | -2.45648100 | -2.14619800 |
| H | 10.32224300 | 3.37710100 | 0.65944300 | H | 9.42263200 | -3.19572900 | 3.31786900 |
| C | 7.46039600 | 2.16445100 | -2.93629000 | H | 10.54697200 | -2.00766900 | 2.51985000 |
| C | 10.32829200 | 2.17705500 | -2.40422900 | H | 9.31861900 | -1.43605000 | 3.72504900 |
| P | 8.68741000 | 1.93067600 | -1.55396200 | H | 5.82338600 | -2.18297600 | 1.64527700 |
| C | 7.33805700 | 2.17850900 | 2.77816000 | H | 6.65420700 | -3.10414300 | 2.97965700 |
| P | 8.80830100 | 1.76101500 | 1.71092600 | H | 6.46152100 | -1.30034300 | 3.08110000 |
| C | 10.19587000 | 1.61238400 | 2.94556800 | H | -10.56834500 | 1.93892600 | -2.54784100 |
| C | 10.52856500 | -0.31484800 | -0.02994000 | H | -9.42943600 | 3.05795600 | -3.42376500 |

| | | | |
|---|---|---|---|
| Ru | 8.48849300 | 0.00447100 | -0.01157800 |
| C | 6.78033900 | -1.59332300 | -2.97467400 |
| P | 8.15981900 | -1.75133100 | -1.73258100 |
| C | 9.63233000 | -2.18306800 | -2.79136700 |
| P | 8.28184100 | -1.92169500 | 1.53270100 |
| C | 6.64513600 | -2.15635600 | 2.39355000 |
| C | 9.51647500 | -2.16392200 | 2.90710000 |
| C | 7.73246100 | -3.36009800 | -0.84516800 |
| H | 6.62928700 | -3.35014000 | -0.67875200 |
| C | 8.48868300 | -3.48292000 | 0.50031400 |
| H | 7.95492200 | -4.22115200 | -1.51821500 |
| H | 9.58391800 | -3.61469400 | 0.33322300 |
| H | 8.13427700 | -4.36336900 | 1.08658300 |
| H | -7.82562600 | 4.24121100 | 1.30217700 |
| H | -6.54789700 | 3.25565000 | 0.51303200 |
| C | -7.64970500 | 3.33489500 | 0.67497100 |
| H | -7.99560600 | 4.25564700 | -1.31269900 |
| C | -8.39344500 | 3.42611500 | -0.68066400 |
| H | -9.48014200 | 3.62533800 | -0.52018500 |
| C | -6.83919900 | 1.69435200 | 2.93969200 |
| C | -9.63597100 | 2.37821300 | 2.62424400 |
| P | -8.16900700 | 1.78199300 | 1.62678100 |
| C | -6.67904300 | 1.96627500 | -2.57401900 |
| P | -8.27935300 | 1.78681200 | -1.61989300 |
| C | -9.54570100 | 2.04510800 | -2.97206200 |
| C | -10.55645400 | 0.31193600 | 0.00971400 |
| Ru | -8.49122600 | -0.00496200 | 0.00930800 |
| C | -7.44235500 | -2.05163300 | 2.99517700 |
| P | -8.70396600 | -1.79625200 | 1.63778600 |
| C | -10.30767800 | -1.97892700 | 2.58525600 |
| P | -8.81404700 | -1.79138600 | -1.60873100 |
| C | -7.34975900 | -2.38215300 | -2.61371800 |
| C | -10.14947700 | -1.70585300 | -2.91584100 |
| C | -8.58327400 | -3.43543500 | 0.69921700 |
| H | -7.49578800 | -3.63096900 | 0.53962400 |
| C | -9.32631600 | -3.34689900 | -0.65697100 |
| H | -8.97905300 | -4.26609300 | 1.33109300 |
| H | -10.42853400 | -3.27236100 | -0.49559900 |
| H | -9.40646700 | 1.28258100 | -3.77094400 |
| H | -6.69091900 | 2.89060500 | -3.19747800 |
| H | -5.82128600 | 1.99971000 | -1.86701800 |
| H | -6.54285900 | 1.08120300 | -3.23675600 |
| H | -11.09527800 | -1.34488700 | -2.45521400 |
| H | -9.84965100 | -0.99722600 | -3.71976800 |
| H | -10.31190500 | -2.71119500 | -3.37004200 |
| H | -7.01164100 | -1.56343900 | -3.28951100 |
| H | -6.50714400 | -2.63708500 | -1.93425800 |
| H | -7.62348700 | -3.27176900 | -3.22762400 |
| H | -7.55632100 | -3.06552200 | 3.44516300 |
| H | -6.41846400 | -1.94024500 | 2.57528200 |
| H | -7.58842600 | -1.29081000 | 3.79445500 |
| H | -11.16245000 | -2.01773500 | 1.87484600 |
| H | -10.29511300 | -2.90149500 | 3.21129600 |
| H | -10.45055200 | -1.09240000 | 3.24456100 |
| H | -10.47305200 | 2.64052000 | 1.94068500 |
| H | -9.98363900 | 1.55976500 | 3.29542900 |
| H | -9.36067400 | 3.26458100 | 3.24211400 |
| H | -6.67367800 | 2.70031200 | 3.39141700 |
| H | -7.14612500 | 0.98995900 | 3.74467800 |
| H | -5.89349200 | 1.32708500 | 2.48385500 |

**Table S13.** Cartesian coordinates of optimized geometry of $[\mathbf{3'^{C4}}]^+$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.88281900 | -0.39130500 | 0.13723700 | H | -9.45134800 | 4.33738000 | 0.75331700 |
| C | -3.77901900 | 0.68525500 | -0.04312000 | C | -11.75289700 | -0.50584700 | -0.02535600 |
| C | -3.22705500 | 2.02067800 | -0.26014400 | C | -13.12594800 | -0.71640300 | -0.02927200 |
| C | -1.86120700 | 2.23229800 | -0.29290800 | C | 11.78742100 | 0.44932000 | -0.14510000 |
| C | -1.45656700 | -0.20366200 | 0.11062000 | C | 13.16391700 | 0.63904400 | -0.20161000 |
| C | -0.92039800 | 1.13975500 | -0.11230100 | C | 14.38392300 | 0.80723700 | -0.25106200 |
| H | -3.92685700 | 2.86431700 | -0.39999700 | C | -14.34227400 | -0.90310500 | -0.03304800 |
| H | -3.28336000 | -1.40845300 | 0.30244900 | H | -15.41648500 | -1.06788400 | -0.03632800 |
| H | -1.46173300 | 3.25054700 | -0.46004400 | H | 15.45868800 | 0.95550400 | -0.29473200 |
| C | -0.54852700 | -1.28626100 | 0.29278200 | H | 6.46291000 | 2.13517100 | -2.61917800 |
| C | 0.85548900 | -1.09317800 | 0.26049300 | H | 6.75237900 | 1.23616500 | -4.16953800 |
| C | 1.39286600 | 0.24734500 | 0.03338800 | H | 5.89011300 | 0.43423400 | -2.77716300 |
| C | 0.48072600 | 1.33091100 | -0.14577800 | H | 9.31397700 | 2.75456200 | -2.88861800 |
| C | 1.79570100 | -2.18103600 | 0.44405100 | H | 10.57229300 | 1.45751300 | -2.86525600 |
| C | 3.16167300 | -1.96346700 | 0.40410200 | H | 9.46097600 | 1.62824900 | -4.29828400 |
| C | 3.72145400 | -0.63338600 | 0.17362700 | H | 10.28717100 | -4.09242000 | -1.37774900 |
| C | 2.82014900 | 0.43408600 | -0.00408400 | H | 11.04816100 | -2.43885100 | -1.45418000 |
| H | 1.40023200 | -3.19990300 | 0.61852600 | H | 10.75405100 | -3.21450000 | 0.14207000 |
| H | 3.85968300 | -2.80815200 | 0.54754200 | H | 6.58878500 | -3.31693200 | 0.07207600 |
| H | 3.21421800 | 1.45204500 | -0.18015200 | H | 7.63751300 | -4.55812200 | -0.75109000 |
| C | 5.15463900 | -0.44550600 | 0.13086100 | H | 8.05178800 | -3.97724100 | 0.91158600 |
| C | -5.20114000 | 0.48049600 | -0.01928000 | H | 6.39320900 | -1.48505600 | 2.85546400 |
| C | 6.39119800 | -0.27578500 | 0.08458500 | H | 7.66418300 | -2.76991200 | 2.88721200 |
| C | -6.44374700 | 0.30874800 | -0.00033000 | H | 7.50120000 | -1.64159100 | 4.29335800 |
| H | 8.40602300 | -3.24663800 | -3.09831700 | H | 10.20653200 | -1.23551700 | 4.16844400 |
| H | 6.97834400 | -2.28071500 | -2.58373600 | H | 10.51200600 | -2.12314800 | 2.61441700 |
| C | 8.09434700 | -2.29611800 | -2.60278400 | H | 11.06556900 | -0.41728100 | 2.78480400 |
| H | 8.20611300 | -0.96406000 | -4.37311200 | H | 9.34505500 | 4.54431300 | 0.75235000 |
| C | 8.64586400 | -1.05705300 | -3.35155900 | H | 10.39327300 | 3.29571400 | -0.05903600 |
| H | 9.75213600 | -1.13893100 | -3.47830200 | H | 8.94260000 | 3.96355500 | -0.91311600 |
| C | 7.63236700 | -3.67237900 | -0.07368900 | H | 5.91160300 | 2.45540800 | 1.42780500 |
| C | 10.34844300 | -3.09244800 | -0.88828500 | H | 6.68989300 | 4.10189100 | 1.36063900 |
| P | 8.66050300 | -2.28805600 | -0.79764300 | H | 6.22787200 | 3.23115500 | -0.16466000 |
| C | 6.70161900 | 1.13995100 | -3.05984700 | H | -10.61972900 | -1.86623600 | 2.55951000 |
| P | 8.33208800 | 0.53409500 | -2.36850700 | H | -9.48453200 | -2.72586000 | 3.69458300 |
| C | 9.53766600 | 1.70664300 | -3.18853100 | H | -9.65397500 | -0.92526200 | 3.76688700 |
| C | 10.54930900 | 0.26801400 | -0.09016800 | H | -6.73788600 | -2.36955900 | 3.64656600 |

| | | | |
|---|---|---|---|
| Ru | 8.48153200 | -0.00365400 | -0.00168500 |
| C | 7.42876300 | -1.72354500 | 3.18356900 |
| P | 8.62583100 | -0.54137000 | 2.36482900 |
| C | 10.26010300 | -1.13312900 | 3.05945600 |
| P | 8.30316400 | 2.28252700 | 0.79314300 |
| C | 6.62237600 | 3.10322400 | 0.86929700 |
| C | 9.35019600 | 3.65719600 | 0.07670300 |
| C | 8.29806900 | 1.04755200 | 3.34630600 |
| H | 7.19040200 | 1.12666100 | 3.46271000 |
| C | 8.85424700 | 2.28792500 | 2.60320100 |
| H | 8.72896000 | 0.95498200 | 4.37169200 |
| H | 9.97040900 | 2.27338200 | 2.59331800 |
| H | 8.53858300 | 3.23774500 | 3.09750000 |
| H | -7.48368900 | -4.33905800 | -0.77495900 |
| H | -6.33545700 | -3.13434700 | -0.09604700 |
| C | -7.41741900 | -3.35110000 | -0.26102900 |
| H | -7.72786200 | -4.06213700 | 1.81308100 |
| C | -8.18987500 | -3.35886500 | 1.08095200 |
| H | -9.24421600 | -3.69056200 | 0.92859600 |
| C | -6.80096700 | -1.96938000 | -2.76962100 |
| C | -9.54765200 | -2.77958700 | -2.23170900 |
| P | -8.06847800 | -2.00234500 | -1.40382700 |
| C | -6.74463000 | -1.53392800 | 2.90927500 |
| P | -8.26883000 | -1.63193500 | 1.83910300 |
| C | -9.64274400 | -1.80508000 | 3.08679400 |
| C | -10.51681400 | -0.31938400 | -0.02847000 |
| Ru | -8.45632400 | 0.00092500 | -0.01047100 |
| C | -7.30502800 | 1.79990700 | -3.11766000 |
| P | -8.67015700 | 1.62968000 | -1.86009200 |
| C | -10.20207500 | 1.53559300 | -2.91976600 |
| P | -8.87479300 | 1.99921800 | 1.38276600 |
| C | -7.40237200 | 2.77383300 | 2.22479100 |
| C | -10.15313400 | 1.96242600 | 2.73837200 |
| C | -8.74380800 | 3.35650400 | -1.10188800 |
| H | -7.68850100 | 3.68398600 | -0.94702700 |
| C | -9.51915500 | 3.35001500 | 0.23845900 |
| H | -9.20203800 | 4.06205300 | -1.83421900 |
| H | -5.83425200 | -1.58376200 | 2.27300900 |
| H | -6.73694800 | -0.56361800 | 3.45549400 |
| H | -11.08046100 | 1.47294000 | 2.36857800 |
| H | -9.76186600 | 1.39278100 | 3.61026700 |
| H | -10.38289900 | 3.00246400 | 3.06655200 |
| H | -6.98862300 | 2.05987800 | 2.97213700 |
| H | -6.60870900 | 2.99073800 | 1.47698700 |
| H | -7.70374400 | 3.71400100 | 2.74171500 |
| H | -7.46518000 | 2.72083700 | -3.72471000 |
| H | -6.32429900 | 1.85832700 | -2.59705000 |
| H | -7.30082200 | 0.91991200 | -3.79760200 |
| H | -11.10871700 | 1.59918500 | -2.27945200 |
| H | -10.20537400 | 2.36596700 | -3.66299300 |
| H | -10.22210300 | 0.56141400 | -3.45866100 |
| H | -10.33271200 | -3.00243800 | -1.47664400 |
| H | -9.97266800 | -2.06579800 | -2.97280900 |
| H | -9.24757100 | -3.71720300 | -2.75400100 |
| H | -6.57831300 | -3.00978800 | -3.10153900 |
| H | -7.19646700 | -1.39650000 | -3.63748700 |
| H | -5.86873000 | -1.48445500 | -2.40614700 |
| H | 0.88240800 | 2.34813200 | -0.31623700 |
| H | -0.95019200 | -2.30357900 | 0.46305000 |
| H | -10.60155900 | 3.13713900 | 0.07105900 |