

Electronic Supplementary Information: Non-Innocent Ligand Flavin and Curcumin Inspired Ruthenium Photosensitizers for Solar Energy Conversion

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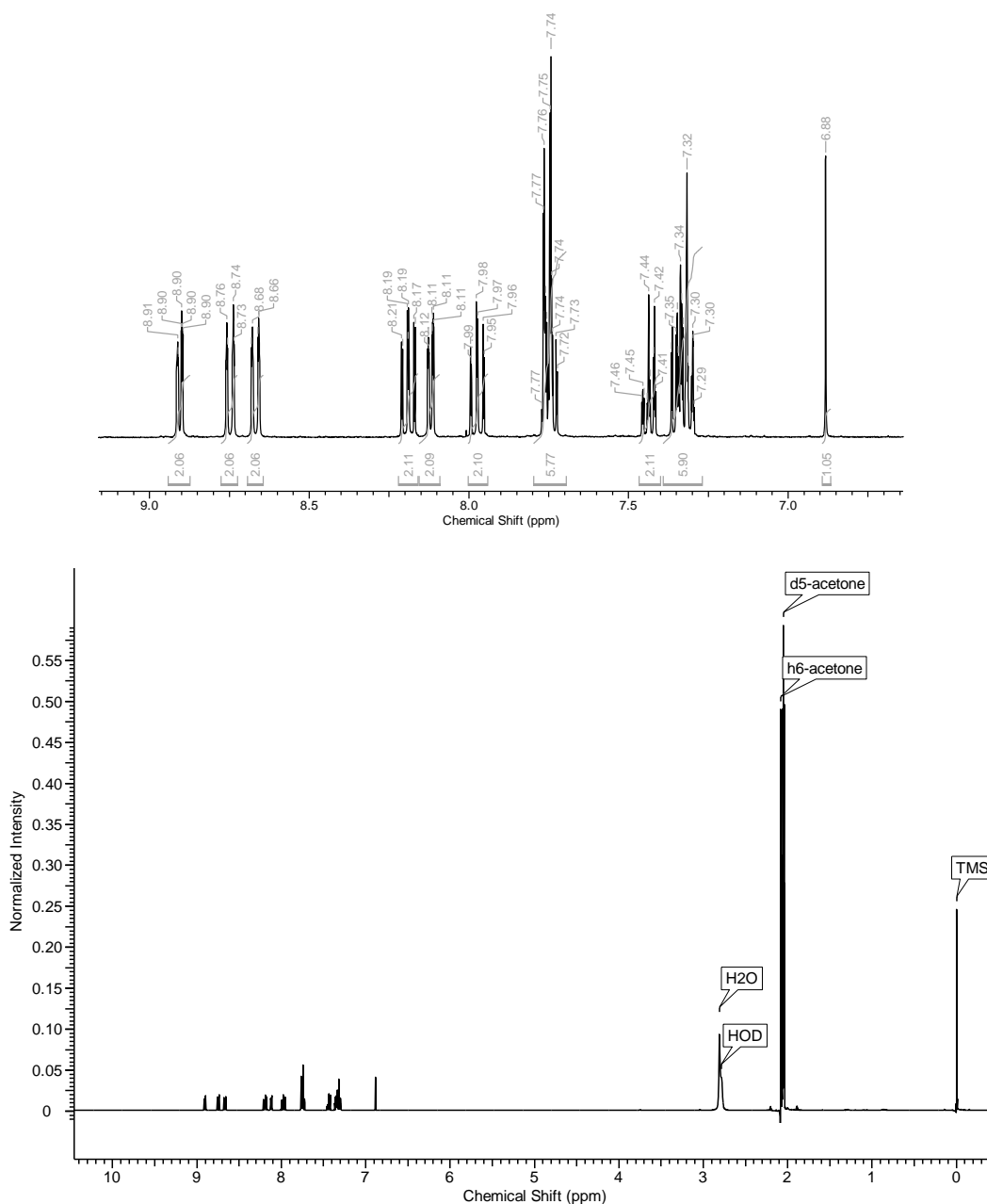


Figure ESI-1. ¹H NMR spectrum for [Ru(Ph₂acac)(bpy)₂][PF₆]₂ (**4**⁺) recorded in *d*⁶-acetone ($\delta = 2.05$ ppm).

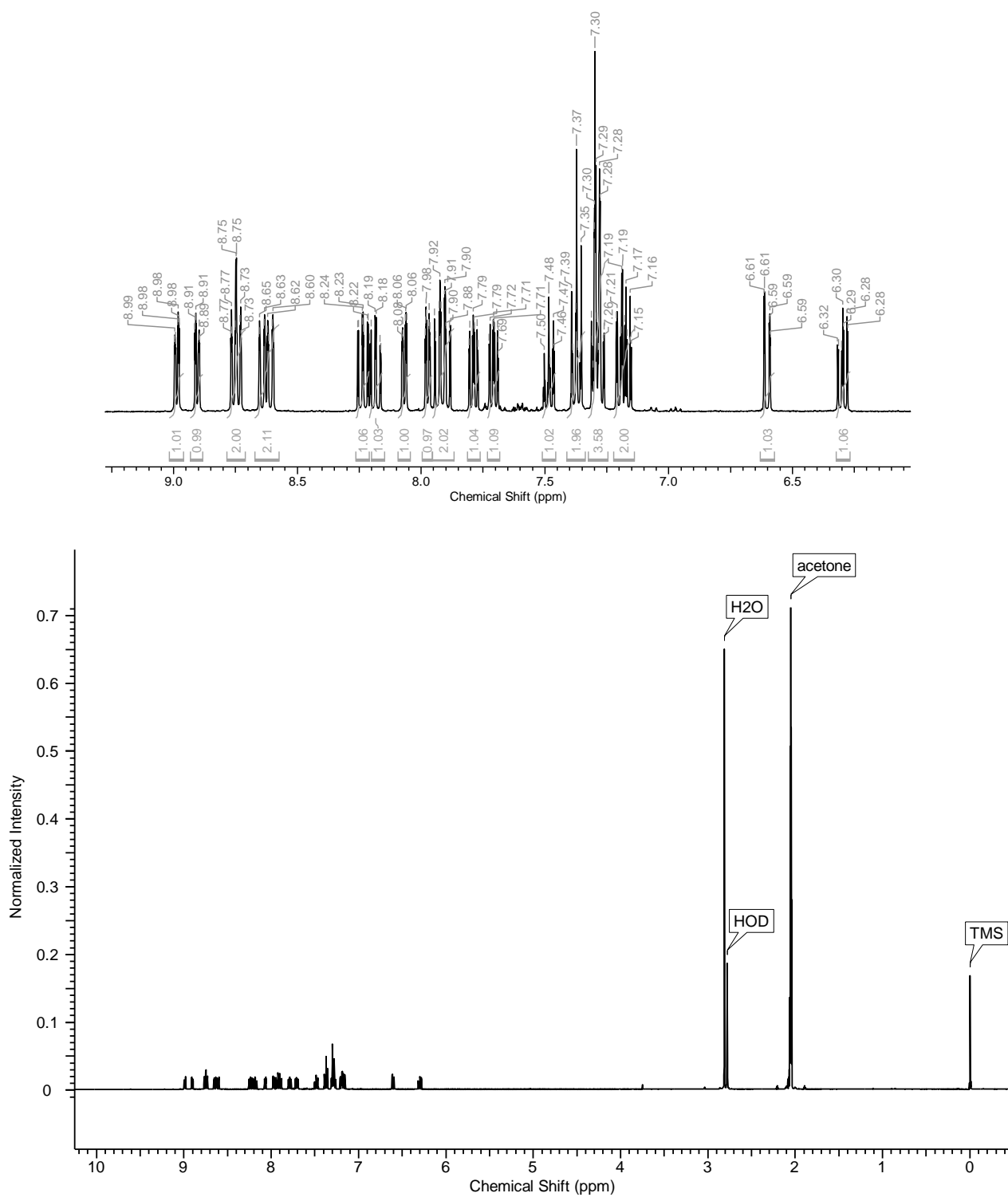


Figure ESI-2. ^1H NMR spectrum for $[\text{Ru}(\text{OBP})(\text{bpy})_2][\text{PF}_6]_2$ (5^+) recorded in d^6 -acetone ($\delta = 2.05$ ppm).

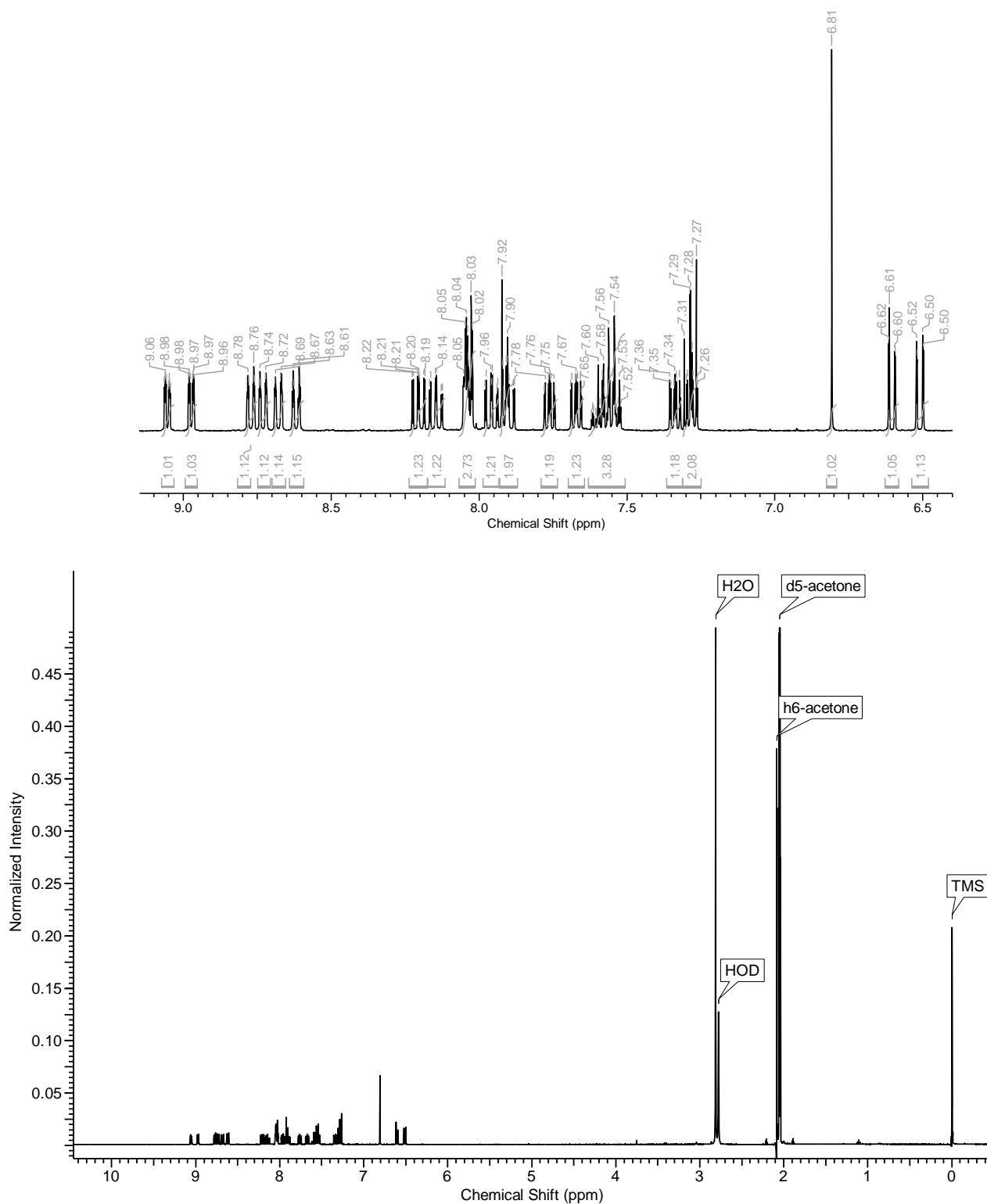


Figure ESI-3. ^1H NMR spectrum for $[\text{Ru}(\text{OFlav})(\text{bpy})_2](\text{PF}_6)_2$ (6^+) recorded in d^6 -acetone ($\delta = 2.05$ ppm).

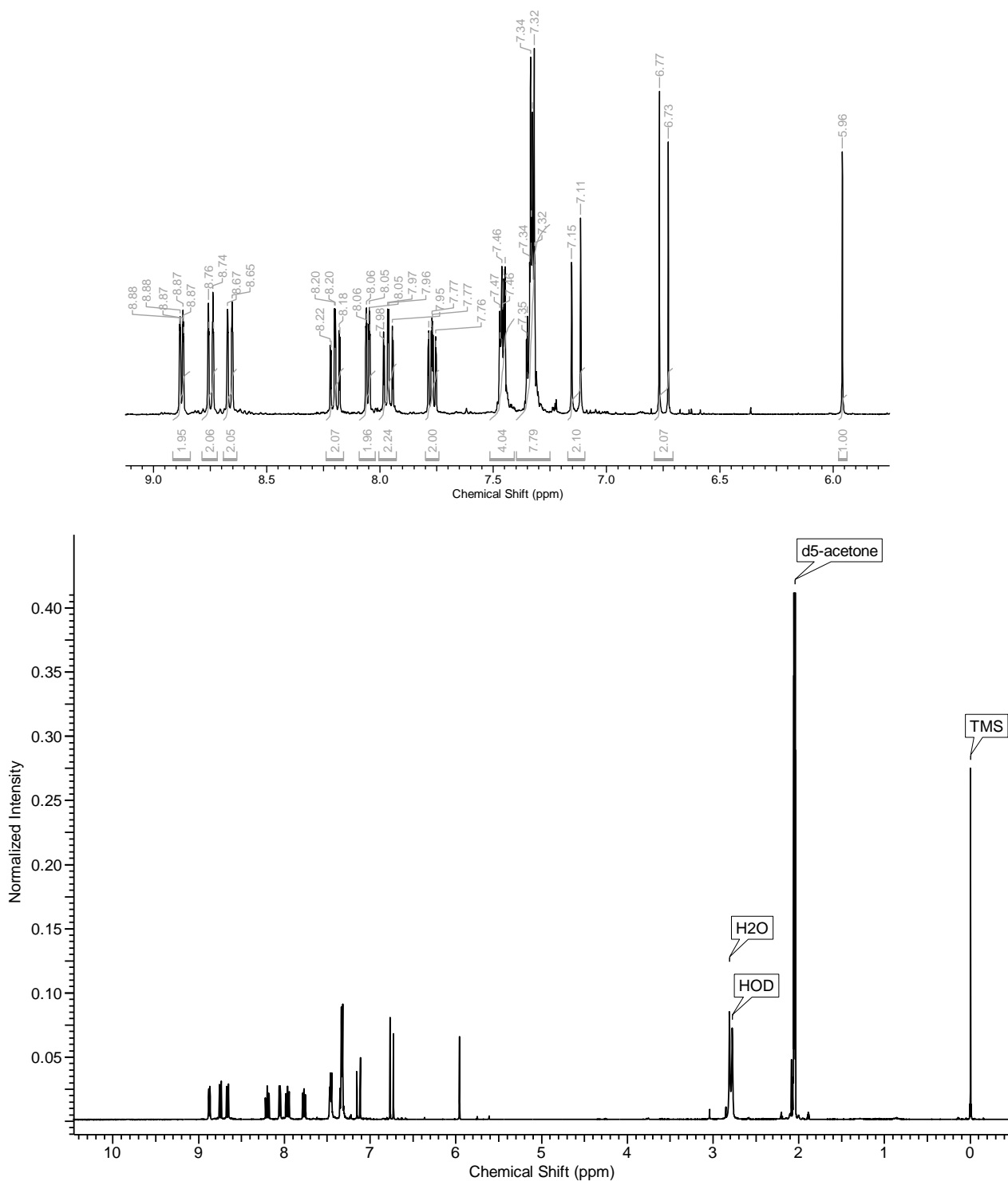


Figure ESI-4. ^1H NMR spectrum for $[\text{Ru}(\text{Ph}_2\text{curc})(\text{bpy})_2][\text{PF}_6]_2$ (7^+) recorded in d^6 -acetone ($\delta = 2.05$ ppm).

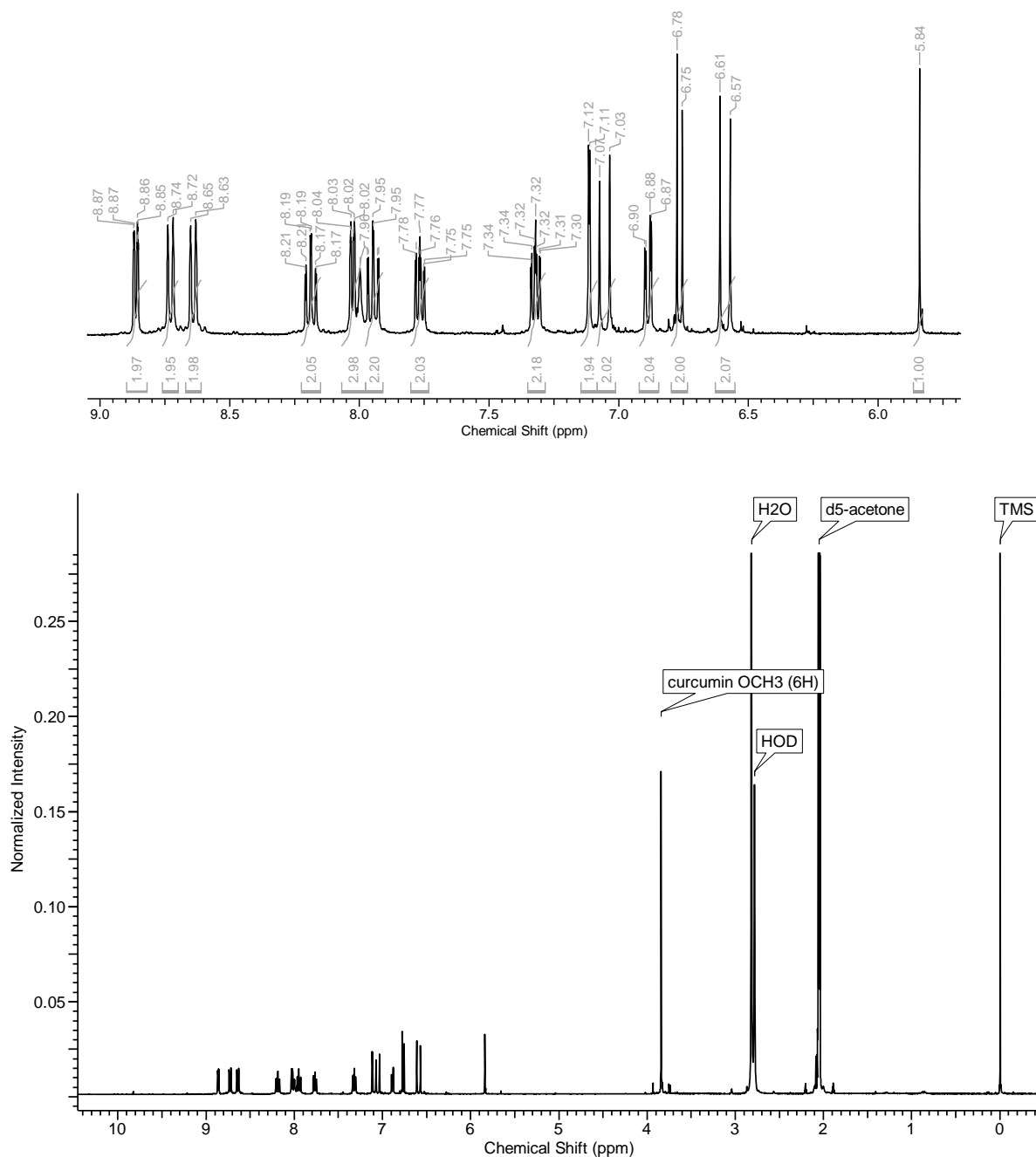


Figure ESI-5. ¹H NMR spectrum for [Ru(curc)(bpy)₂][PF₆]₂ (**8**⁺) recorded in d⁶-acetone (δ = 2.05 ppm). Note: The broad shoulder peak at 8.00 ppm [8.00 – 8.04 (m, 4H)], is assigned to the curcumin -OH peaks and thus has low integration due to proton acidity and H/D exchange in solution. The multiplet occurring at 8.00 – 8.04 ppm is thus attributed to 4H although it integrates as 3H.

Table ESI-1. Percentage contributions (%) of Ru, bpy and NIL to the frontier molecular orbitals of complexes **1**²⁺ - **8**⁺ as determined by Mulliken population analysis.

| | MO | Ru(<i>dπ</i>) | NIL(<i>π</i>) | bpy(<i>π</i>) | Energy (eV) |
|------------------------|------|-----------------|-----------------|-----------------|-------------|
| 1 ²⁺ | LUMO | 1 | ~ | 99 | -2.59 |
| | HOMO | 85 | ~ | 15 | -6.07 |
| 2 | LUMO | 3 | 0 | 97 | -2.27 |
| | HOMO | 51 | 38 | 11 | -5.16 |
| | H-1 | 52 | 40 | 8 | -5.41 |
| | H-2 | 48 | 45 | 7 | -5.45 |
| | H-3 | 0 | 100 | 0 | -5.99 |
| | H-4 | 32 | 60 | 8 | -6.46 |
| | H-5 | 30 | 62 | 8 | -6.49 |
| | H-6 | 26 | 63 | 11 | -6.62 |
| 3 ⁺ | LUMO | 4 | 0 | 96 | -2.25 |
| | HOMO | 67 | 21 | 12 | -5.36 |
| | H-1 | 72 | 14 | 14 | -5.37 |
| | H-2 | 81 | 7 | 13 | -5.37 |
| | H-3 | 19 | 74 | 7 | -6.52 |
| | H-4 | 1 | 1 | 98 | -7.12 |
| | H-5 | 0 | 0 | 99 | -7.14 |
| | H-6 | 4 | 87 | 9 | -7.42 |
| 4 ⁺ | LUMO | 4 | 0 | 96 | -2.27 |
| | HOMO | 69 | 18 | 13 | -5.41 |
| | H-1 | 70 | 17 | 12 | -5.42 |
| | H-2 | 76 | 12 | 4 | -5.72 |
| | H-3 | 14 | 82 | 1 | -6.31 |
| | H-4 | 1 | 99 | 0 | -7.02 |
| | H-5 | 0 | 99 | 95 | -7.03 |
| | H-6 | 0 | 5 | 13 | -7.12 |
| 5 ⁺ | LUMO | 4 | 2 | 95 | -2.29 |
| | HOMO | 46 | 46 | 8 | -5.23 |
| | H-1 | 75 | 9 | 16 | -5.41 |
| | H-2 | 76 | 11 | 12 | -5.74 |
| | H-3 | 34 | 58 | 8 | -6.2 |
| | H-4 | 0 | 97 | 2 | -7.05 |
| | H-5 | 0 | 7 | 93 | -7.13 |
| | H-6 | 0 | 57 | 43 | -7.15 |
| 6 ⁺ | LUMO | 4 | 2 | 94 | -2.26 |
| | HOMO | 43 | 51 | 6 | -5.13 |
| | H-1 | 73 | 10 | 17 | -5.35 |
| | H-2 | 71 | 16 | 13 | -5.58 |
| | H-3 | 43 | 49 | 8 | -6.1 |
| | H-4 | 1 | 98 | 0 | -6.75 |
| | H-5 | 0 | 6 | 93 | -7.1 |
| | H-6 | 0 | 2 | 98 | -7.14 |
| 7 ⁺ | LUMO | 2 | 85 | 13 | -2.35 |
| | HOMO | 76 | 9 | 15 | -5.37 |
| | H-1 | 60 | 30 | 10 | -5.37 |
| | H-2 | 69 | 19 | 12 | -5.62 |
| | H-3 | 11 | 87 | 2 | -5.89 |
| | H-4 | 11 | 86 | 3 | -6.56 |
| | H-5 | 9 | 77 | 13 | -6.94 |
| | H-6 | 0 | 100 | 0 | -7.04 |
| 8 ⁺ | LUMO | 3 | 47 | 50 | -2.26 |
| | HOMO | 51 | 40 | 9 | -5.3 |
| | H-1 | 69 | 19 | 12 | -5.33 |
| | H-2 | 36 | 57 | 8 | -5.47 |
| | H-3 | 40 | 52 | 8 | -5.54 |
| | H-4 | 25 | 71 | 4 | -6.02 |
| | H-5 | 6 | 92 | 2 | -6.47 |
| | H-6 | 6 | 91 | 3 | -6.72 |

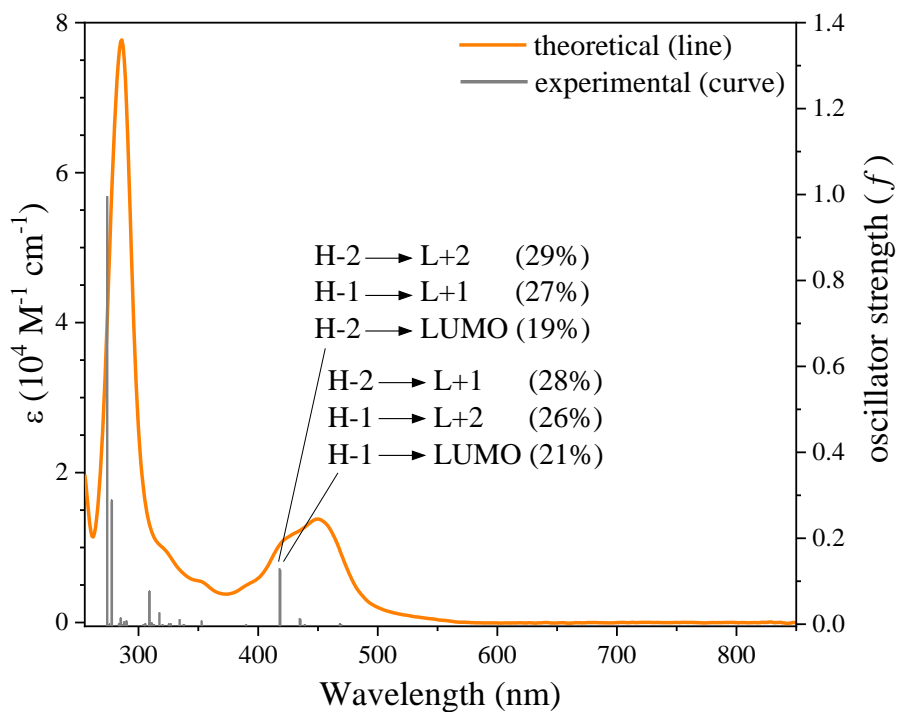


Figure ESI-6. Overlay of experimental (acetonitrile) and theoretical (TDDFT) spectra for 1^+ .

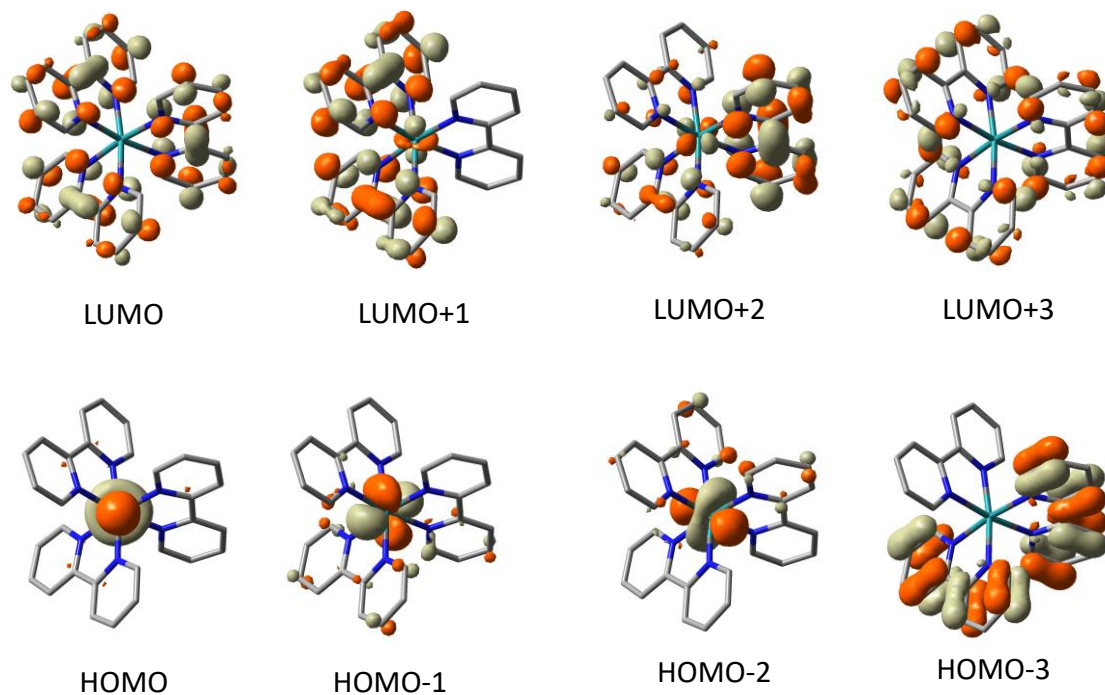


Figure ESI-7. Select frontier molecular orbital surfaces for 1^+ (isofactor = 0.04).

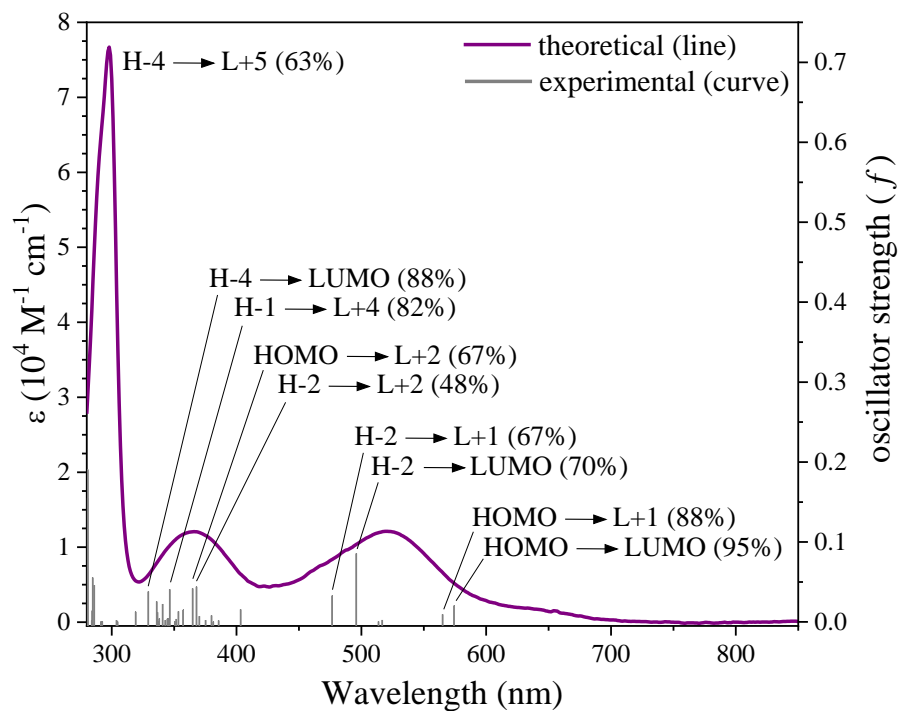


Figure ESI-8. Overlay of experimental (acetonitrile) and theoretical (TDDFT) spectra for **2**.

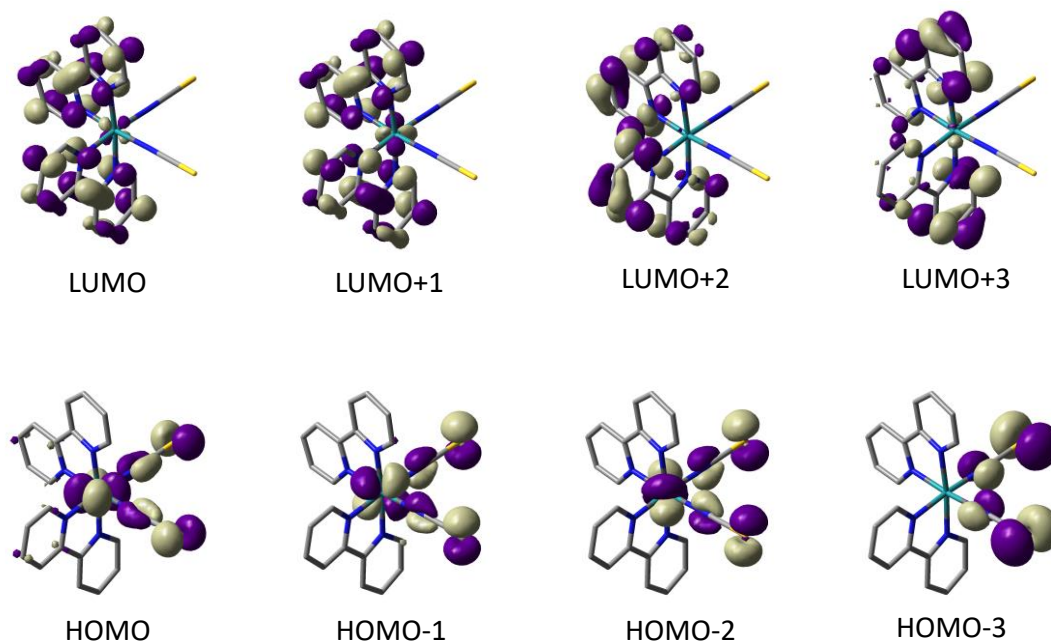


Figure ESI-9. Select frontier molecular orbital surfaces for **2** (isofactor = 0.04).

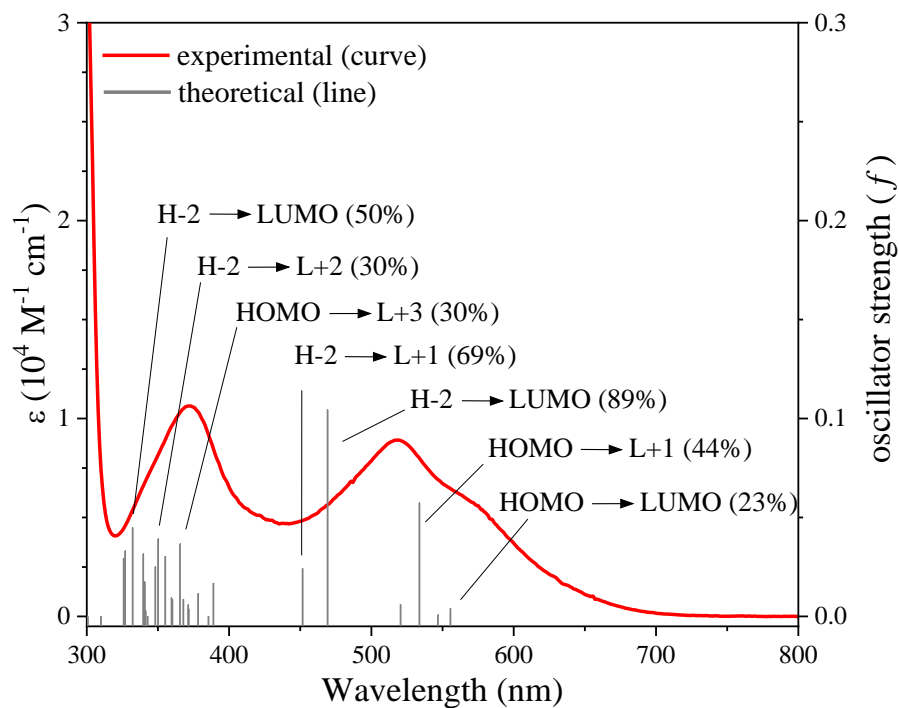


Figure ESI-10. Overlay of experimental (acetone nitrile) and theoretical (TDDFT) spectra for 3^+ .

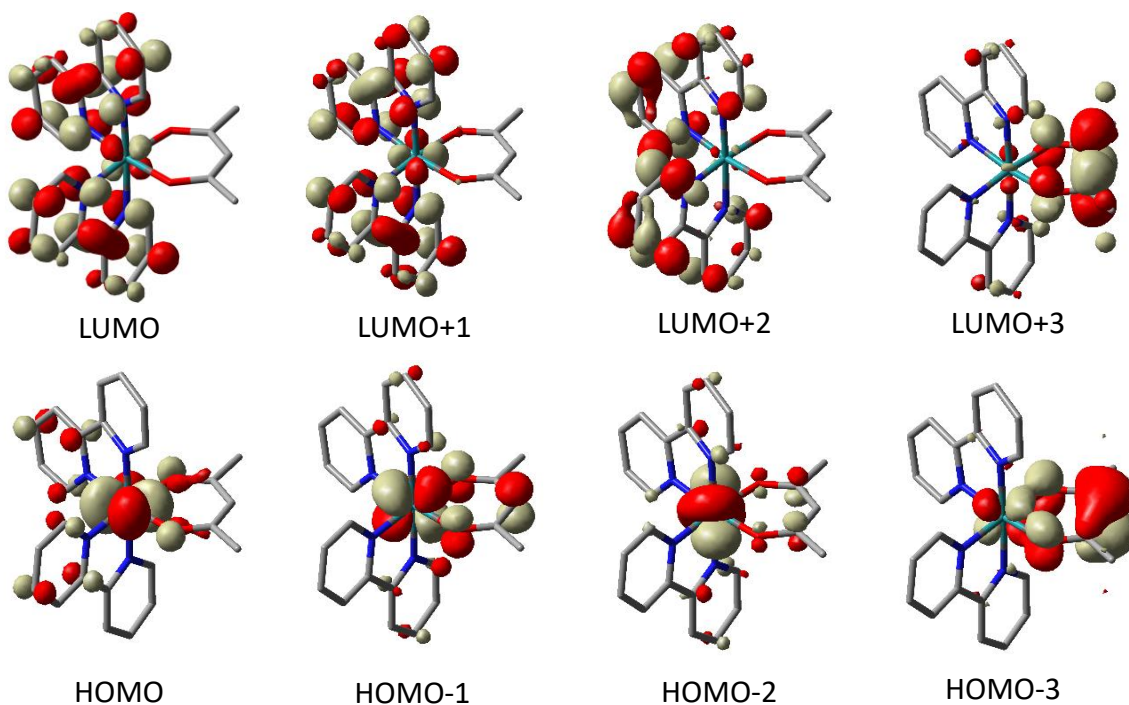


Figure ESI-11. Select frontier molecular orbital surfaces for 3^+ (isofactor = 0.04).

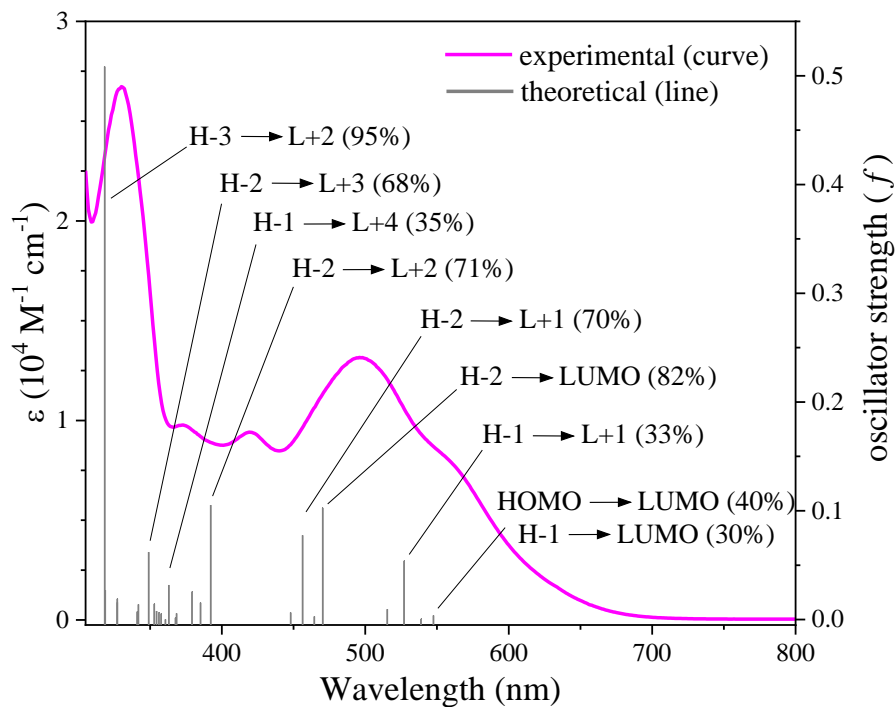


Figure ESI-12. Overlay of experimental (acetonitrile) and theoretical (TDDFT) spectra for 4^+ .

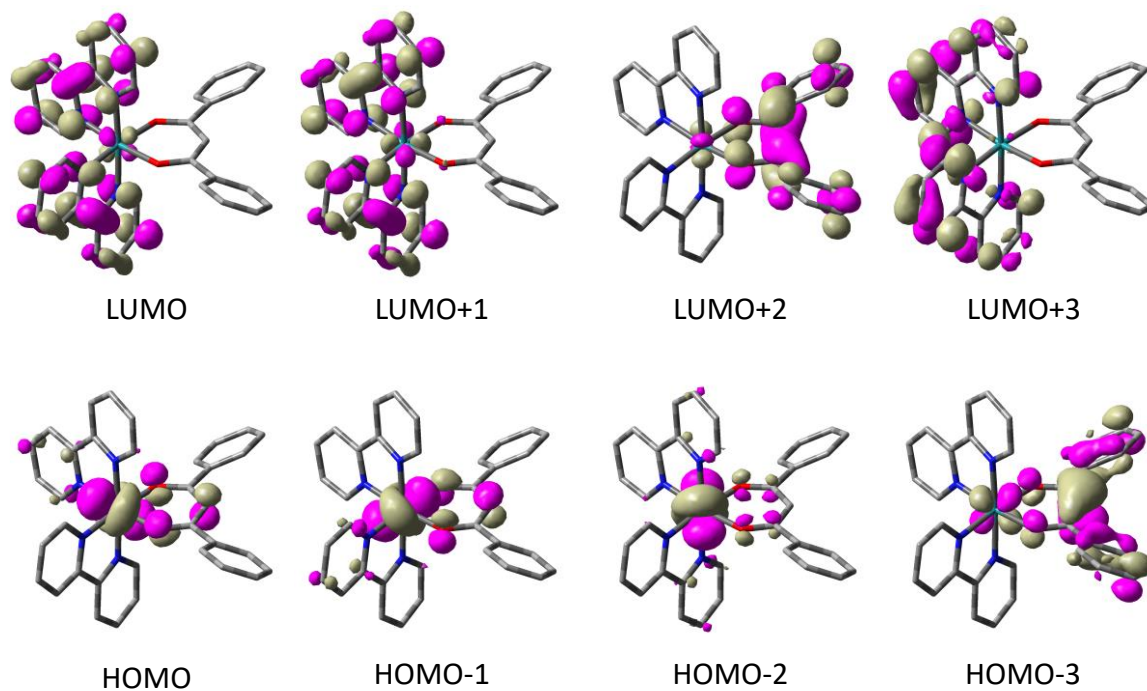


Figure ESI-13. Select frontier molecular orbital surfaces for 4^+ (isofactor = 0.04).

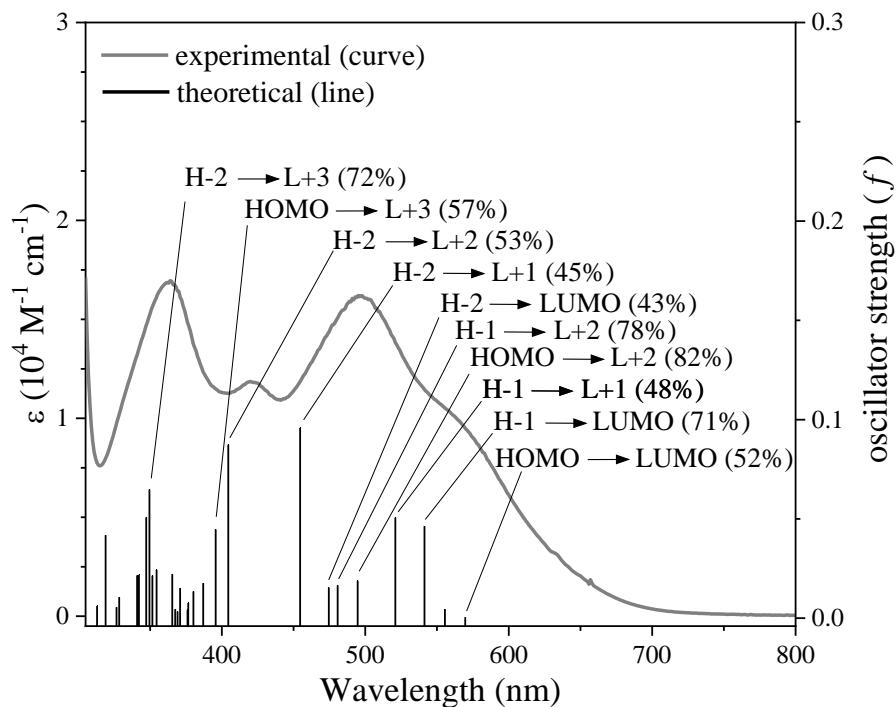


Figure ESI-14. Overlay of experimental (acetone) and theoretical (TDDFT) spectra for 5^+ .

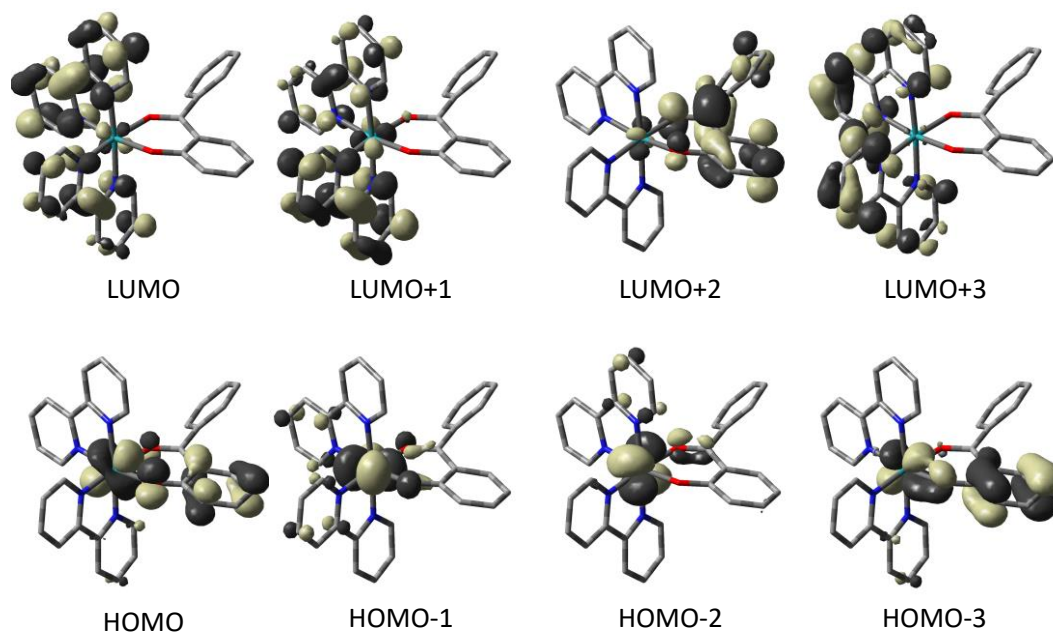


Figure ESI-15. Select frontier molecular orbital surfaces for 5^+ (isofactor = 0.04).

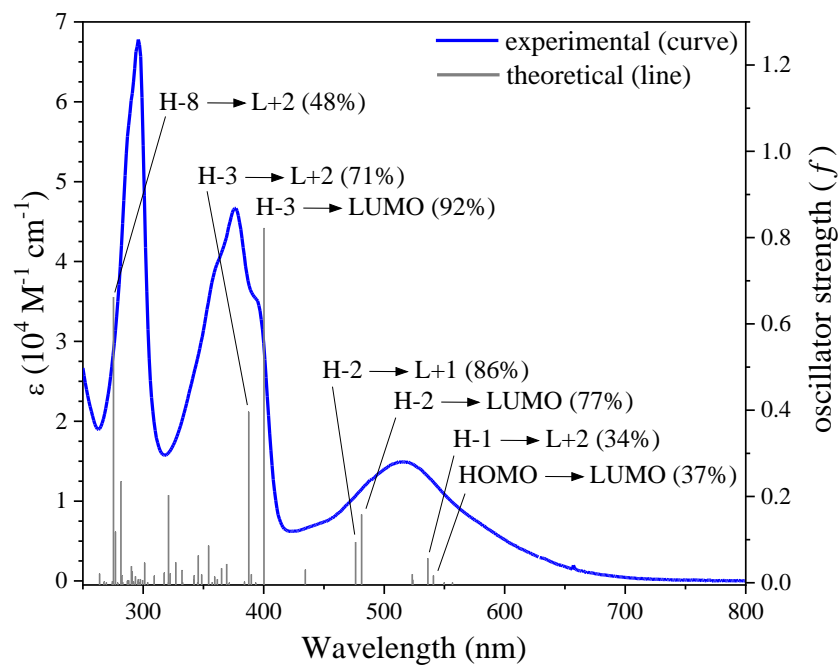


Figure ESI-16. Overlay of experimental (acetonitrile) and theoretical (TDDFT) spectra for 7^+ .

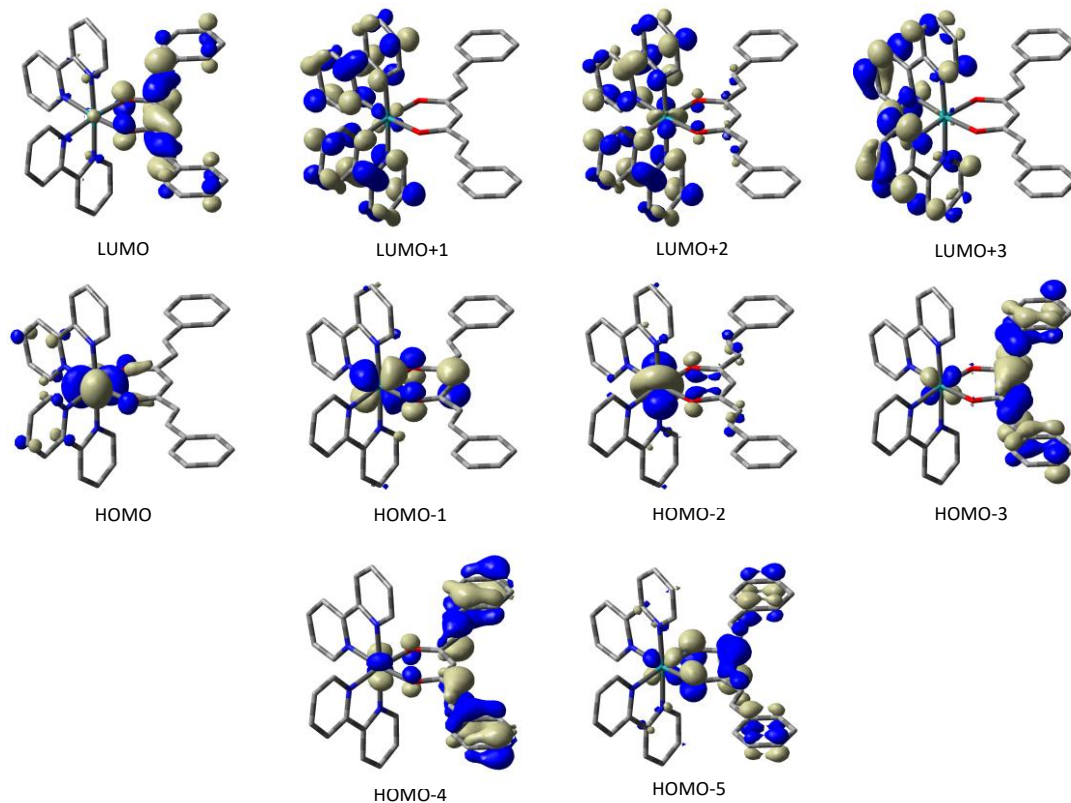


Figure ESI-17. Select frontier molecular orbital surfaces for 7^+ (isofactor = 0.04).

Table ESI-2. DFT cartesian coordinates for $\mathbf{1}^{2+}$.

| Tag | Symbol | X | Y | Z |
|-----|--------|-----------|------------|-----------|
| 1 | Ru | 5.9368523 | 3.4266533 | 3.7487357 |
| 2 | N | 4.2097592 | 2.8477128 | 4.8155180 |
| 3 | N | 4.4041351 | 4.4202648 | 2.6920320 |
| 4 | N | 6.2918120 | 5.2152605 | 4.8115830 |
| 5 | N | 7.5609430 | 4.2646625 | 2.6890249 |
| 6 | N | 7.3153067 | 2.2246154 | 4.8035193 |
| 7 | C | 4.1905473 | 2.0270633 | 5.8834812 |
| 8 | C | 3.0160395 | 1.6733287 | 6.5374395 |
| 9 | C | 1.8075193 | 2.1857302 | 6.0684478 |
| 10 | C | 1.8186472 | 3.0326616 | 4.9645749 |
| 11 | C | 3.0322409 | 3.3527942 | 4.3489590 |
| 12 | C | 3.1422028 | 4.2412518 | 3.1756724 |
| 13 | C | 2.0463207 | 4.8666697 | 2.5737915 |
| 14 | C | 2.2421295 | 5.6836372 | 1.4646137 |
| 15 | C | 3.5358339 | 5.8591794 | 0.9762587 |
| 16 | C | 4.5855776 | 5.2121944 | 1.6175729 |
| 17 | C | 5.5873151 | 5.6386306 | 5.8788327 |
| 18 | C | 5.8530697 | 6.8403508 | 6.5245572 |
| 19 | C | 6.8887104 | 7.6422870 | 6.0479934 |
| 20 | C | 7.6212763 | 7.2119768 | 4.9460027 |
| 21 | C | 7.3079571 | 5.9917739 | 4.3395550 |
| 22 | C | 8.0290064 | 5.4515757 | 3.1705042 |
| 23 | C | 9.1187483 | 6.0907343 | 2.5719340 |
| 24 | C | 9.7360544 | 5.5122561 | 1.4673874 |
| 25 | C | 9.2484661 | 4.3009440 | 0.9800674 |
| 26 | C | 8.1634817 | 3.7116981 | 1.6185748 |
| 27 | C | 8.0399981 | 2.6198774 | 5.8679329 |
| 28 | C | 8.9491379 | 1.7864928 | 6.5089589 |
| 29 | C | 9.1214252 | 0.4887810 | 6.0301727 |
| 30 | C | 8.3772793 | 0.0730956 | 4.9304065 |
| 31 | C | 7.4761025 | 0.9566070 | 4.3291828 |
| 32 | C | 6.6412588 | 0.6034567 | 3.1645001 |
| 33 | C | 6.6469718 | -0.6587153 | 2.5633742 |
| 34 | C | 5.8295723 | -0.9026719 | 1.4641387 |
| 35 | C | 5.0186800 | 0.1250993 | 0.9853738 |
| 36 | C | 5.0543900 | 1.3580296 | 1.6262000 |
| 37 | H | 5.1506525 | 1.6533423 | 6.2164488 |
| 38 | H | 3.0587511 | 1.0103604 | 7.3936594 |
| 39 | H | 0.8704914 | 1.9322267 | 6.5519710 |
| 40 | H | 0.8889973 | 3.4383526 | 4.5868204 |
| 41 | H | 1.0480734 | 4.7199678 | 2.9655187 |

| | | | | |
|----|---|------------|------------|-----------|
| 42 | H | 1.3977126 | 6.1727592 | 0.9915282 |
| 43 | H | 3.7385881 | 6.4843479 | 0.1145524 |
| 44 | H | 5.6054026 | 5.3183696 | 1.2699729 |
| 45 | H | 4.7937231 | 4.9848555 | 6.2179011 |
| 46 | H | 5.2550975 | 7.1322166 | 7.3799429 |
| 47 | H | 7.1242167 | 8.5876265 | 6.5243763 |
| 48 | H | 8.4274519 | 7.8237829 | 4.5622668 |
| 49 | H | 9.4857952 | 7.0305835 | 2.9635220 |
| 50 | H | 10.5824756 | 6.0009516 | 0.9974620 |
| 51 | H | 9.6946815 | 3.8122464 | 0.1218530 |
| 52 | H | 7.7534641 | 2.7720736 | 1.2703120 |
| 53 | H | 7.8740261 | 3.6340631 | 6.2085346 |
| 54 | H | 9.5049112 | 2.1563231 | 7.3626429 |
| 55 | H | 9.8224904 | -0.1904367 | 6.5026486 |
| 56 | H | 8.5004314 | -0.9305037 | 4.5446005 |
| 57 | H | 7.2807929 | -1.4468726 | 2.9488907 |
| 58 | H | 5.8276220 | -1.8789598 | 0.9919655 |
| 59 | H | 4.3659739 | -0.0161178 | 0.1318568 |
| 60 | H | 4.4425519 | 2.1840401 | 1.2862621 |
| 61 | N | 5.8430345 | 1.6020580 | 2.6905240 |

Table ESI-3. DFT cartesian coordinates for **2**.

| Tag | Symbol | X | Y | Z |
|-----|--------|------------|------------|------------|
| 1 | Ru | -1.0603300 | 0.7138940 | 3.9051130 |
| 2 | S | 1.7404390 | 4.1394570 | 1.7747630 |
| 3 | N | 0.1259880 | 2.1816490 | 3.0247760 |
| 4 | N | -0.0022520 | -0.7468030 | 2.8412130 |
| 5 | N | -2.1490810 | 0.6088600 | 2.1106560 |
| 6 | C | 0.7957560 | 2.9959430 | 2.5003350 |
| 7 | C | 1.0831860 | -1.4050550 | 3.2894800 |
| 8 | C | 1.7532040 | -2.3554800 | 2.5284580 |
| 9 | C | 1.2846260 | -2.6401110 | 1.2463530 |
| 10 | C | 0.1643110 | -1.9631130 | 0.7751760 |
| 11 | C | -0.4675500 | -1.0170290 | 1.5879870 |
| 12 | C | -1.6604880 | -0.2531630 | 1.1759910 |
| 13 | C | -2.2758350 | -0.3821890 | -0.0730830 |
| 14 | C | -3.4014940 | 0.3812480 | -0.3671200 |
| 15 | C | -3.8908030 | 1.2629150 | 0.5964770 |
| 16 | C | -3.2358800 | 1.3481560 | 1.8197780 |
| 17 | N | -2.2469030 | 2.1815590 | 4.7852670 |
| 18 | N | -2.1181720 | -0.7468800 | 4.9691590 |
| 19 | N | 0.0284480 | 0.6092100 | 5.6995660 |
| 20 | C | -2.9168960 | 2.9959970 | 5.3091970 |
| 21 | C | -3.2035200 | -1.4053370 | 4.5209790 |

| | | | | |
|----|---|------------|------------|------------|
| 22 | C | -1.6528350 | -1.0168790 | 6.2224200 |
| 23 | C | -0.4599920 | -0.2528070 | 6.6343150 |
| 24 | C | 1.1151410 | 1.3486990 | 5.9903500 |
| 25 | S | -3.8619820 | 4.1396530 | 6.0340300 |
| 26 | C | -3.8734210 | -2.3557400 | 5.2821320 |
| 27 | C | -2.2845850 | -1.9629220 | 7.0353650 |
| 28 | C | 0.1554170 | -0.3816420 | 7.8833790 |
| 29 | C | 1.7701120 | 1.2636580 | 7.2136390 |
| 30 | C | -3.4048150 | -2.6401250 | 6.5642820 |
| 31 | C | 1.2809690 | 0.3819910 | 8.1773190 |
| 32 | H | 1.4154180 | -1.1493400 | 4.2878280 |
| 33 | H | 2.6228500 | -2.8548680 | 2.9397030 |
| 34 | H | 1.7811980 | -3.3752590 | 0.6224580 |
| 35 | H | -0.2146430 | -2.1706230 | -0.2174520 |
| 36 | H | -1.8810650 | -1.0686050 | -0.8113790 |
| 37 | H | -3.8857040 | 0.2889940 | -1.3332810 |
| 38 | H | -4.7628590 | 1.8793430 | 0.4108830 |
| 39 | H | -3.5687450 | 2.0181510 | 2.6030470 |
| 40 | H | -1.9056150 | -2.1702370 | 8.0280270 |
| 41 | H | -3.9013030 | -3.3752400 | 7.1882840 |
| 42 | H | -4.7429990 | -2.8553000 | 4.8709530 |
| 43 | H | -3.5357790 | -1.1498030 | 3.5225930 |
| 44 | H | -0.2392180 | -1.0680640 | 8.6217410 |
| 45 | H | 1.7652250 | 0.2898830 | 9.1434710 |
| 46 | H | 2.6420790 | 1.8802350 | 7.3991580 |
| 47 | H | 1.4478730 | 2.0186810 | 5.2070120 |

Table ESI-4. DFT cartesian coordinates for 3^+ .

| Tag | Symbol | X | Y | Z |
|-----|--------|------------|------------|-----------|
| 1 | Ru | 0.1769170 | -2.8235970 | 2.6736460 |
| 2 | C | -1.1573520 | -0.2339810 | 2.2167520 |
| 3 | C | -1.3459840 | 1.1428600 | 2.0594330 |
| 4 | C | -0.2890580 | 2.0140250 | 2.3050160 |
| 5 | C | 0.9398610 | 1.4908480 | 2.7092280 |
| 6 | C | 1.0678390 | 0.1135140 | 2.8442160 |
| 7 | N | 0.0504230 | -0.7341820 | 2.6010900 |
| 8 | H | -2.3072710 | 1.5332350 | 1.7499110 |
| 9 | H | -0.4250150 | 3.0834810 | 2.1857900 |
| 10 | H | 1.7888910 | 2.1323710 | 2.9155590 |
| 11 | H | 1.9972960 | -0.3494780 | 3.1542600 |
| 12 | C | -2.7615100 | -3.5107470 | 2.1149820 |
| 13 | C | -4.0781020 | -3.2585890 | 1.7498200 |
| 14 | C | -4.4675740 | -1.9413970 | 1.5058400 |
| 15 | C | -3.5259000 | -0.9268680 | 1.6439420 |

| | | | | |
|----|---|------------|------------|------------|
| 16 | C | -2.2155840 | -1.2415850 | 2.0175610 |
| 17 | N | -1.8411360 | -2.5350200 | 2.2449700 |
| 18 | H | -2.4134160 | -4.5180450 | 2.3074980 |
| 19 | H | -4.7757070 | -4.0832090 | 1.6583210 |
| 20 | H | -5.4857910 | -1.7064730 | 1.2153850 |
| 21 | H | -3.8101580 | 0.1023140 | 1.4638050 |
| 22 | C | -0.3249270 | -2.1292080 | 5.6225170 |
| 23 | C | -0.4540880 | -2.3802310 | 6.9830190 |
| 24 | C | -0.3803090 | -3.6984190 | 7.4334080 |
| 25 | C | -0.1870180 | -4.7149830 | 6.5037800 |
| 26 | C | -0.0685930 | -4.4014820 | 5.1462050 |
| 27 | N | -0.1330800 | -3.1071930 | 4.7153950 |
| 28 | H | -0.3680250 | -1.1209700 | 5.2296070 |
| 29 | H | -0.6059390 | -1.5538940 | 7.6679370 |
| 30 | H | -0.4726220 | -3.9325600 | 8.4883550 |
| 31 | H | -0.1291280 | -5.7446020 | 6.8338930 |
| 32 | C | 0.3292580 | -5.7601610 | 1.7854000 |
| 33 | C | 0.4009670 | -7.1378390 | 1.9534610 |
| 34 | C | 0.3270490 | -7.6609170 | 3.2451720 |
| 35 | C | 0.1791970 | -6.7888560 | 4.3194650 |
| 36 | C | 0.1123290 | -5.4112910 | 4.0867860 |
| 37 | N | 0.1916600 | -4.9118590 | 2.8218110 |
| 38 | H | 0.3803330 | -5.2963980 | 0.8073810 |
| 39 | H | 0.5135630 | -7.7797510 | 1.0873020 |
| 40 | H | 0.3808490 | -8.7308370 | 3.4148640 |
| 41 | H | 0.1151590 | -7.1788710 | 5.3273780 |
| 42 | O | 0.5405770 | -2.7798900 | 0.6066560 |
| 43 | C | 1.7057100 | -2.7672200 | 0.0754080 |
| 44 | C | 2.9372460 | -2.8134950 | 0.7555290 |
| 45 | H | 3.8265980 | -2.8067980 | 0.1371410 |
| 46 | C | 3.1457550 | -2.8707700 | 2.1462720 |
| 47 | O | 2.2412140 | -2.8738070 | 3.0523640 |
| 48 | C | 4.5653090 | -2.9234600 | 2.6719910 |
| 49 | C | 1.7084970 | -2.7078150 | -1.4381300 |
| 50 | H | 1.1796130 | -1.8081540 | -1.7703070 |
| 51 | H | 1.1629620 | -3.5685670 | -1.8396420 |
| 52 | H | 2.7172000 | -2.7008590 | -1.8540610 |
| 53 | H | 5.3079880 | -2.9168150 | 1.8726180 |
| 54 | H | 4.6990420 | -3.8275550 | 3.2754440 |
| 55 | H | 4.7435830 | -2.0672620 | 3.3314660 |

Table ESI-5. DFT cartesian coordinates for 4⁺.

| Tag | Symbol | X | Y | Z |
|-----|--------|-----------|------------|-----------|
| 1 | Ru | 0.1838900 | -2.8238530 | 2.6770610 |

| | | | | |
|----|---|------------|------------|------------|
| 2 | C | -1.1385620 | -0.2235360 | 2.2463780 |
| 3 | C | -1.3205740 | 1.1554150 | 2.1013350 |
| 4 | C | -0.2584470 | 2.0189540 | 2.3518030 |
| 5 | C | 0.9689640 | 1.4862750 | 2.7476430 |
| 6 | C | 1.0901340 | 0.1071730 | 2.8710300 |
| 7 | N | 0.0671950 | -0.7326230 | 2.6246440 |
| 8 | H | -2.2802720 | 1.5533160 | 1.7966480 |
| 9 | H | -0.3891650 | 3.0900380 | 2.2418180 |
| 10 | H | 1.8220910 | 2.1216120 | 2.9560590 |
| 11 | H | 2.0185750 | -0.3627490 | 3.1735120 |
| 12 | C | -2.7558980 | -3.4927240 | 2.1033280 |
| 13 | C | -4.0721550 | -3.2303330 | 1.7439420 |
| 14 | C | -4.4568900 | -1.9083980 | 1.5196180 |
| 15 | C | -3.5110430 | -0.8994500 | 1.6701900 |
| 16 | C | -2.2013750 | -1.2244540 | 2.0368370 |
| 17 | N | -1.8318670 | -2.5223390 | 2.2456820 |
| 18 | H | -2.4117540 | -4.5039720 | 2.2814820 |
| 19 | H | -4.7731180 | -4.0508530 | 1.6421000 |
| 20 | H | -5.4747690 | -1.6654100 | 1.2346940 |
| 21 | H | -3.7916860 | 0.1332400 | 1.5052570 |
| 22 | C | -0.3413750 | -2.1579630 | 5.6277870 |
| 23 | C | -0.4901360 | -2.4232060 | 6.9836610 |
| 24 | C | -0.4358010 | -3.7470930 | 7.4194340 |
| 25 | C | -0.2404230 | -4.7549930 | 6.4807560 |
| 26 | C | -0.1010630 | -4.4272600 | 5.1286710 |
| 27 | N | -0.1482680 | -3.1276420 | 4.7122210 |
| 28 | H | -0.3696160 | -1.1448950 | 5.2461270 |
| 29 | H | -0.6422180 | -1.6032680 | 7.6761380 |
| 30 | H | -0.5442670 | -3.9924100 | 8.4702880 |
| 31 | H | -0.1967800 | -5.7887790 | 6.7997970 |
| 32 | C | 0.3410500 | -5.7511500 | 1.7591330 |
| 33 | C | 0.4033510 | -7.1309910 | 1.9131800 |
| 34 | C | 0.3045390 | -7.6677460 | 3.1974680 |
| 35 | C | 0.1435830 | -6.8069130 | 4.2790140 |
| 36 | C | 0.0875060 | -5.4266800 | 4.0605290 |
| 37 | N | 0.1889060 | -4.9142130 | 2.8025150 |
| 38 | H | 0.4118540 | -5.2773510 | 0.7871970 |
| 39 | H | 0.5281410 | -7.7638930 | 1.0421110 |
| 40 | H | 0.3501410 | -8.7397290 | 3.3560890 |
| 41 | H | 0.0620810 | -7.2075900 | 5.2814260 |
| 42 | H | -0.2575640 | -3.2885620 | -4.0733140 |
| 43 | H | 1.6563120 | -2.2616610 | -5.2879020 |
| 44 | C | 0.6042530 | -2.9228470 | -3.5226840 |
| 45 | C | 1.6799270 | -2.3481200 | -4.2055730 |
| 46 | C | 0.6331190 | -3.0280890 | -2.1333100 |

| | | | | |
|----|---|------------|------------|------------|
| 47 | H | -0.2014720 | -3.4682100 | -1.5987640 |
| 48 | C | 2.7833400 | -1.8793440 | -3.4882940 |
| 49 | H | 3.6165520 | -1.4178440 | -4.0099490 |
| 50 | C | 1.7451260 | -2.5757540 | -1.4021940 |
| 51 | C | 2.8184230 | -1.9942420 | -2.0985830 |
| 52 | O | 0.5658110 | -2.7494510 | 0.6191500 |
| 53 | C | 1.7345380 | -2.7072870 | 0.0902360 |
| 54 | H | 3.6726790 | -1.6028550 | -1.5563020 |
| 55 | C | 2.9607950 | -2.8021780 | 0.7783620 |
| 56 | H | 3.8524510 | -2.7910270 | 0.1691060 |
| 57 | C | 3.1581680 | -2.9103300 | 2.1694230 |
| 58 | O | 2.2400330 | -2.8940170 | 3.0656720 |
| 59 | H | 5.4203470 | -3.9583290 | 0.9536290 |
| 60 | C | 4.5543160 | -3.0207140 | 2.7018720 |
| 61 | C | 5.6059070 | -3.5727420 | 1.9506090 |
| 62 | C | 4.8206630 | -2.5748030 | 4.0080250 |
| 63 | C | 6.8897820 | -3.6646100 | 2.4883580 |
| 64 | H | 4.0097260 | -2.1579380 | 4.5950610 |
| 65 | H | 7.6888850 | -4.1031530 | 1.8980760 |
| 66 | C | 6.1062530 | -2.6566040 | 4.5397410 |
| 67 | C | 7.1461060 | -3.2017700 | 3.7813180 |
| 68 | H | 6.2974150 | -2.2958250 | 5.5462150 |
| 69 | H | 8.1473300 | -3.2698590 | 4.1965120 |

Table ESI-6. DFT cartesian coordinates for 5^+ .

| Tag | Symbol | X | Y | Z |
|-----|--------|------------|------------|-----------|
| 1 | Ru | 0.0652200 | -2.5526210 | 2.5238240 |
| 2 | C | -1.5584710 | -0.1234370 | 2.1379370 |
| 3 | C | -1.9043480 | 1.2226710 | 1.9795610 |
| 4 | C | -0.9270570 | 2.2040220 | 2.1111740 |
| 5 | C | 0.3822770 | 1.8196660 | 2.4034640 |
| 6 | C | 0.6650930 | 0.4669160 | 2.5472500 |
| 7 | N | -0.2752550 | -0.4884190 | 2.4170750 |
| 8 | H | -2.9259460 | 1.5040330 | 1.7572240 |
| 9 | H | -1.1849120 | 3.2505270 | 1.9898660 |
| 10 | H | 1.1757110 | 2.5492880 | 2.5173650 |
| 11 | H | 1.6649130 | 0.1160360 | 2.7726170 |
| 12 | C | -2.8124620 | -3.5496880 | 2.2177650 |
| 13 | C | -4.1743290 | -3.4423620 | 1.9659040 |
| 14 | C | -4.7197910 | -2.1780070 | 1.7423260 |
| 15 | C | -3.8811990 | -1.0692860 | 1.7854570 |
| 16 | C | -2.5180130 | -1.2381140 | 2.0474040 |
| 17 | N | -1.9915350 | -2.4808620 | 2.2577410 |
| 18 | H | -2.3473300 | -4.5122520 | 2.3892030 |

| | | | | |
|----|---|------------|------------|------------|
| 19 | H | -4.7862740 | -4.3367920 | 1.9446300 |
| 20 | H | -5.7780750 | -2.0559270 | 1.5391140 |
| 21 | H | -4.2856870 | -0.0793160 | 1.6166110 |
| 22 | C | -0.3066290 | -1.8522860 | 5.4977420 |
| 23 | C | -0.3454990 | -2.0938170 | 6.8656790 |
| 24 | C | -0.1516290 | -3.3969450 | 7.3235920 |
| 25 | C | 0.0682570 | -4.4090060 | 6.3945770 |
| 26 | C | 0.0938980 | -4.1052820 | 5.0301080 |
| 27 | N | -0.0900020 | -2.8250730 | 4.5910230 |
| 28 | H | -0.4480060 | -0.8558010 | 5.0978030 |
| 29 | H | -0.5229080 | -1.2720430 | 7.5499030 |
| 30 | H | -0.1724970 | -3.6235520 | 8.3840030 |
| 31 | H | 0.2180760 | -5.4273550 | 6.7306670 |
| 32 | C | 0.4488220 | -5.4709370 | 1.6652580 |
| 33 | C | 0.6445740 | -6.8357480 | 1.8426530 |
| 34 | C | 0.6693080 | -7.3465240 | 3.1409250 |
| 35 | C | 0.4959060 | -6.4773320 | 4.2142990 |
| 36 | C | 0.3027270 | -5.1135520 | 3.9729380 |
| 37 | N | 0.2814580 | -4.6280510 | 2.7010130 |
| 38 | H | 0.4209280 | -5.0099140 | 0.6844100 |
| 39 | H | 0.7754820 | -7.4771210 | 0.9786830 |
| 40 | H | 0.8200970 | -8.4060500 | 3.3173820 |
| 41 | H | 0.5099460 | -6.8596250 | 5.2270750 |
| 42 | O | 0.3186130 | -2.5545680 | 0.4543590 |
| 43 | C | 1.3933800 | -2.1946320 | -0.1813930 |
| 44 | C | 2.7173760 | -2.0489510 | 0.3914120 |
| 45 | C | 3.0148050 | -2.3357720 | 1.7799160 |
| 46 | O | 2.1488820 | -2.4601590 | 2.6973320 |
| 47 | C | 4.4240850 | -2.5098570 | 2.2575900 |
| 48 | C | 1.2575210 | -1.9525220 | -1.5844390 |
| 49 | C | 3.7716050 | -1.5868510 | -0.4546410 |
| 50 | C | 3.5879760 | -1.3214970 | -1.7928590 |
| 51 | C | 2.3115610 | -1.5288440 | -2.3620910 |
| 52 | C | 5.3454140 | -3.3204030 | 1.5737840 |
| 53 | C | 6.6215170 | -3.5319490 | 2.0974120 |
| 54 | C | 6.9967960 | -2.9265880 | 3.2987550 |
| 55 | C | 6.0844080 | -2.1213670 | 3.9873720 |
| 56 | C | 4.8019570 | -1.9265900 | 3.4787890 |
| 57 | H | 2.1537530 | -1.3379000 | -3.4205080 |
| 58 | H | 0.2685710 | -2.0963370 | -2.0091540 |
| 59 | H | 4.7465280 | -1.4150950 | -0.0146590 |
| 60 | H | 4.4098680 | -0.9551080 | -2.3987870 |
| 61 | H | 5.0564260 | -3.7998650 | 0.6444670 |
| 62 | H | 7.3207810 | -4.1708270 | 1.5665900 |
| 63 | H | 4.0870190 | -1.3136460 | 4.0178830 |

| | | | | |
|----|---|-----------|------------|-----------|
| 64 | H | 7.9936090 | -3.0846530 | 3.6995550 |
| 65 | H | 6.3713110 | -1.6495800 | 4.9223700 |

Table ESI-7. DFT cartesian coordinates for $\mathbf{6}^+$.

| Tag | Symbol | X | Y | Z |
|-----|--------|------------|------------|-----------|
| 1 | Ru | 0.0652200 | -2.5526210 | 2.5238240 |
| 2 | C | -1.5584710 | -0.1234370 | 2.1379370 |
| 3 | C | -1.9043480 | 1.2226710 | 1.9795610 |
| 4 | C | -0.9270570 | 2.2040220 | 2.1111740 |
| 5 | C | 0.3822770 | 1.8196660 | 2.4034640 |
| 6 | C | 0.6650930 | 0.4669160 | 2.5472500 |
| 7 | N | -0.2752550 | -0.4884190 | 2.4170750 |
| 8 | H | -2.9259460 | 1.5040330 | 1.7572240 |
| 9 | H | -1.1849120 | 3.2505270 | 1.9898660 |
| 10 | H | 1.1757110 | 2.5492880 | 2.5173650 |
| 11 | H | 1.6649130 | 0.1160360 | 2.7726170 |
| 12 | C | -2.8124620 | -3.5496880 | 2.2177650 |
| 13 | C | -4.1743290 | -3.4423620 | 1.9659040 |
| 14 | C | -4.7197910 | -2.1780070 | 1.7423260 |
| 15 | C | -3.8811990 | -1.0692860 | 1.7854570 |
| 16 | C | -2.5180130 | -1.2381140 | 2.0474040 |
| 17 | N | -1.9915350 | -2.4808620 | 2.2577410 |
| 18 | H | -2.3473300 | -4.5122520 | 2.3892030 |
| 19 | H | -4.7862740 | -4.3367920 | 1.9446300 |
| 20 | H | -5.7780750 | -2.0559270 | 1.5391140 |
| 21 | H | -4.2856870 | -0.0793160 | 1.6166110 |
| 22 | C | -0.3066290 | -1.8522860 | 5.4977420 |
| 23 | C | -0.3454990 | -2.0938170 | 6.8656790 |
| 24 | C | -0.1516290 | -3.3969450 | 7.3235920 |
| 25 | C | 0.0682570 | -4.4090060 | 6.3945770 |
| 26 | C | 0.0938980 | -4.1052820 | 5.0301080 |
| 27 | N | -0.0900020 | -2.8250730 | 4.5910230 |
| 28 | H | -0.4480060 | -0.8558010 | 5.0978030 |
| 29 | H | -0.5229080 | -1.2720430 | 7.5499030 |
| 30 | H | -0.1724970 | -3.6235520 | 8.3840030 |
| 31 | H | 0.2180760 | -5.4273550 | 6.7306670 |
| 32 | C | 0.4488220 | -5.4709370 | 1.6652580 |
| 33 | C | 0.6445740 | -6.8357480 | 1.8426530 |
| 34 | C | 0.6693080 | -7.3465240 | 3.1409250 |
| 35 | C | 0.4959060 | -6.4773320 | 4.2142990 |
| 36 | C | 0.3027270 | -5.1135520 | 3.9729380 |
| 37 | N | 0.2814580 | -4.6280510 | 2.7010130 |
| 38 | H | 0.4209280 | -5.0099140 | 0.6844100 |
| 39 | H | 0.7754820 | -7.4771210 | 0.9786830 |

| | | | | |
|----|---|-----------|------------|------------|
| 40 | H | 0.8200970 | -8.4060500 | 3.3173820 |
| 41 | H | 0.5099460 | -6.8596250 | 5.2270750 |
| 42 | O | 0.3186130 | -2.5545680 | 0.4543590 |
| 43 | C | 1.3933800 | -2.1946320 | -0.1813930 |
| 44 | C | 2.7173760 | -2.0489510 | 0.3914120 |
| 45 | C | 3.0148050 | -2.3357720 | 1.7799160 |
| 46 | O | 2.1488820 | -2.4601590 | 2.6973320 |
| 47 | C | 4.4240850 | -2.5098570 | 2.2575900 |
| 48 | C | 1.2575210 | -1.9525220 | -1.5844390 |
| 49 | C | 3.7716050 | -1.5868510 | -0.4546410 |
| 50 | C | 3.5879760 | -1.3214970 | -1.7928590 |
| 51 | C | 2.3115610 | -1.5288440 | -2.3620910 |
| 52 | C | 5.3454140 | -3.3204030 | 1.5737840 |
| 53 | C | 6.6215170 | -3.5319490 | 2.0974120 |
| 54 | C | 6.9967960 | -2.9265880 | 3.2987550 |
| 55 | C | 6.0844080 | -2.1213670 | 3.9873720 |
| 56 | C | 4.8019570 | -1.9265900 | 3.4787890 |
| 57 | H | 2.1537530 | -1.3379000 | -3.4205080 |
| 58 | H | 0.2685710 | -2.0963370 | -2.0091540 |
| 59 | H | 4.7465280 | -1.4150950 | -0.0146590 |
| 60 | H | 4.4098680 | -0.9551080 | -2.3987870 |
| 61 | H | 5.0564260 | -3.7998650 | 0.6444670 |
| 62 | H | 7.3207810 | -4.1708270 | 1.5665900 |
| 63 | H | 4.0870190 | -1.3136460 | 4.0178830 |
| 64 | H | 7.9936090 | -3.0846530 | 3.6995550 |
| 65 | H | 6.3713110 | -1.6495800 | 4.9223700 |

Table ESI-8. DFT cartesian coordinates for 7⁺.

| Tag | Symbol | X | Y | Z |
|-----|--------|------------|------------|-----------|
| 1 | Ru | 0.0652200 | -2.5526210 | 2.5238240 |
| 2 | C | -1.5584710 | -0.1234370 | 2.1379370 |
| 3 | C | -1.9043480 | 1.2226710 | 1.9795610 |
| 4 | C | -0.9270570 | 2.2040220 | 2.1111740 |
| 5 | C | 0.3822770 | 1.8196660 | 2.4034640 |
| 6 | C | 0.6650930 | 0.4669160 | 2.5472500 |
| 7 | N | -0.2752550 | -0.4884190 | 2.4170750 |
| 8 | H | -2.9259460 | 1.5040330 | 1.7572240 |
| 9 | H | -1.1849120 | 3.2505270 | 1.9898660 |
| 10 | H | 1.1757110 | 2.5492880 | 2.5173650 |
| 11 | H | 1.6649130 | 0.1160360 | 2.7726170 |
| 12 | C | -2.8124620 | -3.5496880 | 2.2177650 |
| 13 | C | -4.1743290 | -3.4423620 | 1.9659040 |
| 14 | C | -4.7197910 | -2.1780070 | 1.7423260 |
| 15 | C | -3.8811990 | -1.0692860 | 1.7854570 |

| | | | | |
|----|---|------------|------------|------------|
| 16 | C | -2.5180130 | -1.2381140 | 2.0474040 |
| 17 | N | -1.9915350 | -2.4808620 | 2.2577410 |
| 18 | H | -2.3473300 | -4.5122520 | 2.3892030 |
| 19 | H | -4.7862740 | -4.3367920 | 1.9446300 |
| 20 | H | -5.7780750 | -2.0559270 | 1.5391140 |
| 21 | H | -4.2856870 | -0.0793160 | 1.6166110 |
| 22 | C | -0.3066290 | -1.8522860 | 5.4977420 |
| 23 | C | -0.3454990 | -2.0938170 | 6.8656790 |
| 24 | C | -0.1516290 | -3.3969450 | 7.3235920 |
| 25 | C | 0.0682570 | -4.4090060 | 6.3945770 |
| 26 | C | 0.0938980 | -4.1052820 | 5.0301080 |
| 27 | N | -0.0900020 | -2.8250730 | 4.5910230 |
| 28 | H | -0.4480060 | -0.8558010 | 5.0978030 |
| 29 | H | -0.5229080 | -1.2720430 | 7.5499030 |
| 30 | H | -0.1724970 | -3.6235520 | 8.3840030 |
| 31 | H | 0.2180760 | -5.4273550 | 6.7306670 |
| 32 | C | 0.4488220 | -5.4709370 | 1.6652580 |
| 33 | C | 0.6445740 | -6.8357480 | 1.8426530 |
| 34 | C | 0.6693080 | -7.3465240 | 3.1409250 |
| 35 | C | 0.4959060 | -6.4773320 | 4.2142990 |
| 36 | C | 0.3027270 | -5.1135520 | 3.9729380 |
| 37 | N | 0.2814580 | -4.6280510 | 2.7010130 |
| 38 | H | 0.4209280 | -5.0099140 | 0.6844100 |
| 39 | H | 0.7754820 | -7.4771210 | 0.9786830 |
| 40 | H | 0.8200970 | -8.4060500 | 3.3173820 |
| 41 | H | 0.5099460 | -6.8596250 | 5.2270750 |
| 42 | O | 0.3186130 | -2.5545680 | 0.4543590 |
| 43 | C | 1.3933800 | -2.1946320 | -0.1813930 |
| 44 | C | 2.7173760 | -2.0489510 | 0.3914120 |
| 45 | C | 3.0148050 | -2.3357720 | 1.7799160 |
| 46 | O | 2.1488820 | -2.4601590 | 2.6973320 |
| 47 | C | 4.4240850 | -2.5098570 | 2.2575900 |
| 48 | C | 1.2575210 | -1.9525220 | -1.5844390 |
| 49 | C | 3.7716050 | -1.5868510 | -0.4546410 |
| 50 | C | 3.5879760 | -1.3214970 | -1.7928590 |
| 51 | C | 2.3115610 | -1.5288440 | -2.3620910 |
| 52 | C | 5.3454140 | -3.3204030 | 1.5737840 |
| 53 | C | 6.6215170 | -3.5319490 | 2.0974120 |
| 54 | C | 6.9967960 | -2.9265880 | 3.2987550 |
| 55 | C | 6.0844080 | -2.1213670 | 3.9873720 |
| 56 | C | 4.8019570 | -1.9265900 | 3.4787890 |
| 57 | H | 2.1537530 | -1.3379000 | -3.4205080 |
| 58 | H | 0.2685710 | -2.0963370 | -2.0091540 |
| 59 | H | 4.7465280 | -1.4150950 | -0.0146590 |
| 60 | H | 4.4098680 | -0.9551080 | -2.3987870 |

| | | | | |
|----|---|-----------|------------|-----------|
| 61 | H | 5.0564260 | -3.7998650 | 0.6444670 |
| 62 | H | 7.3207810 | -4.1708270 | 1.5665900 |
| 63 | H | 4.0870190 | -1.3136460 | 4.0178830 |
| 64 | H | 7.9936090 | -3.0846530 | 3.6995550 |
| 65 | H | 6.3713110 | -1.6495800 | 4.9223700 |

Table ESI-9. DFT cartesian coordinates for $\mathbf{8}^+$.

| Tag | Symbol | X | Y | Z |
|-----|--------|------------|------------|------------|
| 1 | Ru | 0.1000830 | -1.7727940 | 0.0117300 |
| 2 | C | 1.4541800 | -2.5672170 | -2.4833550 |
| 3 | C | 1.7944400 | -2.6231140 | -3.8389000 |
| 4 | C | 1.0315960 | -1.9224370 | -4.7681620 |
| 5 | C | -0.0639550 | -1.1806830 | -4.3240490 |
| 6 | C | -0.3511160 | -1.1608890 | -2.9644460 |
| 7 | N | 0.3883870 | -1.8312640 | -2.0605910 |
| 8 | H | 2.6441220 | -3.2080420 | -4.1680190 |
| 9 | H | 1.2873230 | -1.9584790 | -5.8216120 |
| 10 | H | -0.6877170 | -0.6230290 | -5.0132180 |
| 11 | H | -1.1882720 | -0.6033420 | -2.5607000 |
| 12 | C | 2.2491760 | -3.7961820 | 0.8602000 |
| 13 | C | 3.3434070 | -4.6346910 | 0.6871970 |
| 14 | C | 3.8686480 | -4.7987310 | -0.5948050 |
| 15 | C | 3.2729710 | -4.1234470 | -1.6550610 |
| 16 | C | 2.1703090 | -3.2960610 | -1.4201060 |
| 17 | N | 1.6696710 | -3.1330770 | -0.1599150 |
| 18 | H | 1.8132930 | -3.6343080 | 1.8383170 |
| 19 | H | 3.7702690 | -5.1419200 | 1.5448440 |
| 20 | H | 4.7245050 | -5.4420470 | -0.7679480 |
| 21 | H | 3.6629590 | -4.2410960 | -2.6582970 |
| 22 | C | -1.8944190 | -3.9514590 | -0.8276260 |
| 23 | C | -2.9209270 | -4.8710190 | -0.6509140 |
| 24 | C | -3.4266120 | -5.0750150 | 0.6331140 |
| 25 | C | -2.8807740 | -4.3558960 | 1.6913920 |
| 26 | C | -1.8455510 | -3.4466200 | 1.4528090 |
| 27 | N | -1.3627610 | -3.2472270 | 0.1909330 |
| 28 | H | -1.4764850 | -3.7551140 | -1.8073280 |
| 29 | H | -3.3115180 | -5.4089620 | -1.5071170 |
| 30 | H | -4.2301780 | -5.7817770 | 0.8093830 |
| 31 | H | -3.2582890 | -4.5030660 | 2.6955460 |
| 32 | C | 0.5023330 | -1.1115910 | 2.9809630 |
| 33 | C | 0.2216420 | -1.1477160 | 4.3415360 |
| 34 | C | -0.8090480 | -1.9737250 | 4.7926210 |
| 35 | C | -1.5158560 | -2.7379400 | 3.8690310 |
| 36 | C | -1.1855300 | -2.6609300 | 2.5120570 |

| | | | | |
|----|---|------------|------------|------------|
| 37 | N | -0.1833020 | -1.8439050 | 2.0829070 |
| 38 | H | 1.2902150 | -0.4912500 | 2.5698200 |
| 39 | H | 0.8003070 | -0.5383530 | 5.0262410 |
| 40 | H | -1.0576930 | -2.0255040 | 5.8471040 |
| 41 | H | -2.3143690 | -3.3881920 | 4.2033770 |
| 42 | H | 8.2749460 | 1.9703370 | 0.4790980 |
| 43 | C | 7.3135700 | 2.4708470 | 0.3963790 |
| 44 | C | 7.2752260 | 3.8616760 | 0.3390970 |
| 45 | C | 6.1343270 | 1.7268060 | 0.3487580 |
| 46 | H | 6.1843740 | 0.6429620 | 0.3933120 |
| 47 | C | 6.0234160 | 4.5233120 | 0.2332840 |
| 48 | C | 4.8868730 | 2.3599580 | 0.2437150 |
| 49 | C | 4.8548240 | 3.7740970 | 0.1872760 |
| 50 | O | 1.5336500 | -0.2465660 | 0.0881490 |
| 51 | C | 1.2639580 | 1.0126510 | 0.0528060 |
| 52 | H | 3.9024370 | 4.2819410 | 0.1048540 |
| 53 | C | -0.0263850 | 1.5811440 | -0.0221240 |
| 54 | H | -0.0671450 | 2.6645510 | -0.0383370 |
| 55 | C | -1.2691420 | 0.9152800 | -0.0783250 |
| 56 | O | -1.4444970 | -0.3610850 | -0.0760650 |
| 57 | H | -4.1606150 | 4.0105650 | -0.2652500 |
| 58 | C | -4.9787680 | 1.9898280 | -0.3256290 |
| 59 | C | -5.0548550 | 3.3992950 | -0.3287120 |
| 60 | C | -6.1852610 | 1.2711010 | -0.4050300 |
| 61 | C | -6.2700440 | 4.0618810 | -0.4214410 |
| 62 | H | -6.1605090 | 0.1851790 | -0.3993580 |
| 63 | C | -7.4121990 | 1.9234010 | -0.4971660 |
| 64 | C | -7.4704910 | 3.3195540 | -0.5143730 |
| 65 | H | -8.3331670 | 1.3498110 | -0.5662500 |
| 66 | C | -2.4714700 | 1.7610560 | -0.1600260 |
| 67 | C | -3.7217750 | 1.2542810 | -0.2378290 |
| 68 | H | -2.3004110 | 2.8337380 | -0.1580890 |
| 69 | H | -3.8129790 | 0.1697030 | -0.2364840 |
| 70 | C | 2.3991170 | 1.9478040 | 0.1031120 |
| 71 | C | 3.6840340 | 1.5371110 | 0.1941880 |
| 72 | H | 2.1477530 | 3.0038040 | 0.0617330 |
| 73 | H | 3.8522220 | 0.4625430 | 0.2347420 |
| 74 | O | -8.6326720 | 4.0170230 | -0.6303040 |
| 75 | H | -9.3767220 | 3.3994370 | -0.6722980 |
| 76 | O | 8.3858910 | 4.6461170 | 0.3786030 |
| 77 | H | 9.1690490 | 4.0814250 | 0.4464170 |
| 78 | O | 6.0889940 | 5.8834710 | 0.1843540 |
| 79 | O | -6.2829880 | 5.4360560 | -0.4867510 |
| 80 | C | -6.8222540 | 6.1005500 | 0.6661780 |
| 81 | H | -6.2432630 | 5.8517950 | 1.5635510 |

| | | | | |
|----|---|------------|-----------|------------|
| 82 | H | -7.8724410 | 5.8385920 | 0.8234190 |
| 83 | H | -6.7392500 | 7.1707130 | 0.4680480 |
| 84 | C | 4.8665260 | 6.6073640 | 0.0730460 |
| 85 | H | 4.3330120 | 6.3534880 | -0.8505530 |
| 86 | H | 5.1440700 | 7.6616290 | 0.0517790 |
| 87 | H | 4.2106940 | 6.4215760 | 0.9318410 |

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