**Supplementary Information**

# Synthetic Exploration of Bis(phenolate) aza-BODIPYs and Heavier Group 13 Chelates

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## Cartesian Coordinates

### 1a

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -1649.987899 | Hartree |
| **Zero-point Energy Correction** | 0.495678 | Hartree |
| **Thermal Correction to Energy** | 0.526563 | Hartree |
| **Thermal Correction to Enthalpy** | 0.527508 | Hartree |
| **Thermal Correction to Free Energy** | 0.431019 | Hartree |
| **EE + Zero-point Energy** | -1649.492221 | Hartree |
| **EE + Thermal Energy Correction** | -1649.461335 | Hartree |
| **EE + Thermal Enthalpy Correction** | -1649.460391 | Hartree |
| **EE + Thermal Free Energy Correction** | -1649.556880 | Hartree |
| **E (Thermal)** | 330.424 | kcal/mol |
| **Heat Capacity (Cv)** | 124.980 | cal/mol-kelvin |
| **Entropy (S)** | 203.077 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| B | -1.999020 | -0.000000 | -0.000007 |
| C | 6.345344 | 4.211769 | -0.888230 |
| O | -2.884194 | -0.386858 | -1.127632 |
| N | 1.005383 | 0.000007 | -0.000017 |
| N | -1.066528 | 1.171658 | -0.232528 |
| N | -1.066520 | -1.171653 | 0.232506 |
| O | -2.884185 | 0.386852 | 1.127627 |
| C | 4.913605 | 3.752410 | -0.760561 |
| C | 3.181050 | -2.062756 | 1.083446 |
| H | 2.893187 | -1.081285 | 1.456653 |
| C | 6.345344 | -4.211786 | 0.888276 |
| C | -2.794884 | -2.703337 | -0.371722 |
| C | -1.454915 | -2.463405 | 0.115456 |
| C | 0.324567 | -1.111237 | 0.268790 |
| C | 4.504009 | -2.489904 | 1.215143 |
| H | 5.232178 | -1.827863 | 1.688475 |
| C | -3.418284 | -3.968123 | -0.345718 |
| H | -2.926753 | -4.789010 | 0.178473 |
| C | 0.811928 | -2.471456 | 0.370739 |
| C | -0.313432 | -3.296866 | 0.266840 |
| H | -0.323951 | -4.381535 | 0.252010 |
| C | 0.324559 | 1.111247 | -0.268819 |
| C | 2.210191 | -2.892499 | 0.489965 |
| C | 4.913615 | -3.752402 | 0.760567 |
| C | 3.943295 | 4.580905 | -0.167782 |
| H | 4.231109 | 5.568200 | 0.200048 |
| C | 2.210178 | 2.892511 | -0.489981 |

| | | | |
|---|---|---|---|
| C | -3.437918 | -1.620095 | -1.051629 |
| C | 2.621401 | 4.163468 | -0.034726 |
| H | 1.900213 | 4.825288 | 0.446451 |
| C | 3.943298 | -4.580915 | 0.167824 |
| H | 4.231105 | -5.568227 | -0.199967 |
| C | 0.811916 | 2.471468 | -0.370761 |
| C | -2.794891 | 2.703333 | 0.371724 |
| C | -1.454926 | 2.463408 | -0.115465 |
| C | -0.313446 | 3.296873 | -0.266849 |
| H | -0.323967 | 4.381543 | -0.252010 |
| C | 4.503989 | 2.489932 | -1.215191 |
| H | 5.232151 | 1.827909 | -1.688558 |
| C | -3.418297 | 3.968117 | 0.345730 |
| H | -2.926773 | 4.789007 | -0.178462 |
| C | -4.640516 | -4.173866 | -0.973314 |
| H | -5.117729 | -5.153302 | -0.937640 |
| C | -4.657876 | -1.851821 | -1.706758 |
| H | -5.131101 | -1.024263 | -2.235816 |
| C | 2.621406 | -4.163476 | 0.034758 |
| H | 1.900214 | -4.825312 | -0.446391 |
| C | 3.181030 | 2.062787 | -1.083503 |
| H | 2.893158 | 1.081333 | -1.456749 |
| C | -5.252999 | 3.110779 | 1.661643 |
| H | -6.209327 | 3.268181 | 2.163024 |
| C | -3.437916 | 1.620086 | 1.051632 |
| C | -4.657868 | 1.851805 | 1.706773 |
| H | -5.131086 | 1.024244 | 2.235832 |
| C | -4.640524 | 4.173853 | 0.973338 |
| H | -5.117741 | 5.153288 | 0.937672 |
| C | -5.253001 | -3.110797 | -1.661618 |
| H | -6.209333 | -3.268204 | -2.162990 |
| H | 6.822596 | 4.294686 | 0.100411 |
| H | 6.936630 | 3.509759 | -1.490435 |
| H | 6.403795 | 5.204794 | -1.357220 |
| H | 6.403772 | -5.204710 | 1.357486 |
| H | 6.822563 | -4.294943 | -0.100359 |
| H | 6.936675 | -3.509669 | 1.490311 |

**1b**

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -1800.426880 | Hartree |
| **Zero-point Energy Correction** | 0.506095 | Hartree |
| **Thermal Correction to Energy** | 0.538360 | Hartree |
| **Thermal Correction to Enthalpy** | 0.539304 | Hartree |
| **Thermal Correction to Free Energy** | 0.441511 | Hartree |
| **EE + Zero-point Energy** | -1799.920786 | Hartree |
| **EE + Thermal Energy Correction** | -1799.888521 | Hartree |
| **EE + Thermal Enthalpy Correction** | -1799.887576 | Hartree |
| **EE + Thermal Free Energy Correction** | -1799.985369 | Hartree |
| **E (Thermal)** | 337.826 | kcal/mol |
| **Heat Capacity (Cv)** | 131.279 | cal/mol-kelvin |
| **Entropy (S)** | 205.823 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| B | 2.358032 | -0.000000 | -0.000000 |
| O | -5.850579 | 4.077891 | 0.852432 |
| O | 3.244540 | -0.370337 | 1.133354 |
| N | -0.645566 | 0.000000 | 0.000000 |
| N | 1.426264 | 1.174739 | 0.215117 |
| N | 1.426263 | -1.174739 | -0.215118 |
| O | 3.244541 | 0.370337 | -1.133354 |
| C | -4.536387 | 3.759744 | 0.690236 |
| C | -2.835577 | -2.060781 | -1.008421 |
| H | -2.557031 | -1.070371 | -1.363805 |
| O | -5.850580 | -4.077890 | -0.852432 |
| C | 3.156964 | -2.696747 | 0.408352 |
| C | 1.814884 | -2.465328 | -0.079340 |
| C | 0.035159 | -1.115608 | -0.251274 |
| C | -4.153513 | -2.480389 | -1.132230 |
| H | -4.906178 | -1.829367 | -1.578094 |
| C | 3.782459 | -3.960437 | 0.397101 |
| H | 3.290577 | -4.788996 | -0.114633 |
| C | -0.452670 | -2.477844 | -0.332963 |
| C | 0.675630 | -3.300968 | -0.217602 |
| H | 0.688008 | -4.385250 | -0.186184 |
| C | 0.035159 | 1.115609 | 0.251274 |
| C | -1.848484 | -2.900476 | -0.443330 |
| C | -4.536388 | -3.759744 | -0.690236 |
| C | -3.574377 | 4.611911 | 0.124042 |
| H | -3.838637 | 5.604193 | -0.234971 |
| C | -1.848483 | 2.900477 | 0.443330 |
| C | 3.800338 | -1.603676 | 1.071662 |
| C | -2.253143 | 4.176874 | 0.009107 |

| | | | |
|---|---|---|---|
| H | -1.526005 | 4.846903 | -0.450844 |
| C | -3.574378 | -4.611910 | -0.124042 |
| H | -3.838637 | -5.604192 | 0.234970 |
| C | -0.452669 | 2.477845 | 0.332963 |
| C | 3.156965 | 2.696747 | -0.408352 |
| C | 1.814885 | 2.465327 | 0.079340 |
| C | 0.675631 | 3.300969 | 0.217602 |
| H | 0.688009 | 4.385251 | 0.186183 |
| C | -4.153512 | 2.480390 | 1.132231 |
| H | -4.906177 | 1.829369 | 1.578096 |
| C | 3.782460 | 3.960436 | -0.397101 |
| H | 3.290579 | 4.788996 | 0.114633 |
| C | 5.007196 | -4.156251 | 1.023596 |
| H | 5.485679 | -5.135449 | 0.999332 |
| C | 5.023064 | -1.824715 | 1.725373 |
| H | 5.496746 | -0.989362 | 2.241685 |
| C | -2.253144 | -4.176874 | -0.009108 |
| H | -1.526006 | -4.846903 | 0.450843 |
| C | -2.835575 | 2.060782 | 1.008422 |
| H | -2.557030 | 1.070373 | 1.363806 |
| C | -6.295041 | 5.371824 | 0.427710 |
| H | -5.775173 | 6.168245 | 0.980227 |
| H | -7.365429 | 5.405110 | 0.654833 |
| H | -6.142716 | 5.505738 | -0.653326 |
| C | 5.620260 | 3.083331 | -1.695500 |
| H | 6.578448 | 3.232426 | -2.195906 |
| C | 3.800339 | 1.603675 | -1.071662 |
| C | 5.023065 | 1.824714 | -1.725372 |
| H | 5.496747 | 0.989360 | -2.241685 |
| C | 5.007198 | 4.156249 | -1.023596 |
| H | 5.485681 | 5.135447 | -0.999332 |
| C | 5.620258 | -3.083333 | 1.695501 |
| H | 6.578446 | -3.232428 | 2.195906 |
| C | -6.295042 | -5.371824 | -0.427711 |
| H | -6.142716 | -5.505738 | 0.653325 |
| H | -7.365430 | -5.405110 | -0.654834 |
| H | -5.775174 | -6.168244 | -0.980228 |

**2a**

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -2364.314438 | Hartree |
| **Zero-point Energy Correction** | 0.671516 | Hartree |
| **Thermal Correction to Energy** | 0.715441 | Hartree |
| **Thermal Correction to Enthalpy** | 0.716385 | Hartree |
| **Thermal Correction to Free Energy** | 0.587331 | Hartree |
| **EE + Zero-point Energy** | -2363.642922 | Hartree |
| **EE + Thermal Energy Correction** | -2363.598997 | Hartree |
| **EE + Thermal Enthalpy Correction** | -2363.598053 | Hartree |
| **EE + Thermal Free Energy Correction** | -2363.727107 | Hartree |
| **E (Thermal)** | 448.946 | kcal/mol |
| **Heat Capacity (Cv)** | 171.962 | cal/mol-kelvin |
| **Entropy (S)** | 271.617 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| Al | -1.918981 | -0.000003 | -0.000322 |
| C | 7.257205 | -3.495261 | 0.198355 |
| O | -3.244461 | 1.288399 | -0.019451 |
| N | 1.472151 | 0.000001 | 0.000201 |
| N | -0.511583 | -1.385720 | 0.024185 |
| N | -0.511578 | 1.385720 | -0.024032 |
| O | -3.244470 | -1.288408 | 0.018023 |
| C | 5.781456 | -3.216364 | 0.183152 |
| N | -1.969754 | 0.033718 | 2.121088 |
| C | 3.889165 | 1.768712 | -0.692892 |
| H | 3.509007 | 0.845655 | -1.126710 |
| C | 7.257213 | 3.495275 | -0.197742 |
| N | -1.968569 | -0.033722 | -2.121765 |
| C | -2.008345 | 3.358851 | -0.025370 |
| C | -0.705089 | 2.725582 | -0.035849 |
| C | 0.858984 | 1.169953 | -0.046411 |
| C | 5.255124 | 2.040147 | -0.727181 |
| H | 5.928794 | 1.319020 | -1.196190 |
| C | -2.099588 | 4.767897 | -0.022061 |
| H | -1.182028 | 5.356454 | -0.024954 |
| C | 1.545983 | 2.438875 | -0.080255 |
| C | 0.552035 | 3.399246 | -0.066973 |
| H | 0.697083 | 4.473557 | -0.109365 |
| C | 0.858977 | -1.169950 | 0.046746 |
| C | 2.990168 | 2.675335 | -0.109171 |
| C | 5.781461 | 3.216394 | -0.182556 |
| C | 4.883419 | -4.122058 | -0.398365 |
| H | 5.261694 | -5.049530 | -0.834766 |
| C | 2.990157 | -2.675332 | 0.109777 |

| | | | |
|---|---|---|---|
| C | -3.214312 | 2.595075 | -0.018331 |
| C | 3.519219 | -3.858805 | -0.435497 |
| H | 2.849141 | -4.576501 | -0.912027 |
| C | 4.883427 | 4.122037 | 0.399042 |
| H | 5.261702 | 5.049488 | 0.835490 |
| C | 1.545972 | -2.438869 | 0.080793 |
| C | -2.008350 | -3.358854 | 0.025587 |
| C | -0.705097 | -2.725581 | 0.036166 |
| C | 0.552023 | -3.399240 | 0.067535 |
| H | 0.697070 | -4.473547 | 0.110026 |
| C | 5.255117 | -2.040084 | 0.727701 |
| H | 5.928791 | -1.318909 | 1.196633 |
| C | -2.099594 | -4.767902 | 0.023056 |
| H | -1.182036 | -5.356458 | 0.026730 |
| C | -0.864160 | -0.072786 | -2.878633 |
| H | 0.087025 | -0.087290 | -2.348713 |
| C | -3.315258 | 5.429497 | -0.014079 |
| H | -3.349404 | 6.519221 | -0.011456 |
| C | -4.445680 | 3.291770 | -0.011222 |
| H | -5.359303 | 2.694937 | -0.006806 |
| C | 3.519228 | 3.858770 | 0.436181 |
| H | 2.849151 | 4.576433 | 0.912760 |
| C | 3.889154 | -1.768662 | 0.693420 |
| H | 3.508998 | -0.845569 | 1.127162 |
| C | -2.146794 | 0.075750 | 4.899589 |
| H | -2.216101 | 0.092067 | 5.988059 |
| C | -4.498932 | -4.675406 | 0.008927 |
| H | -5.468180 | -5.178523 | 0.002654 |
| C | -3.214316 | -2.595083 | 0.017617 |
| C | -4.445680 | -3.291784 | 0.010294 |
| H | -5.359301 | -2.694954 | 0.005114 |
| C | -0.865716 | 0.072682 | 2.878502 |
| H | 0.085730 | 0.087109 | 2.349043 |
| C | -3.161576 | -0.015597 | -2.733165 |
| H | -4.026939 | 0.017026 | -2.073404 |
| C | -3.315259 | -5.429508 | 0.014925 |
| H | -3.349402 | -6.519233 | 0.012948 |
| C | -2.144236 | -0.075763 | -4.900357 |
| H | -2.213006 | -0.092085 | -5.988862 |
| C | -3.296682 | 0.035786 | 4.114700 |
| H | -4.289519 | 0.019870 | 4.562562 |
| C | -3.294509 | -0.035693 | -4.116038 |
| H | -4.287125 | -0.019695 | -4.564389 |
| C | -0.906282 | 0.094470 | 4.267088 |
| H | 0.022367 | 0.125709 | 4.835443 |
| C | -4.498932 | 4.675391 | -0.009086 |

| | | | |
|---|---|---|---|
| H | -5.468183 | 5.178504 | -0.002971 |
| C | -0.904041 | -0.094583 | -4.267240 |
| H | 0.024888 | -0.125907 | -4.835132 |
| C | -3.163069 | 0.015691 | 2.731891 |
| H | -4.028119 | -0.016846 | 2.071710 |
| H | 7.463078 | 4.544665 | -0.449275 |
| H | 7.703745 | 3.306839 | 0.790562 |
| H | 7.776596 | 2.856320 | -0.923336 |
| H | 7.463068 | -4.544569 | 0.450240 |
| H | 7.776627 | -2.856077 | 0.923720 |
| H | 7.703694 | -3.307168 | -0.790031 |

**2b**

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -2514.752698 | Hartree |
| **Zero-point Energy Correction** | 0.681941 | Hartree |
| **Thermal Correction to Energy** | 0.727221 | Hartree |
| **Thermal Correction to Enthalpy** | 0.728166 | Hartree |
| **Thermal Correction to Free Energy** | 0.598381 | Hartree |
| **EE + Zero-point Energy** | -2514.070757 | Hartree |
| **EE + Thermal Energy Correction** | -2514.025477 | Hartree |
| **EE + Thermal Enthalpy Correction** | -2514.024533 | Hartree |
| **EE + Thermal Free Energy Correction** | -2514.154317 | Hartree |
| **E (Thermal)** | 456.338 | kcal/mol |
| **Heat Capacity (Cv)** | 178.257 | cal/mol-kelvin |
| **Entropy (S)** | 273.155 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| Al | 2.237488 | -0.000000 | 0.000000 |
| O | -6.810739 | 3.441466 | 0.392474 |
| O | 3.564831 | -1.295626 | -0.013127 |
| N | -1.165775 | 0.000000 | 0.000000 |
| N | 0.826105 | 1.391940 | 0.018500 |
| N | 0.826105 | -1.391940 | -0.018500 |
| O | 3.564831 | 1.295625 | 0.013128 |
| C | -5.461865 | 3.262600 | 0.274954 |
| N | 2.297958 | -0.024944 | 2.153466 |
| C | -3.585172 | -1.803251 | -0.762602 |
| H | -3.204411 | -0.883382 | -1.200529 |
| O | -6.810739 | -3.441465 | -0.392474 |
| N | 2.297958 | 0.024944 | -2.153465 |
| C | 2.327767 | -3.375492 | -0.004073 |
| C | 1.020461 | -2.738970 | -0.025397 |
| C | -0.552916 | -1.175053 | -0.049048 |
| C | -4.946130 | -2.079586 | -0.831527 |

| | | | |
|---|---|---|---|
| H | -5.630285 | -1.386082 | -1.322050 |
| C | 2.422962 | -4.789104 | 0.012964 |
| H | 1.508319 | -5.381175 | 0.014249 |
| C | -1.239541 | -2.450862 | -0.088831 |
| C | -0.240200 | -3.412201 | -0.065761 |
| H | -0.384313 | -4.485883 | -0.110535 |
| C | -0.552916 | 1.175053 | 0.049048 |
| C | -2.685497 | -2.697361 | -0.140510 |
| C | -5.461866 | -3.262600 | -0.274954 |
| C | -4.590167 | 4.165485 | -0.352436 |
| H | -4.955692 | 5.086098 | -0.802692 |
| C | -2.685497 | 2.697362 | 0.140510 |
| C | 3.538246 | -2.609652 | -0.000429 |
| C | -3.224446 | 3.874660 | -0.410436 |
| H | -2.565056 | 4.580120 | -0.917784 |
| C | -4.590167 | -4.165485 | 0.352436 |
| H | -4.955692 | -5.086098 | 0.802690 |
| C | -1.239540 | 2.450862 | 0.088831 |
| C | 2.327767 | 3.375491 | 0.004072 |
| C | 1.020462 | 2.738970 | 0.025397 |
| C | -0.240199 | 3.412201 | 0.065761 |
| H | -0.384313 | 4.485883 | 0.110535 |
| C | -4.946129 | 2.079587 | 0.831527 |
| H | -5.630284 | 1.386083 | 1.322051 |
| C | 2.422963 | 4.789104 | -0.012964 |
| H | 1.508320 | 5.381175 | -0.014251 |
| C | 1.194000 | 0.060724 | -2.921616 |
| H | 0.239416 | 0.077192 | -2.400873 |
| C | 3.644034 | -5.449528 | 0.030491 |
| H | 3.679898 | -6.539163 | 0.044075 |
| C | 4.774799 | -3.304931 | 0.015774 |
| H | 5.688062 | -2.707759 | 0.016908 |
| C | -3.224447 | -3.874660 | 0.410435 |
| H | -2.565056 | -4.580120 | 0.917783 |
| C | -3.585172 | 1.803251 | 0.762603 |
| H | -3.204410 | 0.883383 | 1.200530 |
| C | 2.487611 | -0.055489 | 4.944086 |
| H | 2.561532 | -0.067290 | 6.032126 |
| C | -7.384385 | 4.635664 | -0.148570 |
| H | -6.965282 | 5.530393 | 0.335501 |
| H | -8.456636 | 4.571845 | 0.063876 |
| H | -7.227391 | 4.692800 | -1.236056 |
| C | 4.830663 | 4.692559 | -0.031014 |
| H | 5.800249 | 5.194650 | -0.044270 |
| C | 3.538246 | 2.609652 | 0.000429 |
| C | 4.774800 | 3.304930 | -0.015773 |

| | | | |
|---|---|---|---|
| H | 5.688062 | 2.707759 | -0.016908 |
| C | 1.194000 | -0.060723 | 2.921616 |
| H | 0.239416 | -0.077192 | 2.400873 |
| C | 3.497722 | 0.004615 | -2.764627 |
| H | 4.362774 | -0.024765 | -2.106199 |
| C | 3.644035 | 5.449527 | -0.030492 |
| H | 3.679899 | 6.539163 | -0.044076 |
| C | 2.487612 | 0.055489 | -4.944085 |
| H | 2.561533 | 0.067290 | -6.032126 |
| C | 3.636714 | -0.018968 | 4.150934 |
| H | 4.631401 | -0.001444 | 4.594709 |
| C | 3.636715 | 0.018967 | -4.150933 |
| H | 4.631401 | 0.001443 | -4.594708 |
| C | 1.241564 | -0.076654 | 4.314105 |
| H | 0.315406 | -0.105436 | 4.886703 |
| C | 4.830663 | -4.692559 | 0.031014 |
| H | 5.800248 | -5.194651 | 0.044270 |
| C | -7.384385 | -4.635664 | 0.148569 |
| H | -7.227391 | -4.692801 | 1.236056 |
| C | 1.241565 | 0.076654 | -4.314104 |
| H | 0.315407 | 0.105437 | -4.886703 |
| C | 3.497721 | -0.004616 | 2.764628 |
| H | 4.362774 | 0.024765 | 2.106200 |
| H | -8.456636 | -4.571845 | -0.063876 |
| H | -6.965282 | -5.530393 | -0.335502 |

**3a**

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -4046.646586 | Hartree |
| **Zero-point Energy Correction** | 0.669446 | Hartree |
| **Thermal Correction to Energy** | 0.714323 | Hartree |
| **Thermal Correction to Enthalpy** | 0.715267 | Hartree |
| **Thermal Correction to Free Energy** | 0.582304 | Hartree |
| **EE + Zero-point Energy** | -4045.977139 | Hartree |
| **EE + Thermal Energy Correction** | -4045.932263 | Hartree |
| **EE + Thermal Enthalpy Correction** | -4045.931318 | Hartree |
| **EE + Thermal Free Energy Correction** | -4046.064282 | Hartree |
| **E (Thermal)** | 448.244 | kcal/mol |
| **Heat Capacity (Cv)** | 173.375 | cal/mol-kelvin |
| **Entropy (S)** | 279.845 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| Ga | -1.832979 | 0.000000 | 0.000000 |
| C | 7.386492 | 3.533959 | -0.344098 |
| O | -3.229624 | -1.346860 | -0.033122 |

| | | | |
|---|---|---|---|
| N | 1.576754 | -0.000000 | -0.000000 |
| N | -0.402449 | 1.414593 | 0.017391 |
| N | -0.402450 | -1.414593 | -0.017391 |
| O | -3.229623 | 1.346861 | 0.033122 |
| C | 5.905371 | 3.247686 | -0.279923 |
| N | -1.926884 | 0.042989 | -2.220100 |
| C | 3.984798 | -1.831027 | 0.804553 |
| H | 3.586183 | -0.941617 | 1.287980 |
| C | 7.386491 | -3.533960 | 0.344098 |
| N | -1.926884 | -0.042989 | 2.220100 |
| C | -1.904728 | -3.397440 | -0.077397 |
| C | -0.598278 | -2.757615 | -0.034413 |
| C | 0.972461 | -1.180151 | 0.028467 |
| C | 5.352031 | -2.108466 | 0.883376 |
| H | 6.002089 | -1.424286 | 1.433395 |
| C | -1.970860 | -4.814013 | -0.125332 |
| H | -1.042411 | -5.383522 | -0.133542 |
| C | 1.662322 | -2.454585 | 0.052338 |
| C | 0.670531 | -3.421905 | 0.004472 |
| H | 0.826161 | -4.494469 | 0.032162 |
| C | 0.972461 | 1.180151 | -0.028467 |
| C | 3.110362 | -2.694262 | 0.117283 |
| C | 5.905371 | -3.247687 | 0.279922 |
| C | 5.032740 | 4.109769 | 0.406977 |
| H | 5.430388 | 5.004830 | 0.890883 |
| C | 3.110363 | 2.694262 | -0.117283 |
| C | -3.137252 | -2.660181 | -0.072819 |
| C | 3.667160 | 3.841164 | 0.487080 |
| H | 3.020870 | 4.523364 | 1.041438 |
| C | 5.032739 | -4.109770 | -0.406977 |
| H | 5.430387 | -5.004830 | -0.890883 |
| C | 1.662322 | 2.454585 | -0.052338 |
| C | -1.904728 | 3.397440 | 0.077397 |
| C | -0.598277 | 2.757615 | 0.034413 |
| C | 0.670532 | 3.421905 | -0.004472 |
| H | 0.826162 | 4.494469 | -0.032162 |
| C | 5.352032 | 2.108465 | -0.883376 |
| H | 6.002089 | 1.424285 | -1.433395 |
| C | -1.970859 | 4.814014 | 0.125332 |
| H | -1.042410 | 5.383523 | 0.133542 |
| C | -0.827587 | 0.031973 | 2.989562 |
| H | 0.125733 | 0.111066 | 2.470654 |
| C | -3.172087 | -5.506092 | -0.165362 |
| H | -3.178634 | -6.595653 | -0.202679 |
| C | -4.354325 | -3.392715 | -0.112226 |
| H | -5.281926 | -2.818138 | -0.106593 |

| | | | |
|---|---|---|---|
| C | 3.667159 | -3.841164 | -0.487080 |
| H | 3.020870 | -4.523365 | -1.041438 |
| C | 3.984798 | 1.831026 | -0.804553 |
| H | 3.586184 | 0.941616 | -1.287980 |
| C | -2.127652 | 0.088319 | -5.004006 |
| H | -2.206207 | 0.105928 | -6.091645 |
| C | -4.377599 | 4.779078 | 0.157514 |
| H | -5.334924 | 5.303449 | 0.187969 |
| C | -3.137251 | 2.660181 | 0.072819 |
| C | -4.354325 | 3.392715 | 0.112226 |
| H | -5.281925 | 2.818139 | 0.106594 |
| C | -0.827587 | -0.031971 | -2.989562 |
| H | 0.125733 | -0.111063 | -2.470654 |
| C | -3.126778 | -0.140710 | 2.819496 |
| H | -3.986057 | -0.202211 | 2.155201 |
| C | -3.172086 | 5.506092 | 0.165362 |
| H | -3.178633 | 6.595654 | 0.202679 |
| C | -2.127651 | -0.088319 | 5.004006 |
| H | -2.206206 | -0.105928 | 6.091645 |
| C | -3.271256 | 0.166086 | -4.205612 |
| H | -4.264791 | 0.245863 | -4.645203 |
| C | -3.271255 | -0.166087 | 4.205613 |
| H | -4.264790 | -0.245865 | 4.645204 |
| C | -0.881067 | -0.012218 | -4.382147 |
| H | 0.039509 | -0.075367 | -4.961057 |
| C | -4.377600 | -4.779078 | -0.157514 |
| H | -5.334925 | -5.303448 | -0.187969 |
| C | -0.881067 | 0.012220 | 4.382147 |
| H | 0.039509 | 0.075370 | 4.961057 |
| C | -3.126779 | 0.140709 | -2.819495 |
| H | -3.986057 | 0.202208 | -2.155200 |
| H | 7.578959 | -4.594986 | 0.557890 |
| H | 7.875814 | -3.303951 | -0.615442 |
| H | 7.875291 | -2.929749 | 1.119861 |
| H | 7.578959 | 4.594985 | -0.557889 |
| H | 7.875291 | 2.929748 | -1.119862 |
| H | 7.875814 | 3.303949 | 0.615441 |

**3b**

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -4197.084828 | Hartree |
| **Zero-point Energy Correction** | 0.679741 | Hartree |
| **Thermal Correction to Energy** | 0.726045 | Hartree |
| **Thermal Correction to Enthalpy** | 0.726989 | Hartree |
| **Thermal Correction to Free Energy** | 0.592356 | Hartree |
| **EE + Zero-point Energy** | -4196.405087 | Hartree |
| **EE + Thermal Energy Correction** | -4196.358783 | Hartree |
| **EE + Thermal Enthalpy Correction** | -4196.357839 | Hartree |
| **EE + Thermal Free Energy Correction** | -4196.492472 | Hartree |
| **E (Thermal)** | 455.600 | kcal/mol |
| **Heat Capacity (Cv)** | 179.724 | cal/mol-kelvin |
| **Entropy (S)** | 283.359 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| Ga | 2.140625 | -0.000001 | 0.000001 |
| O | -6.931023 | -3.415960 | -0.400335 |
| O | 3.538409 | 1.346295 | 0.029011 |
| N | -1.267770 | 0.000000 | -0.000002 |
| N | 0.711317 | -1.414325 | -0.025632 |
| N | 0.711318 | 1.414325 | 0.025630 |
| O | 3.538408 | -1.346297 | -0.029007 |
| C | -5.581231 | -3.244178 | -0.283250 |
| N | 2.235618 | 0.043677 | -2.221085 |
| C | -3.696917 | 1.795329 | 0.772585 |
| H | -3.311441 | 0.877917 | 1.211665 |
| O | -6.931020 | 3.415966 | 0.400333 |
| N | 2.235612 | -0.043678 | 2.221086 |
| C | 2.214497 | 3.397861 | 0.017996 |
| C | 0.907069 | 2.757801 | 0.037597 |
| C | -0.664208 | 1.179731 | 0.054333 |
| C | -5.059330 | 2.064494 | 0.841118 |
| H | -5.739862 | 1.367819 | 1.332168 |
| C | 2.281649 | 4.814967 | 0.001007 |
| H | 1.353454 | 5.384977 | -0.001776 |
| C | -1.354880 | 2.453925 | 0.098649 |
| C | -0.360682 | 3.421372 | 0.080310 |
| H | -0.514910 | 4.493324 | 0.129896 |
| C | -0.664209 | -1.179731 | -0.054336 |
| C | -2.802134 | 2.693679 | 0.149711 |
| C | -5.581229 | 3.244183 | 0.283247 |
| C | -4.714333 | -4.150984 | 0.345133 |
| H | -5.084766 | -5.069049 | 0.796570 |
| C | -2.802135 | -2.693678 | -0.149715 |

| | | | |
|---|---|---|---|
| C | 3.446658 | 2.660229 | 0.015613 |
| C | -3.347058 | -3.867432 | 0.402734 |
| H | -2.691381 | -4.575630 | 0.911081 |
| C | -4.714329 | 4.150989 | -0.345135 |
| H | -5.084761 | 5.069054 | -0.796571 |
| C | -1.354882 | -2.453924 | -0.098652 |
| C | 2.214495 | -3.397863 | -0.017996 |
| C | 0.907067 | -2.757802 | -0.037598 |
| C | -0.360685 | -3.421372 | -0.080312 |
| H | -0.514913 | -4.493324 | -0.129898 |
| C | -5.059331 | -2.064490 | -0.841122 |
| H | -5.739862 | -1.367815 | -1.332172 |
| C | 2.281646 | -4.814969 | -0.001007 |
| H | 1.353450 | -5.384978 | 0.001774 |
| C | 1.133129 | -0.079374 | 2.988768 |
| H | 0.177322 | -0.087295 | 2.468445 |
| C | 3.483444 | 5.507368 | -0.015146 |
| H | 3.490524 | 6.597508 | -0.028926 |
| C | 4.664285 | 3.392825 | 0.001003 |
| H | 5.591529 | 2.817609 | 0.001099 |
| C | -3.347055 | 3.867435 | -0.402737 |
| H | -2.691378 | 4.575633 | -0.911083 |
| C | -3.696918 | -1.795326 | -0.772589 |
| H | -3.311441 | -0.877915 | -1.211670 |
| C | 2.436142 | 0.094601 | -5.004891 |
| H | 2.514603 | 0.114379 | -6.092506 |
| C | -7.511041 | -4.606243 | 0.142601 |
| H | -7.096816 | -5.503948 | -0.340145 |
| H | -8.582953 | -4.536952 | -0.069825 |
| H | -7.354215 | -4.662542 | 1.230155 |
| C | 4.688587 | -4.779898 | 0.014068 |
| H | 5.646331 | -5.304298 | 0.026111 |
| C | 3.446656 | -2.660232 | -0.015610 |
| C | 4.664283 | -3.392829 | -0.000999 |
| H | 5.591527 | -2.817613 | -0.001093 |
| C | 1.133136 | 0.079352 | -2.988769 |
| H | 0.177328 | 0.087257 | -2.468449 |
| C | 3.438522 | -0.033297 | 2.822132 |
| H | 4.300558 | -0.003072 | 2.159279 |
| C | 3.483441 | -5.507370 | 0.015147 |
| H | 3.490520 | -6.597511 | 0.028926 |
| C | 2.436129 | -0.094603 | 5.004894 |
| H | 2.514587 | -0.114382 | 6.092509 |
| C | 3.583047 | 0.058160 | -4.208270 |
| H | 4.579131 | 0.048667 | -4.649233 |
| C | 3.583036 | -0.058140 | 4.208275 |

| | | | |
|---|---|---|---|
| H | 4.579118 | -0.048630 | 4.649242 |
| C | 1.186393 | 0.105228 | -4.381306 |
| H | 0.263212 | 0.133330 | -4.958844 |
| C | 4.688590 | 4.779895 | -0.014065 |
| H | 5.646334 | 5.304294 | -0.026106 |
| C | -7.511037 | 4.606250 | -0.142601 |
| H | -7.354212 | 4.662550 | -1.230156 |
| C | 1.186383 | -0.105251 | 4.381305 |
| H | 0.263201 | -0.133371 | 4.958840 |
| C | 3.438529 | 0.033317 | -2.822126 |
| H | 4.300564 | 0.003109 | -2.159271 |
| H | -8.582949 | 4.536961 | 0.069825 |
| H | -7.096811 | 5.503954 | 0.340145 |

**4a**

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -2123.677773 | Hartree |
| **Zero-point Energy Correction** | 0.668011 | Hartree |
| **Thermal Correction to Energy** | 0.713478 | Hartree |
| **Thermal Correction to Enthalpy** | 0.714423 | Hartree |
| **Thermal Correction to Free Energy** | 0.580827 | Hartree |
| **EE + Zero-point Energy** | -2123.009762 | Hartree |
| **EE + Thermal Energy Correction** | -2122.964295 | Hartree |
| **EE + Thermal Enthalpy Correction** | -2122.963350 | Hartree |
| **EE + Thermal Free Energy Correction** | -2123.096946 | Hartree |
| **E (Thermal)** | 447.714 | kcal/mol |
| **Heat Capacity (Cv)** | 174.185 | cal/mol-kelvin |
| **Entropy (S)** | 281.175 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| In | 1.870064 | -0.000000 | 0.000001 |
| C | -7.528220 | 3.381782 | 0.514950 |
| O | 3.206026 | -1.520672 | -0.002893 |
| N | -1.650367 | 0.000000 | -0.000000 |
| N | 0.303449 | 1.461927 | -0.002767 |
| N | 0.303449 | -1.461927 | 0.002768 |
| O | 3.206026 | 1.520672 | 0.002895 |
| C | -6.042668 | 3.129788 | 0.416172 |
| N | 1.967006 | -0.002528 | 2.354899 |
| C | -4.068044 | -1.789066 | -0.938496 |
| H | -3.630408 | -0.930920 | -1.444936 |
| C | -7.528220 | -3.381782 | -0.514953 |
| N | 1.967008 | 0.002528 | -2.354898 |
| C | 1.756745 | -3.495333 | 0.055207 |
| C | 0.466185 | -2.809255 | 0.003901 |

| | | | |
|---|---|---|---|
| C | -1.065086 | -1.190431 | -0.050744 |
| C | -5.440667 | -2.030152 | -1.045145 |
| H | -6.055817 | -1.348396 | -1.636692 |
| C | 1.752906 | -4.913962 | 0.114843 |
| H | 0.796737 | -5.434651 | 0.128701 |
| C | -1.786145 | -2.447820 | -0.103450 |
| C | -0.821062 | -3.441111 | -0.057959 |
| H | -1.009040 | -4.507841 | -0.106079 |
| C | -1.065086 | 1.190431 | 0.050744 |
| C | -3.238484 | -2.650416 | -0.196628 |
| C | -6.042669 | -3.129787 | -0.416175 |
| C | -5.214196 | 3.990756 | -0.325190 |
| H | -5.651132 | 4.855039 | -0.830828 |
| C | -3.238484 | 2.650416 | 0.196626 |
| C | 3.033533 | -2.827964 | 0.047673 |
| C | -3.843786 | 3.758707 | -0.432476 |
| H | -3.231240 | 4.437660 | -1.027842 |
| C | -5.214196 | -3.990756 | 0.325188 |
| H | -5.651132 | -4.855039 | 0.830826 |
| C | -1.786145 | 2.447820 | 0.103449 |
| C | 1.756746 | 3.495333 | -0.055207 |
| C | 0.466185 | 2.809255 | -0.003900 |
| C | -0.821062 | 3.441111 | 0.057959 |
| H | -1.009040 | 4.507841 | 0.106079 |
| C | -5.440667 | 2.030153 | 1.045143 |
| H | -6.055817 | 1.348396 | 1.636690 |
| C | 1.752906 | 4.913961 | -0.114843 |
| H | 0.796738 | 5.434651 | -0.128701 |
| C | 0.856059 | 0.020452 | -3.113137 |
| H | -0.094925 | 0.036417 | -2.582642 |
| C | 2.913501 | -5.672050 | 0.162257 |
| H | 2.857792 | -6.759892 | 0.209407 |
| C | 4.206306 | -3.629043 | 0.093261 |
| H | 5.163496 | -3.105030 | 0.084117 |
| C | -3.843786 | -3.758706 | 0.432474 |
| H | -3.231241 | -4.437659 | 1.027841 |
| C | -4.068044 | 1.789066 | 0.938494 |
| H | -3.630408 | 0.930921 | 1.444934 |
| C | 2.137620 | 0.001459 | 5.142945 |
| H | 2.204177 | 0.003172 | 6.231508 |
| C | 4.156770 | 5.014268 | -0.149500 |
| H | 5.084469 | 5.589106 | -0.185204 |
| C | 3.033533 | 2.827963 | -0.047671 |
| C | 4.206307 | 3.629043 | -0.093258 |
| H | 5.163496 | 3.105029 | -0.084114 |
| C | 0.856058 | -0.020448 | 3.113138 |

| | | | |
|---|---|---|---|
| H | -0.094927 | -0.036411 | 2.582643 |
| C | 3.163081 | -0.016901 | -2.971347 |
| H | 4.038965 | -0.031019 | -2.323976 |
| C | 2.913502 | 5.672049 | -0.162256 |
| H | 2.857793 | 6.759892 | -0.209406 |
| C | 2.137622 | -0.001458 | -5.142944 |
| H | 2.204180 | -0.003172 | -6.231506 |
| C | 3.293703 | 0.019272 | 4.359005 |
| H | 4.285084 | 0.035127 | 4.810200 |
| C | 3.293705 | -0.019275 | -4.359003 |
| H | 4.285087 | -0.035133 | -4.810197 |
| C | 0.894504 | -0.018701 | 4.506427 |
| H | -0.034720 | -0.033198 | 5.074690 |
| C | 4.156769 | -5.014268 | 0.149502 |
| H | 5.084468 | -5.589106 | 0.185207 |
| C | 0.894506 | 0.018705 | -4.506426 |
| H | -0.034718 | 0.033204 | -5.074689 |
| C | 3.163079 | 0.016898 | 2.971349 |
| H | 4.038964 | 0.031013 | 2.323979 |
| H | -7.737642 | -4.418875 | -0.815063 |
| H | -8.022729 | -3.221825 | 0.455707 |
| H | -7.997862 | -2.710099 | -1.245635 |
| H | -7.737642 | 4.418876 | 0.815058 |
| H | -7.997862 | 2.710101 | 1.245632 |
| H | -8.022729 | 3.221823 | -0.455710 |

**4b**

| | | |
|---|---|---|
| **Imaginary Freq** | 0 | |
| **Temperature** | 298.150 | Kelvin |
| **Pressure** | 1.00000 | atm |
| **Frequencies scaled by** | 1.0000 | |
| **Electronic Energy (EE)** | -2274.115932 | Hartree |
| **Zero-point Energy Correction** | 0.678338 | Hartree |
| **Thermal Correction to Energy** | 0.725240 | Hartree |
| **Thermal Correction to Enthalpy** | 0.726185 | Hartree |
| **Thermal Correction to Free Energy** | 0.590678 | Hartree |
| **EE + Zero-point Energy** | -2273.437595 | Hartree |
| **EE + Thermal Energy Correction** | -2273.390692 | Hartree |
| **EE + Thermal Enthalpy Correction** | -2273.389748 | Hartree |
| **EE + Thermal Free Energy Correction** | -2273.525254 | Hartree |
| **E (Thermal)** | 455.095 | kcal/mol |
| **Heat Capacity (Cv)** | 180.512 | cal/mol-kelvin |
| **Entropy (S)** | 285.198 | cal/mol-kelvin |

| | | | |
|---|---|---|---|
| In | -2.287835 | 0.000005 | 0.000003 |
| O | 6.959919 | -3.270370 | 0.574065 |
| O | -3.626027 | 1.518222 | -0.048641 |

| | | | |
|---|---|---|---|
| N | 1.230054 | -0.000001 | -0.000006 |
| N | -0.723071 | -1.461298 | 0.044851 |
| N | -0.723066 | 1.461303 | -0.044852 |
| O | -3.626032 | -1.518208 | 0.048653 |
| C | 5.608674 | -3.131520 | 0.429209 |
| N | -2.385802 | 0.073950 | 2.354747 |
| C | 3.680432 | 1.727293 | -0.875118 |
| H | 3.263893 | 0.818127 | -1.303024 |
| O | 6.959927 | 3.270347 | -0.574112 |
| N | -2.385813 | -0.073940 | -2.354740 |
| C | -2.177950 | 3.494772 | -0.066539 |
| C | -0.886005 | 2.808413 | -0.085569 |
| C | 0.646110 | 1.189466 | -0.080274 |
| C | 5.047384 | 1.963240 | -0.972426 |
| H | 5.700903 | 1.248654 | -1.474318 |
| C | -2.175691 | 4.914539 | -0.064732 |
| H | -1.220042 | 5.436294 | -0.070857 |
| C | 1.368426 | 2.445647 | -0.161705 |
| C | 0.400000 | 3.438660 | -0.156310 |
| H | 0.585659 | 4.503876 | -0.234971 |
| C | 0.646106 | -1.189467 | 0.080265 |
| C | 2.820349 | 2.649221 | -0.238201 |
| C | 5.608682 | 3.131502 | -0.429248 |
| C | 4.776929 | -4.060990 | -0.213250 |
| H | 5.178669 | -4.971166 | -0.653818 |
| C | 2.820341 | -2.649229 | 0.238179 |
| C | -3.454189 | 2.826701 | -0.050523 |
| C | 3.404424 | -3.810994 | -0.299109 |
| H | 2.775899 | -4.536580 | -0.817244 |
| C | 4.776945 | 4.060975 | 0.213217 |
| H | 5.178690 | 4.971149 | 0.653784 |
| C | 1.368418 | -2.445650 | 0.161691 |
| C | -2.177962 | -3.494762 | 0.066547 |
| C | -0.886015 | -2.808408 | 0.085569 |
| C | 0.399989 | -3.438660 | 0.156303 |
| H | 0.585644 | -4.503876 | 0.234963 |
| C | 5.047383 | -1.963255 | 0.972390 |
| H | 5.700907 | -1.248672 | 1.474278 |
| C | -2.175708 | -4.914530 | 0.064741 |
| H | -1.220061 | -5.436288 | 0.070862 |
| C | -1.275642 | -0.132357 | -3.112019 |
| H | -0.324751 | -0.145093 | -2.581203 |
| C | -3.337014 | 5.673134 | -0.051111 |
| H | -3.282111 | 6.762060 | -0.048840 |
| C | -4.627713 | 3.627970 | -0.039314 |
| H | -5.584396 | 3.102998 | -0.029245 |

| | | | |
|---|---|---|---|
| C | 3.404439 | 3.810983 | 0.299084 |
| H | 2.775920 | 4.536571 | 0.817224 |
| C | 3.680431 | -1.727304 | 0.875090 |
| H | 3.263898 | -0.818136 | 1.302998 |
| C | -2.557766 | 0.157633 | 5.141465 |
| H | -2.624858 | 0.190275 | 6.229510 |
| C | 7.578864 | -4.447818 | 0.046748 |
| H | 7.176748 | -5.353941 | 0.524040 |
| H | 8.644415 | -4.352335 | 0.280094 |
| H | 7.445140 | -4.511133 | -1.043543 |
| C | -4.579709 | -5.014417 | 0.039347 |
| H | -5.508002 | -5.589335 | 0.029076 |
| C | -3.454198 | -2.826687 | 0.050536 |
| C | -4.627726 | -3.627952 | 0.039335 |
| H | -5.584407 | -3.102977 | 0.029270 |
| C | -1.275627 | 0.132365 | 3.112020 |
| H | -0.324738 | 0.145099 | 2.581200 |
| C | -3.581747 | -0.056867 | -2.971430 |
| H | -4.456798 | -0.008095 | -2.324599 |
| C | -3.337033 | -5.673121 | 0.051127 |
| H | -3.282135 | -6.762047 | 0.048857 |
| C | -2.557790 | -0.157623 | -5.141458 |
| H | -2.624887 | -0.190264 | -6.229503 |
| C | -3.713071 | 0.097541 | 4.358468 |
| H | -4.704342 | 0.081773 | 4.809926 |
| C | -3.713092 | -0.097528 | -4.358456 |
| H | -4.704365 | -0.081759 | -4.809909 |
| C | -1.314741 | 0.175148 | 4.504668 |
| H | -0.386120 | 0.221476 | 5.072225 |
| C | -4.579692 | 5.014435 | -0.039325 |
| H | -5.507983 | 5.589356 | -0.029049 |
| C | 7.578879 | 4.447793 | -0.046797 |
| H | 7.445162 | 4.511107 | 1.043494 |
| C | -1.314762 | -0.175140 | -4.504667 |
| H | -0.386144 | -0.221470 | -5.072228 |
| C | -3.581733 | 0.056879 | 2.971442 |
| H | -4.456787 | 0.008108 | 2.324615 |
| H | 8.644428 | 4.352307 | -0.280150 |
| H | 7.176763 | 5.353917 | -0.524087 |

## UV-Vis Calculations with TD-DFT[2]

Theory Level: **1a-b**, **2a-b** and **3a-b:** TD-DFT (B3LYP/jul-cc-pvDz) // DFT(B3LYP/jul-cc-pvDz)
**4a-b**: TD-DFT (B3LYP/LANL2DZ) // DFT (B3LYP/LANL2DZ)

| Structure | Solvent | $\lambda_{max}$ (nm) | Excitation Energy (eV) | Oscillator Strength |
|---|---|---|---|---|
| **1a** | Methanol | 651.99 | 1.9016 | 0.5438 |
| **1a** | Methanol | 664.42 | 1.8661 | 0.5858 |
| **2a** | Methanol | 689.14 | 1.7991 | 0.5213 |
| **2b** | Methanol | 689.19 | 1.7990 | 0.552 |
| **3a** | Methanol | 687.73 | 1.8028 | 0.5241 |
| **3b** | Methanol | 688.02 | 1.8021 | 0.5539 |
| **4a** | Methanol | 661.47 | 1.8744 | 0.6207 |
| **4b** | Methanol | 664.89 | 1.8647 | 0.646 |

**Table S1**. UV-Vis of **1a-b**, **2a-b**, **3a-b**, and **4a-b** in MeOH as implicit solvent.

| Structure | HOMO (eV) | LUMO (eV) |
|---|---|---|
| **1a** | -5.56 | -3.66 |
| **1b** | -5.21 | -3.43 |
| **2a** | -5.00 | -3.20 |
| **2b** | -4.97 | -3.17 |
| **3a** | -5.01 | -3.21 |
| **3b** | -4.98 | -3.17 |
| **4a** | -5.01 | -3.14 |
| **4b** | -4.98 | -3.11 |

**Table S2**. HOMO and LUMO energies of **1a-b**, **2a-b**, **3a-b**, and **4a-b** in MeOH as implicit solvent.

## Molecular Orbital Diagrams

Theory Level: **1a-b**, **2a-b**, and **3a-b:** TD-DFT (B3LYP/jul-cc-pvDz) // DFT(B3LYP/jul-cc-pvDz)
**4a-b**: TD-DFT (B3LYP/LANL2DZ) // DFT (B3LYP/LANL2DZ)

Notes: Natural Transition Orbitals (NTO) calculated for the first excited state during the TD-DFT calculations. HOMO and LUMO visualized using GaussView.

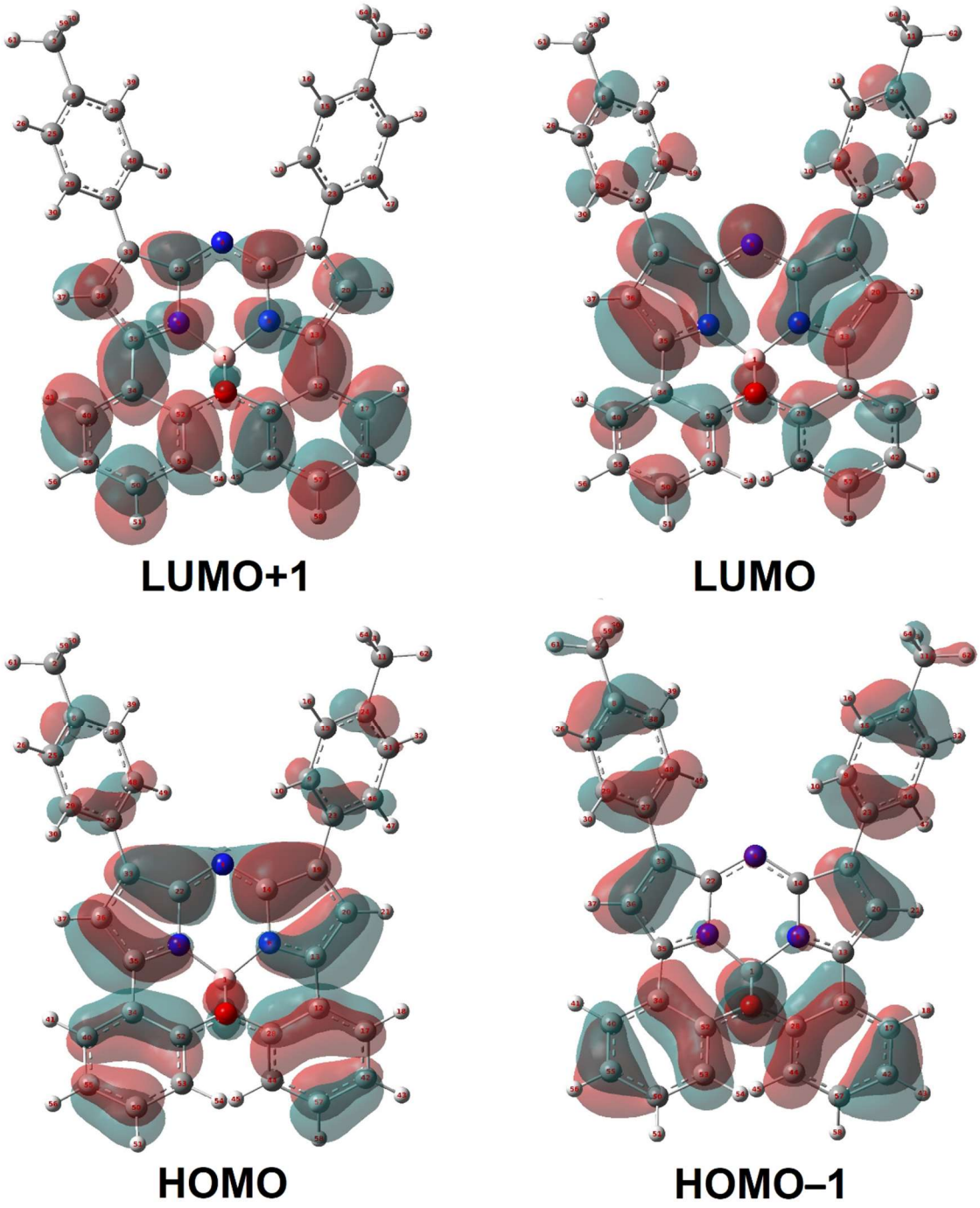



**Figure S1**. Frontier Molecular Orbital Plots of **1a**.

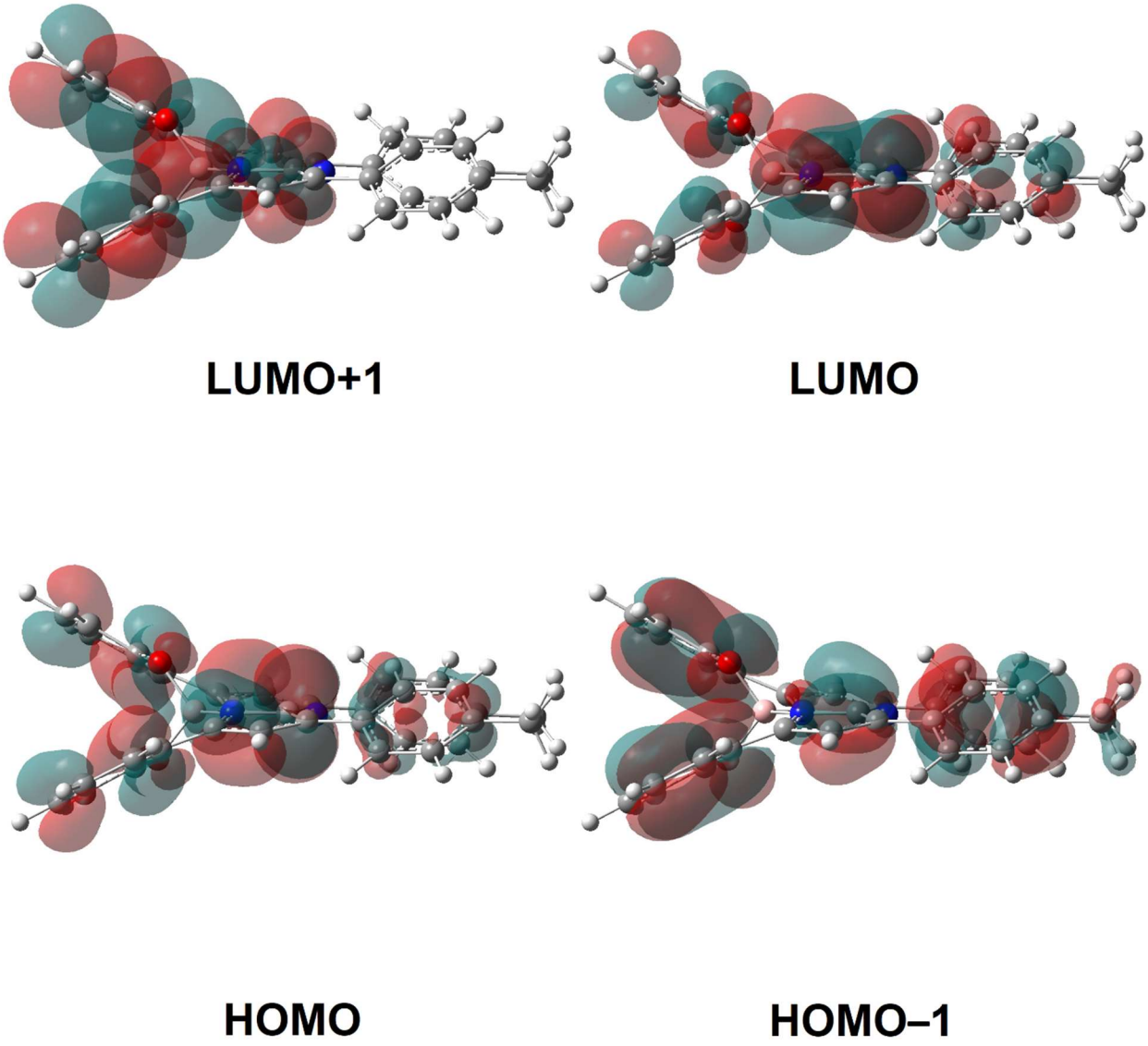



**Figure S2**. Horizontal view of Frontier Molecular Orbital Plots of **1a**.

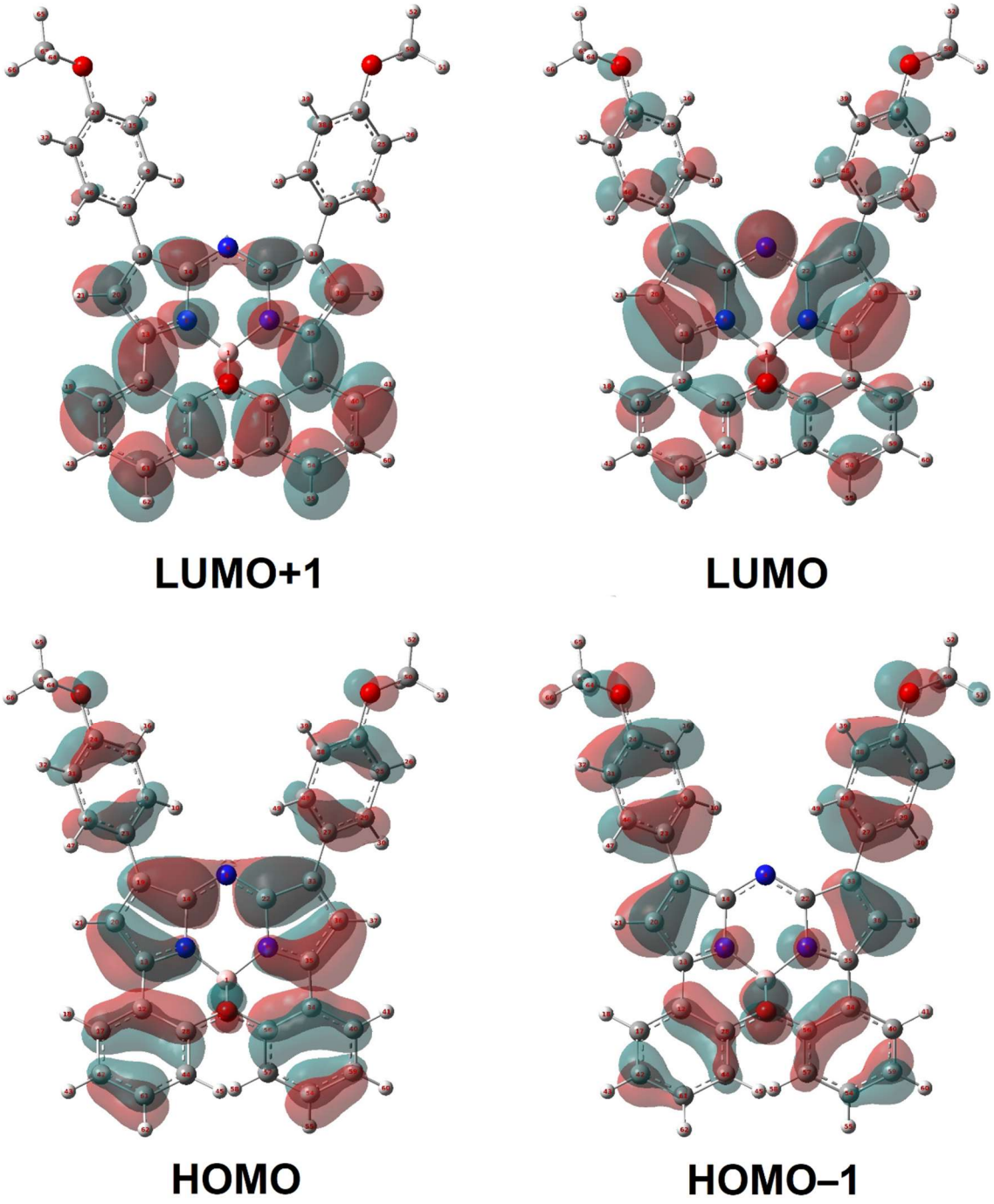



**Figure S3**. Frontier Molecular Orbital Plots of **1b**.

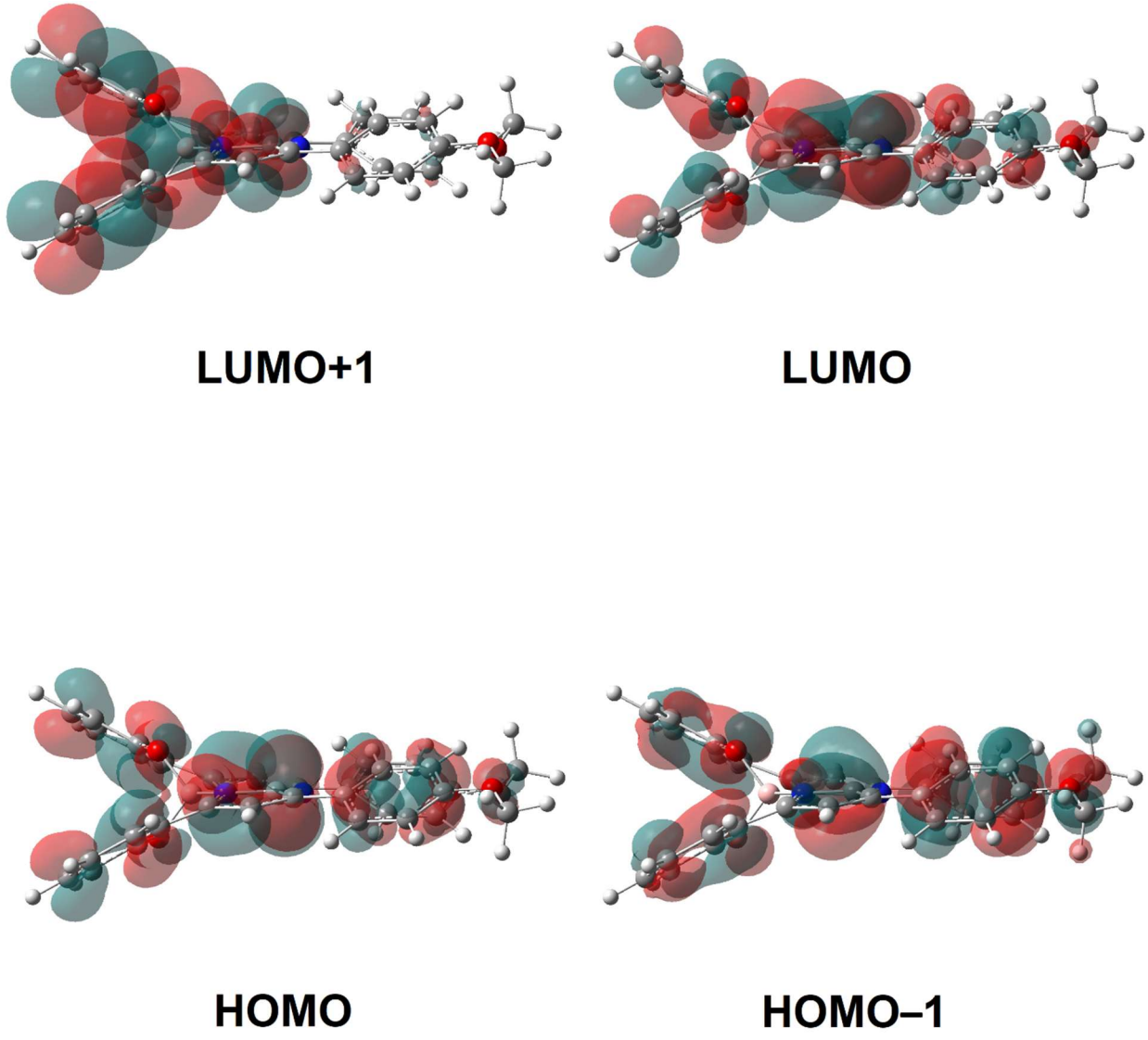



**Figure S4**. Horizontal view of Frontier Molecular Orbital Plots of **1b**.

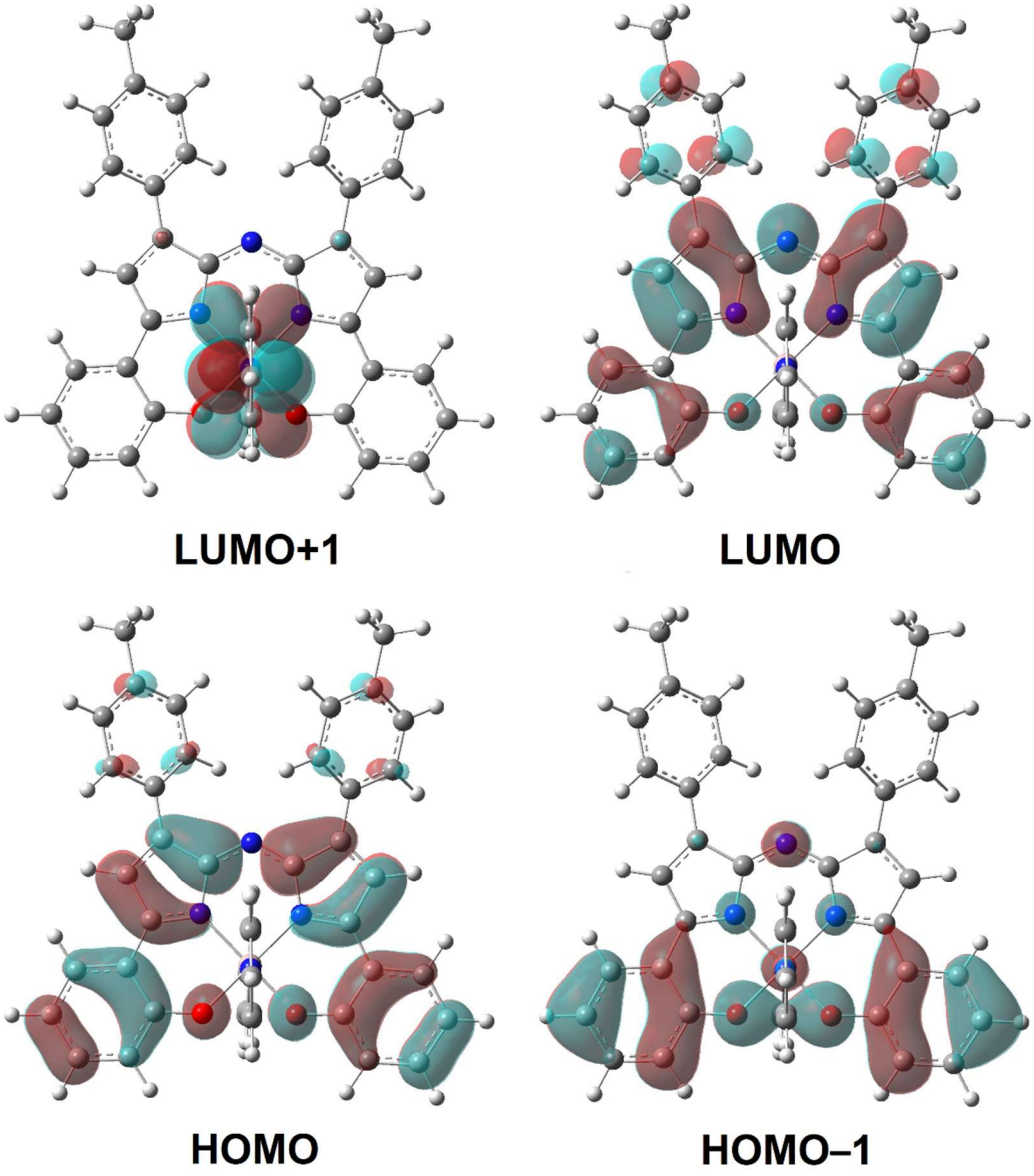



**Figure S5**. Frontier Molecular Orbital Plots of **2a**.

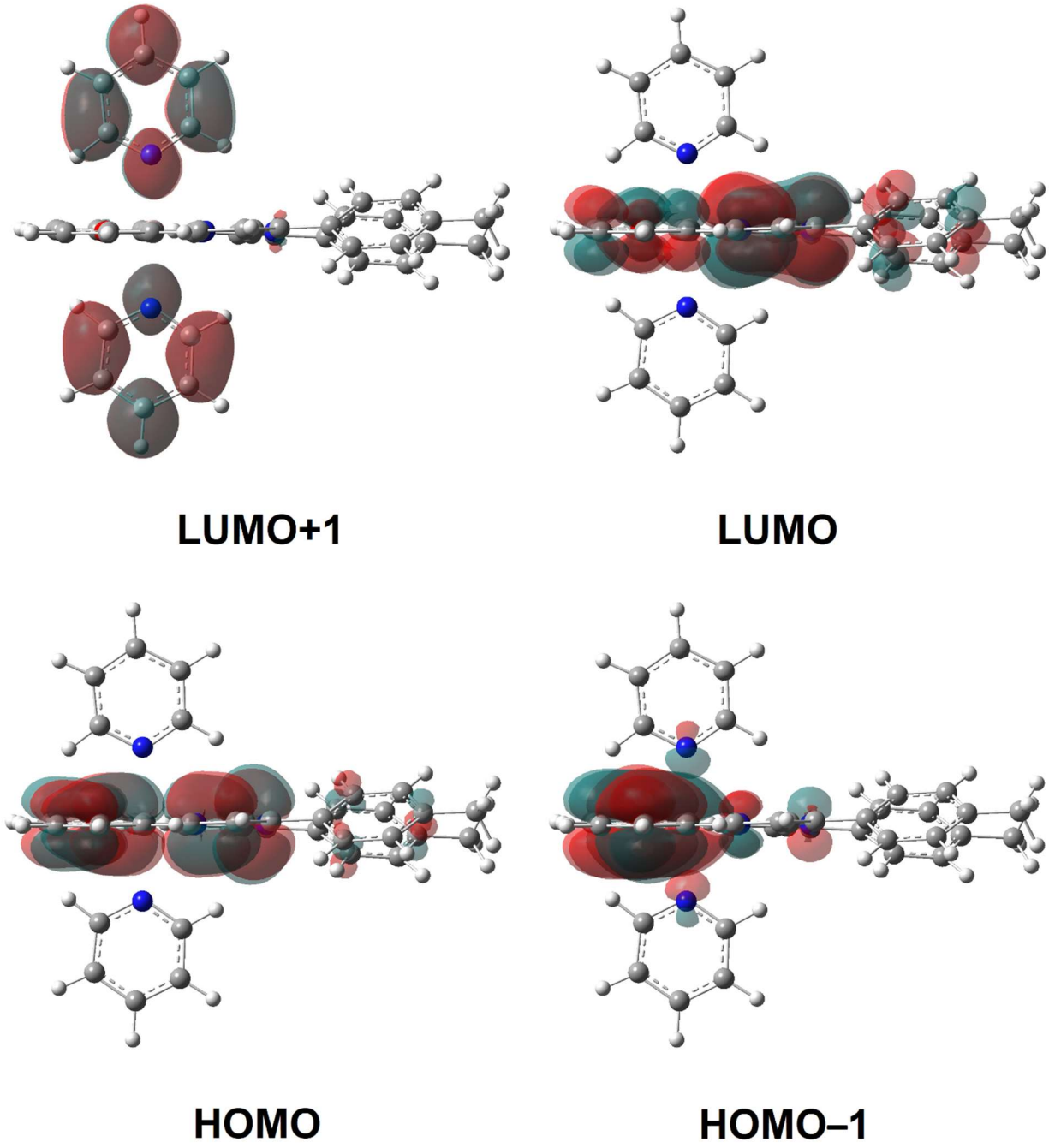



**Figure S6**. Horizontal view of Frontier Molecular Orbital Plots of **2a**.

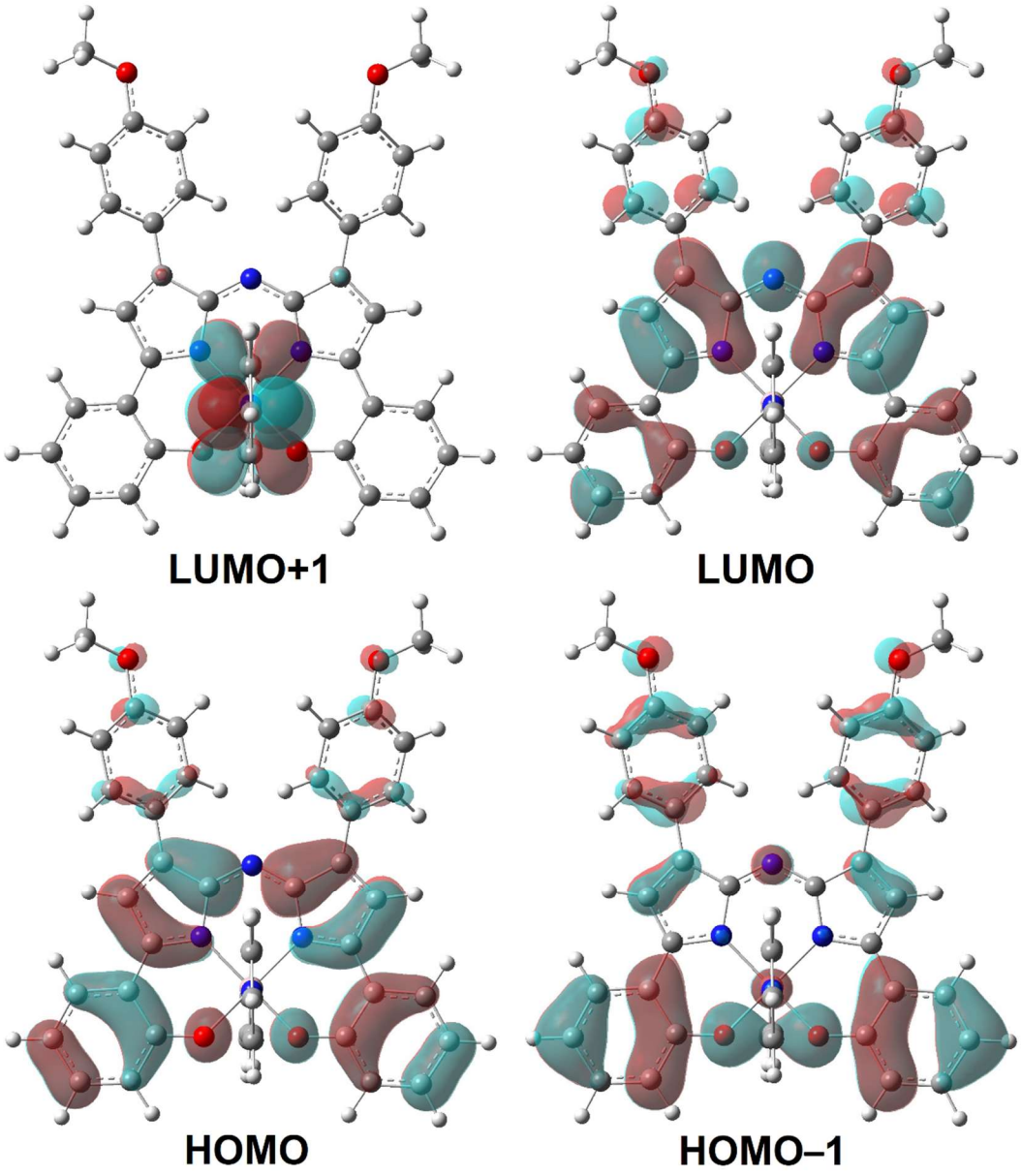



**Figure S7**. Frontier Molecular Orbital Plots of **2b**.

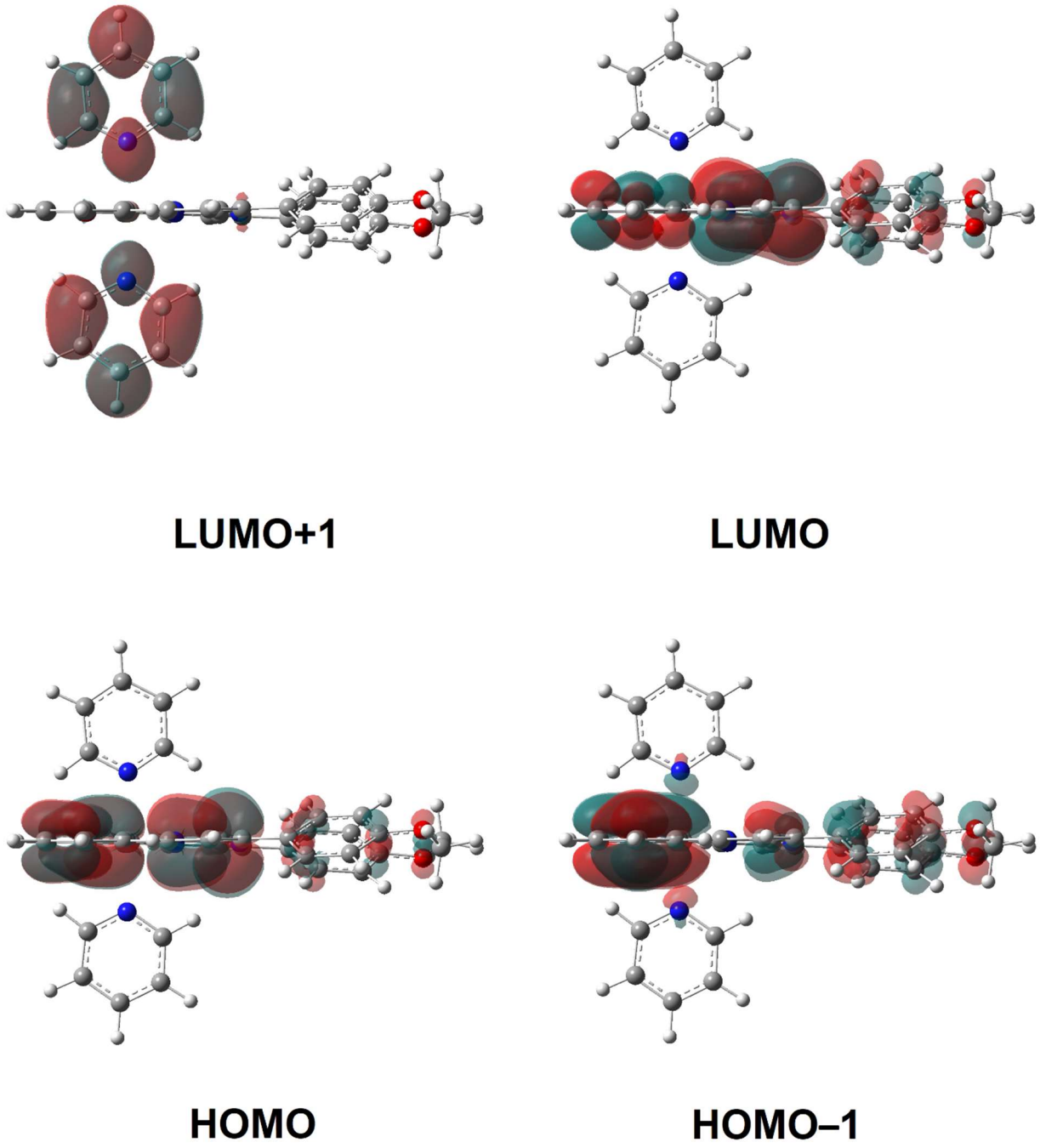



**Figure S8**. Horizontal view of Frontier Molecular Orbital Plots of **2b**.

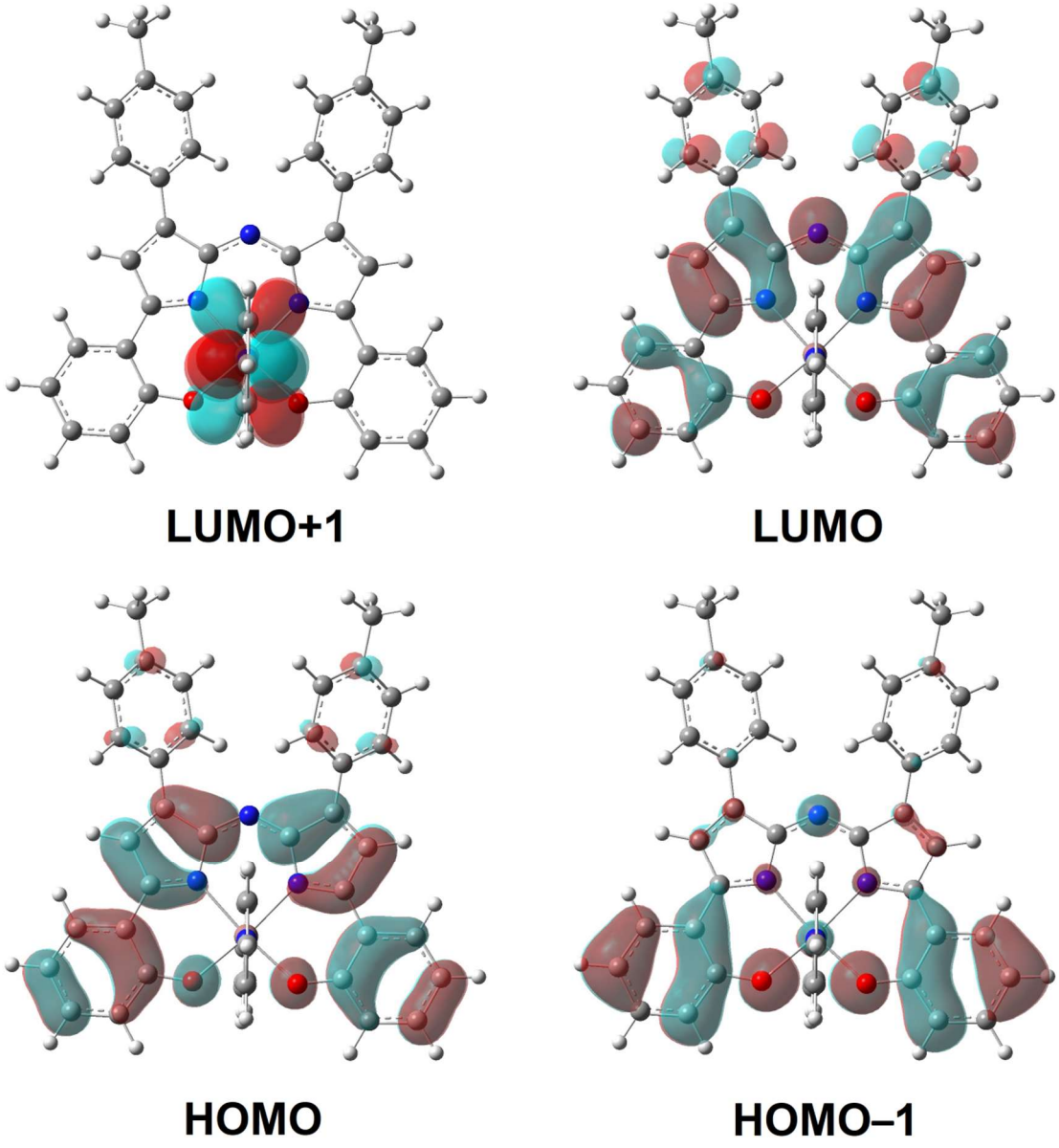



**Figure S9**. Frontier Molecular Orbital Plots of **3a**.

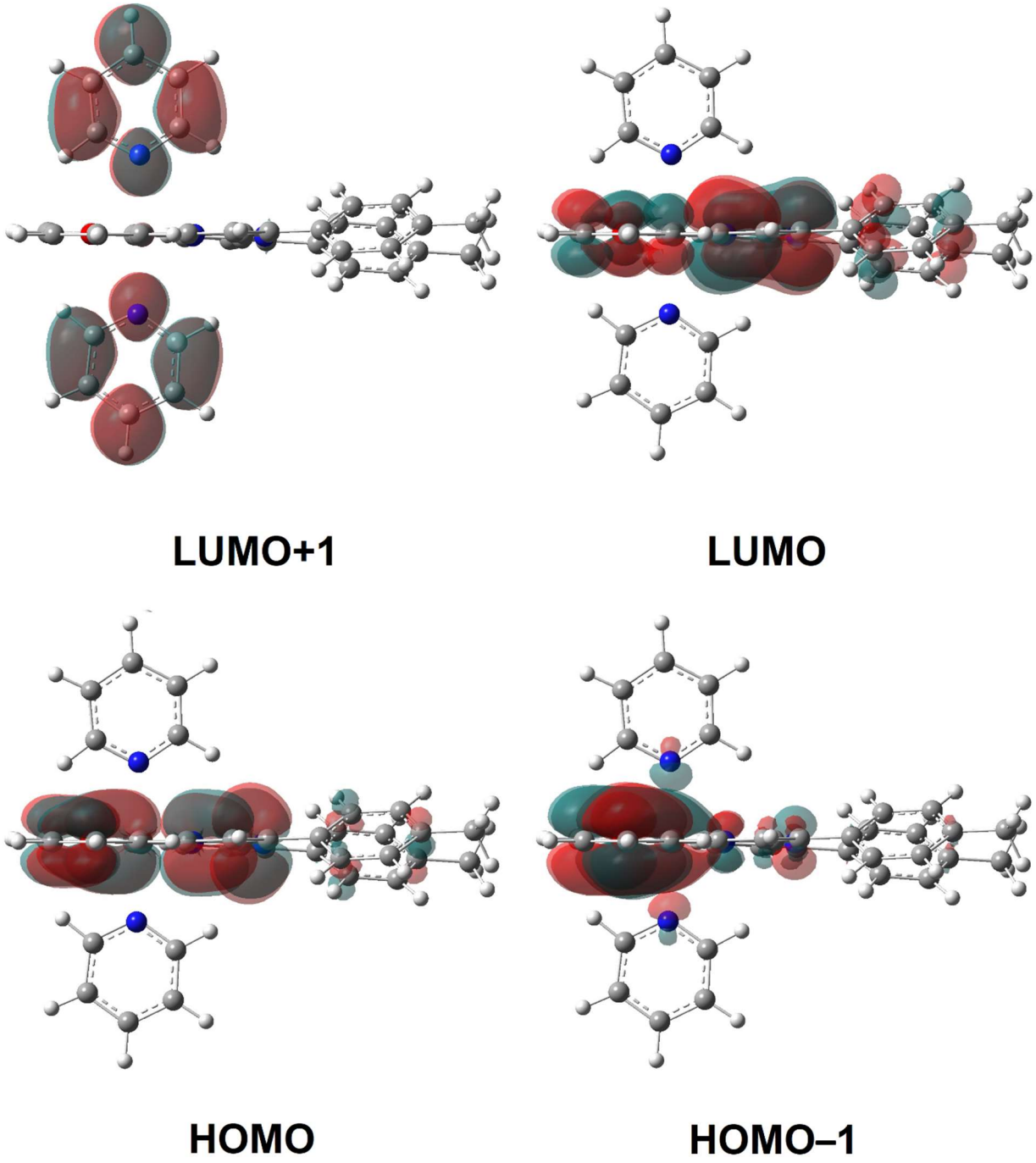



**Figure S10**. Horizontal view of Frontier Molecular Orbital Plots of **3a**.

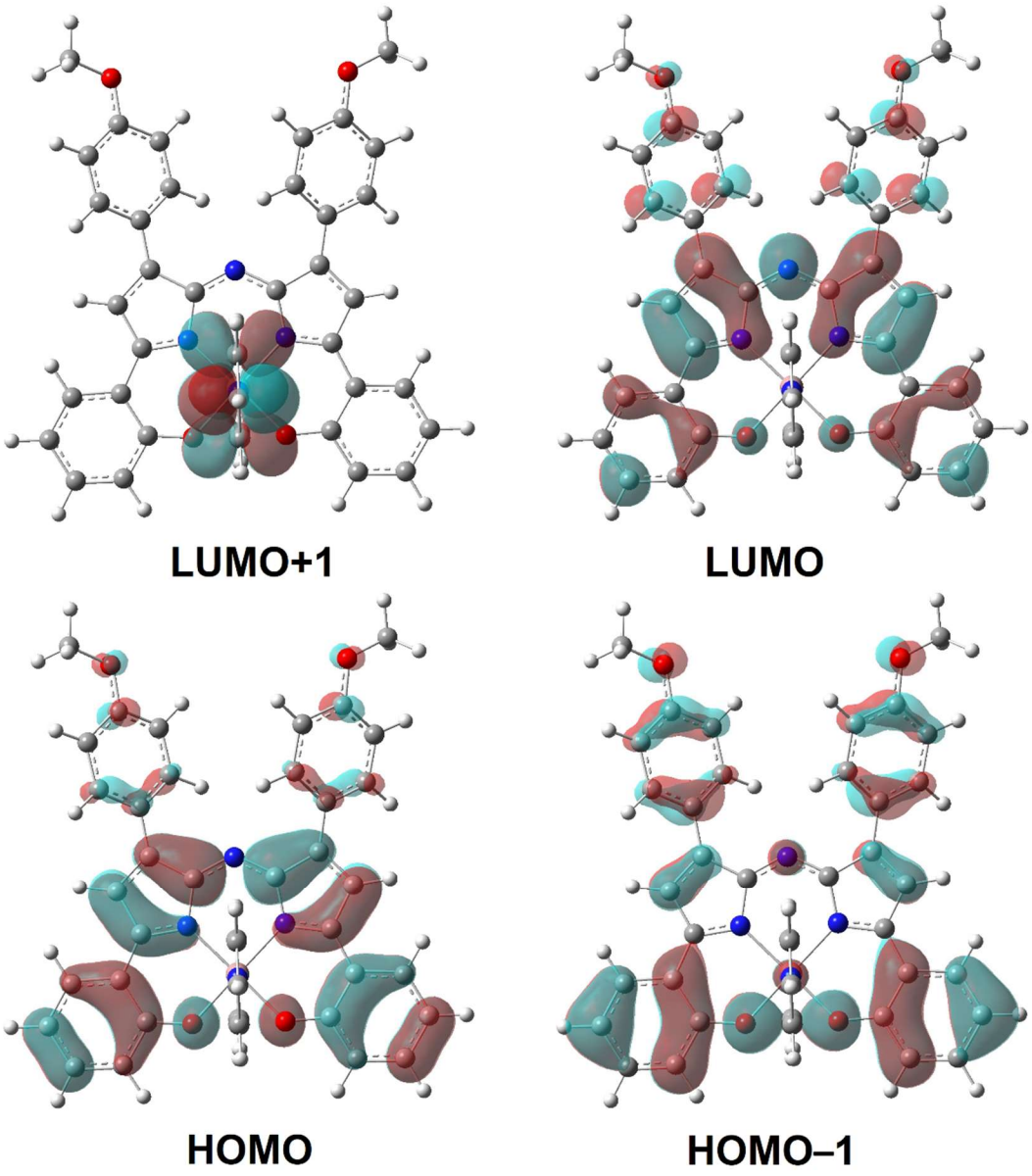



**Figure S11**. Frontier Molecular Orbital Plots of **3b**.

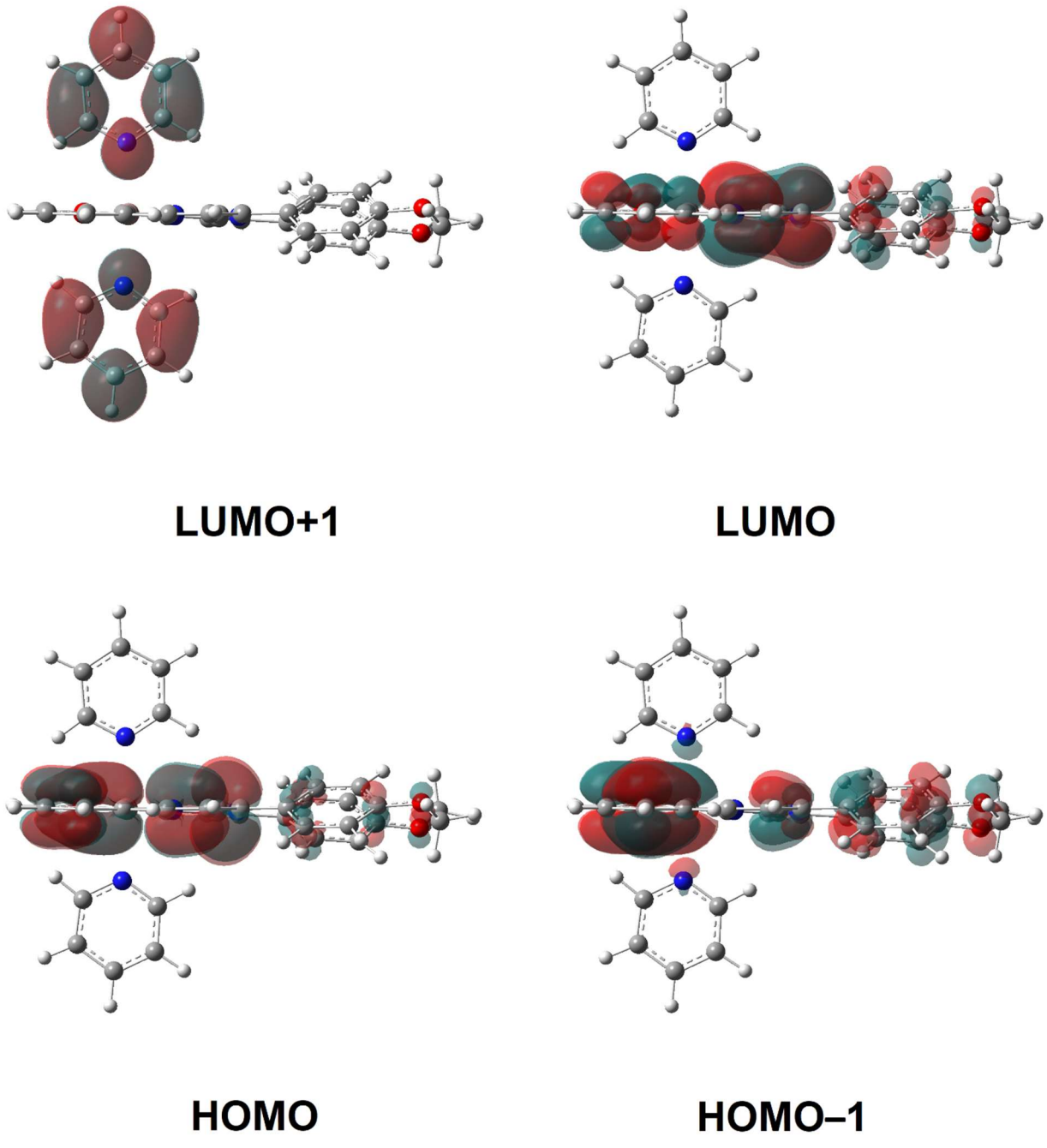



**Figure S12**. Horizontal view of Frontier Molecular Orbital Plots of **3b**.

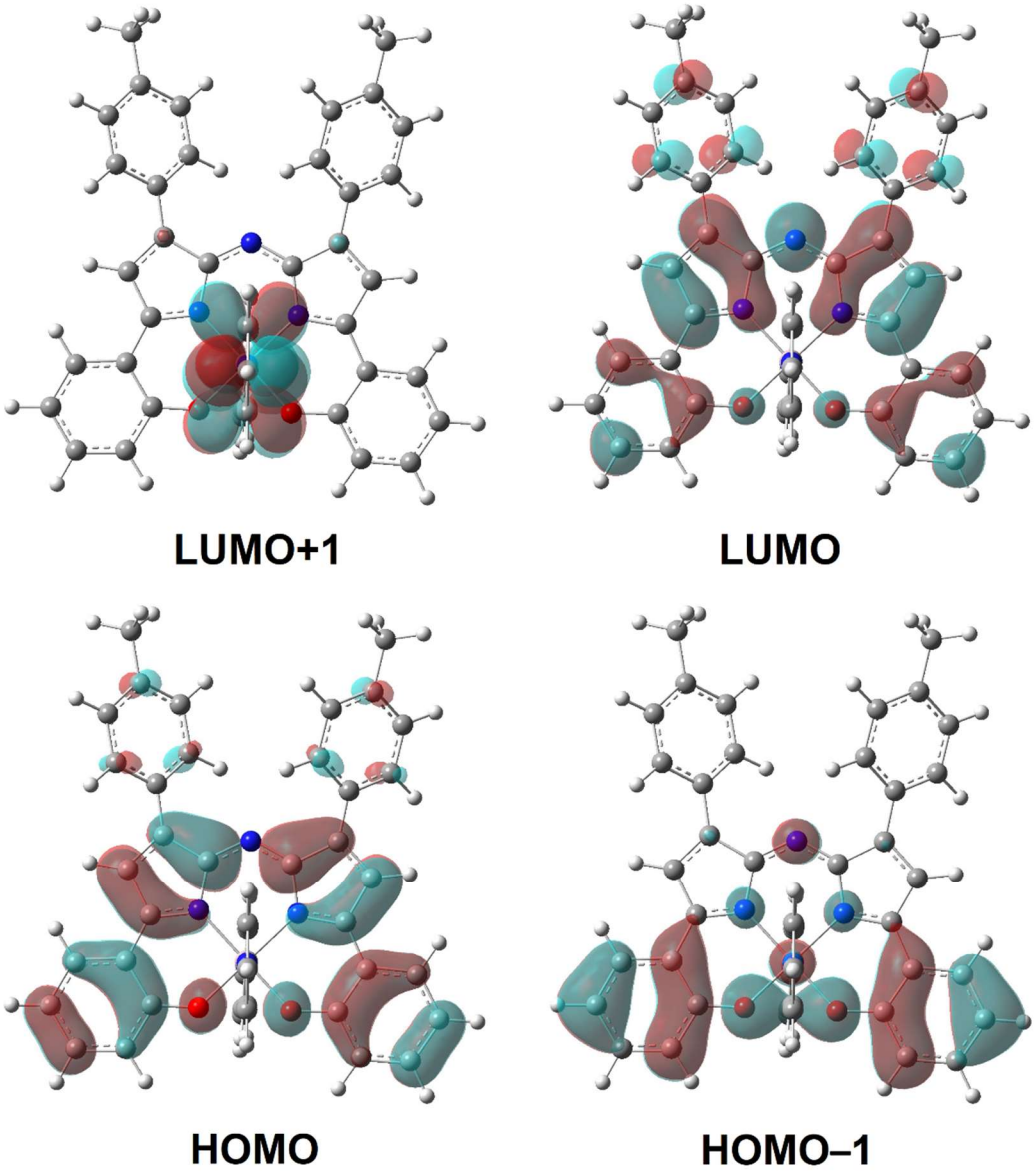



**Figure S13**. Frontier Molecular Orbital Plots of **4a**.

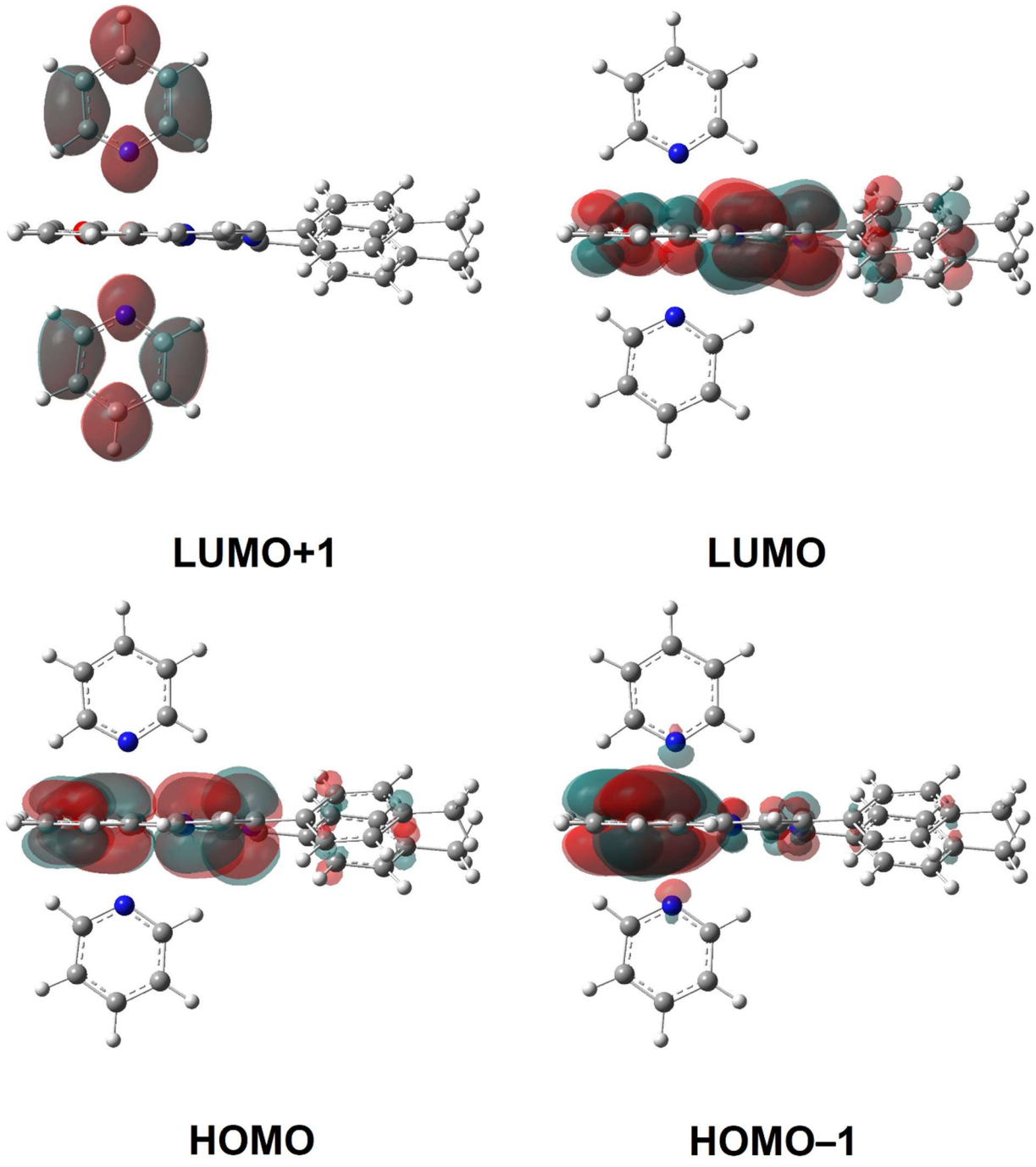



**Figure S14**. Horizontal view of Frontier Molecular Orbital Plots of **4a**.

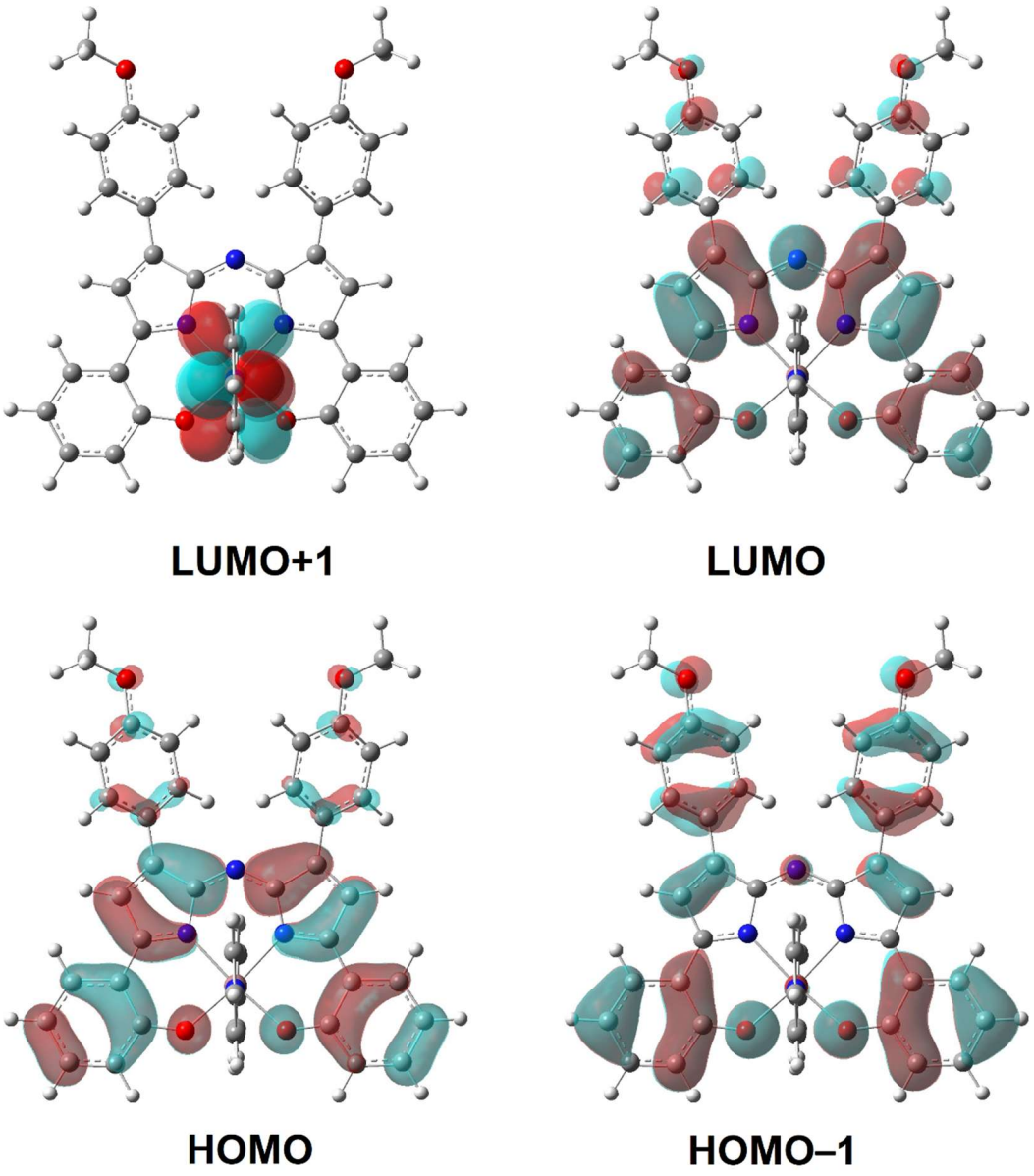



**Figure S15**. Frontier Molecular Orbital Plots of **4b**.

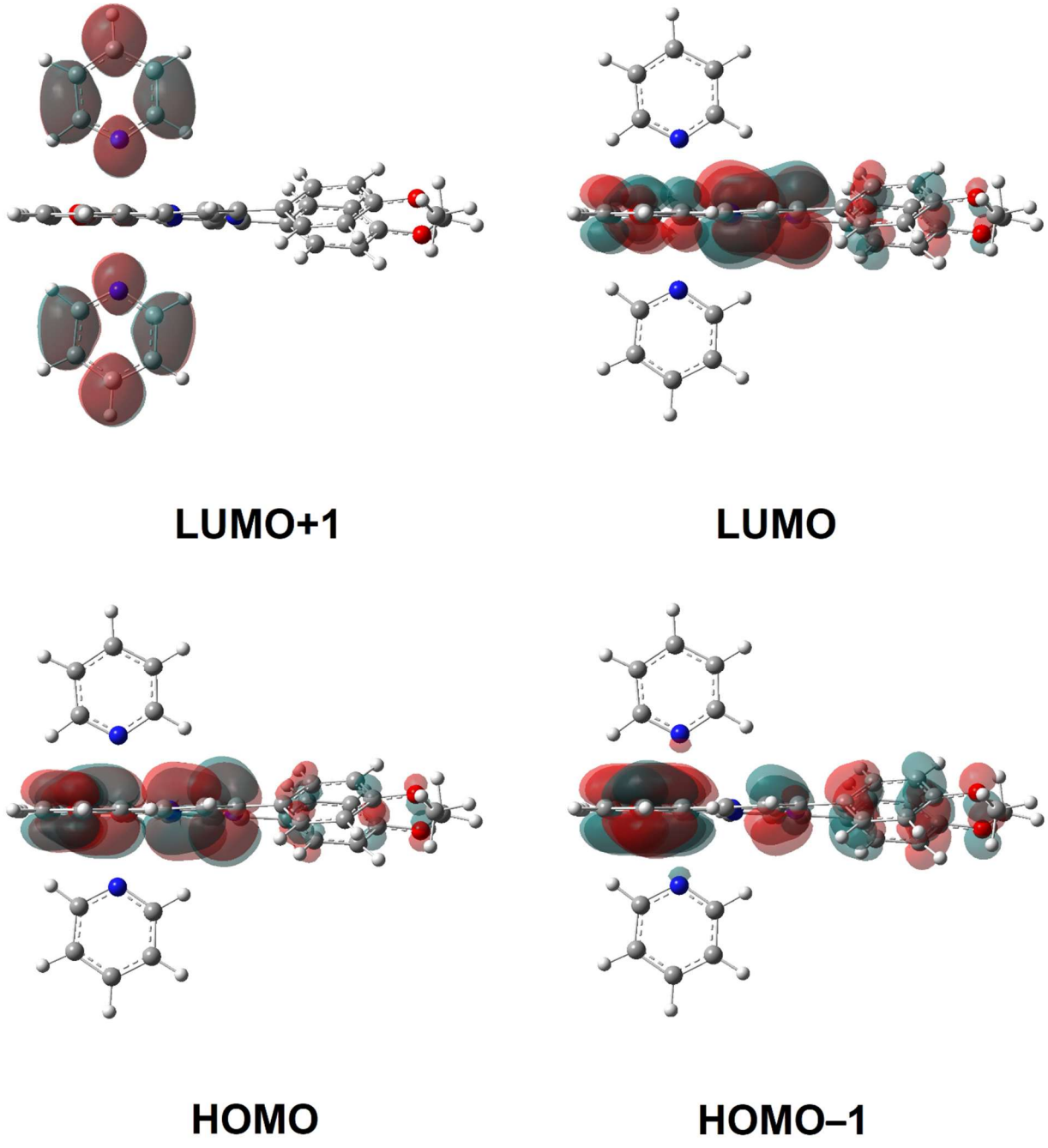



**Figure S16**. Horizontal view of Frontier Molecular Orbital Plots of **4b**.

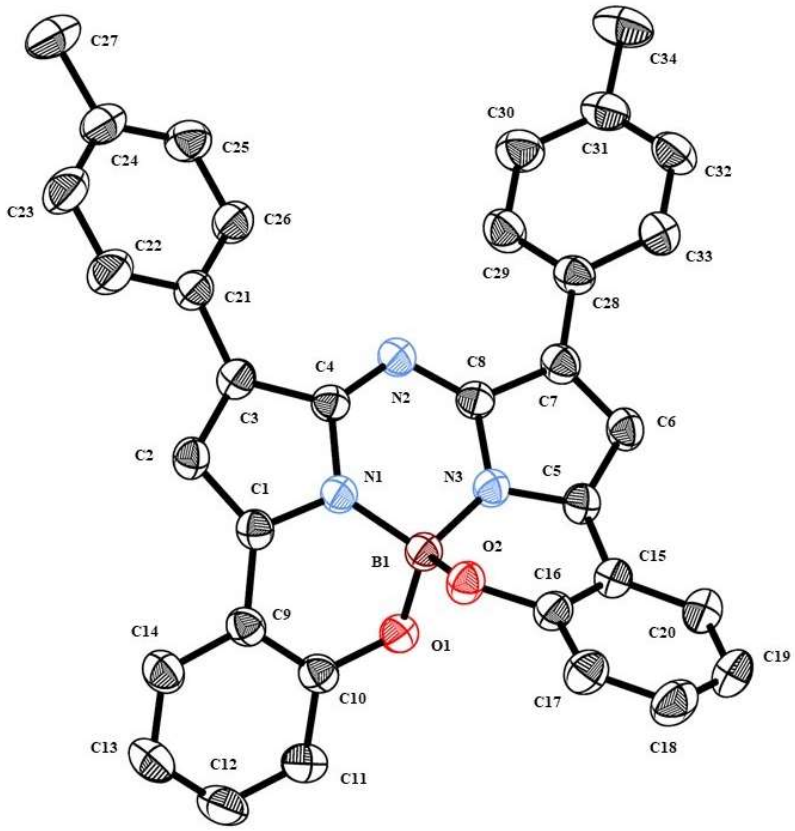



**Figure S17.** Single crystal X-ray diffraction structure of **1a**; ellipsoids are drawn at the 40% probability level. Hydrogen atoms omitted for clarity.

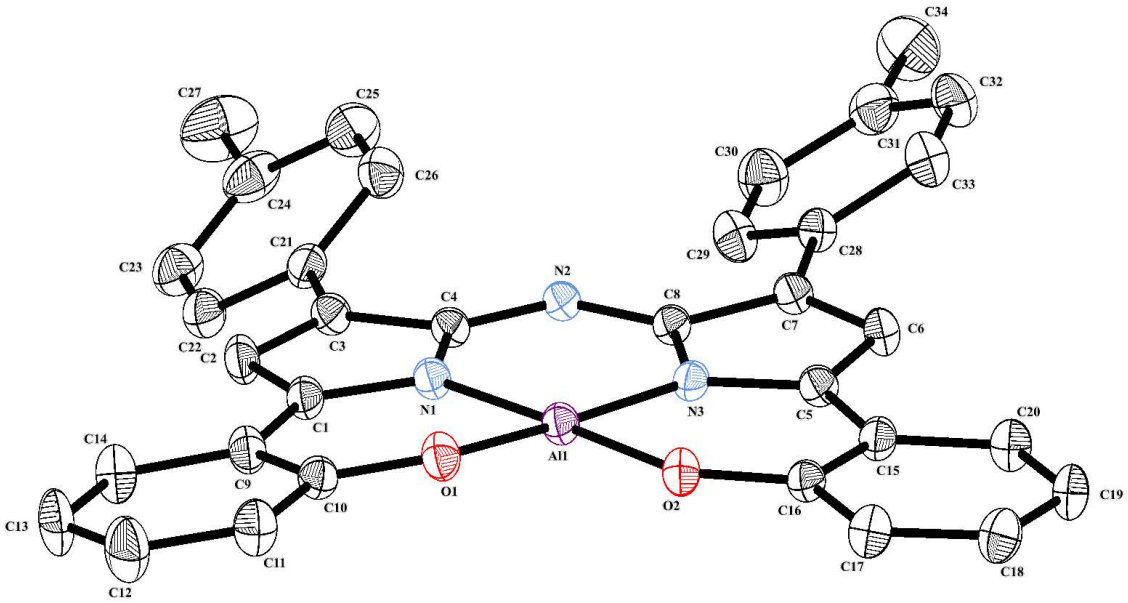



**Figure S18**. Single crystal X-ray diffraction structure of **2a**; ellipsoids are drawn at the 40% probability level. Axial bound pyridine ligands and hydrogen atoms omitted for clarity.

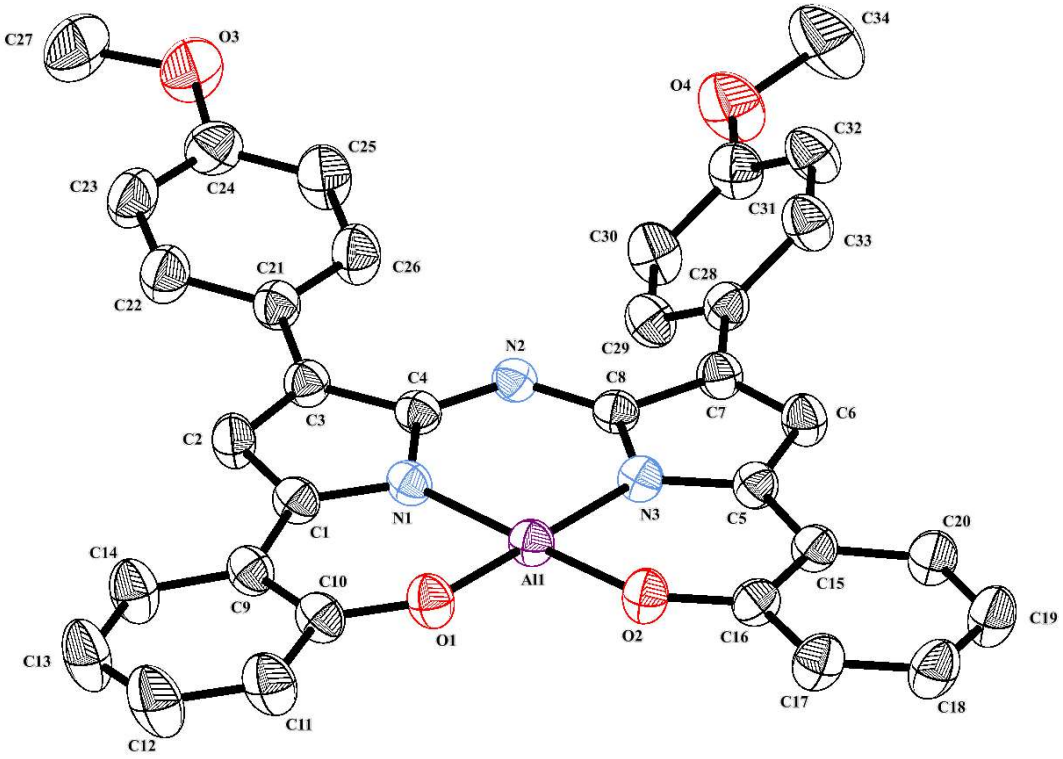



**Figure S19**. Single crystal X-ray diffraction structure of **2b**; ellipsoids are drawn at the 40% probability level. Axial bound pyridine ligands and hydrogen atoms omitted for clarity.

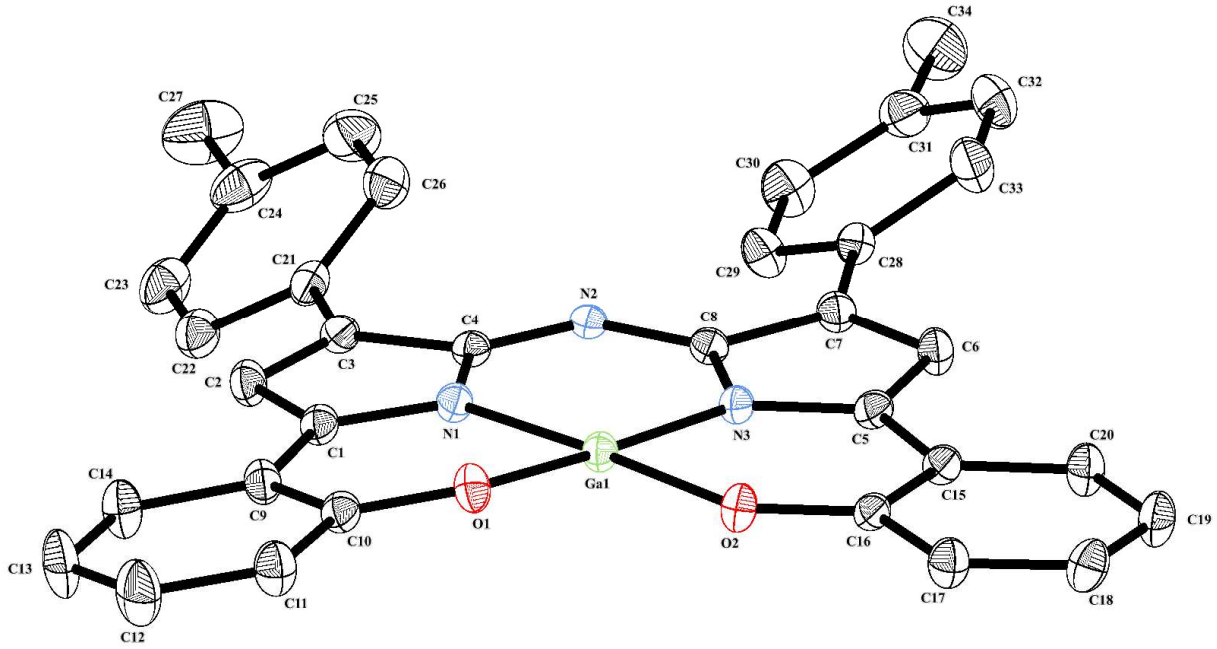



**Figure S20**. Single crystal X-ray diffraction structure of **3a**; ellipsoids are drawn at the 40% probability level. Axial bound pyridine ligands and hydrogen atoms omitted for clarity.

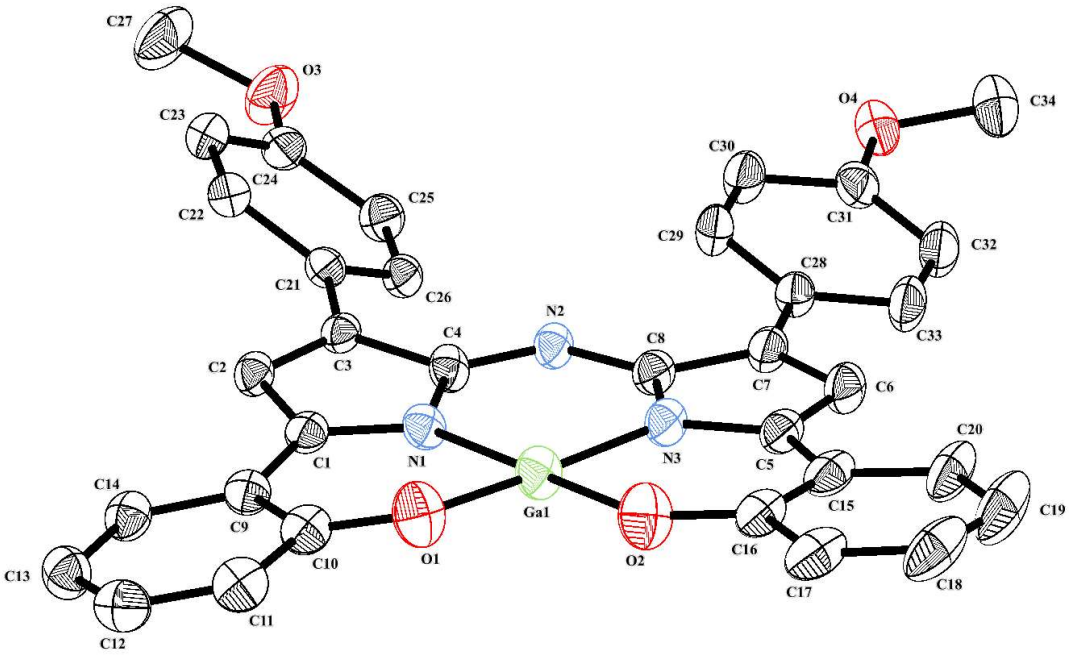



**Figure S21**. Single crystal X-ray diffraction structure of **3b**; ellipsoids are drawn at the 40% probability level. Axial bound pyridine ligands and hydrogen atoms omitted for clarity.

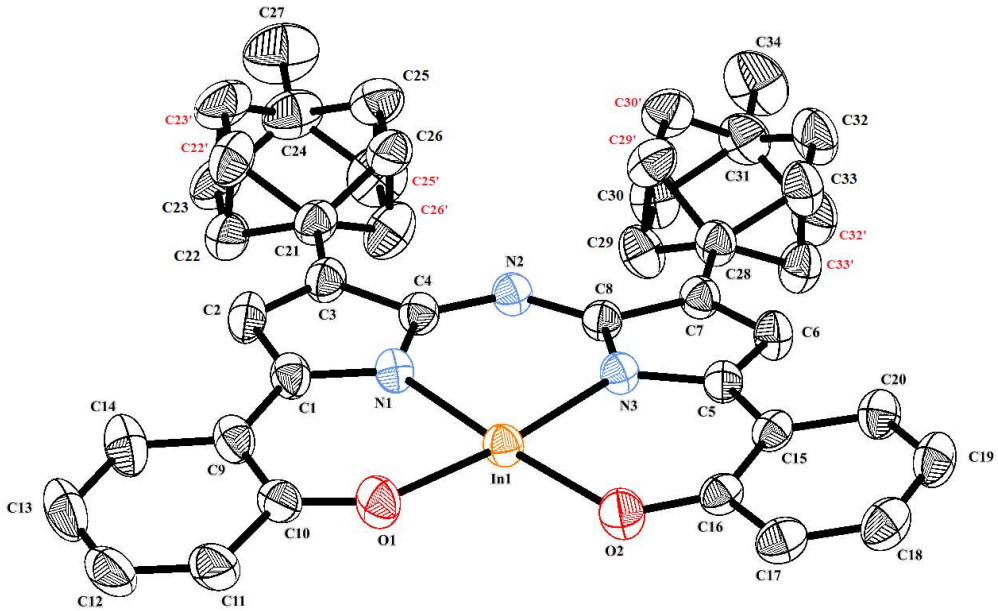



**Figure S22**. Single crystal X-ray diffraction structure of **4a**; ellipsoids are drawn at the 40% probability level. Axial bound pyridine ligands and hydrogen atoms omitted for clarity. Disordered carbon atoms on distal arenes are numbered in red.

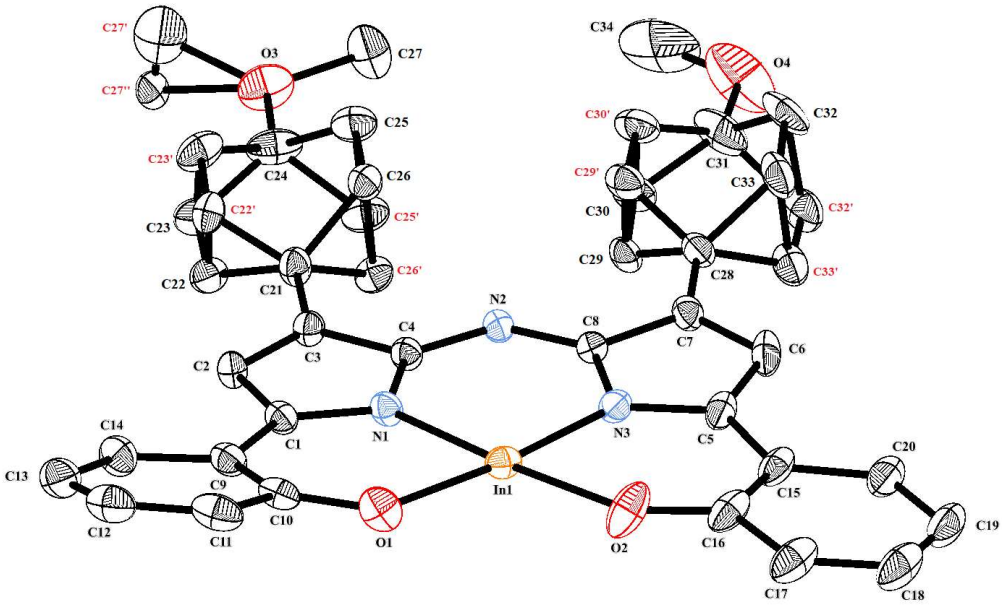



**Figure S23**. Single crystal X-ray diffraction structure of **4b**; ellipsoids are drawn at the 40% probability level. Axial bound pyridine ligands and hydrogen atoms omitted for clarity. Disordered carbon atoms on distal arenes are numbered in red.

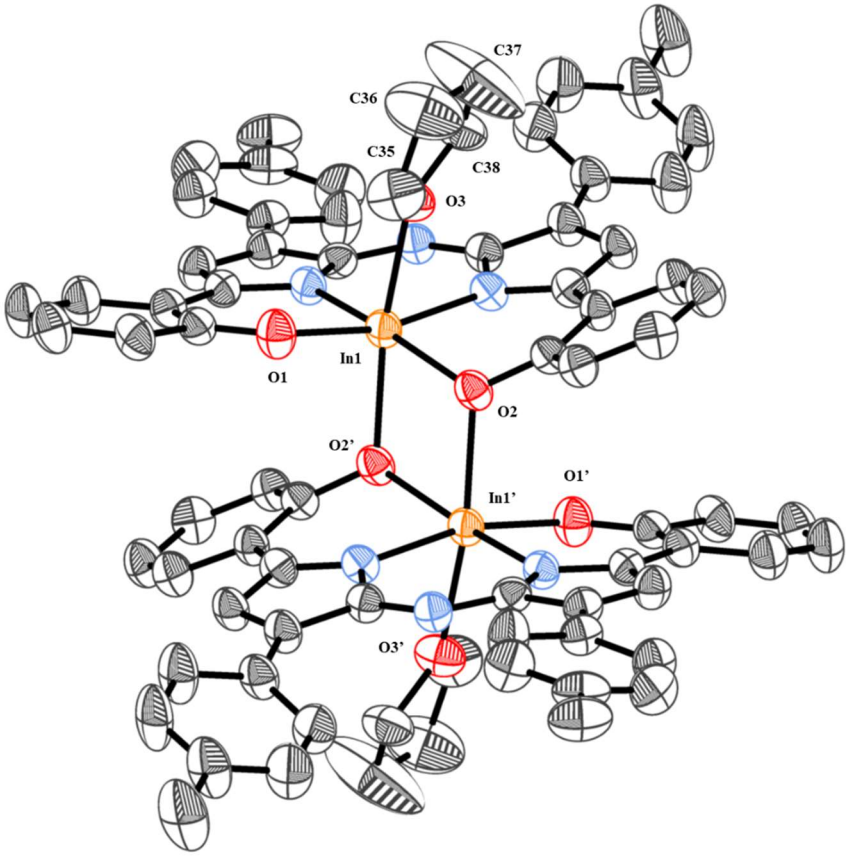



**Figure S24**. Single crystal X-ray diffraction structure of **4a'**; ellipsoids are drawn at the 40% probability level. Axial bound tetrahydrofuran ligands and hydrogen atoms omitted for clarity.

| Description | 1a (B-Me) | 2a (Al-Me) | 2b (Al-OMe) | 3a (Ga-Me) |
|---|---|---|---|---|
| **Empirical Formula** | $C_{34}H_{24}N_3O_2B$ | $C_{44}H_{34}N_5O_2Al$ | $C_{44}H_{34}N_5O_4Al$ | $C_{44}H_{34}N_5O_2Ga$ |
| **Formula Weight** | 517.37 | 691.74 | 723.74 | 734.48 |
| **Wavelength (Å)** | 0.71073 | 0.71073 | 0.71073 | 0.71073 |
| **Temperature (K)** | 293(2) | 150(2) | 293(2) | 150(2) |
| **Crystal system** | Monoclinic | Triclinic | Triclinic | Triclinic |
| **Space Group** | *C* 2/*c* | *P*-1 | *P*-1 | *P*-1 |
| **a (Å)** | 17.8773(13) | 9.5375(13) | 9.4422(3) | 9.5457(2) |
| **b (Å)** | 17.6426(12) | 13.824(2) | 13.9608(4) | 13.7422(3) |
| **c (Å)** | 16.5701(12) | 16.997(2) | 16.9362(5) | 17.0769(4) |
| **α (°)** | 90 | 71.126(2) | 105.914(2) | 71.253(2) |
| **β (°)** | 91.625(5) | 89.184(2) | 100.571(2) | 89.086(2) |
| **γ (°)** | 90 | 69.963(2) | 106.290(2) | 70.313(2) |
| **V (Å$^3$)** | 5224.1(6) | 1980.2(5) | 1977.11(11) | 1986.55(8) |
| **Z** | 8 | 2 | 2 | 2 |
| **Density (g/cm$^3$)** | 1.316 | 1.160 | 1.216 | 1.228 |
| **μ (mm$^{-1}$)** | 0.082 | 0.093 | 0.100 | 0.734 |
| **F (000)** | 2160 | 724 | 756 | 760 |
| **ϴ min., max. (°)** | 1.622, 27.908 | 2.2865, 23.8961 | 1.619, 27.407 | 1.266, 27.515 |
| **Crystal size (mm)** | 0.117 x 0.145 x 0.227 | 0.09 x 0.13 x 0.22 | 0.12 x 0.13 x 0.28 | 0.08 x 0.08 x 0.30 |
| **Index ranges** | -23 < h < 23;<br>-22 < k < 23;<br>-21 < l < 21 | -12 < h < 12;<br>-17 < k < 17;<br>-22 < l < 22 | -12 < h < 12;<br>-18 < k < 18;<br>-21 < l < 21 | -12 < h < 12;<br>-17 < k < 17;<br>-22 < l < 22 |
| **Reflections collected** | 35641 | 19176 | 27131 | 26145 |
| **$R_{int}$ (%)** | 0.0317 | 0.0432 | 0.0420 | 0.0382 |
| **Data/restraints/parameters** | 6163/0/364 | 9025/0/471 | 8924/0/489 | 9069/0/471 |
| **Goodness-of-fit on F$^2$** | 1.036 | 0.999 | 1.024 | 1.053 |
| **$R_1$ [I > 2σ(I)]** | 0.0441 | 0.0476 | 0.0485 | 0.0378 |
| **$wR_2$ [I > 2σ(I)]** | 0.1226 | 0.1245 | 0.1480 | 0.0930 |
| **Largest diff. peak/hole (e Å$^{-3}$)** | 0.285 and -0.225 | 0.263 and -0.255 | 0.211 and -0.328 | 0.470 and -0.572 |
| **Observed data [I > 2.0σ(I)]** | 4163 | 5574 | 5045 | 7000 |

**Table S3**. Crystallographic data and refinement parameters for **1a**, **2a-b** and **3a-b.**

| Description | 3b (Ga-OMe) | 4a (In-Me) | 4b (In-OMe) | 4a' (In-Me-Dimer) |
|---|---|---|---|---|
| **Empirical Formula** | $C_{44}$ $H_{34}$ $N_5$ $O_4$ Ga | $C_{44}$ $H_{34}$ $N_5$ $O_2$ In | $C_{44}$ $H_{34}$ $N_5$ $O_4$ In | $C_{76}$ $H_{64}$ $N_6$ $O_6$ $In_2$ |
| **Formula Weight** | 766.48 | 779.58 | 811.58 | 1386.97 |
| **Wavelength (Å)** | 0.71073 | 0.71073 | 0.71073 | 0.71073 |
| **Temperature (K)** | 215(2) | 293(2) | 150(2) | 293(2) |
| **Crystal system** | Orthorhombic | Triclinic | Triclinic | Triclinic |
| **Space Group** | *Fdd*2 | *P*-1 | *P*-1 | *P*-1 |
| **a (Å)** | 20.9391(10) | 9.7402(16) | 9.7573(4) | 8.7943(8) |
| **b (Å)** | 25.3066(13) | 9.9876(16) | 9.8180(4) | 11.7579(10) |
| **c (Å)** | 29.4364(15) | 19.774(3) | 19.3367(9) | 14.8580(13) |
| **α (°)** | 90 | 104.509(8) | 103.7920(10) | 98.225(6) |
| **β (°)** | 90 | 100.981(8) | 98.2980(10) | 90.613(6) |
| **γ (°)** | 90 | 96.196(9) | 95.5750(10) | 90.271(6) |
| **V (Å$^3$)** | 15598.3(14) | 1803.5(5) | 1763.40(13) | 1520.4(2) |
| **Z** | 16 | 2 | 2 | 1 |
| **Density (g/cm$^3$)** | 1.306 | 1.436 | 1.528 | 1.515 |
| **μ (mm$^{-1}$)** | 0.754 | 0.701 | 0.724 | 0.821 |
| **F (000)** | 6336 | 796 | 828 | 708 |
| **ϴ min., max. (°)** | 2.123, 27.526 | 2.111, 27.749 | 2.129, 27.489 | 1.750, 28.332 |
| **Crystal size (mm)** | 0.26 x 0.26 x 0.28 | 0.08 x 0.24 x 0.55 | 0.07 x 0.19 x 0.24 | 0.038 x 0.082 x 0.085 |
| **Index ranges** | -27 < h < 27;<br>-32 < k < 32;<br>-38 < l < 38 | -12 < h < 12;<br>-13 < k < 12;<br>-25 < l < 25 | -14 < h < 14;<br>-15 < k < 15;<br>-29 < l < 29 | -11 < h < 11;<br>-15 < k < 15;<br>-19 < l < 19 |
| **Reflections collected** | 36867 | 23828 | 17040 | 20853 |
| **$R_{int}$ (%)** | 0.0494 | 0.0247 | 0.0266 | 0.0781 |
| **Data/restraints/parameters** | 8973/1/490 | 8295/0/544 | 8022/1/631 | 7503/0/409 |
| **Goodness-of-fit on F$^2$** | 1.020 | 1.038 | 1.032 | 0.934 |
| **$R_1$ [I > 2σ(I)]** | 0.0359 | 0.0268 | 0.0295 | 0.0529 |
| **w$R_2$ [I > 2σ(I)]** | 0.0816 | 0.0721 | 0.0732 | 0.1379 |
| **Largest diff. peak/hole (e Å$^{-3}$)** | 0.215 and -0.304 | 0.520 and -0.297 | 0.700 and -0.605 | 0.763 and -0.865 |
| **Observed data [I > 2.0σ(I)]** | 7160 | 7473 | 7290 | 4065 |

**Table S4.** Crystallographic data and refinement parameters for **3b**, **4a-b** and **4a'**.

| Compound | Planarity of M Center (°) | | | | |
|---|---|---|---|---|---|
| | N1-M-N3 | N1-M-O1 | O1-M-O2 | N3-M-O2 | Planarity vs 360° |
| 1a (B-Me) | 103.41(11) | 106.91(11) | 107.20(11) | 106.18(11) | 63.70 |
| 2a (Al-Me) | 88.44(6) | 91.70(6) | 89.23(6) | 90.74(6) | 0.13 |
| 2b (Al-OMe) | 88.72(7) | 91.16(7) | 89.45(7) | 90.66(7) | 0.02 |
| 3a (Ga-Me) | 88.97(6) | 91.89(6) | 88.10(6) | 91.18(6) | 0.16 |
| 3b (Ga-OMe) | 88.71(11) | 92.01(12) | 86.65(12) | 92.59(12) | -0.04 |
| 4a (In-Me) | 85.47(6) | 87.32(6) | 99.75(6) | 87.53(6) | 0.09 |
| 4b (In-OMe) | 85.84(6) | 86.75(6) | 99.81(7) | 87.60(7) | 0.03 |
| 4a' (In-Me-Dimer) | 86.64(3) | 87.73(5) | 102.66(4) | 85.20(1) | 2.24 |

**Table S5**. Crystallographic structure bond angles of metal center in **1a**, **2a-b, 3a-b, 4a-b**, and **4a'**.

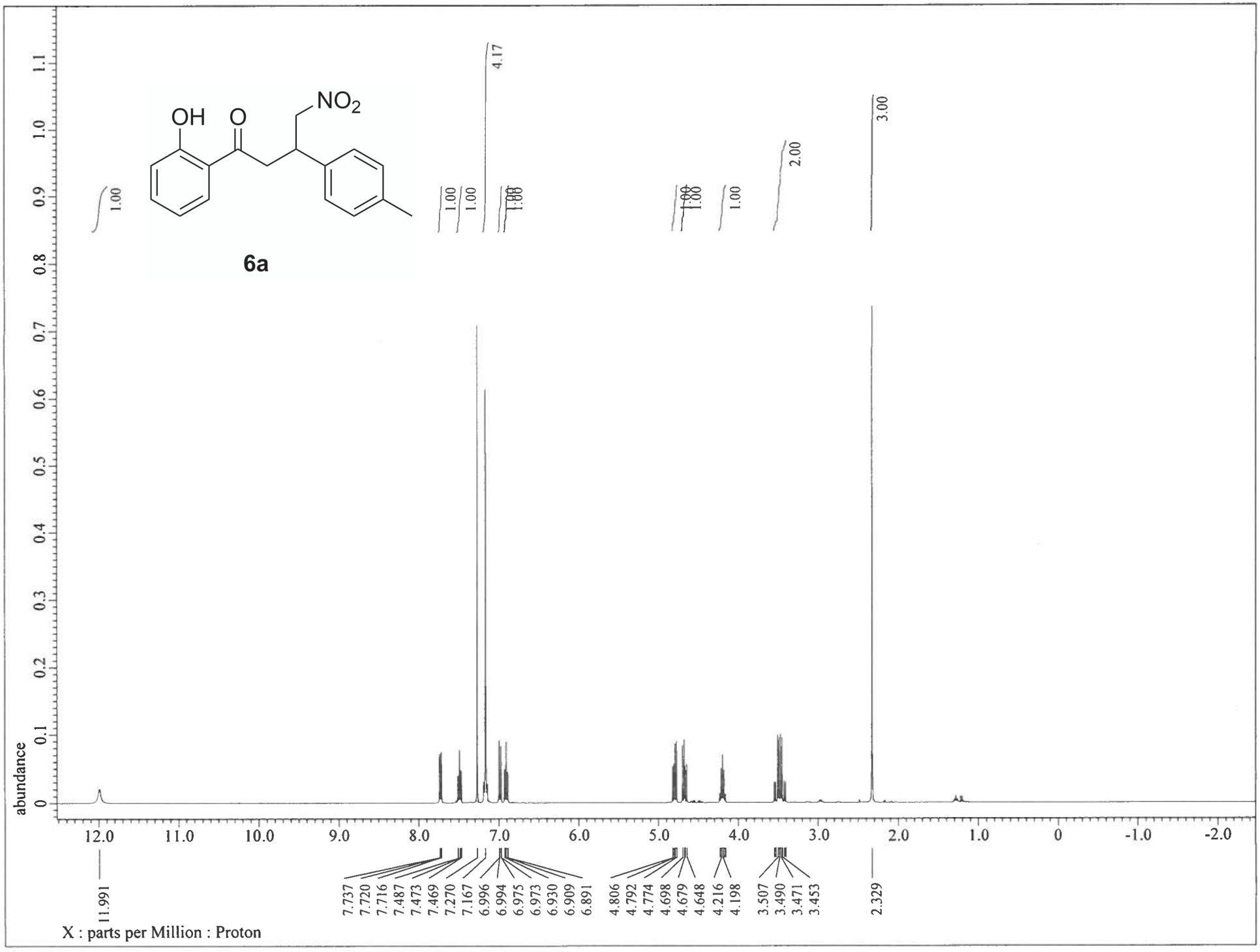
| Compound | Axial Pyridine Ligands (°) | Proximal Dihedral Angles (°) | | Phenolic Puckering (°) |
|---|---|---|---|---|
| | N4-M-N5 | C2-C1-C9-C14 | C6-C5-C15-C20 | O1-N1-N3-O2 |
| 1a (B-Me) | -- | -22.23(9) | -24.41(4) | -66.02(5) |
| 2a (Al-Me) | 176.55(7) | 4.44(5) | -3.62(1) | 3.31(8) |
| 2b (Al-OMe) | 179.07(7) | 5.20(1) | -5.11(7) | -0.23(4) |
| 3a (Ga-Me) | 175.39(6) | 4.35(5) | -3.32(8) | 3.84(1) |
| 3b (Ga-OMe) | 175.3(3) | 12.18(2) | 0.51(1) | 1.31(8) |
| 4a (In-Me) | 171.50(9) | 1.34(1) | 12.69(9) | 2.89(6) |
| 4b (In-OMe) | 170.26(8) | 2.17(4) | -8.81(5) | 0.88(3) |
| 4a' (In-Me-Dimer) | 163.81(12)* | -5.23(9) | 6.05(6) | 17.44(3) |

*Axial THF ligands measured through O3(THF)-In1-O2'.

**Table S6**. Crystallographic structure axial ligand angles and dihedral angles of phenolic puckering in **1a**, **2a-b, 3a-b, 4a-b**, and **4a'**.

## References


1. G. Zhang, C. B. Musgrave, *J. Phys. Chem. A*, 2007, **111**, 1554-1561.
2. P. Ziegler, *Bruker TopSpin 3.2 User Manual,* 2013, 112-131.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O
NO2
6a
abundance
X : parts per Million : Proton
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7.737
7.720
7.716
7.487
7.473
7.469
7.270
7.167
6.996
6.994
6.975
6.973
6.930
6.909
6.891
4.806
4.792
4.774
4.698
4.679
4.648
4.216
4.198
3.507
3.490
3.471
3.453
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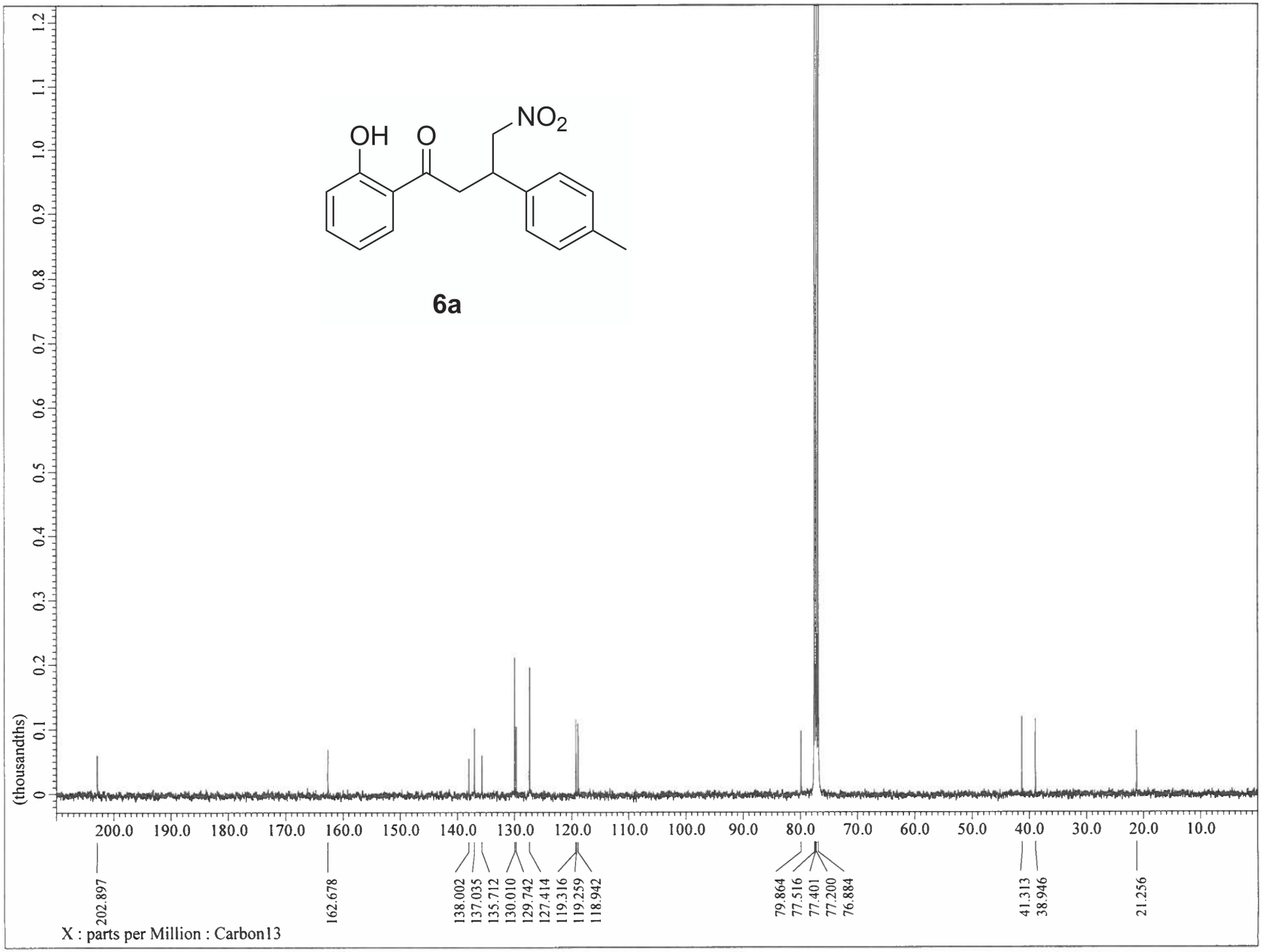
1.00
1.00
1.00
4.17
1.00
1.00
1.00
2.00
3.00


OH
O
NO2
6a
(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
202.897
162.678
138.002
137.035
135.712
130.010
129.742
127.414
119.316
119.259
118.942
79.864
77.516
77.401
77.200
76.884
41.313
38.946
21.256
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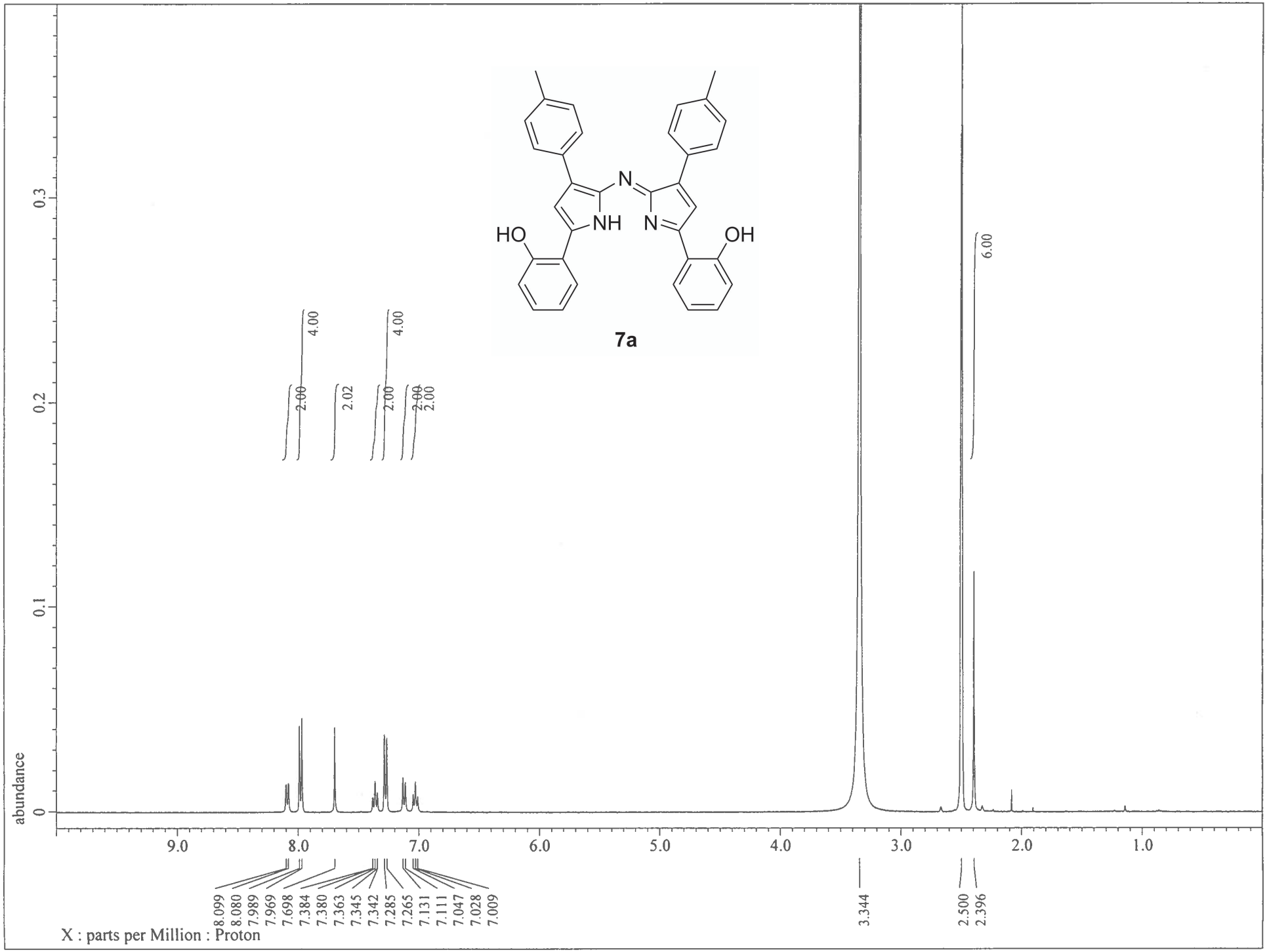
HO
NH
N
N
OH
7a
4.00
2.00
2.02
4.00
2.00
2.00
2.00
6.00
abundance
0
0.1
0.2
0.3
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.099
8.080
7.989
7.969
7.698
7.384
7.380
7.363
7.345
7.342
7.285
7.265
7.131
7.111
7.047
7.028
7.009
3.344
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2.396
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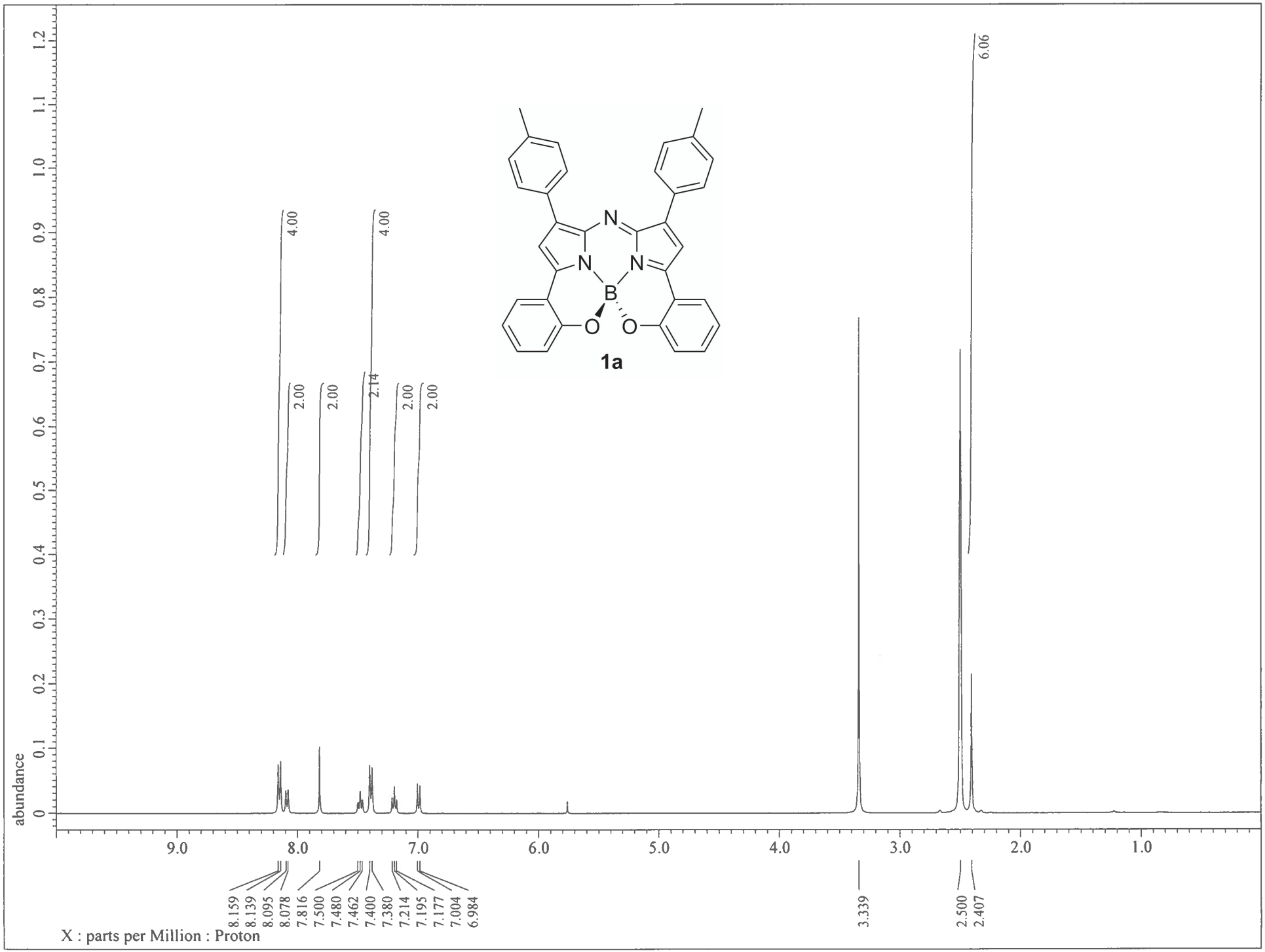
abundance
X : parts per Million : Proton
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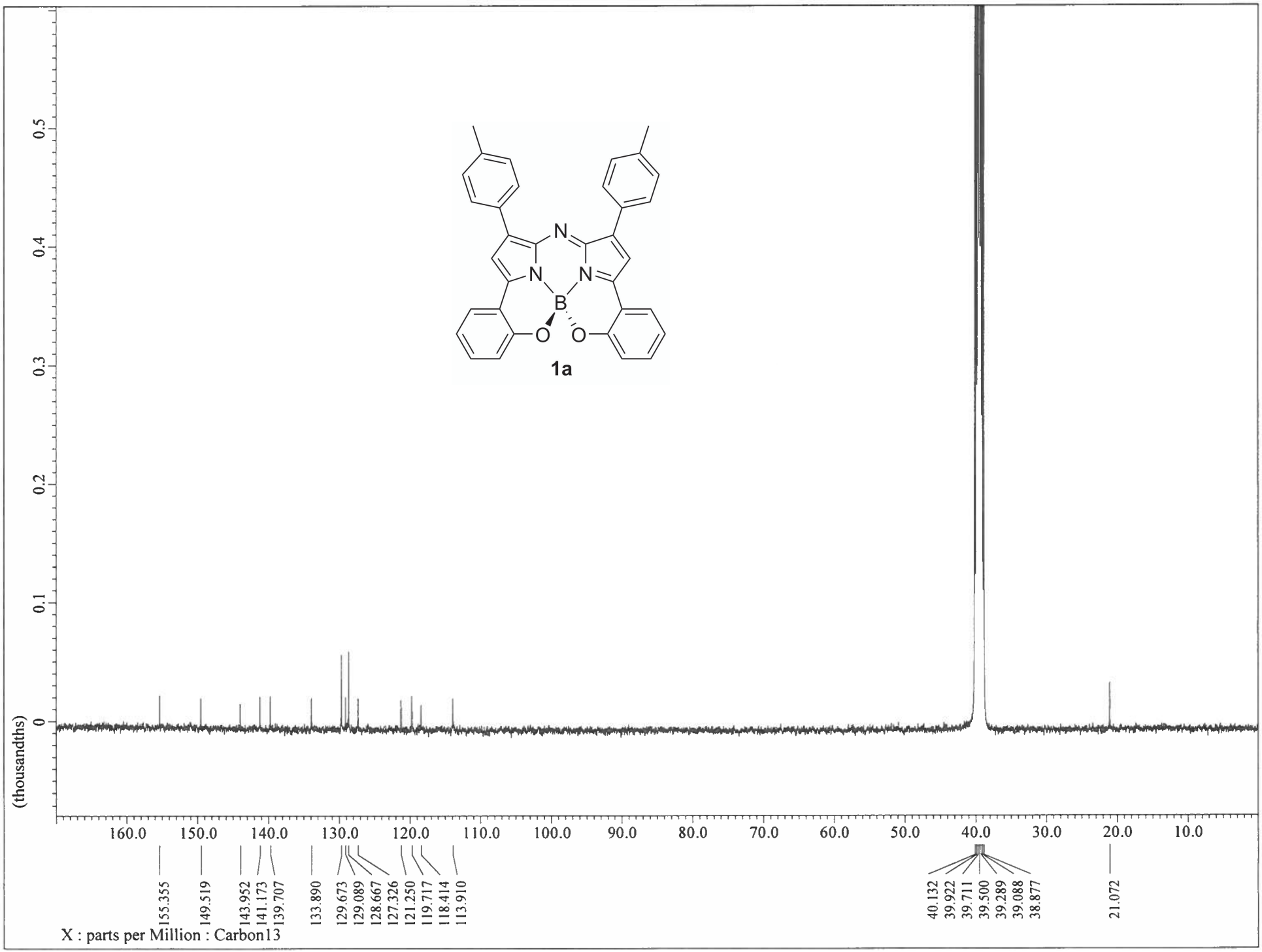
2.00
2.00
2.14
4.00
2.00
2.00
6.06
8.159
8.139
8.095
8.078
7.816
7.500
7.480
7.462
7.400
7.380
7.214
7.195
7.177
7.004
6.984
3.339
2.500
2.407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(thousandths)
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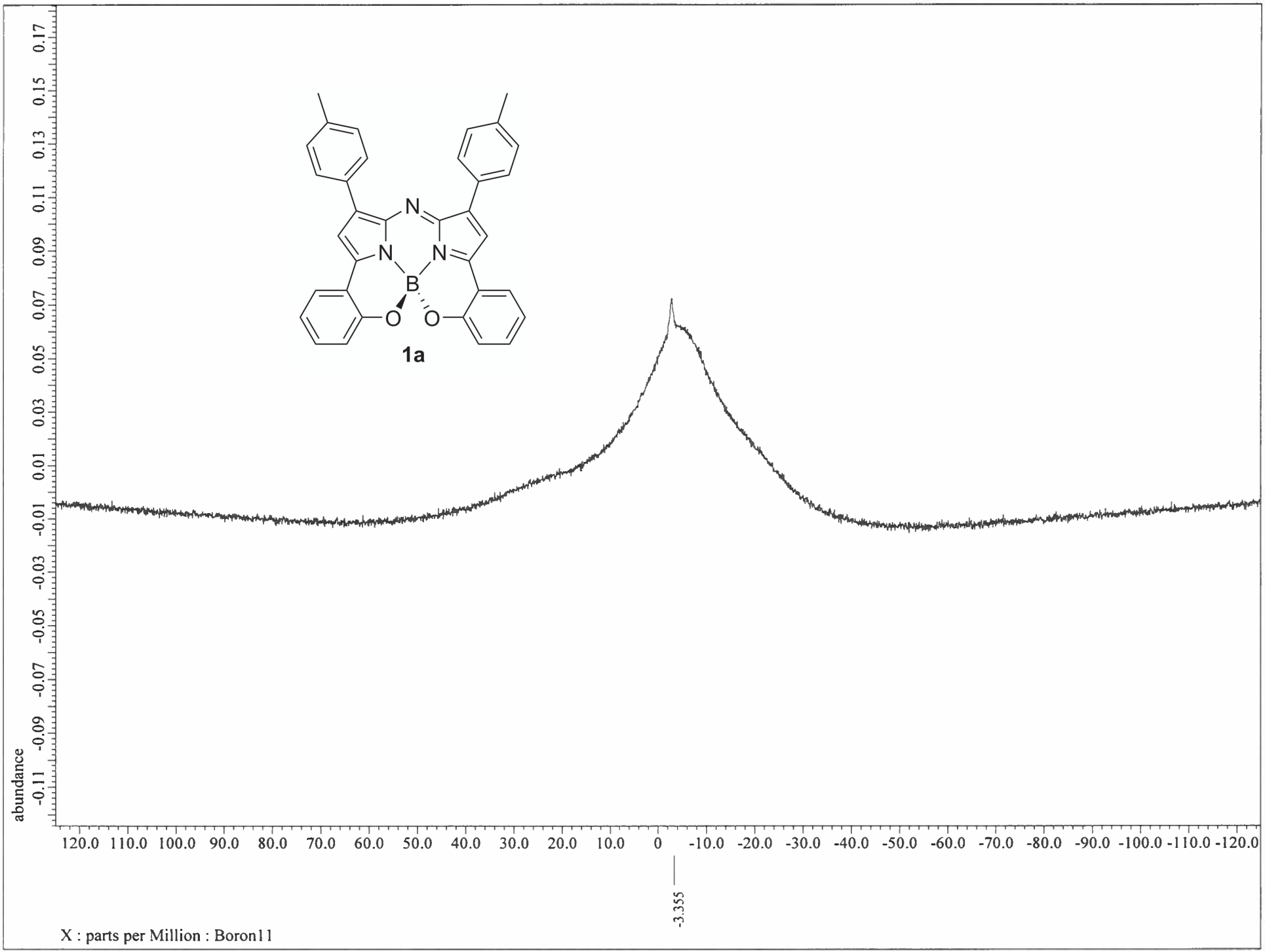
0.4
0.3
0.2
0.1
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
155.355
149.519
143.952
141.173
139.707
133.890
129.673
129.089
128.667
127.326
121.250
119.717
118.414
113.910
40.132
39.922
39.711
39.500
39.289
39.088
38.877
21.072
X : parts per Million : Carbon13


1a
abundance
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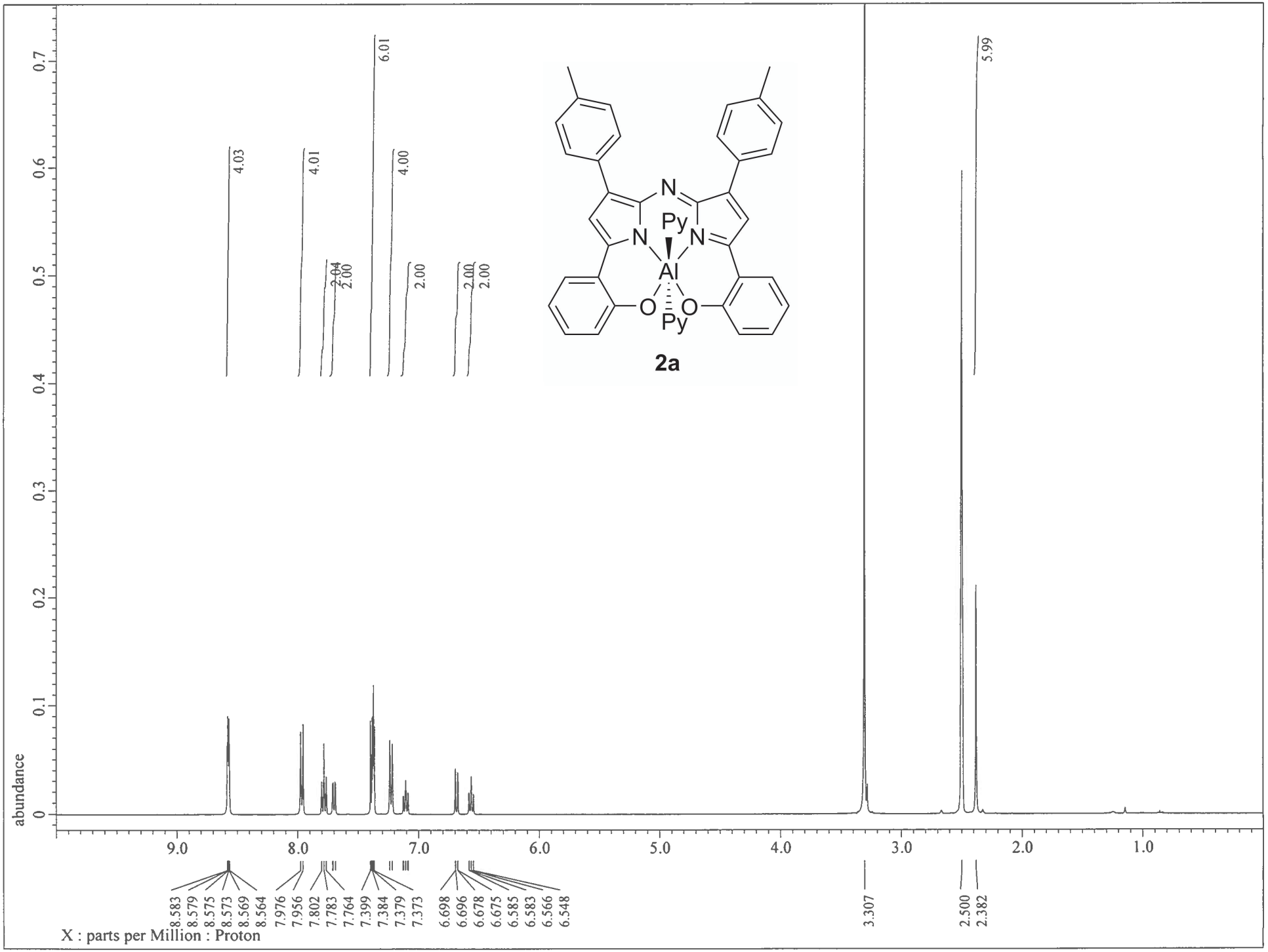
0.15
0.13
0.11
0.09
0.07
0.05
0.03
0.01
-0.01
-0.03
-0.05
-0.07
-0.09
-0.11
120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0
-3.355
X : parts per Million : Boron11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2.04
2.00
6.01
4.00
2.00
2.00
2.00
5.99
N
Py
N
N
Al
O
O
Py
2a
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.583
8.579
8.575
8.573
8.569
8.564
7.976
7.956
7.802
7.783
7.764
7.399
7.384
7.379
7.373
6.698
6.696
6.678
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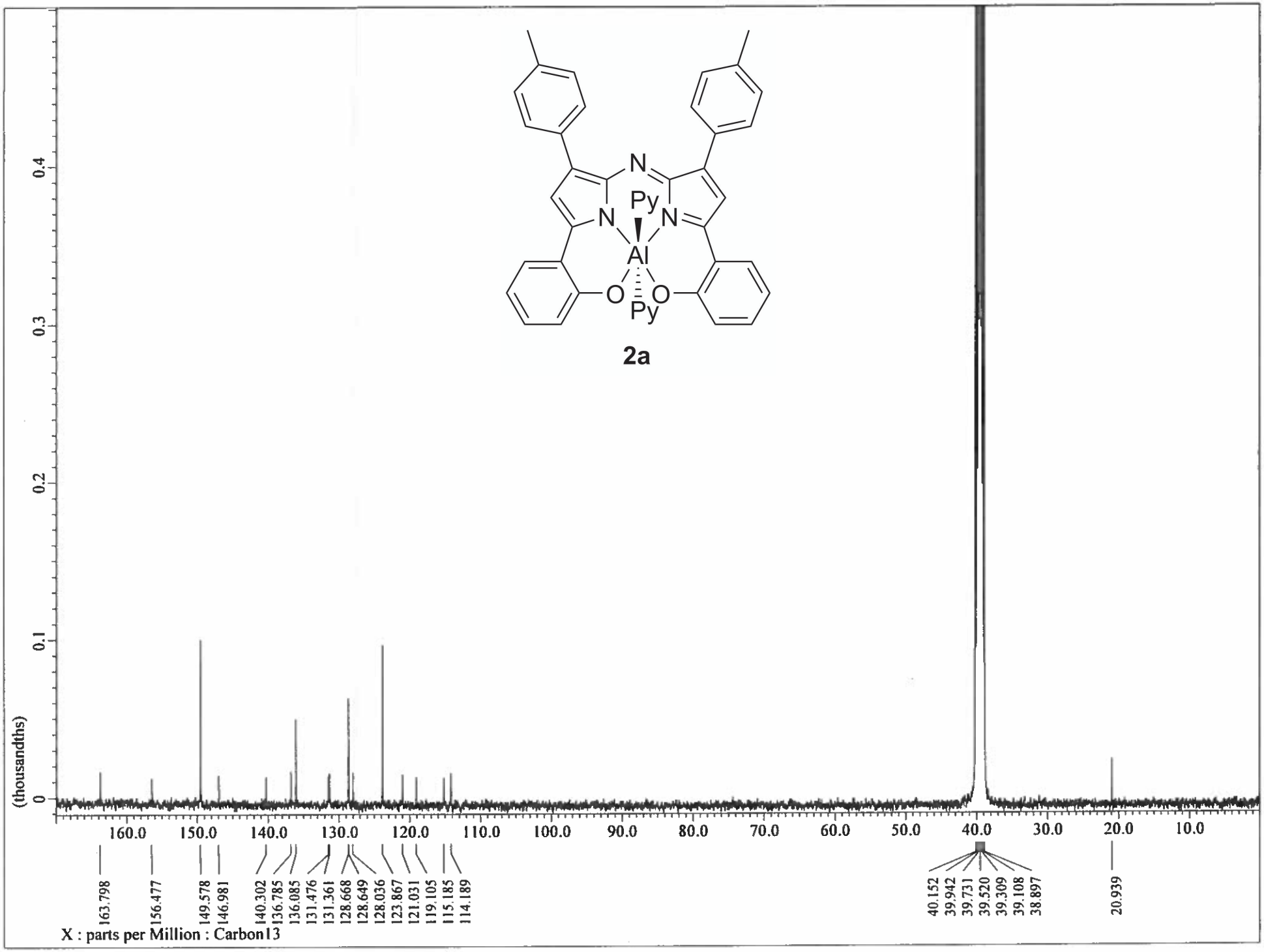
6.585
6.583
6.566
6.548
3.307
2.500
2.382
X : parts per Million : Proton


N
Py
N
N
Al
O
O
Py
2a
(thousandths)
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0.1
0.2
0.3
0.4
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
163.798
156.477
149.578
146.981
140.302
136.785
136.085
131.476
131.361
128.668
128.649
128.036
123.867
121.031
119.105
115.185
114.189
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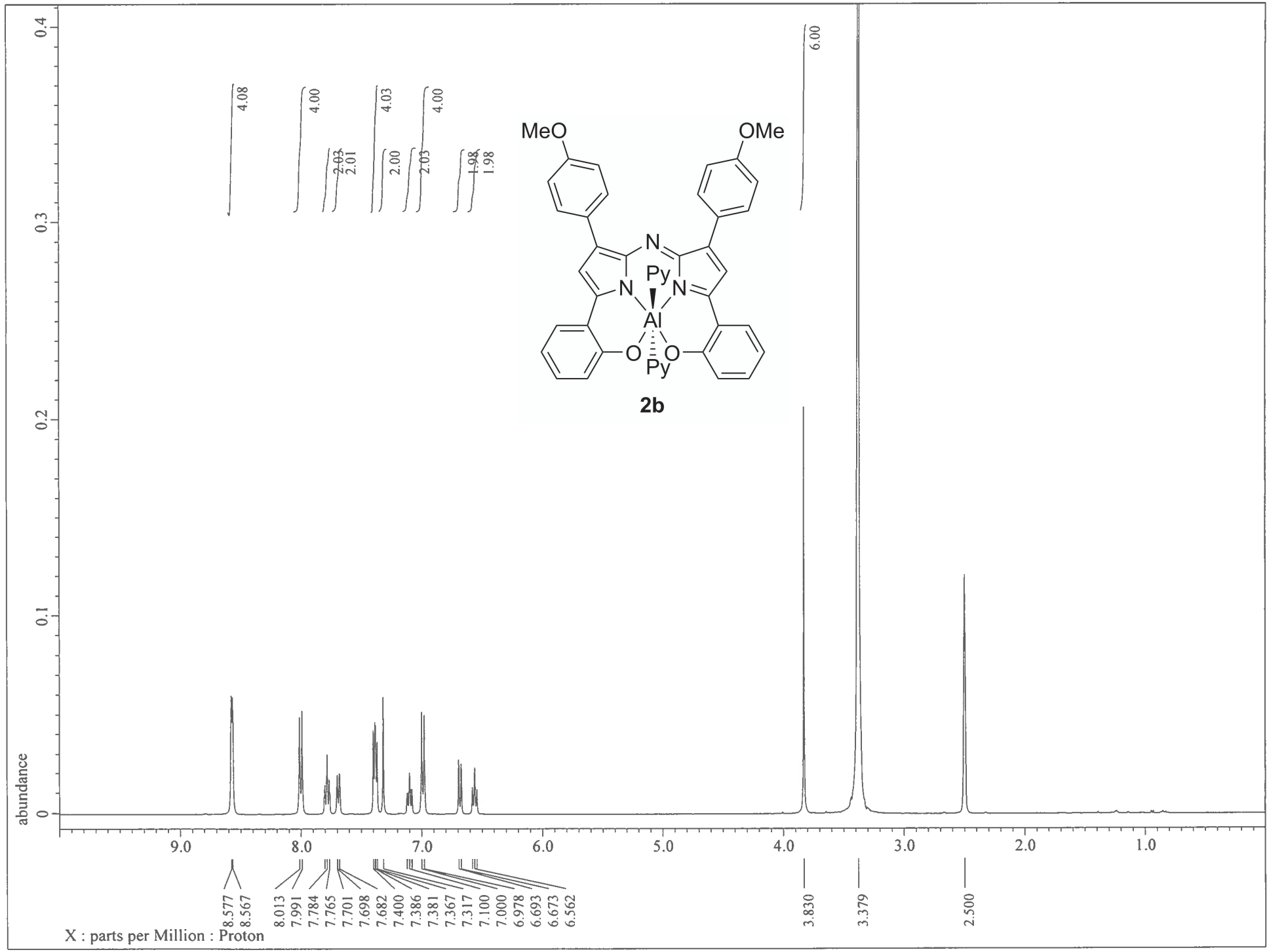
39.309
39.108
38.897
20.939
X : parts per Million : Carbon13


MeO
OMe
N
Py
N
N
Al
O
O
Py
2b
4.08
4.00
2.03
2.01
4.03
2.00
4.00
2.03
1.98
1.98
6.00
abundance
0
0.1
0.2
0.3
0.4
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.577
8.567
8.013
7.991
7.784
7.765
7.701
7.698
7.682
7.400
7.386
7.381
7.367
7.317
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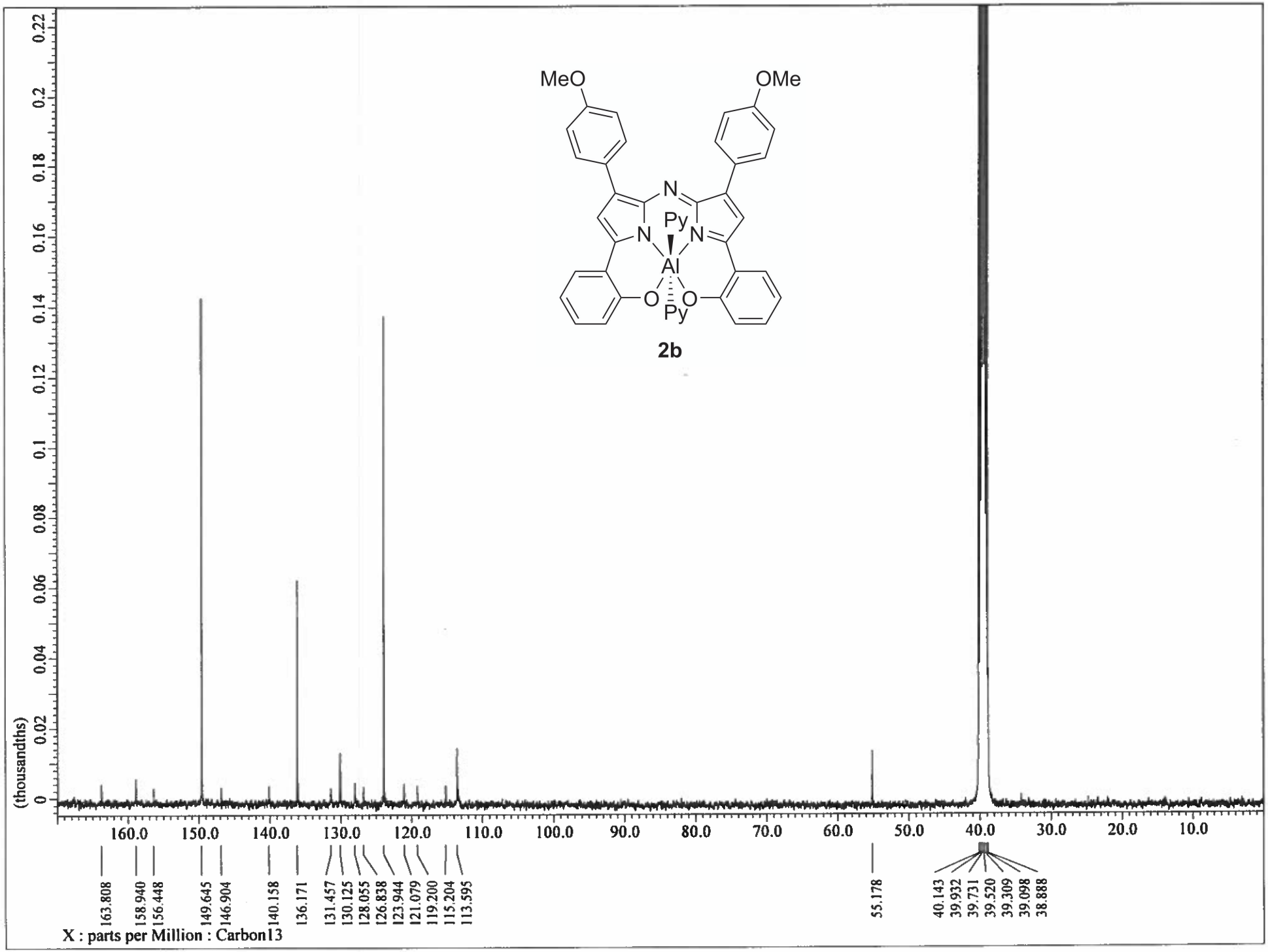
6.673
6.562
3.830
3.379
2.500
X : parts per Million : Proton


MeO
OMe
N
Py
N
N
Al
O
O
Py
2b
(thousandths)
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0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
163.808
158.940
156.448
149.645
146.904
140.158
136.171
131.457
130.125
128.055
126.838
123.944
121.079
119.200
115.204
113.595
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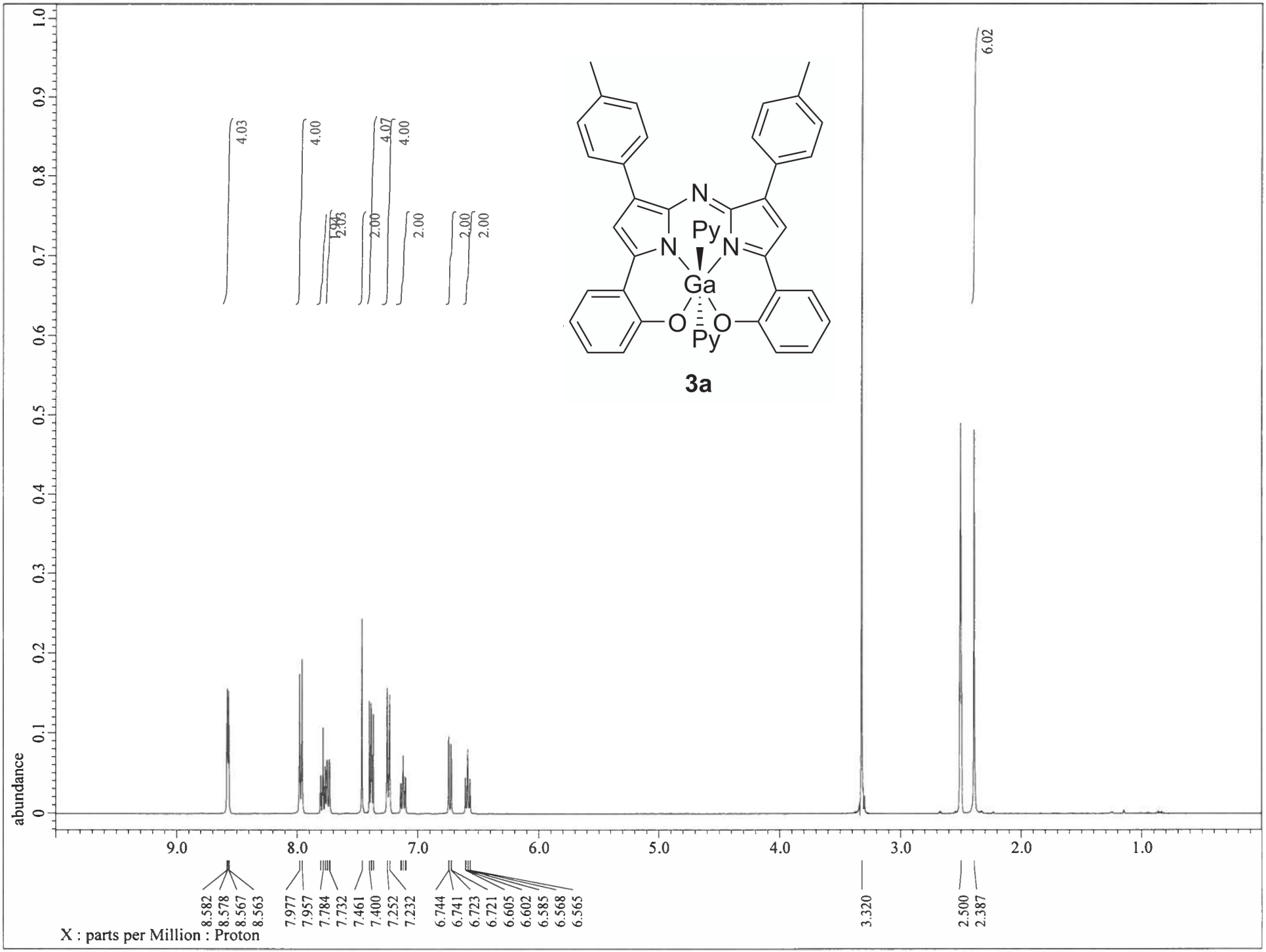
40.143
39.932
39.731
39.520
39.309
39.098
38.888
X : parts per Million : Carbon13


abundance
X : parts per Million : Proton
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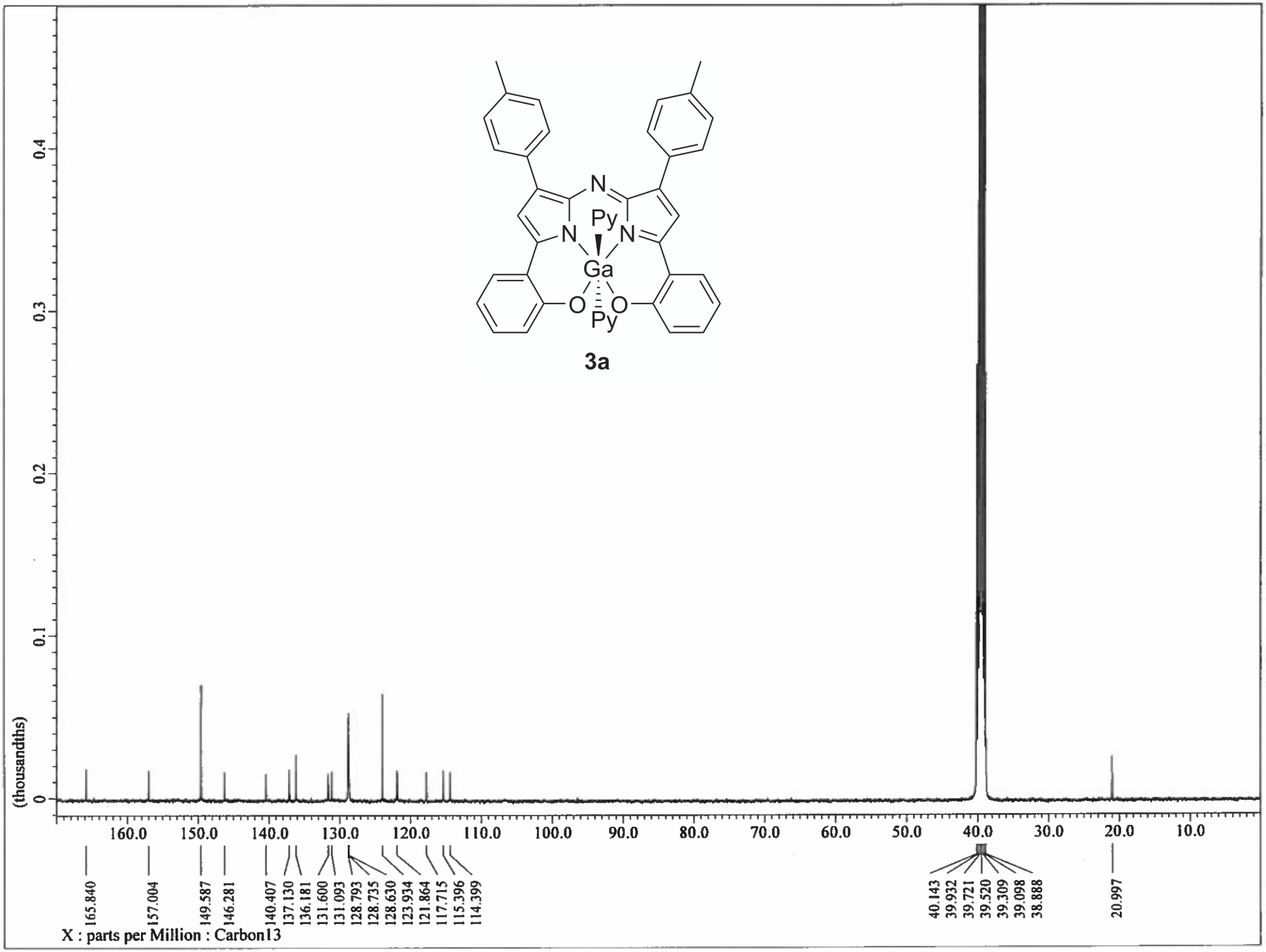
4.00
1.98
2.03
2.00
4.07
4.00
2.00
2.00
2.00
6.02
N
Py
N
N
Ga
O
O
Py
3a
8.582
8.578
8.567
8.563
7.977
7.957
7.784
7.732
7.461
7.400
7.252
7.232
6.744
6.741
6.723
6.721
6.605
6.602
6.585
6.568
6.565
3.320
2.500
2.387


N
Py
N
N
Ga
O
O
Py
3a
(thousandths)
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0.1
0.2
0.3
0.4
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
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157.004
149.587
146.281
140.407
137.130
136.181
131.600
131.093
128.793
128.735
128.630
123.934
121.864
117.715
115.396
114.399
40.143
39.932
39.721
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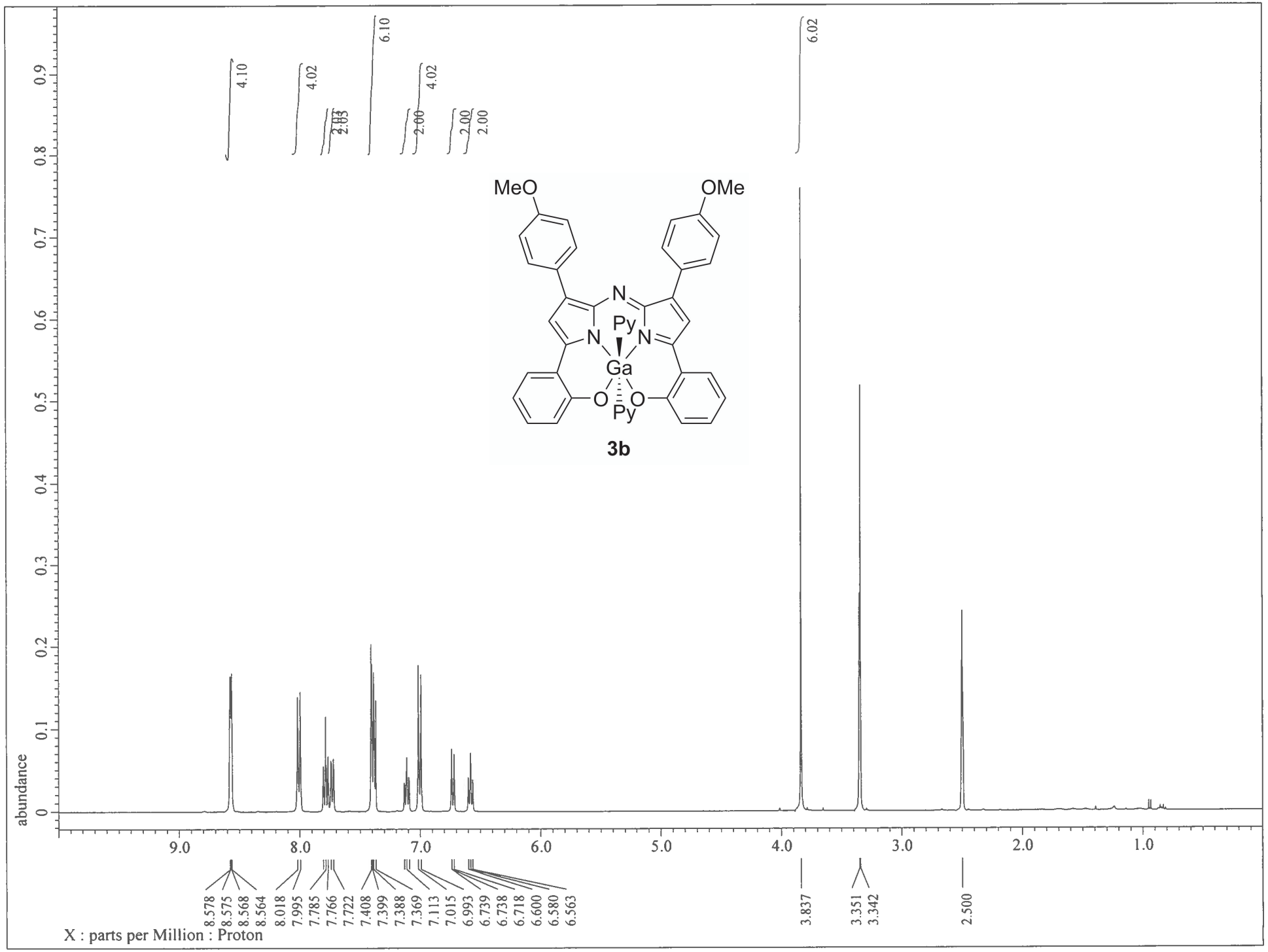
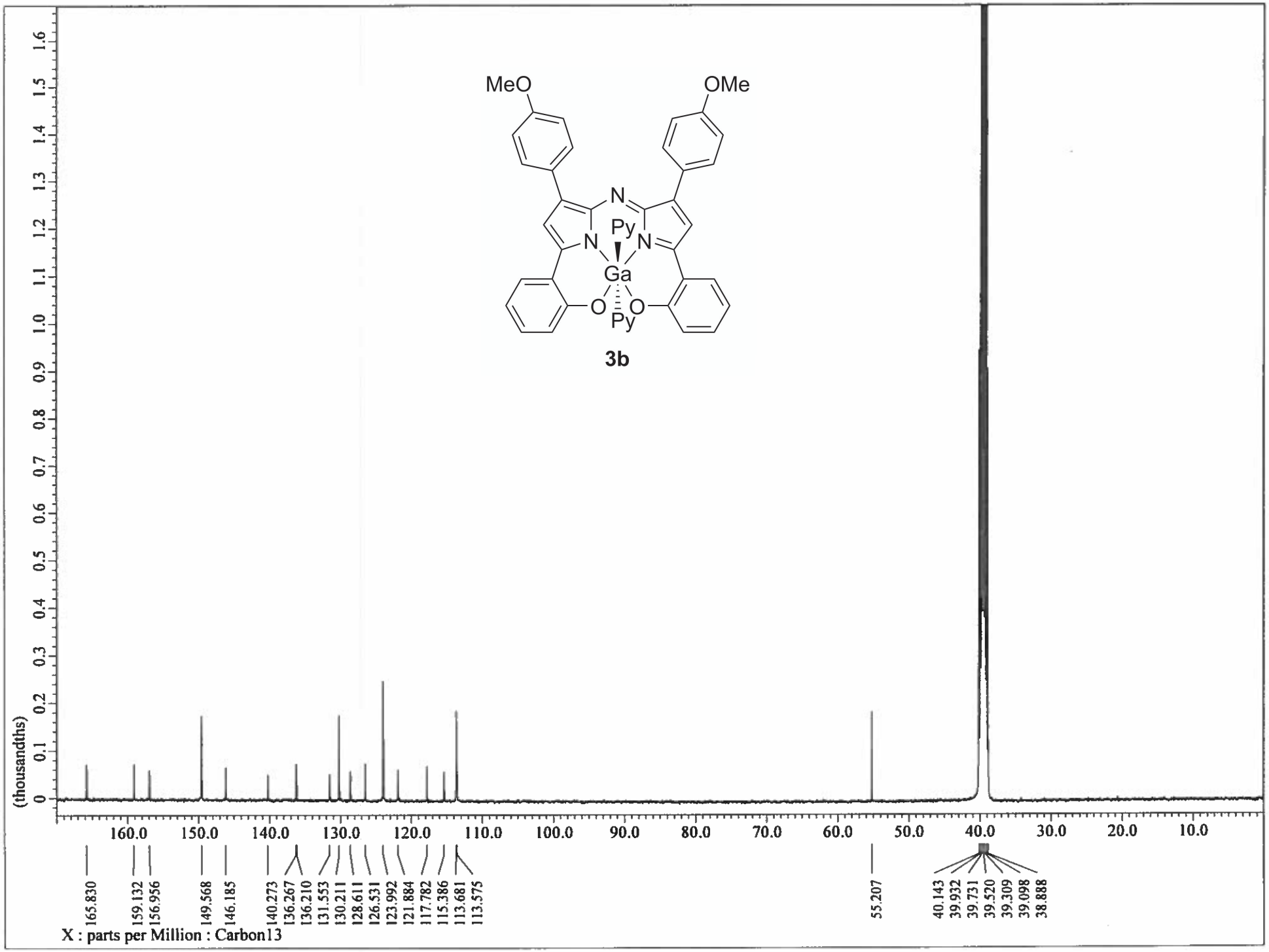
39.309
39.098
38.888
20.997
X : parts per Million : Carbon13


MeO
OMe
N
Py
N
N
Ga
O
O
Py
3b
4.10
4.02
2.03
6.10
2.00
4.02
2.00
2.00
6.02
abundance
X : parts per Million : Proton
8.578
8.575
8.568
8.564
8.018
7.995
7.785
7.766
7.722
7.408
7.399
7.388
7.369
7.113
7.015
6.993
6.739
6.738
6.718
6.600
6.580
6.563
3.837
3.351
3.342
2.500


MeO
OMe
N
Py
N
N
Ga
O
O
Py
3b
(thousandths)
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0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
165.830
159.132
156.956
149.568
146.185
140.273
136.267
136.210
131.553
130.211
128.611
126.531
123.992
121.884
117.782
115.386
113.681
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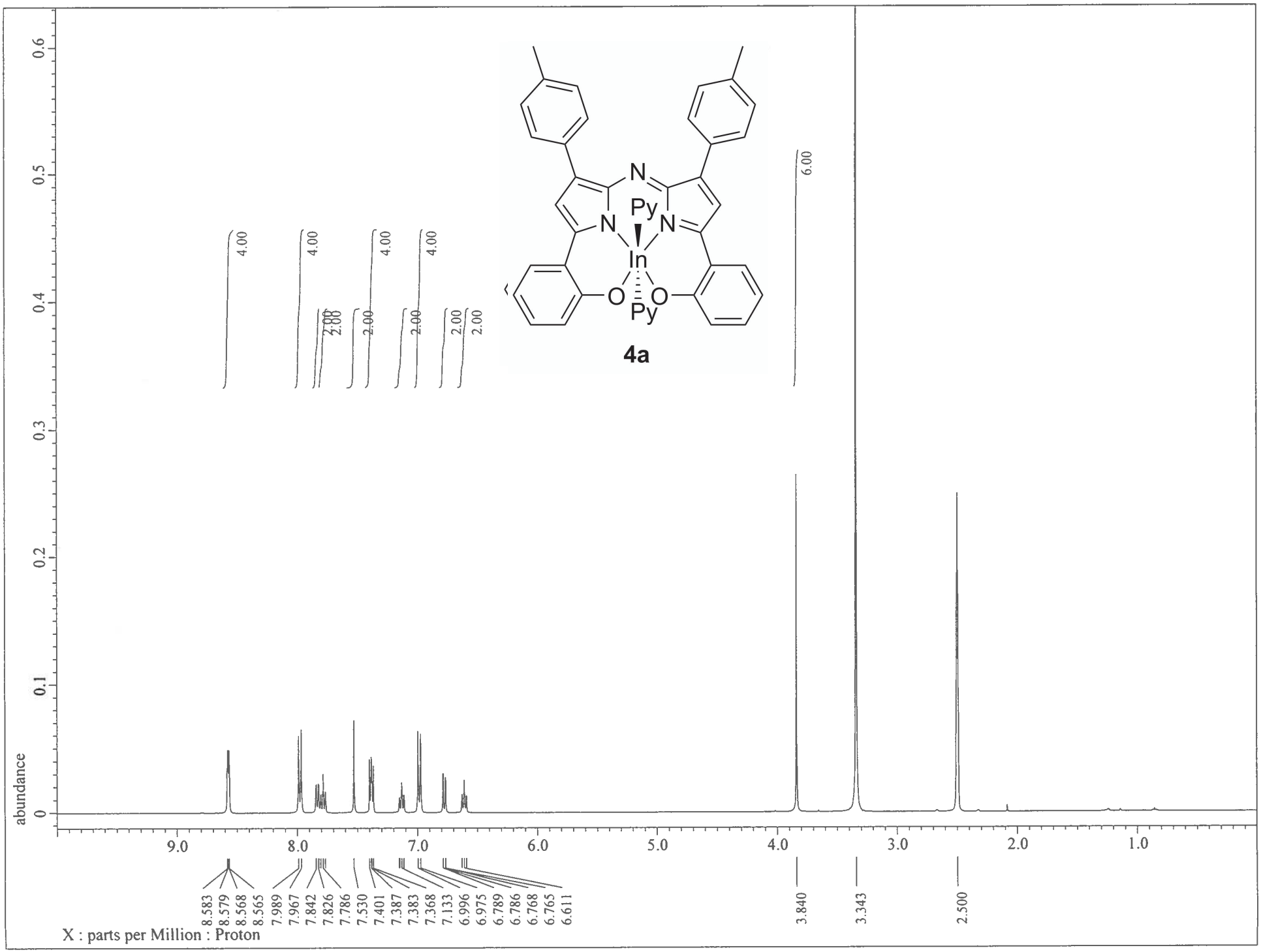
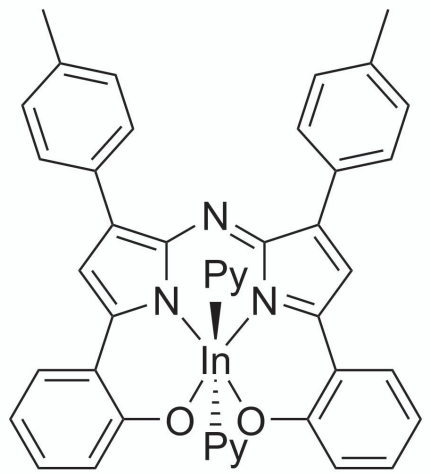
40.143
39.932
39.731
39.520
39.309
39.098
38.888
X : parts per Million : Carbon13


4.00
4.00
2.00
2.00
2.00
2.00
2.00
2.00
6.00
N
Py
N
N
In
O
O
Py
4a
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.583
8.579
8.568
8.565
7.989
7.967
7.842
7.826
7.786
7.530
7.401
7.387
7.383
7.368
7.133
6.996
6.975
6.789
6.786
6.768
6.765
6.611
3.840
3.343
2.500
X : parts per Million : Proton




**4a**

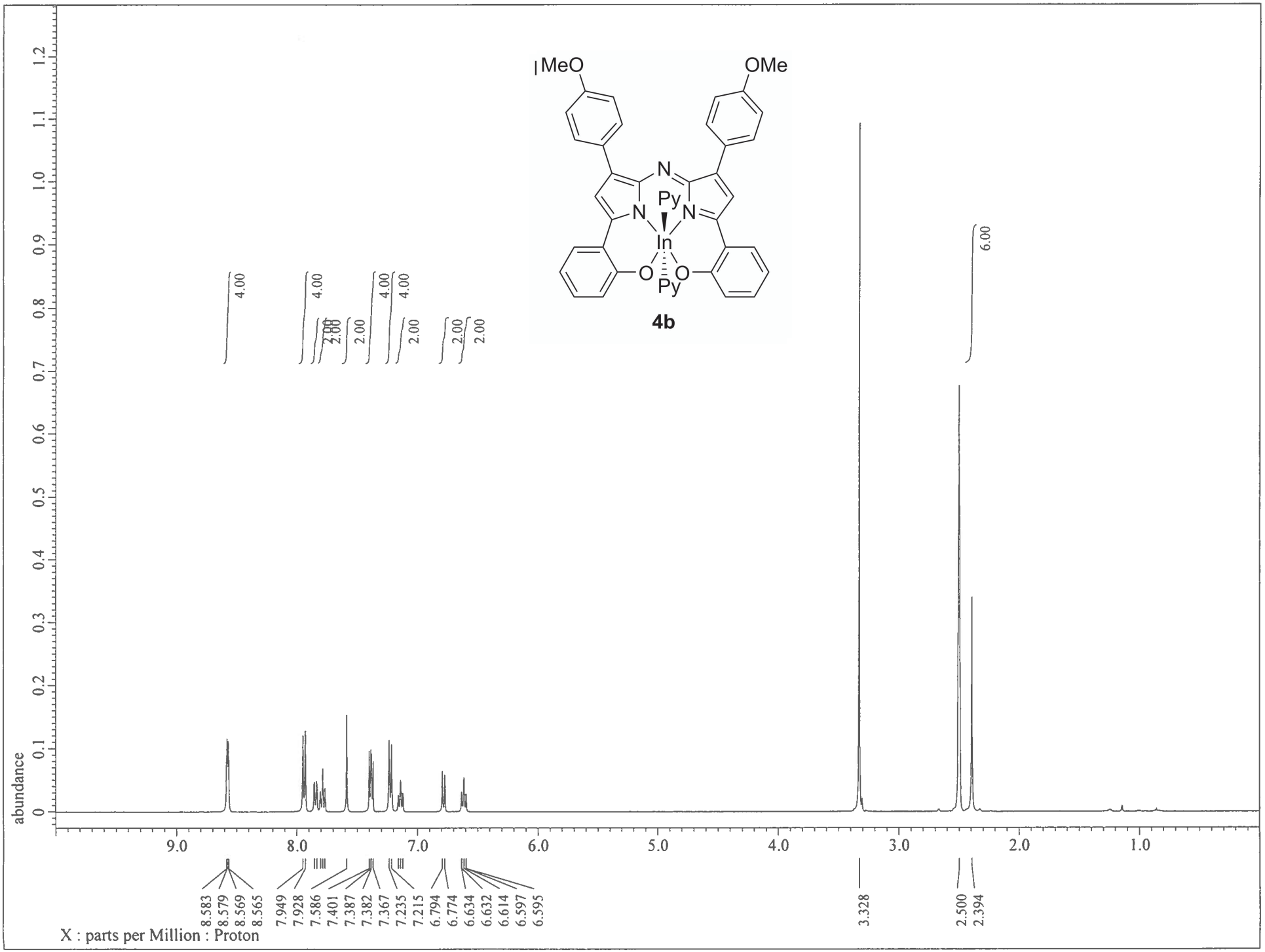
(thousandths)

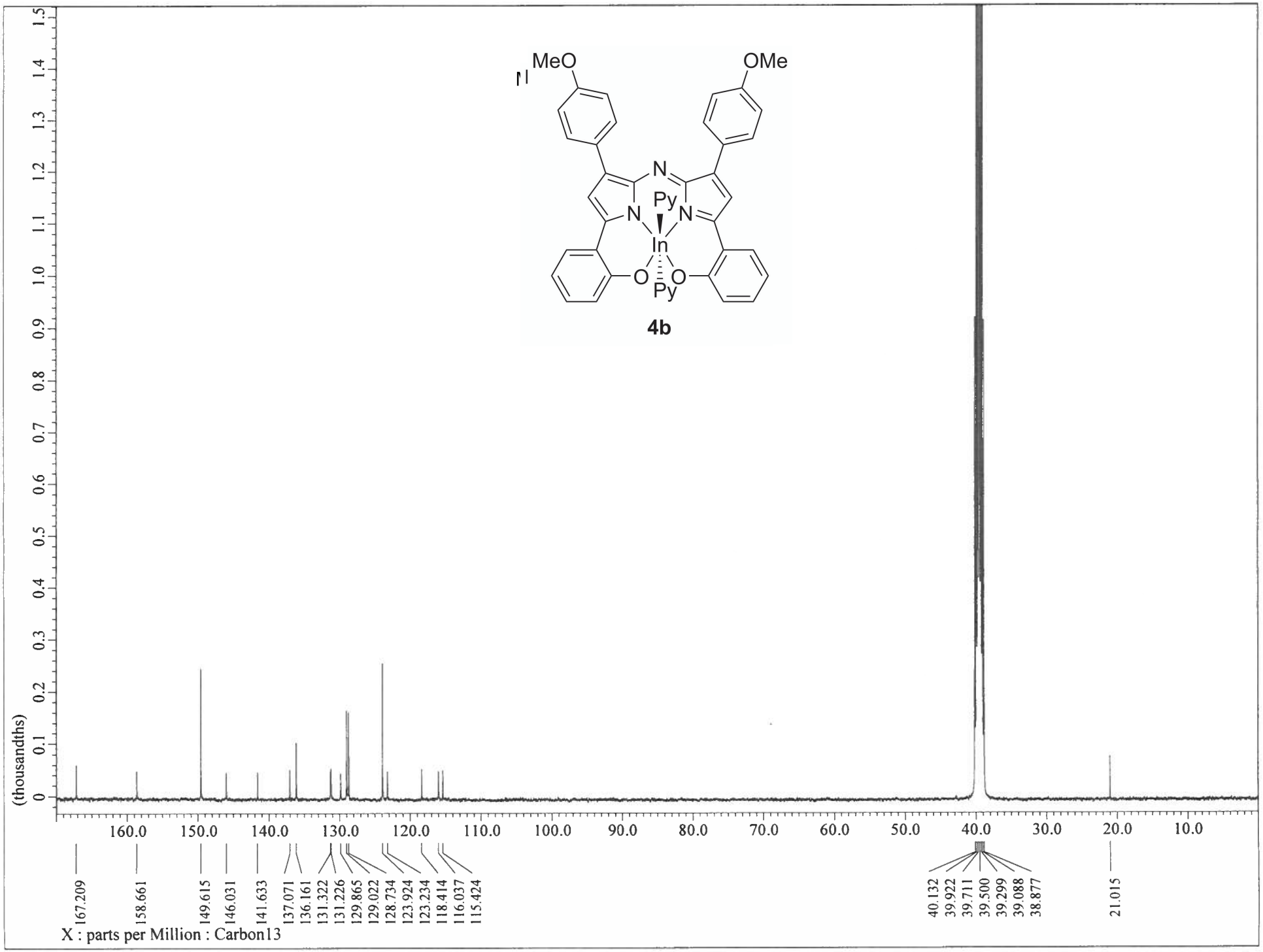
0.3
0.2
0.1
0

160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0

167.171
159.073
158.575
149.625
145.916
141.441
136.171
131.235
130.469
129.817
126.665
123.933
123.234
118.471
115.386
115.175
113.603
55.187
40.132
39.922
39.711
39.500
39.289
39.088
38.877

X : parts per Million : Carbon13


MeO
OMe
N
Py
N
N
In
O
O
Py
4b
4.00
4.00
2.00
2.00
4.00
4.00
2.00
2.00
2.00
6.00
abundance
X : parts per Million : Proton
8.583
8.579
8.569
8.565
7.949
7.928
7.586
7.401
7.387
7.382
7.367
7.235
7.215
6.794
6.774
6.634
6.632
6.614
6.597
6.595
3.328
2.500
2.394


MeO
OMe
N
Py
N
N
In
O
O
Py
4b
(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
167.209
158.661
149.615
146.031
141.633
137.071
136.161
131.322
131.226
129.865
129.022
128.734
123.924
123.234
118.414
116.037
115.424
40.132
39.922
39.711
39.500
39.299
39.088
38.877
21.015
X : parts per Million : Carbon13