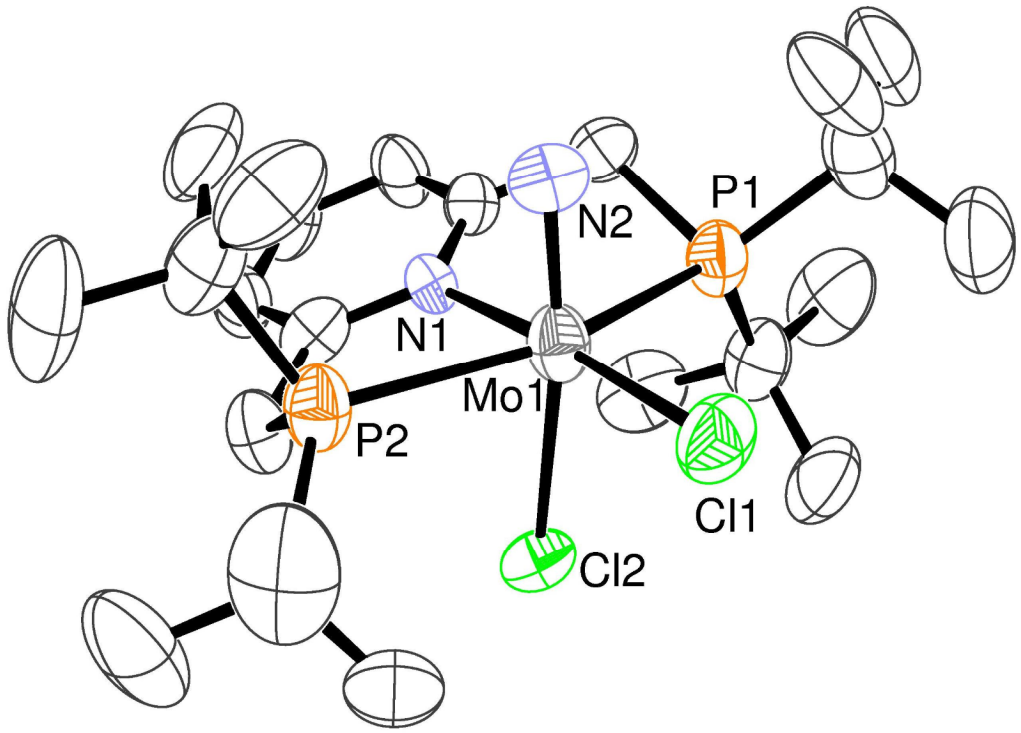
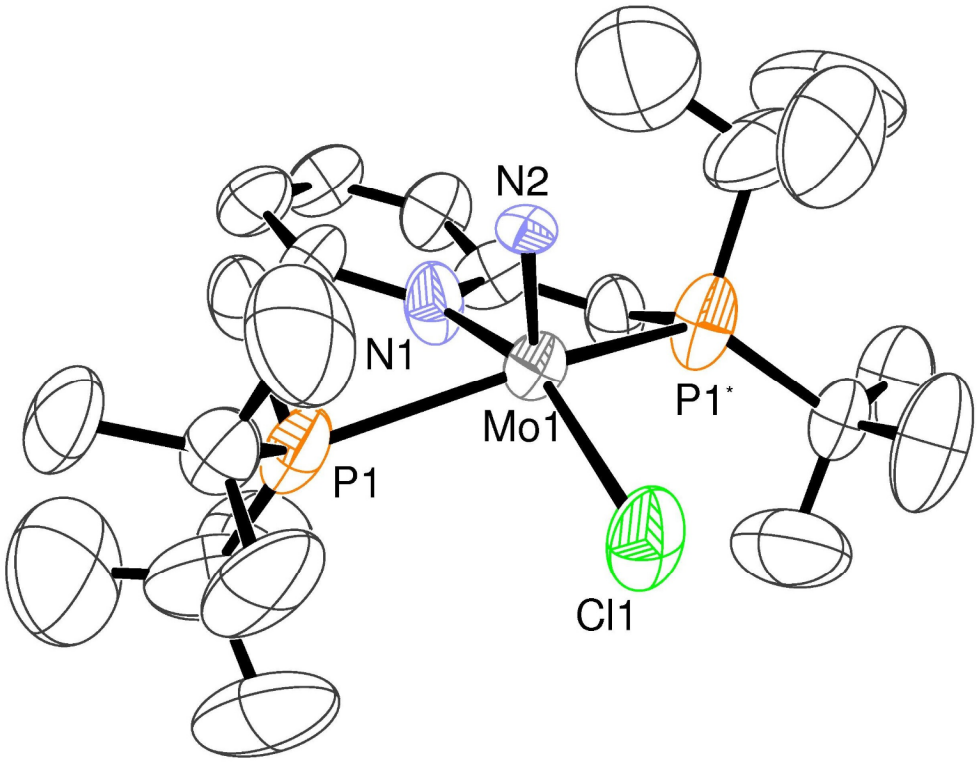
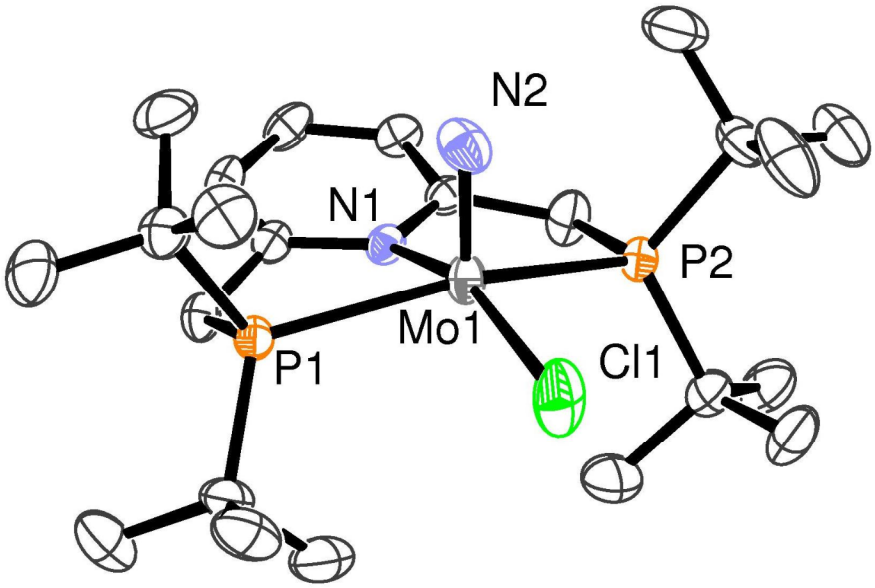


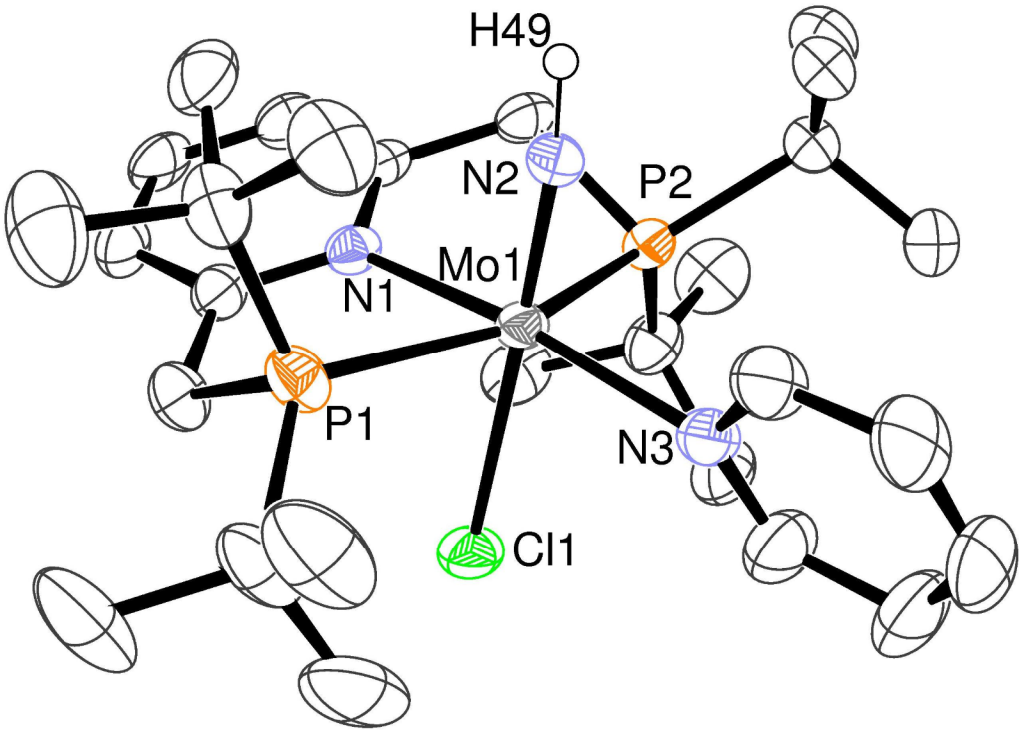

**Supplementary Figure 1 | ORTEP drawing of 2. Thermal ellipsoids are shown at the 50% probability level. One of the two crystallographically disordered molecules is shown. All hydrogen atoms are omitted for clarity.**



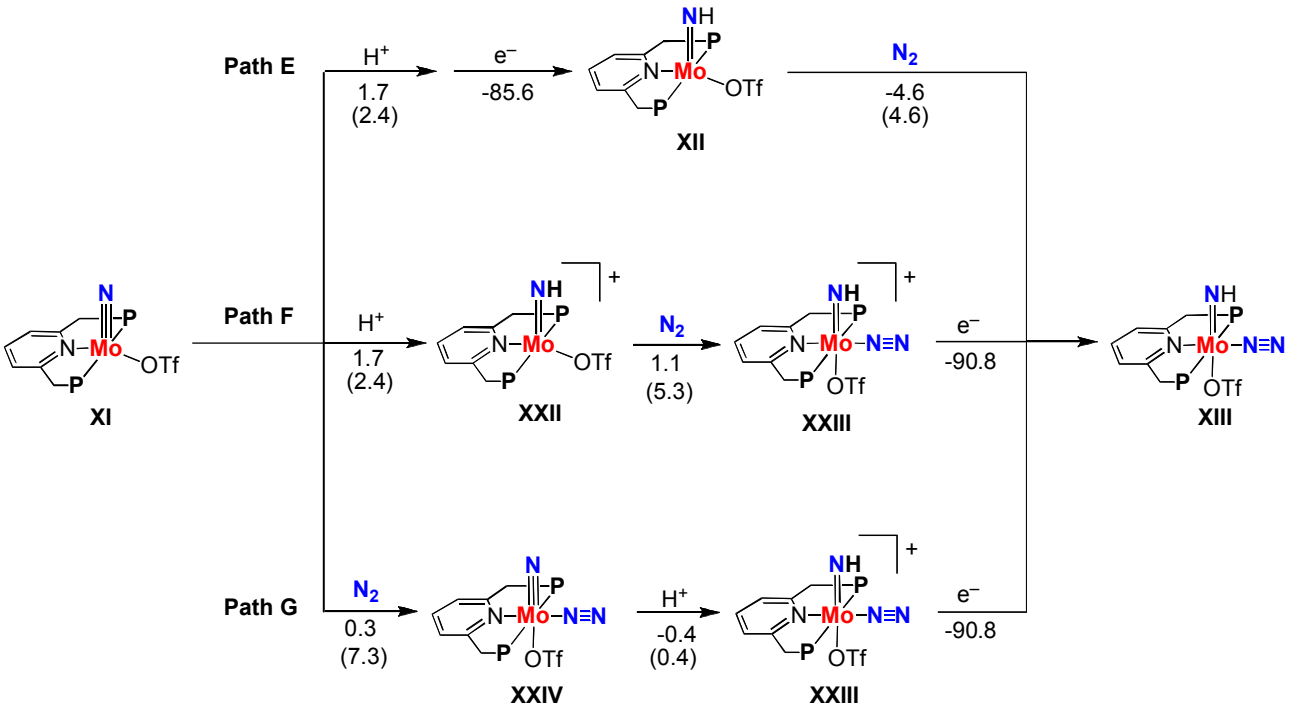

**Supplementary Figure 2 | ORTEP drawing of 3. Thermal ellipsoids are shown at the 50% probability level. One of the two crystallographically disordered molecules is shown. All hydrogen atoms are omitted for clarity.**




**Supplementary Figure 3 | ORTEP drawing of the cationic part of 4. Thermal ellipsoids are shown at the 50% probability level. All hydrogen atoms are omitted for clarity.**




**Supplementary Figure 4 | ORTEP drawing of the cationic part of 5. Thermal ellipsoids are shown at the 50% probability level. All hydrogen atoms except for H(49) are omitted for clarity.**




**Supplementary Figure 5 | Three possible reaction pathways for formation of the six-coordinate imide complex XIII. Protons and electrons are supplied by lutidinium and cobaltocene, respectively. Energy changes and activation energies (in parenthesis) for individual reaction steps were calculated at the B3LYP*/BS2 level of theory (units in kcal/mol).**

**Supplementary Table 1 | X-ray Crystallographic Data for $2\cdot 7/3C_4H_8O$ and $3\cdot 1/6C_6H_{14}$.**

| | $\mathbf{2}\cdot 7/3C_4H_8O$ | $\mathbf{3}\cdot 1/6C_6H_{14}$ |
|---|---|---|
| chemical formula | $C_{32.33}H_{61.67}Cl_2MoN_2O_{2.33}P_2$ | $C_{24}H_{44.33}ClMoN_2P_2$ |
| formula weight | 744.56 | 554.30 |
| dimensions of crystals | 0.30 × 0.20 × 0.15 | 0.35 × 0.15 × 0.15 |
| crystal system | trigonal | hexagonal |
| space group | $R\bar{3}$ | $P6_122$ |
| $a$, Å | 36.248(1) | 16.3159(5) |
| $b$, Å | 36.248(1) | 16.3159(5) |
| $c$, Å | 17.0202(5) | 19.6989(5) |
| $\alpha$, deg | 90 | 90 |
| $\beta$, deg | 90 | 90 |
| $\gamma$, deg | 120 | 120 |
| $V$, Å$^3$ | 19366.9(9) | 4541.4(2) |
| $Z$ | 18 | 6 |
| $\rho_{calcd}$, g cm$^{-3}$ | 1.149 | 1.216 |
| $F(000)$ | 7097.22 | 1747.98 |
| $\mu$, cm$^{-1}$ | 5.291 | 6.387 |
| trans. factors range | 0.518–0.924 | 0.908–0.909 |
| no. reflections measured | 49604 | 44063 |
| no. unique reflections | 9648 ($R_{int}$ = 0.073) | 3467 ($R_{int}$ = 0.053) |
| no. parameters refined | 364 | 168 |
| $R1$ ($I > 2\ \sigma(I)$)[a] | 0.0790 | 0.1103 |
| $wR2$ (all data)[b] | 0.1725 | 0.2165 |
| GOF (all data)[c] | 1.000 | 1.000 |
| Flack parameters | | 0.10(15) |
| max diff peak / hole, e Å$^{-3}$ | 3.11/–1.35 | 1.37/–1.30 |
| CCDC number | 986840 | 986841 |

[a] $R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, $w = 4F_o^2/q\sigma(F_o^2)$ [$q$ = 8.9 ($\mathbf{2}\cdot 7/3C_4H_8O$); $q$ = 62.2 ($\mathbf{3}\cdot 1/6C_6H_{14}$)]. [c] GOF = $[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_{params})]^{1/2}$

**Supplementary Table 2 | X-ray Crystallographic Data for 4 and 5·$C_4H_8O$.**

| | **4** | **5**·$C_4H_8O$ |
|---|---|---|
| chemical formula | $C_{24}H_{43}ClF_3MoN_2O_3P_2S$ | $C_{33}H_{57}ClF_3MoN_3O_4P_2S$ |
| formula weight | 690.01 | 842.23 |
| dimensions of crystals | 0.20 × 0.20 × 0.10 | 0.12 × 0.08 × 0.03 |
| crystal system | monoclinic | monoclinic |
| space group | *C*2/*c* | $P2_1/c$ |
| *a*, Å | 33.3044(7) | 16.4904(4) |
| *b*, Å | 15.2043(3) | 16.7621(3) |
| *c*, Å | 13.0074(3) | 16.7720(4) |
| $\alpha$, deg | 90 | 90 |
| $\beta$, deg | 109.7844(7) | 119.0773(7) |
| $\gamma$, deg | 90 | 90 |
| *V*, Å$^3$ | 6197.8(3) | 4051.7(2) |
| *Z* | 8 | 4 |
| $\rho_{calcd}$, g cm$^{-3}$ | 1.479 | 1.381 |
| *F*(000) | 2856 | 1760 |
| $\mu$, cm$^{-1}$ | 7.250 | 5.707 |
| trans. factors range | 0.692–0.930 | 0.778–0.983 |
| no. reflections measured | 29891 | 39582 |
| no. unique reflections | 7092 ($R_{int}$ = 0.035) | 9260 ($R_{int}$ = 0.055) |
| no. parameters refined | 377 | 493 |
| *R*1 ($I > 2\ \sigma(I)$)[a] | 0.0516 | 0.0449 |
| *wR*2 (all data)[b] | 0.1050 | 0.0718 |
| GOF (all data)[c] | 1.029 | 1.000 |
| Flack parameters | | |
| max diff peak / hole, e Å$^{-3}$ | 4.70/–1.36 | 0.81/–0.78 |
| CCDC number | 973752 | 986842 |

[a] $R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, $w = 4F_o^2/q\sigma(F_o^2)$ [$q$ = 12.0 (**4**); $q$ = 3.545 (**5**·$C_4H_8O$)]. [c] GOF = $[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_{params})]^{1/2}$

**Supplementary Table 3 | Selected Bond Lengths (Å) and Angles (deg) for 2·7/3$C_4H_8O$.**

| | | | |
|---|---|---|---|
| Mo(1)–N(1) | 2.205(6) | P(1)–Mo(1)–N(1) | 77.69(14) |
| Mo(1)–N(2) | 1.745(12) | P(2)–Mo(1)–N(1) | 77.86(14) |
| Mo(1)–P(1) | 2.5971(19) | | |
| Mo(1)–P(2) | 2.591(3) | | |
| Mo(1)–Cl(1) | 2.407(2) | | |
| Mo(1)–Cl(2) | 2.602(4) | | |

**Supplementary Table 4 | Selected Bond Lengths (Å) and Angles (deg) for 3·1/6$C_6H_{14}$.**

| | | | |
|---|---|---|---|
| Mo(1)–N(1) | 2.202(7) | P(1)–Mo(1)–N(1) | 74.92(14) |
| Mo(1)–N(2) | 1.733(9) | P(1)*–Mo(1)–N(1) | 78.14(14) |
| Mo(1)–P(1) | 2.588(3) | | |
| Mo(1)–P(1)* | 2.437(3) | | |
| Mo(1)–Cl(1) | 2.440(3) | | |

**Supplementary Table 5 | Selected Bond Lengths (Å) and Angles (deg) for 4.**

| | | | |
|---|---|---|---|
| Mo(1)–N(1) | 2.227(3) | P(1)–Mo(1)–N(1) | 79.30(8) |
| Mo(1)–N(2) | 1.634(3) | P(2)–Mo(1)–N(1) | 79.08(8) |
| Mo(1)–P(1) | 2.5421(9) | | |
| Mo(1)–P(2) | 2.540(1) | | |
| Mo(1)–Cl(1) | 2.374(1) | | |

**Supplementary Table 6 | Selected Bond lengths (Å) and Angles (deg) for 5·$C_4H_8O$.**

| | | | |
|---|---|---|---|
| Mo(1)–N(1) | 2.184(3) | P(1)–Mo(1)–N(1) | 78.90(6) |
| Mo(1)–N(2) | 1.711(3) | P(2)–Mo(1)–N(1) | 78.98(6) |
| Mo(1)–N(3) | 2.225(3) | Mo(1)–N(2)–H(49) | 172.3(13) |
| Mo(1)–P(1) | 2.5209(7) | | |
| Mo(1)–P(2) | 2.5564(9) | | |
| Mo(1)–Cl(1) | 2.4993(8) | | |

**Supplementary Table 7 | Cartesian coordinate of 1. Units are presented in Å.**

SCF energy (in toluene) = -3962.57531261 hartree

ZPE = 1.284946 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.635377403 | 0.091684026 | -0.007458813 |
| Mo | 2.635380273 | -0.091673298 | -0.007498766 |
| P | 3.257938643 | 2.072237977 | -1.172523258 |
| P | -3.257930861 | -2.072244635 | -1.172454287 |
| N | -4.874109596 | 0.176550058 | 0.016403149 |
| N | 4.874111726 | -0.176565357 | 0.01632513 |
| P | 3.064974045 | -2.293917874 | 1.177333274 |
| P | -3.064977138 | 2.293933267 | 1.17736402 |
| N | -0.575598978 | 0.020135817 | -0.020344925 |
| N | 0.575601843 | -0.020103726 | -0.020353405 |
| N | -2.580942878 | 1.547911994 | -2.823171702 |
| N | -2.60031816 | 1.014326216 | -1.818570178 |
| N | -2.628893009 | -0.833551933 | 1.800962059 |
| N | -2.625965989 | -1.368782601 | 2.805023974 |
| N | 2.580906829 | -1.5479145 | -2.823202544 |
| N | 2.60029284 | -1.014323536 | -1.818603747 |
| N | 2.628930786 | 0.833577163 | 1.800914596 |
| N | 2.626024628 | 1.368817571 | 2.804971252 |
| H | 2.696071696 | 3.652111935 | -4.699098118 |
| H | -2.696117575 | -3.652151969 | -4.699024141 |
| H | -4.060564816 | -2.661077483 | -4.178901924 |
| H | 4.060511247 | 2.661015124 | -4.178997833 |
| C | 3.296519175 | 3.363526531 | -3.822886069 |
| C | -3.296549734 | -3.363569215 | -3.822800781 |
| H | -2.399405059 | -0.7702234 | -3.810361023 |
| H | 2.39932748 | 0.770191107 | -3.810385604 |
| H | -3.801918011 | -4.264748976 | -3.465500605 |
| H | 3.801914063 | 4.264700003 | -3.465607313 |
| H | -1.110738815 | -1.870053953 | -4.317945243 |
| H | 1.11067494 | 1.870040202 | -4.31796489 |
| C | 1.680139036 | 1.511598414 | -3.447297632 |
| C | -1.680194137 | -1.511608973 | -3.447273564 |
| H | 0.624030796 | 3.913124429 | -3.262969456 |
| H | -0.624046911 | -3.913122746 | -3.262942224 |
| C | 2.364157011 | 2.718911257 | -2.774734561 |

| | | | |
|---|---|---|---|
| C | -2.364174858 | -2.718924521 | -2.774678069 |
| H | -4.560176303 | -0.781957407 | -2.729426349 |
| H | 4.56014255 | 0.781924078 | -2.729508188 |
| H | 0.982272273 | 1.007568782 | -2.771137475 |
| H | -0.982325595 | -1.007553569 | -2.771134563 |
| H | 5.549454273 | 2.174134614 | -2.27791347 |
| H | -5.549464254 | -2.174176795 | -2.277804824 |
| C | 1.251025802 | 3.711230504 | -2.382215536 |
| C | -1.251016547 | -3.711218793 | -2.382172596 |
| H | 3.649490071 | 5.267175443 | -1.615209943 |
| H | -3.649479194 | -5.267191698 | -1.615101868 |
| H | 0.597053501 | 3.297948771 | -1.603769292 |
| H | -0.597025166 | -3.297910781 | -1.603756433 |
| C | 4.878942762 | 1.401904473 | -1.878771139 |
| C | -4.878955232 | -1.401935504 | -1.878679698 |
| H | 7.558132831 | 1.083664352 | -1.623890887 |
| H | -7.55814502 | -1.08373068 | -1.623750514 |
| H | 1.641724341 | 4.673412751 | -2.034207479 |
| H | -1.641690018 | -4.673399068 | -2.034131142 |
| H | 5.23316802 | 4.459834436 | -1.64053702 |
| H | -5.233157226 | -4.459849818 | -1.640408925 |
| H | -4.510453255 | 2.624133323 | -1.374739588 |
| H | 4.510481856 | -2.624167541 | -1.374750558 |
| C | 4.406524428 | 4.779202287 | -0.992587811 |
| C | -4.406502457 | -4.779212021 | -0.992471579 |
| H | -2.644473704 | 5.181525873 | -1.315718885 |
| H | 2.644413206 | -5.181506163 | -1.315747379 |
| C | 7.012103477 | 0.498016328 | -0.887594267 |
| C | -7.012109484 | -0.498069449 | -0.887469007 |
| H | 4.808315712 | 5.546514323 | -0.312993051 |
| H | -4.808282015 | -5.546516938 | -0.312861838 |
| C | 5.616357743 | 0.542006718 | -0.883073009 |
| C | -5.616363135 | -0.542040514 | -0.882974261 |
| H | -4.886748773 | 4.351052054 | -1.469889048 |
| H | 4.886711604 | -4.351100028 | -1.469898663 |
| H | -2.028622076 | 3.524102423 | -1.382682391 |
| H | 2.028624899 | -3.524060827 | -1.382738606 |
| C | -4.716922695 | 3.513944395 | -0.775981435 |
| C | 4.716909318 | -3.513987309 | -0.775991204 |
| C | -2.347894097 | 4.317248985 | -0.701537421 |
| C | 2.347854405 | -4.31721247 | -0.701579416 |
| H | -8.775888422 | 0.326640621 | 0.058867799 |
| H | 8.775889217 | -0.326708851 | 0.058716568 |
| C | 3.836256406 | 3.620069643 | -0.150935903 |
| C | -3.836219002 | -3.620071328 | -0.150842088 |
| H | -5.652226727 | 3.350819267 | -0.228012409 |
| H | 5.652212793 | -3.350899953 | -0.228010288 |

| | | | |
|---|---|---|---|
| C | -7.68877878 | 0.284457067 | 0.047334331 |
| C | 7.688779955 | -0.284510562 | 0.047203593 |
| H | -1.484809403 | 4.622456071 | -0.102310626 |
| H | 1.484747214 | -4.622382016 | -0.102365994 |
| H | 1.827338363 | 4.51342771 | 0.078845324 |
| H | -1.827289109 | -4.513414464 | 0.07890149 |
| H | 5.882593937 | 2.921943896 | 0.287569759 |
| H | -5.882551063 | -2.921952434 | 0.28770001 |
| C | -3.549053164 | 3.882315662 | 0.166706126 |
| C | 3.549014495 | -3.882316568 | 0.166681438 |
| C | 2.654673983 | 4.145881878 | 0.693297834 |
| C | -2.654615044 | -4.145872148 | 0.6933691 |
| C | 4.954992006 | 3.170903261 | 0.816182666 |
| C | -4.954936111 | -3.170900142 | 0.816295948 |
| H | 5.181821576 | 4.002417568 | 1.500351588 |
| H | -5.181746191 | -4.002407222 | 1.500480111 |
| H | -4.376991634 | 5.873127686 | 0.339871226 |
| H | 4.376881901 | -5.873156761 | 0.339860036 |
| C | 6.933853621 | -1.011179349 | 0.967138457 |
| C | -6.933844724 | 1.011145081 | 0.967247802 |
| H | 2.264192346 | 3.381338518 | 1.369957816 |
| H | -2.264125452 | -3.381322662 | 1.370017205 |
| C | 5.539351432 | -0.94728827 | 0.932590247 |
| C | -5.539342254 | 0.947272544 | 0.932673741 |
| C | -4.015823922 | 5.082051319 | 1.014854934 |
| C | 4.015733767 | -5.082066774 | 1.014838224 |
| H | -4.847821782 | 4.825111337 | 1.683487594 |
| H | 4.84773233 | -4.825154414 | 1.683480674 |
| H | 3.003867963 | 4.987412041 | 1.311296818 |
| H | -3.0037903 | -4.987402011 | 1.311379037 |
| H | -7.416924854 | 1.635972573 | 1.715285786 |
| H | 7.416939428 | -1.636006822 | 1.715172769 |
| H | 4.665735186 | 2.311453793 | 1.425216117 |
| H | -4.665671558 | -2.311441118 | 1.425312091 |
| H | -1.246113548 | 4.771354575 | 2.012656388 |
| H | 1.24609735 | -4.771315082 | 2.012685706 |
| C | -4.716907816 | 1.743591673 | 1.915265251 |
| C | 4.716924211 | -1.743588558 | 1.915202825 |
| H | -3.211383954 | 5.516749447 | 1.616972266 |
| H | 3.211271746 | -5.516736159 | 1.616947055 |
| H | -5.317474315 | 2.563146789 | 2.33087665 |
| H | 5.317487648 | -2.56314733 | 2.330811386 |
| H | -0.313270445 | 3.323994335 | 1.5615421 |
| H | 0.313266444 | -3.32394941 | 1.561563398 |
| C | -0.921518906 | 3.781618296 | 2.351666744 |
| C | 0.921519909 | -3.781569967 | 2.351686333 |
| H | -4.429302673 | 1.095907809 | 2.75652926 |

| | | | |
|---|---|---|---|
| H | 4.429340797 | -1.095893404 | 2.756465498 |
| C | -2.096540732 | 2.871965886 | 2.762553858 |
| C | 2.096558505 | -2.87192564 | 2.762544115 |
| H | -0.844450964 | 1.066357215 | 2.729603618 |
| H | 0.844487748 | -1.066302923 | 2.729597187 |
| H | -0.266494549 | 3.933147486 | 3.221958516 |
| H | 0.26650521 | -3.933079103 | 3.221989054 |
| C | -1.490711912 | 1.61647054 | 3.42072228 |
| C | 1.49075242 | -1.616418441 | 3.420710838 |
| H | -3.414049403 | 4.51126643 | 3.46856709 |
| H | 3.414062116 | -4.511232835 | 3.468549423 |
| H | -3.764541359 | 2.933715902 | 4.199943545 |
| H | 3.764580596 | -2.933679954 | 4.199908561 |
| C | -2.962559741 | 3.581635653 | 3.824524777 |
| C | 2.962587035 | -3.581594904 | 3.824507218 |
| H | -0.879998808 | 1.929040155 | 4.28097385 |
| H | 0.880048 | -1.928974504 | 4.28097355 |
| H | -2.254595036 | 0.92730038 | 3.795014127 |
| H | 2.254648186 | -0.927253636 | 3.794986817 |
| H | -2.32768707 | 3.834931507 | 4.687340775 |
| H | 2.327724935 | -3.834877829 | 4.687334779 |

**Supplementary Table 8 | Cartesian coordinate of II. Units are presented in Å.**

SCF energy (in toluene) = -3963.00659617 hartree

ZPE = 1.297034 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.98085911 | 1.864639987 | 1.86942464 |
| Mo | 2.220665373 | 1.739301191 | 1.510909153 |
| P | 2.734184325 | -0.686299738 | 2.23904729 |
| P | -3.197099134 | 3.467708845 | 3.860766448 |
| N | -5.229112399 | 1.942802453 | 2.199778669 |
| N | 4.408393943 | 1.559252753 | 1.008597744 |
| P | 2.744380469 | 4.06589171 | 0.584163906 |
| P | -3.869188334 | 0.294304381 | 0.027172426 |
| N | -1.007800911 | 1.811440824 | 1.643876166 |
| N | 0.150379146 | 1.781050891 | 1.576673071 |
| N | -2.75736925 | -0.58357741 | 3.870999807 |
| N | -2.842218067 | 0.296187449 | 3.15965413 |
| N | -3.099896775 | 3.426402951 | 0.563973123 |
| N | -3.161053727 | 4.29728711 | -0.160294839 |
| N | 2.901014311 | 2.626319517 | 4.359790493 |
| N | 2.544020331 | 2.277613717 | 3.233504784 |
| N | 1.820231798 | 1.058343241 | -0.566577203 |
| N | 1.556737193 | 0.710809814 | -1.59607928 |
| H | 2.649923429 | -2.708290659 | 5.556130289 |
| H | -1.999332633 | 3.519133372 | 7.566711604 |
| H | -3.540491407 | 2.923961697 | 6.94918469 |
| H | 4.000191393 | -1.77499332 | 4.910912508 |
| C | 3.105719571 | -2.341843494 | 4.624799699 |
| C | -2.733037333 | 3.640878941 | 6.756104192 |
| H | -2.22433727 | 1.182262978 | 5.651792925 |
| H | 2.557461068 | 0.292657682 | 5.135118625 |
| H | -3.144108524 | 4.649537654 | 6.840697885 |
| H | 3.421856595 | -3.216815027 | 4.052631947 |
| H | -0.741017405 | 1.882464741 | 6.302847438 |
| H | 1.248728228 | -0.731873863 | 5.744322272 |
| C | 1.691567111 | -0.305466642 | 4.832831219 |
| C | -1.455568743 | 1.940004292 | 5.467964545 |
| H | 0.333720112 | -2.552773524 | 4.569172146 |
| H | -0.10192541 | 4.140135152 | 6.017888186 |
| C | 2.07327147 | -1.461468325 | 3.888688276 |

| | | | |
|---|---|---|---|
| C | -2.030202386 | 3.368141406 | 5.40868768 |
| H | -4.451514604 | 1.768438283 | 5.019500283 |
| H | 4.444626678 | 0.284742808 | 3.623235971 |
| H | 0.953157559 | 0.36088145 | 4.375951895 |
| H | -0.929974154 | 1.673017284 | 4.545463672 |
| H | 5.146356763 | -1.145830173 | 2.855407239 |
| H | -5.290917533 | 3.299568061 | 5.26415496 |
| C | 0.788296403 | -2.269236209 | 3.609515044 |
| C | -0.842991465 | 4.335739966 | 5.22755985 |
| H | 2.752604942 | -3.925605828 | 2.164482209 |
| H | -3.096546772 | 6.268604413 | 5.490407632 |
| H | 0.043542094 | -1.677287644 | 3.062305018 |
| H | -0.345950439 | 4.194624454 | 4.258457027 |
| C | 4.518925531 | -0.265029448 | 2.673087499 |
| C | -4.781544548 | 2.685973805 | 4.511042652 |
| H | 7.129046774 | -0.225295572 | 1.927932858 |
| H | -7.491549745 | 2.672447722 | 4.608333866 |
| H | 0.975007516 | -3.195420435 | 3.056308711 |
| H | -1.132718661 | 5.387499701 | 5.316566844 |
| H | 4.413040455 | -3.312092474 | 1.99884435 |
| H | -4.757068401 | 5.630830551 | 5.485473577 |
| H | -4.994702291 | -0.920052766 | 2.500455945 |
| H | 4.597461999 | 3.779453457 | 2.940458551 |
| C | 3.452306465 | -3.433344635 | 1.482895356 |
| C | -3.984806555 | 6.110150437 | 4.870425126 |
| H | -3.477218981 | -3.34821978 | 1.16300632 |
| H | 3.137789099 | 6.429035409 | 3.562750925 |
| C | 6.544153048 | 0.519277858 | 1.393980901 |
| C | -7.121897513 | 2.371647736 | 3.631068085 |
| H | 3.622125449 | -4.122014872 | 0.642432801 |
| H | -4.365354074 | 7.104391137 | 4.593773228 |
| C | 5.175502389 | 0.631471159 | 1.652555065 |
| C | -5.744015603 | 2.320833873 | 3.405849793 |
| H | -5.573119033 | -2.506073112 | 1.978188018 |
| H | 5.273924617 | 5.401426805 | 3.10453438 |
| H | -2.649358149 | -1.89517779 | 1.736822772 |
| H | 2.296900087 | 4.876665899 | 3.445967282 |
| C | -5.383362626 | -1.475959899 | 1.643837099 |
| C | 4.840973263 | 4.68969139 | 2.386991896 |
| C | -3.156435853 | -2.336339888 | 0.874635931 |
| C | 2.621950437 | 5.747463098 | 2.870865723 |
| H | -9.079560869 | 2.079396644 | 2.761338178 |
| H | 8.204030094 | 1.276087892 | 0.236940081 |
| C | 2.911253854 | -2.10119192 | 0.924922545 |
| C | -3.684295208 | 5.320548214 | 3.580299506 |
| H | -6.350671298 | -1.044143315 | 1.362362236 |
| H | 5.620776709 | 4.464872299 | 1.649615794 |

| | | | |
|---|---|---|---|
| C | -8.0038341 | 2.041232199 | 2.60445895 |
| C | 7.141349314 | 1.357577805 | 0.455276912 |
| H | -2.427972391 | -2.444197571 | 0.065240435 |
| H | 1.735420079 | 6.269170122 | 2.498754791 |
| H | 0.804058768 | -2.757993905 | 0.9804819 |
| H | -1.628110648 | 6.106395639 | 3.388847566 |
| H | 4.935419874 | -1.616932406 | 0.201880893 |
| H | -5.841299865 | 4.98880133 | 3.264320932 |
| C | -4.400110962 | -1.522340669 | 0.451230794 |
| C | 3.60123452 | 5.352178337 | 1.742614803 |
| C | 1.533107597 | -2.353061138 | 0.272820587 |
| C | -2.551373875 | 6.030511834 | 2.806187686 |
| C | 3.904270012 | -1.644222784 | -0.168053393 |
| C | -4.96577378 | 5.35618659 | 2.716662011 |
| H | 3.875130665 | -2.369910836 | -0.993310408 |
| H | -5.170520971 | 6.400241176 | 2.43979189 |
| H | -5.485673742 | -3.227095556 | -0.313696349 |
| H | 4.662135485 | 7.232729388 | 1.73310105 |
| C | 6.356050715 | 2.309369259 | -0.19044718 |
| C | -7.47643983 | 1.66164118 | 1.372312631 |
| H | 1.106392333 | -1.443588507 | -0.15994332 |
| H | -2.320629512 | 5.527337229 | 1.863558224 |
| C | 4.994543911 | 2.404262451 | 0.112024015 |
| C | -6.091148161 | 1.614175043 | 1.194666346 |
| C | -5.117897901 | -2.263180003 | -0.694856138 |
| C | 4.080998762 | 6.627976582 | 1.021995701 |
| H | -5.989414779 | -1.711963744 | -1.069991298 |
| H | 4.739966411 | 6.412913826 | 0.170876204 |
| H | 1.647785829 | -3.086517738 | -0.538408777 |
| H | -2.871122636 | 7.055122854 | 2.566054596 |
| H | -8.129551132 | 1.398254219 | 0.543933744 |
| H | 6.790771067 | 2.990663244 | -0.917412355 |
| H | 3.67044992 | -0.662599153 | -0.587466879 |
| H | -4.872258431 | 4.782925416 | 1.791210047 |
| H | -2.494105966 | -1.755994103 | -1.964354549 |
| H | 1.086320584 | 6.769076075 | 0.549461836 |
| C | -5.512218174 | 1.200475542 | -0.136906061 |
| C | 4.145801739 | 3.47059274 | -0.537476974 |
| H | -4.457267254 | -2.483311193 | -1.539311282 |
| H | 3.254030286 | 7.253426037 | 0.671322641 |
| H | -6.259758464 | 0.639245463 | -0.710854363 |
| H | 4.786498843 | 4.285085963 | -0.896858537 |
| H | -1.335441092 | -0.653328522 | -1.187482514 |
| H | 0.098916526 | 5.331028539 | 0.906345808 |
| C | -2.102969597 | -0.733569397 | -1.968604544 |
| C | 0.607169742 | 5.88846879 | 0.108985396 |
| H | -5.27498317 | 2.102703874 | -0.719705214 |

| | | | |
|---|---|---|---|
| H | 3.643950382 | 3.058537561 | -1.425246965 |
| C | -3.206284911 | 0.330557169 | -1.796227296 |
| C | 1.598700636 | 4.999204853 | -0.669230444 |
| H | -1.772032619 | 1.923807687 | -1.305770644 |
| H | 0.194269341 | 3.307451637 | -0.74284433 |
| H | -1.606368778 | -0.580185472 | -2.937394672 |
| H | -0.166701049 | 6.251117774 | -0.582106506 |
| C | -2.560384919 | 1.709405949 | -2.034463556 |
| C | 0.773485917 | 3.938133326 | -1.424656943 |
| H | -4.797985635 | -0.828892398 | -2.820467607 |
| H | 2.919616317 | 6.66787274 | -1.301982623 |
| H | -5.058197785 | 0.92589478 | -2.830383086 |
| H | 3.021785197 | 5.232080489 | -2.338895093 |
| C | -4.295182989 | 0.139122772 | -2.874106868 |
| C | 2.345512128 | 5.841023281 | -1.726016563 |
| H | -2.111811662 | 1.718461773 | -3.038743404 |
| H | 0.064674479 | 4.451176417 | -2.090020123 |
| H | -3.288335104 | 2.526645554 | -1.999329646 |
| H | 1.398303341 | 3.297148051 | -2.057552803 |
| H | -3.823317222 | 0.207974293 | -3.86528051 |
| H | 1.604104465 | 6.27790937 | -2.410644432 |
| H | 2.094948989 | 2.809592234 | 4.989814654 |

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**Supplementary Table 9 | Cartesian coordinate of III. Units are presented in Å.**

SCF energy (in toluene) = -3853.50852839 hartree

ZPE = 1.286557 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.635377403 | 0.091684026 | -0.007458813 |
| Mo | 2.635380273 | -0.091673298 | -0.007498766 |
| P | 3.257938643 | 2.072237977 | -1.172523258 |
| P | -3.257930861 | -2.072244635 | -1.172454287 |
| N | -4.874109596 | 0.176550058 | 0.016403149 |
| N | 4.874111726 | -0.176565357 | 0.01632513 |
| P | 3.064974045 | -2.293917874 | 1.177333274 |
| P | -3.064977138 | 2.293933267 | 1.17736402 |
| N | -0.575598978 | 0.020135817 | -0.020344925 |
| N | 0.575601843 | -0.020103726 | -0.020353405 |
| N | -2.580942878 | 1.547911994 | -2.823171702 |
| N | -2.60031816 | 1.014326216 | -1.818570178 |
| N | -2.628893009 | -0.833551933 | 1.800962059 |
| N | -2.625965989 | -1.368782601 | 2.805023974 |
| N | 2.580906829 | -1.5479145 | -2.823202544 |
| N | 2.60029284 | -1.014323536 | -1.818603747 |
| N | 2.628930786 | 0.833577163 | 1.800914596 |
| N | 2.626024628 | 1.368817571 | 2.804971252 |
| H | 2.696071696 | 3.652111935 | -4.699098118 |
| H | -2.696117575 | -3.652151969 | -4.699024141 |
| H | -4.060564816 | -2.661077483 | -4.178901924 |
| H | 4.060511247 | 2.661015124 | -4.178997833 |
| C | 3.296519175 | 3.363526531 | -3.822886069 |
| C | -3.296549734 | -3.363569215 | -3.822800781 |
| H | -2.399405059 | -0.7702234 | -3.810361023 |
| H | 2.39932748 | 0.770191107 | -3.810385604 |
| H | -3.801918011 | -4.264748976 | -3.465500605 |
| H | 3.801914063 | 4.264700003 | -3.465607313 |
| H | -1.110738815 | -1.870053953 | -4.317945243 |
| H | 1.11067494 | 1.870040202 | -4.31796489 |
| C | 1.680139036 | 1.511598414 | -3.447297632 |
| C | -1.680194137 | -1.511608973 | -3.447273564 |
| H | 0.624030796 | 3.913124429 | -3.262969456 |
| H | -0.624046911 | -3.913122746 | -3.262942224 |
| C | 2.364157011 | 2.718911257 | -2.774734561 |

| | | | |
|---|---|---|---|
| C | -2.364174858 | -2.718924521 | -2.774678069 |
| H | -4.560176303 | -0.781957407 | -2.729426349 |
| H | 4.56014255 | 0.781924078 | -2.729508188 |
| H | 0.982272273 | 1.007568782 | -2.771137475 |
| H | -0.982325595 | -1.007553569 | -2.771134563 |
| H | 5.549454273 | 2.174134614 | -2.27791347 |
| H | -5.549464254 | -2.174176795 | -2.277804824 |
| C | 1.251025802 | 3.711230504 | -2.382215536 |
| C | -1.251016547 | -3.711218793 | -2.382172596 |
| H | 3.649490071 | 5.267175443 | -1.615209943 |
| H | -3.649479194 | -5.267191698 | -1.615101868 |
| H | 0.597053501 | 3.297948771 | -1.603769292 |
| H | -0.597025166 | -3.297910781 | -1.603756433 |
| C | 4.878942762 | 1.401904473 | -1.878771139 |
| C | -4.878955232 | -1.401935504 | -1.878679698 |
| H | 7.558132831 | 1.083664352 | -1.623890887 |
| H | -7.55814502 | -1.08373068 | -1.623750514 |
| H | 1.641724341 | 4.673412751 | -2.034207479 |
| H | -1.641690018 | -4.673399068 | -2.034131142 |
| H | 5.23316802 | 4.459834436 | -1.64053702 |
| H | -5.233157226 | -4.459849818 | -1.640408925 |
| H | -4.510453255 | 2.624133323 | -1.374739588 |
| H | 4.510481856 | -2.624167541 | -1.374750558 |
| C | 4.406524428 | 4.779202287 | -0.992587811 |
| C | -4.406502457 | -4.779212021 | -0.992471579 |
| H | -2.644473704 | 5.181525873 | -1.315718885 |
| H | 2.644413206 | -5.181506163 | -1.315747379 |
| C | 7.012103477 | 0.498016328 | -0.887594267 |
| C | -7.012109484 | -0.498069449 | -0.887469007 |
| H | 4.808315712 | 5.546514323 | -0.312993051 |
| H | -4.808282015 | -5.546516938 | -0.312861838 |
| C | 5.616357743 | 0.542006718 | -0.883073009 |
| C | -5.616363135 | -0.542040514 | -0.882974261 |
| H | -4.886748773 | 4.351052054 | -1.469889048 |
| H | 4.886711604 | -4.351100028 | -1.469898663 |
| H | -2.028622076 | 3.524102423 | -1.382682391 |
| H | 2.028624899 | -3.524060827 | -1.382738606 |
| C | -4.716922695 | 3.513944395 | -0.775981435 |
| C | 4.716909318 | -3.513987309 | -0.775991204 |
| C | -2.347894097 | 4.317248985 | -0.701537421 |
| C | 2.347854405 | -4.31721247 | -0.701579416 |
| H | -8.775888422 | 0.326640621 | 0.058867799 |
| H | 8.775889217 | -0.326708851 | 0.058716568 |
| C | 3.836256406 | 3.620069643 | -0.150935903 |
| C | -3.836219002 | -3.620071328 | -0.150842088 |
| H | -5.652226727 | 3.350819267 | -0.228012409 |
| H | 5.652212793 | -3.350899953 | -0.228010288 |

| | | | |
|---|---|---|---|
| C | -7.68877878 | 0.284457067 | 0.047334331 |
| C | 7.688779955 | -0.284510562 | 0.047203593 |
| H | -1.484809403 | 4.622456071 | -0.102310626 |
| H | 1.484747214 | -4.622382016 | -0.102365994 |
| H | 1.827338363 | 4.51342771 | 0.078845324 |
| H | -1.827289109 | -4.513414464 | 0.07890149 |
| H | 5.882593937 | 2.921943896 | 0.287569759 |
| H | -5.882551063 | -2.921952434 | 0.28770001 |
| C | -3.549053164 | 3.882315662 | 0.166706126 |
| C | 3.549014495 | -3.882316568 | 0.166681438 |
| C | 2.654673983 | 4.145881878 | 0.693297834 |
| C | -2.654615044 | -4.145872148 | 0.6933691 |
| C | 4.954992006 | 3.170903261 | 0.816182666 |
| C | -4.954936111 | -3.170900142 | 0.816295948 |
| H | 5.181821576 | 4.002417568 | 1.500351588 |
| H | -5.181746191 | -4.002407222 | 1.500480111 |
| H | -4.376991634 | 5.873127686 | 0.339871226 |
| H | 4.376881901 | -5.873156761 | 0.339860036 |
| C | 6.933853621 | -1.011179349 | 0.967138457 |
| C | -6.933844724 | 1.011145081 | 0.967247802 |
| H | 2.264192346 | 3.381338518 | 1.369957816 |
| H | -2.264125452 | -3.381322662 | 1.370017205 |
| C | 5.539351432 | -0.94728827 | 0.932590247 |
| C | -5.539342254 | 0.947272544 | 0.932673741 |
| C | -4.015823922 | 5.082051319 | 1.014854934 |
| C | 4.015733767 | -5.082066774 | 1.014838224 |
| H | -4.847821782 | 4.825111337 | 1.683487594 |
| H | 4.84773233 | -4.825154414 | 1.683480674 |
| H | 3.003867963 | 4.987412041 | 1.311296818 |
| H | -3.0037903 | -4.987402011 | 1.311379037 |
| H | -7.416924854 | 1.635972573 | 1.715285786 |
| H | 7.416939428 | -1.636006822 | 1.715172769 |
| H | 4.665735186 | 2.311453793 | 1.425216117 |
| H | -4.665671558 | -2.311441118 | 1.425312091 |
| H | -1.246113548 | 4.771354575 | 2.012656388 |
| H | 1.24609735 | -4.771315082 | 2.012685706 |
| C | -4.716907816 | 1.743591673 | 1.915265251 |
| C | 4.716924211 | -1.743588558 | 1.915202825 |
| H | -3.211383954 | 5.516749447 | 1.616972266 |
| H | 3.211271746 | -5.516736159 | 1.616947055 |
| H | -5.317474315 | 2.563146789 | 2.33087665 |
| H | 5.317487648 | -2.56314733 | 2.330811386 |
| H | -0.313270445 | 3.323994335 | 1.5615421 |
| H | 0.313266444 | -3.32394941 | 1.561563398 |
| C | -0.921518906 | 3.781618296 | 2.351666744 |
| C | 0.921519909 | -3.781569967 | 2.351686333 |
| H | -4.429302673 | 1.095907809 | 2.75652926 |

| | | | |
|---|---|---|---|
| H | 4.429340797 | -1.095893404 | 2.756465498 |
| C | -2.096540732 | 2.871965886 | 2.762553858 |
| C | 2.096558505 | -2.87192564 | 2.762544115 |
| H | -0.844450964 | 1.066357215 | 2.729603618 |
| H | 0.844487748 | -1.066302923 | 2.729597187 |
| H | -0.266494549 | 3.933147486 | 3.221958516 |
| H | 0.26650521 | -3.933079103 | 3.221989054 |
| C | -1.490711912 | 1.61647054 | 3.42072228 |
| C | 1.49075242 | -1.616418441 | 3.420710838 |
| H | -3.414049403 | 4.51126643 | 3.46856709 |
| H | 3.414062116 | -4.511232835 | 3.468549423 |
| H | -3.764541359 | 2.933715902 | 4.199943545 |
| H | 3.764580596 | -2.933679954 | 4.199908561 |
| C | -2.962559741 | 3.581635653 | 3.824524777 |
| C | 2.962587035 | -3.581594904 | 3.824507218 |
| H | -0.879998808 | 1.929040155 | 4.28097385 |
| H | 0.880048 | -1.928974504 | 4.28097355 |
| H | -2.254595036 | 0.92730038 | 3.795014127 |
| H | 2.254648186 | -0.927253636 | 3.794986817 |
| H | -2.32768707 | 3.834931507 | 4.687340775 |
| H | 2.327724935 | -3.834877829 | 4.687334779 |

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**Supplementary Table 10 | Cartesian coordinate of IV. Units are presented in Å.**

SCF energy (in toluene) = -4814.96151136 hartree

ZPE = 1.315695 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.892002857 | -0.043947612 | 0.008716323 |
| Mo | 2.298961332 | 0.581972042 | 0.422737997 |
| P | 2.865370221 | -0.755980831 | 2.56707277 |
| P | -3.572161518 | 2.388794852 | 0.468304394 |
| N | -5.15232017 | -0.141546221 | -0.02188653 |
| N | 4.507776474 | 0.864377112 | 0.55198341 |
| P | 2.743287263 | 2.060776804 | -1.607687564 |
| P | -3.323209889 | -2.515115106 | -0.491316566 |
| N | -0.874523202 | 0.047446495 | 0.076986685 |
| N | 0.275667019 | 0.121685667 | 0.141845048 |
| N | -2.934428929 | -0.595064937 | 3.131652597 |
| N | -2.915948026 | -0.394446364 | 2.013558067 |
| N | -2.855246014 | 0.324839904 | -1.994233371 |
| N | -2.844770586 | 0.547220484 | -3.107823427 |
| N | 1.724720741 | 3.02809401 | 2.141604095 |
| N | 1.99623111 | 2.02177399 | 1.450189986 |
| H | 1.804803082 | -0.494624946 | 6.298779232 |
| H | -3.115085588 | 4.943395904 | 3.375803124 |
| H | -4.453398706 | 3.815486883 | 3.146310785 |
| H | 3.174484108 | 0.296944851 | 5.514588427 |
| C | 2.524495692 | -0.586738482 | 5.471246438 |
| C | -3.692950283 | 4.400038855 | 2.613071771 |
| H | -2.757083296 | 1.954586574 | 3.389835209 |
| H | 1.482625305 | 1.540224763 | 4.039308305 |
| H | -4.203335526 | 5.146932327 | 1.99938395 |
| H | 3.136026524 | -1.47053859 | 5.667687348 |
| H | -1.454046313 | 3.146262848 | 3.528782509 |
| H | 0.206448289 | 0.658412882 | 4.898887559 |
| C | 0.889756747 | 0.621112907 | 4.0371251 |
| C | -2.039731719 | 2.550407246 | 2.814655617 |
| H | 0.015777095 | -1.691364745 | 4.931451388 |
| H | -1.000682204 | 4.80140615 | 1.948357483 |
| C | 1.744758499 | -0.653908595 | 4.141503495 |
| C | -2.725596749 | 3.499946972 | 1.815838669 |
| H | -4.865196874 | 1.573024161 | 2.32252891 |

| | | | |
|---|---|---|---|
| H | 3.830786203 | 1.31086841 | 3.351720114 |
| H | 0.286679806 | 0.626111344 | 3.125303392 |
| H | -1.350482929 | 1.870205017 | 2.308495488 |
| H | 4.960675744 | 0.018759124 | 3.774028735 |
| H | -5.8653867 | 2.764011661 | 1.487388416 |
| C | 0.767245044 | -1.849237614 | 4.144190295 |
| C | -1.622943481 | 4.354282072 | 1.16120257 |
| H | 3.175738777 | -3.322407034 | 4.538389945 |
| H | -4.043867337 | 5.551188133 | -0.070426425 |
| H | 0.227469979 | -1.92757397 | 3.191728057 |
| H | -0.955274653 | 3.745276343 | 0.540685792 |
| C | 4.309631927 | 0.394855303 | 2.975089139 |
| C | -5.183421503 | 1.919055539 | 1.328074325 |
| H | 6.996698251 | 0.806697872 | 2.836974961 |
| H | -7.858577946 | 1.511714942 | 1.165851612 |
| H | 1.253555051 | -2.808968383 | 4.343758549 |
| H | -2.02642596 | 5.170909465 | 0.552244428 |
| H | 4.730669991 | -2.460559708 | 4.486845403 |
| H | -5.609327352 | 4.742993051 | 0.175586785 |
| H | -4.80710113 | -2.08806533 | 2.038742476 |
| H | 3.877104202 | 3.588245963 | 0.670192432 |
| C | 4.048167576 | -3.103526773 | 3.915405809 |
| C | -4.777359334 | 4.879512911 | -0.527537846 |
| H | -2.911052652 | -4.507366697 | 2.754336567 |
| H | 1.935688798 | 5.706292669 | -0.702718721 |
| C | 6.518969719 | 0.916169361 | 1.866476583 |
| C | -7.30137785 | 0.743152235 | 0.635102333 |
| H | 4.572302734 | -4.056252269 | 3.746265785 |
| H | -5.183238734 | 5.397169602 | -1.41006658 |
| C | 5.138795706 | 0.733340535 | 1.755411554 |
| C | -5.9055097 | 0.799527629 | 0.622616365 |
| H | -5.172507994 | -3.716495577 | 2.623494617 |
| H | 4.170481766 | 5.210426597 | 0.015709767 |
| H | -2.294675168 | -2.909656752 | 2.306817651 |
| H | 1.411415319 | 4.215633701 | 0.102968315 |
| C | -4.996326771 | -3.115085678 | 1.719219601 |
| C | 4.114292197 | 4.142050893 | -0.24154955 |
| C | -2.613451122 | -3.874776089 | 1.904218051 |
| C | 1.743871313 | 4.632159451 | -0.853256355 |
| H | -9.048106351 | -0.342802113 | -0.036785068 |
| H | 8.34790918 | 1.339367559 | 0.797016169 |
| C | 3.691867708 | -2.503859585 | 2.540129948 |
| C | -4.162210517 | 3.540285351 | -0.979869094 |
| H | -5.922999813 | -3.128427026 | 1.133538262 |
| H | 5.111954741 | 3.837116243 | -0.577176638 |
| C | -7.961551963 | -0.286553933 | -0.032690393 |
| C | 7.268878328 | 1.213969561 | 0.729576398 |

| | | | |
|---|---|---|---|
| H | -1.748507449 | -4.347937384 | 1.429959378 |
| H | 0.926500175 | 4.547132224 | -1.574591183 |
| H | 1.811412097 | -3.639357899 | 2.351035079 |
| H | -2.186598995 | 4.415481425 | -1.4356143 |
| H | 5.779907178 | -1.855721666 | 2.325746392 |
| H | -6.17612879 | 2.674263599 | -1.214851953 |
| C | -3.812560888 | -3.731274934 | 0.940526324 |
| C | 3.044472163 | 3.95772701 | -1.341724974 |
| C | 2.735161024 | -3.455443549 | 1.790701406 |
| C | -2.971036693 | 3.826890149 | -1.920439638 |
| C | 5.013875199 | -2.394963534 | 1.754408992 |
| C | -5.248910311 | 2.794584083 | -1.78688463 |
| H | 5.396208182 | -3.407493789 | 1.565822817 |
| H | -5.491080574 | 3.389531722 | -2.68012609 |
| H | -4.624190484 | -5.69113494 | 1.357622498 |
| H | 3.818240446 | 5.7265619 | -2.316492193 |
| C | 6.615822051 | 1.356167239 | -0.490940867 |
| C | -7.19372578 | -1.242423169 | -0.694909579 |
| H | 2.470047355 | -3.056497936 | 0.808993835 |
| H | -2.520991094 | 2.907133696 | -2.303020494 |
| C | 5.226512585 | 1.198286207 | -0.558462772 |
| C | -5.799611067 | -1.155091091 | -0.671790633 |
| C | -4.259979369 | -5.133527483 | 0.481442922 |
| C | 3.568775928 | 4.690973432 | -2.593829055 |
| H | -5.085171697 | -5.095537158 | -0.241832966 |
| H | 4.483923457 | 4.234641482 | -2.992712917 |
| H | 3.231454963 | -4.424901139 | 1.638614235 |
| H | -3.330113001 | 4.404819369 | -2.785495469 |
| H | -7.664868315 | -2.06412093 | -1.229376695 |
| H | 7.16739421 | 1.600185415 | -1.395342349 |
| H | 4.891270536 | -1.927803833 | 0.7777166 |
| H | -4.923416993 | 1.808882346 | -2.126597708 |
| H | -1.502987287 | -5.104730729 | -0.550679555 |
| H | 1.01444108 | 3.834034096 | -3.622565842 |
| C | -4.96203239 | -2.1939429 | -1.371350209 |
| C | 4.498845443 | 1.418414782 | -1.863245614 |
| H | -3.444857625 | -5.718716745 | 0.044538334 |
| H | 2.832680344 | 4.74224554 | -3.401378715 |
| H | -5.55645342 | -3.099573619 | -1.545879415 |
| H | 5.10442887 | 2.056886604 | -2.519367949 |
| H | -0.559766185 | -3.595312431 | -0.574359217 |
| H | 0.012969022 | 2.721705819 | -2.659758062 |
| C | -1.179053883 | -4.268422375 | -1.179617061 |
| C | 0.713063523 | 2.788311927 | -3.502188507 |
| H | -4.664877116 | -1.811674068 | -2.358959145 |
| H | 4.378700991 | 0.45474841 | -2.379698483 |
| C | -2.357929841 | -3.524786481 | -1.837659263 |

| | | | |
|---|---|---|---|
| C | 1.899716662 | 1.816268782 | -3.337461119 |
| H | -1.133544132 | -1.7727566 | -2.350327278 |
| H | 0.632568607 | 0.211880047 | -2.531969064 |
| H | -0.530238746 | -4.68099325 | -1.962705926 |
| H | 0.155689595 | 2.505275179 | -4.406854382 |
| C | -1.772206238 | -2.513026258 | -2.8412987 |
| C | 1.317688346 | 0.389254107 | -3.367191744 |
| H | -3.667994741 | -5.306725739 | -2.0221089 |
| H | 3.344072946 | 2.945146826 | -4.586692975 |
| H | -4.035218561 | -4.014221137 | -3.181093834 |
| H | 3.663930032 | 1.19631625 | -4.485510596 |
| C | -3.226844584 | -4.518824075 | -2.637236229 |
| C | 2.876123618 | 1.957515514 | -4.523467965 |
| H | -1.156325429 | -3.055966732 | -3.57083821 |
| H | 0.750459976 | 0.264854724 | -4.30226203 |
| H | -2.549717019 | -1.981737258 | -3.40053394 |
| H | 2.100537067 | -0.369204446 | -3.351426202 |
| H | -2.592175752 | -5.008176758 | -3.391009415 |
| H | 2.319292625 | 1.797603173 | -5.459112633 |
| H | 2.579411752 | 3.560674164 | 2.384499974 |
| S | 3.690710052 | -2.177685502 | -1.883237592 |
| O | 4.049212292 | -1.458647926 | -3.128907923 |
| O | 4.754152107 | -2.982945827 | -1.26294874 |
| O | 2.88557772 | -1.341778779 | -0.912410411 |
| C | 2.43674017 | -3.439418835 | -2.440391205 |
| F | 2.033727222 | -4.199042224 | -1.404122444 |
| F | 1.35229646 | -2.845543614 | -2.971149231 |
| F | 2.977131221 | -4.241022756 | -3.366924845 |

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**Supplementary Table 11 | Cartesian coordinate of V. Units are presented in Å.**

SCF energy (in toluene) = -4815.53322129 hartree

ZPE = 1.328643 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.901799164 | -0.029739246 | 0.132061097 |
| Mo | 2.305167097 | 0.493603219 | 0.501869568 |
| P | 2.871768509 | -1.34334194 | 2.256842318 |
| P | -3.762531934 | 2.331176864 | 0.618290635 |
| N | -5.144147229 | -0.253853427 | -0.095248925 |
| N | 4.534580918 | 0.70342239 | 0.693671936 |
| P | 2.816170713 | 2.419107316 | -1.157128854 |
| P | -3.167444741 | -2.512067701 | -0.444817183 |
| N | -0.870499179 | 0.143639912 | 0.257653796 |
| N | 0.285455193 | 0.241315821 | 0.293560797 |
| N | -3.045300509 | -0.692653297 | 3.22743921 |
| N | -2.999174818 | -0.44885138 | 2.118035266 |
| N | -2.75137532 | 0.386225296 | -1.855772708 |
| N | -2.661787737 | 0.625291237 | -2.962033331 |
| N | 1.020138277 | 2.353469977 | 2.374813166 |
| N | 2.090552171 | 1.720475592 | 1.883883048 |
| H | 1.881365942 | -1.981608017 | 5.963012485 |
| H | -3.822983747 | 4.839262721 | 3.615656367 |
| H | -5.039467891 | 3.62350399 | 3.225672084 |
| H | 3.302055993 | -1.118607965 | 5.366317126 |
| C | 2.584195574 | -1.911359228 | 5.11900173 |
| C | -4.27061166 | 4.270439677 | 2.786415115 |
| H | -3.286940746 | 1.858226346 | 3.607414723 |
| H | 1.706485171 | 0.57859524 | 4.283954684 |
| H | -4.763989735 | 4.989367293 | 2.12807793 |
| H | 3.125603723 | -2.85823892 | 5.06668905 |
| H | -2.121935911 | 3.137078769 | 3.963255135 |
| H | 0.397238752 | -0.390267101 | 4.9877857 |
| C | 1.031878069 | -0.263419632 | 4.097350262 |
| C | -2.544787245 | 2.523329339 | 3.153467709 |
| H | 0.010467707 | -2.688811107 | 4.398426618 |
| H | -1.578909492 | 4.890139132 | 2.472071253 |
| C | 1.786692248 | -1.579660318 | 3.839810072 |
| C | -3.159696789 | 3.454462562 | 2.089991657 |
| H | -5.19297553 | 1.387500827 | 2.313611586 |

| | | | |
|---|---|---|---|
| H | 3.873382367 | 0.44903274 | 3.503221502 |
| H | 0.39009061 | 0.013321613 | 3.25779056 |
| H | -1.745402625 | 1.895808869 | 2.747864522 |
| H | 4.983742549 | -0.933124628 | 3.593748532 |
| H | -6.161935294 | 2.557013512 | 1.412263599 |
| C | 0.728420471 | -2.668145935 | 3.565415877 |
| C | -2.052341012 | 4.410731988 | 1.60194809 |
| H | 3.098355481 | -4.341228043 | 3.497578535 |
| H | -4.349722852 | 5.494534897 | 0.109869756 |
| H | 0.162704721 | -2.451307522 | 2.650562282 |
| H | -1.26788198 | 3.881197608 | 1.045547819 |
| C | 4.338259194 | -0.356713918 | 2.919119374 |
| C | -5.425746575 | 1.750703272 | 1.301568898 |
| H | 7.023231049 | 0.029299561 | 2.881796043 |
| H | -8.040885291 | 1.228799915 | 0.849622807 |
| H | 1.156706559 | -3.671833211 | 3.475335165 |
| H | -2.434139027 | 5.212838649 | 0.961263425 |
| H | 4.679062586 | -3.540126133 | 3.661922421 |
| H | -5.884212036 | 4.599239485 | 0.180431253 |
| H | -4.855733229 | -2.183210918 | 1.991089816 |
| H | 3.74412522 | 3.372608567 | 1.499842163 |
| C | 3.978545923 | -3.99264321 | 2.948011077 |
| C | -4.995563698 | 4.796619189 | -0.432579149 |
| H | -3.006277367 | -4.594104254 | 2.775265781 |
| H | 2.10799783 | 5.811238716 | 0.523249181 |
| C | 6.551136879 | 0.388309755 | 1.970407832 |
| C | -7.395569259 | 0.505807233 | 0.355800303 |
| H | 4.473714743 | -4.884204623 | 2.534882471 |
| H | -5.33890625 | 5.315817393 | -1.340087325 |
| C | 5.168027344 | 0.265191573 | 1.820225713 |
| C | -6.010913585 | 0.625017672 | 0.493041258 |
| H | -5.255814653 | -3.83921292 | 2.467361255 |
| H | 4.230357912 | 5.064293168 | 1.210749505 |
| H | -2.37750821 | -2.975226501 | 2.439596245 |
| H | 1.372237078 | 4.221208957 | 0.798184207 |
| C | -5.006768746 | -3.196005665 | 1.610020041 |
| C | 4.124184197 | 4.071647329 | 0.746366934 |
| C | -2.641862447 | -3.929604219 | 1.977054454 |
| C | 1.862844811 | 4.848669435 | 0.048404293 |
| H | -9.00871081 | -0.630635853 | -0.534349658 |
| H | 8.390127621 | 1.042804086 | 1.041749017 |
| C | 3.642403685 | -3.049004991 | 1.776698388 |
| C | -4.270847158 | 3.501537991 | -0.848882839 |
| H | -5.878781892 | -3.188243926 | 0.945901966 |
| H | 5.127194877 | 3.747931227 | 0.446675907 |
| C | -7.93280372 | -0.525516264 | -0.412144452 |
| C | 7.30960949 | 0.953441269 | 0.94686088 |

| | | | |
|---|---|---|---|
| H | -1.730200117 | -4.37668142 | 1.570193643 |
| H | 1.144495218 | 5.054622087 | -0.749031604 |
| H | 1.716759563 | -4.017176129 | 1.314949157 |
| H | -2.28950756 | 4.452556483 | -1.067405519 |
| H | 5.743454348 | -2.410804618 | 1.71720617 |
| H | -6.214735782 | 2.571317391 | -1.31132083 |
| C | -3.751593516 | -3.770415808 | 0.914173792 |
| C | 3.16676878 | 4.196210817 | -0.461032852 |
| C | 2.657532682 | -3.750699036 | 0.817505482 |
| C | -3.00531458 | 3.868325465 | -1.654442539 |
| C | 4.966652163 | -2.778262744 | 1.034879304 |
| C | -5.236844256 | 2.732766581 | -1.779532584 |
| H | 5.326727484 | -3.721018054 | 0.600582235 |
| H | -5.403228029 | 3.336874518 | -2.683855162 |
| H | -4.558482279 | -5.755941224 | 1.202903822 |
| H | 4.08492207 | 6.083233037 | -0.991503395 |
| C | 6.65833202 | 1.404348688 | -0.19782752 |
| C | -7.051598669 | -1.418529451 | -1.018800844 |
| H | 2.429347629 | -3.124638582 | -0.04899675 |
| H | -2.491688853 | 2.981897914 | -2.035888355 |
| C | 5.268030589 | 1.284110031 | -0.299421582 |
| C | -5.673843633 | -1.270004382 | -0.843036867 |
| C | -4.134019173 | -5.16455773 | 0.377411462 |
| C | 3.833585135 | 5.134140969 | -1.489123636 |
| H | -4.897656989 | -5.11652281 | -0.409853556 |
| H | 4.770093548 | 4.72181476 | -1.88526939 |
| H | 3.11266233 | -4.681549462 | 0.448484674 |
| H | -3.295713905 | 4.481234542 | -2.521110754 |
| H | -7.420938243 | -2.240608052 | -1.627651859 |
| H | 7.213789513 | 1.85629002 | -1.015840119 |
| H | 4.854413981 | -2.083637908 | 0.202686278 |
| H | -4.845589115 | 1.764771303 | -2.099250125 |
| H | -1.271317687 | -5.056013248 | -0.385352447 |
| H | 1.305747368 | 4.696083421 | -2.839774383 |
| C | -4.722135795 | -2.247358645 | -1.479157495 |
| C | 4.556217625 | 1.802276065 | -1.524642669 |
| H | -3.274648048 | -5.721630882 | -0.008727519 |
| H | 3.182912375 | 5.374187328 | -2.335812094 |
| H | -5.249630056 | -3.175962421 | -1.730367467 |
| H | 5.181691772 | 2.551403797 | -2.025827621 |
| H | -0.372150107 | -3.522374717 | -0.273863787 |
| H | 0.175204125 | 3.522188047 | -2.119601653 |
| C | -0.911220402 | -4.192287395 | -0.955020431 |
| C | 0.911687543 | 3.677470039 | -2.918459524 |
| H | -4.347442744 | -1.828133082 | -2.424630823 |
| H | 4.42274026 | 0.976659245 | -2.238667472 |
| C | -2.042357235 | -3.459651821 | -1.703765059 |

| | | | |
|---|---|---|---|
| C | 2.005256348 | 2.590269044 | -2.911915774 |
| H | -0.803778835 | -1.673738722 | -2.061338719 |
| H | 0.562429687 | 0.997649077 | -2.453667818 |
| H | -0.181125572 | -4.561246892 | -1.686402546 |
| H | 0.369288083 | 3.613759434 | -3.872935466 |
| C | -1.39226458 | -2.406767795 | -2.62186459 |
| C | 1.306098328 | 1.251179073 | -3.21744352 |
| H | -3.283249483 | -5.26831242 | -2.066216335 |
| H | 3.609968159 | 3.787413294 | -3.861628848 |
| H | -3.543927173 | -3.961268976 | -3.238602761 |
| H | 3.726432973 | 2.032896711 | -4.152286874 |
| C | -2.792782032 | -4.45857252 | -2.61248475 |
| C | 3.032278477 | 2.871288486 | -4.028344784 |
| H | -0.713587788 | -2.915714297 | -3.316798832 |
| H | 0.784945423 | 1.338880897 | -4.182861967 |
| H | -2.12982781 | -1.866791613 | -3.225763288 |
| H | 2.017890735 | 0.431586173 | -3.298901188 |
| H | -2.064388547 | -4.919268313 | -3.296350425 |
| H | 2.495471185 | 2.989126683 | -4.981855164 |
| H | 1.205340682 | 3.212840142 | 2.8880902 |
| S | 3.693501068 | -1.649522777 | -2.475551835 |
| O | 4.11373025 | -0.642907539 | -3.480785727 |
| O | 4.71829664 | -2.612026722 | -2.038980131 |
| O | 2.850627349 | -1.069101369 | -1.363541247 |
| C | 2.469102981 | -2.702140695 | -3.407898005 |
| F | 1.909961461 | -3.617816469 | -2.590419167 |
| F | 1.484269211 | -1.954612162 | -3.93753438 |
| F | 3.087150051 | -3.350646629 | -4.403733005 |
| H | 0.170862553 | 2.368720271 | 1.806787125 |

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**Supplementary Table 12 | Cartesian coordinate of VI. Units are presented in Å.**

SCF energy (in toluene) = -4815.96314996 hartree

ZPE = 1.342531 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.903339004 | -0.10771704 | 0.028472292 |
| Mo | 2.24707775 | 0.551525093 | 0.30580415 |
| P | 2.820946551 | -0.926364495 | 2.451287231 |
| P | -3.931435105 | 2.229489112 | 0.485401451 |
| N | -5.151093968 | -0.486738959 | -0.156823849 |
| N | 4.492580606 | 0.720469741 | 0.373626793 |
| P | 2.739585736 | 2.14645619 | -1.750841771 |
| P | -3.029814405 | -2.639683167 | -0.486027002 |
| N | -0.923219673 | 0.163845251 | 0.1285249 |
| N | 0.237793023 | 0.306380102 | 0.177640502 |
| N | -2.942706564 | -0.709634757 | 3.135237501 |
| N | -2.940914164 | -0.497788872 | 2.019875988 |
| N | -2.829508312 | 0.286120215 | -1.975026147 |
| N | -2.786378761 | 0.508096364 | -3.084521039 |
| N | 0.864244731 | 2.732051679 | 1.67876216 |
| N | 2.172213107 | 2.006699995 | 1.460534638 |
| H | 2.071642036 | -0.589753588 | 6.244128901 |
| H | -4.082113865 | 4.750906934 | 3.458950284 |
| H | -5.200987317 | 3.427806409 | 3.134012005 |
| H | 3.456795236 | 0.073810974 | 5.372234058 |
| C | 2.711636926 | -0.731477057 | 5.360971088 |
| C | -4.505878729 | 4.128348853 | 2.656945949 |
| H | -3.313146045 | 1.803192942 | 3.462730517 |
| H | 1.866158729 | 1.515748738 | 3.930363884 |
| H | -5.079487088 | 4.787242617 | 2.00140874 |
| H | 3.233828279 | -1.681217085 | 5.488619805 |
| H | -2.234695988 | 3.164977053 | 3.773032565 |
| H | 0.637266963 | 0.858855993 | 5.037915198 |
| C | 1.144081428 | 0.701773084 | 4.075107353 |
| C | -2.640267507 | 2.518431415 | 2.979682907 |
| H | 0.051067483 | -1.490206279 | 5.035976026 |
| H | -1.866684673 | 4.936914666 | 2.261665303 |
| C | 1.827871739 | -0.679257605 | 4.095411716 |
| C | -3.356140044 | 3.394686185 | 1.932973358 |
| H | -5.263144335 | 1.198852931 | 2.21350343 |

| | | | |
|---|---|---|---|
| H | 4.013485642 | 1.021360484 | 3.195256773 |
| H | 0.382537533 | 0.734099252 | 3.287090415 |
| H | -1.820081817 | 1.938170364 | 2.540703122 |
| H | 5.037406284 | -0.388533412 | 3.509458339 |
| H | -6.312903936 | 2.29235148 | 1.30982528 |
| C | 0.696845631 | -1.726762233 | 4.178441699 |
| C | -2.341170245 | 4.430568671 | 1.407629837 |
| H | 2.900137928 | -3.545381 | 4.381884008 |
| H | -4.716392857 | 5.341737767 | -0.040926424 |
| H | 0.066680603 | -1.711725482 | 3.280078673 |
| H | -1.551096548 | 3.964532018 | 0.801855502 |
| C | 4.380053576 | 0.077839579 | 2.766687913 |
| C | -5.528631707 | 1.533887827 | 1.19978213 |
| H | 7.068445277 | 0.188141087 | 2.499126709 |
| H | -8.115198711 | 0.84666251 | 0.789221993 |
| H | 1.067487115 | -2.744954656 | 4.32141065 |
| H | -2.80521908 | 5.207947975 | 0.79365671 |
| H | 4.547141204 | -2.8830282 | 4.247383736 |
| H | -6.192754065 | 4.35599984 | 0.051422666 |
| H | -4.687307337 | -2.336771762 | 1.969846168 |
| H | 3.635715124 | 3.623781374 | 0.702345925 |
| C | 3.755866905 | -3.421912369 | 3.711342237 |
| C | -5.322183182 | 4.599492875 | -0.570253208 |
| H | -2.657781717 | -4.597056017 | 2.790886626 |
| H | 2.086233811 | 5.753598882 | -0.607161621 |
| C | 6.561509329 | 0.44657807 | 1.573012088 |
| C | -7.431625526 | 0.151133077 | 0.308505916 |
| H | 4.144524239 | -4.428212975 | 3.498219436 |
| H | -5.703302009 | 5.088253345 | -1.478451003 |
| C | 5.167330709 | 0.410666146 | 1.518270422 |
| C | -6.054613587 | 0.357410188 | 0.417951522 |
| H | -4.950110143 | -3.997158125 | 2.517105449 |
| H | 4.217354499 | 5.179870016 | 0.049955401 |
| H | -2.131344368 | -2.957836089 | 2.390489541 |
| H | 1.136259579 | 4.257252791 | -0.467176568 |
| C | -4.769760479 | -3.372504144 | 1.630557778 |
| C | 4.055893474 | 4.116756295 | -0.18132809 |
| C | -2.350159609 | -3.940532707 | 1.963714749 |
| C | 1.830349834 | 4.811083708 | -1.111639027 |
| H | -8.98053956 | -1.11282956 | -0.515752063 |
| H | 8.37344855 | 0.841214776 | 0.464215718 |
| C | 3.404785725 | -2.758917025 | 2.364096171 |
| C | -4.525015268 | 3.346482557 | -0.985906246 |
| H | -5.655529337 | -3.457340978 | 0.990594788 |
| H | 5.041649571 | 3.680138145 | -0.375657151 |
| C | -7.911691541 | -0.938269497 | -0.414824707 |
| C | 7.286041193 | 0.815558421 | 0.441603073 |

| | | | |
|---|---|---|---|
| H | -1.424091288 | -4.34952609 | 1.549895991 |
| H | 1.273928054 | 5.06742516 | -2.016022329 |
| H | 1.359887025 | -3.583172562 | 2.254275063 |
| H | -2.62442425 | 4.440530907 | -1.256248817 |
| H | 5.542557047 | -2.380843693 | 2.036699924 |
| H | -6.403723968 | 2.268024956 | -1.394246425 |
| C | -3.492875585 | -3.884452895 | 0.924635558 |
| C | 3.125264676 | 4.018625977 | -1.411602998 |
| C | 2.283833002 | -3.556298007 | 1.664615089 |
| C | -3.293848092 | 3.777543737 | -1.81414063 |
| C | 4.680845037 | -2.800281188 | 1.5020894 |
| C | -5.455673792 | 2.505330092 | -1.889923721 |
| H | 4.919317871 | -3.85021428 | 1.280516888 |
| H | -5.695990457 | 3.096959648 | -2.784819611 |
| H | -4.166673843 | -5.907222087 | 1.276367307 |
| H | 4.054798148 | 5.744147514 | -2.330494376 |
| C | 6.593666733 | 1.157153713 | -0.714488648 |
| C | -6.989324136 | -1.799429042 | -1.003495157 |
| H | 2.05883359 | -3.138599733 | 0.679439185 |
| H | -2.714711778 | 2.919062397 | -2.167210484 |
| C | 5.195720936 | 1.103800921 | -0.729014779 |
| C | -5.620118043 | -1.559923332 | -0.856386452 |
| C | -3.792612274 | -5.314252152 | 0.429047449 |
| C | 3.846621861 | 4.69748735 | -2.596949134 |
| H | -4.569664714 | -5.335955175 | -0.345539797 |
| H | 4.812426464 | 4.228883718 | -2.819176102 |
| H | 2.615226105 | -4.594407611 | 1.521037293 |
| H | -3.635568152 | 4.331684225 | -2.700188176 |
| H | -7.319048037 | -2.662620622 | -1.576308978 |
| H | 7.124862197 | 1.453621282 | -1.615099262 |
| H | 4.584458937 | -2.287247229 | 0.544751177 |
| H | -5.000123409 | 1.572322589 | -2.228713407 |
| H | -0.983685047 | -5.045317981 | -0.401569241 |
| H | 1.337203429 | 4.085357117 | -3.899708329 |
| C | -4.619602499 | -2.499180332 | -1.4802024 |
| C | 4.467773544 | 1.464108465 | -2.006508804 |
| H | -2.905987247 | -5.827421219 | 0.044185278 |
| H | 3.252881568 | 4.706698031 | -3.515872027 |
| H | -5.089964868 | -3.470994754 | -1.673379599 |
| H | 5.090376494 | 2.144960668 | -2.598111161 |
| H | -0.173558042 | -3.462575227 | -0.315062923 |
| H | 0.141020888 | 3.245855002 | -2.878862739 |
| C | -0.67479192 | -4.171910942 | -0.984984045 |
| C | 0.851316027 | 3.123758182 | -3.706918373 |
| H | -4.307242719 | -2.10038354 | -2.456154269 |
| H | 4.347137886 | 0.563767569 | -2.621623033 |
| C | -1.84857665 | -3.51799544 | -1.741035842 |

| | | | |
|---|---|---|---|
| C | 1.84536286 | 1.969421697 | -3.461807338 |
| H | -0.70921505 | -1.67431882 | -2.134110858 |
| H | 0.25682637 | 0.722780756 | -2.607711723 |
| H | 0.071955742 | -4.51112488 | -1.712050537 |
| H | 0.261724578 | 2.876877128 | -4.600550551 |
| C | -1.271096326 | -2.439342254 | -2.679110052 |
| C | 1.01143356 | 0.672816345 | -3.400452251 |
| H | -2.996857843 | -5.39333511 | -2.050102008 |
| H | 3.500844573 | 2.760988705 | -4.699137694 |
| H | -3.335100964 | -4.130432358 | -3.251551774 |
| H | 3.45181022 | 0.980098292 | -4.588620269 |
| C | -2.554468496 | -4.573144291 | -2.620852721 |
| C | 2.841298481 | 1.887114232 | -4.637459544 |
| H | -0.579228926 | -2.921022342 | -3.381844286 |
| H | 0.486281762 | 0.5514281 | -4.359213306 |
| H | -2.04662552 | -1.946076408 | -3.274809093 |
| H | 1.630456368 | -0.210349039 | -3.243470071 |
| H | -1.808667062 | -5.012093714 | -3.29912004 |
| H | 2.270747157 | 1.841731439 | -5.576477775 |
| S | 3.655941962 | -1.87979256 | -2.132702528 |
| O | 3.594794863 | -1.243644992 | -3.466320025 |
| O | 4.997194427 | -2.051428525 | -1.549142089 |
| O | 2.628101099 | -1.313714547 | -1.157252904 |
| C | 3.031038581 | -3.606464368 | -2.463426998 |
| F | 2.873680078 | -4.295627164 | -1.320565911 |
| F | 1.846670291 | -3.559806047 | -3.098992907 |
| F | 3.908877958 | -4.248075437 | -3.235464421 |
| H | 0.954722089 | 3.701248071 | 1.350623511 |
| H | 0.649667075 | 2.747300768 | 2.68449226 |
| H | 0.088180536 | 2.269330419 | 1.17820841 |

**Supplementary Table 13 | Cartesian coordinate of VII. Units are presented in Å.**

SCF energy (in toluene) = -4759.65039062 hartree

ZPE = 1.300929 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.924811878 | -0.084439953 | 0.000810928 |
| Mo | 2.227885423 | 0.737577683 | 0.48241388 |
| P | 2.761924421 | -0.634176434 | 2.619828969 |
| P | -3.636015502 | 2.314840674 | 0.519047444 |
| N | -5.180332744 | -0.222006742 | -0.07852094 |
| N | 4.495025027 | 0.779917131 | 0.496635945 |
| P | 2.742721221 | 2.07986163 | -1.636853994 |
| P | -3.287483054 | -2.552142603 | -0.568057957 |
| N | -0.923507871 | 0.069597987 | 0.091425142 |
| N | 0.222204759 | 0.19020411 | 0.154032495 |
| N | -3.029128698 | -0.74796598 | 3.099067966 |
| N | -2.983549467 | -0.505297437 | 1.989803131 |
| N | -2.866579304 | 0.337906495 | -1.991745443 |
| N | -2.846388381 | 0.584841446 | -3.099606364 |
| N | 1.965140971 | 2.103755598 | 1.409732184 |
| H | 1.996488316 | -0.181225481 | 6.397189141 |
| H | -3.272534669 | 4.787756241 | 3.510057476 |
| H | -4.62578659 | 3.704680381 | 3.175894992 |
| H | 3.50949459 | 0.162364911 | 5.554483669 |
| C | 2.614131549 | -0.472672637 | 5.534548986 |
| C | -3.821565632 | 4.28156452 | 2.701749716 |
| H | -2.973195759 | 1.796432195 | 3.467870397 |
| H | 2.172226808 | 1.914122917 | 4.212426034 |
| H | -4.277923513 | 5.059540694 | 2.084743284 |
| H | 2.925234092 | -1.506851344 | 5.693043483 |
| H | -1.686766311 | 2.982681663 | 3.718332119 |
| H | 0.762333722 | 1.399682071 | 5.156915108 |
| C | 1.331862055 | 1.20973601 | 4.234496399 |
| C | -2.218370445 | 2.399652887 | 2.951894345 |
| H | -0.108154286 | -0.856967451 | 5.117949355 |
| H | -1.122627312 | 4.677153158 | 2.182363098 |
| C | 1.788269147 | -0.263656102 | 4.246071367 |
| C | -2.835037008 | 3.376189041 | 1.931886191 |
| H | -5.006603807 | 1.474142484 | 2.306824413 |
| H | 4.074760664 | 1.243833743 | 3.320843728 |

| | | | |
|---|---|---|---|
| H | 0.696915086 | 1.439256943 | 3.376892112 |
| H | -1.499099792 | 1.722209921 | 2.482961693 |
| H | 5.026059108 | -0.209455429 | 3.667725823 |
| H | -5.974375254 | 2.661248169 | 1.432933665 |
| C | 0.522846042 | -1.145482248 | 4.264840562 |
| C | -1.683158385 | 4.221894685 | 1.352961645 |
| H | 2.564252724 | -3.26661789 | 4.514860401 |
| H | -4.057672879 | 5.501383071 | 0.048784545 |
| H | -0.0741467 | -1.007149413 | 3.355412709 |
| H | -0.974687959 | 3.607271799 | 0.783592721 |
| C | 4.387408504 | 0.270282989 | 2.916072282 |
| C | -5.279004073 | 1.822654239 | 1.300068233 |
| H | 7.079592357 | 0.271646351 | 2.615218548 |
| H | -7.940024186 | 1.380640675 | 1.052912364 |
| H | 0.747207863 | -2.212358597 | 4.370557779 |
| H | -2.035843081 | 5.038036558 | 0.713096358 |
| H | 4.260628381 | -2.725197395 | 4.478419154 |
| H | -5.637564219 | 4.703692234 | 0.235201422 |
| H | -4.830422356 | -2.241797771 | 1.951660371 |
| H | 3.870694811 | 3.549618889 | 0.698773165 |
| C | 3.463697885 | -3.202388741 | 3.893696263 |
| C | -4.78591226 | 4.848181076 | -0.44251633 |
| H | -2.885055235 | -4.631190985 | 2.629586912 |
| H | 2.010920595 | 5.663201558 | -0.512654838 |
| C | 6.569315769 | 0.491304415 | 1.680849202 |
| C | -7.357504999 | 0.625989903 | 0.529429495 |
| H | 3.788731272 | -4.233064403 | 3.688256388 |
| H | -5.162897836 | 5.39039533 | -1.322967482 |
| C | 5.172999192 | 0.513657372 | 1.649395921 |
| C | -5.962763416 | 0.701429442 | 0.556064293 |
| H | -5.167401871 | -3.898050442 | 2.469551539 |
| H | 4.284471057 | 5.141581025 | 0.030062007 |
| H | -2.305543941 | -3.002032578 | 2.254318959 |
| H | 1.447855965 | 4.104819179 | 0.134614611 |
| C | -4.984729204 | -3.261074388 | 1.591254991 |
| C | 4.160511874 | 4.076328114 | -0.215671154 |
| C | -2.585661059 | -3.960622169 | 1.809580258 |
| C | 1.792579423 | 4.615723712 | -0.770993036 |
| H | -9.069673639 | -0.478413147 | -0.19827732 |
| H | 8.375796448 | 0.713582842 | 0.51757116 |
| C | 3.227076955 | -2.500903036 | 2.542150251 |
| C | -4.171186377 | 3.514219989 | -0.910471067 |
| H | -5.896774243 | -3.277781121 | 0.982849126 |
| H | 5.136983627 | 3.70593724 | -0.550308771 |
| C | -7.98452792 | -0.406658688 | -0.165169281 |
| C | 7.287767619 | 0.740532086 | 0.514101069 |
| H | -1.696260871 | -4.392605042 | 1.34103496 |

| | | | |
|---|---|---|---|
| H | 0.979848723 | 4.62106185 | -1.504217648 |
| H | 1.124495404 | -3.13170612 | 2.296312085 |
| H | -2.170414718 | 4.37340489 | -1.280075828 |
| H | 5.396519959 | -2.249450274 | 2.293587425 |
| H | -6.190940986 | 2.688762251 | -1.225774459 |
| C | -3.766289407 | -3.820076136 | 0.822489597 |
| C | 3.077712999 | 3.953443536 | -1.311025368 |
| C | 2.089406901 | -3.21787307 | 1.78060502 |
| C | -2.949198412 | 3.81300631 | -1.806423622 |
| C | 4.53226095 | -2.62706633 | 1.731539769 |
| C | -5.243180786 | 2.800025654 | -1.765551038 |
| H | 4.717368758 | -3.689584171 | 1.521158029 |
| H | -5.445280045 | 3.413744974 | -2.655898695 |
| H | -4.531533649 | -5.812994957 | 1.163668147 |
| H | 3.837208995 | 5.740353127 | -2.263237452 |
| C | 6.591209628 | 1.02701766 | -0.654720185 |
| C | -7.186121697 | -1.344733501 | -0.816417919 |
| H | 1.983531514 | -2.823165276 | 0.765342694 |
| H | -2.500413525 | 2.900336147 | -2.205925216 |
| C | 5.191583273 | 1.049796554 | -0.64305598 |
| C | -5.794196048 | -1.237145773 | -0.757659582 |
| C | -4.162715045 | -5.22010995 | 0.313004506 |
| C | 3.580968733 | 4.710822573 | -2.555302567 |
| H | -4.970586558 | -5.182859376 | -0.429270917 |
| H | 4.487702312 | 4.259683738 | -2.979115333 |
| H | 2.3307156 | -4.288023269 | 1.699852469 |
| H | -3.273918741 | 4.424871636 | -2.661723723 |
| H | -7.631513495 | -2.16695495 | -1.371722852 |
| H | 7.117090836 | 1.228867979 | -1.584187152 |
| H | 4.484470673 | -2.127760374 | 0.763700487 |
| H | -4.926848568 | 1.813410279 | -2.112004253 |
| H | -1.390672634 | -5.081209916 | -0.655552398 |
| H | 0.951483493 | 3.85849289 | -3.556042857 |
| C | -4.926600371 | -2.253370086 | -1.457237389 |
| C | 4.449783741 | 1.363949823 | -1.919939307 |
| H | -3.320691282 | -5.768696374 | -0.120072635 |
| H | 2.828501212 | 4.77627528 | -3.347366924 |
| H | -5.500044804 | -3.170733151 | -1.64172575 |
| H | 5.077053868 | 1.995363185 | -2.562154778 |
| H | -0.492011311 | -3.54494288 | -0.623938275 |
| H | 0.001080689 | 2.724112733 | -2.568566272 |
| C | -1.080092777 | -4.220294657 | -1.257420156 |
| C | 0.660833188 | 2.808325196 | -3.441257504 |
| H | -4.63186816 | -1.858851949 | -2.440533612 |
| H | 4.289007189 | 0.420559051 | -2.465035521 |
| C | -2.267599583 | -3.494483467 | -1.920521488 |
| C | 1.864076981 | 1.849948863 | -3.339291593 |

| | | | |
|---|---|---|---|
| H | -1.077289102 | -1.69978668 | -2.361922621 |
| H | 0.651939393 | 0.208519288 | -2.52393748 |
| H | -0.404491175 | -4.592134162 | -2.037306373 |
| H | 0.066827813 | 2.534851053 | -4.325306269 |
| C | -1.688239961 | -2.441534041 | -2.885228735 |
| C | 1.316201726 | 0.407901037 | -3.37116729 |
| H | -3.513482187 | -5.313677908 | -2.182379247 |
| H | 3.243730463 | 3.031418683 | -4.613009014 |
| H | -3.904414675 | -3.999177534 | -3.308617038 |
| H | 3.608286896 | 1.289101531 | -4.54763319 |
| C | -3.088825699 | -4.492388592 | -2.764863119 |
| C | 2.801890145 | 2.031631479 | -4.550737043 |
| H | -1.04337665 | -2.949376121 | -3.614764785 |
| H | 0.733680598 | 0.279234341 | -4.296075895 |
| H | -2.466870491 | -1.913945001 | -3.446461951 |
| H | 2.114314837 | -0.337269937 | -3.374357293 |
| H | -2.42440106 | -4.936460703 | -3.520792284 |
| H | 2.221248295 | 1.87116782 | -5.471547991 |
| S | 3.793500353 | -2.240781724 | -2.017687932 |
| O | 4.116441824 | -1.511520418 | -3.271243919 |
| O | 4.892320877 | -3.012923286 | -1.409953484 |
| O | 2.979180375 | -1.425719898 | -1.049172953 |
| C | 2.579455875 | -3.540548652 | -2.572245301 |
| F | 2.169762707 | -4.286047399 | -1.525354346 |
| F | 1.489073823 | -2.975675962 | -3.130350565 |
| F | 3.138790646 | -4.357117208 | -3.475358232 |

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**Supplementary Table 14 | Cartesian coordinate of VIII. Units are presented in Å.**

SCF energy (in toluene) = -2036.04242654 hartree

ZPE = 0.646560 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.659031782 | 0.003847832 | 0.008369209 |
| P | 3.167843185 | -2.187772084 | 1.173564489 |
| N | 4.906853844 | -0.007006176 | -0.01577229 |
| P | 3.163919188 | 2.190493396 | -1.168030075 |
| N | -0.508143769 | 0.018982042 | 0.042746851 |
| N | 0.627561218 | 0.013603454 | 0.030405016 |
| N | 2.662630055 | 1.459652118 | 2.825545605 |
| N | 2.660579558 | 0.929070231 | 1.820843475 |
| N | 2.612468294 | -0.921232062 | -1.803679598 |
| N | 2.587683343 | -1.451571597 | -2.808187894 |
| H | 2.567874951 | -3.759688747 | 4.692952513 |
| H | 3.96971534 | -2.823388195 | 4.17194231 |
| C | 3.171438333 | -3.485674866 | 3.814250437 |
| H | 2.425844126 | -0.839078522 | 3.819871772 |
| H | 3.632313823 | -4.402358742 | 3.438180152 |
| H | 1.098194837 | -1.870639728 | 4.362576217 |
| C | 1.660067706 | -1.541287762 | 3.475510079 |
| H | 0.456011328 | -3.865804503 | 3.299453632 |
| C | 2.259907168 | -2.782856672 | 2.785543271 |
| H | 4.583045111 | -0.998852873 | 2.724041302 |
| H | 0.970996805 | -0.999607972 | 2.819495308 |
| H | 5.471467097 | -2.439279022 | 2.222512248 |
| C | 1.08130661 | -3.704834949 | 2.409012857 |
| H | 3.353441261 | -5.407803699 | 1.596245137 |
| H | 0.444785363 | -3.254971913 | 1.636277115 |
| C | 4.840090478 | -1.620427243 | 1.853681776 |
| H | 7.529906315 | -1.428800512 | 1.585164276 |
| H | 1.404826626 | -4.690934288 | 2.059916852 |
| H | 4.985541238 | -4.703605064 | 1.6078241 |
| H | 4.586895642 | 2.510699728 | 1.431443644 |
| C | 4.133138029 | -4.965394645 | 0.967925165 |
| H | 2.77280051 | 5.040841415 | 1.365740974 |
| C | 7.008650439 | -0.800835529 | 0.866373158 |
| H | 4.47570422 | -5.751867209 | 0.278370178 |
| C | 5.611279997 | -0.780771798 | 0.86354941 |

| | | | |
|---|---|---|---|
| H | 5.018219022 | 4.224266167 | 1.477764825 |
| H | 2.082092821 | 3.41146625 | 1.347492285 |
| C | 4.819410149 | 3.375694509 | 0.80638095 |
| C | 2.457890629 | 4.215348003 | 0.709481568 |
| H | 8.804228586 | -0.02636472 | -0.05794856 |
| C | 3.630337868 | -3.765645268 | 0.139930314 |
| H | 5.748505437 | 3.168450972 | 0.262075075 |
| C | 7.716190911 | -0.020951537 | -0.046160799 |
| H | 1.626245933 | 4.58214344 | 0.100421341 |
| H | 1.580611626 | -4.564628207 | -0.061448199 |
| H | 5.711716058 | -3.190246672 | -0.311400994 |
| C | 3.663566063 | 3.76380265 | -0.144816697 |
| C | 2.402374745 | -4.205557804 | -0.688265065 |
| C | 4.769282685 | -3.388475719 | -0.835765944 |
| H | 4.94556586 | -4.238815635 | -1.511195284 |
| H | 4.524550091 | 5.741953761 | -0.301597692 |
| C | 6.996851554 | 0.766030252 | -0.943252353 |
| H | 2.02051792 | -3.398061208 | -1.318039147 |
| C | 5.59974615 | 0.759828074 | -0.910165642 |
| C | 4.160025735 | 4.958740343 | -0.983552035 |
| H | 4.996154122 | 4.688899839 | -1.641330826 |
| H | 2.695264658 | -5.033861188 | -1.351155844 |
| H | 7.508641891 | 1.388893739 | -1.673197316 |
| H | 4.531822864 | -2.52118115 | -1.455774679 |
| H | 1.406482908 | 4.710570111 | -2.017101473 |
| C | 4.815666429 | 1.607112843 | -1.883596421 |
| H | 3.371387409 | 5.408464648 | -1.595298852 |
| H | 5.446844387 | 2.420022884 | -2.265691935 |
| H | 0.442138222 | 3.283842693 | -1.572593809 |
| C | 1.066194707 | 3.727574549 | -2.358924065 |
| H | 4.534452264 | 0.988187275 | -2.748370088 |
| C | 2.227609878 | 2.794386132 | -2.760372986 |
| H | 0.921261607 | 1.023549904 | -2.766721664 |
| H | 0.423508514 | 3.894451565 | -3.23579184 |
| C | 1.601371812 | 1.558706111 | -3.437306025 |
| H | 3.60096828 | 4.400936905 | -3.442397685 |
| H | 3.908025158 | 2.818816169 | -4.182677875 |
| C | 3.123712345 | 3.488556612 | -3.808356499 |
| H | 1.023924249 | 1.893501421 | -4.312250871 |
| H | 2.352915134 | 0.849258126 | -3.797825383 |
| H | 2.504253275 | 3.768088938 | -4.674161249 |

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**Supplementary Table 15 | Cartesian coordinate of IX. Units are presented in Å.**

SCF energy (in toluene) = -2779.48508967 hartree

ZPE = 0.679697 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.543823026 | 0.411087344 | 0.304962972 |
| P | 3.112064197 | -0.816271482 | 2.452595458 |
| N | 4.819973895 | 0.741782854 | 0.396727368 |
| P | 2.885497538 | 2.084537431 | -1.490692965 |
| N | -0.409376143 | 1.153250176 | 0.99823078 |
| N | 0.858593696 | 0.852979878 | 0.679488653 |
| H | 2.343054054 | 0.076753165 | 6.155909035 |
| H | 3.913666948 | -0.029009395 | 5.354473619 |
| C | 2.894183031 | -0.436660801 | 5.353689838 |
| H | 2.927620783 | 1.886310352 | 3.919072874 |
| H | 2.950001762 | -1.492440103 | 5.624122728 |
| H | 1.367080979 | 1.694024606 | 4.726312815 |
| C | 1.97522642 | 1.340154574 | 3.879986472 |
| H | 0.187288856 | -0.442514985 | 4.872072221 |
| C | 2.166797956 | -0.187433479 | 4.014982109 |
| H | 4.629260146 | 0.865316976 | 3.292881454 |
| H | 1.468407628 | 1.606777502 | 2.949194325 |
| H | 5.459758528 | -0.684020981 | 3.369123104 |
| C | 0.772680906 | -0.847426253 | 4.032711912 |
| H | 2.572452585 | -3.270557708 | 4.533092202 |
| H | 0.222080356 | -0.637962716 | 3.107777129 |
| C | 4.817633669 | -0.062392411 | 2.733689199 |
| H | 7.494804204 | -0.04554184 | 2.309701134 |
| H | 0.828440887 | -1.934009354 | 4.167227704 |
| H | 4.310288375 | -2.881166511 | 4.561676825 |
| H | 3.862419376 | 3.255554398 | 1.033470441 |
| C | 3.508540393 | -3.336892515 | 3.966602987 |
| H | 1.669996928 | 5.26699428 | 0.270369266 |
| C | 6.945498746 | 0.313187232 | 1.442761896 |
| H | 3.748283746 | -4.4062851 | 3.865468769 |
| C | 5.549070721 | 0.315306381 | 1.4681052 |
| H | 4.013786769 | 4.99458937 | 0.69436015 |
| H | 1.377496274 | 3.547636677 | 0.617332491 |
| C | 4.035856241 | 3.992599945 | 0.240153112 |
| C | 1.603727927 | 4.265671126 | -0.181114125 |

| | | | |
|---|---|---|---|
| H | 8.703009468 | 0.786173175 | 0.277896343 |
| C | 3.401719698 | -2.728443914 | 2.556973606 |
| H | 5.045604622 | 3.836929945 | -0.158768687 |
| C | 7.615514285 | 0.783279312 | 0.315722283 |
| H | 0.765168737 | 4.276526066 | -0.884502704 |
| H | 1.257327829 | -3.161845281 | 2.254277927 |
| H | 5.596599117 | -2.704582012 | 2.374848479 |
| C | 2.948151823 | 3.915456668 | -0.85404903 |
| C | 2.229752542 | -3.39037626 | 1.798938719 |
| C | 4.715323256 | -3.034915907 | 1.808845588 |
| H | 4.80397298 | -4.124268532 | 1.684858212 |
| H | 3.411565684 | 5.946750689 | -1.452572653 |
| C | 6.866730962 | 1.259349459 | -0.757776777 |
| H | 2.20496844 | -3.072580281 | 0.751920475 |
| C | 5.470964051 | 1.224352686 | -0.699991838 |
| C | 3.286271656 | 4.963368328 | -1.931147348 |
| H | 4.226150364 | 4.734622392 | -2.449946811 |
| H | 2.356694744 | -4.483315778 | 1.820526879 |
| H | 7.352011711 | 1.639035029 | -1.653452535 |
| H | 4.753306378 | -2.601949324 | 0.806683828 |
| H | 0.78074871 | 3.895661883 | -3.031496793 |
| C | 4.667566875 | 1.690899871 | -1.894941765 |
| H | 2.49844638 | 5.069480679 | -2.684063331 |
| H | 5.192863849 | 2.515835564 | -2.39438956 |
| H | 0.039422986 | 2.457206206 | -2.291209632 |
| C | 0.657408883 | 2.811462562 | -3.127333991 |
| H | 4.625101661 | 0.847711487 | -2.601821592 |
| C | 1.99549 | 2.049175729 | -3.207690656 |
| H | 1.059405513 | 0.129618939 | -2.698400073 |
| H | 0.090903237 | 2.629752929 | -4.052480022 |
| C | 1.669007799 | 0.569883302 | -3.496374939 |
| H | 3.102648301 | 3.656824032 | -4.257597772 |
| H | 3.774305361 | 2.029256407 | -4.498770006 |
| C | 2.845890335 | 2.598572549 | -4.371294774 |
| H | 1.100478806 | 0.510302776 | -4.437399403 |
| H | 2.56772968 | -0.042523699 | -3.606283541 |
| H | 2.276699 | 2.498206778 | -5.307878983 |
| H | -0.56781326 | 2.148544079 | 1.167909318 |
| S | 4.056777356 | -2.087775663 | -1.969034381 |
| O | 4.402978764 | -1.19535193 | -3.100475362 |
| O | 5.141784748 | -2.931527722 | -1.442851517 |
| O | 3.218086967 | -1.436336993 | -0.885228582 |
| C | 2.810545059 | -3.2791059 | -2.677410508 |
| F | 2.377470098 | -4.124432748 | -1.726619731 |
| F | 1.748059144 | -2.619723417 | -3.171282095 |
| F | 3.366299123 | -3.99342107 | -3.665039201 |
| H | -1.092194081 | 0.762945582 | 0.346312067 |

**Supplementary Table 16 | Cartesian coordinate of X. Units are presented in Å.**

SCF energy (in toluene) = -2779.89642593 hartree

ZPE = 0.693512 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.087599173 | -0.532788822 | -0.704128949 |
| P | 2.185305993 | -1.37841144 | -0.079536441 |
| N | -0.212800431 | -0.690744436 | 1.694965242 |
| P | -2.575492022 | -0.425750657 | -0.120873092 |
| N | 0.41610222 | 1.048227851 | -3.11315416 |
| N | 0.12803547 | -0.273856939 | -2.524925169 |
| H | 3.23714817 | -5.002836989 | -0.987186835 |
| H | 2.934698861 | -4.340184699 | 0.620785511 |
| C | 3.269186298 | -4.079460144 | -0.391209116 |
| H | 0.486742976 | -3.795512315 | -0.17522473 |
| H | 4.315363847 | -3.766084013 | -0.333646613 |
| H | 0.935991261 | -4.525545502 | -1.718664205 |
| C | 0.928596813 | -3.57988771 | -1.156830927 |
| H | 2.831757967 | -3.657149128 | -3.079164975 |
| C | 2.369095437 | -3.021397641 | -1.059969462 |
| H | 1.537213741 | -2.988266245 | 1.618246485 |
| H | 0.255683377 | -2.904936168 | -1.716225748 |
| H | 2.832837849 | -1.987879916 | 2.248013442 |
| C | 2.872370285 | -2.731237579 | -2.488299229 |
| H | 5.24994675 | -1.823398868 | -0.844594144 |
| H | 2.245035704 | -1.986909203 | -2.994250684 |
| C | 1.898049467 | -1.951785514 | 1.67805799 |
| H | 1.827366916 | -1.296750375 | 4.322530523 |
| H | 3.912069554 | -2.385846525 | -2.498864605 |
| H | 5.074803495 | -1.868900772 | 0.925768175 |
| H | -1.57290243 | -3.00218433 | 1.039706046 |
| C | 5.07945256 | -1.210852156 | 0.047351248 |
| H | -3.719344465 | -3.998279066 | -0.852242877 |
| C | 0.952318118 | -0.939752511 | 3.785605509 |
| H | 5.944606124 | -0.540746909 | 0.151935341 |
| C | 0.856213158 | -1.136122269 | 2.408662796 |
| H | -3.068227132 | -3.856733483 | 1.453762656 |
| H | -2.307741478 | -3.096658699 | -1.430115235 |
| C | -2.626323347 | -2.86109404 | 1.308882428 |
| C | -3.341737303 | -2.990491545 | -1.075395294 |

| | | | |
|---|---|---|---|
| H | -0.033288349 | -0.133082405 | 5.531393691 |
| C | 3.802902063 | -0.354696742 | -0.047128176 |
| H | -2.66659997 | -2.34294592 | 2.273625839 |
| C | -0.0890953 | -0.301246012 | 4.458127557 |
| H | -3.940286552 | -2.592012613 | -1.898809468 |
| H | 3.82151421 | -0.092061469 | -2.242586466 |
| H | 3.871158485 | 0.031000134 | 2.121289663 |
| C | -3.420207052 | -2.128870874 | 0.204029919 |
| C | 3.832845084 | 0.510150369 | -1.325985177 |
| C | 3.740107316 | 0.579708135 | 1.180309678 |
| H | 4.569621492 | 1.297794697 | 1.11314085 |
| H | -5.258096028 | -3.012207646 | 0.927821513 |
| C | -1.206919385 | 0.102405025 | 3.735697931 |
| H | 2.986675031 | 1.20636498 | -1.339657553 |
| C | -1.243898068 | -0.099895752 | 2.352243343 |
| C | -4.882772108 | -2.009796437 | 0.677131408 |
| H | -4.979047201 | -1.395411494 | 1.581840074 |
| H | 4.755146466 | 1.107429493 | -1.335594259 |
| H | -2.044274016 | 0.590041735 | 4.228215721 |
| H | 2.809566809 | 1.152696968 | 1.241571024 |
| H | -5.150431779 | -0.771346913 | -1.963926222 |
| C | -2.450100242 | 0.368460287 | 1.565324044 |
| H | -5.548145378 | -1.599853709 | -0.088800932 |
| H | -3.359436606 | 0.235204067 | 2.165943607 |
| H | -3.672645041 | -0.524933088 | -2.923950754 |
| C | -4.415324139 | -0.027840407 | -2.286625655 |
| H | -2.348096213 | 1.44832154 | 1.382449953 |
| C | -3.760030855 | 0.728627407 | -1.112948186 |
| H | -2.218552547 | 1.472790532 | -2.465844682 |
| H | -4.949493701 | 0.701334009 | -2.911639584 |
| C | -2.913355184 | 1.868747558 | -1.714400543 |
| H | -5.469765526 | 0.602665721 | 0.291598348 |
| H | -4.423268817 | 2.016659088 | 0.546509506 |
| C | -4.849134403 | 1.350036999 | -0.211950666 |
| H | -3.586475472 | 2.574363359 | -2.22237102 |
| H | -2.345277417 | 2.425412077 | -0.964110123 |
| H | -5.514996201 | 1.960233727 | -0.83852727 |
| H | -0.304600157 | 1.289002059 | -3.806076748 |
| S | 0.245349562 | 2.732539455 | 0.557591478 |
| O | -1.10938386 | 3.296970139 | 0.676473625 |
| O | 0.947335655 | 2.350258591 | 1.788379745 |
| O | 0.347574249 | 1.649118777 | -0.54355041 |
| C | 1.28018391 | 4.04161934 | -0.281652863 |
| F | 2.560027031 | 3.646090344 | -0.335807584 |
| F | 0.837094236 | 4.218862134 | -1.544552192 |
| F | 1.193104104 | 5.188141 | 0.380001553 |
| H | 0.435641675 | 1.766558704 | -2.34933828 |

```
  H     1.324037558    1.027603791   -3.595498159
-------------------------------------------------
```

**Supplementary Table 17 | Cartesian coordinate of XI. Units are presented in Å.**

SCF energy (in toluene) = -2723.59879416 hartree

ZPE = 0.652246 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.583513278 | 0.730782997 | 0.409409573 |
| P | 2.995062843 | -0.769789456 | 2.416464735 |
| N | 4.757091388 | 1.126657939 | 0.815022187 |
| P | 3.244896452 | 1.976654377 | -1.679615958 |
| N | 1.879410911 | 1.923562635 | 1.330637526 |
| H | 1.762388891 | -1.619454027 | 5.980769889 |
| H | 3.361986914 | -1.055123373 | 5.481143387 |
| C | 2.476762123 | -1.610966812 | 5.144165766 |
| H | 2.088601597 | 1.046588563 | 4.815384926 |
| H | 2.771805811 | -2.649512006 | 4.959980453 |
| H | 0.490260479 | 0.334297345 | 5.044844567 |
| C | 1.310307485 | 0.450557362 | 4.321788555 |
| H | -0.116999127 | -1.845221245 | 4.355484762 |
| C | 1.802813318 | -0.958598675 | 3.920513181 |
| H | 3.64591389 | 1.279415371 | 3.452814163 |
| H | 0.930210823 | 1.015158552 | 3.463468692 |
| H | 4.820267747 | 0.071392837 | 4.004476248 |
| C | 0.563370005 | -1.773797338 | 3.493667564 |
| H | 4.902285143 | -2.563573034 | 4.115334066 |
| H | 0.019507253 | -1.29046129 | 2.675640766 |
| C | 4.272764212 | 0.438989547 | 3.128152062 |
| H | 6.884999939 | 1.088090122 | 3.450642577 |
| H | 0.80409459 | -2.792233343 | 3.178113665 |
| H | 5.937856171 | -1.740625382 | 2.927227283 |
| H | 3.442912966 | 3.853925235 | 0.576391667 |
| C | 5.200580173 | -2.542380245 | 3.06092807 |
| H | 1.297572487 | 5.214904784 | -1.220843538 |
| C | 6.550870125 | 1.245534546 | 2.428236408 |
| H | 5.712848759 | -3.491964812 | 2.845395877 |
| C | 5.227972755 | 0.944667155 | 2.089368545 |
| H | 3.50558259 | 5.451326728 | -0.194979208 |
| H | 1.100474642 | 3.632067012 | -0.432898949 |
| C | 3.737524951 | 4.385376505 | -0.334878186 |
| C | 1.456907929 | 4.1327868 | -1.339607812 |
| H | 8.44799931 | 1.992736359 | 1.712159273 |

| | | | |
|---|---|---|---|
| C | 3.997308672 | -2.39376266 | 2.108750592 |
| H | 4.824934241 | 4.303419404 | -0.461262911 |
| C | 7.417318648 | 1.749107017 | 1.462441393 |
| H | 0.841466908 | 3.798690014 | -2.18266913 |
| H | 2.772116456 | -3.845316132 | 3.235876429 |
| H | 5.178783886 | -1.464357829 | 0.486204582 |
| C | 2.961933017 | 3.872905698 | -1.568903 |
| C | 3.10008858 | -3.64483715 | 2.210216815 |
| C | 4.514593457 | -2.320981908 | 0.652814615 |
| H | 5.089638867 | -3.231963834 | 0.428337483 |
| H | 3.359102042 | 5.727825947 | -2.604871093 |
| C | 6.936210587 | 1.933785939 | 0.167419716 |
| H | 2.221264661 | -3.566535746 | 1.562336194 |
| C | 5.612409232 | 1.609609717 | -0.136415712 |
| C | 3.440857553 | 4.650105438 | -2.809005804 |
| H | 4.490351469 | 4.444558683 | -3.058567611 |
| H | 3.685800356 | -4.516906212 | 1.88196965 |
| H | 7.580528423 | 2.324616963 | -0.616406577 |
| H | 3.68012728 | -2.275717026 | -0.058999727 |
| H | 1.271737439 | 2.639945432 | -3.98580946 |
| C | 5.116290643 | 1.759780511 | -1.552367055 |
| H | 2.826791799 | 4.440961746 | -3.691775672 |
| H | 5.678560232 | 2.549590504 | -2.06684166 |
| H | 0.760379795 | 1.193670361 | -3.07493594 |
| C | 1.458832188 | 1.570329103 | -3.83173764 |
| H | 5.332855787 | 0.827364578 | -2.09274885 |
| C | 2.924347705 | 1.283406873 | -3.444956342 |
| H | 2.40096366 | -0.700719998 | -2.642543027 |
| H | 1.230640464 | 1.060264005 | -4.779247946 |
| C | 3.102331257 | -0.250811702 | -3.350358867 |
| H | 3.757109609 | 2.877811328 | -4.736355205 |
| H | 4.93229976 | 1.622816835 | -4.298403971 |
| C | 3.877218777 | 1.809410168 | -4.538297683 |
| H | 2.906373231 | -0.687833962 | -4.340550882 |
| H | 4.124880091 | -0.543687207 | -3.073754975 |
| H | 3.66433001 | 1.277011774 | -5.477286327 |
| S | 0.089146906 | -1.419983755 | -0.335890063 |
| O | 0.797085184 | -2.654910767 | 0.055771813 |
| O | -1.021706026 | -0.957066605 | 0.506478993 |
| O | 1.044678771 | -0.29867308 | -0.773504031 |
| C | -0.667275678 | -1.796842083 | -1.997369384 |
| F | -1.227645381 | -0.695393523 | -2.521999249 |
| F | 0.272695625 | -2.243010908 | -2.850573339 |
| F | -1.608103164 | -2.739623976 | -1.867002721 |

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**Supplementary Table 18 | Cartesian coordinate of XII. Units are presented in Å.**

SCF energy (in toluene) = -2724.16007909 hartree

ZPE = 0.659619 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.46557288 | 0.04962626 | -0.09442448 |
| P | -1.424416763 | -2.217968855 | 0.558353543 |
| N | -1.919728212 | -0.23348405 | -1.69912721 |
| P | -0.82598655 | 2.397945233 | -0.859908169 |
| N | 0.943409506 | -0.290738103 | -1.130450282 |
| H | -0.491633022 | -5.855901291 | -0.34949788 |
| H | -2.099859598 | -5.125149911 | -0.275420628 |
| C | -1.085209757 | -5.070401584 | 0.141201108 |
| H | -1.245013406 | -3.612871679 | -2.165986335 |
| H | -1.132461204 | -5.318251039 | 1.206164821 |
| H | 0.369051989 | -4.330838256 | -2.038456797 |
| C | -0.280325784 | -3.533180563 | -1.648939084 |
| H | 1.592839111 | -4.49852419 | 0.077067477 |
| C | -0.413307798 | -3.709117676 | -0.120974804 |
| H | -3.317462342 | -3.155084003 | -0.814102163 |
| H | 0.173894921 | -2.571900504 | -1.907726372 |
| H | -3.722882116 | -1.702866817 | 0.093196441 |
| C | 0.994192337 | -3.681879428 | 0.508806563 |
| H | -3.127304329 | -4.607046965 | 1.781818043 |
| H | 1.503488786 | -2.733466562 | 0.309221165 |
| C | -2.946071656 | -2.160005561 | -0.538726332 |
| H | -4.292092461 | -2.375020553 | -2.847285128 |
| H | 0.970340865 | -3.817823682 | 1.5944459 |
| H | -4.245497191 | -3.249490307 | 1.539333307 |
| H | 1.981340696 | 1.960275954 | -1.448158463 |
| C | -3.424067161 | -3.624892546 | 2.16200653 |
| H | 2.055368391 | 4.52717406 | 0.423260928 |
| C | -3.630403401 | -1.511555484 | -2.855943652 |
| H | -3.834143976 | -3.776624177 | 3.171474023 |
| C | -2.803053432 | -1.291567862 | -1.758392243 |
| H | 2.686801079 | 3.578492705 | -1.655255398 |
| H | 1.502731049 | 2.915882361 | 0.925533548 |
| C | 1.771441027 | 2.983340678 | -1.783188427 |
| C | 1.183334829 | 3.858344958 | 0.473199161 |
| H | -4.270492728 | -0.786053971 | -4.798277729 |

| | | | |
|---|---|---|---|
| C | -2.244144976 | -2.633269065 | 2.260949157 |
| H | 1.547295702 | 2.968628276 | -2.85784695 |
| C | -3.628892539 | -0.624923818 | -3.935399896 |
| H | 0.452285782 | 4.323146764 | 1.14140053 |
| H | -0.885417011 | -4.203987711 | 2.99121723 |
| H | -3.500710461 | -0.816714822 | 2.121707503 |
| C | 0.643065257 | 3.640133658 | -0.956606446 |
| C | -1.200580574 | -3.186580424 | 3.252476935 |
| C | -2.783069024 | -1.290529028 | 2.807505551 |
| H | -3.316351655 | -1.47865398 | 3.75091456 |
| H | 1.19846975 | 5.594423788 | -1.701521561 |
| C | -2.796396217 | 0.49155189 | -3.850787918 |
| H | -0.310037421 | -2.555148615 | 3.321367421 |
| C | -1.965992275 | 0.67218012 | -2.746942706 |
| C | 0.28412816 | 4.989959476 | -1.606983133 |
| H | -0.131178285 | 4.868497604 | -2.616440001 |
| H | -1.656132706 | -3.23382755 | 4.252484781 |
| H | -2.779759536 | 1.233999453 | -4.64592042 |
| H | -1.979191933 | -0.579976765 | 3.024664668 |
| H | -1.584807648 | 5.012589486 | 0.755133866 |
| C | -1.098442751 | 1.901535706 | -2.652437405 |
| H | -0.425898986 | 5.572162492 | -1.009443227 |
| H | -0.088571143 | 1.668879284 | -3.011177282 |
| H | -1.716290879 | 3.536945107 | 1.740066488 |
| C | -2.198511546 | 4.126795484 | 0.950365713 |
| H | -1.492885395 | 2.698920094 | -3.294993983 |
| C | -2.451316513 | 3.285476615 | -0.317427489 |
| H | -3.125040062 | 1.563480931 | 0.880674237 |
| H | -3.164245924 | 4.479581018 | 1.34127845 |
| C | -3.478616395 | 2.190890781 | 0.052308302 |
| H | -2.391868875 | 4.948196698 | -1.776874874 |
| H | -3.371882493 | 3.560167716 | -2.294376012 |
| C | -3.066149528 | 4.160252126 | -1.428092353 |
| H | -4.41086033 | 2.676722146 | 0.377521145 |
| H | -3.719682628 | 1.539228986 | -0.794522129 |
| H | -3.971522721 | 4.649300676 | -1.038466125 |
| S | 0.911540264 | 0.082587539 | 3.048663729 |
| O | 0.126201658 | 0.19068768 | 4.288567084 |
| O | 1.494379867 | -1.226983716 | 2.704960317 |
| O | 0.229262059 | 0.783134816 | 1.863308173 |
| C | 2.374226692 | 1.214759083 | 3.284111025 |
| F | 3.108556601 | 1.270554337 | 2.159482998 |
| F | 1.965146273 | 2.458210342 | 3.585032082 |
| F | 3.145807213 | 0.761752996 | 4.280009104 |
| H | 1.081220374 | -0.500193908 | -2.13643322 |

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**Supplementary Table 19 | Cartesian coordinate of XIII. Units are presented in Å.**

SCF energy (in toluene) = -2833.66915087 hartree

ZPE = 0.670964 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.331746965 | 0.588211857 | 0.384911767 |
| P | 0.345354832 | -0.881270949 | 2.456881255 |
| N | 1.854007513 | 1.031342458 | 0.698688477 |
| P | 0.261712061 | 2.064082234 | -1.653581534 |
| N | -0.76999767 | 1.965947074 | 1.505005982 |
| H | -1.143370689 | -1.778287848 | 5.932414017 |
| H | 0.457495088 | -1.109141695 | 5.587022174 |
| C | -0.347335096 | -1.731565546 | 5.174401428 |
| H | -0.854948492 | 0.911353767 | 4.692297669 |
| H | 0.033347232 | -2.749037652 | 5.042646459 |
| H | -2.380882291 | 0.050995029 | 4.944375337 |
| C | -1.567498189 | 0.220922682 | 4.224117409 |
| H | -2.832499264 | -2.159975587 | 4.102043581 |
| C | -0.933395111 | -1.142276298 | 3.876809772 |
| H | 0.766968332 | 1.334244168 | 3.295971871 |
| H | -1.993467064 | 0.710383486 | 3.343873427 |
| H | 2.032859142 | 0.270637277 | 3.966966041 |
| C | -2.050384032 | -2.06180142 | 3.334270405 |
| H | 2.092822739 | -2.399867048 | 4.551324778 |
| H | -2.508067116 | -1.651458932 | 2.428239782 |
| C | 1.458397299 | 0.514943471 | 3.066921457 |
| H | 4.084501115 | 1.247610592 | 3.231198479 |
| H | -1.69237547 | -3.065494201 | 3.090152047 |
| H | 3.256910049 | -1.522581831 | 3.535054212 |
| H | 0.428987968 | 3.656022738 | 0.87157071 |
| C | 2.574755628 | -2.380854705 | 3.569786047 |
| H | -1.004179601 | 5.610860861 | -1.096087525 |
| C | 3.705945614 | 1.303859399 | 2.213608276 |
| H | 3.197449521 | -3.284438145 | 3.494087018 |
| C | 2.373148843 | 0.967890567 | 1.959706497 |
| H | 0.89947379 | 5.28388236 | 0.310767679 |
| H | -1.688883827 | 4.042463111 | -0.626746671 |
| C | 0.972098093 | 4.206910036 | 0.096302696 |
| C | -1.038353776 | 4.542735816 | -1.355222364 |
| H | 5.572217234 | 1.961849483 | 1.343550131 |

| | | | |
|---|---|---|---|
| C | 1.580583684 | -2.381847868 | 2.385966631 |
| H | 2.033810608 | 3.937631093 | 0.151328153 |
| C | 4.53108108 | 1.701952274 | 1.163138903 |
| H | -1.502102199 | 4.459931047 | -2.345139201 |
| H | 0.334108134 | -3.939810751 | 3.32658823 |
| H | 3.045991798 | -1.384499731 | 1.068920107 |
| C | 0.391240376 | 3.963993676 | -1.31495395 |
| C | 0.81376978 | -3.721129406 | 2.365747015 |
| C | 2.421541801 | -2.284280116 | 1.091095619 |
| H | 3.099112351 | -3.150355016 | 1.062488865 |
| H | 1.417494301 | 5.752631406 | -1.951978653 |
| C | 3.99768979 | 1.759114197 | -0.123610051 |
| H | 0.055223425 | -3.753976391 | 1.578190311 |
| C | 2.656886068 | 1.424945357 | -0.328871704 |
| C | 1.306890487 | 4.717083799 | -2.305502889 |
| H | 2.315805626 | 4.285478988 | -2.341460884 |
| H | 1.533249974 | -4.529604214 | 2.171142381 |
| H | 4.609048703 | 2.06135365 | -0.970253036 |
| H | 1.817492333 | -2.317211998 | 0.182911834 |
| H | -2.444472305 | 2.406385157 | -2.84268436 |
| C | 2.047065113 | 1.466139486 | -1.705973288 |
| H | 0.915828309 | 4.762523268 | -3.322779105 |
| H | 2.68545571 | 2.029433669 | -2.397451236 |
| H | -2.171980764 | 0.664169439 | -2.643608967 |
| C | -1.94706667 | 1.528375142 | -3.273789846 |
| H | 1.979003604 | 0.436459626 | -2.081692135 |
| C | -0.424083861 | 1.73345654 | -3.433525894 |
| H | 0.156749389 | -0.38855284 | -3.247799144 |
| H | -2.390849021 | 1.349233081 | -4.264143371 |
| C | 0.204922946 | 0.429778388 | -3.969236547 |
| H | -0.683899838 | 3.771283602 | -4.258253116 |
| H | 0.892023511 | 3.031205865 | -4.639757598 |
| C | -0.174872842 | 2.828914769 | -4.487797192 |
| H | -0.349686907 | 0.116475651 | -4.86497326 |
| H | 1.250525205 | 0.579085534 | -4.269633305 |
| H | -0.577074906 | 2.472896828 | -5.447869158 |
| S | -0.622915474 | -2.626982622 | -1.090052089 |
| O | 0.398494557 | -3.631796928 | -1.42115567 |
| O | -1.498432953 | -2.87989411 | 0.071027543 |
| O | -0.065006998 | -1.204196454 | -1.12091806 |
| C | -1.794467413 | -2.653843641 | -2.543775011 |
| F | -2.732674872 | -1.69559267 | -2.423550674 |
| F | -1.134329095 | -2.456398797 | -3.698323705 |
| F | -2.405804542 | -3.8420822 | -2.600015272 |
| N | -2.330456562 | 0.207038688 | 0.133964308 |
| N | -3.44526954 | 0.054798279 | 0.046878968 |
| H | -1.744633999 | 2.250447486 | 1.706150778 |

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**Supplementary Table 20 | Cartesian coordinate of XIV. Units are presented in Å.**

SCF energy (in toluene) = -2834.28035937 hartree

ZPE = 0.685336 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.340549375 | 0.6615316 | 0.466625953 |
| P | 0.353693507 | -0.951939655 | 2.440003058 |
| N | 1.823997944 | 1.088307471 | 0.793945033 |
| P | 0.27926516 | 2.09215135 | -1.659110849 |
| H | -0.99841343 | -1.92212065 | 5.944552009 |
| H | 0.5565577 | -1.179556143 | 5.540169397 |
| C | -0.233188045 | -1.840441544 | 5.158161328 |
| H | -0.927865949 | 0.790842413 | 4.636923051 |
| H | 0.191036364 | -2.840194124 | 5.016482096 |
| H | -2.360572177 | -0.179793357 | 4.995583478 |
| C | -1.604507571 | 0.031384684 | 4.22544186 |
| H | -2.733946315 | -2.386828394 | 4.161285395 |
| C | -0.890570624 | -1.292791213 | 3.875987046 |
| H | 0.804961995 | 1.143208991 | 3.54067388 |
| H | -2.122305615 | 0.453801417 | 3.359133077 |
| H | 2.110070593 | 0.03573333 | 3.969382801 |
| C | -1.972560427 | -2.274291269 | 3.374738855 |
| H | 2.219648354 | -2.505714344 | 4.377392885 |
| H | -2.463064152 | -1.908575824 | 2.467708023 |
| C | 1.48485934 | 0.384465926 | 3.140850919 |
| H | 4.025168836 | 1.295077656 | 3.366367667 |
| H | -1.574152026 | -3.266631321 | 3.15132186 |
| H | 3.344132719 | -1.626533777 | 3.316656884 |
| H | -0.136080601 | 4.14435076 | 0.626037113 |
| C | 2.651335681 | -2.474758354 | 3.372529757 |
| H | -1.098679561 | 5.657259688 | -1.614132842 |
| C | 3.654281393 | 1.397257661 | 2.348931014 |
| H | 3.254247857 | -3.386042523 | 3.247967091 |
| C | 2.350553862 | 0.985715069 | 2.057154604 |
| H | 0.757691331 | 5.531219176 | -0.027994835 |
| H | -1.846066693 | 4.098629158 | -1.214061284 |
| C | 0.659145798 | 4.436035767 | -0.062206633 |
| C | -1.077420803 | 4.579444513 | -1.833406688 |
| H | 5.475672323 | 2.258849021 | 1.558565331 |
| C | 1.595856179 | -2.442681228 | 2.243567447 |

| | | | |
|---|---|---|---|
| H | 1.604876012 | 4.00790721 | 0.290570847 |
| C | 4.461082748 | 1.929642262 | 1.345434009 |
| H | -1.360150957 | 4.45548707 | -2.883608541 |
| H | 0.454036959 | -4.064594689 | 3.20284211 |
| H | 2.943678932 | -1.343865254 | 0.889169586 |
| C | 0.326162654 | 4.023805054 | -1.511381921 |
| C | 0.854826216 | -3.79545939 | 2.218235961 |
| C | 2.361050346 | -2.271392925 | 0.911164774 |
| H | 3.06992572 | -3.10744946 | 0.815982517 |
| H | 1.351827207 | 5.769782298 | -2.267346722 |
| C | 3.937056277 | 2.009964143 | 0.054125868 |
| H | 0.04089194 | -3.81249197 | 1.488395136 |
| C | 2.635386168 | 1.57642196 | -0.196725943 |
| C | 1.398152263 | 4.679845121 | -2.409233454 |
| H | 2.410124504 | 4.364940159 | -2.124214015 |
| H | 1.575776626 | -4.577215706 | 1.93791377 |
| H | 4.537593271 | 2.391358609 | -0.76843182 |
| H | 1.707178738 | -2.291130739 | 0.03782556 |
| H | -2.322487306 | 2.375018828 | -3.16129129 |
| C | 2.080399264 | 1.567931243 | -1.595239232 |
| H | 1.265816076 | 4.484872962 | -3.473841745 |
| H | 2.730366198 | 2.123743068 | -2.281628189 |
| H | -2.111889647 | 0.689443502 | -2.660979017 |
| C | -1.810807234 | 1.434625461 | -3.400782958 |
| H | 2.053353175 | 0.523505906 | -1.934134355 |
| C | -0.277772623 | 1.608417043 | -3.457126497 |
| H | 0.290818247 | -0.494182193 | -3.061538158 |
| H | -2.173489662 | 1.101438677 | -4.384056728 |
| C | 0.388220013 | 0.266809673 | -3.837341874 |
| H | -0.408866034 | 3.579054727 | -4.470265781 |
| H | 1.15512793 | 2.752594289 | -4.684138774 |
| C | 0.073321525 | 2.602984457 | -4.581587366 |
| H | -0.096907463 | -0.11662085 | -4.745747823 |
| H | 1.452092565 | 0.402591429 | -4.071966225 |
| H | -0.282170521 | 2.175777123 | -5.531079317 |
| S | -0.854228345 | -2.469012776 | -1.009840774 |
| O | 0.03340331 | -3.500829115 | -1.564363723 |
| O | -1.586116738 | -2.769138646 | 0.235132812 |
| O | -0.16626932 | -1.100927839 | -0.989759217 |
| C | -2.215699416 | -2.29885252 | -2.279507468 |
| F | -3.096005617 | -1.348916646 | -1.921095921 |
| F | -1.717866965 | -1.981490915 | -3.488346856 |
| F | -2.864432973 | -3.464741087 | -2.380235393 |
| N | -2.329628019 | 0.477699137 | 0.424557686 |
| N | -3.462547801 | 0.490416934 | 0.517442512 |
| N | -0.625025822 | 2.120119614 | 1.721326508 |
| H | -1.544679986 | 2.38044182 | 2.091184682 |

```
  H       0.0864368    2.738186956    2.124352349
-------------------------------------------------
```

**Supplementary Table 21 | Cartesian coordinate of XV. Units are presented in Å.**

SCF energy (in toluene) = -2834.87044070 hartree

ZPE = 0.697281 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.291080171 | 0.477582874 | 0.32830479 |
| P | 0.322995639 | -0.91768583 | 2.400825447 |
| N | 1.845790627 | 1.000813457 | 0.672304147 |
| P | 0.285221807 | 2.05195651 | -1.620786606 |
| H | -1.14032503 | -1.728337351 | 5.925175832 |
| H | 0.414353557 | -0.966284835 | 5.553244889 |
| C | -0.340649127 | -1.667067758 | 5.171263512 |
| H | -1.032956102 | 0.922957286 | 4.438339417 |
| H | 0.114805515 | -2.659790408 | 5.102894052 |
| H | -2.450851453 | -0.039104995 | 4.856775937 |
| C | -1.69266364 | 0.121172654 | 4.07656675 |
| H | -2.823246488 | -2.266714655 | 4.058300731 |
| C | -0.944198856 | -1.206800791 | 3.831369249 |
| H | 0.762353333 | 1.309518606 | 3.313927423 |
| H | -2.220335253 | 0.453701821 | 3.176747961 |
| H | 1.998076205 | 0.232115675 | 3.942761348 |
| C | -1.991496275 | -2.231641497 | 3.338198227 |
| H | 2.124475485 | -2.307275083 | 4.547723138 |
| H | -2.393866986 | -1.960984247 | 2.356621018 |
| C | 1.43481728 | 0.486765922 | 3.038294257 |
| H | 4.063057732 | 1.188303756 | 3.233013385 |
| H | -1.582173729 | -3.241512008 | 3.25623328 |
| H | 3.285355082 | -1.475902032 | 3.48855007 |
| H | 0.862879946 | 3.593690546 | 0.820211459 |
| C | 2.604765927 | -2.332454021 | 3.565016739 |
| H | -0.853926613 | 5.665098806 | -1.03692169 |
| C | 3.699100901 | 1.252627369 | 2.209980613 |
| H | 3.230511075 | -3.236576512 | 3.531358927 |
| C | 2.366759911 | 0.933843919 | 1.94138395 |
| H | 1.094000056 | 5.273093895 | 0.28079523 |
| H | -1.572946319 | 4.112419916 | -0.557375552 |
| C | 1.215585649 | 4.217397747 | -0.004437644 |
| C | -0.923483698 | 4.598238187 | -1.297923748 |
| H | 5.590001093 | 1.880859538 | 1.362446777 |
| C | 1.6088021 | -2.392778072 | 2.384042775 |

| | | | |
|---|---|---|---|
| H | 2.290508743 | 4.025993059 | -0.096055381 |
| C | 4.546932272 | 1.638494199 | 1.1717846 |
| H | -1.438013386 | 4.529437228 | -2.263536069 |
| H | 0.43418171 | -3.965925349 | 3.388530981 |
| H | 3.031742759 | -1.393799565 | 1.021887532 |
| C | 0.486878521 | 3.973411031 | -1.350194197 |
| C | 0.883774996 | -3.754870133 | 2.41106456 |
| C | 2.446296996 | -2.31678599 | 1.086276037 |
| H | 3.159267567 | -3.154886293 | 1.095135937 |
| H | 1.560439136 | 5.730750751 | -2.022573279 |
| C | 4.01978838 | 1.70315137 | -0.12031707 |
| H | 0.110581623 | -3.827475155 | 1.640495067 |
| C | 2.678850945 | 1.392563663 | -0.343031677 |
| C | 1.332983994 | 4.723868367 | -2.405035917 |
| H | 2.294673934 | 4.229300084 | -2.592045657 |
| H | 1.624726016 | -4.545141463 | 2.220290114 |
| H | 4.64368045 | 1.991800384 | -0.963208748 |
| H | 1.846806468 | -2.410393339 | 0.179746885 |
| H | -2.434616404 | 2.42995065 | -2.776632799 |
| C | 2.073005514 | 1.464543677 | -1.71737449 |
| H | 0.823233336 | 4.851492445 | -3.36040198 |
| H | 2.712016204 | 2.043809211 | -2.396238397 |
| H | -2.173964477 | 0.688847524 | -2.567753164 |
| C | -1.952272758 | 1.544118926 | -3.211354297 |
| H | 1.997250713 | 0.444577142 | -2.116294135 |
| C | -0.43160655 | 1.743628109 | -3.399393915 |
| H | 0.167384964 | -0.375105303 | -3.244887822 |
| H | -2.417586166 | 1.36217202 | -4.19166732 |
| C | 0.187220436 | 0.447166482 | -3.962121129 |
| H | -0.723932253 | 3.780020059 | -4.215853882 |
| H | 0.850143113 | 3.053672231 | -4.631089241 |
| C | -0.211233641 | 2.842099741 | -4.456671709 |
| H | -0.389234134 | 0.135621634 | -4.844839197 |
| H | 1.223324852 | 0.606745427 | -4.28918717 |
| H | -0.631217845 | 2.485360682 | -5.40901611 |
| S | -0.537410293 | -2.603135125 | -1.112979517 |
| O | 0.454469329 | -3.587225888 | -1.56933912 |
| O | -1.322952576 | -2.907019648 | 0.098116391 |
| O | 0.042754627 | -1.178354175 | -1.138618893 |
| C | -1.823272037 | -2.572933129 | -2.46848966 |
| F | -2.7454495 | -1.621163897 | -2.239491404 |
| F | -1.259837825 | -2.340031043 | -3.666191176 |
| F | -2.439454469 | -3.760077889 | -2.512077947 |
| N | -2.261569627 | 0.116269551 | 0.3222717 |
| N | -3.395243952 | 0.042983002 | 0.433398719 |
| N | -1.122029718 | 2.274780337 | 1.579479064 |
| H | -2.140519907 | 2.171525427 | 1.53375032 |

```
  H    -0.912597668    3.209841216    1.230559055
  H    -0.887600513     2.28018887    2.574241073
-------------------------------------------------
```

**Supplementary Table 22 | Cartesian coordinate of XVI. Units are presented in Å.**

SCF energy (in toluene) = -1873.53202305 hartree

ZPE = 0.663820 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.138937183 | -1.752521887 | -0.401938545 |
| P | -0.268631959 | 0.437173404 | 0.645550084 |
| N | -2.153806962 | -1.847088081 | 0.499827701 |
| P | -0.97716311 | -3.720799675 | -1.526405736 |
| N | 1.755671092 | -1.778846737 | -1.033080221 |
| N | 2.860932423 | -1.823845355 | -1.34436333 |
| H | 1.526897614 | 2.583091887 | 3.399548615 |
| H | 0.007052656 | 1.694390972 | 3.555140659 |
| C | 0.652250271 | 2.218083616 | 2.837893334 |
| H | 1.334791579 | -0.446009364 | 3.042018609 |
| H | 0.110316317 | 3.096229922 | 2.477028892 |
| H | 2.77887849 | 0.560766805 | 2.915616518 |
| C | 1.940623863 | 0.143247874 | 2.337328673 |
| H | 2.985716128 | 2.358167041 | 1.324906019 |
| C | 1.128710373 | 1.291589145 | 1.700180493 |
| H | -0.912676583 | -0.317253995 | 2.838911042 |
| H | 2.355256147 | -0.521085106 | 1.57010795 |
| H | -2.090017988 | 0.901120948 | 2.380040454 |
| C | 2.085713242 | 2.059059911 | 0.765861402 |
| H | -0.444871067 | 3.707213247 | 0.517020265 |
| H | 2.410449836 | 1.437072707 | -0.078234687 |
| C | -1.527384079 | 0.035885927 | 1.997026036 |
| H | -3.887462327 | -0.575166497 | 3.133066699 |
| H | 1.635360866 | 2.975044818 | 0.367039892 |
| H | -1.907298411 | 3.051739184 | 1.286639039 |
| H | -0.809151388 | -5.17012947 | 1.030405785 |
| C | -1.382540497 | 3.172385175 | 0.329674714 |
| H | 0.990420073 | -6.913749363 | -0.743116167 |
| C | -3.681249611 | -1.227269524 | 2.286224777 |
| H | -2.004717497 | 3.826028855 | -0.301670492 |
| C | -2.489899708 | -1.05444621 | 1.57796369 |
| H | -1.048086971 | -6.872604619 | 0.603519675 |
| H | 1.343410259 | -5.197508317 | -0.440978663 |
| C | -1.264958794 | -5.839789426 | 0.290427184 |
| C | 0.808506644 | -5.889698941 | -1.104561735 |

| | | | |
|---|---|---|---|
| H | -5.509368682 | -2.378494488 | 2.471540156 |
| C | -1.162286109 | 1.8277227 | -0.385591771 |
| H | -2.35126798 | -5.700525138 | 0.346297106 |
| C | -4.585465681 | -2.223792539 | 1.9186769 |
| H | 1.268091286 | -5.802804934 | -2.095012425 |
| H | 0.623790599 | 2.501229368 | -1.502216446 |
| H | -3.208561572 | 1.13643358 | 0.081667194 |
| C | -0.707802786 | -5.604796641 | -1.131093868 |
| C | -0.36049628 | 2.05671729 | -1.684702362 |
| C | -2.54805126 | 1.272634365 | -0.783395697 |
| H | -3.039492639 | 1.983000018 | -1.465769227 |
| H | -1.281057666 | -7.622690738 | -1.704839153 |
| C | -4.273953926 | -2.999196756 | 0.797653387 |
| H | -0.202085835 | 1.113963107 | -2.224586996 |
| C | -3.089098084 | -2.781976185 | 0.099310009 |
| C | -1.393566227 | -6.595791993 | -2.087924103 |
| H | -2.469663856 | -6.402084432 | -2.188563692 |
| H | -0.91464293 | 2.737780862 | -2.349078219 |
| H | -4.96371883 | -3.76186834 | 0.441388733 |
| H | -2.468517826 | 0.307726321 | -1.298950876 |
| H | 0.560608448 | -4.986015339 | -4.004362483 |
| C | -2.826801929 | -3.503604663 | -1.198638988 |
| H | -0.947923046 | -6.575504919 | -3.088872503 |
| H | -3.413920572 | -4.429946897 | -1.25422156 |
| H | 1.289380457 | -3.492637516 | -3.364170199 |
| C | 0.469948318 | -3.893010008 | -3.973979058 |
| H | -3.192528576 | -2.860619136 | -2.012748682 |
| C | -0.905655841 | -3.443777592 | -3.443826558 |
| H | -0.204582107 | -1.406909671 | -2.993761805 |
| H | 0.608630237 | -3.529276099 | -5.003797872 |
| C | -0.995496958 | -1.905472841 | -3.582774737 |
| H | -1.978758246 | -5.171407428 | -4.301480748 |
| H | -3.024881471 | -3.783017086 | -3.957903623 |
| C | -2.022613045 | -4.077924389 | -4.294593117 |
| H | -0.841854039 | -1.610713131 | -4.632697857 |
| H | -1.973611348 | -1.512206918 | -3.276893632 |
| H | -1.922434554 | -3.741331046 | -5.338597824 |
| H | 1.220852771 | -2.295904308 | 2.034363338 |
| N | 0.549156108 | -2.823145325 | 1.473963122 |
| H | 0.999966307 | -3.705075772 | 1.227176976 |
| H | -0.24184852 | -3.051980654 | 2.081388699 |

---

**Supplementary Table 23 | Cartesian coordinate of XVII. Units are presented in Å.**

SCF energy (in toluene) = -3909.60899623 hartree

ZPE = 1.314194 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.615071018 | 0.048465227 | -0.107133721 |
| Mo | 2.64334993 | -0.093101933 | -0.030091376 |
| P | 3.259671686 | 2.060792396 | -1.170605418 |
| P | -3.256994285 | -2.111725063 | -1.245982266 |
| N | -4.848854948 | 0.138013293 | -0.057795965 |
| N | 4.859755984 | -0.208053674 | -0.068351916 |
| P | 3.060084175 | -2.296079687 | 1.154199534 |
| P | -3.028481872 | 2.255828683 | 1.079411288 |
| N | -0.539082574 | -0.00448716 | -0.113389541 |
| N | 0.618324799 | -0.026432017 | -0.072525259 |
| N | -2.565028023 | 1.485514588 | -2.929041299 |
| N | -2.587053814 | 0.959030902 | -1.918782154 |
| N | -2.596442958 | -0.869321355 | 1.707510494 |
| N | -2.590413874 | -1.401465744 | 2.712856535 |
| N | 2.715804552 | 0.779442891 | 1.73831046 |
| N | 2.77917287 | 1.291959135 | 2.764130509 |
| H | 2.670606158 | 3.749263408 | -4.664837062 |
| H | -2.737857574 | -3.711293722 | -4.781217592 |
| H | -4.085748856 | -2.702106807 | -4.250865532 |
| H | 4.043696947 | 2.747822903 | -4.184514789 |
| C | 3.279316298 | 3.436678064 | -3.801938873 |
| C | -3.327489908 | -3.413167759 | -3.900310992 |
| H | -2.399561399 | -0.832724694 | -3.902311361 |
| H | 2.385501748 | 0.865280448 | -3.877816529 |
| H | -3.84119839 | -4.30718857 | -3.536990595 |
| H | 3.787036636 | 4.327839965 | -3.425304685 |
| H | -1.118420929 | -1.943914069 | -4.403353488 |
| H | 1.079703626 | 1.964532097 | -4.314091537 |
| C | 1.664322539 | 1.583219432 | -3.463743567 |
| C | -1.689152749 | -1.579770873 | -3.534652487 |
| H | 0.614309032 | 3.975498868 | -3.195610198 |
| H | -0.658395934 | -3.994999368 | -3.353705421 |
| C | 2.362274968 | 2.763386251 | -2.758652014 |
| C | -2.383590862 | -2.777977946 | -2.857151972 |
| H | -4.564392543 | -0.825375709 | -2.802508271 |
| H | 4.548282695 | 0.842455244 | -2.807809054 |
| H | 0.97485274 | 1.061734101 | -2.79150284 |
| H | -1.001399715 | -1.069906091 | -2.850125179 |
| H | 5.545307983 | 2.199153991 | -2.297131279 |

| | | | |
|---|---|---|---|
| H | -5.55690529 | -2.213603769 | -2.341505384 |
| C | 1.250410019 | 3.741287779 | -2.328831806 |
| C | -1.279923356 | -3.782624363 | -2.470261575 |
| H | 3.64713027 | 5.277220248 | -1.557106387 |
| H | -3.672779631 | -5.30895293 | -1.681075153 |
| H | 0.60581025 | 3.302521092 | -1.556855597 |
| H | -0.623951697 | -3.378523885 | -1.687496956 |
| C | 4.873572269 | 1.413828583 | -1.925001941 |
| C | -4.880992843 | -1.442537661 | -1.948938477 |
| H | 7.546201341 | 1.039736 | -1.728260567 |
| H | -7.556705234 | -1.117784467 | -1.665611154 |
| H | 1.645942677 | 4.689555988 | -1.951107198 |
| H | -1.678486963 | -4.740239958 | -2.120155646 |
| H | 5.228644144 | 4.467560491 | -1.636418974 |
| H | -5.251030671 | -4.490685893 | -1.687062983 |
| H | -4.495205052 | 2.574187776 | -1.462595771 |
| H | 4.467199025 | -2.627259757 | -1.371215465 |
| C | 4.416138753 | 4.771745561 | -0.963463104 |
| C | -4.418269425 | -4.814581761 | -1.049310373 |
| H | -2.641680416 | 5.136582727 | -1.425955411 |
| H | 2.66629935 | -5.189537974 | -1.350287028 |
| C | 7.004360979 | 0.45012711 | -0.991290275 |
| C | -7.001158541 | -0.533092973 | -0.935530757 |
| H | 4.834036012 | 5.521979406 | -0.274535866 |
| H | -4.816258872 | -5.578773594 | -0.36401783 |
| C | 5.610814165 | 0.514012537 | -0.965938373 |
| C | -5.606112714 | -0.578733347 | -0.948112745 |
| H | -4.881990735 | 4.299397294 | -1.556954777 |
| H | 4.827749733 | -4.365033394 | -1.52505583 |
| H | -2.023140271 | 3.479813303 | -1.494492596 |
| H | 1.808715149 | -3.645894121 | -1.147344948 |
| C | -4.702292933 | 3.463805805 | -0.863559562 |
| C | 4.679129653 | -3.542227404 | -0.808950839 |
| C | -2.336873086 | 4.274545507 | -0.812491113 |
| C | 2.33815956 | -4.442212517 | -0.61142559 |
| H | -8.752980667 | 0.29211965 | 0.034265933 |
| H | 8.774024357 | -0.408095093 | -0.079749999 |
| C | 3.863181995 | 3.594325974 | -0.136273297 |
| C | -3.831788581 | -3.656983879 | -0.216739127 |
| H | -5.632261412 | 3.296094749 | -0.30804012 |
| H | 5.633292231 | -3.378724948 | -0.296493258 |
| C | -7.666225046 | 0.248699129 | 0.008825547 |
| C | 7.687807868 | -0.350480253 | -0.075374554 |
| H | -1.468556189 | 4.582934077 | -0.222778084 |
| H | 1.597537961 | -4.925641806 | 0.032273278 |
| H | 1.861143167 | 4.48440967 | 0.158117612 |
| H | -1.832176254 | -4.576689176 | -0.001339418 |
| H | 5.909662007 | 2.858096505 | 0.242069736 |
| H | -5.868936571 | -2.943332544 | 0.238983814 |
| C | -3.528073702 | 3.838632123 | 0.068438391 |
| C | 3.556008635 | -3.921661089 | 0.185023363 |
| C | 2.699937147 | 4.09738419 | 0.745393674 |

| | | | |
|---|---|---|---|
| C | -2.645121131 | -4.186096113 | 0.618447239 |
| C | 5.002074211 | 3.123946303 | 0.796981831 |
| C | -4.93895794 | -3.198997468 | 0.759848304 |
| H | 5.262662981 | 3.953378626 | 1.471863155 |
| H | -5.165585265 | -4.028525283 | 1.44647694 |
| H | -4.3593475 | 5.828036895 | 0.245926563 |
| H | 4.454159247 | -5.887364223 | 0.381811914 |
| C | 6.931171863 | -1.063329949 | 0.857312054 |
| C | -6.897633607 | 0.972896396 | 0.91990406 |
| H | 2.326760218 | 3.311864474 | 1.407309944 |
| H | -2.233025277 | -3.416168523 | 1.276028122 |
| C | 5.539195403 | -0.979569453 | 0.846273711 |
| C | -5.504065298 | 0.908389742 | 0.868039249 |
| C | -3.990477814 | 5.03850437 | 0.918651409 |
| C | 4.102310215 | -5.079762475 | 1.043545277 |
| H | -4.816077471 | 4.780323887 | 1.594719976 |
| H | 4.958188929 | -4.773264368 | 1.658226266 |
| H | 3.062932514 | 4.921240577 | 1.379521644 |
| H | -2.99629284 | -5.012288003 | 1.255653381 |
| H | -7.37007062 | 1.597483945 | 1.675003459 |
| H | 7.415333889 | -1.689224079 | 1.604326286 |
| H | 4.711343583 | 2.273396972 | 1.416794934 |
| H | -4.638415615 | -2.341214881 | 1.36544488 |
| H | -1.208964972 | 4.742080608 | 1.886608845 |
| H | 1.362694904 | -4.846277118 | 2.116308427 |
| C | -4.669095165 | 1.704467815 | 1.839642859 |
| C | 4.723283345 | -1.743905491 | 1.858323598 |
| H | -3.181889032 | 5.475293127 | 1.51357181 |
| H | 3.343922176 | -5.513172287 | 1.70335908 |
| H | -5.264286551 | 2.523285936 | 2.264475019 |
| H | 5.323612987 | -2.553467943 | 2.293961752 |
| H | -0.273171342 | 3.298243018 | 1.425881901 |
| H | 0.353218061 | -3.478371137 | 1.58291911 |
| C | -0.874641242 | 3.754146385 | 2.221814894 |
| C | 0.98646355 | -3.855826686 | 2.395722857 |
| H | -4.367905454 | 1.057400696 | 2.676609116 |
| H | 4.445047306 | -1.066903291 | 2.679065524 |
| C | -2.038760074 | 2.838627768 | 2.649291162 |
| C | 2.110672392 | -2.864043749 | 2.757275212 |
| H | -0.772967134 | 1.042408053 | 2.599574723 |
| H | 0.768830988 | -1.128678299 | 2.640573478 |
| H | -0.208856174 | 3.909074499 | 3.083107638 |
| H | 0.338453532 | -3.992051299 | 3.273814817 |
| C | -1.41632173 | 1.586253612 | 3.298166725 |
| C | 1.437495132 | -1.614096566 | 3.358707048 |
| H | -3.360625284 | 4.468144251 | 3.36973786 |
| H | 3.531671172 | -4.389183268 | 3.517496799 |
| H | -3.684813948 | 2.889821525 | 4.111996143 |
| H | 3.765527246 | -2.770431755 | 4.205862028 |
| C | -2.894891821 | 3.543964524 | 3.721987946 |
| C | 3.013761797 | -3.482740573 | 3.844784283 |
| H | -0.796388785 | 1.902386529 | 4.150295144 |

```
 H     0.839544574   -1.921137468    4.230341363
 H    -2.171326047    0.892396465    3.681967469
 H     2.161604027   -0.867715873    3.698283634
 H    -2.248844647    3.806043097    4.573732743
 H      2.39108964   -3.755957265    4.710517817
 N     2.431015879   -1.197238412   -2.134082584
 H     2.636854754   -2.193617533   -2.088620738
 H     2.973660841   -0.828016373   -2.915339023
 H     1.448015151   -1.113562321   -2.400858067
---------------------------------------------------
```

**Supplementary Table 24 | Cartesian coordinate of XVIII. Units are presented in Å.**

SCF energy (in toluene) = -3853.04790381 hartree

ZPE = 1.273448 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.562034206 | 0.030977988 | -0.006149736 |
| Mo | 2.674593022 | -0.228681369 | -0.238041528 |
| P | 3.181279597 | 1.820472758 | -1.522609474 |
| P | -3.133965873 | -1.954366333 | -1.497529218 |
| N | -4.796945202 | 0.121279208 | -0.0581995 |
| N | 4.920084413 | -0.281036126 | -0.278739324 |
| P | 3.111200153 | -2.066975571 | 1.338869504 |
| P | -3.03903636 | 2.046858694 | 1.459635426 |
| N | -0.499927308 | -0.059403703 | -0.024084473 |
| N | 0.655918576 | -0.116024817 | -0.103156886 |
| N | -2.477766836 | 1.857854676 | -2.593965847 |
| N | -2.495189973 | 1.195493906 | -1.66892309 |
| N | -2.646458056 | -1.139463827 | 1.650471637 |
| N | -2.719601641 | -1.806876582 | 2.569989335 |
| N | 2.664683627 | -2.010707006 | -2.762065512 |
| N | 2.672045774 | -1.339543785 | -1.830061928 |
| H | 2.582679774 | 3.382708752 | -5.043390273 |
| H | -2.448621458 | -3.024624839 | -5.185622197 |
| H | -3.826053538 | -2.100005635 | -4.580376097 |
| H | 4.032852646 | 2.546656128 | -4.482711941 |
| C | 3.178634245 | 3.148273652 | -4.147950293 |
| C | -3.08067144 | -2.855451188 | -4.300681927 |
| H | -2.1825315 | -0.303763754 | -3.895943189 |
| H | 2.610309078 | 0.418526515 | -4.106146486 |
| H | -3.60520792 | -3.791166945 | -4.091155671 |
| H | 3.561676623 | 4.094737883 | -3.75542262 |
| H | -0.854477243 | -1.319415328 | -4.476554727 |
| H | 1.255854903 | 1.362892373 | -4.748924296 |
| C | 1.793676185 | 1.094833707 | -3.826941732 |
| C | -1.476938735 | -1.087230596 | -3.599936845 |
| H | 0.440761704 | 3.379447555 | -3.691535299 |
| H | -0.421447652 | -3.493461989 | -3.722768151 |
| C | 2.290101317 | 2.385444637 | -3.14373915 |
| C | -2.184265718 | -2.375968846 | -3.139163671 |
| H | -4.373713512 | -0.442997444 | -2.900498717 |
| H | 4.582674913 | 0.67322177 | -3.088745097 |
| H | 1.111316726 | 0.535780541 | -3.180458628 |
| H | -0.825402141 | -0.684482407 | -2.818834695 |
| H | 5.484612331 | 2.094803442 | -2.560220254 |

| | | | |
|---|---|---|---|
| H | -5.378006029 | -1.879117538 | -2.686916239 |
| C | 1.053641227 | 3.234756203 | -2.789896297 |
| C | -1.086156023 | -3.420293738 | -2.850282698 |
| H | 3.292287046 | 5.050752624 | -1.858078279 |
| H | -3.499530323 | -5.052622466 | -2.388233404 |
| H | 0.421889432 | 2.73564872 | -2.045022975 |
| H | -0.463246929 | -3.127384081 | -1.996125964 |
| C | 4.848305161 | 1.272420146 | -2.205374625 |
| C | -4.722866546 | -1.174980397 | -2.158028922 |
| H | 7.505747658 | 0.870134497 | -2.150836826 |
| H | -7.408225449 | -0.875577296 | -1.974154691 |
| H | 1.319544856 | 4.229739459 | -2.413306815 |
| H | -1.490208567 | -4.420768794 | -2.661001676 |
| H | 4.946240453 | 4.400890802 | -1.859016823 |
| H | -5.077853828 | -4.234320118 | -2.384448478 |
| H | -4.369769965 | 2.811171634 | -1.105530047 |
| H | 4.153280567 | -3.378625977 | -1.064415006 |
| C | 4.076858096 | 4.621143546 | -1.225662812 |
| C | -4.288148511 | -4.649899922 | -1.745281945 |
| H | -2.482930938 | 5.217840729 | -0.619359602 |
| H | 1.862124104 | -5.332537165 | -0.179346409 |
| C | 7.006412881 | 0.307610667 | -1.364586486 |
| C | -6.894389079 | -0.402905396 | -1.140007966 |
| H | 4.382756223 | 5.402124647 | -0.512064346 |
| H | -4.725514469 | -5.498865222 | -1.19802921 |
| C | 5.619226613 | 0.402947568 | -1.243057798 |
| C | -5.500369599 | -0.458600851 | -1.081163447 |
| H | -4.757505595 | 4.522478543 | -0.889614153 |
| H | 4.274311986 | -5.090251972 | -0.623462007 |
| H | -1.852402127 | 3.574672425 | -0.817955059 |
| H | 1.644837824 | -3.653478433 | -0.715848735 |
| C | -4.59936922 | 3.572642247 | -0.357106251 |
| C | 4.291117801 | -4.065134713 | -0.223334481 |
| C | -2.216377894 | 4.295367547 | -0.081101475 |
| C | 1.829095943 | -4.285456304 | 0.159283606 |
| H | -8.697543043 | 0.294958582 | -0.165826747 |
| H | 8.813174538 | -0.606275838 | -0.592583059 |
| C | 3.596519219 | 3.381154615 | -0.450646934 |
| C | -3.758318954 | -3.622811367 | -0.725314537 |
| H | -5.547263671 | 3.307726455 | 0.125759258 |
| H | 5.2886901 | -3.898216465 | 0.202056639 |
| C | -7.611065149 | 0.246924308 | -0.135873049 |
| C | 7.733657004 | -0.509112466 | -0.499542441 |
| H | -1.390319374 | 4.538017266 | 0.594861514 |
| H | 0.977337473 | -4.184751247 | 0.841656204 |
| H | 1.50710575 | 4.07340421 | -0.238095301 |
| H | -1.767855439 | -4.565400333 | -0.542304391 |
| H | 5.664768671 | 2.773266168 | 0.033241815 |
| H | -5.823525812 | -2.983992279 | -0.292297237 |
| C | -3.460482441 | 3.771097169 | 0.669310693 |
| C | 3.170570452 | -3.925376001 | 0.831879741 |
| C | 2.346325348 | 3.741303606 | 0.381732658 |

| | | | |
|---|---|---|---|
| C | -2.611635536 | -4.266416858 | 0.08674989 |
| C | 4.712041467 | 2.974864708 | 0.537195516 |
| C | -4.922118248 | -3.306647919 | 0.241810413 |
| H | 4.88086382 | 3.796182254 | 1.250188312 |
| H | -5.179345064 | -4.224021511 | 0.792595266 |
| H | -4.246112227 | 5.740713637 | 1.097690328 |
| H | 3.584269373 | -5.921086336 | 1.566271511 |
| C | 7.031729521 | -1.188629483 | 0.495949042 |
| C | -6.89603104 | 0.833769649 | 0.9075279 |
| H | 2.000345697 | 2.884415108 | 0.975823771 |
| H | -2.234590942 | -3.597237872 | 0.864794288 |
| C | 5.648206861 | -1.046321148 | 0.599513429 |
| C | -5.501693512 | 0.764880155 | 0.924634857 |
| C | -3.939203388 | 4.847819034 | 1.663653552 |
| C | 3.455387867 | -4.909251375 | 1.980601941 |
| H | -4.810785776 | 4.521391844 | 2.245808264 |
| H | 4.376018756 | -4.661829999 | 2.525418523 |
| H | 2.590150758 | 4.557174787 | 1.079566625 |
| H | -2.990253951 | -5.173246196 | 0.582981459 |
| H | -7.410708502 | 1.35290664 | 1.713120864 |
| H | 7.552394821 | -1.819747319 | 1.21315523 |
| H | 4.442763362 | 2.078766616 | 1.111036943 |
| H | -4.667110267 | -2.540135546 | 0.977049395 |
| H | -1.24205839 | 4.353951294 | 2.725602495 |
| H | 0.883707914 | -3.546695968 | 3.01620785 |
| C | -4.722326846 | 1.415362469 | 2.040312191 |
| C | 4.91179582 | -1.678084832 | 1.752189728 |
| H | -3.156338918 | 5.163257298 | 2.360479787 |
| H | 2.631789002 | -4.957441405 | 2.701956393 |
| H | -5.340092931 | 2.175207209 | 2.536351219 |
| H | 5.474514933 | -2.534318142 | 2.147055778 |
| H | -0.303890602 | 2.968234821 | 2.127626294 |
| H | 0.304436282 | -2.085477714 | 2.186007268 |
| C | -0.947848184 | 3.321807683 | 2.94322607 |
| C | 0.875515414 | -2.450580418 | 3.047665998 |
| H | -4.474521182 | 0.658712644 | 2.799033797 |
| H | 4.865373555 | -0.9388189 | 2.566323646 |
| C | -2.152073856 | 2.382997181 | 3.160509815 |
| C | 2.298991614 | -1.862054009 | 3.080265886 |
| H | -0.936484141 | 0.570141058 | 2.917521243 |
| H | 1.578625389 | 0.129256885 | 2.489336961 |
| H | -0.339294301 | 3.345362333 | 3.859815285 |
| H | 0.327950899 | -2.155702592 | 3.955087277 |
| C | -1.592284817 | 1.036654599 | 3.659241047 |
| C | 2.183365088 | -0.333071243 | 3.281138216 |
| H | -3.496456122 | 3.91794627 | 4.034751795 |
| H | 3.162736642 | -3.536776464 | 4.23442205 |
| H | -3.886860604 | 2.253966218 | 4.507758967 |
| H | 4.095417104 | -2.033645744 | 4.350122241 |
| C | -3.065637452 | 2.942216219 | 4.271848932 |
| C | 3.081356239 | -2.446707046 | 4.273377423 |
| H | -1.008908453 | 1.213901949 | 4.575801552 |

```
   H     1.689731212   -0.120574025    4.241509963
   H    -2.380928914    0.319936328    3.910427325
   H     3.163551972    0.164132583    3.304690655
   H     -2.47305567    3.060686925    5.192039808
   H     2.558421211   -2.191713211    5.208132432
---------------------------------------------------
```

**Supplementary Table 25 | Cartesian coordinate of XIX. Units are presented in Å.**

SCF energy (in toluene) = -1926.49168292 hartree

ZPE = 0.636867 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.710355514 | -0.010499466 | -0.00026362 |
| P | -3.176757357 | 2.166886364 | 1.162682403 |
| N | -4.8657873 | -0.019120168 | -0.000685088 |
| P | -3.159000725 | -2.191597472 | -1.164680654 |
| N | -2.523750295 | -1.460698013 | 2.804388677 |
| N | -2.612751224 | -0.922188471 | 1.802535277 |
| N | -2.617934544 | 0.901819174 | -1.802945522 |
| N | -2.531898127 | 1.440739355 | -2.804842053 |
| H | -2.505526961 | 3.733237914 | 4.681119516 |
| H | -3.889101192 | 2.752011255 | 4.194297878 |
| C | -3.12765102 | 3.446950467 | 3.819125764 |
| H | -2.271231142 | 0.837921248 | 3.771264127 |
| H | -3.633920982 | 4.350900708 | 3.469867974 |
| H | -0.947398821 | 1.908455319 | 4.250811946 |
| C | -1.550741423 | 1.57032626 | 3.39457229 |
| H | -0.464693686 | 3.958422477 | 3.21805025 |
| C | -2.229373517 | 2.793951202 | 2.74755613 |
| H | -4.484121327 | 0.918543104 | 2.746460515 |
| H | -0.885355729 | 1.055231298 | 2.691648757 |
| H | -5.451500265 | 2.336579151 | 2.320536768 |
| C | -1.107507473 | 3.772528465 | 2.344813988 |
| H | -3.473770083 | 5.372498092 | 1.614986764 |

| | | | |
|---|---|---|---|
| H | -0.471365409 | 3.359037459 | 1.550701867 |
| C | -4.80610366 | 1.550808618 | 1.90604522 |
| H | -7.490224229 | 1.318663234 | 1.678437978 |
| H | -1.487103803 | 4.743542979 | 2.010890417 |
| H | -5.079287841 | 4.610333132 | 1.644050261 |
| H | -4.567031198 | -2.479780223 | 1.415232324 |
| C | -4.246159414 | 4.907401171 | 0.993596999 |
| H | -2.814203372 | -5.086930144 | 1.331196024 |
| C | -6.973898815 | 0.718991229 | 0.932019921 |
| H | -4.628001817 | 5.68782011 | 0.317613317 |
| C | -5.578396805 | 0.71750554 | 0.916163225 |
| H | -5.021889288 | -4.188728637 | 1.497327165 |
| H | -2.12265031 | -3.459283747 | 1.371690052 |
| C | -4.822829951 | -3.352563343 | 0.810197346 |
| C | -2.488341477 | -4.24359986 | 0.703208507 |
| H | -8.776665226 | -0.035404818 | -0.000643399 |
| C | -3.71295986 | 3.733847815 | 0.147881231 |
| H | -5.756548389 | -3.140413052 | 0.276719694 |
| C | -7.688892651 | -0.030822594 | -0.000703991 |
| H | -1.649148501 | -4.59537999 | 0.095940285 |
| H | -1.685636919 | 4.58446332 | -0.09710577 |
| H | -5.779866381 | 3.092075646 | -0.280337526 |
| C | -3.68366227 | -3.762852918 | -0.150092863 |
| C | -2.521017686 | 4.224212032 | -0.704681884 |
| C | -4.848376029 | 3.315162378 | -0.813275252 |
| H | -5.055792152 | 4.151476324 | -1.497736172 |
| H | -4.584392139 | -5.723383154 | -0.319550379 |
| C | -6.967689877 | -0.774547882 | -0.933524281 |
| H | -2.147467158 | 3.442355375 | -1.371700655 |
| C | -5.572250921 | -0.761388932 | -0.91769891 |

| | | | |
|---|---|---|---|
| C | -4.207235611 | -4.940802606 | -0.995650521 |
| H | -5.041496099 | -4.650211856 | -1.647581789 |
| H | -2.853771953 | 5.063735337 | -1.334140504 |
| H | -7.47899307 | -1.378463222 | -1.679982107 |
| H | -4.584088201 | 2.44692935 | -1.421236657 |
| H | -1.448027874 | -4.754207834 | -2.013124364 |
| C | -4.79301649 | -1.587876592 | -1.907915466 |
| H | -3.430556418 | -5.400769563 | -1.615496241 |
| H | -5.431889939 | -2.378695898 | -2.322870017 |
| H | -0.444117025 | -3.360960876 | -1.553236321 |
| C | -1.07684293 | -3.779965414 | -2.347184382 |
| H | -4.476023204 | -0.9524521 | -2.747846258 |
| C | -2.207104069 | -2.811051265 | -2.749725667 |
| H | -0.878135376 | -1.060907385 | -2.694540012 |
| H | -0.432746536 | -3.960275434 | -3.220628454 |
| C | -1.539308908 | -1.58172858 | -3.397210187 |
| H | -3.598725454 | -4.379951624 | -3.470449678 |
| H | -3.86808666 | -2.783729598 | -4.195463936 |
| C | -3.100424096 | -3.471942732 | -3.820549121 |
| H | -0.93345711 | -1.914690094 | -4.253708004 |
| H | -2.266257698 | -0.855541253 | -3.773558624 |
| H | -2.47648974 | -3.753225505 | -4.682885984 |

---

**Supplementary Table 26 | Cartesian coordinate of XIX'. Units are presented in Å.**

SCF energy (in toluene) = -1926.51501551 hartree

ZPE = 0.635509 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.823392577 | -0.297373761 | -0.117155257 |
| P | -2.959511308 | 1.956761547 | 0.86075548 |
| N | -5.001449443 | -0.213743216 | 0.428289921 |
| P | -3.620596518 | -2.327617328 | -1.232000062 |
| N | -2.297791738 | -1.631859269 | 2.62445636 |
| N | -2.471778093 | -1.131754545 | 1.608633977 |
| N | -0.881421448 | -0.369678098 | -0.642125623 |
| N | 0.213264266 | -0.405531562 | -0.962860586 |
| H | -1.514545657 | 4.025236012 | 3.826078923 |
| H | -3.04726976 | 3.150071315 | 3.78539391 |
| C | -2.309298209 | 3.662899398 | 3.156267944 |
| H | -1.776654846 | 0.922657469 | 3.398079498 |
| H | -2.790572459 | 4.541307665 | 2.71518575 |
| H | -0.310969982 | 1.90265722 | 3.566438366 |
| C | -1.047424783 | 1.522976041 | 2.841975403 |
| H | 0.235636256 | 3.709096655 | 2.038523457 |
| C | -1.689812456 | 2.718119032 | 2.106525937 |
| H | -3.9936812 | 1.173757488 | 2.875788499 |
| H | -0.532564386 | 0.852689564 | 2.145562331 |
| H | -4.962365231 | 2.540346148 | 2.323443024 |
| C | -0.571718268 | 3.449431446 | 1.337761425 |
| H | -2.930942395 | 5.190956471 | 0.649498483 |
| H | -0.136908071 | 2.815008099 | 0.554984814 |
| C | -4.441065031 | 1.634808992 | 1.982937003 |
| H | -7.052223231 | 1.37739734 | 2.607869315 |
| H | -0.915333769 | 4.38343806 | 0.878438011 |
| H | -4.561890225 | 4.653272354 | 1.105056503 |
| H | -4.043972741 | -3.240937205 | 1.508906791 |
| C | -3.843194261 | 4.71280073 | 0.277066644 |
| H | -2.004155088 | -5.338663046 | 0.437054946 |
| C | -6.756055073 | 0.664761356 | 1.841283974 |
| H | -4.275282849 | 5.384198327 | -0.481159943 |
| C | -5.434191583 | 0.662599685 | 1.388597937 |
| H | -4.241407956 | -4.995637652 | 1.372556632 |
| H | -1.670190398 | -3.600697082 | 0.591040264 |
| C | -4.368143649 | -4.042515474 | 0.837801687 |
| C | -2.063568287 | -4.370115043 | -0.082131025 |
| H | -8.700720535 | -0.270772741 | 1.679318847 |
| C | -3.571017091 | 3.335898799 | -0.354445777 |

| | | | |
|---|---|---|---|
| H | -5.441178464 | -3.919939414 | 0.642421726 |
| C | -7.672216697 | -0.249569364 | 1.324958935 |
| H | -1.406772722 | -4.425230489 | -0.957936189 |
| H | -1.572165752 | 3.874242941 | -1.134482668 |
| H | -5.706311589 | 2.768402853 | -0.268611932 |
| C | -3.53315967 | -4.087169167 | -0.462597865 |
| C | -2.529532934 | 3.477196743 | -1.486555003 |
| C | -4.885526115 | 2.83529198 | -0.99254541 |
| H | -5.195291546 | 3.538530145 | -1.780226176 |
| H | -4.072977813 | -6.161346717 | -0.778643566 |
| C | -7.237618948 | -1.129922645 | 0.335005598 |
| H | -2.329171165 | 2.510992691 | -1.969088033 |
| C | -5.915076396 | -1.081749166 | -0.108900588 |
| C | -4.069185409 | -5.222203431 | -1.352774514 |
| H | -5.099708069 | -5.041687556 | -1.686701954 |
| H | -2.912172052 | 4.164955662 | -2.255861911 |
| H | -7.922052587 | -1.847199052 | -0.112367131 |
| H | -4.766743919 | 1.846543749 | -1.454285425 |
| H | -1.805573566 | -4.051389262 | -3.134654351 |
| C | -5.474332064 | -1.947953707 | -1.264040273 |
| H | -3.444445799 | -5.386996842 | -2.238078596 |
| H | -6.109475832 | -2.840271384 | -1.339624317 |
| H | -1.075412889 | -2.488898823 | -2.699896615 |
| C | -1.826201316 | -2.973704507 | -3.335881683 |
| H | -5.639227496 | -1.378287781 | -2.190699586 |
| C | -3.229608947 | -2.372114328 | -3.122205721 |
| H | -2.4163292 | -0.333845827 | -2.978460214 |
| H | -1.5203477 | -2.831908202 | -4.383430411 |
| C | -3.181710955 | -0.884923524 | -3.544389498 |
| H | -4.315009819 | -4.171907105 | -3.796486672 |
| H | -5.260735605 | -2.678514218 | -3.930352826 |
| C | -4.251622817 | -3.102045487 | -4.015752133 |
| H | -2.918497685 | -0.807095824 | -4.610139746 |
| H | -4.148427002 | -0.378057884 | -3.41487108 |
| H | -3.949673803 | -3.001264587 | -5.069695012 |

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**Supplementary Table 27 | Cartesian coordinate of XX. Units are presented in Å.**

SCF energy (in toluene) = -1983.07761485 hartree

ZPE = 0.675588 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.152898577 | -1.480244295 | -0.773851492 |
| P | -0.293363018 | 0.56371018 | 0.679897559 |
| N | -2.117150883 | -1.775287798 | 0.22775867 |
| P | -0.926135757 | -3.642730945 | -1.828355833 |
| N | 1.667860116 | -1.272300771 | -1.592632524 |
| N | 2.738927203 | -1.206767523 | -1.989093174 |
| H | 1.696616676 | 2.144426273 | 3.671088457 |
| H | 0.271251533 | 1.103765114 | 3.761007759 |
| C | 0.784678227 | 1.842951393 | 3.132206875 |
| H | 1.728491836 | -0.643515682 | 2.724657716 |
| H | 0.145727289 | 2.725057384 | 3.058213011 |
| H | 3.056027236 | 0.491711701 | 2.532730438 |
| C | 2.158336491 | 0.097420811 | 2.033832068 |
| H | 2.895703519 | 2.556589541 | 1.463458821 |
| C | 1.18009505 | 1.257351935 | 1.760305656 |
| H | -0.667202549 | -0.845217785 | 2.612024423 |
| H | 2.476097891 | -0.396447933 | 1.1091428 |
| H | -1.844887202 | 0.463070274 | 2.707063875 |
| C | 1.959864093 | 2.3073353 | 0.940749836 |
| H | -0.599790581 | 3.74060149 | 1.400602016 |
| H | 2.225718287 | 1.926362877 | -0.053935936 |
| C | -1.37345518 | -0.247158259 | 2.014677089 |
| H | -3.841790757 | -0.816775823 | 2.986477192 |
| H | 1.403599868 | 3.241334999 | 0.813939862 |
| H | -1.933357318 | 2.823497835 | 2.140181792 |
| H | -1.136567655 | -4.278406005 | 1.024912104 |
| C | -1.53130542 | 3.204257666 | 1.191862223 |
| H | 0.697792331 | -6.648862888 | -0.047226735 |
| C | -3.652027215 | -1.326891287 | 2.044419224 |
| H | -2.249915026 | 3.946268585 | 0.811680557 |
| C | -2.419747256 | -1.152018667 | 1.411248456 |
| H | -1.251759196 | -6.050849571 | 1.125822998 |
| H | 1.247300985 | -4.977023624 | -0.271307832 |
| C | -1.481963771 | -5.175253961 | 0.500015394 |
| C | 0.638007848 | -5.773495083 | -0.712127733 |
| H | -5.590776107 | -2.286033364 | 1.944703891 |
| C | -1.363588911 | 2.095247588 | 0.133219231 |
| H | -2.57315677 | -5.096883898 | 0.437680468 |
| C | -4.624803442 | -2.141367572 | 1.465493314 |

| | | | |
|---|---|---|---|
| H | 1.113954922 | -6.049203497 | -1.657566982 |
| H | 0.247808946 | 3.133159603 | -0.970320685 |
| H | -3.330537282 | 1.262791036 | 0.684592354 |
| C | -0.839976557 | -5.360656901 | -0.895666896 |
| C | -0.746628536 | 2.709450582 | -1.143749415 |
| C | -2.784249285 | 1.589544878 | -0.208414267 |
| H | -3.351607015 | 2.422626609 | -0.64996662 |
| H | -1.568073827 | -7.404029374 | -0.892476724 |
| C | -4.328676845 | -2.756156846 | 0.24825998 |
| H | -0.673340387 | 1.979553722 | -1.95366815 |
| C | -3.08213177 | -2.562324169 | -0.349369403 |
| C | -1.588881951 | -6.531235287 | -1.564220555 |
| H | -2.643648501 | -6.294388852 | -1.752242842 |
| H | -1.394747465 | 3.528487721 | -1.491741803 |
| H | -5.061990978 | -3.387347709 | -0.249033201 |
| H | -2.782377872 | 0.774086547 | -0.934133946 |
| H | 0.386013753 | -5.928818612 | -3.636530283 |
| C | -2.761630125 | -3.215768624 | -1.672427561 |
| H | -1.132904032 | -6.843124234 | -2.509103834 |
| H | -3.441722778 | -4.059634824 | -1.850784449 |
| H | 1.39651782 | -4.470378166 | -3.491309571 |
| C | 0.506730732 | -4.894219173 | -3.9749009 |
| H | -2.932098588 | -2.487185804 | -2.478181352 |
| C | -0.74458018 | -4.025749706 | -3.728369373 |
| H | 0.354968758 | -2.149394674 | -4.057467101 |
| H | 0.707994567 | -4.930278229 | -5.055744278 |
| C | -0.51355914 | -2.685049045 | -4.454234309 |
| H | -2.222552436 | -5.669006797 | -3.933766161 |
| H | -2.871539434 | -4.056661371 | -4.28733501 |
| C | -1.981745281 | -4.693504813 | -4.364707048 |
| H | -0.335868503 | -2.891266677 | -5.520845449 |
| H | -1.37593985 | -2.015810835 | -4.387517013 |
| H | -1.790743589 | -4.847083672 | -5.437823897 |
| H | 1.951926439 | -2.876479332 | 0.463522012 |
| N | 1.040804884 | -2.683171438 | 0.886691685 |
| H | 0.645497827 | -3.586270324 | 1.145833123 |
| H | 1.233799028 | -2.1872557 | 1.75545544 |
| N | -1.072707171 | -0.528709531 | -2.245503266 |
| N | -1.642862429 | 0.013915347 | -3.079168521 |

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**Supplementary Table 28 | Cartesian coordinate of XXI. Units are presented in Å.**

SCF energy = -2035.41892234 hartree (BS1)

ZPE = 0.654866 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.253304433 | 1.763908953 | 1.595322264 |
| P | 2.772655486 | -0.70658602 | 2.231955693 |
| N | 4.449473132 | 1.570339988 | 1.08363936 |
| P | 2.757593984 | 4.085394413 | 0.560093557 |
| N | -0.889984676 | 2.121920524 | 2.035342973 |
| N | 0.217937739 | 1.988401951 | 1.881983029 |
| N | 2.652641221 | 2.802006608 | 4.43711244 |
| N | 2.508855014 | 2.315256905 | 3.327044459 |
| N | 1.630656224 | 1.032561112 | -0.385463841 |
| N | 1.230547961 | 0.669679351 | -1.363482858 |
| H | 2.632835199 | -2.792849247 | 5.495508699 |
| H | 4.00783804 | -1.874833761 | 4.880940157 |
| C | 3.098831868 | -2.408320364 | 4.577123275 |
| H | 2.664290115 | 0.23176081 | 5.122513846 |
| H | 3.392332569 | -3.272110277 | 3.977449064 |
| H | 1.356528672 | -0.760517751 | 5.769003383 |
| C | 1.764080142 | -0.329364679 | 4.844153204 |
| H | 0.298256784 | -2.486113343 | 4.544970017 |
| C | 2.088717389 | -1.47848684 | 3.8695263 |
| H | 4.511173932 | 0.167765136 | 3.652431527 |
| H | 1.015284289 | 0.358721611 | 4.43483356 |
| H | 5.17579971 | -1.221817451 | 2.793596627 |
| C | 0.77563096 | -2.237395471 | 3.58716655 |
| H | 2.812254593 | -3.935723327 | 2.082984539 |
| H | 0.062395003 | -1.633116151 | 3.011712556 |
| C | 4.561263367 | -0.322352899 | 2.669402146 |
| H | 7.167280755 | -0.255001621 | 1.936728632 |
| H | 0.939662285 | -3.181375174 | 3.058103987 |
| H | 4.457459499 | -3.286574869 | 1.893186522 |
| H | 4.545469314 | 3.821589588 | 2.938723071 |
| C | 3.487283676 | -3.414236411 | 1.39763748 |
| H | 3.031980573 | 6.518929346 | 3.494108681 |
| C | 6.585578339 | 0.509380284 | 1.428073501 |
| H | 3.649052941 | -4.080765087 | 0.538619352 |
| C | 5.217412394 | 0.618452275 | 1.688804695 |
| H | 5.177333243 | 5.454973238 | 3.160020478 |
| H | 2.240274802 | 4.941603069 | 3.432563169 |
| C | 4.791309614 | 4.747370507 | 2.413261155 |
| C | 2.548524184 | 5.795005041 | 2.822698269 |

| | | | |
|---|---|---|---|
| H | 8.251483271 | 1.306988624 | 0.30676734 |
| C | 2.899856182 | -2.084631627 | 0.87956114 |
| H | 5.605002945 | 4.549818647 | 1.705499437 |
| C | 7.187730218 | 1.379110487 | 0.522144411 |
| H | 1.65543538 | 6.277047085 | 2.415640703 |
| H | 0.834868895 | -2.85842376 | 0.992597209 |
| H | 4.881115711 | -1.512876794 | 0.094393233 |
| C | 3.564712643 | 5.391377626 | 1.730474865 |
| C | 1.502714518 | -2.366506974 | 0.280716558 |
| C | 3.83989899 | -1.580544929 | -0.240891594 |
| H | 3.813127008 | -2.303924407 | -1.067440029 |
| H | 4.605887416 | 7.278785672 | 1.708673216 |
| C | 6.399841129 | 2.341129207 | -0.103423533 |
| H | 1.000023564 | -1.464753751 | -0.077550223 |
| C | 5.036065404 | 2.420830112 | 0.19315459 |
| C | 4.052571047 | 6.65490776 | 0.992738362 |
| H | 4.738788064 | 6.427553701 | 0.167231669 |
| H | 1.616235597 | -3.042549738 | -0.578247621 |
| H | 6.831693393 | 3.034310164 | -0.82058407 |
| H | 3.5516981 | -0.608196112 | -0.649791392 |
| H | 1.114010324 | 6.791714956 | 0.411252579 |
| C | 4.179196682 | 3.452351936 | -0.501617032 |
| H | 3.231634303 | 7.265557677 | 0.604577944 |
| H | 4.808208047 | 4.264541907 | -0.884133545 |
| H | 0.092669396 | 5.388104146 | 0.799899074 |
| C | 0.631410531 | 5.902528902 | -0.006052401 |
| H | 3.702781253 | 2.989315157 | -1.379290995 |
| C | 1.622897099 | 4.96886757 | -0.732135908 |
| H | 0.167457021 | 3.316003315 | -0.777447504 |
| H | -0.117139759 | 6.251640751 | -0.730498274 |
| C | 0.796042625 | 3.893301654 | -1.463863204 |
| H | 3.022390752 | 6.562607116 | -1.387845103 |
| H | 3.053718289 | 5.10885359 | -2.405460905 |
| C | 2.409051489 | 5.759090193 | -1.801278505 |
| H | 0.129532244 | 4.393021441 | -2.180378668 |
| H | 1.421051598 | 3.203846655 | -2.042962316 |
| H | 1.688591307 | 6.220618182 | -2.491383069 |
| H | 2.206802864 | 2.273621368 | 5.205239783 |

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**Supplementary Table 29 | Cartesian coordinate of XXII. Units are presented in Å.**

SCF energy (in toluene) = -2724.02957112 hartree

ZPE = 0.662558 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.486151315 | 0.056417154 | -0.130749294 |
| P | -1.45945757 | -2.257989173 | 0.536902636 |
| N | -2.046892262 | -0.219131363 | -1.729957396 |
| P | -0.760522602 | 2.413786967 | -0.937488039 |
| N | 0.9976722 | -0.296171455 | -0.917103535 |
| H | -0.370321203 | -5.83904272 | -0.370268801 |
| H | -2.00500484 | -5.171977535 | -0.33639149 |
| C | -1.006336107 | -5.082038684 | 0.109586797 |
| H | -1.12253424 | -3.610736726 | -2.199044246 |
| H | -1.071858257 | -5.342079855 | 1.17037295 |
| H | 0.499152454 | -4.282028222 | -2.011636692 |
| C | -0.182239756 | -3.502584096 | -1.64347656 |
| H | 1.65168359 | -4.418628213 | 0.147188815 |
| C | -0.368690029 | -3.697571626 | -0.12322723 |
| H | -3.228234012 | -3.247449981 | -0.92680791 |
| H | 0.259675184 | -2.531277365 | -1.888830877 |
| H | -3.786572549 | -1.876913215 | 0.007189718 |
| C | 1.006509978 | -3.637649599 | 0.57357894 |
| H | -3.077753604 | -4.69059879 | 1.718626582 |
| H | 1.496066707 | -2.668773919 | 0.432497225 |
| C | -2.947332636 | -2.237775571 | -0.604827019 |
| H | -4.275878986 | -2.465826179 | -2.926371262 |
| H | 0.937118984 | -3.812358196 | 1.651450262 |
| H | -4.266508509 | -3.398325131 | 1.451186088 |
| H | 1.944088901 | 1.917538311 | -1.97058863 |
| C | -3.435100895 | -3.725613312 | 2.087249986 |
| H | 2.329917254 | 4.398243104 | 0.04163856 |
| C | -3.665881812 | -1.566737752 | -2.903017502 |
| H | -3.853056935 | -3.894366328 | 3.089333904 |
| C | -2.850366805 | -1.322988283 | -1.794800927 |
| H | 2.646747935 | 3.527651131 | -2.174812486 |
| H | 1.884776941 | 2.745178958 | 0.49986376 |
| C | 1.705403423 | 2.962777082 | -2.200906699 |
| C | 1.484171918 | 3.708941256 | 0.173124278 |
| H | -4.346801003 | -0.818964363 | -4.811125975 |
| C | -2.314939683 | -2.668307669 | 2.215069365 |
| H | 1.327532205 | 3.021794908 | -3.228759615 |
| C | -3.711160643 | -0.646277305 | -3.945333983 |
| H | 0.86093345 | 4.103648194 | 0.979672017 |

| | | | |
|---|---|---|---|
| H | -0.924588426 | -4.16557313 | 3.028673948 |
| H | -3.662525049 | -0.926791824 | 1.975444232 |
| C | 0.738287875 | 3.589094314 | -1.17215884 |
| C | -1.280954442 | -3.15331396 | 3.251559739 |
| C | -2.949838398 | -1.345181599 | 2.701819037 |
| H | -3.517034071 | -1.544153993 | 3.621544781 |
| H | 1.224864982 | 5.567353056 | -1.888828975 |
| C | -2.943412989 | 0.510911761 | -3.848151407 |
| H | -0.41630097 | -2.490083409 | 3.3338496 |
| C | -2.1163067 | 0.705596393 | -2.739990515 |
| C | 0.31772453 | 4.981903378 | -1.684144481 |
| H | -0.253106921 | 4.931032072 | -2.620281878 |
| H | -1.766552279 | -3.189111299 | 4.236356624 |
| H | -2.968334466 | 1.262840285 | -4.632351138 |
| H | -2.199539653 | -0.588080526 | 2.946233848 |
| H | -1.213176924 | 4.913983591 | 0.89919684 |
| C | -1.259768117 | 1.947072164 | -2.679011042 |
| H | -0.268154496 | 5.542496635 | -0.948782436 |
| H | -0.312034193 | 1.728835899 | -3.188423622 |
| H | -1.254061692 | 3.385708303 | 1.813493472 |
| C | -1.819209607 | 4.032101727 | 1.131295702 |
| H | -1.738041416 | 2.759377878 | -3.239467796 |
| C | -2.27346943 | 3.27578807 | -0.135642939 |
| H | -2.784215586 | 1.479076541 | 1.039200522 |
| H | -2.711482352 | 4.38386577 | 1.667596725 |
| C | -3.246145929 | 2.15747385 | 0.30688722 |
| H | -2.391082892 | 5.042008061 | -1.460429812 |
| H | -3.428296139 | 3.689518336 | -1.965713448 |
| C | -3.017335655 | 4.22141125 | -1.098002261 |
| H | -4.108651056 | 2.616021813 | 0.810453091 |
| H | -3.633578379 | 1.575273006 | -0.536865135 |
| H | -3.867483782 | 4.669097019 | -0.564328759 |
| S | 0.596732523 | 0.195775147 | 3.032455166 |
| O | -0.302971076 | 0.203826611 | 4.188613143 |
| O | 1.335662879 | -1.02633891 | 2.683596075 |
| O | -0.084375006 | 0.841786218 | 1.773926055 |
| C | 1.88456513 | 1.508701595 | 3.362653105 |
| F | 2.787319998 | 1.516657246 | 2.367153922 |
| F | 1.305187712 | 2.713525841 | 3.43505734 |
| F | 2.498106588 | 1.236906069 | 4.510534833 |
| H | 1.990107042 | -0.468265333 | -1.085707351 |

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**Supplementary Table 30 | Cartesian coordinate of XXIII. Units are presented in Å.**

SCF energy (in toluene) = -2833.53000327 hartree

ZPE = 0.673437 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.308541516 | 0.577312982 | 0.365987468 |
| P | 0.352379363 | -0.912459408 | 2.466752952 |
| N | 1.843437955 | 0.992223993 | 0.661296892 |
| P | 0.260058095 | 2.066632293 | -1.69182129 |
| N | -0.944556502 | 1.829436646 | 1.391572068 |
| H | -1.146593795 | -1.700615145 | 5.9413488 |
| H | 0.432896082 | -0.996863934 | 5.574005145 |
| C | -0.349918554 | -1.660921546 | 5.185399744 |
| H | -0.960887802 | 0.96570834 | 4.521828766 |
| H | 0.059953749 | -2.671040614 | 5.096862707 |
| H | -2.411335529 | 0.040014512 | 4.912379482 |
| C | -1.647022065 | 0.199348119 | 4.139763648 |
| H | -2.820995124 | -2.213318928 | 4.116928746 |
| C | -0.955539235 | -1.151864378 | 3.861873414 |
| H | 0.76798474 | 1.333013449 | 3.294253886 |
| H | -2.158916137 | 0.585397854 | 3.252516859 |
| H | 2.031366126 | 0.274245119 | 3.940151878 |
| C | -2.031580923 | -2.138222647 | 3.355876424 |
| H | 2.088511664 | -2.384725556 | 4.586950904 |
| H | -2.490526457 | -1.800950165 | 2.420883316 |
| C | 1.448835017 | 0.509811528 | 3.044200029 |
| H | 4.073439237 | 1.249542218 | 3.186745021 |
| H | -1.639972107 | -3.143421325 | 3.183820909 |
| H | 3.264140683 | -1.508436865 | 3.581165701 |
| H | 0.394224554 | 3.652715838 | 0.89433081 |
| C | 2.584107543 | -2.368262725 | 3.613019542 |
| H | -0.944431913 | 5.626216144 | -1.078405018 |
| C | 3.69113435 | 1.285682844 | 2.170316573 |
| H | 3.2126533 | -3.267679876 | 3.55312784 |
| C | 2.358867368 | 0.943755824 | 1.926330165 |
| H | 0.947342645 | 5.2440645 | 0.343008491 |
| H | -1.684882783 | 4.073315074 | -0.653441755 |
| C | 0.977576899 | 4.167190847 | 0.126809114 |
| C | -1.000158718 | 4.564935019 | -1.356875363 |
| H | 5.556913199 | 1.913469668 | 1.283111258 |
| C | 1.610705405 | -2.394561086 | 2.411787918 |
| H | 2.023768678 | 3.852376 | 0.21187304 |
| C | 4.514254925 | 1.656616787 | 1.109007495 |
| H | -1.442902797 | 4.513991041 | -2.357076116 |

| | | | |
|---|---|---|---|
| H | 0.380494945 | -3.956637951 | 3.362135623 |
| H | 3.112499264 | -1.402231893 | 1.132531419 |
| C | 0.415489467 | 3.952991001 | -1.296274635 |
| C | 0.855558146 | -3.740767305 | 2.398988969 |
| C | 2.467906498 | -2.287832399 | 1.12937482 |
| H | 3.129586204 | -3.164407037 | 1.094685852 |
| H | 1.471004197 | 5.729751671 | -1.915259127 |
| C | 3.982963302 | 1.694438578 | -0.17881286 |
| H | 0.098003799 | -3.793270831 | 1.612401105 |
| C | 2.639527187 | 1.371084881 | -0.379946977 |
| C | 1.369313902 | 4.692000778 | -2.262126435 |
| H | 2.377082695 | 4.257216366 | -2.259507272 |
| H | 1.584759898 | -4.540854238 | 2.212395063 |
| H | 4.597624789 | 1.978122464 | -1.028705097 |
| H | 1.877907565 | -2.299985163 | 0.211904619 |
| H | -2.463474692 | 2.480347581 | -2.817445883 |
| C | 2.024985674 | 1.421637985 | -1.752928306 |
| H | 1.01179804 | 4.729287101 | -3.291285169 |
| H | 2.666868946 | 1.98140143 | -2.44249129 |
| H | -2.235776703 | 0.721690018 | -2.67965678 |
| C | -1.993626532 | 1.603290439 | -3.279067076 |
| H | 1.941390059 | 0.397354185 | -2.139955551 |
| C | -0.467803559 | 1.769859355 | -3.45491127 |
| H | 0.06343085 | -0.37221306 | -3.317441286 |
| H | -2.452034685 | 1.46839865 | -4.268423314 |
| C | 0.127704668 | 0.461714596 | -4.017927504 |
| H | -0.674251399 | 3.832704612 | -4.24013929 |
| H | 0.875368309 | 3.051320519 | -4.651131905 |
| C | -0.194918061 | 2.880441732 | -4.488682191 |
| H | -0.439630702 | 0.182784088 | -4.916161599 |
| H | 1.173566108 | 0.589302938 | -4.324635882 |
| H | -0.617364227 | 2.551710626 | -5.448550838 |
| S | -0.610542241 | -2.548957281 | -1.020730469 |
| O | 0.508036683 | -3.446855253 | -1.309188476 |
| O | -1.488025265 | -2.809676771 | 0.129734708 |
| O | -0.141383906 | -1.055049073 | -1.045703781 |
| C | -1.731300949 | -2.646473925 | -2.517275576 |
| F | -2.670383773 | -1.685922817 | -2.458932502 |
| F | -1.023000485 | -2.49525207 | -3.640387326 |
| F | -2.321559667 | -3.837189715 | -2.51817273 |
| N | -2.394738056 | 0.092709835 | 0.041427658 |
| N | -3.484341038 | -0.112317893 | -0.074081377 |
| H | -1.622429529 | 2.409917649 | 1.89103253 |

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**Supplementary Table 31 | Cartesian coordinate of XXIV. Units are presented in Å.**

SCF energy (in toluene) = -2833.09807794 hartree

ZPE = 0.661422 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.309247343 | 0.541421146 | 0.380043695 |
| P | 0.371213047 | -0.83705176 | 2.501938319 |
| N | 1.877811881 | 1.000307405 | 0.635794674 |
| P | 0.201848281 | 2.051524522 | -1.640906701 |
| N | -0.918300621 | 1.734522416 | 1.389615658 |
| H | -1.184236674 | -1.606485458 | 5.979082064 |
| H | 0.48803385 | -1.147316597 | 5.63425705 |
| C | -0.393175893 | -1.650701909 | 5.215872865 |
| H | -0.598036849 | 1.009287036 | 4.881416609 |
| H | -0.152134069 | -2.70691116 | 5.06204036 |
| H | -2.237802578 | 0.363414099 | 5.003939539 |
| C | -1.373264505 | 0.459845349 | 4.330922859 |
| H | -2.878281389 | -1.836752957 | 4.173318918 |
| C | -0.908438185 | -0.959936326 | 3.938548635 |
| H | 0.883523139 | 1.388250852 | 3.268857442 |
| H | -1.677273845 | 1.058905886 | 3.466282226 |
| H | 2.145886012 | 0.319027979 | 3.914815479 |
| C | -2.124939185 | -1.730900827 | 3.378628665 |
| H | 1.957553012 | -2.557176454 | 4.649610319 |
| H | -2.585809434 | -1.191141282 | 2.544894216 |
| C | 1.546296577 | 0.547343387 | 3.026408453 |
| H | 4.186923363 | 1.251298809 | 3.090173121 |
| H | -1.86867549 | -2.733826942 | 3.022220523 |
| H | 3.162535062 | -1.618876809 | 3.741965416 |
| H | 0.262463857 | 3.611682988 | 0.94467736 |
| C | 2.475448194 | -2.473121274 | 3.690957641 |
| H | -1.010747717 | 5.604503326 | -0.994106177 |
| C | 3.774326175 | 1.291011528 | 2.085417965 |
| H | 3.097303908 | -3.373082752 | 3.57565677 |
| C | 2.432057471 | 0.955396815 | 1.881061521 |
| H | 0.863440466 | 5.205032309 | 0.431193415 |
| H | -1.747599378 | 4.037887751 | -0.610095473 |
| C | 0.880568839 | 4.128332451 | 0.205875247 |
| C | -1.062557417 | 4.548956298 | -1.298204495 |
| H | 5.611827978 | 1.922176664 | 1.142613968 |
| C | 1.525501157 | -2.388649392 | 2.476338231 |
| H | 1.918523027 | 3.79261971 | 0.313703006 |
| C | 4.563804083 | 1.665574584 | 1.000779856 |
| H | -1.494088233 | 4.519958479 | -2.304857514 |

| | | | |
|---|---|---|---|
| H | 0.120143957 | -3.861174381 | 3.326018742 |
| H | 3.131409398 | -1.48020901 | 1.269409772 |
| C | 0.352627702 | 3.935503428 | -1.233707304 |
| C | 0.669802038 | -3.671045025 | 2.396716563 |
| C | 2.412894926 | -2.306557376 | 1.212083254 |
| H | 2.992992505 | -3.237553548 | 1.138349484 |
| H | 1.392414169 | 5.734691777 | -1.824840453 |
| C | 3.990474248 | 1.709445311 | -0.268744563 |
| H | -0.043263995 | -3.646142376 | 1.566042121 |
| C | 2.641679571 | 1.380135387 | -0.426411779 |
| C | 1.319319851 | 4.692767727 | -2.169509328 |
| H | 2.333429444 | 4.273503702 | -2.131757909 |
| H | 1.339206366 | -4.528024113 | 2.233891307 |
| H | 4.575116038 | 1.999895073 | -1.137741404 |
| H | 1.838706032 | -2.21190403 | 0.288693342 |
| H | -2.518151129 | 2.51493695 | -2.733753866 |
| C | 1.9796032 | 1.432426127 | -1.777217291 |
| H | 0.996794259 | 4.717612835 | -3.211682404 |
| H | 2.597572105 | 1.990555592 | -2.490656902 |
| H | -2.305324239 | 0.754570296 | -2.652308251 |
| C | -2.061588237 | 1.650265505 | -3.230299666 |
| H | 1.87662833 | 0.405674438 | -2.153801473 |
| C | -0.53404074 | 1.802771809 | -3.411839018 |
| H | -0.016989745 | -0.336497613 | -3.267778098 |
| H | -2.530849835 | 1.548164263 | -4.219701041 |
| C | 0.026800016 | 0.484881025 | -3.985342286 |
| H | -0.713004376 | 3.872489712 | -4.182211911 |
| H | 0.820106935 | 3.069924598 | -4.606982035 |
| C | -0.252890619 | 2.913096303 | -4.442309947 |
| H | -0.573092499 | 0.197381831 | -4.860323689 |
| H | 1.064428178 | 0.599232668 | -4.326267788 |
| H | -0.684261285 | 2.600349429 | -5.404764395 |
| S | -0.390202435 | -2.767070801 | -1.258427365 |
| O | 0.708991278 | -3.723189607 | -1.463900115 |
| O | -1.383991824 | -3.071225987 | -0.207835819 |
| O | 0.080389284 | -1.318512526 | -1.229624614 |
| C | -1.382577425 | -2.83937384 | -2.838979976 |
| F | -2.322066615 | -1.871435498 | -2.857608415 |
| F | -0.588254357 | -2.670654778 | -3.911736846 |
| F | -1.99253343 | -4.024963771 | -2.94367346 |
| N | -2.28340505 | -0.122304973 | -0.047009194 |
| N | -3.342578068 | -0.429361928 | -0.240102938 |

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**Supplementary Table 32 | Cartesian coordinate of the reactant complex for protonation of 1 by lutidinium. Units are presented in Å.**

SCF energy (in toluene) = -4289.81340546 hartree

ZPE = 1.442197 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 3.00651646 | 0.426313984 | -0.109637676 |
| Mo | -1.970290333 | -1.092783803 | 0.614780896 |
| P | -2.387603348 | -2.562062225 | -1.432904872 |
| P | 2.843615817 | 2.968193782 | -0.107032579 |
| N | 5.156738659 | 1.051406235 | -0.396855324 |
| N | -4.040947467 | -1.861543037 | 1.011212457 |
| P | -2.499914572 | -0.03231846 | 2.873953907 |
| P | 4.229284241 | -1.825875227 | -0.236404882 |
| N | 1.066447593 | -0.128304261 | 0.143991107 |
| N | -0.03401148 | -0.445874064 | 0.289112553 |
| N | 2.547333806 | 0.419440637 | -3.245052665 |
| N | 2.716500385 | 0.431309469 | -2.12128003 |
| N | 3.253162218 | 0.405044462 | 1.910678403 |
| N | 3.379089323 | 0.407618222 | 3.039418561 |
| N | -3.268201364 | 1.291353849 | -0.935451595 |
| N | -2.755564482 | 0.424256168 | -0.374770992 |
| N | -1.195693387 | -2.710888444 | 1.647014803 |
| N | -0.784077955 | -3.610903794 | 2.19402028 |
| H | -2.584843671 | -2.007244753 | -5.28751913 |
| H | 1.099779417 | 5.688998808 | -2.290150321 |
| H | 2.689496063 | 4.970980927 | -2.556124564 |
| H | -3.910825546 | -1.917265579 | -4.12321335 |
| C | -2.936123393 | -2.384961683 | -4.315600823 |
| C | 1.951237441 | 5.211301342 | -1.781480179 |
| H | 1.584592614 | 2.71931118 | -2.882130294 |
| H | -2.688231172 | 0.029435763 | -3.031501913 |
| H | 2.38911852 | 5.955790974 | -1.11173771 |
| H | -3.09362852 | -3.460802853 | -4.423364973 |
| H | 0.029026668 | 3.514474777 | -2.623586795 |
| H | -1.394371444 | -0.165059799 | -4.226651936 |
| C | -1.742335581 | -0.485552701 | -3.233537744 |
| C | 0.857323145 | 2.998043081 | -2.113516256 |
| H | -0.169287728 | -2.154041982 | -4.53210471 |
| H | -0.53274448 | 4.710662971 | -0.668911351 |
| C | -1.897942631 | -2.01888756 | -3.234122975 |
| C | 1.451318142 | 3.94557307 | -1.053029355 |
| H | 3.941471216 | 2.954848806 | -2.251432174 |
| H | -4.362267499 | -1.259190936 | -1.838042533 |

| | | | |
|---|---|---|---|
| H | -1.011369988 | -0.150058601 | -2.490908092 |
| H | 0.464972964 | 2.078154959 | -1.66635647 |
| H | -4.816128944 | -2.950525226 | -2.067425573 |
| H | 4.680625277 | 4.243967236 | -1.30047163 |
| C | -0.523362923 | -2.615535293 | -3.599073056 |
| C | 0.312103954 | 4.316076629 | -0.083247074 |
| H | -2.126763048 | -5.096605233 | -3.454450243 |
| H | 2.453497418 | 5.983919917 | 1.037025228 |
| H | 0.228100317 | -2.407560238 | -2.826910601 |
| H | -0.049518408 | 3.442394171 | 0.474206132 |
| C | -4.253855312 | -2.268681565 | -1.416761363 |
| C | 4.322216305 | 3.2082866 | -1.251588787 |
| H | -6.719029838 | -3.104596063 | -0.648477128 |
| H | 6.982158192 | 3.67708545 | -1.510762976 |
| H | -0.560688549 | -3.69666846 | -3.76567699 |
| H | 0.595277691 | 5.092890802 | 0.633584932 |
| H | -3.790092117 | -4.992391557 | -2.831591362 |
| H | 4.108823506 | 5.780308966 | 0.419958169 |
| H | 4.998960631 | -0.520216805 | -2.804989808 |
| H | -4.730569416 | 0.922632401 | 1.149394156 |
| C | -2.755719674 | -5.25243756 | -2.572219043 |
| C | 3.424668852 | 5.520082499 | 1.237895665 |
| H | 3.850901262 | -3.257568228 | -3.773157719 |
| H | -3.535985643 | 3.595087428 | 2.244686294 |
| C | -6.126218147 | -2.766140359 | 0.198256047 |
| C | 6.784460264 | 2.690635457 | -1.097984167 |
| H | -2.74155204 | -6.33087759 | -2.355429887 |
| H | 3.821576461 | 5.989141869 | 2.150462898 |
| C | -4.829360947 | -2.29534947 | -0.019680628 |
| C | 5.462812649 | 2.282369146 | -0.904987416 |
| H | 5.757945836 | -1.81794245 | -3.735278396 |
| H | -5.49261528 | 2.210885324 | 2.10051997 |
| H | 2.860206226 | -2.075798126 | -2.905155414 |
| H | -2.578090187 | 2.468076072 | 1.254940076 |
| C | 5.558460186 | -1.454601541 | -2.71655203 |
| C | -4.919006191 | 1.273594675 | 2.166686793 |
| C | 3.533559747 | -2.927462011 | -2.7726645 |
| C | -2.87199223 | 2.716345102 | 2.279277188 |
| H | 8.86655095 | 2.14176083 | -0.891505516 |
| H | -7.644250438 | -3.187814838 | 1.68135316 |
| C | -2.249348804 | -4.494624683 | -1.327964184 |
| C | 3.332531237 | 3.997114304 | 1.46550925 |
| H | 6.528333782 | -1.23480788 | -2.255829367 |
| H | -5.560116084 | 0.541193221 | 2.670225277 |
| C | 7.831308187 | 1.837395556 | -0.753919229 |
| C | -6.639684172 | -2.815031084 | 1.493739816 |
| H | 2.966408177 | -3.748307706 | -2.32336073 |
| H | -1.972621796 | 3.014103132 | 2.826706606 |
| H | -0.120680035 | -4.624837001 | -1.903557302 |
| H | 1.311349276 | 4.074775393 | 2.356517801 |
| H | -4.177120694 | -4.877909087 | -0.330082215 |
| H | 5.521470493 | 3.837409153 | 1.24960319 |

| | | | |
|---|---|---|---|
| C | 4.785065611 | -2.551173248 | -1.948711556 |
| C | -3.620708082 | 1.548521142 | 2.958288451 |
| C | -0.777879569 | -4.885433733 | -1.06849278 |
| C | 2.316767308 | 3.713886995 | 2.594422758 |
| C | -3.103342562 | -4.975024661 | -0.132161381 |
| C | 4.72837925 | 3.530794416 | 1.941084613 |
| H | -2.898827523 | -6.041861754 | 0.038388883 |
| H | 4.940808904 | 4.004629726 | 2.910443235 |
| H | 6.063666745 | -4.03500165 | -2.865158277 |
| H | -4.749139914 | 2.817787546 | 4.298797686 |
| C | -5.833222414 | -2.378312428 | 2.543110495 |
| C | 7.519089355 | 0.585342837 | -0.22853795 |
| H | -0.380184952 | -4.416796383 | -0.164790478 |
| H | 2.251369151 | 2.648026979 | 2.828946488 |
| C | -4.545827187 | -1.902532528 | 2.281788844 |
| C | 6.182613679 | 0.211681129 | -0.066263061 |
| C | 5.716847354 | -3.77617967 | -1.853717282 |
| C | -4.044802521 | 1.975870269 | 4.377877847 |
| H | 6.609978032 | -3.576419194 | -1.247949162 |
| H | -4.563915625 | 1.173382357 | 4.917249106 |
| H | -0.716504903 | -5.975068949 | -0.930408205 |
| H | 2.642786252 | 4.234157354 | 3.507376491 |
| H | 8.30414996 | -0.111827654 | 0.054380886 |
| H | -6.193798818 | -2.401099245 | 3.568785107 |
| H | -2.877938866 | -4.443862327 | 0.795376687 |
| H | 4.794881489 | 2.449418434 | 2.082297596 |
| H | 3.337528564 | -4.864697997 | -0.529216271 |
| H | -1.133526415 | 2.229360679 | 4.644104665 |
| C | 5.8356822 | -1.1498964 | 0.482759005 |
| C | -3.67144575 | -1.413907449 | 3.411337687 |
| H | 5.217117781 | -4.661855632 | -1.449406882 |
| H | -3.204576597 | 2.3155291 | 4.990751326 |
| H | 6.687694093 | -1.830824188 | 0.36481045 |
| H | -4.289611721 | -1.155267585 | 4.28005558 |
| H | 1.991896935 | -3.775804489 | -0.121152592 |
| H | -0.067857446 | 1.600270035 | 3.363687254 |
| C | 2.872847552 | -4.291918482 | 0.28002079 |
| C | -0.501551482 | 1.385279008 | 4.348791147 |
| H | 5.640892875 | -1.06652923 | 1.561608009 |
| H | -3.004966258 | -2.22848087 | 3.730954481 |
| C | 3.849643725 | -3.311366696 | 0.958721274 |
| C | -1.250163755 | 0.035886067 | 4.359195833 |
| H | 2.234596631 | -2.183638102 | 1.934637669 |
| H | 0.308308956 | -0.959287293 | 3.169726153 |
| H | 2.516875644 | -5.015490563 | 1.027630296 |
| H | 0.329222409 | 1.335446498 | 5.066714246 |
| C | 3.139197573 | -2.74015698 | 2.20118184 |
| C | -0.194542785 | -1.065384043 | 4.136187157 |
| H | 5.668992549 | -4.539400582 | 0.63492376 |
| H | -2.631944701 | 0.54591419 | 6.021326869 |
| H | 5.782402264 | -3.423191001 | 2.00918403 |
| H | -2.362310711 | -1.194401699 | 5.80934469 |

| | | | |
|---|---|---|---|
| C | 5.102178438 | -4.071679578 | 1.443939419 |
| C | -1.889720772 | -0.206376815 | 5.743247071 |
| H | 2.846270733 | -3.574816549 | 2.854834407 |
| H | 0.568720688 | -0.983299057 | 4.923130106 |
| H | 3.785325417 | -2.079590978 | 2.788226746 |
| H | -0.618035041 | -2.072957986 | 4.201050797 |
| H | 4.784797427 | -4.873079956 | 2.127481799 |
| H | -1.097549429 | -0.180147999 | 6.505912546 |
| H | -4.381845322 | 2.466847176 | -1.845213731 |
| C | -6.777405615 | 3.515194032 | -3.8522425 |
| C | -6.642772516 | 4.893061987 | -3.634472155 |
| C | -5.663242663 | 5.363896191 | -2.750449513 |
| C | -4.831635732 | 4.467775383 | -2.093898617 |
| N | -4.99771554 | 3.132599594 | -2.344155611 |
| C | -5.939712526 | 2.624818729 | -3.197224646 |
| H | -7.530995283 | 3.127801894 | -4.531988951 |
| H | -7.296673841 | 5.593152065 | -4.148222522 |
| H | -5.541444035 | 6.42746318 | -2.566168069 |
| C | -3.761456242 | 4.85107529 | -1.119401824 |
| H | -2.791397048 | 4.423964253 | -1.408817964 |
| H | -3.664878791 | 5.939158854 | -1.062449278 |
| H | -3.98819719 | 4.468401571 | -0.114502612 |
| C | -5.985625696 | 1.13567696 | -3.35729762 |
| H | -5.065037415 | 0.761121529 | -3.826945045 |
| H | -6.079806797 | 0.638691792 | -2.381525451 |
| H | -6.833856411 | 0.842427487 | -3.982724651 |

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**Supplementary Table 33 | Cartesian coordinate of the transition state for protonation of a terminal dinitrogen ligand in 1 by lutidinium. Units are presented in Å.**

SCF energy (in toluene) = -4289.79497531 hartree

ZPE = 1.437074 hartree

imaginary frequency: 1033*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 3.064380177 | 0.378827923 | -0.091650051 |
| Mo | -2.009976507 | -0.940106368 | 0.382749833 |
| P | -2.342611027 | -2.366704275 | -1.726725403 |
| P | 2.930735153 | 2.913517979 | -0.320532506 |
| N | 5.246651898 | 0.969717769 | -0.307424952 |
| N | -4.051660231 | -1.806081108 | 0.727119494 |
| P | -2.589942961 | 0.017618685 | 2.676546675 |
| P | 4.277834618 | -1.884571907 | 0.012855615 |
| N | 1.119338427 | -0.100354354 | 0.089298971 |
| N | -0.00494368 | -0.34980282 | 0.175784782 |
| N | 2.748330246 | 0.094915286 | -3.233060783 |
| N | 2.872746988 | 0.20900963 | -2.109717063 |
| N | 3.193539952 | 0.515220618 | 1.936210238 |
| N | 3.244633693 | 0.594714386 | 3.068199453 |
| N | -2.95370604 | 1.593272217 | -1.096683767 |
| N | -2.665308657 | 0.591921438 | -0.528363392 |
| N | -1.169202828 | -2.62480041 | 1.383242245 |
| N | -0.70591427 | -3.512035024 | 1.895041779 |
| H | -2.529687847 | -1.678223533 | -5.554671811 |
| H | 1.361738729 | 5.461643288 | -2.816596873 |
| H | 2.975093896 | 4.754807444 | -2.896696636 |
| H | -3.86576525 | -1.668543872 | -4.402169935 |
| C | -2.878035396 | -2.10365028 | -4.601988333 |
| C | 2.170921597 | 5.034251282 | -2.205176405 |
| H | 1.897951778 | 2.480650808 | -3.177456152 |
| H | -2.711977995 | 0.267817312 | -3.224032883 |
| H | 2.54173242 | 5.830373332 | -1.555034908 |
| H | -3.003483759 | -3.178310402 | -4.753569375 |
| H | 0.326649701 | 3.280911657 | -3.084647821 |
| H | -1.413539408 | 0.156102143 | -4.420140839 |
| C | -1.751343566 | -0.211611922 | -3.440220593 |
| C | 1.113308782 | 2.799824397 | -2.48409636 |
| H | -0.117108857 | -1.781528746 | -4.788114872 |
| H | -0.391954959 | 4.580302558 | -1.260513359 |
| C | -1.85665578 | -1.747208878 | -3.50100051 |
| C | 1.62039785 | 3.812734314 | -1.438182304 |

| | | | |
|---|---|---|---|
| H | 4.175809809 | 2.733349984 | -2.37585097 |
| H | -4.357733046 | -1.122221103 | -2.095600885 |
| H | -1.032896226 | 0.119571602 | -2.684175846 |
| H | 0.685817701 | 1.907166036 | -2.016199226 |
| H | -4.75163748 | -2.817271507 | -2.397634576 |
| H | 4.857394883 | 4.087446443 | -1.472187937 |
| C | -0.461703359 | -2.28849476 | -3.875844452 |
| C | 0.405210384 | 4.23330398 | -0.586768864 |
| H | -2.003693524 | -4.817543482 | -3.826618901 |
| H | 2.468807073 | 6.00167041 | 0.558711279 |
| H | 0.279113855 | -2.084309642 | -3.092443905 |
| H | 0.003916393 | 3.391210106 | -0.008179762 |
| C | -4.217515558 | -2.144003994 | -1.71520709 |
| C | 4.487869902 | 3.059500265 | -1.372500248 |
| H | -6.653370076 | -3.105814772 | -1.006343621 |
| H | 7.158795727 | 3.498798991 | -1.495470031 |
| H | -0.464671436 | -3.363234708 | -4.083331571 |
| H | 0.627846308 | 5.056682135 | 0.099672726 |
| H | -3.671319139 | -4.762558723 | -3.211142741 |
| H | 4.169462534 | 5.767670935 | 0.097146182 |
| H | 5.174655833 | -0.750491523 | -2.590060728 |
| H | -4.713361548 | 0.960906662 | 0.895820244 |
| C | -2.634738119 | -5.016772541 | -2.95514834 |
| C | 3.420390983 | 5.560948945 | 0.872509045 |
| H | 4.061152669 | -3.580460918 | -3.417963589 |
| H | -3.682046689 | 3.638035714 | 2.139406912 |
| C | -6.085223708 | -2.769824582 | -0.142130294 |
| C | 6.928621405 | 2.545405475 | -1.025844742 |
| H | -2.604417352 | -6.101973362 | -2.778113011 |
| H | 3.740575729 | 6.096399989 | 1.778664682 |
| C | -4.804470046 | -2.243642762 | -0.328506652 |
| C | 5.593901745 | 2.158372231 | -0.88326434 |
| H | 5.946643007 | -2.11207544 | -3.41266029 |
| H | -5.569295628 | 2.218058766 | 1.813924743 |
| H | 3.033686108 | -2.332259479 | -2.700742379 |
| H | -2.630082128 | 2.579907364 | 1.171098317 |
| C | 5.717902318 | -1.684105274 | -2.425728832 |
| C | -4.984201364 | 1.290782286 | 1.902287977 |
| C | 3.697104732 | -3.168502953 | -2.465059967 |
| C | -2.991400415 | 2.781574652 | 2.184343139 |
| H | 8.989720202 | 2.000251937 | -0.661725932 |
| H | -7.605500874 | -3.290893952 | 1.305911003 |
| C | -2.146309186 | -4.296272966 | -1.681493261 |
| C | 3.3088442 | 4.058395288 | 1.200829854 |
| H | 6.674833671 | -1.445743703 | -1.947139327 |
| H | -5.641190632 | 0.534319654 | 2.347178095 |
| C | 7.945271157 | 1.712471791 | -0.563457027 |
| C | -6.613744625 | -2.874191883 | 1.144044228 |
| H | 3.106642272 | -3.94996027 | -1.977193429 |
| H | -2.137216986 | 3.087432089 | 2.795032143 |
| H | -0.012052785 | -4.340864869 | -2.257214373 |
| H | 1.232106254 | 4.210135179 | 1.941493904 |

| | | | |
|---|---|---|---|
| H | -4.061403468 | -4.790135825 | -0.707560923 |
| H | 5.505786624 | 3.873196031 | 1.148886426 |
| C | 4.910131418 | -2.725491266 | -1.616427023 |
| C | -3.741574493 | 1.567477533 | 2.776713542 |
| C | -0.664295944 | -4.660258914 | -1.439322524 |
| C | 2.213150612 | 3.854627222 | 2.271012404 |
| C | -2.985675321 | -4.849229768 | -0.506685698 |
| C | 4.664497597 | 3.628726458 | 1.807314533 |
| H | -2.739455961 | -5.911989739 | -0.369593268 |
| H | 4.816646107 | 4.181045063 | 2.746233296 |
| H | 6.225682167 | -4.263530379 | -2.37536123 |
| H | -4.983576702 | 2.735537103 | 4.106607148 |
| C | -5.841150441 | -2.436315255 | 2.21753731 |
| C | 7.590872591 | 0.501701214 | 0.027221506 |
| H | -0.278133561 | -4.228024886 | -0.512540433 |
| H | 2.116968189 | 2.805086595 | 2.561465347 |
| C | -4.570017409 | -1.901952157 | 1.988685844 |
| C | 6.242959398 | 0.149866599 | 0.13789888 |
| C | 5.836423067 | -3.93874085 | -1.399029779 |
| C | -4.24753709 | 1.921746193 | 4.188592407 |
| H | 6.704675055 | -3.698431043 | -0.772383067 |
| H | -4.753239179 | 1.079724618 | 4.678107239 |
| H | -0.57506591 | -5.753286607 | -1.355735381 |
| H | 2.482821719 | 4.425344465 | 3.172039202 |
| H | 8.35095966 | -0.179627396 | 0.401992562 |
| H | -6.215783734 | -2.501407848 | 3.236207053 |
| H | -2.78822492 | -4.341330295 | 0.440379299 |
| H | 4.709577647 | 2.562864025 | 2.042976654 |
| H | 3.36796547 | -4.930627962 | -0.101566564 |
| H | -1.31606629 | 2.242514385 | 4.557945945 |
| C | 5.852830963 | -1.165370139 | 0.762816928 |
| C | -3.73525654 | -1.412259089 | 3.147291735 |
| H | 5.318840761 | -4.796766133 | -0.958733619 |
| H | -3.450453312 | 2.276865909 | 4.848615596 |
| H | 6.703038885 | -1.858261873 | 0.740138215 |
| H | -4.381054492 | -1.194622352 | 4.007251863 |
| H | 2.022544818 | -3.805202202 | 0.192420261 |
| H | -0.209102768 | 1.687971667 | 3.277382387 |
| C | 2.886001591 | -4.301046471 | 0.653760259 |
| C | -0.657595212 | 1.425653219 | 4.244019622 |
| H | 5.604281371 | -1.001266273 | 1.821976886 |
| H | -3.052447858 | -2.213636989 | 3.466855043 |
| C | 3.852759218 | -3.282140329 | 1.29137024 |
| C | -1.377968339 | 0.062084414 | 4.192181915 |
| H | 2.218238871 | -2.084359262 | 2.141539349 |
| H | 0.2193893 | -0.876952404 | 3.006988204 |
| H | 2.502200997 | -4.969924332 | 1.437560683 |
| H | 0.159264402 | 1.367877649 | 4.976928666 |
| C | 3.114036746 | -2.620015347 | 2.471053391 |
| C | -0.299783186 | -1.015251676 | 3.960813994 |
| H | 5.669344115 | -4.55068977 | 1.120740129 |
| H | -2.811002633 | 0.497911589 | 5.830309881 |

| | | | |
|---|---|---|---|
| H | 5.746688468 | -3.341400789 | 2.416626396 |
| H | -2.499606591 | -1.230954325 | 5.582169836 |
| C | 5.079102317 | -4.019929286 | 1.871682396 |
| C | -2.046810215 | -0.232006172 | 5.552155682 |
| H | 2.805420629 | -3.40347663 | 3.178753941 |
| H | 0.447886292 | -0.943363143 | 4.763309763 |
| H | 3.747557899 | -1.916615515 | 3.02146906 |
| H | -0.709810719 | -2.03070838 | 3.994839377 |
| H | 4.72672031 | -4.768067774 | 2.597438723 |
| H | -1.274192591 | -0.209551346 | 6.334617108 |
| H | -4.03357622 | 2.131847686 | -1.302594369 |
| C | -7.432950301 | 3.290432513 | -2.060170629 |
| C | -7.226023318 | 4.669557844 | -2.059902323 |
| C | -5.944238822 | 5.166318973 | -1.832060735 |
| C | -4.893036288 | 4.274824166 | -1.598401018 |
| N | -5.11888892 | 2.939861009 | -1.595060973 |
| C | -6.352619017 | 2.436650319 | -1.827654011 |
| H | -8.418679078 | 2.871315746 | -2.244338091 |
| H | -8.0556173 | 5.349891176 | -2.241398684 |
| H | -5.748416996 | 6.235377307 | -1.8356395 |
| C | -3.487798943 | 4.748377615 | -1.34277426 |
| H | -2.771170996 | 4.218124191 | -1.980475421 |
| H | -3.403362779 | 5.82392422 | -1.527849784 |
| H | -3.192148001 | 4.552132218 | -0.303875614 |
| C | -6.50290552 | 0.93989519 | -1.848273016 |
| H | -5.923927339 | 0.506629649 | -2.675013962 |
| H | -6.142219179 | 0.487505624 | -0.916369065 |
| H | -7.5511875 | 0.655236569 | -1.983823039 |

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**Supplementary Table 34 | Cartesian coordinate of the product complex for protonation of a terminal dinitrogen ligand in 1 by lutidinium. Units are presented in Å.**

SCF energy (in toluene) = -4289.80099118 hartree

ZPE = 1.440119 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 3.100398543 | 0.180335551 | -0.078324009 |
| Mo | -2.017931589 | -0.787138268 | 0.411176457 |
| P | -2.476997113 | -2.191986341 | -1.698619099 |
| P | 3.022877386 | 2.708983878 | -0.479872388 |
| N | 5.296438377 | 0.694925753 | -0.381901787 |
| N | -4.073999507 | -1.607397128 | 0.843217929 |
| P | -2.509366549 | 0.232182789 | 2.703238721 |
| P | 4.249569909 | -2.112657042 | 0.188766238 |
| N | 1.157545909 | -0.207552284 | 0.13477316 |
| N | 0.016221037 | -0.387885059 | 0.216995385 |
| N | 2.764000568 | -0.312147213 | -3.193520629 |
| N | 2.892679153 | -0.126229383 | -2.081511285 |
| N | 3.278933182 | 0.46603051 | 1.930821032 |
| N | 3.37064321 | 0.630353543 | 3.050212044 |
| N | -2.772858447 | 1.819824859 | -1.008105127 |
| N | -2.586752431 | 0.752033523 | -0.457106901 |
| N | -1.237964232 | -2.551338734 | 1.441499423 |
| N | -0.786334857 | -3.434889153 | 1.96169808 |
| H | -2.84838236 | -1.507721776 | -5.508514194 |
| H | 1.44877867 | 5.107487338 | -3.108021378 |
| H | 3.066346458 | 4.405412616 | -3.140906038 |
| H | -4.129905321 | -1.52005167 | -4.297000498 |
| C | -3.14696933 | -1.941437873 | -4.542912357 |
| C | 2.257967791 | 4.721855339 | -2.470218069 |
| H | 1.968384475 | 2.11640159 | -3.293105404 |
| H | -2.947474241 | 0.433479915 | -3.179672669 |
| H | 2.622130048 | 5.557470654 | -1.867724482 |
| H | -3.263402103 | -3.016986753 | -4.693446047 |
| H | 0.399431895 | 2.927589414 | -3.234307227 |
| H | -1.707845186 | 0.333149829 | -4.434489993 |
| C | -1.99172259 | -0.034974922 | -3.437854234 |
| C | 1.189361106 | 2.478977951 | -2.614457887 |
| H | -0.410586764 | -1.599486766 | -4.865601715 |
| H | -0.306765489 | 4.321233185 | -1.470873614 |
| C | -2.080010594 | -1.571492811 | -3.490322832 |
| C | 1.707160405 | 3.547786249 | -1.632596378 |
| H | 4.235532814 | 2.380278602 | -2.536550409 |
| H | -4.505682069 | -0.926143751 | -1.958855809 |

| | | | |
|---|---|---|---|
| H | -1.242390151 | 0.31017947 | -2.719967762 |
| H | 0.760226381 | 1.619321529 | -2.090719723 |
| H | -4.914215041 | -2.619942901 | -2.246195706 |
| H | 4.968767583 | 3.753968689 | -1.709328373 |
| C | -0.697148145 | -2.097055351 | -3.928559111 |
| C | 0.503356729 | 4.019778042 | -0.791651081 |
| H | -2.195585096 | -4.640253824 | -3.811556493 |
| H | 2.616756658 | 5.849692752 | 0.230903969 |
| H | 0.080655526 | -1.867363239 | -3.189632098 |
| H | 0.108300935 | 3.216026844 | -0.157729852 |
| C | -4.344944737 | -1.949720487 | -1.590082078 |
| C | 4.570175047 | 2.743783223 | -1.553846913 |
| H | -6.759927306 | -2.876742035 | -0.774704533 |
| H | 7.247530526 | 3.085454574 | -1.77194024 |
| H | -0.690903869 | -3.174801758 | -4.120023366 |
| H | 0.738733047 | 4.88344601 | -0.160929026 |
| H | -3.846279438 | -4.600192742 | -3.151088374 |
| H | 4.299436657 | 5.559379769 | -0.264980557 |
| H | 5.11897928 | -1.239498953 | -2.49388697 |
| H | -4.654457089 | 1.184792942 | 0.942781412 |
| C | -2.801016951 | -4.845196768 | -2.923644818 |
| C | 3.570646348 | 5.412163991 | 0.542118653 |
| H | 3.833764819 | -4.074800343 | -3.072561514 |
| H | -3.553199406 | 3.873723642 | 2.166951828 |
| C | -6.151441938 | -2.543678639 | 0.062327887 |
| C | 7.001475384 | 2.168997289 | -1.241065199 |
| H | -2.756203194 | -5.930052587 | -2.747809982 |
| H | 3.92539204 | 5.993038894 | 1.406372601 |
| C | -4.869878015 | -2.041101881 | -0.178858208 |
| C | 5.659890849 | 1.835906567 | -1.037045156 |
| H | 5.782655585 | -2.693373664 | -3.2507762 |
| H | -5.459904486 | 2.473660376 | 1.85235753 |
| H | 2.899529595 | -2.716582325 | -2.429861772 |
| H | -2.560711928 | 2.81029289 | 1.15213601 |
| C | 5.6191054 | -2.188162445 | -2.287983377 |
| C | -4.894102199 | 1.536237335 | 1.949990515 |
| C | 3.526686321 | -3.566262814 | -2.146742307 |
| C | -2.876380092 | 3.005912297 | 2.181045823 |
| H | 9.054004513 | 1.574387448 | -0.911477695 |
| H | -7.623058106 | -3.016407337 | 1.572849871 |
| C | -2.285496874 | -4.12123348 | -1.662530422 |
| C | 3.444421917 | 3.933925283 | 0.961607127 |
| H | 6.606314106 | -1.972390486 | -1.862998025 |
| H | -5.558826797 | 0.803791634 | 2.423558842 |
| C | 8.004651919 | 1.328696519 | -0.76365948 |
| C | -6.630622598 | -2.620180016 | 1.36850817 |
| H | 2.913268581 | -4.269852925 | -1.575408454 |
| H | -1.995411633 | 3.293621537 | 2.761789332 |
| H | -0.174846856 | -4.175377551 | -2.310574821 |
| H | 1.382538021 | 4.159395246 | 1.719363304 |
| H | -4.178331407 | -4.621652554 | -0.651984294 |
| H | 5.637143452 | 3.72146901 | 0.880780695 |

| | | | |
|---|---|---|---|
| C | 4.790222167 | -3.121690392 | -1.376712231 |
| C | -3.630094727 | 1.80516401 | 2.797200962 |
| C | -0.79447877 | -4.474943654 | -1.460097311 |
| C | 2.363541947 | 3.813605291 | 2.058743208 |
| C | -3.098698507 | -4.679361007 | -0.471787401 |
| C | 4.804762127 | 3.514404123 | 1.563478078 |
| H | -2.848789987 | -5.7422406 | -0.343241375 |
| H | 4.9801881 | 4.101539108 | 2.476596054 |
| H | 6.0057595 | -4.777215674 | -2.046509841 |
| H | -4.830344334 | 2.998698672 | 4.138938731 |
| C | -5.81565972 | -2.176866692 | 2.407188158 |
| C | 7.632116388 | 0.167057843 | -0.091107508 |
| H | -0.373865372 | -4.011680317 | -0.56307875 |
| H | 2.258267855 | 2.787327788 | 2.41991709 |
| C | -4.545309757 | -1.666702402 | 2.123304188 |
| C | 6.278003175 | -0.129641083 | 0.085002214 |
| C | 5.664112036 | -4.359140063 | -1.088021964 |
| C | -4.098177429 | 2.181491045 | 4.216801982 |
| H | 6.563094198 | -4.11385933 | -0.508413815 |
| H | -4.597168108 | 1.352398923 | 4.734840502 |
| H | -0.696464446 | -5.564705403 | -1.349465462 |
| H | 2.653948066 | 4.439472629 | 2.915564998 |
| H | 8.382439238 | -0.515126568 | 0.301205917 |
| H | -6.157094468 | -2.215646703 | 3.43856288 |
| H | -2.88698745 | -4.176721364 | 0.474801141 |
| H | 4.840180992 | 2.457878482 | 1.839311996 |
| H | 3.226855625 | -5.115123382 | 0.381380119 |
| H | -1.0895688 | 2.460771057 | 4.465425738 |
| C | 5.867595234 | -1.381248886 | 0.820952168 |
| C | -3.66692433 | -1.162690116 | 3.242843438 |
| H | 5.122785387 | -5.15553067 | -0.567495365 |
| H | -3.28086209 | 2.543482653 | 4.848193992 |
| H | 6.695287532 | -2.101031291 | 0.825352819 |
| H | -4.285300316 | -0.902934045 | 4.11064283 |
| H | 1.928776258 | -3.925831247 | 0.625899641 |
| H | -0.069132954 | 1.833290302 | 3.147505783 |
| C | 2.796477396 | -4.406472006 | 1.095731154 |
| C | -0.473879611 | 1.614286861 | 4.14390129 |
| H | 5.663589017 | -1.124906457 | 1.871288 |
| H | -2.996360672 | -1.970218746 | 3.57230553 |
| C | 3.821357618 | -3.372215131 | 1.603567887 |
| C | -1.242379723 | 0.276949258 | 4.169626821 |
| H | 2.265731788 | -2.04502193 | 2.410628119 |
| H | 0.270925672 | -0.758243022 | 2.957386988 |
| H | 2.426357319 | -4.991130187 | 1.950068979 |
| H | 0.377329426 | 1.549341169 | 4.83601336 |
| C | 3.15504684 | -2.585756671 | 2.749153537 |
| C | -0.21594508 | -0.848512795 | 3.933461554 |
| H | 5.577461986 | -4.725941331 | 1.476620099 |
| H | -2.589220858 | 0.823925821 | 5.845505492 |
| H | 5.765242439 | -3.402221744 | 2.643218667 |
| H | -2.355449816 | -0.923875516 | 5.64744746 |

| | | | |
|---|---|---|---|
| C | 5.046214919 | -4.101263543 | 2.198499779 |
| C | -1.866399024 | 0.054770661 | 5.563717391 |
| H | 2.847186696 | -3.295750085 | 3.53097441 |
| H | 0.564053739 | -0.782133184 | 4.704856777 |
| H | 3.834667942 | -1.865627727 | 3.216032252 |
| H | -0.663188271 | -1.845710312 | 4.015860954 |
| H | 4.701471388 | -4.76119452 | 3.008370671 |
| H | -1.062171315 | 0.072847783 | 6.313728486 |
| H | -3.769238433 | 2.13087495 | -1.178245935 |
| C | -7.635343464 | 3.499691381 | -2.381594502 |
| C | -7.40211243 | 4.865348124 | -2.536514309 |
| C | -6.129092198 | 5.366166384 | -2.272336599 |
| C | -5.121694538 | 4.485812317 | -1.856621954 |
| N | -5.353945603 | 3.164590766 | -1.708871921 |
| C | -6.582921317 | 2.675088672 | -1.967416022 |
| H | -8.615571127 | 3.072553814 | -2.580360648 |
| H | -8.201703214 | 5.529437383 | -2.859664352 |
| H | -5.910350685 | 6.425523725 | -2.3839598 |
| C | -3.730215763 | 4.978918327 | -1.546574235 |
| H | -2.978043115 | 4.404532544 | -2.101068008 |
| H | -3.620159464 | 6.039581373 | -1.797084507 |
| H | -3.501928759 | 4.852296437 | -0.479597566 |
| C | -6.772672566 | 1.187046304 | -1.807360003 |
| H | -6.199821968 | 0.642692199 | -2.571651056 |
| H | -6.418078194 | 0.850377771 | -0.824809806 |
| H | -7.825766732 | 0.903096105 | -1.911693258 |

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**Supplementary Table 35 | Cartesian coordinate of the transition state for elimination of a terminal dinitrogen ligand trans to the NNH group in II. Units are presented in Å.**

SCF energy (in toluene) = -3962.99773733 hartree

ZPE = 1.295192 hartree

imaginary frequency: 70*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.926412567 | 1.815830106 | 1.787003454 |
| Mo | 2.236463706 | 1.832097899 | 1.71627339 |
| P | 2.690803741 | -0.589994917 | 2.410247608 |
| P | -3.161018178 | 3.408472139 | 3.793269838 |
| N | -5.181803854 | 1.875816967 | 2.124578634 |
| N | 4.382039313 | 1.559029539 | 1.056095458 |
| P | 2.746308082 | 4.11587768 | 0.703325688 |
| P | -3.825764201 | 0.241503198 | -0.061295426 |
| N | -0.964337859 | 1.792003761 | 1.591458566 |
| N | 0.203038537 | 1.776251132 | 1.540915579 |
| N | -2.716671521 | -0.642211858 | 3.776352354 |
| N | -2.790828278 | 0.241504279 | 3.069525937 |
| N | -3.053977579 | 3.383286141 | 0.490194413 |
| N | -3.121486253 | 4.256022353 | -0.230956986 |
| N | 2.434787222 | 2.893329603 | 4.544131472 |
| N | 2.493132798 | 2.430446612 | 3.390261479 |
| N | 1.760969851 | 0.930815442 | -1.279456563 |
| N | 1.338290282 | 0.572623766 | -2.239194878 |
| H | 2.807566652 | -2.713517564 | 5.659081574 |
| H | -1.927207529 | 3.442035906 | 7.475443755 |
| H | -3.453922369 | 2.796628983 | 6.870380005 |
| H | 4.16792484 | -1.9429596 | 4.843617813 |
| C | 3.174247843 | -2.378163161 | 4.678118477 |
| C | -2.674828517 | 3.544272743 | 6.675377296 |
| H | -2.110515439 | 1.118251075 | 5.534182993 |
| H | 3.037458373 | 0.32802041 | 5.266981546 |
| H | -3.120764755 | 4.537014745 | 6.774125927 |
| H | 3.288512374 | -3.267224612 | 4.054467597 |
| H | -0.635191224 | 1.852638279 | 6.174481825 |
| H | 1.785386396 | -0.599700679 | 6.099388134 |
| C | 2.080575698 | -0.187334148 | 5.123331594 |
| C | -1.362043127 | 1.896749977 | 5.351238047 |
| H | 0.410825228 | -2.23848729 | 4.992622658 |
| H | -0.045879459 | 4.108349529 | 5.894679553 |
| C | 2.175034899 | -1.345702783 | 4.112513392 |
| C | -1.97417844 | 3.310970957 | 5.319316297 |

| | | | |
|---|---|---|---|
| H | -4.38723445 | 1.679001261 | 4.93730858 |
| H | 4.625339942 | 0.153342793 | 3.630816102 |
| H | 1.340060322 | 0.560554943 | 4.831439295 |
| H | -0.832150488 | 1.659029639 | 4.423453637 |
| H | 5.113693423 | -1.266664883 | 2.707749439 |
| H | -5.241847981 | 3.197357482 | 5.203923126 |
| C | 0.771394728 | -1.972488846 | 3.989010864 |
| C | -0.816827411 | 4.314046604 | 5.140298087 |
| H | 2.290997865 | -3.810204757 | 2.250518017 |
| H | -3.11346862 | 6.186775459 | 5.445758578 |
| H | 0.045869499 | -1.271166714 | 3.559170826 |
| H | -0.331785003 | 4.208276537 | 4.162326204 |
| C | 4.543081589 | -0.331641011 | 2.646708467 |
| C | -4.730703471 | 2.598076697 | 4.440796199 |
| H | 7.077808218 | -0.3812268 | 1.702557733 |
| H | -7.440740545 | 2.555853782 | 4.549894764 |
| H | 0.764822331 | -2.890135816 | 3.391471958 |
| H | -1.136774665 | 5.353578997 | 5.267771104 |
| H | 3.99769207 | -3.432953664 | 1.919711112 |
| H | -4.762699493 | 5.520787539 | 5.432261716 |
| H | -4.942551817 | -0.985151912 | 2.413783514 |
| H | 4.635040992 | 3.769932566 | 2.966686137 |
| C | 2.979945961 | -3.390885181 | 1.511607199 |
| C | -3.998725724 | 6.021431361 | 4.823728437 |
| H | -3.440498611 | -3.405569284 | 1.060813238 |
| H | 3.311144568 | 6.519009629 | 3.623806765 |
| C | 6.491636637 | 0.408325841 | 1.23913122 |
| C | -7.072400409 | 2.270512371 | 3.567543288 |
| H | 2.957806709 | -4.056717776 | 0.63608838 |
| H | -4.397055498 | 7.011900111 | 4.558601511 |
| C | 5.154188068 | 0.574872048 | 1.607838606 |
| C | -5.694744947 | 2.235400248 | 3.336816147 |
| H | -5.527158013 | -2.565860511 | 1.883585819 |
| H | 5.369691026 | 5.373912638 | 3.157235211 |
| H | -2.600914796 | -1.956044848 | 1.627326414 |
| H | 2.375490896 | 5.013921966 | 3.552576953 |
| C | -5.337105261 | -1.533886899 | 1.555339754 |
| C | 4.903945913 | 4.688250363 | 2.435091241 |
| C | -3.117331973 | -2.395333153 | 0.769513415 |
| C | 2.744630291 | 5.853331221 | 2.955484378 |
| H | -9.030691883 | 1.972568079 | 2.701373469 |
| H | 8.096562 | 1.130813807 | -0.014145419 |
| C | 2.586977033 | -1.97093372 | 1.058443179 |
| C | -3.683316503 | 5.253148312 | 3.524066742 |
| H | -6.304909879 | -1.098309265 | 1.282113434 |
| H | 5.666752266 | 4.44220348 | 1.686389845 |
| C | -7.955262709 | 1.94546753 | 2.540178532 |
| C | 7.057520885 | 1.250810838 | 0.285197905 |
| H | -2.396500199 | -2.506987659 | -0.045968193 |
| H | 1.884440249 | 6.421492572 | 2.589979025 |
| H | 0.428992815 | -2.365049141 | 1.276944789 |
| H | -1.642133875 | 6.076242925 | 3.33804161 |

| | | | |
|---|---|---|---|
| H | 4.596785055 | -1.738135855 | 0.190304548 |
| H | -5.834585952 | 4.887724132 | 3.201791029 |
| C | -4.360599613 | -1.57533332 | 0.356951207 |
| C | 3.677852724 | 5.394399658 | 1.811644691 |
| C | 1.136498374 | -1.99399904 | 0.528037766 |
| C | -2.565385608 | 5.993386831 | 2.7573188 |
| C | 3.547012788 | -1.595330011 | -0.092614017 |
| C | -4.964264658 | 5.274401513 | 2.659280692 |
| H | 3.350210078 | -2.253247293 | -0.951333941 |
| H | -5.186187393 | 6.317306189 | 2.391423671 |
| H | -5.454633794 | -3.272031735 | -0.413671778 |
| H | 4.823525752 | 7.224926845 | 1.735369363 |
| C | 6.268300579 | 2.251852108 | -0.275503277 |
| C | -7.429306444 | 1.585329031 | 1.301501139 |
| H | 0.796260564 | -0.99886796 | 0.222000713 |
| H | -2.329844487 | 5.507521045 | 1.806765669 |
| C | 4.937492097 | 2.393939633 | 0.12734709 |
| C | -6.044352736 | 1.550954485 | 1.119473645 |
| C | -5.08842343 | -2.305607337 | -0.789886324 |
| C | 4.190674576 | 6.635717807 | 1.055712233 |
| H | -5.962412687 | -1.750058404 | -1.152767963 |
| H | 4.805243587 | 6.382805301 | 0.18221529 |
| H | 1.075320491 | -2.661308183 | -0.344282132 |
| H | -2.904668194 | 7.015231017 | 2.532285737 |
| H | -8.082932199 | 1.32623445 | 0.472168349 |
| H | 6.675717366 | 2.931249304 | -1.019889416 |
| H | 3.430213183 | -0.562875813 | -0.432488408 |
| H | -4.859189166 | 4.711120626 | 1.728670385 |
| H | -2.494718333 | -1.812803353 | -2.084126373 |
| H | 1.087333964 | 6.826853134 | 0.70130288 |
| C | -5.465286126 | 1.153389315 | -0.216794973 |
| C | 4.086140412 | 3.48632984 | -0.471662946 |
| H | -4.436149532 | -2.519845663 | -1.642241421 |
| H | 3.376641093 | 7.290939048 | 0.729803478 |
| H | -6.212336282 | 0.598691166 | -0.797496007 |
| H | 4.729088138 | 4.284668118 | -0.861785836 |
| H | -1.314444149 | -0.74670785 | -1.29150485 |
| H | 0.131018536 | 5.382215775 | 1.112215606 |
| C | -2.083301867 | -0.798543937 | -2.073276377 |
| C | 0.599545471 | 5.936807222 | 0.28924335 |
| H | -5.226688211 | 2.061884912 | -0.789183476 |
| H | 3.537274264 | 3.084627406 | -1.335901611 |
| C | -3.165396187 | 0.284248201 | -1.884577624 |
| C | 1.571112622 | 5.052504282 | -0.518595207 |
| H | -1.704784854 | 1.848050339 | -1.376330431 |
| H | 0.217399068 | 3.31659804 | -0.547650645 |
| H | -1.584789376 | -0.640493565 | -3.040296834 |
| H | -0.204901247 | 6.285446192 | -0.373764463 |
| C | -2.495834012 | 1.654381907 | -2.108374899 |
| C | 0.736401241 | 3.980152514 | -1.246627613 |
| H | -4.786161945 | -0.835005325 | -2.906227884 |
| H | 2.841125232 | 6.743137422 | -1.188300207 |

```
   H     -5.006129208   0.925408721  -2.912224842
   H      2.959410004   5.302608296  -2.216882012
   C     -4.261431523   0.121616584   -2.95982221
   C      2.279203619   5.899834542  -1.596530704
   H     -2.047910233   1.667154207  -3.112974891
   H     -0.022766411   4.478525123  -1.866123034
   H     -3.210139165    2.48298835  -2.063754322
   H      1.350486417   3.374084635  -1.922557283
   H     -3.791110057   0.181597687  -3.952315153
   H      1.516546447   6.314773614  -2.271592143
   H      3.381404546   3.084613821   4.919469486
-----------------------------------------------
```

**Supplementary Table 36 | Cartesian coordinate of the product complex for elimination of a terminal dinitrogen ligand trans to the NNH group in II. Units are presented in Å.**

SCF energy (in toluene) = -3963.00710453 hartree

ZPE = 1.293303 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.891301886 | 1.870391597 | 1.874668552 |
| Mo | 2.263664809 | 1.830721043 | 1.847080226 |
| P | 2.630525452 | -0.574090615 | 2.464391344 |
| P | -3.099531237 | 3.431187606 | 3.912849801 |
| N | -5.147550979 | 1.942451959 | 2.234405731 |
| N | 4.440876927 | 1.527724934 | 1.214582499 |
| P | 2.721635809 | 4.008210978 | 0.668236855 |
| P | -3.825480965 | 0.340063683 | 0.001198951 |
| N | -0.92935363 | 1.831325869 | 1.678947083 |
| N | 0.240913287 | 1.796831211 | 1.645469056 |
| N | -2.721753866 | -0.61551171 | 3.830611227 |
| N | -2.773309791 | 0.277544739 | 3.133540779 |
| N | -3.036709133 | 3.458971345 | 0.606209041 |
| N | -3.135868901 | 4.34265886 | -0.097451143 |
| N | 2.483400472 | 2.918754185 | 4.661965574 |
| N | 2.549078294 | 2.455395844 | 3.507343728 |
| N | 4.072921928 | 0.955776187 | -3.135101657 |
| N | 4.149145115 | 0.091915234 | -3.823969524 |
| H | 2.699333943 | -2.946515369 | 5.533220509 |
| H | -1.837901867 | 3.387928 | 7.583777961 |
| H | -3.366679037 | 2.747105199 | 6.97912682 |
| H | 4.086029382 | -2.161835998 | 4.778042667 |
| C | 3.0745965 | -2.539046386 | 4.583258777 |
| C | -2.592040391 | 3.50119102 | 6.791423661 |
| H | -2.043015832 | 1.099076832 | 5.592165787 |
| H | 3.085819455 | 0.143047888 | 5.335368802 |
| H | -3.040997195 | 4.490266587 | 6.910536774 |
| H | 3.149107808 | -3.373020883 | 3.879733308 |
| H | -0.562526258 | 1.814288921 | 6.242356251 |
| H | 1.810051966 | -0.766496657 | 6.152590079 |
| C | 2.100935201 | -0.318485611 | 5.191181853 |
| C | -1.292581102 | 1.878727419 | 5.423337913 |
| H | 0.333682125 | -2.290730636 | 4.989766368 |
| H | 0.036757329 | 4.072415045 | 5.999364869 |
| C | 2.113776883 | -1.424204068 | 4.115586351 |
| C | -1.900382533 | 3.295110061 | 5.426439565 |
| H | -4.3296573 | 1.692697851 | 5.037045263 |
| H | 4.617529385 | -0.09786011 | 3.720280797 |

| | | | |
|---|---|---|---|
| H | 1.3938939 | 0.482018198 | 4.957497212 |
| H | -0.766819552 | 1.660238053 | 4.488493405 |
| H | 5.001630925 | -1.436414536 | 2.643975319 |
| H | -5.169060398 | 3.213317086 | 5.335911387 |
| C | 0.685636151 | -1.990374655 | 3.992747628 |
| C | -0.742897699 | 4.299530632 | 5.260506959 |
| H | 2.237211033 | -3.743157225 | 1.989247495 |
| H | -3.010131315 | 6.176354713 | 5.613499744 |
| H | -0.023209158 | -1.24791808 | 3.608182334 |
| H | -0.269815536 | 4.218270489 | 4.274916993 |
| C | 4.494699596 | -0.464082178 | 2.690434184 |
| C | -4.669717476 | 2.622550144 | 4.558527898 |
| H | 7.080561766 | -0.462763274 | 1.938322144 |
| H | -7.377137234 | 2.602438768 | 4.692367908 |
| H | 0.640618739 | -2.880284888 | 3.354582832 |
| H | -1.05905696 | 5.336079966 | 5.417951799 |
| H | 3.906593967 | -3.282982075 | 1.588303203 |
| H | -4.668320518 | 5.53322447 | 5.598583128 |
| H | -4.934249839 | -0.929850155 | 2.458077622 |
| H | 4.459792489 | 4.122998247 | 3.005066313 |
| C | 2.863577455 | -3.233009911 | 1.250095796 |
| C | -3.901151988 | 6.03393608 | 4.994064908 |
| H | -3.436064464 | -3.32786657 | 1.045177139 |
| H | 2.632589548 | 6.715045763 | 3.346544809 |
| C | 6.533549479 | 0.360245283 | 1.485272678 |
| C | -7.021113739 | 2.32944244 | 3.702020224 |
| H | 2.796604329 | -3.809530935 | 0.315704334 |
| H | -4.287605921 | 7.034250393 | 4.74912296 |
| C | 5.17019973 | 0.508180754 | 1.75672242 |
| C | -5.646108727 | 2.286395998 | 3.457178384 |
| H | -5.521699433 | -2.500001201 | 1.901335127 |
| H | 4.927742135 | 5.829077809 | 3.144639525 |
| H | -2.599592022 | -1.890188067 | 1.646161234 |
| H | 2.078972047 | 5.032297439 | 3.432674717 |
| C | -5.332470365 | -1.462348815 | 1.591179489 |
| C | 4.625317612 | 5.044112589 | 2.4367828 |
| C | -3.115969542 | -2.309827921 | 0.778659008 |
| C | 2.27415666 | 5.864126467 | 2.748005772 |
| H | -8.990277716 | 2.061390846 | 2.850863865 |
| H | 8.238381895 | 1.174227803 | 0.436686515 |
| C | 2.399881662 | -1.788744106 | 0.985652616 |
| C | -3.605482835 | 5.284990023 | 3.678607813 |
| H | -6.301261271 | -1.021657157 | 1.329735035 |
| H | 5.467686412 | 4.882925686 | 1.752315307 |
| C | -7.916736498 | 2.027799667 | 2.678732494 |
| C | 7.175910084 | 1.270560057 | 0.65034891 |
| H | -2.395820315 | -2.398507317 | -0.040413084 |
| H | 1.327015544 | 6.165996895 | 2.28772715 |
| H | 0.260318911 | -2.218344654 | 1.343908099 |
| H | -1.559241537 | 6.094939532 | 3.490398311 |
| H | 4.291496412 | -1.24943526 | -0.028182512 |
| H | -5.763484541 | 4.947371806 | 3.375371482 |

| | | | |
|---|---|---|---|
| C | -4.361227438 | -1.48270762 | 0.388132559 |
| C | 3.348937943 | 5.5053263 | 1.698611076 |
| C | 0.910357562 | -1.787204669 | 0.576821374 |
| C | -2.486280938 | 6.026205745 | 2.913872559 |
| C | 3.209878696 | -1.233676764 | -0.206983997 |
| C | -4.895236445 | 5.332456862 | 2.828315332 |
| H | 3.013646365 | -1.856813664 | -1.091370758 |
| H | -5.108694215 | 6.381388595 | 2.577878607 |
| H | -5.460423209 | -3.164504043 | -0.406389303 |
| H | 4.173957786 | 7.496053851 | 1.529030176 |
| C | 6.428488408 | 2.302253195 | 0.089309519 |
| C | -7.405639386 | 1.682506828 | 1.429751716 |
| H | 0.550369547 | -0.772170204 | 0.36648437 |
| H | -2.259090554 | 5.550103788 | 1.956160944 |
| C | 5.064040758 | 2.405632175 | 0.374000675 |
| C | -6.022878998 | 1.640342904 | 1.233388207 |
| C | -5.093855617 | -2.192822476 | -0.768389847 |
| C | 3.694777489 | 6.757102225 | 0.870472118 |
| H | -5.968051518 | -1.630615732 | -1.120266823 |
| H | 4.397619312 | 6.548145424 | 0.053606188 |
| H | 0.787586244 | -2.387770733 | -0.336590042 |
| H | -2.819621984 | 7.052963113 | 2.703173047 |
| H | -8.069216569 | 1.441785897 | 0.602795497 |
| H | 6.889437928 | 3.025687587 | -0.578333748 |
| H | 2.922230746 | -0.204682526 | -0.461564182 |
| H | -4.807544578 | 4.781572343 | 1.888653168 |
| H | -2.490527006 | -1.661963824 | -2.058372699 |
| H | 0.65705907 | 6.339956908 | 0.17968481 |
| C | -5.461972706 | 1.261649976 | -0.115904552 |
| C | 4.242505575 | 3.469313999 | -0.306160884 |
| H | -4.443806456 | -2.394754593 | -1.625580606 |
| H | 2.804385439 | 7.233909776 | 0.446777046 |
| H | -6.218215931 | 0.718931633 | -0.696103073 |
| H | 4.882402305 | 4.312068166 | -0.595698742 |
| H | -1.310693683 | -0.579510198 | -1.284443471 |
| H | -0.091331804 | 4.792716403 | 0.641808834 |
| C | -2.095513769 | -0.641106483 | -2.049250799 |
| C | 0.37576099 | 5.344352157 | -0.18330696 |
| H | -5.228505963 | 2.178642269 | -0.676802918 |
| H | 3.856993526 | 3.044155038 | -1.243313448 |
| C | -3.189913585 | 0.422829222 | -1.830284158 |
| C | 1.57784325 | 4.580004044 | -0.771701263 |
| H | -1.741540032 | 1.995830905 | -1.318240015 |
| H | 0.507471203 | 2.658116374 | -0.725568009 |
| H | -1.621742002 | -0.468818504 | -3.02652436 |
| H | -0.38894232 | 5.484542048 | -0.960194562 |
| C | -2.541393955 | 1.804597596 | -2.040490188 |
| C | 1.053357963 | 3.287242444 | -1.436342655 |
| H | -4.808028951 | -0.699556756 | -2.854253945 |
| H | 2.613195982 | 6.398883835 | -1.491177959 |
| H | -5.052568553 | 1.057212086 | -2.822274522 |
| H | 3.1114525 | 4.915754394 | -2.32647976 |

```
   C    -4.297524894   0.265024976   -2.894244398
   C     2.262365683   5.432325821   -1.860906566
   H    -2.107838413   1.838315746   -3.050976724
   H     0.362334388   3.556684049   -2.247881304
   H    -3.264908185   2.623651112   -1.973337191
   H       1.8555347   2.686468328   -1.887448823
   H    -3.840244915   0.351835236      -3.890839
   H     1.534018451   5.634065925   -2.659911857
   H     3.428982681    3.09464447    5.045905097
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**Supplementary Table 37 | Cartesian coordinate of the reactant complex for protonation of IV. Units are presented in Å.**

SCF energy (in toluene) = -5142.20480431 hartree

ZPE = 1.474342 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 3.160798658 | 0.5710895 | -0.068883044 |
| Mo | -1.963312028 | -0.560294953 | 0.076507263 |
| P | -2.198341933 | -1.669476812 | -2.275643903 |
| P | 3.022235276 | 3.048066629 | 0.55634873 |
| N | 5.336829767 | 1.263528973 | -0.210970985 |
| N | -4.093581278 | -1.219439106 | 0.10648629 |
| P | -2.710712268 | 0.214835178 | 2.43146639 |
| P | 4.421310451 | -1.572545176 | -0.771022973 |
| N | 1.246300676 | 0.006998414 | 0.050784863 |
| N | 0.127412926 | -0.279426172 | 0.120242033 |
| N | 2.705673903 | 1.352636034 | -3.102656844 |
| N | 2.875184465 | 1.070113866 | -2.015160905 |
| N | 3.399493931 | 0.061183487 | 1.900352707 |
| N | 3.510296855 | -0.213178895 | 2.99360162 |
| N | -2.638205396 | 2.172483193 | -1.133249057 |
| N | -2.350757245 | 1.023811958 | -0.636264793 |
| H | -1.792112998 | -0.352758089 | -5.91135348 |
| H | 1.307416226 | 6.24121724 | -0.888308958 |
| H | 2.901646429 | 5.612355094 | -1.305177764 |
| H | -3.264740902 | -0.369503941 | -4.936253726 |
| C | -2.306259183 | -0.881215436 | -5.095011271 |
| C | 2.153476835 | 5.650533516 | -0.504509121 |
| H | 1.778009243 | 3.527342873 | -2.20774532 |
| H | -2.074188624 | 1.206136172 | -3.313884366 |
| H | 2.580983385 | 6.203697659 | 0.335101042 |
| H | -2.515349119 | -1.89411936 | -5.444893891 |
| H | 0.228543807 | 4.235593762 | -1.751224436 |
| H | -0.65603789 | 1.115433876 | -4.377057829 |
| C | -1.151963312 | 0.650298315 | -3.512527735 |
| C | 1.0543055 | 3.601221872 | -1.389918023 |
| H | 0.476661345 | -0.895930665 | -4.88397284 |
| H | -0.335193748 | 4.903783242 | 0.443268147 |
| C | -1.416085251 | -0.831885675 | -3.835260689 |
| C | 1.646663635 | 4.24406628 | -0.120266892 |
| H | 4.106158931 | 3.552532502 | -1.53790197 |
| H | -3.983569452 | -0.093671738 | -2.563382577 |
| H | -0.491522589 | 0.760978546 | -2.646245957 |
| H | 0.666618513 | 2.595327479 | -1.192845872 |

| | | | |
|---|---|---|---|
| H | -4.55695091 | -1.642773994 | -3.201633943 |
| H | 4.850276423 | 4.574034181 | -0.304525318 |
| C | -0.044757201 | -1.481893349 | -4.11370995 |
| C | 0.50427433 | 4.363622448 | 0.906858124 |
| H | -1.685956675 | -3.752680958 | -4.711058847 |
| H | 2.669502484 | 5.698738679 | 2.406202949 |
| H | 0.588165078 | -1.480603758 | -3.217901218 |
| H | 0.133096218 | 3.379305336 | 1.218911255 |
| C | -4.016065632 | -1.175058768 | -2.36945814 |
| C | 4.493199495 | 3.556871982 | -0.5083257 |
| H | -6.582389965 | -2.01775058 | -2.03601144 |
| H | 7.145897291 | 4.08683339 | -0.676903336 |
| H | -0.119782551 | -2.509736503 | -4.480112578 |
| H | 0.78863867 | 4.927394532 | 1.80075271 |
| H | -3.437494851 | -3.623811895 | -4.423001339 |
| H | 4.317177289 | 5.63528343 | 1.742110303 |
| H | 5.154624738 | 0.36714793 | -2.90761038 |
| H | -4.534652496 | 1.538967496 | 0.526828758 |
| C | -2.494322821 | -4.019157207 | -4.023806813 |
| C | 3.636016856 | 5.189830751 | 2.478183644 |
| H | 4.005315663 | -2.074576044 | -4.54542304 |
| H | -3.552050231 | 3.955659275 | 2.261909715 |
| C | -6.082542964 | -1.852206022 | -1.08484019 |
| C | 6.954768089 | 3.028984542 | -0.513272668 |
| H | -2.577756233 | -5.115635245 | -4.035346573 |
| H | 4.044934062 | 5.417434615 | 3.473612777 |
| C | -4.75255508 | -1.42653952 | -1.071786168 |
| C | 5.636170143 | 2.579850838 | -0.406852195 |
| H | 5.876122508 | -0.633048076 | -4.17465625 |
| H | -5.444902093 | 2.711725903 | 1.509149257 |
| H | 3.026573443 | -1.134060616 | -3.410783714 |
| H | -2.490802789 | 2.968499371 | 1.227708768 |
| C | 5.711446836 | -0.555327474 | -3.090088086 |
| C | -4.919839453 | 1.744298214 | 1.529018683 |
| C | 3.699295358 | -1.991831882 | -3.491882394 |
| C | -2.917528759 | 3.055436214 | 2.232296356 |
| H | 9.039056573 | 2.453103236 | -0.475680342 |
| H | -7.769474726 | -2.451178061 | 0.126186949 |
| C | -2.242335248 | -3.578639987 | -2.567592266 |
| C | 3.524519254 | 3.659340015 | 2.329012905 |
| H | 6.697453258 | -0.462516504 | -2.620228624 |
| H | -5.662255784 | 0.979722299 | 1.783600279 |
| C | 8.005712465 | 2.121127597 | -0.402401204 |
| C | -6.741426074 | -2.094471903 | 0.12068302 |
| H | 3.13375642 | -2.895441834 | -3.244731459 |
| H | -2.103301251 | 3.212245955 | 2.943872029 |
| H | -0.0568356 | -3.8329326 | -2.692611044 |
| H | 1.509117244 | 3.537932934 | 3.229845544 |
| H | -4.373660274 | -3.915014242 | -2.158410635 |
| H | 5.708704293 | 3.523404383 | 2.058225301 |
| C | 4.960366236 | -1.821232761 | -2.616939584 |
| C | -3.782603283 | 1.822160838 | 2.570089298 |

| | | | |
|---|---|---|---|
| C | -0.900705738 | -4.158562261 | -2.07376175 |
| C | 2.511817893 | 3.121381198 | 3.363961389 |
| C | -3.395700768 | -4.16689015 | -1.729777724 |
| C | 4.914262448 | 3.070019296 | 2.661759509 |
| H | -3.308460737 | -5.261532329 | -1.736464558 |
| H | 5.141806312 | 3.286041483 | 3.715630463 |
| H | 6.2377429 | -2.998185171 | -3.902449198 |
| H | -5.112203476 | 2.884139899 | 3.908067754 |
| C | -6.06513837 | -1.871173689 | 1.315447252 |
| C | 7.700571411 | 0.778001552 | -0.196492102 |
| H | -0.701515712 | -3.875530919 | -1.038386217 |
| H | 2.435027378 | 2.031073953 | 3.337604633 |
| C | -4.741297589 | -1.413732328 | 1.290876109 |
| C | 6.365470976 | 0.37255504 | -0.11342345 |
| C | 5.901971661 | -3.018780295 | -2.855072312 |
| C | -4.44343811 | 2.011185559 | 3.950766352 |
| H | 6.801837028 | -2.977130629 | -2.228557778 |
| H | -5.057373994 | 1.149110716 | 4.239616168 |
| H | -0.942629679 | -5.255785439 | -2.120505314 |
| H | 2.84975941 | 3.404110454 | 4.371792297 |
| H | 8.488317588 | 0.034203736 | -0.105073748 |
| H | -6.55061274 | -2.043240631 | 2.272540015 |
| H | -3.363793174 | -3.867510196 | -0.682728685 |
| H | 4.957923182 | 1.986283715 | 2.531190304 |
| H | 3.529309678 | -4.422449739 | -1.806390534 |
| H | -1.696380371 | 2.153682557 | 4.763522591 |
| C | 6.02576878 | -1.081297835 | 0.084211668 |
| C | -4.021425585 | -1.128867564 | 2.586921988 |
| H | 5.413296166 | -3.984654939 | -2.69411175 |
| H | -3.720784685 | 2.196401165 | 4.749890988 |
| H | 6.876678254 | -1.70925712 | -0.206239853 |
| H | -4.754582048 | -0.919978461 | 3.375857238 |
| H | 2.188449762 | -3.513229589 | -1.06703907 |
| H | -0.416935465 | 1.811134039 | 3.570910393 |
| C | 3.093505367 | -4.096774698 | -0.856322333 |
| C | -0.989931652 | 1.395900424 | 4.409848725 |
| H | 5.840954656 | -1.269813645 | 1.151756398 |
| H | -3.473222543 | -2.031892642 | 2.895735006 |
| C | 4.093073532 | -3.310280874 | 0.015345017 |
| C | -1.648885432 | 0.050310556 | 4.043112462 |
| H | 2.520003131 | -2.483545652 | 1.31180005 |
| H | 0.093194063 | -0.618981114 | 2.877132759 |
| H | 2.778242522 | -4.997737687 | -0.314374131 |
| H | -0.277552541 | 1.215192716 | 5.227109516 |
| C | 3.439187885 | -3.071388639 | 1.389035575 |
| C | -0.508612509 | -0.938615273 | 3.734991816 |
| H | 5.893222188 | -4.420031159 | -0.67040599 |
| H | -3.300040451 | 0.137590903 | 5.523887164 |
| H | 6.070110899 | -3.665840096 | 0.926237355 |
| H | -2.812269339 | -1.511162744 | 5.058457143 |
| C | 5.362510705 | -4.159415365 | 0.248567364 |
| C | -2.450259937 | -0.493835924 | 5.244005404 |

| | | | |
|---|---|---|---|
| H | 3.180530906 | -4.042365614 | 1.831416948 |
| H | 0.153743668 | -0.993009203 | 4.611543221 |
| H | 4.113834951 | -2.567431231 | 2.089974004 |
| H | -0.888489834 | -1.941521125 | 3.547176687 |
| H | 5.064580903 | -5.101573103 | 0.731566715 |
| H | -1.781392259 | -0.547085121 | 6.115413749 |
| S | -1.79241797 | -3.941325311 | 1.794873097 |
| O | -2.30498577 | -3.657102944 | 3.154805281 |
| O | -2.449828412 | -5.021428326 | 1.047999508 |
| O | -1.548605079 | -2.683792364 | 0.972044005 |
| C | -0.060455894 | -4.571484831 | 2.085649634 |
| F | 0.558949296 | -4.790871077 | 0.910822895 |
| F | 0.667590649 | -3.689933895 | 2.789376386 |
| F | -0.115484025 | -5.72090871 | 2.762399969 |
| C | -5.962205539 | 3.366469924 | -2.073797646 |
| N | -4.737541612 | 3.787688511 | -1.664839118 |
| C | -4.423653348 | 5.09812797 | -1.493525824 |
| C | -5.400639479 | 6.063560623 | -1.731602019 |
| C | -6.67283374 | 5.669708747 | -2.145711644 |
| C | -6.953786455 | 4.314293489 | -2.320116083 |
| H | -7.935345132 | 3.982461109 | -2.646187753 |
| H | -7.442144297 | 6.415658452 | -2.333279534 |
| H | -5.155349833 | 7.112502066 | -1.591948122 |
| C | -6.17751858 | 1.893561268 | -2.251694269 |
| H | -7.219485351 | 1.688981677 | -2.514857443 |
| H | -5.536879148 | 1.503930111 | -3.053404855 |
| H | -5.934934616 | 1.34070728 | -1.336629899 |
| C | -3.024483771 | 5.43579507 | -1.070142859 |
| H | -2.951166709 | 6.493055628 | -0.798722596 |
| H | -2.713088061 | 4.82250517 | -0.216933062 |
| H | -2.316830645 | 5.245416606 | -1.889428128 |
| H | -3.945581077 | 3.036097097 | -1.43876798 |
| H | -1.769121093 | 2.656831473 | -1.406157877 |

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**Supplementary Table 38 | Cartesian coordinate of the transition state for protonation of IV. Units are presented in Å.**

SCF energy (in toluene) = -5142.20262299 hartree

ZPE = 1.471585 hartree

imaginary frequency: 537*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 3.154649901 | 0.500927421 | -0.06880634 |
| Mo | -1.993262882 | -0.505088168 | 0.05806155 |
| P | -2.231402687 | -1.607259229 | -2.301379536 |
| P | 3.074149155 | 2.974492595 | 0.585762497 |
| N | 5.347696133 | 1.147857442 | -0.205961381 |
| N | -4.129487925 | -1.147410873 | 0.080999696 |
| P | -2.737167216 | 0.268035649 | 2.420349745 |
| P | 4.372173815 | -1.664018333 | -0.794665576 |
| N | 1.228160883 | -0.012995619 | 0.044976348 |
| N | 0.10016882 | -0.265769931 | 0.109502562 |
| N | 2.714291868 | 1.323505284 | -3.094176489 |
| N | 2.879467522 | 1.026308472 | -2.010120863 |
| N | 3.382876889 | -0.035589288 | 1.894848032 |
| N | 3.488496245 | -0.324977848 | 2.984541302 |
| N | -2.583131882 | 2.26108672 | -1.125546694 |
| N | -2.352913204 | 1.090030151 | -0.641498649 |
| H | -1.81443358 | -0.27748375 | -5.930245389 |
| H | 1.427053884 | 6.220207482 | -0.817626088 |
| H | 3.007993694 | 5.563921501 | -1.242497172 |
| H | -3.288492668 | -0.292912862 | -4.957646784 |
| C | -2.331603027 | -0.807440184 | -5.116844066 |
| C | 2.260614863 | 5.607495526 | -0.441364225 |
| H | 1.841302495 | 3.514299601 | -2.171314012 |
| H | -2.097076999 | 1.271484728 | -3.325249858 |
| H | 2.699194078 | 6.141164716 | 0.405066705 |
| H | -2.543812063 | -1.818083201 | -5.4710748 |
| H | 0.307656762 | 4.250050525 | -1.706172578 |
| H | -0.681398762 | 1.182520694 | -4.390510559 |
| C | -1.176259478 | 0.714581461 | -3.526938162 |
| C | 1.119020202 | 3.593320063 | -1.352675971 |
| H | 0.451797818 | -0.830364126 | -4.900134212 |
| H | -0.241282362 | 4.903942479 | 0.500001377 |
| C | -1.443080752 | -0.765663067 | -3.855530546 |
| C | 1.724432103 | 4.207120752 | -0.074772012 |
| H | 4.165280678 | 3.4784205 | -1.504812626 |
| H | -4.014071537 | -0.029352485 | -2.597188523 |

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H -0.513698869       0.8206412   -2.661675529
H  0.710198485       2.5933257   -1.168440667
H -4.585768723     -1.58060106   -3.227179131
H  4.933372789     4.468824189   -0.260874361
C -0.072765545    -1.417974191   -4.133322147
C  0.585293533     4.337532651    0.954653179
H -1.714546064    -3.680062237   -4.742964482
H  2.782614197     5.609032511     2.46753048
H  0.558119118    -1.421372932    -3.23614494
H  0.191588534     3.357383595    1.252257982
C -4.046310645    -1.109022328   -2.396510641
C  4.553842406     3.462201613   -0.475924891
H -6.616909066    -1.933990765   -2.067405466
H  7.216570803     3.936310896   -0.644223087
H  -0.14930674    -2.444197241   -4.503827048
H  0.883114168     4.881068708    1.856606063
H -3.467594098    -3.552062351   -4.463278285
H  4.427160678     5.517568483    1.798852621
H  5.142686519      0.28389773   -2.908200229
H -4.539081047     1.626385876    0.521386584
C -2.526288019    -3.948689487   -4.060758459
C  3.737979238     5.078493945    2.531259306
H  3.939634583     -2.11694926   -4.572705892
H -3.538768095     4.018979725     2.27149342
C  -6.11841619    -1.770794699   -1.115198597
C  7.002976242     2.881115019   -0.491752552
H -2.610227922    -5.045078533    -4.07698251
H  4.153836262     5.285386591    3.528295854
C  -4.78592377    -1.353670697   -1.099072921
C  5.675155033     2.459358744   -0.387661918
H   5.83882722    -0.715377884   -4.190139023
H -5.440871472     2.799925737    1.508259956
H  2.982901944    -1.168475543   -3.426023128
H  -2.47448908     3.028326317    1.244961227
C  5.679344277    -0.647728447   -3.104152272
C -4.924688301     1.828066158    1.524035242
C  3.637645495    -2.038938445   -3.517672987
C -2.911419775     3.113952253    2.245181812
H   9.07432516     2.259972553    -0.46458076
H -7.813573153     -2.35356565    0.091681464
C -2.281097527    -3.515067588   -2.601263457
C  3.592612889     3.552607931     2.36475172
H  6.668585704    -0.581470081   -2.636595156
H -5.674582319     1.067962995    1.769695441
C  8.034174259     1.949644545   -0.392831583
C -6.782807312    -2.004830628    0.088658647
H  3.054243467    -2.933331204   -3.278490887
H -2.103507754     3.260625151    2.965939567
H -0.095914022    -3.771860788   -2.713196288
H  1.575936034     3.464203907    3.266884372
H -4.416155393    -3.844325069   -2.206596412
H  5.772856707     3.371496113    2.088478121
```

| | | | |
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| C | 4.903585067 | -1.903440279 | -2.643833438 |
| C | -3.790238132 | 1.886795615 | 2.568836273 |
| C | -0.944259262 | -4.1005739 | -2.10209491 |
| C | 2.569843945 | 3.025524217 | 3.39546663 |
| C | -3.441845523 | -4.101779111 | -1.772897197 |
| C | 4.969455169 | 2.928790625 | 2.688058893 |
| H | -3.359126155 | -5.196763471 | -1.783418503 |
| H | 5.203284496 | 3.127540108 | 3.743919877 |
| H | 6.154406727 | -3.091192599 | -3.94504817 |
| H | -5.111527513 | 2.951637381 | 3.911971015 |
| C | -6.108885036 | -1.783669301 | 1.285009071 |
| C | 7.700396285 | 0.61136255 | -0.200699366 |
| H | -0.751499311 | -3.823876592 | -1.063733257 |
| H | 2.47022118 | 1.937402206 | 3.358807379 |
| C | -4.781758076 | -1.335787342 | 1.263886189 |
| C | 6.356908583 | 0.234101305 | -0.119618872 |
| C | 5.820169985 | -3.117112379 | -2.89731439 |
| C | -4.453248306 | 2.070614296 | 3.94929052 |
| H | 6.721844753 | -3.100919268 | -2.272283239 |
| H | -5.078566856 | 1.213564563 | 4.228388839 |
| H | -0.987282263 | -5.197402654 | -2.156388783 |
| H | 2.914823681 | 3.291308544 | 4.405495088 |
| H | 8.47197381 | -0.150229997 | -0.118553552 |
| H | -6.598670286 | -1.950352595 | 2.240831231 |
| H | -3.415608272 | -3.806768211 | -0.72455987 |
| H | 4.988954848 | 1.845893449 | 2.545059801 |
| H | 3.420129138 | -4.485434075 | -1.855163005 |
| H | -1.709139312 | 2.178183946 | 4.770029574 |
| C | 5.986502192 | -1.213894603 | 0.063739563 |
| C | -4.064609202 | -1.059242161 | 2.563573838 |
| H | 5.312199638 | -4.074679905 | -2.746677857 |
| H | -3.731341192 | 2.240407208 | 4.752556713 |
| H | 6.823582434 | -1.856732934 | -0.234061868 |
| H | -4.799588917 | -0.841645245 | 3.34831545 |
| H | 2.100354886 | -3.556584838 | -1.102613188 |
| H | -0.431163621 | 1.836732422 | 3.575563942 |
| C | 2.994013949 | -4.1602348 | -0.900520949 |
| C | -1.008329833 | 1.418357661 | 4.410077595 |
| H | 5.798994742 | -1.409193116 | 1.129586795 |
| H | -3.530709131 | -1.969630568 | 2.875239927 |
| C | 4.012195219 | -3.402678158 | -0.024896757 |
| C | -1.676751337 | 0.08107248 | 4.030595822 |
| H | 2.461322875 | -2.55758441 | 1.286400092 |
| H | 0.062426906 | -0.588571433 | 2.861403426 |
| H | 2.662375939 | -5.059924287 | -0.366191346 |
| H | -0.298404458 | 1.224764177 | 5.226489329 |
| C | 3.368983773 | -3.164070615 | 1.353830164 |
| C | -0.542648872 | -0.912525773 | 3.715280384 |
| H | 5.787442969 | -4.540913936 | -0.728817107 |
| H | -3.331302522 | 0.166516908 | 5.507395624 |
| H | 5.984797952 | -3.80770016 | 0.875201736 |
| H | -2.851355494 | -1.481434777 | 5.030691833 |

| | | | |
|---|---|---|---|
| C | 5.265184899 | -4.279464429 | 0.194702092 |
| C | -2.484322917 | -0.467656182 | 5.225222998 |
| H | 3.093438237 | -4.134011594 | 1.788299319 |
| H | 0.118039717 | -0.979491532 | 4.592230837 |
| H | 4.056504509 | -2.680235274 | 2.056503386 |
| H | -0.928417639 | -1.911112944 | 3.517784935 |
| H | 4.949784014 | -5.220515716 | 0.668623349 |
| H | -1.818116058 | -0.530993863 | 6.097949575 |
| S | -1.878004001 | -3.890382961 | 1.77293125 |
| O | -2.381530445 | -3.601293536 | 3.135030495 |
| O | -2.558370425 | -4.954192775 | 1.023493847 |
| O | -1.611965143 | -2.633797547 | 0.954142281 |
| C | -0.158437882 | -4.555206442 | 2.06003324 |
| F | 0.454517694 | -4.787266572 | 0.884336399 |
| F | 0.58779623 | -3.688276365 | 2.762655742 |
| F | -0.236177431 | -5.703070287 | 2.736892961 |
| C | -5.826412434 | 3.474712813 | -2.052049203 |
| N | -4.596667712 | 3.86556426 | -1.633678374 |
| C | -4.280333637 | 5.171114029 | -1.440576066 |
| C | -5.246400964 | 6.153744917 | -1.658167683 |
| C | -6.523161333 | 5.782683631 | -2.077515984 |
| C | -6.813641055 | 4.433801118 | -2.278657558 |
| H | -7.797794936 | 4.11570967 | -2.611202916 |
| H | -7.285896546 | 6.539306476 | -2.248774953 |
| H | -4.989386283 | 7.197228015 | -1.498746453 |
| C | -6.063647723 | 2.009462909 | -2.272123016 |
| H | -7.116099763 | 1.821864596 | -2.50544794 |
| H | -5.457413757 | 1.64348257 | -3.111192188 |
| H | -5.7951192 | 1.42228799 | -1.386696617 |
| C | -2.878877743 | 5.500772722 | -1.012064458 |
| H | -2.793758032 | 6.562696843 | -0.762649174 |
| H | -2.582482079 | 4.905450655 | -0.141162445 |
| H | -2.16542076 | 5.284356927 | -1.819616775 |
| H | -3.758130795 | 3.055913267 | -1.397567138 |
| H | -1.699268308 | 2.720960492 | -1.385974066 |

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**Supplementary Table 39 | Cartesian coordinate of the product complex for protonation of IV. Units are presented in Å.**

SCF energy (in toluene) = -5142.21833182 hartree

ZPE = 1.476087 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 3.153544859 | 0.543933102 | 0.004532361 |
| Mo | -1.947133053 | -0.500454003 | 0.248402179 |
| P | -2.291335435 | -1.500804232 | -2.182243582 |
| P | 3.036953631 | 3.005906401 | 0.724675169 |
| N | 5.326984365 | 1.247519101 | -0.176049063 |
| N | -4.095683236 | -1.134646471 | 0.306183341 |
| P | -2.63973349 | 0.194279156 | 2.667982601 |
| P | 4.403738242 | -1.582339241 | -0.812000454 |
| N | 1.25317507 | -0.008055086 | 0.167748754 |
| N | 0.12874594 | -0.284623376 | 0.250404603 |
| N | 2.592813509 | 1.398319684 | -2.996190968 |
| N | 2.802865657 | 1.092178857 | -1.923480314 |
| N | 3.46880915 | -0.029902021 | 1.943421364 |
| N | 3.628095371 | -0.348336726 | 3.017828444 |
| N | -2.454486612 | 2.380615074 | -0.689604239 |
| N | -2.308679873 | 1.117028803 | -0.358134121 |
| H | -2.013380993 | 0.023732747 | -5.741394924 |
| H | 1.245215549 | 6.228246669 | -0.537535475 |
| H | 2.839219827 | 5.646088777 | -1.022603726 |
| H | -3.456545208 | -0.09083338 | -4.73052171 |
| C | -2.490983837 | -0.566776054 | -4.94576411 |
| C | 2.110209752 | 5.635915269 | -0.203309456 |
| H | 1.741663647 | 3.57677716 | -1.987484826 |
| H | -2.25961399 | 1.425400268 | -3.098439642 |
| H | 2.548757261 | 6.157770676 | 0.650076282 |
| H | -2.68218802 | -1.561686172 | -5.350918495 |
| H | 0.193735569 | 4.248074827 | -1.479081285 |
| H | -0.847371014 | 1.413372884 | -4.165287305 |
| C | -1.324009793 | 0.899375323 | -3.317901861 |
| C | 1.030481993 | 3.608525696 | -1.156042929 |
| H | 0.302720719 | -0.552921575 | -4.807202112 |
| H | -0.356004292 | 4.783510595 | 0.764124194 |
| C | -1.565576354 | -0.569408 | -3.710675601 |
| C | 1.633835262 | 4.205671991 | 0.129327513 |
| H | 4.066627764 | 3.592543999 | -1.376582178 |
| H | -4.091109161 | 0.101512565 | -2.326976112 |
| H | -0.657100687 | 0.984119287 | -2.45413677 |
| H | 0.664888102 | 2.58783589 | -0.993383103 |

| | | | |
|---|---|---|---|
| H | -4.676627204 | -1.424288183 | -2.995742498 |
| H | 4.838169656 | 4.559605612 | -0.119012395 |
| C | -0.19233506 | -1.182754953 | -4.054706888 |
| C | 0.513228812 | 4.256925055 | 1.185728704 |
| H | -1.849122096 | -3.455610031 | -4.736471161 |
| H | 2.715135537 | 5.575129412 | 2.681173778 |
| H | 0.462235596 | -1.218789403 | -3.175107438 |
| H | 0.182836539 | 3.251930272 | 1.478479757 |
| C | -4.104348957 | -0.986538494 | -2.169199477 |
| C | 4.477477135 | 3.552054256 | -0.357215668 |
| H | -6.660690939 | -1.812932319 | -1.785659996 |
| H | 7.126714122 | 4.088159563 | -0.561945636 |
| H | -0.266255736 | -2.191854751 | -4.4705406 |
| H | 0.806561267 | 4.80008803 | 2.089154279 |
| H | -3.593401893 | -3.321924902 | -4.404933826 |
| H | 4.35027103 | 5.552955521 | 1.980672482 |
| H | 5.068286847 | 0.436702669 | -2.893345786 |
| H | -4.49868538 | 1.656642904 | 0.861229743 |
| C | -2.647225367 | -3.747786415 | -4.047604396 |
| C | 3.687452162 | 5.073074951 | 2.712051315 |
| H | 3.881735956 | -1.938667414 | -4.588620238 |
| H | -3.460121952 | 3.947787121 | 2.70548353 |
| C | -6.128398547 | -1.695852973 | -0.845293787 |
| C | 6.938133371 | 3.024560112 | -0.438135395 |
| H | -2.744379988 | -4.840978974 | -4.114012485 |
| H | 4.116179354 | 5.263427871 | 3.706818809 |
| C | -4.793091164 | -1.287276506 | -0.856508661 |
| C | 5.62172906 | 2.571139895 | -0.322891694 |
| H | 5.763074691 | -0.511893594 | -4.213911419 |
| H | -5.363857263 | 2.763962984 | 1.941739542 |
| H | 2.924492919 | -1.066108499 | -3.383559439 |
| H | -2.400558036 | 3.031257621 | 1.622028407 |
| C | 5.624711116 | -0.474858708 | -3.123823531 |
| C | -4.84677854 | 1.794562811 | 1.88805848 |
| C | 3.60660806 | -1.90871919 | -3.523900646 |
| C | -2.822329798 | 3.054257973 | 2.630557354 |
| H | 9.021992237 | 2.448265328 | -0.465918894 |
| H | -7.788479612 | -2.30819457 | 0.393587667 |
| C | -2.358294491 | -3.390299344 | -2.575388341 |
| C | 3.583758185 | 3.547936826 | 2.506293282 |
| H | 6.620827854 | -0.394739345 | -2.673821013 |
| H | -5.590106838 | 1.020548344 | 2.110340017 |
| C | 7.990242646 | 2.113114767 | -0.385405205 |
| C | -6.754550535 | -1.970094297 | 0.369386666 |
| H | 3.062639017 | -2.83126984 | -3.3007662 |
| H | -2.009593381 | 3.175968982 | 3.35091455 |
| H | -0.176376942 | -3.634219374 | -2.760451615 |
| H | 1.596498541 | 3.389145619 | 3.461887319 |
| H | -4.483254432 | -3.725532515 | -2.1326821 |
| H | 5.763911767 | 3.444191443 | 2.182153096 |
| C | 4.89149254 | -1.760821743 | -2.679230305 |
| C | -3.686608952 | 1.805462744 | 2.907136008 |

| | | | |
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| C | -1.008521306 | -4.005542316 | -2.150640948 |
| C | 2.601648396 | 2.96579423 | 3.547072849 |
| C | -3.498482695 | -4.011748713 | -1.743268296 |
| C | 4.986142527 | 2.956572273 | 2.780677491 |
| H | -3.425342446 | -5.105162323 | -1.814280679 |
| H | 5.234622747 | 3.128473968 | 3.837690197 |
| H | 6.138193182 | -2.886827736 | -4.038106172 |
| H | -4.975982485 | 2.794410558 | 4.330517163 |
| C | -6.03955092 | -1.800268963 | 1.550211762 |
| C | 7.689541425 | 0.762851051 | -0.226677112 |
| H | -0.785867702 | -3.805207815 | -1.100878544 |
| H | 2.522170548 | 1.877517886 | 3.479075258 |
| C | -4.710377065 | -1.363273888 | 1.501748434 |
| C | 6.356137718 | 0.353690771 | -0.133261755 |
| C | 5.832031234 | -2.944020326 | -2.983196767 |
| C | -4.315065828 | 1.915441805 | 4.312149751 |
| H | 6.748388226 | -2.916696725 | -2.380552803 |
| H | -4.931898956 | 1.045000236 | 4.568222248 |
| H | -1.053821677 | -5.095732499 | -2.28058629 |
| H | 2.970411034 | 3.2063905 | 4.554939545 |
| H | 8.479391004 | 0.01731606 | -0.178742816 |
| H | -6.49973258 | -1.99726131 | 2.514825235 |
| H | -3.438511507 | -3.77220545 | -0.682089514 |
| H | 5.037789889 | 1.879890623 | 2.601847883 |
| H | 3.500903615 | -4.402282412 | -1.926012623 |
| H | -1.524906471 | 1.989245904 | 5.05946249 |
| C | 6.024616231 | -1.107980828 | 0.019848811 |
| C | -3.94618348 | -1.148243608 | 2.785119771 |
| H | 5.35292992 | -3.917191129 | -2.839926251 |
| H | -3.572991821 | 2.053516652 | 5.10377013 |
| H | 6.872782039 | -1.719759299 | -0.310716697 |
| H | -4.651517853 | -0.974559411 | 3.606052906 |
| H | 2.174853996 | -3.508079072 | -1.142744751 |
| H | -0.295815774 | 1.694873747 | 3.804022446 |
| C | 3.079381352 | -4.102093792 | -0.961151897 |
| C | -0.841151057 | 1.243406662 | 4.64241905 |
| H | 5.868013209 | -1.334133642 | 1.084860491 |
| H | -3.398910093 | -2.070499379 | 3.02964046 |
| C | 4.094935972 | -3.346640935 | -0.080495314 |
| C | -1.534940789 | -0.07178031 | 4.234823078 |
| H | 2.551553251 | -2.567620217 | 1.279202773 |
| H | 0.154500287 | -0.732761951 | 2.989343415 |
| H | 2.768092047 | -5.017917033 | -0.442086086 |
| H | -0.101883431 | 1.012643925 | 5.42218791 |
| C | 3.471374974 | -3.157870822 | 1.314861687 |
| C | -0.427104413 | -1.071142912 | 3.853516426 |
| H | 5.885436846 | -4.417250286 | -0.845523137 |
| H | -3.138661798 | -0.010380337 | 5.766283903 |
| H | 6.087237941 | -3.73763128 | 0.78191444 |
| H | -2.719049862 | -1.647853804 | 5.205884969 |
| C | 5.37003246 | -4.200480321 | 0.093129193 |
| C | -2.318810909 | -0.652857135 | 5.43049315 |

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|---|---|---|---|
| H | 3.221935763 | -4.144178171 | 1.728279575 |
| H | 0.261337652 | -1.172041004 | 4.705432759 |
| H | 4.162344584 | -2.679455748 | 2.017747845 |
| H | -0.832944069 | -2.059246486 | 3.642952523 |
| H | 5.081539157 | -5.164368138 | 0.53694178 |
| H | -1.626120373 | -0.769987519 | 6.276360082 |
| S | -1.794485586 | -3.932513599 | 1.78905173 |
| O | -2.28240069 | -3.751793002 | 3.172888263 |
| O | -2.457108946 | -4.951218195 | 0.966908085 |
| O | -1.577445531 | -2.606438729 | 1.061525784 |
| C | -0.050428015 | -4.565331422 | 1.99203578 |
| F | 0.5380873 | -4.693936349 | 0.788978139 |
| F | 0.689327039 | -3.731461089 | 2.738487433 |
| F | -0.085538078 | -5.759871645 | 2.584727602 |
| C | -5.904254269 | 3.428408454 | -2.52935725 |
| N | -4.57231706 | 3.639833041 | -2.472123279 |
| C | -4.026762826 | 4.602509359 | -3.245962843 |
| C | -4.798969676 | 5.378172105 | -4.118668305 |
| C | -6.172541331 | 5.154399619 | -4.188207435 |
| C | -6.73460635 | 4.168363049 | -3.38016384 |
| H | -7.803709283 | 3.970949551 | -3.400425563 |
| H | -6.796058478 | 5.743163526 | -4.858351509 |
| H | -4.325057525 | 6.144166867 | -4.727820397 |
| C | -6.473119879 | 2.366292868 | -1.622583081 |
| H | -7.55563702 | 2.265444521 | -1.756158101 |
| H | -6.01336797 | 1.388835731 | -1.818503301 |
| H | -6.279362322 | 2.610247767 | -0.570072147 |
| C | -2.53822047 | 4.823678742 | -3.126053298 |
| H | -2.20100476 | 5.631487388 | -3.784143591 |
| H | -2.269604989 | 5.094944061 | -2.095302716 |
| H | -1.980186295 | 3.915780198 | -3.391610845 |
| H | -3.289576066 | 2.663430688 | -1.241406448 |
| H | -1.588545365 | 2.836300562 | -0.983778172 |

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**Supplementary Table 40 | Cartesian coordinate of the reactant complex for protonation of V. Units are presented in Å.**

SCF energy (in toluene) = -5142.76298601 hartree

ZPE = 1.486976 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -3.149402713 | 0.420766827 | 0.02396704 |
| Mo | 1.997880702 | -0.355821831 | 0.095769749 |
| P | 2.220975083 | -1.503612389 | 2.497478942 |
| P | -3.411488849 | 2.973931214 | -0.125872433 |
| N | -5.416131898 | 0.716219723 | 0.016843084 |
| N | 4.143722218 | -1.026548593 | 0.082493022 |
| P | 2.734070925 | 0.362049674 | -2.289040295 |
| P | -4.065650379 | -2.004013786 | 0.170308959 |
| N | -1.162284024 | 0.146051537 | 0.014873031 |
| N | -0.007568151 | -0.012967307 | 0.021338258 |
| N | -3.062217663 | 0.624749637 | 3.183174259 |
| N | -3.104292093 | 0.551110377 | 2.050550188 |
| N | -3.152871415 | 0.281972147 | -2.014031823 |
| N | -3.149374338 | 0.211577915 | -3.14485736 |
| N | 1.753321476 | 2.48653866 | 0.992870937 |
| N | 2.405792925 | 1.241273226 | 0.891960779 |
| H | 1.953361183 | -0.192357778 | 6.149168817 |
| H | -2.466580852 | 6.045016555 | 2.088789057 |
| H | -3.936765977 | 5.077453102 | 2.192877453 |
| H | 3.403414722 | -0.269908445 | 5.142828776 |
| C | 2.424167149 | -0.734817549 | 5.315849306 |
| C | -3.150053776 | 5.40944562 | 1.505292058 |
| H | -2.532522603 | 3.081031771 | 2.805195281 |
| H | 2.27520706 | 1.350232614 | 3.500836227 |
| H | -3.608501071 | 6.041780304 | 0.740865268 |
| H | 2.589622126 | -1.760541629 | 5.649553564 |
| H | -1.095413997 | 4.098281633 | 2.68470661 |
| H | 0.935070024 | 1.367912935 | 4.667731592 |
| C | 1.326768433 | 0.868451601 | 3.769529309 |
| C | -1.762791644 | 3.435058287 | 2.112558722 |
| H | -0.359853925 | -0.575708599 | 5.168914719 |
| H | -0.483243632 | 5.294413733 | 0.752894971 |
| C | 1.510873099 | -0.628574455 | 4.075470193 |
| C | -2.352169736 | 4.221393962 | 0.925189068 |

| | | | |
|---|---|---|---|
| H | -4.75755407 | 2.866651804 | 1.869578644 |
| H | 4.076342403 | -0.008974724 | 2.806251076 |
| H | 0.608241922 | 1.015134987 | 2.956937781 |
| H | -1.19193874 | 2.560770394 | 1.780153677 |
| H | 4.577576747 | -1.607013196 | 3.373680658 |
| H | -5.554900883 | 3.978143094 | 0.755736336 |
| C | 0.106622124 | -1.190322001 | 4.385739097 |
| C | -1.175257391 | 4.756682072 | 0.087394988 |
| H | 1.603557631 | -3.558833655 | 4.949172814 |
| H | -3.387744301 | 5.955740737 | -1.399528204 |
| H | -0.548092078 | -1.148512492 | 3.506590245 |
| H | -0.613104324 | 3.949668153 | -0.401207436 |
| C | 4.053877537 | -1.080773617 | 2.566600748 |
| C | -5.040003489 | 3.011925874 | 0.816774678 |
| H | 6.580206683 | -1.981474794 | 2.224852106 |
| H | -7.747539001 | 3.068375015 | 0.721180449 |
| H | 0.126337679 | -2.220669862 | 4.751115739 |
| H | -1.491685711 | 5.462440765 | -0.68651199 |
| H | 3.357206506 | -3.542430708 | 4.642117465 |
| H | -5.055975532 | 5.487355924 | -1.000679152 |
| H | -5.292590917 | -0.653160576 | 2.52326146 |
| H | 4.454702902 | 1.830551747 | -0.407919073 |
| C | 2.385540697 | -3.870221422 | 4.250544867 |
| C | -4.22579362 | 5.318160168 | -1.698664497 |
| H | -3.927092858 | -3.164612384 | 3.817033247 |
| H | 3.482489543 | 4.128927005 | -2.267474897 |
| C | 6.100760899 | -1.763175512 | 1.273833309 |
| C | -7.351759494 | 2.106938251 | 0.402813832 |
| H | 2.397757346 | -4.96986505 | 4.252491854 |
| H | -4.55999623 | 5.671067115 | -2.685306984 |
| C | 4.782933002 | -1.30405845 | 1.257250015 |
| C | -5.969963525 | 1.90360337 | 0.396746966 |
| H | -5.969226213 | -1.978424438 | 3.478469559 |
| H | 5.358328575 | 2.98521971 | -1.42436212 |
| H | -3.005660558 | -1.902676444 | 2.986383805 |
| H | 2.363777468 | 3.168345493 | -1.270951383 |
| C | -5.712510192 | -1.659777802 | 2.457883844 |
| C | 4.861248442 | 2.003596934 | -1.40934708 |
| C | -3.539848735 | -2.845385047 | 2.838087713 |
| C | 2.854856458 | 3.224600911 | -2.247698215 |
| H | -9.281966675 | 1.222817253 | -0.010042937 |
| H | 7.806018391 | -2.318058452 | 0.067718752 |
| C | 2.151557744 | -3.405579568 | 2.798828054 |
| C | -3.845189712 | 3.827656911 | -1.811814303 |
| H | -6.648551188 | -1.608443067 | 1.890146612 |
| H | 5.633916006 | 1.250790771 | -1.601310789 |
| C | -8.203438306 | 1.081685013 | -0.00255677 |

| | | | |
|---|---|---|---|
| C | 6.782730759 | -1.948329094 | 0.072237454 |
| H | -2.819541765 | -3.59930016 | 2.508649735 |
| H | 2.087236325 | 3.347831547 | -3.015125464 |
| H | -0.050817015 | -3.463807949 | 2.902394423 |
| H | -1.770775104 | 4.244846365 | -2.453985846 |
| H | 4.250407187 | -3.890119509 | 2.376728144 |
| H | -5.982489911 | 3.282894419 | -1.860947676 |
| C | -4.72515212 | -2.687426326 | 1.85963212 |
| C | 3.753600404 | 1.99388906 | -2.485130782 |
| C | 0.769262176 | -3.886490945 | 2.31150807 |
| C | -2.649304323 | 3.67875827 | -2.779694476 |
| C | 3.25488654 | -4.060981632 | 1.946969089 |
| C | -5.063548968 | 3.101921487 | -2.429931854 |
| H | 3.09080543 | -5.147807184 | 1.936082838 |
| H | -5.22486891 | 3.499138855 | -3.44236843 |
| H | -5.907273677 | -4.269528324 | 2.737122772 |
| H | 5.06155995 | 3.026271505 | -3.865081825 |
| C | 6.130278105 | -1.65644133 | -1.119772256 |
| C | -7.638769572 | -0.128226328 | -0.397878391 |
| H | 0.614778087 | -3.627849612 | 1.260833744 |
| H | -2.354524647 | 2.63367333 | -2.912435735 |
| C | 4.808931868 | -1.197082242 | -1.09529378 |
| C | -6.25065892 | -0.290490621 | -0.373018758 |
| C | -5.479013147 | -4.028719433 | 1.752886954 |
| C | 4.438477726 | 2.11940694 | -3.862213359 |
| H | -6.313587072 | -3.984466471 | 1.041602668 |
| H | 5.103476873 | 1.274673865 | -4.077566078 |
| H | 0.714189725 | -4.980439882 | 2.40109134 |
| H | -2.938760464 | 4.068431868 | -3.766597957 |
| H | -8.264192924 | -0.955944796 | -0.723106187 |
| H | 6.627235743 | -1.796634448 | -2.07610971 |
| H | 3.2653821 | -3.732034093 | 0.908740789 |
| H | -4.920737846 | 2.022838723 | -2.521133541 |
| H | -2.843276809 | -4.84724543 | 0.791220945 |
| H | 1.720787776 | 2.144474858 | -4.754651087 |
| C | -5.636996093 | -1.602394729 | -0.783772546 |
| C | 4.114094148 | -0.90744282 | -2.409378885 |
| H | -4.82953906 | -4.863440664 | 1.47250716 |
| H | 3.728477641 | 2.209601532 | -4.688769462 |
| H | -6.388402797 | -2.399453612 | -0.731478908 |
| H | 4.862678281 | -0.626442269 | -3.159831547 |
| H | -1.590056242 | -3.632283412 | 0.442651782 |
| H | 0.449019746 | 1.939060255 | -3.521994392 |
| C | -2.353553274 | -4.278959657 | -0.005971828 |
| C | 0.999979922 | 1.438994654 | -4.329174548 |
| H | -5.314528304 | -1.540075171 | -1.833383924 |
| H | 3.653322132 | -1.82872652 | -2.78604886 |

| | | | |
|---|---|---|---|
| C | -3.349601108 | -3.474056434 | -0.863110277 |
| C | 1.629778554 | 0.108452318 | -3.863863117 |
| H | -1.776098193 | -2.196925274 | -1.714326323 |
| H | -0.143652833 | -0.366071182 | -2.663285328 |
| H | -1.830556519 | -4.997783655 | -0.646665327 |
| H | 0.271222988 | 1.208091157 | -5.118603879 |
| C | -2.572048686 | -2.869694861 | -2.04896077 |
| C | 0.45929513 | -0.812422933 | -3.461008912 |
| H | -5.02717464 | -4.914501204 | -0.66930753 |
| H | 3.286647568 | 0.04284302 | -5.334598837 |
| H | -5.103845466 | -3.906965537 | -2.129615922 |
| H | 2.719364481 | -1.558829684 | -4.786399747 |
| C | -4.425840853 | -4.420404132 | -1.436935164 |
| C | 2.408063236 | -0.537810578 | -5.029115698 |
| H | -2.103972197 | -3.683878646 | -2.617457172 |
| H | -0.190015637 | -0.947428348 | -4.338587956 |
| H | -3.222534707 | -2.322467067 | -2.739813584 |
| H | 0.799763589 | -1.797634075 | -3.142576916 |
| H | -3.920510172 | -5.208535639 | -2.013668788 |
| H | 1.740994738 | -0.603419483 | -5.901208623 |
| S | 2.329702468 | -3.723755405 | -1.707434426 |
| O | 2.281089867 | -3.424820968 | -3.157002035 |
| O | 3.636744661 | -4.162270546 | -1.183226277 |
| O | 1.646173079 | -2.672271143 | -0.849048929 |
| C | 1.224877923 | -5.222089975 | -1.566348773 |
| F | 1.005102014 | -5.554276002 | -0.282080861 |
| F | 0.036952571 | -4.984441363 | -2.15236362 |
| F | 1.805705684 | -6.254539044 | -2.181289596 |
| C | 4.956983233 | 4.243002292 | 1.750806706 |
| N | 3.823447417 | 4.67504263 | 1.108485177 |
| C | 3.71821857 | 5.900365293 | 0.499324698 |
| C | 4.825062763 | 6.732788206 | 0.499891277 |
| C | 6.018195018 | 6.319579668 | 1.113260839 |
| C | 6.07154156 | 5.070950393 | 1.743155541 |
| H | 6.97620481 | 4.735643637 | 2.24281953 |
| H | 6.88990963 | 6.968807567 | 1.107244692 |
| H | 4.7517713 | 7.705712746 | 0.02208426 |
| C | 4.892359031 | 2.925050819 | 2.454730907 |
| H | 5.900336965 | 2.542983899 | 2.645868162 |
| H | 4.388305607 | 3.03632559 | 3.427384907 |
| H | 4.31970736 | 2.180669791 | 1.875715616 |
| C | 2.392143226 | 6.269948447 | -0.09396659 |
| H | 2.481212326 | 7.183578404 | -0.689328274 |
| H | 2.00099693 | 5.471760234 | -0.736307093 |
| H | 1.64889527 | 6.452743044 | 0.69545652 |
| H | 3.035684679 | 3.996340621 | 1.008281217 |
| H | 1.57232267 | 2.661695437 | 1.988395341 |

```
  H     0.829648488    2.443052918    0.539934561
-------------------------------------------------
```

**Supplementary Table 41 | Cartesian coordinate of the transition state for protonation of V. Units are presented in Å.**

SCF energy (in toluene) = -5142.75689633 hartree

ZPE = 1.483863 hartree

imaginary frequency: 1073*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -3.166950834 | 0.264719998 | 0.037267371 |
| Mo | 2.029435834 | -0.195665343 | 0.086184158 |
| P | 2.311630419 | -1.36186074 | 2.471784185 |
| P | -3.612358092 | 2.78043877 | -0.136807538 |
| N | -5.451946485 | 0.406746569 | 0.077323519 |
| N | 4.197382594 | -0.814123341 | 0.046747822 |
| P | 2.723813658 | 0.534894237 | -2.327075892 |
| P | -3.928119796 | -2.216701882 | 0.224555572 |
| N | -1.153965395 | 0.145566495 | 0.013484433 |
| N | 0.009428618 | 0.082603746 | 0.027925851 |
| N | -3.045776238 | 0.525863975 | 3.189435782 |
| N | -3.100344596 | 0.429279634 | 2.058535249 |
| N | -3.190546227 | 0.098990088 | -1.99772073 |
| N | -3.200870373 | 0.017018573 | -3.127967863 |
| N | 1.808139055 | 2.664865739 | 1.017349076 |
| N | 2.514668085 | 1.386793146 | 0.908119217 |
| H | 2.01714333 | -0.051833393 | 6.122276933 |
| H | -2.809158516 | 5.931228867 | 2.018473378 |
| H | -4.200306364 | 4.860594401 | 2.185901503 |
| H | 3.460419409 | -0.072030939 | 5.102916883 |
| C | 2.502739687 | -0.576275763 | 5.285914941 |
| C | -3.466027096 | 5.241656281 | 1.466509799 |
| H | -2.616225703 | 2.982975211 | 2.763512584 |
| H | 2.245203342 | 1.49699761 | 3.469950764 |
| H | -3.998069906 | 5.83130473 | 0.715594808 |
| H | 2.713356546 | -1.593756048 | 5.62014284 |
| H | -1.267927549 | 4.103965028 | 2.564108042 |
| H | 0.907863815 | 1.456678385 | 4.641538755 |
| C | 1.321622474 | 0.973377945 | 3.744517684 |
| C | -1.908121449 | 3.383030352 | 2.031523318 |
| H | -0.28542612 | -0.538270047 | 5.163603383 |
| H | -0.852927402 | 5.336727365 | 0.602606522 |

| | | | |
|---|---|---|---|
| C | 1.575533022 | -0.513488266 | 4.053142932 |
| C | -2.607632692 | 4.108144944 | 0.863712432 |
| H | -4.886151744 | 2.604383458 | 1.902242751 |
| H | 4.122967197 | 0.181964687 | 2.783567367 |
| H | 0.59064309 | 1.076699448 | 2.934126406 |
| H | -1.289395815 | 2.547911337 | 1.682467518 |
| H | 4.674133717 | -1.407334014 | 3.329039285 |
| H | -5.787554678 | 3.65473187 | 0.806883569 |
| C | 0.199402782 | -1.134041641 | 4.377027952 |
| C | -1.509102406 | 4.718186563 | -0.025909053 |
| H | 1.786189402 | -3.4375327 | 4.926039392 |
| H | -3.833916314 | 5.744475052 | -1.443928709 |
| H | -0.464722315 | -1.121128568 | 3.504182324 |
| H | -0.892700048 | 3.944436161 | -0.505036451 |
| C | 4.13007312 | -0.886402717 | 2.532048424 |
| C | -5.208780916 | 2.7245847 | 0.857783937 |
| H | 6.683467274 | -1.692455179 | 2.164434197 |
| H | -7.916126585 | 2.601074246 | 0.837769636 |
| H | 0.265421987 | -2.161910629 | 4.743524656 |
| H | -1.90598571 | 5.367352154 | -0.811732687 |
| H | 3.535012116 | -3.355256241 | 4.604188433 |
| H | -5.445565612 | 5.166933348 | -0.966650603 |
| H | -5.196704855 | -0.917887306 | 2.590156793 |
| H | 4.426514747 | 2.069551264 | -0.486601645 |
| C | 2.57319096 | -3.719716 | 4.220770838 |
| C | -4.637981139 | 5.047043219 | -1.7000351 |
| H | -3.644721833 | -3.32095087 | 3.879667517 |
| H | 3.369504039 | 4.323878789 | -2.334411453 |
| C | 6.189076826 | -1.485641269 | 1.218477159 |
| C | -7.466046327 | 1.666839884 | 0.510679794 |
| H | 2.626961094 | -4.818094719 | 4.223056316 |
| H | -5.039089643 | 5.364555111 | -2.673618565 |
| C | 4.855284252 | -1.074588716 | 1.214395787 |
| C | -6.074465139 | 1.555464285 | 0.469165432 |
| H | -5.769850044 | -2.273433423 | 3.570164897 |
| H | 5.283124623 | 3.242643756 | -1.523564573 |
| H | -2.830116937 | -2.007235534 | 3.018363065 |
| H | 2.263805895 | 3.331060194 | -1.364742327 |
| C | -5.552821856 | -1.949727427 | 2.541900392 |
| C | 4.815963052 | 2.246729578 | -1.49428853 |
| C | -3.300800466 | -2.986104358 | 2.88977748 |
| C | 2.769035578 | 3.401742981 | -2.332440757 |
| H | -9.343236636 | 0.655961537 | 0.146457877 |
| H | 7.904564299 | -1.969106458 | -0.003833559 |
| C | 2.310107782 | -3.265241705 | 2.770703567 |
| C | -4.160562511 | 3.584833799 | -1.816517988 |
| H | -6.500680183 | -1.963568812 | 1.9919915 |

| | | | |
|---|---|---|---|
| H | 5.608018356 | 1.515163859 | -1.688591833 |
| C | -8.257859855 | 0.586622945 | 0.127445512 |
| C | 6.868302165 | -1.637673987 | 0.010692 |
| H | -2.537447466 | -3.692275518 | 2.551372431 |
| H | 2.006274335 | 3.506241879 | -3.10723343 |
| H | 0.111683957 | -3.400896219 | 2.886306383 |
| H | -2.130043556 | 4.104007074 | -2.529070689 |
| H | 4.421446759 | -3.678351045 | 2.332916214 |
| H | -6.259893964 | 2.905624321 | -1.793477974 |
| C | -4.513247173 | -2.9188248 | 1.934754406 |
| C | 3.697936853 | 2.192571659 | -2.557970407 |
| C | 0.943578439 | -3.795616411 | 2.292844149 |
| C | -2.996544673 | 3.507176998 | -2.830265851 |
| C | 3.429241209 | -3.881050395 | 1.909597261 |
| C | -5.347441814 | 2.771196323 | -2.385082747 |
| H | 3.301257448 | -4.972677531 | 1.897222217 |
| H | -5.561760125 | 3.136683675 | -3.399709865 |
| H | -5.568043366 | -4.563307873 | 2.858094285 |
| H | 4.959387019 | 3.244473679 | -3.966598398 |
| C | 6.19605877 | -1.363875171 | -1.174213993 |
| C | -7.62388748 | -0.584052235 | -0.280610575 |
| H | 0.776355064 | -3.544144438 | 1.242476535 |
| H | -2.664584721 | 2.478690876 | -2.99658535 |
| C | 4.857969391 | -0.95508957 | -1.136338109 |
| C | -6.227844654 | -0.653994438 | -0.28872563 |
| C | -5.180244377 | -4.30733779 | 1.860985615 |
| C | 4.36287041 | 2.320186532 | -3.944726027 |
| H | -6.032770866 | -4.325926763 | 1.170487691 |
| H | 5.04959926 | 1.492455157 | -4.156922611 |
| H | 0.927282363 | -4.890722023 | 2.383892043 |
| H | -3.341274815 | 3.901937547 | -3.797212923 |
| H | -8.200506274 | -1.452625236 | -0.589071497 |
| H | 6.68994877 | -1.481498464 | -2.135182497 |
| H | 3.422044397 | -3.549049857 | 0.872169474 |
| H | -5.139930524 | 1.701045276 | -2.459964977 |
| H | -2.530780825 | -4.972847866 | 0.851262364 |
| H | 1.626529295 | 2.253288919 | -4.800668345 |
| C | -5.537348566 | -1.923759976 | -0.70568307 |
| C | 4.142860263 | -0.691516135 | -2.445697551 |
| H | -4.484800354 | -5.101374705 | 1.573095572 |
| H | 3.640919182 | 2.378685495 | -4.763788394 |
| H | -6.232757933 | -2.768742653 | -0.637907582 |
| H | 4.875991082 | -0.388866745 | -3.202832592 |
| H | -1.357805782 | -3.694612088 | 0.456162269 |
| H | 0.382564263 | 2.026201074 | -3.542773425 |
| C | -2.092343073 | -4.390381237 | 0.034569508 |
| C | 0.933715262 | 1.532700225 | -4.354078077 |

| | | | |
|---|---|---|---|
| H | -5.235169738 | -1.844983395 | -1.760246564 |
| H | 3.71091233 | -1.628289024 | -2.817506312 |
| C | -3.150730951 | -3.655229894 | -0.809164685 |
| C | 1.611460637 | 0.22709555 | -3.885684495 |
| H | -1.672002104 | -2.298094714 | -1.704435186 |
| H | -0.126623115 | -0.297505202 | -2.652772676 |
| H | -1.544238849 | -5.088519647 | -0.607759458 |
| H | 0.198224099 | 1.271764198 | -5.127656959 |
| C | -2.435039132 | -3.018370522 | -2.01676286 |
| C | 0.478305848 | -0.728515838 | -3.457402378 |
| H | -4.734987572 | -5.19068625 | -0.564778794 |
| H | 3.249410854 | 0.202163651 | -5.378684017 |
| H | -4.901254008 | -4.20736163 | -2.034112127 |
| H | 2.744514584 | -1.411970063 | -4.805561916 |
| C | -4.179984402 | -4.670659805 | -1.350089426 |
| C | 2.395670639 | -0.404848636 | -5.054779344 |
| H | -1.933802985 | -3.809276378 | -2.589448146 |
| H | -0.179638632 | -0.891969983 | -4.323576043 |
| H | -3.130336082 | -2.514700558 | -2.697026075 |
| H | 0.856636435 | -1.699115797 | -3.137046248 |
| H | -3.64003229 | -5.43406968 | -1.928701822 |
| H | 1.719118125 | -0.502655483 | -5.916492923 |
| S | 2.480999967 | -3.566284897 | -1.743578865 |
| O | 2.40934114 | -3.281786165 | -3.19539852 |
| O | 3.812182353 | -3.933320735 | -1.224038012 |
| O | 1.749702978 | -2.543315729 | -0.891640308 |
| C | 1.462774513 | -5.123701474 | -1.587310088 |
| F | 1.254841294 | -5.451387068 | -0.299429063 |
| F | 0.266822586 | -4.964556086 | -2.182807632 |
| F | 2.106589764 | -6.12903062 | -2.184414074 |
| C | 4.772297591 | 4.345899268 | 1.743679553 |
| N | 3.572094085 | 4.631556797 | 1.17893222 |
| C | 3.306227094 | 5.858613947 | 0.659973205 |
| C | 4.2888658 | 6.846979277 | 0.660820643 |
| C | 5.542331758 | 6.569277586 | 1.208079807 |
| C | 5.78146493 | 5.313789867 | 1.758681701 |
| H | 6.741830508 | 5.070742456 | 2.205457112 |
| H | 6.321280313 | 7.328908458 | 1.20996915 |
| H | 4.065646276 | 7.822111454 | 0.236704728 |
| C | 4.961808722 | 2.99785884 | 2.37615415 |
| H | 6.015852509 | 2.701083009 | 2.342048231 |
| H | 4.666898171 | 3.040180353 | 3.436016854 |
| H | 4.345255359 | 2.233792244 | 1.882758319 |
| C | 1.923571082 | 6.115681118 | 0.130492057 |
| H | 1.87351363 | 7.09203919 | -0.361070646 |
| H | 1.614637731 | 5.351626278 | -0.591357817 |
| H | 1.193719119 | 6.115211998 | 0.950831152 |

```
  H     2.706974839   3.717296108   1.069586307
  H     1.343291406   2.664520304   1.934727545
  H     1.047215793   2.726141596     0.3255895
-----------------------------------------------
```

**Supplementary Table 42 | Cartesian coordinate of the product complex for protonation of V. Units are presented in Å.**

SCF energy (in toluene) = -5142.76598702 hartree

ZPE = 1.487369 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.908412705 | -0.143291308 | -0.042507989 |
| Mo | 2.216046337 | 0.675570716 | 0.412347894 |
| P | 2.780739776 | -1.003377369 | 2.426723672 |
| P | -3.937054422 | 2.190009014 | 0.222617886 |
| N | -5.153961586 | -0.550947642 | -0.123596205 |
| N | 4.472126682 | 0.703068712 | 0.423775733 |
| P | 2.746264938 | 2.338589984 | -1.565966977 |
| P | -3.027927046 | -2.709580196 | -0.397962372 |
| N | -0.932776224 | 0.23076755 | 0.096261848 |
| N | 0.203533584 | 0.454546107 | 0.235937121 |
| N | -2.95237981 | -0.503168843 | 3.102145227 |
| N | -2.946488716 | -0.383542728 | 1.972517393 |
| N | -2.844150679 | 0.124272124 | -2.068045231 |
| N | -2.814665301 | 0.285508149 | -3.18834917 |
| N | 1.119590864 | 2.936761001 | 2.022242222 |
| N | 2.270210838 | 2.031597472 | 1.675405569 |
| H | 2.081812222 | -0.869985625 | 6.247756144 |
| H | -3.888709878 | 4.977578967 | 2.947305085 |
| H | -5.021514646 | 3.629478414 | 2.833162189 |
| H | 3.466231228 | -0.183113177 | 5.391894367 |
| C | 2.709341343 | -0.976594054 | 5.350545254 |
| C | -4.365970392 | 4.280268537 | 2.24243597 |
| H | -3.10965618 | 2.036727926 | 3.176691218 |
| H | 1.859037597 | 1.349847804 | 4.103285993 |
| H | -4.990315262 | 4.87253798 | 1.569696762 |
| H | 3.220269567 | -1.938519602 | 5.424577586 |
| H | -2.00981455 | 3.413610788 | 3.270344427 |
| H | 0.594432944 | 0.618230302 | 5.116109514 |
| C | 1.133701344 | 0.530836388 | 4.161992794 |
| C | -2.475736526 | 2.696468939 | 2.57615319 |
| H | 0.041339083 | -1.699208029 | 5.011238703 |
| H | -1.770746173 | 5.038060254 | 1.575566456 |
| C | 1.813548146 | -0.849776159 | 4.099423287 |
| C | -3.269997807 | 3.476979398 | 1.510670746 |

| | | | |
|---|---|---|---|
| H | -5.176808748 | 1.338261144 | 2.107400721 |
| H | 4.061840629 | 0.843496321 | 3.274112957 |
| H | 0.399320205 | 0.624899532 | 3.351916849 |
| H | -1.697641093 | 2.073371797 | 2.120097209 |
| H | 5.036671393 | -0.621194853 | 3.470931026 |
| H | -6.281031925 | 2.332730676 | 1.154790506 |
| C | 0.67704893 | -1.8937655 | 4.135776129 |
| C | -2.294256059 | 4.445041604 | 0.812870926 |
| H | 2.855703151 | -3.721446969 | 4.210515979 |
| H | -4.806191524 | 5.228945424 | -0.521123776 |
| H | 0.0393237 | -1.823940715 | 3.24581791 |
| H | -1.540624002 | 3.9102889 | 0.216523223 |
| C | 4.382737031 | -0.08092362 | 2.776112529 |
| C | -5.493967538 | 1.572303041 | 1.08062398 |
| H | 7.068322956 | -0.070560119 | 2.447126222 |
| H | -8.08592229 | 0.811717782 | 0.882321062 |
| H | 1.039299718 | -2.921401674 | 4.218285978 |
| H | -2.799375844 | 5.15405654 | 0.150223831 |
| H | 4.507708634 | -3.07560388 | 4.067336186 |
| H | -6.254786961 | 4.229393958 | -0.269149907 |
| H | -4.634075973 | -2.30750931 | 2.085065569 |
| H | 3.951816819 | 3.592367345 | 0.842421939 |
| C | 3.695927756 | -3.576666973 | 3.525136183 |
| C | -5.423074778 | 4.435249177 | -0.954777536 |
| H | -2.47676738 | -4.443788207 | 2.971699621 |
| H | 2.446325214 | 6.027873336 | -0.457361965 |
| C | 6.552130008 | 0.263290431 | 1.550550435 |
| C | -7.417718264 | 0.090564539 | 0.417944977 |
| H | 4.064783458 | -4.576395549 | 3.253563627 |
| H | -5.861379093 | 4.839861507 | -1.878587057 |
| C | 5.156888668 | 0.29680584 | 1.531388178 |
| C | -6.040776293 | 0.323678079 | 0.434911349 |
| H | -4.817689491 | -3.93695948 | 2.743725614 |
| H | 4.539718683 | 5.17133417 | 0.267698214 |
| H | -2.066882975 | -2.79874496 | 2.466068855 |
| H | 1.651078399 | 4.612141833 | 0.223585747 |
| C | -4.686574636 | -3.364758363 | 1.813924947 |
| C | 4.321430534 | 4.136230088 | -0.033524919 |
| C | -2.237689609 | -3.815113812 | 2.101193624 |
| C | 2.087360161 | 5.015897473 | -0.694787331 |
| H | -8.987748972 | -1.250175913 | -0.225972913 |
| H | 8.353969123 | 0.623525648 | 0.413461591 |
| C | 3.322745378 | -2.841712883 | 2.221148616 |
| C | -4.618390507 | 3.167513858 | -1.307084233 |
| H | -5.586921974 | -3.521986028 | 1.208978175 |
| H | 5.268810939 | 3.684849116 | -0.347366427 |
| C | -7.918086102 | -1.05486227 | -0.197214455 |

| | | | |
|---|---|---|---|
| C | 7.266383136 | 0.653892651 | 0.41937553 |
| H | -1.302241646 | -4.189055553 | 1.674037257 |
| H | 1.29480765 | 5.114154722 | -1.439738077 |
| H | 1.26056325 | -3.621508448 | 2.123214176 |
| H | -2.790440918 | 4.312234912 | -1.796817085 |
| H | 5.461536294 | -2.501552304 | 1.85797283 |
| H | -6.494169946 | 2.027795813 | -1.533531667 |
| C | -3.413338761 | -3.875766319 | 1.101852585 |
| C | 3.280819 | 4.164882861 | -1.174637509 |
| C | 2.169481448 | -3.580305075 | 1.512508765 |
| C | -3.447219829 | 3.556423653 | -2.238225518 |
| C | 4.576510835 | -2.871958858 | 1.325441614 |
| C | -5.570669367 | 2.231215196 | -2.087314458 |
| H | 4.781452577 | -3.916262866 | 1.049747368 |
| H | -5.85708202 | 2.729907996 | -3.024217298 |
| H | -3.990327258 | -5.89256871 | 1.618233008 |
| H | 4.291934221 | 5.850276514 | -2.077215275 |
| C | 6.564360496 | 1.085450765 | -0.699739627 |
| C | -7.014511217 | -1.943066842 | -0.774603066 |
| H | 1.929193666 | -3.104323414 | 0.558381499 |
| H | -2.836405788 | 2.694668197 | -2.519681506 |
| C | 5.165274714 | 1.104385507 | -0.677667298 |
| C | -5.643610629 | -1.676498642 | -0.719600776 |
| C | -3.673105636 | -5.346543677 | 0.717652821 |
| C | 3.928936102 | 4.860668607 | -2.391413726 |
| H | -4.476889975 | -5.451938823 | -0.021696492 |
| H | 4.796312495 | 4.311265278 | -2.775507751 |
| H | 2.475830482 | -4.615046083 | 1.303772666 |
| H | -3.857631921 | 3.986086511 | -3.163408158 |
| H | -7.360031783 | -2.848769835 | -1.266904773 |
| H | 7.087322511 | 1.397150387 | -1.600013505 |
| H | 4.473433313 | -2.311274226 | 0.396180809 |
| H | -5.109840801 | 1.276739061 | -2.351578646 |
| H | -0.925751095 | -5.058308513 | -0.266829165 |
| H | 1.310859759 | 4.45270173 | -3.494644873 |
| C | -4.661290026 | -2.642253775 | -1.328685669 |
| C | 4.424519279 | 1.569778559 | -1.913662785 |
| H | -2.781812163 | -5.851164618 | 0.332807211 |
| H | 3.232104258 | 5.017804773 | -3.220023689 |
| H | -5.127119224 | -3.628459956 | -1.442668238 |
| H | 5.068959714 | 2.247526743 | -2.485652174 |
| H | -0.162301235 | -3.453218855 | -0.345677023 |
| H | 0.134245978 | 3.555278559 | -2.49993547 |
| C | -0.675848262 | -4.224628526 | -0.931306141 |
| C | 0.810315985 | 3.488462661 | -3.362852966 |
| H | -4.394504139 | -2.298503029 | -2.338687945 |
| H | 4.238006156 | 0.714082467 | -2.573751734 |

| | | | |
|---|---|---|---|
| C | -1.908330668 | -3.656448138 | -1.660194619 |
| C | 1.779360781 | 2.293672373 | -3.245286193 |
| H | -0.83420766 | -1.82580781 | -2.254254512 |
| H | 0.190855843 | 1.036916925 | -2.403912582 |
| H | 0.040808347 | -4.597297134 | -1.672630926 |
| H | 0.18145732 | 3.328715575 | -4.249787121 |
| C | -1.417765257 | -2.635262188 | -2.70579687 |
| C | 0.907823798 | 1.019981642 | -3.231731702 |
| H | -3.023192205 | -5.576184624 | -1.77604076 |
| H | 3.401108882 | 3.112644175 | -4.511294052 |
| H | -3.462739088 | -4.404625398 | -3.034544901 |
| H | 3.3039485 | 1.330684369 | -4.49642754 |
| C | -2.635333 | -4.785819294 | -2.423339293 |
| C | 2.719261144 | 2.255621769 | -4.467804322 |
| H | -0.76923923 | -3.153225356 | -3.423309477 |
| H | 0.33755019 | 0.979780776 | -4.171567417 |
| H | -2.242330628 | -2.195235721 | -3.276174767 |
| H | 1.504773313 | 0.109792831 | -3.165743527 |
| H | -1.918464144 | -5.25201304 | -3.114579352 |
| H | 2.106991094 | 2.278097062 | -5.381051954 |
| S | 3.505845047 | -1.7025246 | -2.191003381 |
| O | 3.382143536 | -1.017096174 | -3.496511876 |
| O | 4.875878049 | -1.891205812 | -1.680362094 |
| O | 2.528259586 | -1.179069985 | -1.146784158 |
| C | 2.891064662 | -3.423507754 | -2.567208957 |
| F | 2.827926269 | -4.176231156 | -1.454573327 |
| F | 1.665542514 | -3.374346736 | -3.116816122 |
| F | 3.72676606 | -4.00408297 | -3.42989492 |
| C | 3.377190137 | 5.167925002 | 4.064066389 |
| N | 2.217697026 | 5.332213052 | 3.388955151 |
| C | 1.687845185 | 6.572003767 | 3.282662441 |
| C | 2.312460485 | 7.6935647 | 3.835512408 |
| C | 3.516956955 | 7.530987359 | 4.519598477 |
| C | 4.054463722 | 6.252741457 | 4.636917737 |
| H | 4.988339152 | 6.085034133 | 5.168034431 |
| H | 4.025991778 | 8.38851869 | 4.955149402 |
| H | 1.857996422 | 8.675297667 | 3.727659673 |
| C | 3.905877722 | 3.764698253 | 4.213312168 |
| H | 4.984807709 | 3.767198914 | 4.406985016 |
| H | 3.42132397 | 3.264890523 | 5.066324912 |
| H | 3.700844298 | 3.166890923 | 3.316736585 |
| C | 0.376599573 | 6.698526753 | 2.549973416 |
| H | 0.048382683 | 7.741908748 | 2.49567186 |
| H | 0.455639397 | 6.314426936 | 1.524439292 |
| H | -0.408072113 | 6.125291177 | 3.062774282 |
| H | 1.485512965 | 3.833154007 | 2.460277924 |
| H | 0.531771598 | 2.460674404 | 2.719096065 |

```
 H     0.526437286    3.135915037    1.205880385
-------------------------------------------------
```

**Supplementary Table 43 | Cartesian coordinate of the reactant complex for protonation of IX. Units are presented in Å.**

SCF energy (in toluene) = -3106.71020800 hartree

ZPE = 0.837539 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 0.441189 | 0.058288165 | -0.686129409 |
| P | -0.670861103 | 2.341608145 | -0.683735007 |
| N | 2.28185543 | 1.534548221 | -0.200360327 |
| P | 2.549116342 | -1.308007536 | -1.041167246 |
| N | -1.536374521 | -2.178873005 | -0.423003632 |
| N | -0.806031229 | -1.192990266 | -1.119394879 |
| H | -2.144801775 | 4.248179523 | -3.730378306 |
| H | -0.635593109 | 4.587837994 | -2.881923712 |
| C | -1.641301611 | 4.168315184 | -2.755874355 |
| H | 0.184001014 | 2.172312589 | -3.527690624 |
| H | -2.188254721 | 4.801946112 | -2.053816414 |
| H | -1.348467256 | 2.086897493 | -4.403860278 |
| C | -0.871998904 | 1.886275488 | -3.432571392 |
| H | -3.528724187 | 2.180818408 | -3.207946194 |
| C | -1.606931025 | 2.685068639 | -2.331687411 |
| H | 1.076415923 | 3.44498845 | -1.948979063 |
| H | -0.918991705 | 0.805038095 | -3.253252285 |
| H | 0.660085728 | 4.45338353 | -0.570962034 |
| C | -3.044103768 | 2.13786502 | -2.221412996 |
| H | -3.167317058 | 4.335888594 | -0.160193982 |
| H | -3.046061638 | 1.091680587 | -1.888058379 |
| C | 0.854065501 | 3.417486906 | -0.872376685 |
| H | 2.811450803 | 4.818486474 | 0.412210999 |
| H | -3.660507136 | 2.722034138 | -1.529134119 |
| H | -1.643326486 | 5.211533337 | 0.11592477 |
| H | 2.652807645 | 1.090007785 | -2.831015332 |
| C | -2.318748023 | 4.449169974 | 0.524278377 |
| H | 2.593903418 | -1.154358163 | -4.860758412 |
| C | 3.012876174 | 3.750419252 | 0.391236956 |
| H | -2.717172914 | 4.846223893 | 1.469386443 |
| C | 2.07769936 | 2.879316889 | -0.169297331 |
| H | 3.908799851 | 0.66633968 | -4.008961293 |
| H | 1.279817756 | -0.905865792 | -3.694004045 |
| C | 3.55757331 | 0.489389327 | -2.982353327 |

| | | | |
|---|---|---|---|
| C | 2.232378966 | -1.427482548 | -3.858838266 |
| H | 4.946985616 | 3.895955633 | 1.345078665 |
| C | -1.595951971 | 3.120979175 | 0.816030375 |
| H | 4.333019528 | 0.862146056 | -2.302888271 |
| C | 4.206215947 | 3.236594547 | 0.897804964 |
| H | 2.027237186 | -2.501976923 | -3.865743771 |
| H | -3.367470272 | 1.81977877 | 0.589341924 |
| H | 0.135984709 | 4.193224302 | 1.660607778 |
| C | 3.289481899 | -1.022320854 | -2.807725585 |
| C | -2.607161482 | 2.077278275 | 1.338526622 |
| C | -0.546797312 | 3.374758493 | 1.919982969 |
| H | -1.0719949 | 3.676111186 | 2.837609257 |
| H | 4.997581749 | -1.454867478 | -4.066001391 |
| C | 4.443846815 | 1.869058763 | 0.796914567 |
| H | -2.086743688 | 1.165619597 | 1.652427144 |
| C | 3.466974696 | 1.037578368 | 0.238347488 |
| C | 4.614315101 | -1.761547687 | -3.081792482 |
| H | 5.38848984 | -1.514429156 | -2.343905508 |
| H | -3.130335034 | 2.490260764 | 2.213151607 |
| H | 5.374301449 | 1.435126417 | 1.154431842 |
| H | 0.037904928 | 2.485624813 | 2.170479833 |
| H | 2.853297636 | -4.065482107 | -2.598088398 |
| C | 3.7332333 | -0.446340303 | 0.115711723 |
| H | 4.4993859 | -2.849573601 | -3.107174146 |
| H | 4.785496718 | -0.611951467 | -0.151995196 |
| H | 1.194498794 | -3.774978772 | -2.032677057 |
| C | 2.205053316 | -4.066786265 | -1.716314493 |
| H | 3.567757331 | -0.901595786 | 1.101958284 |
| C | 2.730691796 | -3.172369066 | -0.574700484 |
| H | 0.793515214 | -3.237961532 | 0.444280165 |
| H | 2.153541984 | -5.103561987 | -1.354412747 |
| C | 1.849338284 | -3.428230089 | 0.662960152 |
| H | 4.884933502 | -3.407031283 | -1.040885774 |
| H | 4.545964384 | -3.023054214 | 0.659358725 |
| C | 4.180281598 | -3.565673923 | -0.220248609 |
| H | 1.949207171 | -4.484525601 | 0.953978392 |
| H | 2.129438787 | -2.809887577 | 1.519088145 |
| H | 4.203231539 | -4.636083737 | 0.030857615 |
| H | -1.395781979 | -3.089146969 | -0.874929185 |
| S | 0.750285544 | -0.337556486 | 2.845008783 |
| O | 2.063500185 | -1.00306126 | 2.758026235 |
| O | 0.635920419 | 0.834611018 | 3.720360378 |
| O | 0.048178772 | -0.146031339 | 1.499250939 |
| C | -0.404607965 | -1.603881323 | 3.591911934 |
| F | -1.60804616 | -1.050864275 | 3.835949995 |
| F | -0.603900685 | -2.639588318 | 2.732475435 |
| F | 0.089775038 | -2.09078707 | 4.725526236 |

| | | | |
|---|---|---|---|
| H | -1.182031781 | -2.247594072 | 0.540750236 |
| C | -4.917888017 | -1.493342218 | 0.713899619 |
| N | -4.245035033 | -1.6302212 | -0.458835757 |
| C | -4.821487924 | -1.555182449 | -1.685162888 |
| C | -6.191394915 | -1.30759556 | -1.756914485 |
| C | -6.925615043 | -1.159783707 | -0.579188218 |
| C | -6.289372419 | -1.254688189 | 0.660682674 |
| H | -6.845462796 | -1.143177199 | 1.586960703 |
| H | -7.995967871 | -0.970738529 | -0.626533676 |
| H | -6.669858736 | -1.237797103 | -2.729725593 |
| C | -3.943158959 | -1.77406094 | -2.884069533 |
| H | -4.367915739 | -1.280689034 | -3.764053326 |
| H | -2.92577369 | -1.397958666 | -2.716399699 |
| H | -3.872491589 | -2.848141204 | -3.110791445 |
| C | -4.130229597 | -1.593385298 | 1.986692608 |
| H | -4.796765607 | -1.558323698 | 2.853222079 |
| H | -3.554400455 | -2.526269784 | 2.033915023 |
| H | -3.41388032 | -0.767167819 | 2.072841808 |
| H | -3.178528865 | -1.8318016 | -0.419023097 |

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**Supplementary Table 44 | Cartesian coordinate of the transition state for protonation of IX. Units are presented in Å.**

SCF energy (in toluene) = -3106.70281635 hartree

ZPE = 0.833893 hartree

imaginary frequency: 967*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 0.417341928 | 0.03430861 | -0.671770101 |
| P | -0.650227024 | 2.333915248 | -0.648112727 |
| N | 2.2802417 | 1.476518709 | -0.137754061 |
| P | 2.517312022 | -1.34674811 | -1.047040955 |
| N | -1.629562098 | -2.044454827 | -0.18687632 |
| N | -0.907014647 | -1.166138092 | -1.062173401 |
| H | -2.028743645 | 4.226656119 | -3.741486408 |
| H | -0.552401129 | 4.57472311 | -2.839592147 |
| C | -1.559696628 | 4.149251059 | -2.749941139 |
| H | 0.305083308 | 2.147723452 | -3.444505968 |
| H | -2.13540778 | 4.778972913 | -2.067491451 |
| H | -1.189343698 | 2.063537274 | -4.382775947 |
| C | -0.755109585 | 1.86543679 | -3.391666337 |
| H | -3.424593792 | 2.162877002 | -3.263232417 |
| C | -1.534967344 | 2.666875923 | -2.323643467 |
| H | 1.133713288 | 3.450575914 | -1.85283438 |
| H | -0.820368361 | 0.783143192 | -3.217301664 |
| H | 0.700083389 | 4.425085881 | -0.456629015 |
| C | -2.972031673 | 2.111242794 | -2.262279156 |
| H | -3.178954562 | 4.283943063 | -0.197893399 |
| H | -2.982540187 | 1.061307824 | -1.942400996 |
| C | 0.889374862 | 3.395961502 | -0.782167677 |
| H | 2.834366523 | 4.731517639 | 0.594093312 |
| H | -3.613079485 | 2.686451489 | -1.58517603 |
| H | -1.679432509 | 5.182217627 | 0.137985501 |
| H | 2.702902664 | 1.105303021 | -2.757527022 |
| C | -2.357425873 | 4.406665354 | 0.516658292 |
| H | 2.604984602 | -1.08402812 | -4.858829515 |
| C | 3.02329183 | 3.662346791 | 0.541299695 |
| H | -2.79511759 | 4.790658544 | 1.44949552 |
| C | 2.091034968 | 2.822234587 | -0.068204728 |
| H | 3.952817314 | 0.680272183 | -3.940259571 |

| | | | |
|---|---|---|---|
| H | 1.28356651 | -0.833200861 | -3.703479118 |
| C | 3.589745149 | 0.482096304 | -2.921881906 |
| C | 2.224667309 | -1.375296204 | -3.869236689 |
| H | 4.936374661 | 3.751233933 | 1.542984051 |
| C | -1.623118331 | 3.089374814 | 0.828568464 |
| H | 4.370948496 | 0.811907221 | -2.227034013 |
| C | 4.198637023 | 3.116458756 | 1.056897521 |
| H | 1.990623526 | -2.44304348 | -3.908920528 |
| H | -3.34752939 | 1.73597188 | 0.538162895 |
| H | 0.056979943 | 4.19627526 | 1.729493467 |
| C | 3.279876826 | -1.026755376 | -2.796020674 |
| C | -2.628989222 | 2.023927639 | 1.316013005 |
| C | -0.609951609 | 3.356710937 | 1.96132703 |
| H | -1.167151819 | 3.634220069 | 2.867598539 |
| H | 4.989836876 | -1.466410485 | -4.048098281 |
| C | 4.423297757 | 1.750498089 | 0.915749803 |
| H | -2.099671893 | 1.129148066 | 1.662438284 |
| C | 3.449214661 | 0.949835053 | 0.309113477 |
| C | 4.589000964 | -1.791231484 | -3.076955503 |
| H | 5.360755698 | -1.583851634 | -2.324534788 |
| H | -3.200669422 | 2.430984965 | 2.162482699 |
| H | 5.34047249 | 1.293973292 | 1.279344125 |
| H | -0.006952551 | 2.48086573 | 2.216996929 |
| H | 2.772567671 | -4.061536482 | -2.677245143 |
| C | 3.701827226 | -0.53359855 | 0.143990407 |
| H | 4.447369612 | -2.87477469 | -3.134154849 |
| H | 4.753780833 | -0.70135968 | -0.12384341 |
| H | 1.111467086 | -3.752536803 | -2.125606421 |
| C | 2.111586761 | -4.074195254 | -1.805142085 |
| H | 3.529251753 | -1.017409707 | 1.115282045 |
| C | 2.639425437 | -3.226644703 | -0.629036501 |
| H | 0.681680898 | -3.309640139 | 0.352828826 |
| H | 2.033761826 | -5.119735873 | -1.47491688 |
| C | 1.734126206 | -3.504419676 | 0.587606806 |
| H | 4.796140702 | -3.486681289 | -1.069599835 |
| H | 4.43727866 | -3.153253194 | 0.637521631 |
| C | 4.075901739 | -3.659208424 | -0.265410149 |
| H | 1.825614614 | -4.567371806 | 0.855278103 |
| H | 1.998220854 | -2.90691239 | 1.463370792 |
| H | 4.074566087 | -4.737612291 | -0.051102347 |
| H | -1.441237151 | -3.016638449 | -0.461394504 |
| S | 0.769907524 | -0.38984772 | 2.827399015 |
| O | 2.019690274 | -1.168232865 | 2.755333935 |
| O | 0.798871986 | 0.87380118 | 3.57205102 |
| O | 0.015620394 | -0.286999271 | 1.493045218 |
| C | -0.449161436 | -1.478589735 | 3.732431895 |
| F | -1.594649327 | -0.812100052 | 3.953901017 |

| | | | |
|---|---|---|---|
| F | -0.748725677 | -2.569419344 | 2.979214454 |
| F | 0.055151619 | -1.888089991 | 4.890764946 |
| H | -1.281078983 | -1.916178187 | 0.777792922 |
| C | -4.931701546 | -1.612332985 | 0.817549804 |
| N | -4.212792795 | -1.736822331 | -0.325219153 |
| C | -4.798204472 | -1.753610481 | -1.545525231 |
| C | -6.184876317 | -1.61774181 | -1.651723867 |
| C | -6.949170358 | -1.484256591 | -0.493781642 |
| C | -6.319547949 | -1.485121835 | 0.752041929 |
| H | -6.89290647 | -1.387165723 | 1.669860246 |
| H | -8.030454413 | -1.382400698 | -0.55988765 |
| H | -6.650593335 | -1.624508166 | -2.633743084 |
| C | -3.912591503 | -1.957785503 | -2.746540079 |
| H | -4.362990097 | -1.511701044 | -3.639700773 |
| H | -2.914624537 | -1.527061557 | -2.596244593 |
| H | -3.787367704 | -3.032229779 | -2.948267827 |
| C | -4.177752717 | -1.605126739 | 2.120138407 |
| H | -4.870319901 | -1.608199087 | 2.967365582 |
| H | -3.523174465 | -2.480795167 | 2.217539441 |
| H | -3.544537824 | -0.713293936 | 2.206801283 |
| H | -2.919732451 | -1.867493875 | -0.24879658 |

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**Supplementary Table 45 | Cartesian coordinate of the product complex for protonation of IX. Units are presented in Å.**

SCF energy (in toluene) = -3106.70689941 hartree

ZPE = 0.837796 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 0.464455677 | 0.043523483 | -0.797841915 |
| P | -0.608292433 | 2.330498394 | -0.749918236 |
| N | 2.2929667 | 1.486654742 | -0.157234007 |
| P | 2.604846735 | -1.291491334 | -1.170116891 |
| N | -1.615530555 | -1.923081533 | -0.153415157 |
| N | -0.927947667 | -1.10948394 | -1.145365567 |
| H | -1.861347726 | 4.20216564 | -3.906046314 |
| H | -0.436147289 | 4.5731272 | -2.933750199 |
| C | -1.439280761 | 4.130496046 | -2.893305481 |
| H | 0.496998317 | 2.160237055 | -3.479915468 |
| H | -2.05822207 | 4.749007188 | -2.238261876 |
| H | -0.940946486 | 2.031009496 | -4.497668727 |
| C | -0.558336699 | 1.8555603 | -3.481440823 |
| H | -3.23419376 | 2.10957707 | -3.511401104 |
| C | -1.41398172 | 2.649047744 | -2.465882035 |
| H | 1.199982948 | 3.520937851 | -1.8438969 |
| H | -0.614392596 | 0.771158859 | -3.304108815 |
| H | 0.699409294 | 4.430645646 | -0.426003799 |
| C | -2.842816517 | 2.070378224 | -2.484674038 |
| H | -3.188208946 | 4.210868121 | -0.408196361 |
| H | -2.859574185 | 1.022457024 | -2.160651622 |
| C | 0.916388403 | 3.418831122 | -0.786578224 |
| H | 2.798917406 | 4.715059977 | 0.710268681 |
| H | -3.531461106 | 2.641255869 | -1.85235848 |
| H | -1.728710024 | 5.125889577 | 0.038925194 |
| H | 2.87870641 | 1.240091 | -2.746244297 |
| C | -2.415378265 | 4.33138546 | 0.358457521 |
| H | 2.950565723 | -0.870324688 | -4.952862459 |
| C | 2.995136269 | 3.649057637 | 0.628878835 |
| H | -2.915943469 | 4.68689824 | 1.270549395 |
| C | 2.094124002 | 2.82745882 | -0.048047299 |
| H | 4.198484365 | 0.877139689 | -3.872366735 |
| H | 1.552939377 | -0.631205184 | -3.890887503 |
| C | 3.779368773 | 0.631280878 | -2.886494616 |

| | | | |
|---|---|---|---|
| C | 2.494706242 | -1.185711736 | -4.003617936 |
| H | 4.862314531 | 3.709701052 | 1.715234355 |
| C | -1.677752601 | 3.019671631 | 0.685949132 |
| H | 4.517251443 | 0.933967767 | -2.134477971 |
| C | 4.149146079 | 3.089469223 | 1.176640102 |
| H | 2.249003785 | -2.24720901 | -4.094642164 |
| H | -3.345468845 | 1.631180738 | 0.253256804 |
| H | -0.085210261 | 4.142727107 | 1.713622739 |
| C | 3.474010596 | -0.882796659 | -2.847802559 |
| C | -2.687310709 | 1.921257779 | 1.080403926 |
| C | -0.735452829 | 3.27508745 | 1.881047394 |
| H | -1.348189974 | 3.501514883 | 2.765338461 |
| H | 5.26478881 | -1.269677257 | -3.998597791 |
| C | 4.383990459 | 1.729310692 | 1.003370079 |
| H | -2.162936539 | 1.030229473 | 1.442194618 |
| C | 3.439807223 | 0.94735899 | 0.329881793 |
| C | 4.803994799 | -1.630033076 | -3.06766541 |
| H | 5.522225598 | -1.443505976 | -2.25911761 |
| H | -3.322917701 | 2.293987551 | 1.896533868 |
| H | 5.283926103 | 1.262573178 | 1.395762108 |
| H | -0.108107444 | 2.41386547 | 2.129506843 |
| H | 3.019907291 | -3.916473424 | -2.90886025 |
| C | 3.69474905 | -0.533497013 | 0.141698668 |
| H | 4.67483392 | -2.711494472 | -3.169180316 |
| H | 4.764304611 | -0.705343414 | -0.038606817 |
| H | 1.311950481 | -3.661099116 | -2.482329395 |
| C | 2.288787937 | -3.982366195 | -2.097442267 |
| H | 3.437673939 | -1.052075523 | 1.077199415 |
| C | 2.699960043 | -3.190753591 | -0.838646053 |
| H | 0.663142287 | -3.342361268 | -0.067506832 |
| H | 2.20336402 | -5.044312697 | -1.827177462 |
| C | 1.687553156 | -3.537131694 | 0.271527877 |
| H | 4.891260493 | -3.400376757 | -1.092591132 |
| H | 4.372313591 | -3.173915026 | 0.592045078 |
| C | 4.103740219 | -3.628544353 | -0.368576118 |
| H | 1.765893909 | -4.611636479 | 0.492117428 |
| H | 1.854784485 | -2.98710808 | 1.201511292 |
| H | 4.100132602 | -4.717662562 | -0.219419084 |
| H | -1.442222114 | -2.917186969 | -0.350955373 |
| S | 0.895628223 | -0.392952064 | 2.673845793 |
| O | 1.9166446 | -1.454219199 | 2.738347349 |
| O | 1.280197776 | 0.950363022 | 3.123130651 |
| O | 0.098143694 | -0.378006761 | 1.35447176 |
| C | -0.494371794 | -0.964154257 | 3.782659173 |
| F | -1.465748867 | -0.038201744 | 3.824206721 |
| F | -1.025961664 | -2.105453331 | 3.285818557 |
| F | -0.046467464 | -1.19355589 | 5.011195831 |

| | | | |
|---|---|---|---|
| H | -1.234403658 | -1.702278421 | 0.788957507 |
| C | -5.087172974 | -1.571516329 | 0.991114597 |
| N | -4.403556904 | -1.678529369 | -0.171305276 |
| C | -5.061820069 | -1.659606358 | -1.350346065 |
| C | -6.452479956 | -1.505378408 | -1.401241306 |
| C | -7.166233187 | -1.386384246 | -0.210990125 |
| C | -6.477252581 | -1.424630886 | 1.001441335 |
| H | -7.005410432 | -1.34182971 | 1.94801552 |
| H | -8.248014864 | -1.268564029 | -0.226002243 |
| H | -6.95974913 | -1.487265266 | -2.362885236 |
| C | -4.24776529 | -1.855340404 | -2.60574639 |
| H | -4.742175849 | -1.403837765 | -3.473176664 |
| H | -3.242869746 | -1.42634362 | -2.50931001 |
| H | -4.130591004 | -2.927986229 | -2.821932061 |
| C | -4.289581091 | -1.61819945 | 2.270598596 |
| H | -4.949088119 | -1.631927235 | 3.144601349 |
| H | -3.658300015 | -2.515626145 | 2.314183004 |
| H | -3.628476164 | -0.746877039 | 2.366692406 |
| H | -2.692126078 | -1.777629651 | -0.17304515 |

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**Supplementary Table 46 | Cartesian coordinate of the reactant complex for protonation of XI. Units are presented in Å.**

SCF energy (in toluene) = -3050.84437788 hartree

ZPE = 0.810189 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 0.445715914 | 0.162627326 | -0.0993269 |
| P | 0.27710922 | 2.54576064 | 0.871507359 |
| N | 1.919020395 | 1.278522297 | -1.421247794 |
| P | 1.766347114 | -1.726317333 | -1.086496071 |
| N | -0.918204086 | 0.001174918 | -1.066088275 |
| H | -1.994867291 | 5.560177769 | 0.035464751 |
| H | -0.260478216 | 5.56453439 | 0.372390039 |
| C | -1.198844574 | 5.036278051 | 0.584363547 |
| H | -0.136629594 | 4.091636985 | -1.751497272 |
| H | -1.42128268 | 5.137471002 | 1.651224831 |
| H | -1.89811631 | 4.031735428 | -1.855797702 |
| C | -1.02109183 | 3.53936047 | -1.409378171 |
| H | -3.332850677 | 3.43024549 | 0.050296786 |
| C | -1.171003117 | 3.565211178 | 0.126950322 |
| H | 1.724973518 | 4.35091378 | -0.109812048 |
| H | -0.962487666 | 2.515266533 | -1.793252977 |
| H | 2.616328142 | 3.135438729 | 0.78202672 |
| C | -2.499608969 | 2.882023432 | 0.514974166 |
| H | 0.512667638 | 5.237041239 | 2.583368809 |
| H | -2.529102171 | 1.842269782 | 0.172286594 |
| C | 1.807239472 | 3.268779425 | 0.049418763 |
| H | 3.276887192 | 4.335595599 | -1.933063156 |
| H | -2.666356929 | 2.878882859 | 1.59690088 |
| H | 2.155219713 | 4.594834172 | 2.380191236 |
| H | -0.796824063 | -2.235072583 | -2.354372779 |
| C | 1.19925101 | 4.446600133 | 2.897511469 |
| H | -0.256923958 | -4.928290032 | -0.791217428 |
| C | 3.055526691 | 3.287934898 | -2.120046443 |
| H | 1.394295783 | 4.593163883 | 3.969355245 |
| C | 2.245951854 | 2.58844365 | -1.219887036 |
| H | -0.73851301 | -3.932050025 | -2.880815277 |
| H | -0.451477014 | -3.350169897 | 0.005571262 |
| C | -0.131989707 | -3.031821549 | -2.709045761 |
| C | 0.274654514 | -4.025717255 | -0.456618198 |

| | | | |
|---|---|---|---|
| H | 4.228527647 | 3.159455843 | -3.929577159 |
| C | 0.626892132 | 3.025128317 | 2.704734576 |
| H | 0.285371025 | -2.739681299 | -3.680740166 |
| C | 3.589605957 | 2.63134953 | -3.224905032 |
| H | 0.980180596 | -4.332133257 | 0.320405532 |
| H | -1.383741998 | 3.670685425 | 3.32170705 |
| H | 2.622489978 | 2.068806291 | 2.63829437 |
| C | 0.96288177 | -3.371265682 | -1.673073789 |
| C | -0.660700864 | 2.875725581 | 3.541437553 |
| C | 1.682137142 | 2.011948389 | 3.206006764 |
| H | 1.929075056 | 2.246543997 | 4.250853743 |
| H | 1.408912367 | -5.22354601 | -2.700010819 |
| C | 3.308242478 | 1.278721631 | -3.396361791 |
| H | -1.151030593 | 1.90786349 | 3.399279511 |
| C | 2.472775692 | 0.621803911 | -2.489029169 |
| C | 1.960033995 | -4.350765194 | -2.321078516 |
| H | 2.4876823 | -3.904900127 | -3.174398434 |
| H | -0.402593053 | 2.955544038 | 4.606401978 |
| H | 3.726515771 | 0.725050115 | -4.232961886 |
| H | 1.31231315 | 0.984059927 | 3.187102112 |
| H | 3.169792686 | -4.124167722 | 0.411826135 |
| C | 2.158137908 | -0.83754271 | -2.697090754 |
| H | 2.704848967 | -4.723648859 | -1.610694559 |
| H | 1.223585039 | -0.9089734 | -3.268283626 |
| H | 2.458214035 | -2.931605349 | 1.527975518 |
| C | 3.29894771 | -3.129663179 | 0.851604475 |
| H | 2.941585492 | -1.309352183 | -3.303226453 |
| C | 3.453444666 | -2.023577666 | -0.21509947 |
| H | 3.068193978 | -0.457144134 | 1.288508183 |
| H | 4.214257723 | -3.161731235 | 1.459540908 |
| C | 3.819647066 | -0.717815285 | 0.530019059 |
| H | 4.393698472 | -3.271551472 | -1.777810832 |
| H | 4.798950673 | -1.545355417 | -1.888260559 |
| C | 4.593056992 | -2.368630685 | -1.192180907 |
| H | 4.770196397 | -0.868630885 | 1.06132638 |
| H | 3.957040749 | 0.132192223 | -0.147836423 |
| H | 5.515032097 | -2.544338982 | -0.619695931 |
| S | -0.816564167 | -0.961908867 | 2.867696662 |
| O | -0.210424595 | -0.564461812 | 4.143750283 |
| O | -2.090144747 | -0.327907372 | 2.470174394 |
| O | 0.197832978 | -1.030235567 | 1.711602926 |
| C | -1.192602951 | -2.780881252 | 3.058288959 |
| F | -1.885001585 | -3.231492734 | 1.987672163 |
| F | -0.058406342 | -3.486029316 | 3.152698292 |
| F | -1.929525742 | -2.976144244 | 4.151297191 |
| C | -3.931394463 | 0.19703417 | -3.081604478 |
| N | -3.569179563 | -0.398430242 | -1.914690534 |

| | | | |
|---|---|---|---|
| C | -4.408741031 | -1.128772268 | -1.132372825 |
| C | -5.734563375 | -1.261468017 | -1.546444063 |
| C | -6.154027294 | -0.664231072 | -2.734575046 |
| C | -5.2483879 | 0.063234444 | -3.510497831 |
| H | -5.553789043 | 0.528041475 | -4.443477529 |
| H | -7.186311776 | -0.770127745 | -3.061490074 |
| H | -6.421826834 | -1.838148131 | -0.934559048 |
| C | -2.887678326 | 0.978518524 | -3.824661441 |
| H | -3.19855527 | 1.139721771 | -4.861327447 |
| H | -2.737341172 | 1.960427835 | -3.355920907 |
| H | -1.920576036 | 0.463507328 | -3.813857881 |
| C | -3.8494525 | -1.755580275 | 0.103792165 |
| H | -3.043449737 | -2.454985026 | -0.150714746 |
| H | -3.413174818 | -1.015230488 | 0.788513191 |
| H | -4.629122761 | -2.30810875 | 0.636055702 |
| H | -2.56272041 | -0.275656922 | -1.589097802 |

**Supplementary Table 47 | Cartesian coordinate of the transition state for protonation of XI. Units are presented in Å.**

SCF energy (in toluene) = -3050.83593497 hartree

ZPE = 0.805643 hartree

imaginary frequency: 117*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.43292601 | 0.172783684 | -0.166609727 |
| P | -2.163636581 | -1.610250788 | 0.553805765 |
| N | -1.964768605 | 0.380300523 | -1.812692517 |
| P | 0.183469921 | 2.408980752 | -1.124911682 |
| N | 0.815608805 | -0.727130542 | -0.883942499 |
| H | -2.429579563 | -5.383104323 | -0.218375699 |
| H | -3.72697618 | -4.184658909 | -0.161947474 |
| C | -2.741540606 | -4.438331714 | 0.249026948 |
| H | -2.425515238 | -3.118570608 | -2.116586097 |
| H | -2.848801443 | -4.628315363 | 1.321178928 |
| H | -1.109459768 | -4.282023567 | -1.9301323 |
| C | -1.48310014 | -3.306880482 | -1.586378673 |
| H | -0.049997619 | -4.763693527 | 0.257560166 |
| C | -1.675507713 | -3.367901779 | -0.055402478 |
| H | -4.187793512 | -1.941296426 | -0.885999078 |
| H | -0.757167909 | -2.541829505 | -1.881844039 |
| H | -4.190593889 | -0.423507526 | -0.012343022 |
| C | -0.342222955 | -3.764609274 | 0.611856392 |
| H | -4.48595471 | -3.362346727 | 1.874360381 |
| H | 0.458855334 | -3.063036418 | 0.358353111 |
| C | -3.551131669 | -1.094367866 | -0.603961358 |
| H | -4.900468676 | -0.891447991 | -2.9150707 |
| H | -0.415679366 | -3.806372694 | 1.703502997 |
| H | -5.183885137 | -1.790563929 | 1.431984006 |
| H | 2.551405888 | 0.888140897 | -1.940292453 |
| C | -4.517422882 | -2.302230555 | 2.137527999 |
| H | 3.762837278 | 3.169305825 | -0.115173964 |
| C | -3.991232984 | -0.296229852 | -2.931891169 |
| H | -4.989415183 | -2.227818424 | 3.127348269 |
| C | -3.130169942 | -0.332099454 | -1.831080674 |
| H | 3.788886944 | 2.115442186 | -2.2573098 |
| H | 2.655203175 | 1.904463894 | 0.456732939 |

| | | | |
|---|---|---|---|
| C | 2.70816529 | 1.919097468 | -2.279191117 |
| C | 2.704027544 | 2.903856922 | 0.014713108 |
| H | -4.356032591 | 0.561623292 | -4.880011591 |
| C | -3.119166784 | -1.649668036 | 2.22683422 |
| H | 2.391798651 | 2.003214852 | -3.326408141 |
| C | -3.69152842 | 0.517328499 | -4.019744199 |
| H | 2.275641907 | 3.605721751 | 0.735188155 |
| H | -2.251456172 | -3.463000915 | 3.118866203 |
| H | -3.878698867 | 0.407773451 | 1.906786693 |
| C | 2.009897749 | 2.948096346 | -1.362952873 |
| C | -2.280255869 | -2.381127707 | 3.294857504 |
| C | -3.309934527 | -0.173435518 | 2.647442029 |
| H | -3.891782541 | -0.148514699 | 3.579367815 |
| H | 3.222142156 | 4.543110298 | -2.17330546 |
| C | -2.534285716 | 1.289896318 | -3.975825413 |
| H | -1.252999651 | -2.009865067 | 3.357893278 |
| C | -1.684170592 | 1.206480812 | -2.870612709 |
| C | 2.155218139 | 4.345735786 | -1.997241124 |
| H | 1.646855775 | 4.42079686 | -2.967155953 |
| H | -2.745943384 | -2.223946094 | 4.277406351 |
| H | -2.276325948 | 1.953481495 | -4.796930638 |
| H | -2.3620693 | 0.330003779 | 2.853646888 |
| H | 0.635841759 | 5.0745809 | 0.489183611 |
| C | -0.417354445 | 2.026641123 | -2.858618997 |
| H | 1.783193393 | 5.144472974 | -1.347644663 |
| H | 0.386987651 | 1.419211478 | -3.29375939 |
| H | 0.045745556 | 3.742425328 | 1.513877134 |
| C | -0.245426306 | 4.484788806 | 0.761038307 |
| H | -0.533907691 | 2.907115054 | -3.502100814 |
| C | -0.921174728 | 3.830606088 | -0.463728715 |
| H | -2.072155307 | 2.471296304 | 0.83817459 |
| H | -0.963014547 | 5.172345443 | 1.230048041 |
| C | -2.243359306 | 3.19100918 | 0.024814873 |
| H | -0.363781609 | 5.379462991 | -1.939542481 |
| H | -1.830757287 | 4.470030803 | -2.36466371 |
| C | -1.253621527 | 4.890676123 | -1.531053527 |
| H | -2.887689837 | 3.981694831 | 0.434755261 |
| H | -2.801766662 | 2.702694338 | -0.782024384 |
| H | -1.875615254 | 5.672823095 | -1.072934426 |
| S | 0.560910643 | 0.263348439 | 3.087109605 |
| O | -0.435729719 | 0.55147207 | 4.124447147 |
| O | 1.045930351 | -1.11715813 | 2.922336086 |
| O | 0.209087144 | 0.929032611 | 1.727926047 |
| C | 2.053724433 | 1.291423026 | 3.538450324 |
| F | 3.076767008 | 1.018895134 | 2.70661543 |
| F | 1.761575784 | 2.596515906 | 3.443660494 |
| F | 2.423992179 | 1.009301415 | 4.785673721 |

| | | | |
|---|---|---|---|
| C | 3.110127496 | -2.711236714 | -2.640474017 |
| N | 2.978440007 | -2.131082245 | -1.425608131 |
| C | 3.901877422 | -2.323327855 | -0.454926314 |
| C | 5.011186625 | -3.14352492 | -0.690639454 |
| C | 5.161850116 | -3.752958005 | -1.934095858 |
| C | 4.203788427 | -3.531716818 | -2.923968351 |
| H | 4.296186071 | -3.988071819 | -3.906176099 |
| H | 6.01943071 | -4.39275194 | -2.132743063 |
| H | 5.742950821 | -3.293031158 | 0.098935938 |
| C | 2.034403495 | -2.43864644 | -3.660599533 |
| H | 2.299865549 | -2.867141771 | -4.632349638 |
| H | 1.075810955 | -2.873073511 | -3.347101273 |
| H | 1.878120406 | -1.359892855 | -3.78937099 |
| C | 3.701973282 | -1.611388944 | 0.854020603 |
| H | 3.810903118 | -0.52667406 | 0.723495983 |
| H | 2.704350671 | -1.780803516 | 1.276084459 |
| H | 4.444978389 | -1.935016426 | 1.589983449 |
| H | 1.773293139 | -1.347993706 | -1.128198114 |

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**Supplementary Table 48 | Cartesian coordinate of the product complex for protonation of XI. Units are presented in Å.**

SCF energy (in toluene) = -3050.83838305 hartree

ZPE = 0.806890 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.487588874 | 0.042074193 | -0.106607041 |
| P | -1.449439632 | -2.277831768 | 0.523800724 |
| N | -2.046256271 | -0.22265206 | -1.717345387 |
| P | -0.732831082 | 2.400121757 | -0.924097019 |
| N | 0.969405829 | -0.312715066 | -0.90629951 |
| H | -0.422424807 | -5.862204588 | -0.459432505 |
| H | -2.050085219 | -5.184940452 | -0.343132865 |
| C | -1.031719522 | -5.108195935 | 0.058776713 |
| H | -1.207429439 | -3.619763282 | -2.233936794 |
| H | -1.052856568 | -5.382782397 | 1.117820363 |
| H | 0.419550812 | -4.291896421 | -2.095237898 |
| C | -0.25293835 | -3.516293012 | -1.702145166 |
| H | 1.615378782 | -4.482591704 | 0.048513197 |
| C | -0.398313462 | -3.723480519 | -0.179185511 |
| H | -3.268067105 | -3.231540156 | -0.914215027 |
| H | 0.180006859 | -2.540240298 | -1.944799699 |
| H | -3.783315473 | -1.864438497 | 0.050340385 |
| C | 1.000136003 | -3.675579774 | 0.471494842 |
| H | -3.011804406 | -4.758382527 | 1.762070307 |
| H | 1.501490877 | -2.722483471 | 0.276007768 |
| C | -2.964870375 | -2.229891862 | -0.586680842 |
| H | -4.366638915 | -2.399472962 | -2.868716008 |
| H | 0.963596032 | -3.816157508 | 1.556361867 |
| H | -4.211949636 | -3.486301354 | 1.45517297 |
| H | 2.023326696 | 1.885143037 | -1.822163619 |
| C | -3.38101944 | -3.788444184 | 2.104198922 |
| H | 2.356161327 | 4.403734907 | 0.032033905 |
| C | -3.731685845 | -1.517400292 | -2.856841344 |
| H | -3.803465758 | -3.937839921 | 3.107789893 |
| C | -2.88013826 | -1.303259216 | -1.769026587 |
| H | 2.692182555 | 3.493616235 | -2.135827513 |
| H | 1.810430399 | 2.813795176 | 0.598635442 |
| C | 1.765638517 | 2.903420364 | -2.135872579 |
| C | 1.472596607 | 3.767788186 | 0.184329589 |

| | | | |
|---|---|---|---|
| H | -4.443882602 | -0.737835765 | -4.740717842 |
| C | -2.27522836 | -2.715036635 | 2.208889782 |
| H | 1.407443419 | 2.878680954 | -3.172618229 |
| C | -3.779365147 | -0.58950506 | -3.892205239 |
| H | 0.845197902 | 4.255721983 | 0.934808048 |
| H | -0.830944899 | -4.184644544 | 2.979778477 |
| H | -3.686480949 | -1.017238359 | 2.025369026 |
| C | 0.763750369 | 3.578529183 | -1.173256086 |
| C | -1.206169874 | -3.182276987 | 3.218101657 |
| C | -2.922939084 | -1.405314905 | 2.715781306 |
| H | -3.434243624 | -1.611438784 | 3.666314796 |
| H | 1.268284884 | 5.52679641 | -1.962366848 |
| C | -2.974461355 | 0.543479884 | -3.810055048 |
| H | -0.355297183 | -2.498497492 | 3.28411476 |
| C | -2.114202534 | 0.708305558 | -2.722057809 |
| C | 0.358194186 | 4.942731599 | -1.766020816 |
| H | -0.174793059 | 4.843106298 | -2.720647748 |
| H | -1.663165481 | -3.235024643 | 4.21574418 |
| H | -2.998586775 | 1.300728094 | -4.589211235 |
| H | -2.184993427 | -0.623650651 | 2.913663731 |
| H | -1.218271134 | 4.984147314 | 0.809941968 |
| C | -1.223329983 | 1.924580564 | -2.670323835 |
| H | -0.261442234 | 5.531678497 | -1.081958751 |
| H | -0.272549644 | 1.672375776 | -3.157892981 |
| H | -1.218476033 | 3.490135565 | 1.781348803 |
| C | -1.802734298 | 4.09889016 | 1.080419212 |
| H | -1.669609134 | 2.740666998 | -3.251235052 |
| C | -2.250432354 | 3.290349232 | -0.156169515 |
| H | -2.758916917 | 1.549017562 | 1.098267283 |
| H | -2.698047603 | 4.451263247 | 1.611479476 |
| C | -3.221572384 | 2.190057061 | 0.334212119 |
| H | -2.364766872 | 4.989696839 | -1.56445049 |
| H | -3.421291317 | 3.624600824 | -1.989606275 |
| C | -2.996467295 | 4.195817418 | -1.154278359 |
| H | -4.088864042 | 2.669141374 | 0.810209114 |
| H | -3.60266621 | 1.567026703 | -0.482922362 |
| H | -3.836071579 | 4.679217615 | -0.635080332 |
| S | 0.593599231 | 0.22627369 | 3.095204394 |
| O | -0.33633815 | 0.111553389 | 4.22331046 |
| O | 1.463772527 | -0.914108337 | 2.76117136 |
| O | -0.085679439 | 0.835394957 | 1.835509176 |
| C | 1.731992114 | 1.642085874 | 3.528619612 |
| F | 2.694946888 | 1.764264932 | 2.594461274 |
| F | 1.042456604 | 2.789128758 | 3.585227975 |
| F | 2.302314729 | 1.40615207 | 4.708015492 |
| C | 3.70909668 | -1.27450467 | -2.960461609 |
| N | 3.480070701 | -0.873582653 | -1.690200385 |

| | | | |
|---|---|---|---|
| C | 4.478887491 | -0.862647394 | -0.77858559 |
| C | 5.767751508 | -1.281601508 | -1.130354456 |
| C | 6.018286644 | -1.70308325 | -2.43416428 |
| C | 4.978354785 | -1.695873861 | -3.364133304 |
| H | 5.141992717 | -2.012401288 | -4.391187821 |
| H | 7.014299916 | -2.030931328 | -2.725396919 |
| H | 6.557717548 | -1.269365996 | -0.383890371 |
| C | 2.542650955 | -1.246634681 | -3.915967745 |
| H | 2.858688545 | -1.509857856 | -4.930627123 |
| H | 1.763071306 | -1.955914441 | -3.607464441 |
| H | 2.084800274 | -0.249163652 | -3.945985989 |
| C | 4.157204147 | -0.362123066 | 0.603393183 |
| H | 3.910614311 | 0.707360455 | 0.577840184 |
| H | 3.293857384 | -0.875413547 | 1.043748632 |
| H | 5.012341653 | -0.491967259 | 1.274672846 |
| H | 2.023651307 | -0.526018499 | -1.234353702 |

**Supplementary Table 49 | Cartesian coordinate of the reactant complex for coordination of dinitrogen to XII. Units are presented in Å.**

SCF energy (in toluene) = -2833.65797456 hartree

ZPE = 0.667056 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.098363812 | 0.589512026 | 0.342224076 |
| P | 0.447304354 | -0.857238664 | 2.399874949 |
| N | 1.94945628 | 1.097831266 | 0.76690574 |
| P | 0.460438132 | 2.027091404 | -1.665961838 |
| N | -1.357752767 | 1.547878619 | 1.113655134 |
| H | -0.881831866 | -1.768744088 | 5.921656369 |
| H | 0.659357657 | -1.013673703 | 5.49114931 |
| C | -0.124800964 | -1.690720389 | 5.126984971 |
| H | -0.839075639 | 0.935136494 | 4.5380186 |
| H | 0.311594621 | -2.686949227 | 4.999239898 |
| H | -2.247898814 | -0.036424278 | 4.972344426 |
| C | -1.517414562 | 0.154216585 | 4.172870151 |
| H | -2.658755125 | -2.232136419 | 4.17117396 |
| C | -0.803321352 | -1.173760206 | 3.841903396 |
| H | 0.846880086 | 1.278208715 | 3.421057713 |
| H | -2.069506828 | 0.532106785 | 3.307493891 |
| H | 2.117732464 | 0.189457806 | 4.002539399 |
| C | -1.89272615 | -2.165726987 | 3.383884735 |
| H | 2.356549349 | -2.401290297 | 4.31481073 |
| H | -2.372587287 | -1.83983158 | 2.45671613 |
| C | 1.548306691 | 0.489637438 | 3.115361041 |
| H | 4.080970125 | 1.398082087 | 3.400869112 |
| H | -1.506141198 | -3.172857405 | 3.212470015 |
| H | 3.426915804 | -1.519189429 | 3.202508968 |
| H | -0.036262467 | 3.705539473 | 0.792251666 |
| C | 2.753513504 | -2.379786168 | 3.294771355 |
| H | -1.109336695 | 5.491657739 | -1.354103022 |
| C | 3.744446632 | 1.467664959 | 2.3685446 |
| H | 3.365099052 | -3.284418061 | 3.162090036 |
| C | 2.463513534 | 1.032806267 | 2.057564718 |
| H | 0.614294466 | 5.290965537 | 0.3067107 |
| H | -1.787337441 | 3.87208149 | -1.098682738 |
| C | 0.683378366 | 4.205718586 | 0.138227875 |
| C | -1.032031036 | 4.437544304 | -1.659118219 |

| | | | |
|---|---|---|---|
| H | 5.587852551 | 2.338194583 | 1.612522793 |
| C | 1.654350903 | -2.368092048 | 2.211734419 |
| H | 1.690995526 | 3.888898487 | 0.42834763 |
| C | 4.584801684 | 1.992271163 | 1.377630306 |
| H | -1.283245644 | 4.388195263 | -2.724245095 |
| H | 0.504867333 | -3.947419898 | 3.238146267 |
| H | 2.915130567 | -1.319373662 | 0.732622011 |
| C | 0.392036035 | 3.928532392 | -1.353758047 |
| C | 0.887414359 | -3.706201856 | 2.239879059 |
| C | 2.347147531 | -2.250262239 | 0.834386939 |
| H | 3.057085088 | -3.084815536 | 0.732456376 |
| H | 1.332237567 | 5.782720401 | -1.952045562 |
| C | 4.085022312 | 2.043161279 | 0.070845073 |
| H | 0.055554155 | -3.724450606 | 1.528420057 |
| C | 2.802957217 | 1.596429719 | -0.215877972 |
| C | 1.435048678 | 4.711340468 | -2.179359063 |
| H | 2.459738497 | 4.424599021 | -1.910794184 |
| H | 1.582119114 | -4.510018612 | 1.955588268 |
| H | 4.699599933 | 2.420879618 | -0.743937365 |
| H | 1.635373776 | -2.329453607 | 0.006905275 |
| H | -2.157490361 | 2.367126713 | -3.147717874 |
| C | 2.282062211 | 1.584517868 | -1.626117577 |
| H | 1.316152769 | 4.593676025 | -3.259164529 |
| H | 2.905042454 | 2.202314146 | -2.283564292 |
| H | -1.948270723 | 0.662113692 | -2.701943168 |
| C | -1.646106587 | 1.435124871 | -3.414731308 |
| H | 2.319762029 | 0.555834794 | -2.014689259 |
| C | -0.110341654 | 1.599415471 | -3.459701566 |
| H | 0.364826877 | -0.525782771 | -3.089983632 |
| H | -2.00461652 | 1.135409458 | -4.41055899 |
| C | 0.520532772 | 0.243374222 | -3.851336888 |
| H | -0.221313109 | 3.593027122 | -4.409883839 |
| H | 1.354092416 | 2.786843254 | -4.603668739 |
| C | 0.270206737 | 2.623700032 | -4.545455588 |
| H | 0.041271696 | -0.107857163 | -4.776352046 |
| H | 1.594121624 | 0.336989762 | -4.059684211 |
| H | -0.051432327 | 2.232475766 | -5.522292052 |
| S | -1.166219253 | -2.442028051 | -0.971121596 |
| O | -0.168233994 | -3.4519462 | -1.35571261 |
| O | -1.967298603 | -2.675501309 | 0.241914767 |
| O | -0.617618147 | -1.006729539 | -1.077746593 |
| C | -2.400105277 | -2.40559762 | -2.369676441 |
| F | -3.320299135 | -1.449796826 | -2.159874514 |
| F | -1.783819256 | -2.153373326 | -3.536519827 |
| F | -3.018310394 | -3.588869047 | -2.45409848 |
| N | -4.752720167 | -0.266405128 | 0.235804597 |
| N | -4.455154026 | 0.187694818 | 1.201045521 |

```
  H    -1.817341005    2.047980795    1.883695759
-------------------------------------------------
```

**Supplementary Table 50 | Cartesian coordinate of the transition state for coordination of dinitrogen to XII. Units are presented in Å.**

SCF energy (in toluene) = -2833.65137694 hartree

ZPE = 0.667834 hartree

imaginary frequency: 78*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.180974764 | 0.62120118 | 0.392570568 |
| P | 0.386508949 | -0.87039605 | 2.432900129 |
| N | 1.87792231 | 1.063713035 | 0.736695598 |
| P | 0.356645565 | 2.051864656 | -1.647176161 |
| N | -1.068403126 | 1.8299693 | 1.350514135 |
| H | -1.067824633 | -1.786848316 | 5.908143398 |
| H | 0.525066683 | -1.112431274 | 5.535101021 |
| C | -0.285894746 | -1.735767647 | 5.135814497 |
| H | -0.833556838 | 0.89103199 | 4.701679244 |
| H | 0.096050463 | -2.751908672 | 4.994651866 |
| H | -2.365057115 | 0.033791895 | 4.90253165 |
| C | -1.536943674 | 0.212344754 | 4.201434394 |
| H | -2.788022618 | -2.168176146 | 4.10005513 |
| C | -0.896286216 | -1.147454703 | 3.84841496 |
| H | 0.801349059 | 1.291628146 | 3.392461234 |
| H | -1.943130838 | 0.714582699 | 3.316945971 |
| H | 2.07318505 | 0.215878365 | 3.99380788 |
| C | -2.01430726 | -2.073384684 | 3.323307671 |
| H | 2.180793361 | -2.446897871 | 4.444627409 |
| H | -2.480782171 | -1.673177358 | 2.418156028 |
| C | 1.496582084 | 0.494369703 | 3.104289732 |
| H | 4.074878994 | 1.287644433 | 3.321111304 |
| H | -1.655877727 | -3.077459293 | 3.082973156 |
| H | 3.314379386 | -1.551425095 | 3.407542936 |
| H | 0.4119794 | 3.661538912 | 0.852967774 |
| C | 2.632257139 | -2.409230512 | 3.448444371 |
| H | -1.123821868 | 5.517132802 | -1.103259841 |
| C | 3.719366981 | 1.361471801 | 2.295672411 |
| H | 3.24848338 | -3.313295385 | 3.334608797 |
| C | 2.407212162 | 0.992557984 | 2.017242283 |
| H | 0.814344273 | 5.303205884 | 0.298386697 |
| H | -1.722525719 | 3.899991506 | -0.671537104 |

| | | | |
|---|---|---|---|
| C | 0.933419874 | 4.23115603 | 0.081219864 |
| C | -1.091646565 | 4.452814657 | -1.379197412 |
| H | 5.590802806 | 2.104101014 | 1.485927331 |
| C | 1.597990319 | -2.381045219 | 2.301978284 |
| H | 2.002369287 | 3.998787997 | 0.147301131 |
| C | 4.563130523 | 1.816624882 | 1.27896572 |
| H | -1.532675342 | 4.361563018 | -2.378916725 |
| H | 0.375061327 | -3.94876765 | 3.255724746 |
| H | 3.00361687 | -1.351679837 | 0.949093274 |
| C | 0.367755268 | 3.956432694 | -1.330610315 |
| C | 0.82066452 | -3.713778859 | 2.282254122 |
| C | 2.380274952 | -2.25221898 | 0.974093229 |
| H | 3.050887394 | -3.119745746 | 0.885065312 |
| H | 1.282007216 | 5.804155743 | -1.975530019 |
| C | 4.038668679 | 1.884344057 | -0.015597538 |
| H | 0.033425511 | -3.728709813 | 1.523020281 |
| C | 2.723127712 | 1.51280726 | -0.265891416 |
| C | 1.244130233 | 4.759076633 | -2.316756298 |
| H | 2.279240687 | 4.394157057 | -2.338430198 |
| H | 1.52590122 | -4.522914739 | 2.043384935 |
| H | 4.653564075 | 2.220753703 | -0.847574619 |
| H | 1.725797185 | -2.257079265 | 0.099387457 |
| H | -2.338708842 | 2.292172928 | -2.931557407 |
| C | 2.16327265 | 1.548445096 | -1.661466143 |
| H | 0.860538683 | 4.766054049 | -3.337890766 |
| H | 2.796563829 | 2.153585421 | -2.321747966 |
| H | -2.022555203 | 0.573197835 | -2.622211781 |
| C | -1.805347067 | 1.405534033 | -3.296968836 |
| H | 2.155317316 | 0.524719241 | -2.061406353 |
| C | -0.285875505 | 1.648498774 | -3.428207052 |
| H | 0.330716473 | -0.454458779 | -3.160895809 |
| H | -2.217321333 | 1.156363466 | -4.286038191 |
| C | 0.391298516 | 0.34432994 | -3.904485433 |
| H | -0.594833582 | 3.64661176 | -4.320769243 |
| H | 1.023159486 | 2.963321722 | -4.623802622 |
| C | -0.039954199 | 2.72030817 | -4.5064251 |
| H | -0.126331759 | -0.006635449 | -4.808498863 |
| H | 1.442650662 | 0.507956382 | -4.175258632 |
| H | -0.39125753 | 2.324078886 | -5.470849202 |
| S | -0.885373245 | -2.570130071 | -1.020013867 |
| O | 0.137528402 | -3.581626342 | -1.326360195 |
| O | -1.770286049 | -2.804613301 | 0.136733045 |
| O | -0.337480873 | -1.144110039 | -1.081655875 |
| C | -2.033057546 | -2.600874473 | -2.4915284 |
| F | -3.003579493 | -1.675844306 | -2.361688091 |
| F | -1.362899079 | -2.351256969 | -3.62900986 |
| F | -2.606225764 | -3.805783034 | -2.586135966 |

```
  N    -3.046455975      0.0422315    0.048373638
  N    -4.133412639     0.12750276    0.247774175
  H    -1.039124668    2.612776969    2.020340571
-------------------------------------------------
```

**Supplementary Table 51 | Cartesian coordinate of the reactant complex for protonation of XIV. Units are presented in Å.**

SCF energy (in toluene) = -3161.50806660 hartree

ZPE = 0.842892 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.591757089 | 0.540795729 | 0.610906259 |
| P | 0.050652003 | -0.99675011 | 2.552221543 |
| N | 1.521457456 | 1.150166406 | 1.00062542 |
| P | -0.061602743 | 2.398500607 | -1.240937682 |
| H | -1.200459949 | -2.133586295 | 6.038292077 |
| H | 0.30078494 | -1.287225343 | 5.645453757 |
| C | -0.447999906 | -1.98643249 | 5.250378351 |
| H | -1.302218141 | 0.614794917 | 4.77579524 |
| H | 0.033661224 | -2.955207106 | 5.085947351 |
| H | -2.647534305 | -0.445310288 | 5.179517955 |
| C | -1.94260665 | -0.184840516 | 4.378368106 |
| H | -2.944627172 | -2.638858162 | 4.253042335 |
| C | -1.153684874 | -1.454799509 | 3.986697919 |
| H | 0.441128321 | 1.155936939 | 3.664321076 |
| H | -2.542329152 | 0.196841909 | 3.54497426 |
| H | 1.703374679 | 0.041260026 | 4.166349674 |
| C | -2.176140247 | -2.498540923 | 3.47975008 |
| H | 2.012594472 | -2.517295582 | 4.41223417 |
| H | -2.675731061 | -2.179990906 | 2.560314811 |
| C | 1.127523425 | 0.381533931 | 3.29971111 |
| H | 3.749902696 | 1.111737086 | 3.549226819 |
| H | -1.721958788 | -3.473167403 | 3.289956092 |
| H | 3.087074181 | -1.556106501 | 3.370683645 |
| H | 0.591228984 | 3.756881286 | 1.316477053 |
| C | 2.432397934 | -2.434920953 | 3.406001778 |
| H | -1.205389834 | 5.943846513 | -0.37629213 |
| C | 3.373904993 | 1.263385248 | 2.540832509 |
| H | 3.074417488 | -3.31298885 | 3.24907875 |
| C | 2.042590711 | 0.955995932 | 2.251763696 |
| H | 0.788104939 | 5.462120248 | 0.883015913 |
| H | -1.876857063 | 4.384331648 | 0.128642827 |
| C | 0.908848032 | 4.432573654 | 0.518365347 |
| C | -1.286677512 | 4.881882662 | -0.650145756 |
| H | 5.247424138 | 1.977487583 | 1.735333574 |

| | | | |
|---|---|---|---|
| C | 1.367126256 | -2.416346573 | 2.288431291 |
| H | 1.981855514 | 4.264365913 | 0.37534091 |
| C | 4.204121989 | 1.746756549 | 1.531541774 |
| H | -1.861670866 | 4.833066188 | -1.582311663 |
| H | 0.293297048 | -4.110690069 | 3.203431843 |
| H | 2.651132703 | -1.240718355 | 0.92573857 |
| C | 0.126465402 | 4.282830317 | -0.809902619 |
| C | 0.667986709 | -3.790366818 | 2.225516911 |
| C | 2.10121117 | -2.187047741 | 0.948521515 |
| H | 2.84028334 | -2.991570907 | 0.826175332 |
| H | 1.183063336 | 6.082988364 | -1.371332193 |
| C | 3.674709224 | 1.925878089 | 0.254223518 |
| H | -0.154002798 | -3.808091186 | 1.503217725 |
| C | 2.329584369 | 1.638727671 | 0.012155594 |
| C | 0.924778061 | 5.121096593 | -1.837081408 |
| H | 1.870035422 | 4.645323943 | -2.127614243 |
| H | 1.409259118 | -4.536433065 | 1.90667345 |
| H | 4.29559673 | 2.288507143 | -0.560485141 |
| H | 1.438323121 | -2.231611834 | 0.081152984 |
| H | -2.803712242 | 2.743318477 | -2.442094553 |
| C | 1.726408388 | 1.822027689 | -1.352159341 |
| H | 0.361401451 | 5.346205844 | -2.74198757 |
| H | 2.362141249 | 2.468259937 | -1.969255028 |
| H | -2.453962311 | 1.014752068 | -2.248004524 |
| C | -2.268774161 | 1.888861684 | -2.877255079 |
| H | 1.679014915 | 0.843159526 | -1.847640368 |
| C | -0.763641688 | 2.188893597 | -3.043298034 |
| H | -0.063065903 | 0.089796726 | -3.135549278 |
| H | -2.711353817 | 1.696248178 | -3.864685906 |
| C | -0.057307318 | 1.001504457 | -3.73415782 |
| H | -1.172821091 | 4.280423093 | -3.640224811 |
| H | 0.42168709 | 3.678252949 | -4.166613444 |
| C | -0.621971745 | 3.399532966 | -3.986295686 |
| H | -0.584977398 | 0.785400589 | -4.673367719 |
| H | 0.978401185 | 1.249900599 | -3.998564716 |
| H | -1.052608562 | 3.116973608 | -4.957485177 |
| S | -1.053856625 | -2.188264675 | -1.185703006 |
| O | 0.0003516 | -2.952027685 | -1.851606366 |
| O | -1.674112309 | -2.688697658 | 0.047398792 |
| O | -0.560013347 | -0.675239704 | -1.053070242 |
| C | -2.455791647 | -2.022865209 | -2.418153833 |
| F | -3.405211227 | -1.213666185 | -1.923820596 |
| F | -2.005675376 | -1.517450921 | -3.569980345 |
| F | -2.969729334 | -3.23113778 | -2.62849271 |
| N | -2.563408531 | 0.018026103 | 0.81657294 |
| N | -3.645499389 | -0.242441875 | 0.997188664 |
| N | -1.43218539 | 2.220119465 | 1.931231594 |

| | | | |
|---|---|---|---|
| H | -0.81129501 | 3.024891788 | 2.024198432 |
| H | -1.605264192 | 1.883893709 | 2.881521027 |
| C | -5.130087821 | 3.750826582 | 1.033542335 |
| N | -4.036430609 | 3.870847176 | 1.817168233 |
| C | -4.044855353 | 4.778420213 | 2.818805216 |
| C | -5.150676063 | 5.5975835 | 3.069573927 |
| C | -6.279725016 | 5.477536634 | 2.260348856 |
| C | -6.269252068 | 4.543648784 | 1.227770831 |
| H | -7.129918126 | 4.422056931 | 0.574467884 |
| H | -7.152432728 | 6.105054423 | 2.431398249 |
| H | -5.120968683 | 6.316856514 | 3.88431568 |
| C | -2.801303885 | 4.883262322 | 3.670214896 |
| H | -2.91237147 | 5.64921674 | 4.445076365 |
| H | -2.585268722 | 3.930194955 | 4.173211238 |
| H | -1.925963499 | 5.14800678 | 3.060300846 |
| C | -5.087346235 | 2.713120156 | -0.058167018 |
| H | -5.894446926 | 2.862238044 | -0.783756573 |
| H | -4.128308669 | 2.747400638 | -0.589353396 |
| H | -5.191691727 | 1.701725206 | 0.357908227 |
| H | -2.345988924 | 2.634430897 | 1.648508596 |

---

**Supplementary Table 52 | Cartesian coordinate of the transition state for protonation of XIV. Units are presented in Å.**

SCF energy (in toluene) = -3161.48814983 hartree

ZPE = 0.840082 hartree

imaginary frequency: 361*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.670013889 | 0.730333195 | 0.634886974 |
| P | -0.027769099 | -0.830962002 | 2.57640244 |
| N | 1.49234963 | 1.232271616 | 0.948777458 |
| P | -0.062980416 | 2.442456158 | -1.333781766 |
| H | -1.30016617 | -1.875439944 | 6.089938372 |
| H | 0.228737842 | -1.088029796 | 5.676183721 |
| C | -0.545701416 | -1.768037153 | 5.297004606 |
| H | -1.310421077 | 0.843143626 | 4.787645543 |
| H | -0.09746535 | -2.755359196 | 5.147779516 |
| H | -2.706216085 | -0.159971383 | 5.187022319 |
| C | -1.980557308 | 0.066509109 | 4.39318215 |
| H | -3.065868197 | -2.353753492 | 4.304343715 |
| C | -1.234253149 | -1.235019246 | 4.0252004 |
| H | 0.439684909 | 1.330627619 | 3.621971825 |
| H | -2.544109537 | 0.462612144 | 3.541479413 |
| H | 1.685658324 | 0.197059698 | 4.144869828 |
| C | -2.289687055 | -2.251505942 | 3.531902646 |
| H | 1.887897011 | -2.387634889 | 4.456999142 |
| H | -2.772172968 | -1.931045042 | 2.604013114 |
| C | 1.103202784 | 0.528272224 | 3.278749395 |
| H | 3.746365381 | 1.160426133 | 3.475074138 |
| H | -1.866822873 | -3.243457146 | 3.359633923 |
| H | 2.990701464 | -1.475288632 | 3.401642638 |
| H | 0.657801662 | 3.865391421 | 1.147939529 |
| C | 2.308554355 | -2.332426553 | 3.449219359 |
| H | -1.094958609 | 6.047093075 | -0.598385608 |
| C | 3.365890287 | 1.304541903 | 2.467191086 |
| H | 2.922202526 | -3.232557679 | 3.303439611 |
| C | 2.018721093 | 1.045686049 | 2.19960361 |
| H | 0.913795261 | 5.550475868 | 0.658219963 |
| H | -1.757143532 | 4.516298373 | 0.00965459 |
| C | 0.995013332 | 4.504761498 | 0.328296619 |

| | | | |
|---|---|---|---|
| C | -1.200566272 | 4.974365579 | -0.817181766 |
| H | 5.25885012 | 1.922077591 | 1.628585303 |
| C | 1.242987847 | -2.29614213 | 2.332012506 |
| H | 2.060081573 | 4.296638303 | 0.178430421 |
| C | 4.205276594 | 1.72847242 | 1.439506774 |
| H | -1.808867343 | 4.885321622 | -1.725672634 |
| H | 0.124180085 | -3.946013581 | 3.274044613 |
| H | 2.561656799 | -1.180715409 | 0.953000348 |
| C | 0.193677095 | 4.336883217 | -0.986489545 |
| C | 0.503084818 | -3.649484141 | 2.289918166 |
| C | 1.986041967 | -2.111020105 | 0.989943275 |
| H | 2.703047651 | -2.937869383 | 0.885271478 |
| H | 1.29766679 | 6.08626752 | -1.617300988 |
| C | 3.671125384 | 1.892403588 | 0.161635308 |
| H | -0.321965183 | -3.650955495 | 1.57120572 |
| C | 2.313842606 | 1.651475107 | -0.057644497 |
| C | 0.994351277 | 5.122410673 | -2.051519072 |
| H | 1.914839443 | 4.605355743 | -2.351258661 |
| H | 1.220849269 | -4.420926477 | 1.977325028 |
| H | 4.29799486 | 2.206143591 | -0.669030326 |
| H | 1.325181742 | -2.153338468 | 0.121414431 |
| H | -2.783520922 | 2.79448643 | -2.63967392 |
| C | 1.704687533 | 1.80621195 | -1.421578119 |
| H | 0.418371043 | 5.34374037 | -2.950035844 |
| H | 2.356020621 | 2.40532109 | -2.069520333 |
| H | -2.460615511 | 1.075447284 | -2.321918321 |
| C | -2.2502407 | 1.905206279 | -3.001191672 |
| H | 1.621521262 | 0.809223674 | -1.872707187 |
| C | -0.738005683 | 2.175189945 | -3.144324187 |
| H | -0.084482481 | 0.060579866 | -3.13960123 |
| H | -2.669570705 | 1.652934416 | -3.985469194 |
| C | -0.047938515 | 0.945849332 | -3.776255073 |
| H | -1.097649892 | 4.248056404 | -3.830906257 |
| H | 0.492778946 | 3.596489724 | -4.306108932 |
| C | -0.558606917 | 3.343432123 | -4.133020692 |
| H | -0.567593427 | 0.702551288 | -4.713262697 |
| H | 0.996588227 | 1.160057378 | -4.035407827 |
| H | -0.978396826 | 3.031060038 | -5.100076462 |
| S | -1.153682804 | -2.089511462 | -1.11468473 |
| O | -0.131179722 | -2.920858924 | -1.753752491 |
| O | -1.804505711 | -2.548830494 | 0.121077381 |
| O | -0.630508692 | -0.609491868 | -1.020848854 |
| C | -2.542779193 | -1.939494639 | -2.359410969 |
| F | -3.484856014 | -1.093889346 | -1.905176721 |
| F | -2.081656272 | -1.481604727 | -3.529434273 |
| F | -3.08661 | -3.141680633 | -2.537512688 |
| N | -2.638226393 | 0.211690337 | 0.801881195 |

| | | | |
|---|---|---|---|
| N | -3.719755097 | -0.054442225 | 0.994929608 |
| N | -1.404377736 | 2.367735252 | 1.834785308 |
| H | -0.80966558 | 3.197710848 | 1.831416127 |
| H | -1.467558398 | 2.060747353 | 2.80830082 |
| C | -4.791504536 | 3.526880425 | 1.052472431 |
| N | -3.829696385 | 3.543705078 | 2.008009354 |
| C | -4.00232223 | 4.167358746 | 3.206279925 |
| C | -5.207002534 | 4.809516616 | 3.475319277 |
| C | -6.221795947 | 4.806007385 | 2.515042046 |
| C | -6.010749861 | 4.165441733 | 1.298760886 |
| H | -6.778700059 | 4.150533209 | 0.529949225 |
| H | -7.167241549 | 5.305074401 | 2.716476204 |
| H | -5.342397765 | 5.308842384 | 4.430572268 |
| C | -2.875151409 | 4.135581677 | 4.20237902 |
| H | -3.107502659 | 4.780846523 | 5.054824326 |
| H | -2.713567163 | 3.119117385 | 4.585883978 |
| H | -1.934030459 | 4.481012807 | 3.757701409 |
| C | -4.521514293 | 2.813655624 | -0.237793481 |
| H | -4.883416349 | 3.411302838 | -1.08267616 |
| H | -3.458540892 | 2.603666085 | -0.374583128 |
| H | -5.05341453 | 1.853233706 | -0.257006893 |
| H | -2.814259351 | 3.007278402 | 1.825859164 |

**Supplementary Table 53 | Cartesian coordinate of the product complex for protonation of XIV. Units are presented in Å.**

SCF energy (in toluene) = -3161.50809391 hartree

ZPE = 0.843324 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.551514869 | 0.641235399 | 0.569535989 |
| P | 0.042143238 | -0.845332904 | 2.561690192 |
| N | 1.589756008 | 1.179481236 | 0.91626541 |
| P | 0.027560862 | 2.407821275 | -1.351935219 |
| H | -1.248149996 | -1.788587626 | 6.091914379 |
| H | 0.29589136 | -1.042074721 | 5.662619932 |
| C | -0.493809559 | -1.711128781 | 5.295851469 |
| H | -1.194616175 | 0.908076776 | 4.751612108 |
| H | -0.067705868 | -2.71026552 | 5.160861024 |
| H | -2.61635942 | -0.047380241 | 5.159109367 |
| C | -1.883948598 | 0.14536774 | 4.363148241 |
| H | -3.027051101 | -2.258770167 | 4.327872059 |
| C | -1.175601389 | -1.183430904 | 4.017826894 |
| H | 0.559918182 | 1.320655783 | 3.604286002 |
| H | -2.438380315 | 0.549932006 | 3.509886292 |
| H | 1.7729373 | 0.159506907 | 4.112431417 |
| C | -2.255310815 | -2.185164459 | 3.548361856 |
| H | 1.932458452 | -2.404872128 | 4.469270737 |
| H | -2.740587039 | -1.870219648 | 2.620286378 |
| C | 1.198245591 | 0.502598031 | 3.246086117 |
| H | 3.850509321 | 1.119943156 | 3.436561506 |
| H | -1.853637285 | -3.188111324 | 3.388862061 |
| H | 3.052553952 | -1.535113404 | 3.395408901 |
| H | 0.777059772 | 3.796048874 | 1.157082197 |
| C | 2.351666442 | -2.3760736 | 3.459809527 |
| H | -1.005863413 | 6.005566607 | -0.56140065 |
| C | 3.467520558 | 1.25867944 | 2.428981079 |
| H | 2.945816504 | -3.291362944 | 3.32907678 |
| C | 2.12060687 | 1.000719997 | 2.166155008 |
| H | 0.987055282 | 5.492935027 | 0.689497013 |
| H | -1.723761771 | 4.477475984 | -0.025660587 |
| C | 1.082949899 | 4.455377228 | 0.340273924 |
| C | -1.119547992 | 4.941902684 | -0.815297673 |
| H | 5.35803523 | 1.871658586 | 1.580419005 |

| | | | |
|---|---|---|---|
| C | 1.284334817 | -2.338005143 | 2.344488455 |
| H | 2.149838465 | 4.2681139 | 0.175937841 |
| C | 4.303564232 | 1.678875593 | 1.396265708 |
| H | -1.701399481 | 4.890743678 | -1.742963741 |
| H | 0.131149923 | -3.946981583 | 3.316735455 |
| H | 2.608914941 | -1.262700034 | 0.938470917 |
| C | 0.274529235 | 4.296291679 | -0.973071653 |
| C | 0.516207072 | -3.676190293 | 2.327621819 |
| C | 2.025281347 | -2.187321884 | 0.997240281 |
| H | 2.73443451 | -3.022384116 | 0.906477027 |
| H | 1.377048205 | 6.049852733 | -1.593607599 |
| C | 3.763596864 | 1.844329236 | 0.121555685 |
| H | -0.309316147 | -3.673952774 | 1.609451821 |
| C | 2.405238574 | 1.605296897 | -0.095325104 |
| C | 1.080103169 | 5.086426619 | -2.032465619 |
| H | 2.004123003 | 4.573420788 | -2.327993177 |
| H | 1.217169418 | -4.468109197 | 2.028644459 |
| H | 4.387522178 | 2.158415578 | -0.711115648 |
| H | 1.360802675 | -2.241666894 | 0.131902344 |
| H | -2.71342639 | 2.801251488 | -2.53599041 |
| C | 1.794303236 | 1.771783164 | -1.458519283 |
| H | 0.507977398 | 5.308322879 | -2.932927967 |
| H | 2.44552699 | 2.37799652 | -2.099660182 |
| H | -2.415418572 | 1.067517835 | -2.307980825 |
| C | -2.208324016 | 1.921938071 | -2.956764721 |
| H | 1.708293885 | 0.781414033 | -1.924573912 |
| C | -0.695480244 | 2.167874374 | -3.141140684 |
| H | -0.062011625 | 0.046089467 | -3.167083705 |
| H | -2.66422963 | 1.721866939 | -3.936657347 |
| C | -0.034545477 | 0.935674633 | -3.797811237 |
| H | -1.045163539 | 4.249902364 | -3.806136652 |
| H | 0.53126597 | 3.585840682 | -4.312229398 |
| C | -0.519814068 | 3.342756993 | -4.123026756 |
| H | -0.580250091 | 0.70369874 | -4.722701379 |
| H | 1.005047151 | 1.14192921 | -4.082332602 |
| H | -0.95910788 | 3.041006649 | -5.084501674 |
| S | -1.123429613 | -2.132674711 | -1.135000969 |
| O | -0.100693807 | -2.961610728 | -1.771969642 |
| O | -1.76548885 | -2.564408177 | 0.112467689 |
| O | -0.569054859 | -0.638674194 | -1.053005132 |
| C | -2.516432766 | -1.961533448 | -2.376700872 |
| F | -3.442847966 | -1.109182637 | -1.912052641 |
| F | -2.048935648 | -1.506568687 | -3.542611698 |
| F | -3.066511689 | -3.159655353 | -2.550937968 |
| N | -2.545714215 | 0.190098449 | 0.780825026 |
| N | -3.637627315 | -0.028496199 | 0.952600532 |
| N | -1.333596341 | 2.411863694 | 1.786075917 |

| | | | |
|---|---|---|---|
| H | -0.87614645 | 3.297331736 | 1.569146524 |
| H | -1.194753004 | 2.261970987 | 2.788604514 |
| C | -5.14114145 | 3.632799449 | 1.118339645 |
| N | -4.144618436 | 3.585138495 | 2.026986241 |
| C | -4.315497759 | 4.197542909 | 3.220231851 |
| C | -5.492827944 | 4.878929255 | 3.542722507 |
| C | -6.523836001 | 4.931250338 | 2.604500537 |
| C | -6.345608831 | 4.302529208 | 1.376067232 |
| H | -7.124863338 | 4.323319067 | 0.617782264 |
| H | -7.449506208 | 5.45775665 | 2.82882413 |
| H | -5.59382778 | 5.361540305 | 4.511877361 |
| C | -3.175348263 | 4.120032966 | 4.208167977 |
| H | -3.401271787 | 4.681061341 | 5.12109012 |
| H | -2.976111166 | 3.078429778 | 4.49761385 |
| H | -2.252156285 | 4.535042135 | 3.780202248 |
| C | -4.929230865 | 2.913566517 | -0.189027169 |
| H | -5.527696986 | 3.360241181 | -0.991390517 |
| H | -3.873879666 | 2.93463082 | -0.481862752 |
| H | -5.223255556 | 1.858265711 | -0.10264844 |
| H | -2.353931748 | 2.622843413 | 1.708400136 |

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**Supplementary Table 54 | Cartesian coordinate of the transition state for elimination of the ammonia ligand from XVII. Units are presented in Å.**

SCF energy (in toluene) = -3909.60899623 hartree

ZPE = 1.310831 hartree

imaginary frequency: 51*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.58903079 | 0.070012599 | -0.046776179 |
| Mo | 2.657553379 | 0.023549409 | 0.171806494 |
| P | 3.271924049 | 2.116711781 | -1.055686633 |
| P | -3.231564893 | -2.073008172 | -1.228988968 |
| N | -4.82580549 | 0.157140233 | 0.003526994 |
| N | 4.876214688 | -0.116770939 | 0.130922574 |
| P | 3.042692367 | -2.163790721 | 1.328428754 |
| P | -3.00736197 | 2.259788254 | 1.176122604 |
| N | -0.519990422 | 0.035574895 | -0.03269409 |
| N | 0.636391075 | 0.035272928 | 0.041643107 |
| N | -2.558952102 | 1.552876705 | -2.844890528 |
| N | -2.568482667 | 1.011030631 | -1.843112597 |
| N | -2.574491809 | -0.879256747 | 1.751514672 |
| N | -2.571196262 | -1.427712257 | 2.747842661 |
| N | 2.688595597 | 0.921893736 | 1.886163761 |
| N | 2.726768769 | 1.47321419 | 2.895008633 |
| H | 2.622580609 | 3.542367364 | -4.637799778 |
| H | -2.720890414 | -3.587575148 | -4.800772257 |
| H | -4.064647941 | -2.587499828 | -4.242867676 |
| H | 4.016461019 | 2.595977661 | -4.106038556 |
| C | 3.244282922 | 3.296417285 | -3.76290893 |
| C | -3.308011695 | -3.309472309 | -3.911728748 |
| H | -2.368610442 | -0.739242746 | -3.863118099 |
| H | 2.45233542 | 0.640904965 | -3.479113081 |
| H | -3.823522704 | -4.210715545 | -3.569017706 |
| H | 3.74002036 | 4.218181787 | -3.446808565 |
| H | -1.081893721 | -1.838726017 | -4.373502926 |
| H | 1.173560018 | 1.658744356 | -4.179638432 |
| C | 1.703699687 | 1.406709068 | -3.248279961 |
| C | -1.660331657 | -1.49191432 | -3.502646953 |
| H | 0.558562328 | 3.788272559 | -3.185595421 |
| H | -0.639992111 | -3.915178425 | -3.381138682 |

| | | | |
|---|---|---|---|
| C | 2.349431984 | 2.679647552 | -2.667960674 |
| C | -2.359803577 | -2.703816645 | -2.85528689 |
| H | -4.541143798 | -0.755055885 | -2.757383008 |
| H | 4.544843872 | 0.795257832 | -2.614042557 |
| H | 0.980423745 | 0.972201956 | -2.549609369 |
| H | -0.979431863 | -0.993804347 | -2.802822538 |
| H | 5.549235701 | 2.192876369 | -2.205967484 |
| H | -5.531091403 | -2.153173948 | -2.322704167 |
| C | 1.211424672 | 3.654688621 | -2.310117118 |
| C | -1.261286425 | -3.722878201 | -2.49287733 |
| H | 3.609060386 | 5.290916456 | -1.61494054 |
| H | -3.647887178 | -5.259779345 | -1.728921494 |
| H | 0.590130563 | 3.265265537 | -1.493928662 |
| H | -0.60283414 | -3.342771926 | -1.700986487 |
| C | 4.881495718 | 1.431575536 | -1.781098256 |
| C | -4.855651049 | -1.389367394 | -1.915640424 |
| H | 7.560358144 | 1.085737477 | -1.560473742 |
| H | -7.531744074 | -1.074948599 | -1.624879162 |
| H | 1.579939054 | 4.646018179 | -2.023357312 |
| H | -1.664477849 | -4.687476101 | -2.16807122 |
| H | 5.208737654 | 4.514296709 | -1.640111614 |
| H | -5.227532817 | -4.444288415 | -1.713069949 |
| H | -4.48034249 | 2.615456874 | -1.359932006 |
| H | 4.229839451 | -2.475326926 | -1.351672058 |
| C | 4.386172934 | 4.838934926 | -0.989024417 |
| C | -4.391761841 | -4.779098903 | -1.08484066 |
| H | -2.619987042 | 5.179919767 | -1.283207016 |
| H | 2.414765438 | -4.857800632 | -1.300759149 |
| C | 7.017506806 | 0.511019655 | -0.812926764 |
| C | -6.976847184 | -0.501936039 | -0.88516363 |
| H | 4.783148438 | 5.636559399 | -0.342289727 |
| H | -4.786251325 | -5.557533921 | -0.41375997 |
| C | 5.624243561 | 0.581812537 | -0.784410826 |
| C | -5.581646669 | -0.545464095 | -0.898445099 |
| H | -4.862550572 | 4.342530447 | -1.428717088 |
| H | 4.67832562 | -4.192509586 | -1.451115764 |
| H | -2.008234749 | 3.522733326 | -1.386835067 |
| H | 1.720465499 | -3.244009871 | -0.995615805 |
| C | -4.683628171 | 3.496842001 | -0.747532787 |
| C | 4.521658573 | -3.349470412 | -0.759288524 |
| C | -2.316633606 | 4.304703558 | -0.6880401 |
| C | 2.162834093 | -4.125390022 | -0.51699184 |
| H | -8.729382274 | 0.304977203 | 0.098218821 |
| H | 8.783393158 | -0.349162284 | 0.101324361 |
| C | 3.850027159 | 3.699879404 | -0.100347817 |
| C | -3.804675282 | -3.637793764 | -0.230219389 |
| H | -5.613050971 | 3.323850358 | -0.19265639 |

| | | | |
|---|---|---|---|
| H | 5.485511333 | -3.138004078 | -0.283004344 |
| C | -7.642570335 | 0.263509535 | 0.071894452 |
| C | 7.697351232 | -0.286211613 | 0.107883853 |
| H | -1.445270624 | 4.597923451 | -0.095054318 |
| H | 1.39535377 | -4.579776591 | 0.116544811 |
| H | 1.829235895 | 4.562114784 | 0.138071885 |
| H | -1.801131887 | -4.553344186 | -0.034387147 |
| H | 5.895342681 | 2.986254111 | 0.323342691 |
| H | -5.841417638 | -2.93296865 | 0.240264478 |
| C | -3.507024461 | 3.85645552 | 0.187640896 |
| C | 3.436389702 | -3.743641277 | 0.267193349 |
| C | 2.673826762 | 4.227813277 | 0.749479271 |
| C | -2.616793798 | -4.181973842 | 0.593505485 |
| C | 4.987273145 | 3.285581098 | 0.860377313 |
| C | -4.911306102 | -3.199066883 | 0.755657777 |
| H | 5.248064938 | 4.151551739 | 1.487894578 |
| H | -5.137943219 | -4.04199953 | 1.425748986 |
| H | -4.337440531 | 5.842967832 | 0.395217227 |
| H | 4.235663313 | -5.757987761 | 0.335132187 |
| C | 6.940989675 | -0.999124732 | 1.039730353 |
| C | -6.875031122 | 0.974309089 | 0.994079183 |
| H | 2.315298904 | 3.471951294 | 1.454006798 |
| H | -2.209174926 | -3.426215125 | 1.270264594 |
| C | 5.549440136 | -0.903354539 | 1.034085676 |
| C | -5.481294461 | 0.912453738 | 0.94091637 |
| C | -3.966986551 | 5.044244648 | 1.056018168 |
| C | 3.949648523 | -4.967932487 | 1.047258666 |
| H | -4.790802596 | 4.777214973 | 1.730836511 |
| H | 4.840579531 | -4.733742459 | 1.644595838 |
| H | 3.017448762 | 5.093815407 | 1.336429679 |
| H | -2.965526322 | -5.024677098 | 1.209979307 |
| H | -7.34820586 | 1.586189227 | 1.759017442 |
| H | 7.423298863 | -1.634881467 | 1.779339219 |
| H | 4.692995101 | 2.471179138 | 1.527145917 |
| H | -4.610366774 | -2.353646986 | 1.378319101 |
| H | -1.1811479 | 4.728029791 | 2.021645736 |
| H | 1.22124453 | -4.640298687 | 2.223648884 |
| C | -4.647785299 | 1.694437969 | 1.925194987 |
| C | 4.727337427 | -1.678272955 | 2.031163248 |
| H | -3.156390103 | 5.472493333 | 1.654305358 |
| H | 3.192618457 | -5.394139276 | 1.714192825 |
| H | -5.244287311 | 2.506362914 | 2.361161232 |
| H | 5.310447028 | -2.517378533 | 2.432570624 |
| H | -0.251633066 | 3.287642873 | 1.53817763 |
| H | 0.285554711 | -3.187032485 | 1.791803293 |
| C | -0.850764721 | 3.733601392 | 2.341326805 |
| C | 0.915850175 | -3.64442871 | 2.564397442 |

| | | | |
|---|---|---|---|
| H | -4.348106188 | 1.034942344 | 2.752982093 |
| H | 4.475056154 | -1.022240023 | 2.877286733 |
| C | -2.019205021 | 2.817070568 | 2.755037933 |
| C | 2.111978656 | -2.744049543 | 2.932289836 |
| H | -0.764419797 | 1.015269601 | 2.680539125 |
| H | 0.859429199 | -0.941151225 | 2.945089621 |
| H | -0.183654698 | 3.871404928 | 3.204323216 |
| H | 0.287439294 | -3.784055547 | 3.456132154 |
| C | -1.403990538 | 1.552798284 | 3.387066289 |
| C | 1.542024412 | -1.481388497 | 3.608697001 |
| H | -3.334715565 | 4.442177077 | 3.496577843 |
| H | 3.456434499 | -4.388795447 | 3.572648595 |
| H | -3.668254943 | 2.854820731 | 4.215142476 |
| H | 3.812872289 | -2.824283071 | 4.329800919 |
| C | -2.874376467 | 3.510668925 | 3.836099801 |
| C | 3.006732162 | -3.46937635 | 3.959497446 |
| H | -0.781392836 | 1.853888147 | 4.242479192 |
| H | 0.980174677 | -1.784390866 | 4.505357591 |
| H | -2.163000348 | 0.858242512 | 3.761885263 |
| H | 2.32019176 | -0.780415944 | 3.926757771 |
| H | -2.228483346 | 3.756814399 | 4.692617877 |
| H | 2.393926794 | -3.745982516 | 4.831232969 |
| N | 2.36947968 | -1.815523547 | -3.124763629 |
| H | 2.478102686 | -2.829155618 | -3.078251846 |
| H | 2.577321469 | -1.546304176 | -4.087868262 |
| H | 1.375778131 | -1.624474772 | -2.987212004 |

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**Supplementary Table 55 | Cartesian coordinate of the product complex for elimination of the ammonia ligand from XVII. Units are presented in Å.**

SCF energy (in toluene) = -3909.59414048 hartree

ZPE = 1.309396 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.624288372 | 0.136416637 | 0.053949422 |
| Mo | 2.623528343 | 0.01263996 | 0.18633786 |
| P | 3.168858121 | 1.803472654 | -1.417443345 |
| P | -3.297214154 | -1.843014158 | -1.391566767 |
| N | -4.857790983 | 0.267611985 | 0.102144851 |
| N | 4.864338105 | -0.104892158 | 0.191124275 |
| P | 2.988704416 | -2.067085365 | 1.461473112 |
| P | -2.999971883 | 2.177635102 | 1.519161591 |
| N | -0.559062058 | 0.068871314 | 0.048563771 |
| N | 0.599513768 | 0.050174655 | 0.098505687 |
| N | -2.646582241 | 1.927573127 | -2.557856373 |
| N | -2.617964202 | 1.27967235 | -1.621999226 |
| N | -2.651600293 | -1.025228268 | 1.72086341 |
| N | -2.684655192 | -1.692478296 | 2.642079024 |
| N | 2.745487107 | 1.11374055 | 1.780243644 |
| N | 2.821399087 | 1.780816991 | 2.712271664 |
| H | 2.597416181 | 1.891143881 | -5.278712933 |
| H | -2.835569232 | -2.938433074 | -5.114677923 |
| H | -4.157815552 | -1.987161935 | -4.433795826 |
| H | 4.126797395 | 1.657776209 | -4.424091301 |
| C | 3.140458249 | 2.132538681 | -4.35169859 |
| C | -3.412339009 | -2.755760014 | -4.194884039 |
| H | -2.441533956 | -0.226805715 | -3.861317933 |
| H | 3.086240955 | -0.455569114 | -3.36267065 |
| H | -3.942022903 | -3.680742928 | -3.953449426 |
| H | 3.283560289 | 3.217242164 | -4.333050231 |
| H | -1.16285487 | -1.270581146 | -4.496283408 |
| H | 1.601130686 | -0.105571934 | -4.262534119 |
| C | 2.133818863 | 0.089482478 | -3.318877727 |
| C | -1.736974624 | -1.020026994 | -3.591026122 |
| H | 0.3786047 | 2.005092377 | -4.018782125 |
| H | -0.754780184 | -3.459763298 | -3.771844289 |
| C | 2.331816271 | 1.614428157 | -3.145315801 |
| C | -2.445371688 | -2.291500875 | -3.085170915 |

| | | | |
|---|---|---|---|
| H | -4.578228315 | -0.324251534 | -2.749439788 |
| H | 4.855668425 | 0.56867648 | -2.649529224 |
| H | 1.519179899 | -0.327634032 | -2.50798316 |
| H | -1.045785515 | -0.616293511 | -2.844490668 |
| H | 5.548790264 | 2.130934946 | -2.215932649 |
| H | -5.593396067 | -1.7432284 | -2.479095446 |
| C | 0.945406305 | 2.285743981 | -3.118581934 |
| C | -1.356810475 | -3.359918188 | -2.856276012 |
| H | 2.847773909 | 4.695925149 | -2.816169743 |
| H | -3.772096231 | -4.946477366 | -2.250643712 |
| H | 0.356367428 | 1.972306888 | -2.248725195 |
| H | -0.676689186 | -3.076183153 | -2.042794092 |
| C | 4.934941456 | 1.304079467 | -1.834293973 |
| C | -4.903928159 | -1.0455427 | -1.985993524 |
| H | 7.583862138 | 1.229451837 | -1.340121281 |
| H | -7.573038497 | -0.699724889 | -1.680992663 |
| H | 1.015908032 | 3.380268926 | -3.109761861 |
| H | -1.769646023 | -4.349087186 | -2.631193483 |
| H | 4.573719848 | 4.312315362 | -2.630036764 |
| H | -5.332237864 | -4.098420943 | -2.163469119 |
| H | -4.443855119 | 2.935689707 | -0.989371932 |
| H | 4.234214561 | -2.45746324 | -1.187566636 |
| C | 3.665667234 | 4.61441583 | -2.091624306 |
| C | -4.514671046 | -4.5231999 | -1.566720806 |
| H | -2.494544615 | 5.325790187 | -0.608795009 |
| H | 2.137786464 | -4.715406043 | -1.154097514 |
| C | 7.028005257 | 0.630934518 | -0.621050158 |
| C | -7.01294922 | -0.228780316 | -0.876063532 |
| H | 3.846049933 | 5.623311752 | -1.689332813 |
| H | -4.935892518 | -5.360784753 | -0.989983615 |
| C | 5.634013364 | 0.609033547 | -0.695937287 |
| C | -5.61899695 | -0.307900303 | -0.880979151 |
| H | -4.789036315 | 4.65629891 | -0.77445309 |
| H | 4.509963094 | -4.212327722 | -1.296606507 |
| H | -1.907634006 | 3.670792593 | -0.841321462 |
| H | 1.721794688 | -2.991376075 | -1.030688215 |
| C | -4.622333143 | 3.709434954 | -0.239231168 |
| C | 4.414081979 | -3.365502333 | -0.598545609 |
| C | -2.217814552 | 4.39741048 | -0.085885178 |
| C | 1.980263091 | -3.88544915 | -0.44772606 |
| H | -8.756445583 | 0.509976507 | 0.17414082 |
| H | 8.778208329 | -0.10894346 | 0.424085719 |
| C | 3.327494814 | 3.660688163 | -0.932294786 |
| C | -3.910421415 | -3.500851836 | -0.584225087 |
| H | -5.550575708 | 3.467850094 | 0.291760616 |
| H | 5.376995703 | -3.24882947 | -0.086523907 |
| C | -7.6707545 | 0.442838375 | 0.153884419 |

| | | | |
|---|---|---|---|
| C | 7.692528762 | -0.115703132 | 0.353061307 |
| H | -1.352647992 | 4.621728889 | 0.545097507 |
| H | 1.113507087 | -4.136751789 | 0.172598916 |
| H | 1.153946499 | 4.044988747 | -0.950556998 |
| H | -1.938777943 | -4.494060911 | -0.504166402 |
| H | 5.438715273 | 3.512808271 | -0.297882542 |
| H | -5.934785129 | -2.813839159 | -0.045177726 |
| C | -3.431579072 | 3.89790039 | 0.728301497 |
| C | 3.26001345 | -3.65827182 | 0.385562676 |
| C | 2.007292819 | 4.098874707 | -0.264975694 |
| C | -2.734632744 | -4.161779525 | 0.169798268 |
| C | 4.453382203 | 3.750705373 | 0.122428402 |
| C | -5.01549899 | -3.15912483 | 0.442012994 |
| H | 4.500968206 | 4.782350186 | 0.503273717 |
| H | -5.266131449 | -4.071916611 | 1.003414875 |
| H | -4.168834093 | 5.881503063 | 1.178308924 |
| H | 3.834632748 | -5.749354037 | 0.432954109 |
| C | 6.917305497 | -0.872850034 | 1.231072368 |
| C | -6.897349682 | 1.026485122 | 1.156513956 |
| H | 1.783733241 | 3.477801703 | 0.609021361 |
| H | -2.294722025 | -3.49020005 | 0.911934394 |
| C | 5.524812018 | -0.848435256 | 1.140046227 |
| C | -5.504981398 | 0.933348943 | 1.110255368 |
| C | -3.843973285 | 4.989742254 | 1.736154826 |
| C | 3.612566796 | -4.945463574 | 1.152415541 |
| H | -4.687626541 | 4.679895876 | 2.366567244 |
| H | 4.501799811 | -4.821726247 | 1.784389225 |
| H | 2.098106037 | 5.142686482 | 0.073504956 |
| H | -3.105096934 | -5.050376884 | 0.703669214 |
| H | -7.364416408 | 1.562822519 | 1.979682294 |
| H | 7.383859673 | -1.478916896 | 2.005065502 |
| H | 4.27138011 | 3.09061285 | 0.976204579 |
| H | -4.705694232 | -2.401816526 | 1.165434561 |
| H | -1.097703461 | 4.457810581 | 2.66746985 |
| H | 0.934414602 | -4.31351267 | 2.377974942 |
| C | -4.664730077 | 1.580319867 | 2.182396149 |
| C | 4.703441978 | -1.650930325 | 2.119136939 |
| H | -3.021599998 | 5.300859027 | 2.388004289 |
| H | 2.789533377 | -5.296792212 | 1.783422571 |
| H | -5.245471621 | 2.356214166 | 2.697918274 |
| H | 5.281171136 | -2.515881581 | 2.473876535 |
| H | -0.21243308 | 3.046781468 | 2.039483051 |
| H | 0.1724217 | -2.744757967 | 2.017191864 |
| C | -0.811267888 | 3.421739012 | 2.87826739 |
| C | 0.765165711 | -3.298130173 | 2.755874505 |
| H | -4.396960472 | 0.826801872 | 2.937529668 |
| H | 4.497585167 | -1.026204001 | 3.00089102 |

| | | | |
|---|---|---|---|
| C | -2.021223327 | 2.508417005 | 3.163789987 |
| C | 2.077295871 | -2.5627272 | 3.094486665 |
| H | -0.840217002 | 0.681246236 | 2.878616364 |
| H | 1.070275247 | -0.613877572 | 3.151889261 |
| H | -0.154834089 | 3.436402006 | 3.76015787 |
| H | 0.151827539 | -3.38667488 | 3.664571946 |
| C | -1.461862041 | 1.155413573 | 3.6437557 |
| C | 1.705151532 | -1.236269339 | 3.788878024 |
| H | -3.2922653 | 4.075026497 | 4.094416863 |
| H | 3.220252364 | -4.369293777 | 3.677100185 |
| H | -3.68725663 | 2.422028386 | 4.602292445 |
| H | 3.814743582 | -2.867595724 | 4.410895303 |
| C | -2.867297612 | 3.092703331 | 4.315331669 |
| C | 2.913830342 | -3.400860214 | 4.082232781 |
| H | -0.836348009 | 1.327559443 | 4.53204118 |
| H | 1.15441068 | -1.460269973 | 4.715124775 |
| H | -2.24986169 | 0.451036669 | 3.930476827 |
| H | 2.583104679 | -0.639228259 | 4.062190715 |
| H | -2.223620239 | 3.207091963 | 5.200748716 |
| H | 2.311880695 | -3.597700341 | 4.98273522 |
| N | 5.738326139 | -1.588227478 | -3.562863119 |
| H | 6.431825385 | -1.446853034 | -2.826341683 |
| H | 6.2432537 | -1.546968428 | -4.449537206 |
| H | 5.410789713 | -2.549688133 | -3.461486605 |

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**Supplementary Table 56 | Cartesian coordinate of the reactant complex for coordination of dinitrogen to XVIII. Units are presented in Å.**

SCF energy (in toluene) = -3962.54624778 hartree

ZPE = 1.279297 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.569491425 | 0.015759051 | -0.025604302 |
| Mo | 2.665364896 | -0.256928488 | -0.267710335 |
| P | 3.173001668 | 1.796826612 | -1.546120374 |
| P | -3.148728274 | -1.970577322 | -1.512868268 |
| N | -4.804146263 | 0.109582542 | -0.071052502 |
| N | 4.910244065 | -0.311762461 | -0.31178691 |
| P | 3.104118882 | -2.11623662 | 1.288443214 |
| P | -3.03878986 | 2.034661691 | 1.437834707 |
| N | -0.508206622 | -0.07853243 | -0.047687047 |
| N | 0.647403364 | -0.138387035 | -0.127958946 |
| N | -2.488768716 | 1.838967353 | -2.616185552 |
| N | -2.504953917 | 1.177867588 | -1.690233886 |
| N | -2.651367338 | -1.152247241 | 1.632892129 |
| N | -2.722923561 | -1.818143309 | 2.553624124 |
| N | 2.641225143 | -2.017519677 | -2.806253865 |
| N | 2.653958336 | -1.353891252 | -1.868809524 |
| N | 3.529336901 | 2.839731891 | 4.299313224 |
| N | 2.598398304 | 3.292742638 | 4.693324644 |
| H | 2.568366143 | 3.368848346 | -5.061496226 |
| H | -2.475633742 | -3.045028989 | -5.20201285 |
| H | -3.848886382 | -2.116148197 | -4.593695441 |
| H | 4.01716115 | 2.5263859 | -4.507039812 |
| C | 3.166199111 | 3.130418823 | -4.168370289 |
| C | -3.104803493 | -2.873419767 | -4.315493359 |
| H | -2.198840513 | -0.323987916 | -3.91544483 |
| H | 2.586239594 | 0.403572248 | -4.133923929 |
| H | -3.631344588 | -3.807499395 | -4.103681397 |
| H | 3.553875731 | 4.074672115 | -3.775152793 |
| H | -0.874317681 | -1.343410127 | -4.497760101 |
| H | 1.234101792 | 1.356463151 | -4.768499036 |
| C | 1.773710862 | 1.082438452 | -3.84930992 |
| C | -1.494525035 | -1.108875362 | -3.620170585 |
| H | 0.431032055 | 3.371053061 | -3.70275502 |
| H | -0.445263601 | -3.517327474 | -3.744066466 |

| | | | |
|---|---|---|---|
| C | 2.277913428 | 2.368442722 | -3.163225824 |
| C | -2.204022287 | -2.395465177 | -3.156748998 |
| H | -4.389597153 | -0.458092637 | -2.91353395 |
| H | 4.56711697 | 0.64661428 | -3.116795758 |
| H | 1.090669216 | 0.524020579 | -3.203030281 |
| H | -0.840345502 | -0.70705823 | -2.840799463 |
| H | 5.473309168 | 2.067095754 | -2.591644411 |
| H | -5.395847798 | -1.892340738 | -2.696365319 |
| C | 1.045891473 | 3.221633516 | -2.803259088 |
| C | -1.107760121 | -3.442336315 | -2.870045617 |
| H | 3.291499356 | 5.0288456 | -1.876798308 |
| H | -3.523329431 | -5.069058407 | -2.399697642 |
| H | 0.414311885 | 2.722883704 | -2.057984913 |
| H | -0.482161545 | -3.150506023 | -2.0175017 |
| C | 4.836856476 | 1.245799461 | -2.234625939 |
| C | -4.738136442 | -1.188953257 | -2.169668293 |
| H | 7.495683364 | 0.848911689 | -2.178263862 |
| H | -7.42280959 | -0.885770993 | -1.977628765 |
| H | 1.31668054 | 4.214557878 | -2.424800781 |
| H | -1.513636964 | -4.441824634 | -2.679450466 |
| H | 4.943630755 | 4.374380606 | -1.884378576 |
| H | -5.100027528 | -4.247685754 | -2.391892778 |
| H | -4.377586883 | 2.796631692 | -1.12449701 |
| H | 4.158430484 | -3.374212292 | -1.134151108 |
| C | 4.076836622 | 4.595576307 | -1.247854897 |
| C | -4.309145637 | -4.664110833 | -1.754723006 |
| H | -2.48927203 | 5.201334597 | -0.650265076 |
| H | 1.880218387 | -5.365561097 | -0.282791012 |
| C | 6.996517697 | 0.283666625 | -1.393865362 |
| C | -6.905636802 | -0.412975857 | -1.145614682 |
| H | 4.387230408 | 5.374061514 | -0.53344353 |
| H | -4.746485898 | -5.511659921 | -1.205263695 |
| C | 5.609033689 | 0.375725198 | -1.273939812 |
| C | -5.511517763 | -0.470449424 | -1.091186153 |
| H | -4.764025876 | 4.50826184 | -0.908810717 |
| H | 4.287945131 | -5.094068193 | -0.729341748 |
| H | -1.857306141 | 3.558286184 | -0.844916277 |
| H | 1.649781998 | -3.679954435 | -0.792163022 |
| C | -4.604249504 | 3.558896549 | -0.375955924 |
| C | 4.299779959 | -4.077457068 | -0.307880283 |
| C | -2.220131064 | 4.281058588 | -0.109539892 |
| C | 1.83949963 | -4.324327173 | 0.072628857 |
| H | -8.704713636 | 0.288090928 | -0.16622826 |
| H | 8.804436377 | -0.626822524 | -0.620494456 |
| C | 3.596094781 | 3.355139585 | -0.473833753 |
| C | -3.774151482 | -3.637152519 | -0.737375989 |
| H | -5.550500472 | 3.294765479 | 0.110508161 |

| | | | |
|---|---|---|---|
| H | 5.296434998 | -3.914404537 | 0.121161708 |
| C | -7.618204093 | 0.238729787 | -0.139747375 |
| C | 7.724493459 | -0.532853868 | -0.529143941 |
| H | -1.392631924 | 4.527068629 | 0.563362908 |
| H | 0.987776636 | -4.240935249 | 0.757429232 |
| H | 1.509687621 | 4.054108116 | -0.253721861 |
| H | -1.784691979 | -4.582847393 | -0.558981361 |
| H | 5.665113392 | 2.744069285 | 0.001538512 |
| H | -5.836763993 | -2.9937592 | -0.298615126 |
| C | -3.461589251 | 3.758093299 | 0.646132417 |
| C | 3.178775235 | -3.964907348 | 0.750009263 |
| C | 2.349151743 | 3.716465262 | 0.362733291 |
| C | -2.626462092 | -4.282321812 | 0.072039644 |
| C | 4.71402525 | 2.944307003 | 0.509181971 |
| C | -4.9343736 | -3.317738529 | 0.233017988 |
| H | 4.886254537 | 3.762436864 | 1.224921228 |
| H | -5.191783733 | -4.234089294 | 0.785433616 |
| H | -4.245181182 | 5.728463038 | 1.074941002 |
| H | 3.611646876 | -5.969193782 | 1.447182737 |
| C | 7.022744732 | -1.216811629 | 0.463388414 |
| C | -6.899093924 | 0.825704516 | 0.900787425 |
| H | 2.001172729 | 2.858080908 | 0.953377332 |
| H | -2.246529986 | -3.613489324 | 0.848994199 |
| C | 5.638611223 | -1.078658853 | 0.564759887 |
| C | -5.504787318 | 0.755206436 | 0.913438073 |
| C | -3.936056283 | 4.836312067 | 1.640889947 |
| C | 3.47326433 | -4.966663545 | 1.880571026 |
| H | -4.805210367 | 4.510869186 | 2.227206604 |
| H | 4.391721726 | -4.720938976 | 2.429793965 |
| H | 2.597077108 | 4.528948388 | 1.063120767 |
| H | -3.005310072 | -5.18837998 | 0.569503763 |
| H | -7.410543638 | 1.346331271 | 1.707479786 |
| H | 7.543811258 | -1.848728921 | 1.179586952 |
| H | 4.44657993 | 2.046678252 | 1.081083599 |
| H | -4.675585652 | -2.551110291 | 0.966823434 |
| H | -1.234181193 | 4.342046537 | 2.693350204 |
| H | 0.885392762 | -3.646144635 | 2.940652963 |
| C | -4.720837642 | 1.406295543 | 2.02565275 |
| C | 4.900838506 | -1.719310461 | 1.711552713 |
| H | -3.150188171 | 5.152553797 | 2.333963749 |
| H | 2.650251772 | -5.036315776 | 2.600628836 |
| H | -5.335882148 | 2.167794545 | 2.522523837 |
| H | 5.466655826 | -2.574172818 | 2.104965565 |
| H | -0.304252444 | 2.955660155 | 2.084890327 |
| H | 0.295008316 | -2.176070451 | 2.133563507 |
| C | -0.939299562 | 3.309314639 | 2.907521317 |
| C | 0.869107931 | -2.550734305 | 2.989184798 |

| | | | |
|---|---|---|---|
| H | -4.471596289 | 0.650473349 | 2.784735288 |
| H | 4.845689749 | -0.983723131 | 2.528544678 |
| C | -2.143453566 | 2.372368665 | 3.133586199 |
| C | 2.287739887 | -1.950775465 | 3.032020771 |
| H | -0.931289228 | 0.557506229 | 2.887722532 |
| H | 1.548691125 | 0.042806883 | 2.476628024 |
| H | -0.321014915 | 3.331698246 | 3.817455752 |
| H | 0.319094356 | -2.274229958 | 3.900910557 |
| C | -1.582966898 | 1.026115194 | 3.631821238 |
| C | 2.157605175 | -0.427475521 | 3.260332513 |
| H | -3.481623107 | 3.910447252 | 4.01181062 |
| H | 3.165785045 | -3.637971598 | 4.156574336 |
| H | -3.871178433 | 2.247838635 | 4.490423594 |
| H | 4.085889567 | -2.129302851 | 4.298326835 |
| C | -3.050493029 | 2.934780029 | 4.248642175 |
| C | 3.075342557 | -2.549532047 | 4.214753608 |
| H | -0.99523727 | 1.204296932 | 4.545336464 |
| H | 1.662051553 | -0.237663337 | 4.224580106 |
| H | -2.37128864 | 0.310733283 | 3.887795564 |
| H | 3.132856928 | 0.078156629 | 3.292610272 |
| H | -2.4526975 | 3.054732048 | 5.165216449 |
| H | 2.550471044 | -2.315487098 | 5.153905244 |

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**Supplementary Table 57 | Cartesian coordinate of the transition state for coordination of dinitrogen to XVIII. Units are presented in Å.**

SCF energy (in toluene) = -3962.53971198 hartree

ZPE = 1.281230 hartree

imaginary frequency: 64*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.592612699 | 0.105627233 | 0.035617467 |
| Mo | 2.649526078 | -0.176206421 | -0.1251175 |
| P | 3.223020507 | 1.969125262 | -1.297632057 |
| P | -3.191539086 | -2.033983317 | -1.198971721 |
| N | -4.83303084 | 0.179464493 | 0.027468642 |
| N | 4.872901856 | -0.217137021 | -0.050575836 |
| P | 3.07038783 | -2.296429285 | 1.137488114 |
| P | -3.056870872 | 2.276368472 | 1.267329669 |
| N | -0.533389453 | 0.014049 | 0.008763732 |
| N | 0.621712063 | -0.052356284 | -0.042758633 |
| N | -2.531876371 | 1.632843098 | -2.74224589 |
| N | -2.549808938 | 1.074089836 | -1.751807107 |
| N | -2.604819357 | -0.861019432 | 1.819023546 |
| N | -2.614475518 | -1.417714416 | 2.812031109 |
| N | 2.714453328 | -1.64376359 | -2.838191493 |
| N | 2.679030712 | -1.087652789 | -1.832583523 |
| N | 2.553729741 | 1.610279071 | 2.922644821 |
| N | 2.469502998 | 2.192376208 | 3.862287186 |
| H | 2.708225661 | 3.503938698 | -4.844983344 |
| H | -2.569020542 | -3.517955801 | -4.75367097 |
| H | -3.942746955 | -2.54012044 | -4.232693002 |
| H | 4.064804899 | 2.517329689 | -4.294923133 |
| C | 3.294054779 | 3.221011445 | -3.95703397 |
| C | -3.184237471 | -3.25086756 | -3.881053292 |
| H | -2.297775942 | -0.656554706 | -3.786642467 |
| H | 2.418148869 | 0.600409818 | -3.893730896 |
| H | -3.694543577 | -4.16026697 | -3.552978777 |
| H | 3.79219022 | 4.125383159 | -3.595287786 |
| H | -0.993601339 | -1.736113749 | -4.299716247 |
| H | 1.140791699 | 1.682531023 | -4.472864381 |
| C | 1.688634035 | 1.3525261 | -3.577064796 |
| C | -1.580598915 | -1.403569427 | -3.430746492 |

| | | | |
|---|---|---|---|
| H | 0.600934927 | 3.742849556 | -3.464681903 |
| H | -0.515761499 | -3.802875499 | -3.29527235 |
| C | 2.346078957 | 2.582717706 | -2.919696693 |
| C | -2.269307876 | -2.631896964 | -2.802880866 |
| H | -4.47304503 | -0.703580984 | -2.738386445 |
| H | 4.580985959 | 0.699470013 | -2.812189531 |
| H | 0.977717528 | 0.864673152 | -2.902543216 |
| H | -0.896139276 | -0.915870247 | -2.72990642 |
| H | 5.528895993 | 2.124392239 | -2.364691621 |
| H | -5.464105181 | -2.110291705 | -2.340514317 |
| C | 1.216515831 | 3.572206437 | -2.569467579 |
| C | -1.158486635 | -3.630299448 | -2.419967251 |
| H | 3.597528207 | 5.172783919 | -1.755330369 |
| H | -3.565757957 | -5.217077404 | -1.725519729 |
| H | 0.554027052 | 3.17371454 | -1.790655004 |
| H | -0.518189984 | -3.236679501 | -1.620828887 |
| C | 4.872613422 | 1.339380433 | -1.966397822 |
| C | -4.802324677 | -1.347704168 | -1.90979083 |
| H | 7.550071805 | 1.075835449 | -1.685431781 |
| H | -7.484832711 | -1.048117752 | -1.688772283 |
| H | 1.59239331 | 4.548328613 | -2.243109208 |
| H | -1.55085388 | -4.60391776 | -2.106783823 |
| H | 5.193298759 | 4.393411135 | -1.688059149 |
| H | -5.152466488 | -4.415776595 | -1.756410725 |
| H | -4.466901336 | 2.662998652 | -1.300367703 |
| H | 4.535713195 | -2.778734471 | -1.377500313 |
| C | 4.328900155 | 4.705446282 | -1.087592408 |
| C | -4.334316516 | -4.746834709 | -1.10344158 |
| H | -2.61595707 | 5.22350496 | -1.150133764 |
| H | 2.564475797 | -5.249535911 | -1.248447653 |
| C | 7.010714211 | 0.485420869 | -0.947690882 |
| C | -6.953910554 | -0.47965768 | -0.928336041 |
| H | 4.680816666 | 5.486733748 | -0.395712899 |
| H | -4.74312632 | -5.5314509 | -0.448298277 |
| C | 5.616078245 | 0.506786049 | -0.952740162 |
| C | -5.558385456 | -0.518066599 | -0.90249674 |
| H | -4.851375384 | 4.389528726 | -1.354345499 |
| H | 4.868634359 | -4.516972133 | -1.379887666 |
| H | -1.984756793 | 3.572699216 | -1.239612973 |
| H | 2.05049669 | -3.562417285 | -1.405803509 |
| C | -4.686606909 | 3.535061883 | -0.680767008 |
| C | 4.706128437 | -3.642997494 | -0.73100971 |
| C | -2.322872382 | 4.349412067 | -0.548453667 |
| C | 2.302640271 | -4.342144521 | -0.68211966 |
| H | -8.737312988 | 0.312138627 | 0.010074448 |
| H | 8.78606918 | -0.314785714 | 0.003535272 |
| C | 3.734747653 | 3.539912578 | -0.274456441 |

| | | | |
|---|---|---|---|
| C | -3.780317131 | -3.607279219 | -0.224887683 |
| H | -5.628492279 | 3.352057859 | -0.150791697 |
| H | 5.632484373 | -3.479367242 | -0.167384933 |
| C | -7.650012204 | 0.275135874 | 0.01514261 |
| C | 7.698697803 | -0.286846406 | -0.010362335 |
| H | -1.47278621 | 4.649533386 | 0.071828831 |
| H | 1.409717225 | -4.571930406 | -0.091011358 |
| H | 1.759113653 | 4.515683068 | -0.13716053 |
| H | -1.76838336 | -4.491730093 | 0.012410346 |
| H | 5.761001036 | 2.854641758 | 0.261681466 |
| H | -5.833880033 | -2.922701227 | 0.201651536 |
| C | -3.535332847 | 3.886346977 | 0.288991305 |
| C | 3.505281869 | -3.935815016 | 0.196729024 |
| C | 2.502835566 | 4.039986559 | 0.509171863 |
| C | -2.609850007 | -4.151394569 | 0.623233226 |
| C | 4.807363405 | 3.095753066 | 0.744621959 |
| C | -4.913676789 | -3.184482416 | 0.736959461 |
| H | 4.994869312 | 3.917080951 | 1.452984418 |
| H | -5.149190225 | -4.033479421 | 1.396360594 |
| H | -4.378790933 | 5.867195418 | 0.497746042 |
| H | 4.242529624 | -5.951842185 | 0.460411698 |
| C | 6.948252503 | -1.025427639 | 0.904529665 |
| C | -6.912919418 | 0.980620261 | 0.965634559 |
| H | 2.004866533 | 3.219771464 | 1.037312779 |
| H | -2.238515713 | -3.406396987 | 1.331794879 |
| C | 5.554404771 | -0.977915372 | 0.86800881 |
| C | -5.518037613 | 0.923424662 | 0.951693171 |
| C | -4.025456504 | 5.061069318 | 1.158822975 |
| C | 3.896128314 | -5.123207279 | 1.096957632 |
| H | -4.868772686 | 4.78217801 | 1.804108964 |
| H | 4.717265127 | -4.878253866 | 1.783389641 |
| H | 2.815151197 | 4.785620609 | 1.256542996 |
| H | -2.963753451 | -5.015418399 | 1.206515469 |
| H | -7.410584552 | 1.583630007 | 1.722039811 |
| H | 7.43594899 | -1.645036297 | 1.654277686 |
| H | 4.495733175 | 2.217708482 | 1.320004373 |
| H | -4.633805207 | -2.340554988 | 1.371865196 |
| H | -1.293179964 | 4.75987209 | 2.21298891 |
| H | 1.071063045 | -4.57874058 | 2.051083598 |
| C | -4.715484743 | 1.697737339 | 1.967062243 |
| C | 4.738363128 | -1.764708768 | 1.860956572 |
| H | -3.236375653 | 5.485708479 | 1.787798375 |
| H | 3.053559306 | -5.500868479 | 1.686071041 |
| H | -5.326673608 | 2.503274437 | 2.394205919 |
| H | 5.333898426 | -2.590249244 | 2.272824799 |
| H | -0.329814313 | 3.345041838 | 1.734261434 |
| H | 0.277568615 | -3.065965039 | 1.554763911 |

| | | | |
|---|---|---|---|
| C | -0.959158634 | 3.765841514 | 2.528517652 |
| C | 0.833603065 | -3.555547714 | 2.363735085 |
| H | -4.437198135 | 1.029227599 | 2.795136189 |
| H | 4.470842695 | -1.113117915 | 2.70759967 |
| C | -2.126329613 | 2.824585259 | 2.887617147 |
| C | 2.0903206 | -2.750502964 | 2.748240764 |
| H | -0.864148611 | 1.028192359 | 2.811633015 |
| H | 1.049513039 | -0.821465694 | 2.627720833 |
| H | -0.324496755 | 3.903788575 | 3.416650503 |
| H | 0.161706998 | -3.624385245 | 3.231992087 |
| C | -1.51340212 | 1.557793962 | 3.516713203 |
| C | 1.620662806 | -1.413321514 | 3.351846591 |
| H | -3.479675287 | 4.422049333 | 3.618791388 |
| H | 3.224422961 | -4.489956965 | 3.519044015 |
| H | -3.819115311 | 2.818596385 | 4.297278238 |
| H | 3.768112775 | -2.930656226 | 4.164242849 |
| C | -3.020650998 | 3.488855422 | 3.955614848 |
| C | 2.888776501 | -3.499119832 | 3.834837208 |
| H | -0.911553727 | 1.851428158 | 4.390487821 |
| H | 0.972665759 | -1.610354599 | 4.219026529 |
| H | -2.273494762 | 0.852483158 | 3.867399894 |
| H | 2.464489074 | -0.809690794 | 3.707654928 |
| H | -2.40492936 | 3.726058308 | 4.836884499 |
| H | 2.247174374 | -3.63760415 | 4.718827268 |

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**Supplementary Table 58 | Cartesian coordinate of the reactant complex for coordination of dinirogen to XVI. Units are presented in Å.**

SCF energy (in toluene) = -1983.03005450 hartree

ZPE = 0.670536 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 0.421011816 | -0.172212312 | 0.086856761 |
| P | 0.279975163 | 2.008794371 | 1.155932205 |
| N | -1.547014002 | -0.319852552 | 1.082737875 |
| P | -0.427752961 | -2.14991007 | -1.011812183 |
| N | 2.299759907 | -0.185474602 | -0.583161413 |
| N | 3.407398453 | -0.240153754 | -0.886725898 |
| H | 2.188014266 | 4.20354791 | 3.793076154 |
| H | 0.710764301 | 3.268296464 | 4.048411865 |
| C | 1.289190755 | 3.812380518 | 3.290444432 |
| H | 2.056543259 | 1.173072471 | 3.447709577 |
| H | 0.697146229 | 4.673306972 | 2.969354581 |
| H | 3.462648559 | 2.215285658 | 3.22389607 |
| C | 2.598943764 | 1.774806322 | 2.702879409 |
| H | 3.50866541 | 4.024439475 | 1.619090665 |
| C | 1.715992917 | 2.900465075 | 2.122094253 |
| H | -0.205273797 | 1.202188661 | 3.37354324 |
| H | 2.978588346 | 1.118143495 | 1.911301594 |
| H | -1.439443325 | 2.395952127 | 3.008169797 |
| C | 2.583259484 | 3.692524593 | 1.12389559 |
| H | 0.008485363 | 5.271278406 | 1.044735135 |
| H | 2.869545897 | 3.074002601 | 0.263626409 |
| C | -0.879618308 | 1.552162544 | 2.576713424 |
| H | -3.15687215 | 0.861474371 | 3.833763391 |
| H | 2.075317938 | 4.589231467 | 0.751407366 |
| H | -1.385374623 | 4.585655935 | 1.910139583 |
| H | -0.153684215 | -3.580531614 | 1.5266373 |
| C | -0.926991677 | 4.714646149 | 0.920584262 |
| H | 1.65808964 | -5.280906118 | -0.311268405 |
| C | -2.984323137 | 0.230946914 | 2.963425292 |
| H | -1.604324542 | 5.352019395 | 0.330703303 |
| C | -1.838425241 | 0.444638061 | 2.193692525 |
| H | -0.32613159 | -5.296977009 | 1.118426312 |
| H | 1.963858167 | -3.553804653 | -0.012973232 |
| C | -0.598434442 | -4.277375325 | 0.805393104 |

| | | | |
|---|---|---|---|
| C | 1.429405074 | -4.261897091 | -0.660135772 |
| H | -4.775972526 | -0.961830878 | 3.223012392 |
| C | -0.725432716 | 3.37333134 | 0.193162084 |
| H | -1.687869195 | -4.186549963 | 0.891396407 |
| C | -3.886842256 | -0.776905781 | 2.624288664 |
| H | 1.848760201 | -4.153907167 | -1.666237626 |
| H | 0.958423376 | 4.079212326 | -1.052782039 |
| H | -2.718795701 | 2.648635001 | 0.812697448 |
| C | -0.09522697 | -4.026549869 | -0.63283604 |
| C | -0.028711243 | 3.617310772 | -1.161674394 |
| C | -2.1230755 | 2.783203369 | -0.098611445 |
| H | -2.675674365 | 3.47217264 | -0.755565014 |
| H | -0.628533717 | -6.059202849 | -1.192451612 |
| C | -3.621237575 | -1.524849052 | 1.473129152 |
| H | 0.105345989 | 2.679406853 | -1.71562562 |
| C | -2.480225113 | -1.270088774 | 0.716852704 |
| C | -0.783535379 | -5.035329643 | -1.568811304 |
| H | -1.867586748 | -4.872655942 | -1.632187967 |
| H | -0.643227426 | 4.289430452 | -1.780514463 |
| H | -4.312965393 | -2.296365233 | 1.140695929 |
| H | -2.059408086 | 1.810897978 | -0.602139012 |
| H | 1.028160057 | -3.372099724 | -3.562048842 |
| C | -2.265271145 | -1.971454636 | -0.600957064 |
| H | -0.373105177 | -5.000214241 | -2.584414547 |
| H | -2.836767097 | -2.908477614 | -0.640010532 |
| H | 1.750102703 | -1.868203634 | -2.940446591 |
| C | 0.914681091 | -2.281563652 | -3.519081554 |
| H | -2.678636487 | -1.327594618 | -1.391424133 |
| C | -0.446528355 | -1.865742467 | -2.928218632 |
| H | 0.232471276 | 0.186119082 | -2.511020971 |
| H | 1.002200958 | -1.907655782 | -4.550917063 |
| C | -0.578451666 | -0.329536278 | -3.055995161 |
| H | -1.515148553 | -3.616850333 | -3.742063192 |
| H | -2.577537323 | -2.253599867 | -3.349199937 |
| C | -1.584565815 | -2.52471038 | -3.730303454 |
| H | -0.488474304 | -0.027749012 | -4.111154838 |
| H | -1.546596748 | 0.04089027 | -2.694760483 |
| H | -1.538718021 | -2.184144778 | -4.77683016 |
| H | 1.898543176 | -0.681387419 | 2.459343395 |
| N | 1.208358182 | -1.223979337 | 1.936441696 |
| H | 1.660997406 | -2.101945743 | 1.677907112 |
| H | 0.450883609 | -1.458298711 | 2.583745862 |
| N | 2.524016653 | 2.073817502 | -3.455317036 |
| N | 3.597920113 | 2.028093967 | -3.185851039 |

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**Supplementary Table 59 | Cartesian coordinate of the transition state for coordination of dinirogen to XVI. Units are presented in Å.**

SCF energy (in toluene) = -1983.02333356 hartree

ZPE = 0.672276 hartree

imaginary frequency: 94*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.159339036 | -1.67018422 | -0.546120201 |
| P | -0.293237701 | 0.491081506 | 0.644161216 |
| N | -2.164276933 | -1.811162776 | 0.414485239 |
| P | -1.046224076 | -3.661243359 | -1.673843903 |
| N | 1.773117526 | -1.834372114 | -0.985546098 |
| N | 2.905677563 | -1.991853244 | -1.097506526 |
| H | 1.660832414 | 2.426408584 | 3.445900695 |
| H | 0.20563844 | 1.443773192 | 3.640906858 |
| C | 0.752460529 | 2.077025391 | 2.930388196 |
| H | 1.591413673 | -0.518971851 | 2.815965419 |
| H | 0.139401887 | 2.958109224 | 2.723992856 |
| H | 2.967040154 | 0.559806424 | 2.608320711 |
| C | 2.085618894 | 0.148315483 | 2.093427407 |
| H | 2.909210982 | 2.524490971 | 1.241270602 |
| C | 1.159662854 | 1.305493499 | 1.658382477 |
| H | -0.742055826 | -0.51379947 | 2.785078631 |
| H | 2.437836025 | -0.438091835 | 1.237002061 |
| H | -1.958455929 | 0.729798238 | 2.565945339 |
| C | 1.980342613 | 2.225017286 | 0.732468981 |
| H | -0.683721822 | 3.726842289 | 0.960589522 |
| H | 2.262244729 | 1.71569676 | -0.198063241 |
| C | -1.42787267 | -0.078811923 | 2.041787599 |
| H | -3.703507569 | -0.791127046 | 3.270134627 |
| H | 1.441993272 | 3.143818066 | 0.474129455 |
| H | -2.011628846 | 2.853332312 | 1.757789259 |
| H | -1.024244604 | -4.75408791 | 1.008699214 |
| C | -1.594584082 | 3.14398791 | 0.784902615 |
| H | 1.054657543 | -6.621619313 | -0.472924183 |
| C | -3.559699677 | -1.364937582 | 2.356444846 |
| H | -2.321716352 | 3.82147555 | 0.310650975 |
| C | -2.420433587 | -1.124582463 | 1.582906065 |
| H | -0.957444548 | -6.520251676 | 0.842636126 |

| | | | |
|---|---|---|---|
| H | 1.308151083 | -4.856888703 | -0.444683013 |
| C | -1.308795145 | -5.592618846 | 0.365546896 |
| C | 0.814608202 | -5.675431274 | -0.98229345 |
| H | -5.379481414 | -2.524178785 | 2.558663385 |
| C | -1.3518128 | 1.93697964 | -0.139627592 |
| H | -2.404946895 | -5.627532736 | 0.350237856 |
| C | -4.490893622 | -2.324178384 | 1.964014204 |
| H | 1.273169306 | -5.71232633 | -1.977143367 |
| H | 0.292841642 | 2.868215319 | -1.292924768 |
| H | -3.314514417 | 1.046478354 | 0.361731462 |
| C | -0.715323085 | -5.48575671 | -1.056799959 |
| C | -0.69814506 | 2.428307101 | -1.44656658 |
| C | -2.727304194 | 1.341326361 | -0.515847562 |
| H | -3.308077291 | 2.101007435 | -1.061047891 |
| H | -1.149810971 | -7.590166204 | -1.35280609 |
| C | -4.24701379 | -3.012558536 | 0.772107466 |
| H | -0.596661144 | 1.614621827 | -2.171378337 |
| C | -3.106612622 | -2.738695397 | 0.021223622 |
| C | -1.316174457 | -6.637931892 | -1.88175879 |
| H | -2.399242619 | -6.529483201 | -2.021422785 |
| H | -1.335599602 | 3.2022448 | -1.901252924 |
| H | -4.949606099 | -3.759661911 | 0.408773963 |
| H | -2.625898878 | 0.462535875 | -1.16422654 |
| H | 0.446280917 | -5.212504498 | -3.96463044 |
| C | -2.884099518 | -3.429457509 | -1.296982738 |
| H | -0.848869211 | -6.734708759 | -2.867690541 |
| H | -3.475218576 | -4.353487536 | -1.351483442 |
| H | 1.07557244 | -3.568414024 | -3.715729767 |
| C | 0.256370296 | -4.149714002 | -4.157965251 |
| H | -3.258422175 | -2.772054348 | -2.095921852 |
| C | -1.113475427 | -3.694437591 | -3.618572732 |
| H | -0.563066019 | -1.570257026 | -3.667230555 |
| H | 0.293407932 | -4.006960128 | -5.248687118 |
| C | -1.337636022 | -2.233337036 | -4.061123381 |
| H | -2.114039947 | -5.615030523 | -4.096294447 |
| H | -3.230294207 | -4.255496809 | -3.880350055 |
| C | -2.237692801 | -4.540871233 | -4.251673998 |
| H | -1.304227922 | -2.175214767 | -5.160083721 |
| H | -2.315457668 | -1.842671445 | -3.748279917 |
| H | -2.242429504 | -4.370195 | -5.33960547 |
| H | 1.219623315 | -2.241479633 | 1.826475999 |
| N | 0.475703583 | -2.754403933 | 1.350170192 |
| H | 0.846652482 | -3.686977188 | 1.160716961 |
| H | -0.28876905 | -2.872985724 | 2.020622347 |
| N | 0.99802532 | -0.022426159 | -2.947895534 |
| N | 2.015649555 | 0.210281206 | -3.336060334 |

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**Supplementary Table 60 | Cartesian coordinate of the transition state for elimination of the ammonia ligand from XX. Units are presented in Å.**

SCF energy (in toluene) = -1983.06187392 hartree

ZPE = 0.673637 hartree

imaginary frequency: 50*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.291584638 | -1.415184887 | -0.836062705 |
| P | -0.43524808 | 0.590889669 | 0.65135552 |
| N | -2.298051447 | -1.701446266 | 0.113342805 |
| P | -1.00468225 | -3.599856001 | -1.844233151 |
| N | 1.577434974 | -1.267625864 | -1.531131887 |
| N | 2.678156405 | -1.242440973 | -1.84475295 |
| H | 1.552945281 | 1.89214834 | 3.755499048 |
| H | 0.115166176 | 0.866675483 | 3.774010536 |
| C | 0.640845049 | 1.636079132 | 3.1945581 |
| H | 1.34186102 | -0.975743834 | 2.370218158 |
| H | 0.011579366 | 2.529494715 | 3.16968293 |
| H | 2.733110413 | 0.090151748 | 2.660027724 |
| C | 1.907997345 | -0.127585911 | 1.963467103 |
| H | 2.842281805 | 2.327379912 | 1.629786704 |
| C | 1.038694373 | 1.132858346 | 1.791557983 |
| H | -0.930798535 | -0.830810294 | 2.542757549 |
| H | 2.338351742 | -0.437748117 | 1.006021554 |
| H | -2.064384308 | 0.518622179 | 2.611117052 |
| C | 1.90071175 | 2.191898467 | 1.076239601 |
| H | -0.608751982 | 3.711895984 | 1.492745974 |
| H | 2.158600671 | 1.879967745 | 0.055915271 |
| C | -1.591571651 | -0.199685129 | 1.928714943 |
| H | -4.111364204 | -0.712121307 | 2.800116464 |
| H | 1.411043239 | 3.170430813 | 1.025062153 |
| H | -2.035022133 | 2.853923257 | 2.118712346 |
| H | -0.703584822 | -4.074606791 | 1.072970443 |
| C | -1.560624853 | 3.249492617 | 1.210810892 |
| H | 0.739356453 | -6.446125737 | 0.034172304 |
| C | -3.890358606 | -1.233176122 | 1.871287125 |
| H | -2.209459621 | 4.053388543 | 0.831200043 |
| C | -2.635167301 | -1.07144058 | 1.280549446 |
| H | -1.161744121 | -5.774336614 | 1.275701426 |

| | | | |
|---|---|---|---|
| H | 1.247716509 | -4.795782435 | -0.376323837 |
| C | -1.302998424 | -4.885770744 | 0.641439365 |
| C | 0.635545247 | -5.639580876 | -0.708370504 |
| H | -5.823862945 | -2.192879188 | 1.716226608 |
| C | -1.404563201 | 2.178690225 | 0.112999259 |
| H | -2.361291642 | -4.607881121 | 0.697464278 |
| C | -4.840568834 | -2.05731453 | 1.270544305 |
| H | 1.034749005 | -6.014865034 | -1.654348748 |
| H | 0.311236299 | 3.159352407 | -0.877081577 |
| H | -3.42213405 | 1.384587335 | 0.527527332 |
| C | -0.8486145 | -5.225150286 | -0.796597869 |
| C | -0.696294596 | 2.800770398 | -1.1112268 |
| C | -2.825382565 | 1.749017779 | -0.317473995 |
| H | -3.345405129 | 2.627506813 | -0.728255087 |
| H | -1.613362853 | -7.242450086 | -0.584241849 |
| C | -4.498172282 | -2.703119205 | 0.082908967 |
| H | -0.625166455 | 2.091424372 | -1.940579189 |
| C | -3.231491349 | -2.513840694 | -0.474034334 |
| C | -1.685617209 | -6.41303707 | -1.30482295 |
| H | -2.750522743 | -6.165839573 | -1.406256514 |
| H | -1.280518385 | 3.665866952 | -1.460237087 |
| H | -5.207618237 | -3.354543572 | -0.42230003 |
| H | -2.815028766 | 0.980715675 | -1.094643057 |
| H | 0.331833018 | -5.943414908 | -3.595430958 |
| C | -2.852730789 | -3.20486191 | -1.757655617 |
| H | -1.329051712 | -6.792669387 | -2.2685983 |
| H | -3.510196249 | -4.066726827 | -1.929699548 |
| H | 1.332695869 | -4.474930354 | -3.478251811 |
| C | 0.446806741 | -4.914480931 | -3.954069782 |
| H | -3.00661762 | -2.508991647 | -2.595246438 |
| C | -0.815578525 | -4.059479601 | -3.72455484 |
| H | 0.251020622 | -2.18271143 | -4.136672686 |
| H | 0.647047887 | -4.969154904 | -5.034472851 |
| C | -0.623569105 | -2.736948206 | -4.493604072 |
| H | -2.270498974 | -5.730821937 | -3.821825458 |
| H | -2.939699597 | -4.158391057 | -4.297941439 |
| C | -2.039995051 | -4.78501627 | -4.321901142 |
| H | -0.476830601 | -2.966677384 | -5.560030343 |
| H | -1.489834965 | -2.072391652 | -4.416526201 |
| H | -1.837536187 | -5.013073587 | -5.37954741 |
| H | 2.788929247 | -2.808640875 | 0.185504987 |
| N | 2.373498798 | -3.203208005 | 1.0320066 |
| H | 2.733558292 | -4.15582624 | 1.111867675 |
| H | 2.774579519 | -2.680506741 | 1.811447834 |
| N | -1.079645977 | -0.455390455 | -2.32900385 |
| N | -1.579405287 | 0.113954283 | -3.190925296 |

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**Supplementary Table 61 | Cartesian coordinate of the product complex for elimination of the ammonia ligand from XX. Units are presented in Å.**

SCF energy (in toluene) = -1983.06752402 hartree

ZPE = 0.671638 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.568818136 | -1.327413488 | -0.890349162 |
| P | -0.662912932 | 0.574765171 | 0.666283436 |
| N | -2.592810543 | -1.666964014 | 0.035610161 |
| P | -1.112554855 | -3.558400974 | -1.793993879 |
| N | 1.244467134 | -1.029102405 | -1.669123381 |
| N | 2.299588878 | -0.870383478 | -2.085393539 |
| H | 1.39943353 | 1.224752065 | 3.919691119 |
| H | -0.311426233 | 0.803190034 | 3.800147431 |
| C | 0.509258134 | 1.311538558 | 3.277717671 |
| H | 0.465899447 | -1.387910326 | 2.623078566 |
| H | 0.26005059 | 2.374285876 | 3.210423569 |
| H | 2.124671752 | -0.813281823 | 2.796846753 |
| C | 1.246580578 | -0.788376925 | 2.133757564 |
| H | 2.882180698 | 1.337914832 | 1.861287052 |
| C | 0.813113789 | 0.677656271 | 1.905447376 |
| H | -1.533899776 | -0.635157043 | 2.578528662 |
| H | 1.539280525 | -1.290389924 | 1.202072386 |
| H | -2.562688594 | 0.768293741 | 2.340128839 |
| C | 1.982504024 | 1.424799149 | 1.233244457 |
| H | -0.191807303 | 3.646072237 | 1.559524435 |
| H | 2.220637225 | 1.006169806 | 0.247372717 |
| C | -2.040580981 | -0.03719626 | 1.80727077 |
| H | -4.639226341 | -0.434974242 | 2.440218703 |
| H | 1.77326751 | 2.49432572 | 1.112431134 |
| H | -1.777130717 | 3.092253598 | 2.146672539 |
| H | -0.938733727 | -3.751939654 | 1.153489111 |
| C | -1.214553277 | 3.397252324 | 1.254207198 |
| H | 1.04301682 | -5.895993376 | 0.325393349 |
| C | -4.333908727 | -1.04797989 | 1.595234732 |
| H | -1.675526633 | 4.324536186 | 0.880646514 |
| C | -3.031170848 | -0.934174066 | 1.106085999 |
| H | -1.030137513 | -5.491444149 | 1.478386263 |
| H | 1.267179971 | -4.19582646 | -0.125173632 |
| C | -1.315914157 | -4.705915532 | 0.762904557 |

| | | | |
|---|---|---|---|
| C | 0.816478782 | -5.144228882 | -0.446484179 |
| H | -6.235607472 | -2.060079439 | 1.386215063 |
| C | -1.252220036 | 2.332754537 | 0.143774841 |
| H | -2.411232026 | -4.655014093 | 0.747946427 |
| C | -5.218475527 | -1.955078183 | 1.014229404 |
| H | 1.321848777 | -5.45972745 | -1.365239047 |
| H | 0.668566446 | 2.932240791 | -0.763066914 |
| H | -3.401194326 | 1.925896804 | 0.463958569 |
| C | -0.715400448 | -5.044169739 | -0.620420494 |
| C | -0.380686498 | 2.788682317 | -1.045823458 |
| C | -2.711209325 | 2.191806867 | -0.347050082 |
| H | -3.041756983 | 3.160637145 | -0.750539237 |
| H | -1.094620135 | -7.149956942 | -0.268435464 |
| C | -4.763169218 | -2.728711436 | -0.051426359 |
| H | -0.415551857 | 2.063601227 | -1.865379606 |
| C | -3.459168923 | -2.56558666 | -0.526965218 |
| C | -1.277866456 | -6.407859021 | -1.06080568 |
| H | -2.362123918 | -6.377435349 | -1.232315132 |
| H | -0.7564966 | 3.751111037 | -1.425008397 |
| H | -5.415679055 | -3.454156167 | -0.532046126 |
| H | -2.81195332 | 1.45158358 | -1.146423106 |
| H | 0.620831354 | -5.716446963 | -3.375085513 |
| C | -2.98989908 | -3.380675183 | -1.709296486 |
| H | -0.797110509 | -6.78441803 | -1.970365187 |
| H | -3.542400251 | -4.329556438 | -1.750612694 |
| H | 1.315609333 | -4.077028117 | -3.401985873 |
| C | 0.531814405 | -4.719958349 | -3.822620397 |
| H | -3.238076322 | -2.830987095 | -2.629464812 |
| C | -0.870502866 | -4.108518567 | -3.63306771 |
| H | -0.1509413 | -2.111429618 | -4.20325298 |
| H | 0.73368299 | -4.827624575 | -4.898699852 |
| C | -0.936933625 | -2.821036631 | -4.482587454 |
| H | -1.9665751 | -6.031688433 | -3.600147041 |
| H | -2.946448751 | -4.650768579 | -4.129555224 |
| C | -1.941012249 | -5.088892188 | -4.154535018 |
| H | -0.80260637 | -3.086650183 | -5.542338928 |
| H | -1.897529664 | -2.300876224 | -4.393945515 |
| H | -1.723515166 | -5.331019829 | -5.206045425 |
| H | 3.44126741 | -2.20339538 | -0.603128558 |
| N | 3.588476838 | -2.825552915 | 0.195165083 |
| H | 4.025351138 | -3.6690848 | -0.18046725 |
| H | 4.298388296 | -2.377723041 | 0.77751622 |
| N | -1.446542726 | -0.409362175 | -2.367332611 |
| N | -1.989989222 | 0.132280873 | -3.218305805 |

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**Supplementary Table 62 | Cartesian coordinate of the reactant complex for coordination of dinitrogen to XIX'. Units are presented in Å.**

SCF energy (in toluene) = -2036.01364113 hartree

ZPE = 0.640838 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.897435293 | -0.190280519 | -0.259172779 |
| P | 3.431585504 | -2.227810116 | 0.998045567 |
| N | 5.140787208 | -0.093022779 | -0.283616928 |
| P | 3.248497387 | 2.063312315 | -1.190648159 |
| N | -0.249202745 | -0.350957241 | -0.163627671 |
| N | 0.889900355 | -0.291853159 | -0.210922777 |
| N | -1.515602513 | 2.214990789 | 2.001332891 |
| N | -0.656535393 | 1.713906732 | 2.488729382 |
| N | 2.976080795 | -1.015407686 | -2.021787137 |
| N | 3.058913729 | -1.505991966 | -3.053850624 |
| H | 2.85513776 | -3.01693181 | 4.780095008 |
| H | 4.388334763 | -2.628215063 | 3.993505539 |
| C | 3.400971466 | -3.07685873 | 3.825828187 |
| H | 3.364163169 | -0.334252847 | 3.283848795 |
| H | 3.546036723 | -4.137006538 | 3.599605725 |
| H | 1.914437136 | -0.83784463 | 4.160141699 |
| C | 2.409730178 | -0.869124634 | 3.177867134 |
| H | 0.652707528 | -2.87516907 | 3.536439442 |
| C | 2.600037762 | -2.338941608 | 2.735397494 |
| H | 5.130754744 | -1.227094287 | 2.411042251 |
| H | 1.771893214 | -0.315232673 | 2.475044015 |
| H | 5.827434501 | -2.689167222 | 1.728558559 |
| C | 1.203861679 | -2.977410265 | 2.589429964 |
| H | 3.099598295 | -5.326362106 | 1.857598143 |
| H | 0.61308076 | -2.488780646 | 1.804536404 |
| C | 5.214426072 | -1.811875322 | 1.483170133 |
| H | 7.865188359 | -1.700421545 | 0.935199688 |
| H | 1.262797061 | -4.048262445 | 2.361169165 |
| H | 4.82755132 | -4.921589385 | 1.738806056 |
| H | 4.48630062 | 1.991313649 | 1.486464683 |
| C | 3.91658001 | -5.117016555 | 1.157565494 |
| H | 2.517945766 | 4.331483512 | 1.796318188 |
| C | 7.299333427 | -0.993030208 | 0.333156651 |
| H | 4.09087517 | -6.036852701 | 0.57864131 |

| | | | |
|---|---|---|---|
| C | 5.90980464 | -0.949929333 | 0.458614349 |
| H | 4.842008707 | 3.689450039 | 1.859644054 |
| H | 2.004536031 | 2.671394498 | 1.428344477 |
| C | 4.71293482 | 2.967699408 | 1.039198031 |
| C | 2.312216769 | 3.624608157 | 0.978093054 |
| H | 9.028790146 | -0.139567339 | -0.649821703 |
| C | 3.580006315 | -3.968093894 | 0.190368201 |
| H | 5.674811437 | 2.882283846 | 0.520077208 |
| C | 7.946237081 | -0.121662562 | -0.542086586 |
| H | 1.459675258 | 4.01328221 | 0.412446476 |
| H | 1.408957129 | -4.367541283 | 0.154439226 |
| H | 5.692606941 | -3.734094961 | -0.412421235 |
| C | 3.579269611 | 3.457194282 | 0.110623997 |
| C | 2.252885673 | -4.271269183 | -0.538242892 |
| C | 4.703393338 | -3.871866268 | -0.86687388 |
| H | 4.734588359 | -4.813161546 | -1.435776605 |
| H | 4.263399804 | 5.502029014 | 0.358321049 |
| C | 7.169652678 | 0.778595435 | -1.26904554 |
| H | 2.008689666 | -3.490002368 | -1.265814143 |
| C | 5.77915771 | 0.77345097 | -1.131487716 |
| C | 3.997951372 | 4.82234862 | -0.466203205 |
| H | 4.878024673 | 4.743807296 | -1.11810974 |
| H | 2.346548335 | -5.224196377 | -1.08077292 |
| H | 7.631232802 | 1.482661057 | -1.957808801 |
| H | 4.53242598 | -3.060343626 | -1.580934675 |
| H | 1.27083624 | 4.4941808 | -1.698490029 |
| C | 4.944456337 | 1.7319574 | -1.949121849 |
| H | 3.193967599 | 5.303290573 | -1.033752845 |
| H | 5.526668146 | 2.635706931 | -2.176816392 |
| H | 0.430363611 | 2.931223691 | -1.543413469 |
| C | 1.036031201 | 3.555192107 | -2.213030585 |
| H | 4.710516493 | 1.257132215 | -2.913272024 |
| C | 2.294929648 | 2.809917783 | -2.699691182 |
| H | 1.174356924 | 0.940366671 | -2.973726235 |
| H | 0.410761584 | 3.808869234 | -3.081921848 |
| C | 1.823823068 | 1.609225869 | -3.548208307 |
| H | 3.508944057 | 4.625226606 | -3.075289741 |
| H | 3.997301929 | 3.216127284 | -4.036451212 |
| C | 3.1378708 | 3.738225328 | -3.597809848 |
| H | 1.255751273 | 1.985692283 | -4.412481267 |
| H | 2.654255055 | 1.009342711 | -3.937585519 |
| H | 2.514523665 | 4.087602802 | -4.434920386 |

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**Supplementary Table 63 | Cartesian coordinate of the transition state for coordination of dinitrogen to XIX'. Units are presented in Å.**

SCF energy (in toluene) = -2036.00646998 hartree

ZPE = 0.643386 hartree

imaginary frequency: 67*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.7152904 | -0.080353185 | -0.077384972 |
| P | 3.266365356 | -2.211728179 | 1.100749262 |
| N | 4.955788968 | -0.031272329 | -0.085684379 |
| P | 3.159868234 | 2.148604965 | -1.163361172 |
| N | -0.439130874 | -0.134069408 | 0.009503869 |
| N | 0.700359877 | -0.116769364 | -0.027136369 |
| N | 0.275814525 | 1.878339381 | 2.903685239 |
| N | 1.284899412 | 1.621139104 | 2.522092138 |
| N | 2.732920037 | -0.924478411 | -1.825057814 |
| N | 2.783892233 | -1.42514229 | -2.855858999 |
| H | 2.692538878 | -3.61215703 | 4.705177984 |
| H | 4.123873551 | -2.762785362 | 4.118245717 |
| C | 3.28990522 | -3.403211742 | 3.804471638 |
| H | 2.670155355 | -0.668069524 | 3.550265263 |
| H | 3.704358814 | -4.354909055 | 3.461716446 |
| H | 1.395285002 | -1.60744145 | 4.341462623 |
| C | 1.869328325 | -1.398959068 | 3.370160488 |
| H | 0.557877372 | -3.698703758 | 3.37247459 |
| C | 2.390281208 | -2.713027238 | 2.757708275 |
| H | 4.716931189 | -1.04893924 | 2.644827085 |
| H | 1.122267717 | -0.935837494 | 2.719951072 |
| H | 5.59067694 | -2.482601841 | 2.106671903 |
| C | 1.16164674 | -3.595822206 | 2.458237483 |
| H | 3.359750855 | -5.401374325 | 1.625163541 |
| H | 0.520775444 | -3.149151238 | 1.687315754 |
| C | 4.954379023 | -1.658169623 | 1.758983433 |
| H | 7.639460683 | -1.450705028 | 1.420459709 |
| H | 1.436140174 | -4.606357735 | 2.136100194 |
| H | 5.018423594 | -4.761701142 | 1.59280402 |
| H | 4.224742988 | 2.326398307 | 1.575912554 |
| C | 4.148001381 | -5.012025035 | 0.972031227 |
| H | 2.816124419 | 4.980096119 | 1.415313429 |

| | | | |
|---|---|---|---|
| C | 7.093914517 | -0.816227961 | 0.725620185 |
| H | 4.45135583 | -5.834307211 | 0.306335864 |
| C | 5.69790486 | -0.808182256 | 0.762043197 |
| H | 4.903994917 | 3.961284524 | 1.693324573 |
| H | 1.895105562 | 3.487636599 | 1.16872733 |
| C | 4.664536864 | 3.146317672 | 0.993883305 |
| C | 2.468603799 | 4.264175786 | 0.655135088 |
| H | 8.856889924 | -0.010838036 | -0.237119695 |
| C | 3.679487316 | -3.822990866 | 0.111916546 |
| H | 5.608873709 | 2.789912415 | 0.568193304 |
| C | 7.769733649 | -0.015841661 | -0.1939916 |
| H | 1.787123086 | 4.801407801 | -0.00936721 |
| H | 1.589923295 | -4.520304352 | -0.055546974 |
| H | 5.760812471 | -3.266995608 | -0.373308589 |
| C | 3.690203413 | 3.676359339 | -0.082678535 |
| C | 2.42950777 | -4.233484531 | -0.69727344 |
| C | 4.815926472 | -3.493397858 | -0.882507737 |
| H | 4.991250499 | -4.375779082 | -1.51628383 |
| H | 4.756455544 | 5.563355121 | -0.145166217 |
| C | 7.015886757 | 0.77641733 | -1.059016948 |
| H | 2.095689451 | -3.430013001 | -1.360088574 |
| C | 5.6209401 | 0.753058459 | -0.989970292 |
| C | 4.394752522 | 4.805715547 | -0.857548517 |
| H | 5.266820723 | 4.452173299 | -1.422588568 |
| H | 2.677470552 | -5.103483192 | -1.323996725 |
| H | 7.499999037 | 1.413500564 | -1.795635469 |
| H | 4.567048218 | -2.659882951 | -1.544000935 |
| H | 1.488722381 | 4.762092889 | -2.023746125 |
| C | 4.798542501 | 1.596082941 | -1.929176209 |
| H | 3.719237708 | 5.315239152 | -1.553124586 |
| H | 5.408478795 | 2.415137385 | -2.330674389 |
| H | 0.473447923 | 3.38718193 | -1.52136649 |
| C | 1.100193638 | 3.784574151 | -2.329958846 |
| H | 4.489601223 | 0.97770878 | -2.784280965 |
| C | 2.217362616 | 2.801651629 | -2.733213674 |
| H | 0.85661501 | 1.072993738 | -2.704658797 |
| H | 0.446809954 | 3.95435244 | -3.198325268 |
| C | 1.54247102 | 1.580339779 | -3.39162641 |
| H | 3.656785378 | 4.348471655 | -3.408400925 |
| H | 3.86845912 | 2.770684643 | -4.192656206 |
| C | 3.126358091 | 3.469042369 | -3.787310693 |
| H | 0.965371596 | 1.925322299 | -4.263169639 |
| H | 2.263755445 | 0.838591062 | -3.748804538 |
| H | 2.504783708 | 3.800731311 | -4.632897774 |

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**Supplementary Table 64 | Cartesian coordinate of the transition state for protonation of the bridging dinitrogen ligand in 1 by LutH$^+$ [TS(BR)]. Units are presented in Å.**

SCF energy (in toluene) = -4289.74738262 hartree

ZPE = 1.440997 hartree

imaginary frequency: 1040*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.700799535 | 0.204071548 | -0.131785265 |
| Mo | -2.634300315 | -0.145041435 | -0.258835441 |
| P | -4.007879695 | 1.879560104 | 0.909538014 |
| P | 3.910625461 | -2.080975256 | 0.532455069 |
| N | 4.991898665 | 0.609248018 | -0.41999196 |
| N | -4.747129207 | -0.232206945 | -1.180515939 |
| P | -2.57699827 | -2.175214857 | -1.851704631 |
| P | 2.817364429 | 2.665490096 | -0.987967022 |
| N | 0.767612254 | -0.073181483 | 0.125552058 |
| N | -0.417979133 | -0.240025297 | 0.352393235 |
| N | 3.341408566 | 1.125646766 | 2.830853111 |
| N | 3.028312252 | 0.817206701 | 1.785645085 |
| N | 2.715520768 | -0.425754993 | -2.077879067 |
| N | 2.858482857 | -0.740519672 | -3.155019205 |
| N | -3.735020531 | -1.89102989 | 2.124558243 |
| N | -3.283392961 | -1.273202897 | 1.277811262 |
| N | -2.139091857 | 1.033395095 | -1.824265042 |
| N | -1.964661395 | 1.691402797 | -2.735714356 |
| H | -5.451004726 | 2.89564964 | 4.404313744 |
| H | 4.25432866 | -4.275337018 | 3.73088798 |
| H | 5.352050957 | -3.002781831 | 3.203342629 |
| H | -6.215714973 | 1.822891921 | 3.235545306 |
| C | -5.523474402 | 2.667038317 | 3.330460317 |
| C | 4.640936116 | -3.755143546 | 2.842217404 |
| H | 3.453400237 | -1.391603979 | 3.463673323 |
| H | -4.351174274 | 0.242170942 | 3.478989356 |
| H | 5.189919795 | -4.491116956 | 2.251864381 |
| H | -5.971417768 | 3.536593025 | 2.845106074 |
| H | 2.405832846 | -2.724015714 | 3.954661859 |
| H | -3.586835815 | 1.314885135 | 4.657637533 |
| C | -3.647287903 | 1.074640382 | 3.585767511 |
| C | 2.763363219 | -2.153858037 | 3.085118378 |

| | | | |
|---|---|---|---|
| H | -3.078801682 | 3.586252614 | 4.245143878 |
| H | 2.054307159 | -4.693887438 | 2.620039685 |
| C | -4.107407011 | 2.326048996 | 2.812584253 |
| C | 3.4455876 | -3.118843893 | 2.098338069 |
| H | 5.211948317 | -0.82418671 | 2.130958362 |
| H | -5.596029918 | 0.197782945 | 1.568190346 |
| H | -2.669405718 | 0.716904633 | 3.260415489 |
| H | 1.90834149 | -1.64365435 | 2.635402499 |
| H | -6.497570658 | 1.603395223 | 0.999208242 |
| H | 6.288797325 | -1.945974958 | 1.30479301 |
| C | -3.168900473 | 3.502633853 | 3.151934403 |
| C | 2.437138166 | -4.216395628 | 1.706546895 |
| H | -5.038662419 | 4.919327232 | 1.47442613 |
| H | 4.832431123 | -5.182352091 | 0.288859709 |
| H | -2.160362751 | 3.371125788 | 2.748621469 |
| H | 1.578401272 | -3.809261088 | 1.158334367 |
| C | -5.638615197 | 0.959981838 | 0.778009636 |
| C | 5.469828539 | -1.23491473 | 1.144678142 |
| H | -7.948130083 | 0.686420463 | -0.548655244 |
| H | 8.007477138 | -0.478267545 | 0.670079005 |
| H | -3.552653293 | 4.461190578 | 2.788123968 |
| H | 2.88844571 | -5.006574561 | 1.098329016 |
| H | -6.342960839 | 3.996331167 | 0.694535739 |
| H | 6.267829997 | -4.131453954 | 0.311478575 |
| H | 4.612587412 | 2.806895759 | 1.399937845 |
| H | -4.89883992 | -2.794965392 | -0.066218674 |
| C | -5.369895194 | 4.476204518 | 0.530606571 |
| C | 5.417465868 | -4.465571455 | -0.295665049 |
| H | 2.398038708 | 5.063210099 | 1.971727994 |
| H | -3.114139043 | -5.407033958 | 0.144608836 |
| C | -7.119072296 | 0.257303523 | -1.106074198 |
| C | 7.299955184 | 0.128425727 | 0.110340058 |
| H | -5.536567164 | 5.30597121 | -0.172111603 |
| H | 5.831991546 | -5.014189205 | -1.153890356 |
| C | -5.836751881 | 0.296671478 | -0.550418893 |
| C | 5.931661667 | -0.122657948 | 0.244086723 |
| H | 4.763587845 | 4.537105295 | 1.718196019 |
| H | -5.268637187 | -4.489002288 | -0.412875779 |
| H | 2.1013474 | 3.32176126 | 1.915115481 |
| H | -2.64368595 | -3.799817854 | 0.712600072 |
| C | 4.598478539 | 3.791293211 | 0.927274077 |
| C | -4.857916837 | -3.563267066 | -0.842290463 |
| C | 2.158910794 | 4.224156914 | 1.302064162 |
| C | -2.634793022 | -4.462803045 | -0.154541082 |
| H | 8.801215612 | 1.343924789 | -0.862087524 |
| H | -8.306822488 | -0.336358031 | -2.814710346 |
| C | -4.336422223 | 3.513601892 | -0.090004459 |

| | | | |
|---|---|---|---|
| C | 4.576422453 | -3.289783592 | -0.833158023 |
| H | 5.449346743 | 3.857841864 | 0.239757594 |
| H | -5.521348635 | -3.266246548 | -1.662059833 |
| C | 7.74003508 | 1.139363709 | -0.738979729 |
| C | -7.318676016 | -0.308658222 | -2.360921542 |
| H | 1.16848997 | 4.414472718 | 0.87598142 |
| H | -1.593885492 | -4.690788488 | -0.407242868 |
| H | -2.551281833 | 4.541695074 | 0.70931444 |
| H | 2.701528357 | -4.443402638 | -0.997041121 |
| H | -5.89291987 | 2.774624005 | -1.46247642 |
| H | 6.439376705 | -2.225684138 | -1.341845296 |
| C | 3.259428169 | 4.113458813 | 0.226043082 |
| C | -3.419744864 | -3.849820306 | -1.331734716 |
| C | -2.989213997 | 4.247177915 | -0.250937091 |
| C | 3.376307044 | -3.849693982 | -1.622102007 |
| C | -4.866068844 | 3.155058606 | -1.497535412 |
| C | 5.485771983 | -2.503610601 | -1.805136738 |
| H | -4.88015096 | 4.072092686 | -2.104879959 |
| H | 5.718895008 | -3.153891918 | -2.660236016 |
| H | 3.796069005 | 6.201417323 | 0.298316537 |
| H | -4.125568367 | -5.74284461 | -2.096059535 |
| C | -6.211789046 | -0.840777752 | -3.01396944 |
| C | 6.783663309 | 1.880780562 | -1.42648682 |
| H | -2.263386717 | 3.629980485 | -0.787592192 |
| H | 2.792751526 | -3.054964894 | -2.091441184 |
| C | -4.955190214 | -0.806894416 | -2.403043222 |
| C | 5.425613356 | 1.606186444 | -1.244098315 |
| C | 3.431929882 | 5.486723329 | -0.454150466 |
| C | -3.527082454 | -4.89501639 | -2.460755485 |
| H | 4.173029592 | 5.466210069 | -1.262493695 |
| H | -4.034302558 | -4.504698821 | -3.351948273 |
| H | -3.143753473 | 5.165610823 | -0.836796653 |
| H | 3.747178705 | -4.507587954 | -2.421635886 |
| H | 7.07647402 | 2.679895256 | -2.102906959 |
| H | -6.308570886 | -1.301958135 | -3.993818881 |
| H | -4.245425387 | 2.425725017 | -2.020690209 |
| H | 5.019350219 | -1.599681514 | -2.201657906 |
| H | 0.609224396 | 4.892285196 | -1.195964902 |
| H | -0.580663593 | -4.582833449 | -2.287901657 |
| C | 4.398630285 | 2.429635497 | -1.969821269 |
| C | -3.789971394 | -1.457497764 | -3.086745154 |
| H | 2.494355902 | 5.888272613 | -0.850626392 |
| H | -2.555338683 | -5.297325446 | -2.764510885 |
| H | 4.838258958 | 3.383385466 | -2.284508469 |
| H | -4.149849728 | -2.192846289 | -3.816131377 |
| H | -0.059321381 | 3.256245991 | -0.987630297 |
| H | 0.176490016 | -3.231964746 | -1.411162495 |

| | | | |
|---|---|---|---|
| C | 0.395146995 | 3.947072782 | -1.707227351 |
| C | -0.150306094 | -3.581998006 | -2.398873948 |
| H | 4.091180227 | 1.906558727 | -2.88616744 |
| H | -3.217003352 | -0.705460239 | -3.646665685 |
| C | 1.64425449 | 3.335237856 | -2.367416026 |
| C | -1.119899825 | -2.587648114 | -3.061181907 |
| H | 0.734873851 | 1.349662406 | -2.619057773 |
| H | -0.024022901 | -0.833211076 | -2.346894948 |
| H | -0.356788263 | 4.153189017 | -2.480273832 |
| H | 0.744256851 | -3.682797964 | -3.028940953 |
| C | 1.205411805 | 2.130004911 | -3.220231738 |
| C | -0.370712386 | -1.264775974 | -3.289928499 |
| H | 2.585213324 | 5.292530968 | -2.853682057 |
| H | -2.073907414 | -4.075988334 | -4.408037518 |
| H | 3.154422602 | 3.944583059 | -3.858053498 |
| H | -2.159277885 | -2.405982738 | -4.998137756 |
| C | 2.285458136 | 4.358327949 | -3.331962967 |
| C | -1.54062318 | -3.124066856 | -4.447428 |
| H | 0.466307918 | 2.472089638 | -3.956535376 |
| H | 0.504488484 | -1.453044463 | -3.926656936 |
| H | 2.03947453 | 1.687942187 | -3.777374805 |
| H | -0.9865124 | -0.516607919 | -3.801198392 |
| H | 1.541866113 | 4.61168536 | -4.101360248 |
| H | -0.631695138 | -3.283005778 | -5.046691304 |
| H | -0.544134685 | -0.597836299 | 1.51092636 |
| C | -0.132347848 | 0.343849791 | 5.052443942 |
| C | -0.343698984 | -0.857577695 | 5.730042301 |
| C | -0.615556429 | -2.007898307 | 4.996787835 |
| C | -0.660138672 | -1.940473871 | 3.598580488 |
| N | -0.462588853 | -0.7673833 | 2.959088488 |
| C | -0.209059425 | 0.367799343 | 3.659356076 |
| H | 0.081310414 | 1.262846489 | 5.592011856 |
| H | -0.296578671 | -0.893384036 | 6.816711888 |
| H | -0.786252218 | -2.962104005 | 5.489804819 |
| C | -0.907631775 | -3.174751904 | 2.779240179 |
| H | -0.225060942 | -3.97964271 | 3.077101751 |
| H | -1.932636018 | -3.532341488 | 2.932084138 |
| H | -0.775297858 | -2.973978764 | 1.712880309 |
| C | -0.044703451 | 1.636138365 | 2.875448844 |
| H | 0.802119272 | 1.572667083 | 2.189879242 |
| H | -0.926527319 | 1.810748771 | 2.24884147 |
| H | 0.102161698 | 2.491455805 | 3.542269813 |

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**Supplementary Table 65 | Cartesian coordinate of the product complex for protonation of the bridging dinitrogen ligand in 1 by LutH$^+$ [II-Lut(BR)]. Units are presented in Å.**

SCF energy (in toluene) = -4289.79412988 hartree

ZPE = 1.442022 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.590250588 | -0.450952706 | 0.084540188 |
| Mo | -2.475131633 | -0.792813423 | 0.390298689 |
| P | -3.127700808 | -0.91979797 | -2.100287945 |
| P | 3.078677683 | 1.960376976 | 0.948044322 |
| N | 4.895584048 | -0.228076257 | -0.114872935 |
| N | -4.628436304 | -1.506728999 | 0.476563923 |
| P | -2.901047841 | -0.994441756 | 2.907935941 |
| P | 3.368249838 | -2.78643514 | -0.902000557 |
| N | 0.721567174 | -0.355281395 | 0.296392812 |
| N | -0.496723315 | -0.042314692 | 0.403662612 |
| N | 2.283367976 | 0.660670779 | -2.874733902 |
| N | 2.389187194 | 0.268983397 | -1.820365417 |
| N | 2.831324809 | -1.196375522 | 1.973911328 |
| N | 2.984273546 | -1.613852753 | 3.013000529 |
| N | -3.264853619 | 2.26122789 | 0.457658704 |
| N | -3.030263025 | 1.145515423 | 0.422175099 |
| N | -1.791763151 | -2.689766688 | 0.351450792 |
| N | -1.404647113 | -3.760146188 | 0.320973226 |
| H | -3.497228903 | 1.551543664 | -5.089803732 |
| H | 1.94152665 | 5.506706854 | -0.102534342 |
| H | 3.449397336 | 4.695192276 | -0.535094463 |
| H | -4.743131467 | 1.098334379 | -3.926254847 |
| C | -3.827428381 | 0.746344518 | -4.416900033 |
| C | 2.675584481 | 4.763769578 | 0.239832946 |
| H | 1.99688853 | 2.990413054 | -1.726547167 |
| H | -3.317201078 | 2.136534337 | -2.103434532 |
| H | 3.136569562 | 5.144761405 | 1.153824687 |
| H | -4.082351768 | -0.113881064 | -5.040326173 |
| H | 0.586880077 | 3.904285312 | -1.179511457 |
| H | -2.133084002 | 2.546127744 | -3.348678231 |
| C | -2.431827373 | 1.767744294 | -2.631241326 |
| C | 1.265753749 | 3.081357756 | -0.915154229 |
| H | -1.081672156 | 0.957158997 | -4.751589891 |
| H | 0.071066998 | 4.310461251 | 1.084896492 |

| | | | |
|---|---|---|---|
| C | -2.699725375 | 0.460583451 | -3.401230039 |
| C | 1.92934862 | 3.42431756 | 0.433821182 |
| H | 4.202342336 | 2.435185271 | -1.124077439 |
| H | -4.996912755 | 0.512115571 | -1.597858605 |
| H | -1.624028852 | 1.651752467 | -1.901380758 |
| H | 0.688996728 | 2.152208986 | -0.877545566 |
| H | -5.592836558 | -0.774369045 | -2.648357372 |
| H | 5.176421655 | 3.097956228 | 0.187611111 |
| C | -1.402879696 | 0.093902417 | -4.150879144 |
| C | 0.812881711 | 3.607367272 | 1.483807257 |
| H | -3.208688028 | -2.038835413 | -5.148528942 |
| H | 3.256233001 | 4.354478704 | 3.097218311 |
| H | -0.585650054 | -0.145427802 | -3.458585089 |
| H | 0.290170397 | 2.668186587 | 1.711003114 |
| C | -4.952123273 | -0.571739967 | -1.781250404 |
| C | 4.593225155 | 2.221334951 | -0.118298082 |
| H | -7.450053909 | -1.539959174 | -1.394570747 |
| H | 7.283158822 | 2.158000541 | -0.368055119 |
| H | -1.532378137 | -0.747516569 | -4.839262092 |
| H | 1.183234368 | 4.022637018 | 2.427079239 |
| H | -4.815354698 | -2.201242196 | -4.404683234 |
| H | 4.848904686 | 4.07072961 | 2.357889316 |
| H | 4.401054294 | -0.826621446 | -2.888822159 |
| H | -5.0027343 | 0.896412556 | 2.007642616 |
| C | -3.795369969 | -2.605548547 | -4.418594678 |
| C | 4.112953766 | 3.674134422 | 3.068664745 |
| H | 2.670592087 | -2.765786285 | -4.658866276 |
| H | -3.623272826 | 2.483522217 | 4.361472799 |
| C | -6.80740685 | -1.733472252 | -0.538997361 |
| C | 6.862339671 | 1.157002509 | -0.314003988 |
| H | -3.864636096 | -3.637913 | -4.792466881 |
| H | 4.57903153 | 3.699054198 | 4.064144125 |
| C | -5.479860827 | -1.2983335 | -0.569982345 |
| C | 5.481222986 | 1.003319464 | -0.179986106 |
| H | 4.828402009 | -1.819938832 | -4.285369033 |
| H | -5.668497927 | 1.559254964 | 3.507092038 |
| H | 1.938423979 | -1.822158485 | -3.353671277 |
| H | -2.789816825 | 2.044434535 | 2.866668289 |
| C | 4.73401222 | -1.822221991 | -3.190357458 |
| C | -5.180097979 | 0.679149803 | 3.063878852 |
| C | 2.436797915 | -2.767706317 | -3.584563949 |
| C | -3.036320342 | 1.692042792 | 3.872188358 |
| H | 8.760677923 | 0.133255018 | -0.477426369 |
| H | -8.319769169 | -2.758511437 | 0.618870171 |
| C | -3.152315784 | -2.629514583 | -3.018302545 |
| C | 3.707966624 | 2.219445903 | 2.755251975 |
| H | 5.736385768 | -1.990261966 | -2.780193329 |

| | | | |
|---|---|---|---|
| H | -5.890200759 | -0.153089103 | 3.131069747 |
| C | 7.68252664 | 0.032667138 | -0.376591122 |
| C | -7.290499901 | -2.408879713 | 0.579268726 |
| H | 1.72526321 | -3.578784548 | -3.405912978 |
| H | -2.106638105 | 1.580614936 | 4.438386776 |
| H | -1.073875828 | -2.521174838 | -3.761718785 |
| H | 1.725484938 | 2.4128283 | 3.708142941 |
| H | -5.036086148 | -3.393085956 | -2.164541645 |
| H | 5.821338235 | 1.702504149 | 2.392845648 |
| C | 3.749810481 | -2.945048277 | -2.789491602 |
| C | -3.876639526 | 0.395117655 | 3.844767873 |
| C | -1.706094064 | -3.158069496 | -3.135456062 |
| C | 2.613928334 | 1.776459382 | 3.752300569 |
| C | -3.965323205 | -3.626783391 | -2.161634447 |
| C | 4.960423845 | 1.337553363 | 2.964913758 |
| H | -3.85075386 | -4.631818379 | -2.593255569 |
| H | 5.236952568 | 1.37596703 | 4.027871306 |
| H | 4.678726445 | -4.233353262 | -4.251071679 |
| H | -4.936266112 | 0.821005074 | 5.680273762 |
| C | -6.421434655 | -2.622986846 | 1.646870276 |
| C | 7.085305138 | -1.223912235 | -0.305504224 |
| H | -1.232063821 | -3.255950139 | -2.155251928 |
| H | 2.300712215 | 0.740797719 | 3.597426395 |
| C | -5.104752788 | -2.161257238 | 1.57656653 |
| C | 5.698445474 | -1.329881767 | -0.17923349 |
| C | 4.408920237 | -4.282172897 | -3.186248931 |
| C | -4.280440004 | 0.030180312 | 5.287418791 |
| H | 5.334851042 | -4.47610608 | -2.629756068 |
| H | -4.842691183 | -0.910832352 | 5.341449366 |
| H | -1.727414662 | -4.157137311 | -3.596129111 |
| H | 3.016854991 | 1.849878316 | 4.772539627 |
| H | 7.685520043 | -2.129481132 | -0.345792245 |
| H | -6.754844083 | -3.144011099 | 2.541203185 |
| H | -3.625709646 | -3.672413194 | -1.124110414 |
| H | 4.796193194 | 0.288336207 | 2.706987951 |
| H | 1.869297698 | -5.296241646 | -2.116649137 |
| H | -1.297801027 | -0.06369919 | 5.497603129 |
| C | 5.057871246 | -2.692904491 | -0.09351153 |
| C | -4.166341823 | -2.377950602 | 2.738219656 |
| H | 3.74278914 | -5.140692468 | -3.062314155 |
| H | -3.422875737 | -0.040851935 | 5.964176395 |
| H | 5.745373292 | -3.451083738 | -0.486428425 |
| H | -4.741647585 | -2.560815606 | 3.654202077 |
| H | 0.756210224 | -4.193951238 | -1.264953407 |
| H | -0.318188854 | -0.018699195 | 4.013109164 |
| C | 1.528505873 | -4.959228472 | -1.13274876 |
| C | -0.752065496 | -0.679619179 | 4.775358429 |

| | | | |
|---|---|---|---|
| H | 4.882909741 | -2.943128823 | 0.963228139 |
| H | -3.565069982 | -3.280103305 | 2.554303511 |
| C | 2.681611998 | -4.467059779 | -0.236538346 |
| C | -1.626617169 | -1.781921371 | 4.144738485 |
| H | 1.312602985 | -3.476217637 | 1.168475139 |
| H | -0.184564163 | -2.142217183 | 2.529416226 |
| H | 1.046206538 | -5.816262964 | -0.643243463 |
| H | 0.081794256 | -1.151753484 | 5.314862946 |
| C | 2.113368233 | -4.221181565 | 1.174022886 |
| C | -0.695155392 | -2.694200211 | 3.32440002 |
| H | 4.240895849 | -5.808457605 | -1.078122327 |
| H | -2.912161806 | -2.079667359 | 5.929135614 |
| H | 4.551516414 | -5.295238897 | 0.593094715 |
| H | -2.836349029 | -3.485202563 | 4.850373149 |
| C | 3.766415044 | -5.561151809 | -0.12515381 |
| C | -2.261281894 | -2.64451662 | 5.257617912 |
| H | 1.688012224 | -5.163858462 | 1.545702716 |
| H | 0.069078373 | -3.113068521 | 3.995733275 |
| H | 2.882687414 | -3.909781013 | 1.888618263 |
| H | -1.224873729 | -3.536731207 | 2.867839778 |
| H | 3.290246247 | -6.478283936 | 0.2499455 |
| H | -1.455773038 | -3.076668159 | 5.870070278 |
| H | -0.564696022 | 0.9658088 | 0.622041161 |
| C | -0.852633952 | 7.772790063 | -3.533314328 |
| C | -2.095895362 | 8.159214856 | -3.03508955 |
| C | -2.535558955 | 7.617710441 | -1.82868177 |
| C | -1.714444533 | 6.701988271 | -1.155927395 |
| N | -0.513279786 | 6.329484512 | -1.638732756 |
| C | -0.087143734 | 6.852982281 | -2.80446584 |
| H | -0.475165769 | 8.176586207 | -4.470257648 |
| H | -2.712002241 | 8.873891434 | -3.578264884 |
| H | -3.498709657 | 7.897488724 | -1.407447733 |
| C | -2.14484369 | 6.084972595 | 0.152718456 |
| H | -1.385449072 | 6.258460005 | 0.926737872 |
| H | -3.093883814 | 6.505991722 | 0.503381024 |
| H | -2.273537302 | 4.998292001 | 0.053048037 |
| C | 1.268300044 | 6.403505851 | -3.295648503 |
| H | 2.047810718 | 6.654842716 | -2.563959662 |
| H | 1.29047617 | 5.313942501 | -3.431159939 |
| H | 1.528093838 | 6.875199915 | -4.25005274 |

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**Supplementary Table 66 | Cartesian coordinate of the transition state for protonation of the pyridine nitrogen atom in 1 by LutH$^+$ [TS(PY)]. Units are presented in Å.**

SCF energy (in toluene) = -4289.74661785 hartree

ZPE = 1.437743 hartree

imaginary frequency: 1314*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.008275243 | -0.351635214 | 0.15699937 |
| Mo | 3.172117341 | 0.178217323 | -0.136480457 |
| P | 3.955004592 | -2.120868773 | 0.721394614 |
| P | -2.408588027 | 0.819088555 | 2.511765679 |
| N | -4.517466253 | -0.690967679 | 0.2044093 |
| N | 5.43606197 | 0.405128314 | -0.068823967 |
| P | 3.526194956 | 2.577304343 | -0.988886663 |
| P | -2.482179163 | -1.412205276 | -2.200741146 |
| N | 0.019660785 | -0.174012001 | -0.001017612 |
| N | 1.162944422 | -0.026912678 | -0.105445805 |
| N | -1.473610607 | -3.238301834 | 1.350053248 |
| N | -1.686595535 | -2.208839815 | 0.925492339 |
| N | -1.945716143 | 1.526256918 | -0.624479636 |
| N | -1.702440701 | 2.549883272 | -1.052190737 |
| N | 2.906498244 | 1.197435365 | 2.850745194 |
| N | 3.02943072 | 0.833422744 | 1.78135311 |
| N | 3.210847635 | -0.507207599 | -2.053574569 |
| N | 3.199973588 | -0.907114985 | -3.11619715 |
| H | 3.487544468 | -4.262532966 | 3.940262779 |
| H | -2.389953238 | -0.228827529 | 6.268385088 |
| H | -3.747355622 | -0.413876968 | 5.161484983 |
| H | 4.731389932 | -3.043998309 | 3.659149503 |
| C | 4.07217028 | -3.760961554 | 3.154732769 |
| C | -2.839828707 | 0.174726037 | 5.349464806 |
| H | -2.423610105 | -2.0099256 | 3.624998715 |
| H | 2.931984821 | -1.279001424 | 3.461360965 |
| H | -3.14020741 | 1.203609396 | 5.559439796 |
| H | 4.695309403 | -4.520890557 | 2.6772556 |
| H | -1.259819615 | -1.90429548 | 4.952165688 |
| H | 1.743804832 | -2.546994379 | 3.783821409 |
| C | 2.292141056 | -2.028306006 | 2.983672172 |
| C | -1.55025666 | -1.461473701 | 3.987648271 |

| | | | |
|---|---|---|---|
| H | 1.479387186 | -4.480258188 | 2.454805781 |
| H | -0.059952227 | 0.089968028 | 5.456806174 |
| C | 3.096305652 | -3.067841647 | 2.180035394 |
| C | -1.818112567 | 0.040408683 | 4.201186486 |
| H | -4.744645584 | 0.345460621 | 3.392591066 |
| H | 5.111706801 | -0.970374563 | 2.494876638 |
| H | 1.566980779 | -1.503846045 | 2.352677236 |
| H | -0.728835588 | -1.627355759 | 3.287052511 |
| H | 6.203473093 | -2.210059011 | 1.877192196 |
| H | -4.740775928 | 1.296606286 | 1.903635378 |
| C | 2.095524691 | -4.102460276 | 1.626457527 |
| C | -0.464909713 | 0.663763792 | 4.610680821 |
| H | 4.655287727 | -5.291604543 | 0.689569761 |
| H | -2.019973084 | 2.976195483 | 4.929248618 |
| H | 1.412985459 | -3.661216268 | 0.889858118 |
| H | 0.274510584 | 0.611238786 | 3.802298658 |
| C | 5.489671327 | -1.434786791 | 1.572604194 |
| C | -4.262280009 | 0.454406836 | 2.413972447 |
| H | 8.140722774 | -0.903329635 | 1.49191125 |
| H | -4.637711663 | -2.056667969 | 3.3325544 |
| H | 2.588629257 | -4.966972233 | 1.16988098 |
| H | -0.541229916 | 1.704039116 | 4.937242519 |
| H | 6.143616961 | -4.339099314 | 0.884351238 |
| H | -3.727090899 | 2.983730616 | 4.436804927 |
| H | -2.360871354 | -4.007294871 | -0.703476386 |
| H | 4.805917735 | 2.616316564 | 1.708661293 |
| C | 5.365192128 | -4.639190289 | 0.171126191 |
| C | -2.71294105 | 3.283019212 | 4.142330524 |
| H | 0.382936085 | -3.913605698 | -2.355493238 |
| H | 2.787566415 | 4.981283631 | 1.894673386 |
| C | 7.580299602 | -0.251948969 | 0.825580005 |
| C | -4.641988495 | -2.035283243 | 2.24576767 |
| H | 5.855971472 | -5.248007792 | -0.602530036 |
| H | -2.69818722 | 4.382890593 | 4.114130493 |
| C | 6.192051312 | -0.388980993 | 0.744953092 |
| C | -4.41371787 | -0.808951188 | 1.596192978 |
| H | -1.646635657 | -5.145838754 | -1.843990138 |
| H | 5.088146373 | 4.332783442 | 2.02002462 |
| H | -0.039455081 | -2.699020764 | -1.130125712 |
| H | 2.247319041 | 3.319449113 | 1.609530374 |
| C | -2.272013233 | -4.244938066 | -1.762700376 |
| C | 4.992471418 | 3.578162191 | 1.225622622 |
| C | -0.143950752 | -2.963295918 | -2.185846139 |
| C | 2.575699779 | 4.236538151 | 1.112953671 |
| H | -5.083123346 | -4.135265433 | 2.014706934 |
| H | 9.309365031 | 0.825072347 | 0.099104068 |
| C | 4.686170337 | -3.432978801 | -0.508241329 |

| | | | |
|---|---|---|---|
| C | -2.338035953 | 2.757471563 | 2.74087783 |
| H | -3.264265637 | -4.513613395 | -2.148488198 |
| H | 5.959453573 | 3.525268367 | 0.712101858 |
| C | -4.878857663 | -3.19028918 | 1.517845245 |
| C | 8.228822479 | 0.70827984 | 0.052668369 |
| H | 0.37183164 | -2.193537405 | -2.772574887 |
| H | 1.742311648 | 4.61798457 | 0.514910917 |
| H | 2.779881408 | -4.479339309 | -0.901216315 |
| H | -0.14977304 | 2.805907377 | 3.052677093 |
| H | 6.660144474 | -2.495363725 | -0.801051459 |
| H | -4.36997634 | 3.319824942 | 2.101487246 |
| C | -1.621797105 | -3.125710289 | -2.602692563 |
| C | 3.85298742 | 4.011281624 | 0.274485542 |
| C | 3.567003235 | -3.945585604 | -1.441513791 |
| C | -0.907145069 | 3.213057734 | 2.376212755 |
| C | 5.757938349 | -2.734444002 | -1.375469073 |
| C | -3.3300067 | 3.428424683 | 1.766031383 |
| H | 6.057779786 | -3.419799773 | -2.181613421 |
| H | -3.116124281 | 4.506759992 | 1.73965338 |
| H | -1.166783274 | -4.602511535 | -4.09713969 |
| H | 4.542837265 | 6.052956965 | 0.444288333 |
| C | 7.458392855 | 1.514913788 | -0.781593813 |
| C | -4.81463021 | -3.113083164 | 0.112167139 |
| H | 3.104029386 | -3.135260702 | -2.010627254 |
| H | -0.635811101 | 2.923665904 | 1.356062074 |
| C | 6.071298084 | 1.350703082 | -0.820724919 |
| C | -4.587204803 | -1.902239789 | -0.511882967 |
| C | -1.659418635 | -3.619578184 | -4.062218949 |
| C | 4.285487427 | 5.348062121 | -0.360278095 |
| H | -2.681272442 | -3.759789307 | -4.433125322 |
| H | 5.177932174 | 5.242980775 | -0.990543492 |
| H | 4.004388405 | -4.649225637 | -2.165666168 |
| H | -0.850202318 | 4.309733893 | 2.440386161 |
| H | -4.904263834 | -4.010154552 | -0.493072159 |
| H | 7.921385951 | 2.277057626 | -1.403746792 |
| H | 5.39329985 | -1.815501052 | -1.841261026 |
| H | -3.246632411 | 3.057115985 | 0.745893623 |
| H | -0.499437768 | -0.957820081 | -4.515462195 |
| H | 1.629234173 | 5.05551842 | -1.578401178 |
| C | -4.342665002 | -1.805590965 | -1.985218668 |
| C | 5.231091091 | 2.227912005 | -1.711931778 |
| H | -1.11579631 | -2.969491599 | -4.754189033 |
| H | 3.494670085 | 5.815546086 | -0.955124229 |
| H | -4.647502071 | -2.720890763 | -2.503161745 |
| H | 5.786957657 | 3.135256177 | -1.978778548 |
| H | -0.549627858 | 0.471807203 | -3.468692132 |
| H | 0.722715922 | 3.531243699 | -1.433023828 |

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| C | -1.078749984 | -0.062664636 | -4.26644265 |
| C | 1.375501908 | 4.120431456 | -2.088005315 |
| H | -4.894344757 | -0.966783112 | -2.427270479 |
| H | 5.024705762 | 1.693559913 | -2.651089773 |
| C | -2.528519573 | -0.386133744 | -3.857524352 |
| C | 2.619253547 | 3.327181192 | -2.534415047 |
| H | -2.77801342 | 1.562019652 | -2.851362692 |
| H | 1.489820522 | 1.466833281 | -2.827825085 |
| H | -1.081883934 | 0.583220249 | -5.156720549 |
| H | 0.787126776 | 4.387793736 | -2.97794447 |
| C | -3.262532308 | 0.945310199 | -3.605213992 |
| C | 2.130438981 | 2.147653076 | -3.397444884 |
| H | -2.75156608 | -1.916156814 | -5.452955718 |
| H | 3.891668029 | 5.10602906 | -2.919450281 |
| H | -4.284526298 | -1.416102987 | -4.719245984 |
| H | 4.363368021 | 3.664803129 | -3.841297768 |
| C | -3.285432541 | -1.072548166 | -5.018724307 |
| C | 3.510455011 | 4.217168481 | -3.428564051 |
| H | -3.269569159 | 1.518793599 | -4.543745493 |
| H | 1.548002564 | 2.544728178 | -4.242204992 |
| H | -4.311888622 | 0.795553014 | -3.321214054 |
| H | 2.955288867 | 1.563846268 | -3.819760522 |
| H | -3.429249284 | -0.335732155 | -5.822381027 |
| H | 2.911680946 | 4.56335313 | -4.284210543 |
| H | -5.52407758 | 0.15099868 | -0.161470683 |
| C | -8.986672738 | 2.115345813 | -0.943808229 |
| C | -9.003609756 | 0.846658544 | -0.363629133 |
| C | -7.803663073 | 0.185126365 | -0.105415388 |
| N | -6.617267165 | 0.780124038 | -0.415665842 |
| C | -6.578073379 | 2.016469958 | -0.97112513 |
| C | -7.764238697 | 2.703021837 | -1.249181408 |
| H | -9.918179482 | 2.637483439 | -1.152269561 |
| H | -9.941667342 | 0.36073191 | -0.109806289 |
| H | -7.710778697 | 3.691311358 | -1.698881833 |
| C | -5.242801128 | 2.634324006 | -1.262270268 |
| H | -5.092139953 | 3.524169505 | -0.637652093 |
| H | -4.425460873 | 1.937583938 | -1.073337355 |
| H | -5.187003377 | 2.961951362 | -2.307568133 |
| C | -7.788988239 | -1.18504005 | 0.509961465 |
| H | -7.204697861 | -1.205092282 | 1.437773181 |
| H | -8.80911646 | -1.507107915 | 0.739496547 |
| H | -7.339620705 | -1.921881835 | -0.166858851 |

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**Supplementary Table 67 | Cartesian coordinate of the product complex for protonation of the pyridine nitrogen atom in 1 by LutH$^+$ [II-Lut(PY)]. Units are presented in Å.**

SCF energy (in toluene) = -4289.76769226 hartree

ZPE = 1.441601 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -2.042672051 | -0.591944169 | 0.205448605 |
| Mo | 3.125715073 | 0.2184401 | -0.076894958 |
| P | 4.04835294 | -2.038031725 | 0.760056994 |
| P | -2.337587734 | 0.654659753 | 2.628047179 |
| N | -4.292557075 | -0.747668009 | -0.021783706 |
| N | 5.379445205 | 0.559020699 | -0.109471295 |
| P | 3.321312824 | 2.641963239 | -0.922070289 |
| P | -2.372036119 | -1.660032687 | -2.267604159 |
| N | 0.02768783 | -0.283023791 | 0.051669931 |
| N | 1.167241197 | -0.09038185 | -0.019268718 |
| N | -1.263144392 | -3.482539033 | 1.262026528 |
| N | -1.573800135 | -2.466703494 | 0.878013084 |
| N | -2.230503418 | 1.321280176 | -0.458711943 |
| N | -2.202071625 | 2.389395188 | -0.834282414 |
| N | 2.916742244 | 1.248901094 | 2.916976921 |
| N | 3.01407523 | 0.879848316 | 1.848813181 |
| N | 3.167783975 | -0.455263928 | -2.003152105 |
| N | 3.166770038 | -0.839714584 | -3.070135586 |
| H | 3.827498394 | -4.122084923 | 4.040076766 |
| H | -2.472316777 | -0.623920652 | 6.295334093 |
| H | -3.807811411 | -0.541288152 | 5.146415674 |
| H | 5.019717571 | -2.884195118 | 3.641191664 |
| C | 4.348756439 | -3.633459032 | 3.203719524 |
| C | -2.84561651 | -0.084404582 | 5.412614792 |
| H | -2.50447972 | -2.215192609 | 3.612803122 |
| H | 3.114948142 | -1.214317682 | 3.561679676 |
| H | -3.03208079 | 0.946983171 | 5.717981579 |
| H | 4.959480425 | -4.395259144 | 2.713056809 |
| H | -1.344002639 | -2.216229768 | 4.944072272 |
| H | 1.985051244 | -2.522728682 | 3.92224883 |
| C | 2.485627605 | -1.984753708 | 3.103827617 |
| C | -1.60860584 | -1.720705426 | 3.998352053 |
| H | 1.768517112 | -4.484060527 | 2.641362808 |
| H | -0.065444514 | -0.288112923 | 5.553317269 |

| | | | |
|---|---|---|---|
| C | 3.29633326 | -2.996478065 | 2.271257481 |
| C | -1.811265382 | -0.21841423 | 4.27645954 |
| H | -4.744334223 | 0.044841978 | 3.208635531 |
| H | 5.245897736 | -0.820340864 | 2.462089293 |
| H | 1.7187955 | -1.486473582 | 2.501035304 |
| H | -0.790500432 | -1.89500088 | 3.295303085 |
| H | 6.354445953 | -2.018141072 | 1.795606394 |
| H | -4.597088415 | 1.097093448 | 1.801037319 |
| C | 2.315025155 | -4.079108714 | 1.777739431 |
| C | -0.43307643 | 0.325609563 | 4.718390794 |
| H | 4.843630409 | -5.186244698 | 0.721698475 |
| H | -1.804172549 | 2.706437444 | 5.094351599 |
| H | 1.568225285 | -3.672718575 | 1.084781909 |
| H | 0.308621517 | 0.257242405 | 3.912922666 |
| C | 5.595060675 | -1.275171624 | 1.523758952 |
| C | -4.137966478 | 0.244418883 | 2.314597282 |
| H | 8.220007546 | -0.641506066 | 1.283373734 |
| H | -4.53645251 | -2.336706867 | 2.998622729 |
| H | 2.818467398 | -4.920905601 | 1.291871072 |
| H | -0.45734465 | 1.360524601 | 5.068782433 |
| H | 6.312523492 | -4.191429689 | 0.838089805 |
| H | -3.542752509 | 2.767219213 | 4.729129923 |
| H | -2.643145866 | -4.172089892 | -0.639971628 |
| H | 4.741517421 | 2.74211407 | 1.700230408 |
| C | 5.508798407 | -4.51794137 | 0.165685839 |
| C | -2.546308277 | 3.054722065 | 4.372856712 |
| H | -0.015605458 | -4.655795879 | -2.385227226 |
| H | 2.654606371 | 5.064119375 | 1.970999122 |
| C | 7.59383377 | -0.014008061 | 0.653873854 |
| C | -4.575654498 | -2.212604154 | 1.919294689 |
| H | 5.978864366 | -5.118929013 | -0.626661394 |
| H | -2.508719117 | 4.154102718 | 4.382878801 |
| C | 6.209469764 | -0.205896038 | 0.656171092 |
| C | -4.085887649 | -0.961859457 | 1.379011289 |
| H | -2.174882734 | -5.455979888 | -1.756958504 |
| H | 4.978453617 | 4.468931272 | 1.991339823 |
| H | -0.139734198 | -3.341523343 | -1.202953582 |
| H | 2.183557888 | 3.369598063 | 1.779354618 |
| C | -2.634644475 | -4.459255882 | -1.69129075 |
| C | 4.867995103 | 3.707904189 | 1.20528533 |
| C | -0.335570294 | -3.613011601 | -2.244515163 |
| C | 2.430657886 | 4.282224652 | 1.230318566 |
| H | -5.562130086 | -4.076358429 | 1.579833709 |
| H | 9.230075454 | 1.132059187 | -0.172358432 |
| C | 4.766555107 | -3.33537414 | -0.489627141 |
| C | -2.290254032 | 2.584377487 | 2.924283771 |
| H | -3.67022642 | -4.563181061 | -2.033558579 |

| | | | |
|---|---|---|---|
| H | 5.80736987 | 3.687794196 | 0.640967433 |
| C | -5.15019563 | -3.170806393 | 1.141899998 |
| C | 8.154188267 | 0.972099153 | -0.154689997 |
| H | 0.29814762 | -2.987273622 | -2.880377225 |
| H | 1.541243241 | 4.600269667 | 0.678741401 |
| H | 2.873962644 | -4.435607139 | -0.792916766 |
| H | -0.089727467 | 2.612911121 | 3.059066549 |
| H | 6.701754277 | -2.351323069 | -0.866579126 |
| H | -4.383100371 | 3.112397441 | 2.494302469 |
| C | -1.835833261 | -3.500120227 | -2.599597339 |
| C | 3.662084114 | 4.092663982 | 0.317872094 |
| C | 3.620640116 | -3.882333422 | -1.369836473 |
| C | -0.895381969 | 3.06304683 | 2.467798417 |
| C | 5.781990767 | -2.612099897 | -1.402523241 |
| C | -3.381261854 | 3.283712281 | 2.080639323 |
| H | 6.063517674 | -3.290941073 | -2.220341165 |
| H | -3.201995547 | 4.36776237 | 2.119943687 |
| H | -1.791200198 | -5.073987836 | -4.071629394 |
| H | 4.291664996 | 6.157171147 | 0.429011006 |
| C | 7.30556626 | 1.748481919 | -0.940353649 |
| C | -5.159765423 | -2.995253364 | -0.284797752 |
| H | 3.108556006 | -3.086607479 | -1.917920897 |
| H | -0.710134698 | 2.827964527 | 1.414467591 |
| C | 5.926048473 | 1.528739273 | -0.897494008 |
| C | -4.691715637 | -1.855792526 | -0.850858792 |
| C | -2.058732191 | -4.007628218 | -4.040180079 |
| C | 4.006149012 | 5.43791556 | -0.352738105 |
| H | -3.108830051 | -3.932738286 | -4.349786418 |
| H | 4.857157343 | 5.359559293 | -1.041492469 |
| H | 4.042895117 | -4.575851596 | -2.11208184 |
| H | -0.823445254 | 4.153846996 | 2.587969253 |
| H | -5.460305224 | -3.81714011 | -0.928073868 |
| H | 7.701488365 | 2.527921036 | -1.586785544 |
| H | 5.377044891 | -1.702758164 | -1.852969856 |
| H | -3.385681974 | 3.000185766 | 1.028534874 |
| H | -0.306241132 | -1.86278518 | -4.701348008 |
| H | 1.269803086 | 5.027333548 | -1.39217853 |
| C | -4.289585096 | -1.68558774 | -2.275512163 |
| C | 4.998518486 | 2.368994144 | -1.738742062 |
| H | -1.438948492 | -3.502214242 | -4.785056007 |
| H | 3.161035116 | 5.87364878 | -0.894812197 |
| H | -4.700176043 | -2.473254073 | -2.91578752 |
| H | 5.498757327 | 3.30144844 | -2.027791125 |
| H | 0.188167212 | -0.671413167 | -3.483877662 |
| H | 0.457032546 | 3.461022227 | -1.167570289 |
| C | -0.508429426 | -0.862633581 | -4.308628747 |
| C | 1.029549627 | 4.07462803 | -1.874488803 |

| | | | |
|---|---|---|---|
| H | -4.610659675 | -0.713787525 | -2.675036393 |
| H | 4.769673327 | 1.830088683 | -2.67006316 |
| C | -1.978242738 | -0.657655784 | -3.886792461 |
| C | 2.27706648 | 3.33877901 | -2.403113861 |
| H | -1.393899666 | 1.189216624 | -2.865478537 |
| H | 1.218050966 | 1.428454649 | -2.602362689 |
| H | -0.269041166 | -0.148102289 | -5.10936469 |
| H | 0.364994983 | 4.30088481 | -2.720791125 |
| C | -2.152135972 | 0.837311044 | -3.567584997 |
| C | 1.78515563 | 2.130418766 | -3.222345531 |
| H | -2.869331466 | -2.031364637 | -5.390933777 |
| H | 3.419792799 | 5.179523343 | -2.885518165 |
| H | -3.969733024 | -0.761070074 | -4.830031118 |
| H | 3.919521176 | 3.752566518 | -3.814680272 |
| C | -2.922866247 | -0.992074137 | -5.062786351 |
| C | 3.06157243 | 4.262494922 | -3.359982978 |
| H | -2.039241298 | 1.413071235 | -4.497687602 |
| H | 1.126353208 | 2.491401407 | -4.025820695 |
| H | -3.140167159 | 1.076335552 | -3.157817107 |
| H | 2.60437615 | 1.581003247 | -3.698077918 |
| H | -2.641781233 | -0.364541786 | -5.921021422 |
| H | 2.395704379 | 4.560908591 | -4.183262266 |
| H | -4.793199413 | 0.124380653 | -0.278542667 |
| C | -8.994510301 | 2.853000001 | -0.835004935 |
| C | -8.934959985 | 1.732257634 | -0.010658696 |
| C | -7.740266729 | 1.004971185 | 0.070420612 |
| N | -6.637566238 | 1.356004912 | -0.628309176 |
| C | -6.69971547 | 2.435934071 | -1.43823322 |
| C | -7.860926597 | 3.209012491 | -1.561832518 |
| H | -9.910291644 | 3.435968818 | -0.914116733 |
| H | -9.800448767 | 1.415734935 | 0.566682448 |
| H | -7.868224414 | 4.071924806 | -2.223518832 |
| C | -5.468499176 | 2.774115179 | -2.239018816 |
| H | -5.593569333 | 3.715425282 | -2.785223153 |
| H | -4.583654576 | 2.864394885 | -1.598463646 |
| H | -5.26078367 | 1.986208472 | -2.976796189 |
| C | -7.64880436 | -0.212198453 | 0.956521976 |
| H | -6.991489002 | -0.026587981 | 1.817070648 |
| H | -8.633827906 | -0.492009271 | 1.34581122 |
| H | -7.237458167 | -1.068303041 | 0.408814819 |

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**Supplementary Table 68 | Cartesian coordinate of the reactant complex for coordination of dinitrogen to XXII. Units are presented in Å.**

SCF energy (in toluene) = -2833.52870426 hartree

ZPE = 0.670416 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.166437016 | 0.495192316 | 0.319616191 |
| P | 0.401533206 | -0.965165018 | 2.397683631 |
| N | 1.886034836 | 1.13740604 | 0.806901809 |
| P | 0.368551253 | 1.996082139 | -1.684918994 |
| N | -1.31748157 | 1.490038416 | 1.129143317 |
| H | -0.939310269 | -1.940819456 | 5.876810026 |
| H | 0.610550112 | -1.201786857 | 5.462383292 |
| C | -0.183904798 | -1.857432111 | 5.082894672 |
| H | -0.886535701 | 0.741558751 | 4.689852214 |
| H | 0.232736032 | -2.857845756 | 4.929879572 |
| H | -2.367826877 | -0.191703436 | 4.897138879 |
| C | -1.557040893 | 0.031759696 | 4.190564461 |
| H | -2.672666841 | -2.428570629 | 4.148041114 |
| C | -0.867597979 | -1.297583205 | 3.817196604 |
| H | 0.684236574 | 1.20695687 | 3.412088597 |
| H | -2.005339018 | 0.522143615 | 3.320564064 |
| H | 1.981919352 | 0.173291686 | 4.019450127 |
| C | -1.957264306 | -2.272747182 | 3.328252354 |
| H | 2.329841135 | -2.490684008 | 4.305886879 |
| H | -2.500653967 | -1.877355722 | 2.465563127 |
| C | 1.423140324 | 0.450436435 | 3.119357154 |
| H | 3.955432787 | 1.404843863 | 3.467688342 |
| H | -1.560777157 | -3.249708056 | 3.042806914 |
| H | 3.384465987 | -1.522833065 | 3.250189887 |
| H | -0.196154983 | 3.673085418 | 0.795630583 |
| C | 2.74412401 | -2.412585284 | 3.296367188 |
| H | -1.347427987 | 5.387345775 | -1.382455058 |
| C | 3.62458281 | 1.481347773 | 2.435574383 |
| H | 3.396844858 | -3.283283036 | 3.143103101 |
| C | 2.343250873 | 1.041836218 | 2.093053316 |
| H | 0.383976524 | 5.270996096 | 0.286650056 |
| H | -1.966363994 | 3.748117802 | -1.123633705 |
| C | 0.498441571 | 4.189669928 | 0.127630871 |
| C | -1.22548015 | 4.336649662 | -1.679916414 |

| | | | |
|---|---|---|---|
| H | 5.460146298 | 2.352416752 | 1.705661826 |
| C | 1.666111331 | -2.412640336 | 2.193544081 |
| H | 1.522311183 | 3.928312714 | 0.418632678 |
| C | 4.459864469 | 2.007231867 | 1.453515768 |
| H | -1.46336639 | 4.271607257 | -2.746698715 |
| H | 0.526575718 | -4.037143728 | 3.159950231 |
| H | 2.942178596 | -1.297693325 | 0.771746156 |
| C | 0.217744989 | 3.892705286 | -1.361734978 |
| C | 0.931859578 | -3.770413255 | 2.178269937 |
| C | 2.368239149 | -2.230264726 | 0.827146626 |
| H | 3.081667747 | -3.055037081 | 0.690206603 |
| H | 1.062374803 | 5.780995504 | -1.976377088 |
| C | 3.999561039 | 2.073980497 | 0.138907526 |
| H | 0.122204051 | -3.801845094 | 1.442405464 |
| C | 2.712208521 | 1.632837197 | -0.166818252 |
| C | 1.22514743 | 4.716071175 | -2.193504595 |
| H | 2.264051659 | 4.493633341 | -1.91941815 |
| H | 1.656275272 | -4.54961927 | 1.903761876 |
| H | 4.632921081 | 2.461446625 | -0.654537719 |
| H | 1.664718414 | -2.281097823 | -0.012048629 |
| H | -2.211539456 | 2.256024064 | -3.248706465 |
| C | 2.212522009 | 1.643804373 | -1.587870529 |
| H | 1.116066683 | 4.583562003 | -3.271525622 |
| H | 2.816263991 | 2.321447284 | -2.201978479 |
| H | -1.989847465 | 0.562328681 | -2.758411612 |
| C | -1.675851167 | 1.32727694 | -3.473846212 |
| H | 2.340944688 | 0.638286583 | -2.012929355 |
| C | -0.14222532 | 1.520353089 | -3.479434577 |
| H | 0.391967566 | -0.590763363 | -3.069346882 |
| H | -1.99382257 | 1.001246709 | -4.473857966 |
| C | 0.538093481 | 0.177419449 | -3.833505806 |
| H | -0.291506991 | 3.49630546 | -4.459076625 |
| H | 1.32275138 | 2.75159954 | -4.582307066 |
| C | 0.24499264 | 2.547267179 | -4.560985228 |
| H | 0.089129156 | -0.199979101 | -4.762341591 |
| H | 1.611048852 | 0.299829947 | -4.028191512 |
| H | -0.023629777 | 2.130076753 | -5.541713902 |
| S | -1.217834038 | -2.438970717 | -0.96159332 |
| O | -0.123841572 | -3.314752271 | -1.390088596 |
| O | -1.9508965 | -2.727935039 | 0.274958494 |
| O | -0.77440974 | -0.9234811 | -1.056252527 |
| C | -2.48644718 | -2.429377482 | -2.335122533 |
| F | -3.425704471 | -1.51194419 | -2.068146939 |
| F | -1.898463454 | -2.130401773 | -3.498474074 |
| F | -3.045495702 | -3.633480791 | -2.409118804 |
| N | -5.591815474 | 2.087873758 | 1.201388853 |
| N | -4.491273542 | 2.089619161 | 1.320142287 |

```
 H    -2.268086065    1.807945783    1.344789289
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**Supplementary Table 69 | Cartesian coordinate of the transition state for coordination of dinitrogen to XXII. Units are presented in Å.**

SCF energy (in toluene) = 2833.52111384 hartree

ZPE = 0.671330 hartree

Imaginary frequency: 73*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.179897479 | 0.598195977 | 0.369873802 |
| P | 0.389240015 | -0.923617925 | 2.439437557 |
| N | 1.902994268 | 1.068236769 | 0.742476868 |
| P | 0.363182843 | 2.070693848 | -1.679404289 |
| N | -0.96571857 | 1.785008657 | 1.358886644 |
| H | -0.998043382 | -1.764517736 | 5.942828017 |
| H | 0.55181017 | -1.024447763 | 5.526822561 |
| C | -0.228081347 | -1.704937981 | 5.160856729 |
| H | -0.937555865 | 0.90513188 | 4.536327974 |
| H | 0.202287523 | -2.705699548 | 5.056815791 |
| H | -2.36104106 | -0.058306523 | 4.931454078 |
| C | -1.606753234 | 0.124602107 | 4.154153018 |
| H | -2.71984976 | -2.306806584 | 4.178444007 |
| C | -0.889336527 | -1.20929288 | 3.85833174 |
| H | 0.765181639 | 1.281365248 | 3.365737534 |
| H | -2.133576111 | 0.504403662 | 3.27289057 |
| H | 2.035909346 | 0.217003787 | 3.990555827 |
| C | -1.959576628 | -2.217810728 | 3.389652613 |
| H | 2.239298779 | -2.415872916 | 4.437675802 |
| H | -2.454250579 | -1.891067692 | 2.470380001 |
| C | 1.46630867 | 0.482442387 | 3.094349297 |
| H | 4.0601848 | 1.282194178 | 3.335868515 |
| H | -1.554918136 | -3.215529297 | 3.206327818 |
| H | 3.35444479 | -1.519144995 | 3.381917137 |
| H | 0.284292844 | 3.727036432 | 0.846124163 |
| C | 2.684030854 | -2.385382648 | 3.439156503 |
| H | -1.06781375 | 5.566652374 | -1.222276817 |
| C | 3.705302493 | 1.347244533 | 2.311001168 |
| H | 3.31375852 | -3.280048536 | 3.335966802 |
| C | 2.388705899 | 0.983171656 | 2.020650119 |
| H | 0.798360802 | 5.327298322 | 0.278082337 |
| H | -1.741519447 | 3.979606978 | -0.813083415 |

| | | | |
|---|---|---|---|
| C | 0.880554964 | 4.247249273 | 0.092174271 |
| C | -1.049732274 | 4.500680075 | -1.487596123 |
| H | 5.576948029 | 2.056175654 | 1.500560203 |
| C | 1.644135358 | -2.397115394 | 2.297679642 |
| H | 1.934205929 | 3.977929307 | 0.231350214 |
| C | 4.547163607 | 1.777485387 | 1.288186946 |
| H | -1.43500201 | 4.413655985 | -2.508993795 |
| H | 0.473439868 | -3.985932691 | 3.280462595 |
| H | 3.009920626 | -1.348400591 | 0.910980697 |
| C | 0.393108629 | 3.971789026 | -1.347806215 |
| C | 0.894997547 | -3.746508271 | 2.298299048 |
| C | 2.409779126 | -2.263880088 | 0.960949512 |
| H | 3.108395036 | -3.108826123 | 0.883560955 |
| H | 1.350388403 | 5.793163842 | -1.994741064 |
| C | 4.051545124 | 1.840787487 | -0.012819236 |
| H | 0.096456239 | -3.785844492 | 1.551450018 |
| C | 2.724952718 | 1.490700982 | -0.267539616 |
| C | 1.342016703 | 4.736597119 | -2.296839534 |
| H | 2.37717336 | 4.379253226 | -2.223408893 |
| H | 1.615432109 | -4.538977904 | 2.053429022 |
| H | 4.683358152 | 2.163754593 | -0.835725837 |
| H | 1.751305304 | -2.317591475 | 0.089420893 |
| H | -2.313619471 | 2.354307789 | -3.002791117 |
| C | 2.168152879 | 1.543357819 | -1.664357594 |
| H | 1.03792309 | 4.701240388 | -3.343497616 |
| H | 2.806661277 | 2.158939007 | -2.308027854 |
| H | -2.046020224 | 0.633579118 | -2.649570532 |
| C | -1.796024902 | 1.446617145 | -3.336370411 |
| H | 2.175824906 | 0.529368992 | -2.086720837 |
| C | -0.269642528 | 1.652489753 | -3.455684277 |
| H | 0.318152017 | -0.463115586 | -3.177192187 |
| H | -2.198412551 | 1.186658836 | -4.325267018 |
| C | 0.396033001 | 0.33628007 | -3.917275074 |
| H | -0.513146368 | 3.659957676 | -4.356562918 |
| H | 1.085981126 | 2.926183028 | -4.646406401 |
| C | 0.015756295 | 2.717556946 | -4.532252002 |
| H | -0.116153509 | -0.007303502 | -4.826008279 |
| H | 1.450904077 | 0.484124634 | -4.181526549 |
| H | -0.34104273 | 2.32620791 | -5.495438937 |
| S | -0.960021492 | -2.4326099 | -0.971404531 |
| O | 0.136858196 | -3.334160534 | -1.328761073 |
| O | -1.768682346 | -2.693210192 | 0.225801811 |
| O | -0.490502063 | -0.933917615 | -1.036044788 |
| C | -2.157046893 | -2.474209058 | -2.408129534 |
| F | -3.127201463 | -1.565324079 | -2.22134658 |
| F | -1.52062678 | -2.203374501 | -3.55172035 |
| F | -2.695098811 | -3.688213496 | -2.469433896 |

```
 N    -3.118615827   0.165043661   0.164969935
 N    -4.216952629    0.11818306   0.299266111
 H    -1.749265864   2.280649503   1.788778385
---------------------------------------------------
```

**Supplementary Table 70 | Cartesian coordinate of the reactant complex for coordination of dinitrogen to XI. Units are presented in Å.**

SCF energy (in toluene) = -2833.09593003 hartree

ZPE = 0.658862 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.090846858 | 0.515515465 | 0.350721653 |
| P | 0.503696831 | -0.938863679 | 2.368875807 |
| N | 1.984347419 | 1.161492734 | 0.808302074 |
| P | 0.428787188 | 2.013627905 | -1.62789221 |
| N | -1.037481938 | 1.511163978 | 1.28777066 |
| H | -0.793426309 | -1.953547806 | 5.868777711 |
| H | 0.732294809 | -1.16188553 | 5.453877486 |
| C | -0.039387027 | -1.845614907 | 5.074916499 |
| H | -0.802500982 | 0.717493096 | 4.696219142 |
| H | 0.416816907 | -2.830360404 | 4.927255188 |
| H | -2.281580729 | -0.234900808 | 4.852946906 |
| C | -1.454708003 | 0.00827203 | 4.170147397 |
| H | -2.522085709 | -2.473632006 | 4.111684295 |
| C | -0.728733573 | -1.305857322 | 3.805104382 |
| H | 0.766248175 | 1.214525813 | 3.391244484 |
| H | -1.872106712 | 0.508748158 | 3.290609089 |
| H | 2.085825759 | 0.212208835 | 4.025549191 |
| C | -1.793996543 | -2.3042444 | 3.304313659 |
| H | 2.564897853 | -2.363516577 | 4.226739793 |
| H | -2.33842605 | -1.919190484 | 2.435554256 |
| C | 1.531141142 | 0.4769902 | 3.117824516 |
| H | 4.051507904 | 1.472039844 | 3.470237439 |
| H | -1.374006053 | -3.275763678 | 3.03009089 |
| H | 3.532487952 | -1.407995054 | 3.0800297 |
| H | -0.226726527 | 3.703987153 | 0.78270022 |
| C | 2.924815392 | -2.314376261 | 3.192745549 |
| H | -1.249255618 | 5.434094009 | -1.406047691 |
| C | 3.721711726 | 1.540794262 | 2.436593293 |
| H | 3.594206743 | -3.173413451 | 3.036861784 |
| C | 2.445213228 | 1.081986621 | 2.095940322 |
| H | 0.415083907 | 5.298369179 | 0.308945183 |
| H | -1.895390442 | 3.793856495 | -1.213240584 |
| C | 0.510238538 | 4.213010312 | 0.155374077 |
| C | -1.125578402 | 4.387679935 | -1.72124742 |

| | | | |
|---|---|---|---|
| H | 5.548226846 | 2.434448486 | 1.706009568 |
| C | 1.780798442 | -2.379660834 | 2.161854846 |
| H | 1.511436064 | 3.921209843 | 0.49405193 |
| C | 4.553308267 | 2.073010126 | 1.454461828 |
| H | -1.31057369 | 4.34881412 | -2.800711609 |
| H | 0.732268025 | -3.996894023 | 3.244520969 |
| H | 2.904655784 | -1.296947585 | 0.594100538 |
| C | 0.295014588 | 3.917783004 | -1.345138032 |
| C | 1.096018901 | -3.760718987 | 2.238859645 |
| C | 2.376157945 | -2.246277466 | 0.740333527 |
| H | 3.104944923 | -3.05509995 | 0.580087822 |
| H | 1.18417939 | 5.79425717 | -1.945351552 |
| C | 4.090387464 | 2.124585688 | 0.138184994 |
| H | 0.268238702 | -3.841872017 | 1.527706098 |
| C | 2.80999616 | 1.661832481 | -0.162862828 |
| C | 1.346984502 | 4.723354188 | -2.136207997 |
| H | 2.368529217 | 4.494133404 | -1.806743321 |
| H | 1.840294715 | -4.52800007 | 1.976947808 |
| H | 4.714947128 | 2.521442514 | -0.658360341 |
| H | 1.595376581 | -2.350143496 | -0.023390534 |
| H | -2.092235224 | 2.405673128 | -3.296003214 |
| C | 2.289263806 | 1.670312297 | -1.574914932 |
| H | 1.292041632 | 4.571872977 | -3.217483492 |
| H | 2.888631653 | 2.335516178 | -2.207368248 |
| H | -1.982986646 | 0.719876408 | -2.749404489 |
| C | -1.604194357 | 1.443098014 | -3.478516515 |
| H | 2.39391976 | 0.659060628 | -1.991594698 |
| C | -0.061587757 | 1.538594427 | -3.431380372 |
| H | 0.242220839 | -0.588360044 | -2.92316341 |
| H | -1.906635893 | 1.105878997 | -4.481241211 |
| C | 0.506002552 | 0.127646158 | -3.708811703 |
| H | -0.023631502 | 3.479626999 | -4.477537855 |
| H | 1.532613158 | 2.616412548 | -4.511654085 |
| C | 0.44181156 | 2.489296623 | -4.532836451 |
| H | 0.065652637 | -0.247317354 | -4.643866636 |
| H | 1.594429476 | 0.133851832 | -3.8505577 |
| H | 0.182891786 | 2.065001165 | -5.514499989 |
| S | -1.926991501 | -2.13705718 | -0.644058947 |
| O | -0.943064314 | -3.160586562 | -0.239920235 |
| O | -3.175783088 | -2.027786108 | 0.122087024 |
| O | -1.278860205 | -0.778542643 | -0.961384036 |
| C | -2.43743701 | -2.615427015 | -2.371816105 |
| F | -3.277134075 | -1.704002024 | -2.885386897 |
| F | -1.359887025 | -2.703018362 | -3.172451406 |
| F | -3.050736389 | -3.804594342 | -2.348887171 |
| N | -4.169274275 | 1.451549002 | -0.293987996 |
| N | -4.472260442 | 1.023067971 | 0.68092562 |

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**Supplementary Table 71 | Cartesian coordinate of the transition state for coordination of dinitrogen to XI. Units are presented in Å.**

SCF energy (in toluene) = -2833.08497954 hartree

ZPE = 0.659524 hartree

Imaginary frequency: 107*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | 2.492520234 | 0.539474458 | 0.38796536 |
| P | 3.076442863 | -0.895522673 | 2.443344282 |
| N | 4.596948531 | 1.081767523 | 0.760714246 |
| P | 3.003995907 | 2.012261367 | -1.6275705 |
| N | 1.721135995 | 1.641960782 | 1.378025992 |
| H | 1.661204676 | -1.8424376 | 5.929188772 |
| H | 3.269089656 | -1.213884577 | 5.545593638 |
| C | 2.432029329 | -1.801055983 | 5.145222765 |
| H | 1.960349161 | 0.829303868 | 4.834681251 |
| H | 2.777327728 | -2.826247598 | 4.976908097 |
| H | 0.382293092 | 0.044840674 | 4.95201009 |
| C | 1.237559389 | 0.214736792 | 4.281984495 |
| H | -0.093264165 | -2.137273464 | 4.13854386 |
| C | 1.821265828 | -1.159721431 | 3.884031015 |
| H | 3.479752224 | 1.275721314 | 3.378272492 |
| H | 0.888618676 | 0.787227881 | 3.416002356 |
| H | 4.765096859 | 0.219653164 | 4.004003445 |
| C | 0.666024623 | -2.032901346 | 3.349043723 |
| H | 4.91068307 | -2.50241632 | 4.405911562 |
| H | 0.192032035 | -1.580348936 | 2.472489043 |
| C | 4.191162854 | 0.485128232 | 3.108548537 |
| H | 6.77737336 | 1.314011504 | 3.337478938 |
| H | 0.988505814 | -3.036302692 | 3.058156176 |
| H | 6.019748953 | -1.593076547 | 3.355988455 |
| H | 2.666640005 | 3.69158841 | 0.853281412 |
| C | 5.339016624 | -2.452779403 | 3.399945563 |
| H | 1.471697993 | 5.480957187 | -1.264988678 |
| C | 6.413822676 | 1.384180853 | 2.315472445 |
| H | 5.952826823 | -3.354766011 | 3.259600921 |
| C | 5.099472065 | 1.001681699 | 2.032339413 |
| H | 3.262494935 | 5.285267134 | 0.32515701 |
| H | 0.813125131 | 3.869275959 | -0.929979788 |

| | | | |
|---|---|---|---|
| C | 3.338919895 | 4.200460166 | 0.157334016 |
| C | 1.532151625 | 4.420148438 | -1.549184789 |
| H | 8.265679526 | 2.140229405 | 1.498037011 |
| C | 4.273661443 | -2.404079919 | 2.285014164 |
| H | 4.369736175 | 3.907621284 | 0.390470257 |
| C | 7.239886561 | 1.841791769 | 1.291723838 |
| H | 1.218870622 | 4.344980823 | -2.596428903 |
| H | 3.039731061 | -3.962238234 | 3.244735647 |
| H | 5.629280855 | -1.37489881 | 0.876345044 |
| C | 2.97260225 | 3.916711683 | -1.316495856 |
| C | 3.477753302 | -3.72663086 | 2.268557717 |
| C | 5.00839925 | -2.276852405 | 0.929551299 |
| H | 5.678195125 | -3.141794867 | 0.813544236 |
| H | 3.899564202 | 5.769416031 | -1.931801318 |
| C | 6.729474963 | 1.903855668 | -0.004433249 |
| H | 2.680739351 | -3.723418681 | 1.518393558 |
| C | 5.40961522 | 1.520884158 | -0.248501451 |
| C | 3.967922209 | 4.703689669 | -2.195184038 |
| H | 5.005762253 | 4.397472395 | -2.009745573 |
| H | 4.166986472 | -4.54474562 | 2.013872805 |
| H | 7.344803384 | 2.247771995 | -0.831959347 |
| H | 4.316794319 | -2.289860929 | 0.081386947 |
| H | 0.371297541 | 2.291518364 | -3.020763744 |
| C | 4.837741533 | 1.558258373 | -1.638902275 |
| H | 3.771442185 | 4.619717637 | -3.266019849 |
| H | 5.453813038 | 2.184325898 | -2.295389758 |
| H | 0.637284009 | 0.5633425 | -2.709635827 |
| C | 0.900886205 | 1.396265661 | -3.367778434 |
| H | 4.859950259 | 0.541424202 | -2.053762098 |
| C | 2.431036353 | 1.600794503 | -3.432388629 |
| H | 2.968637239 | -0.514531929 | -3.100072048 |
| H | 0.527274811 | 1.161138434 | -4.375291493 |
| C | 3.084194185 | 0.266111218 | -3.85744831 |
| H | 2.242459666 | 3.600489557 | -4.358878515 |
| H | 3.839945765 | 2.846727539 | -4.585955665 |
| C | 2.763200106 | 2.648840001 | -4.511037226 |
| H | 2.586943725 | -0.088471628 | -4.771531648 |
| H | 4.148525298 | 0.388896022 | -4.09766509 |
| H | 2.437990362 | 2.2567766 | -5.486343439 |
| S | 1.60571777 | -2.613241158 | -1.033667952 |
| O | 2.648543907 | -3.602079896 | -1.351522801 |
| O | 0.743539798 | -2.866293117 | 0.135547933 |
| O | 2.119660394 | -1.176257384 | -1.107593106 |
| C | 0.447740226 | -2.646089289 | -2.495657317 |
| F | -0.516955778 | -1.716664802 | -2.355221636 |
| F | 1.114205261 | -2.390573333 | -3.634774437 |
| F | -0.130567518 | -3.848220864 | -2.595805102 |

```
  N     -0.30274668    0.126739695     0.05701126
  N    -1.398103237    0.259662925    0.163431744
-------------------------------------------------
```

**Supplementary Table 72 | Cartesian coordinate of the reactant complex for protonation of XXIV by LutH$^+$. Units are presented in Å.**

SCF energy (in toluene) = -3160.33583475 hartree

ZPE = 0.819388 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.668729425 | 0.76408586 | 0.649305018 |
| P | 0.17206536 | -0.723862687 | 2.669594978 |
| N | 1.479063577 | 1.338569209 | 0.925011559 |
| P | -0.220211709 | 2.286539423 | -1.405337272 |
| N | -1.38343517 | 1.915908552 | 1.674620274 |
| H | -1.23111363 | -1.812113895 | 6.119427867 |
| H | 0.312569987 | -1.014167378 | 5.788849624 |
| C | -0.443110618 | -1.686934099 | 5.362786774 |
| H | -1.176360017 | 0.908428792 | 4.94663945 |
| H | 0.013130099 | -2.669399522 | 5.210416941 |
| H | -2.618660719 | -0.08595654 | 5.179290811 |
| C | -1.830387923 | 0.173088635 | 4.458206827 |
| H | -2.889808569 | -2.293603767 | 4.268839877 |
| C | -1.078713713 | -1.119545677 | 4.077912605 |
| H | 0.422706644 | 1.509975818 | 3.568025467 |
| H | -2.301346644 | 0.643291292 | 3.589357945 |
| H | 1.780884076 | 0.54234306 | 4.176038675 |
| C | -2.111272563 | -2.120946618 | 3.511573132 |
| H | 2.038256342 | -2.136501257 | 4.719792374 |
| H | -2.589694283 | -1.742368441 | 2.602327946 |
| C | 1.169059667 | 0.754890503 | 3.292985354 |
| H | 3.740123947 | 1.684101145 | 3.413757963 |
| H | -1.668830192 | -3.088712577 | 3.262638531 |
| H | 3.136577223 | -1.151047476 | 3.728408586 |
| H | -0.178371144 | 3.832780191 | 1.147374867 |
| C | 2.518023886 | -2.057064007 | 3.740874854 |
| H | -1.687175409 | 5.752298915 | -0.81655162 |
| C | 3.333926095 | 1.722926467 | 2.406470932 |
| H | 3.206106999 | -2.908792349 | 3.645479361 |
| C | 2.023776953 | 1.294793384 | 2.17615696 |
| H | 0.210987542 | 5.496245825 | 0.633129045 |
| H | -2.287719979 | 4.150116558 | -0.342541201 |
| C | 0.345215567 | 4.430255881 | 0.395781919 |
| C | -1.662887482 | 4.683018187 | -1.071307434 |

| | | | |
|---|---|---|---|
| H | 5.133088814 | 2.503390537 | 1.501555373 |
| C | 1.530553624 | -2.109289436 | 2.552889451 |
| H | 1.418184165 | 4.218584901 | 0.466779343 |
| C | 4.107675918 | 2.177553167 | 1.34014071 |
| H | -2.121012683 | 4.573061951 | -2.059771045 |
| H | 0.423506286 | -3.794838567 | 3.448904148 |
| H | 2.909075114 | -0.953873847 | 1.271792335 |
| C | -0.204016016 | 4.182378085 | -1.027368029 |
| C | 0.872359691 | -3.504387529 | 2.492368615 |
| C | 2.356386089 | -1.899389895 | 1.262862485 |
| H | 3.101103938 | -2.705903217 | 1.206626745 |
| H | 0.697721139 | 6.048380767 | -1.635913876 |
| C | 3.55130584 | 2.20146539 | 0.062984063 |
| H | 0.11344583 | -3.576385194 | 1.708006219 |
| C | 2.23030621 | 1.783489197 | -0.120697751 |
| C | 0.677747883 | 5.007627843 | -1.990027041 |
| H | 1.717303245 | 4.656065796 | -1.997864361 |
| H | 1.65428886 | -4.242310723 | 2.265746509 |
| H | 4.129424264 | 2.540298265 | -0.79251737 |
| H | 1.756459618 | -1.958264413 | 0.353483019 |
| H | -2.967392524 | 2.436526945 | -2.541584292 |
| C | 1.594816961 | 1.792721872 | -1.484988146 |
| H | 0.311876614 | 5.022699756 | -3.016858585 |
| H | 2.18415419 | 2.396594106 | -2.184416999 |
| H | -2.554605752 | 0.707633015 | -2.428762591 |
| C | -2.408340751 | 1.618792682 | -3.015196866 |
| H | 1.583047177 | 0.763024463 | -1.867324994 |
| C | -0.907825272 | 1.945411908 | -3.183598044 |
| H | -0.172071557 | -0.133855482 | -3.07002501 |
| H | -2.850556068 | 1.451674033 | -4.007389826 |
| C | -0.186890468 | 0.709402503 | -3.762436301 |
| H | -1.312533891 | 3.989314719 | -3.946453739 |
| H | 0.300910466 | 3.360018736 | -4.370115947 |
| C | -0.748125679 | 3.087460426 | -4.206270109 |
| H | -0.722759402 | 0.388294633 | -4.666159763 |
| H | 0.84213218 | 0.944302753 | -4.06344354 |
| H | -1.141184839 | 2.731456458 | -5.169105631 |
| S | -0.65236241 | -2.446209663 | -0.921823905 |
| O | 0.520712251 | -3.285204579 | -1.196932589 |
| O | -1.528599668 | -2.808812004 | 0.209859514 |
| O | -0.313460144 | -0.947726714 | -0.933741955 |
| C | -1.741504034 | -2.630106463 | -2.428810402 |
| F | -2.776552289 | -1.766877127 | -2.370648087 |
| F | -1.045006393 | -2.380730104 | -3.547478606 |
| F | -2.221119773 | -3.872347755 | -2.479812314 |
| N | -2.627940924 | 0.010282803 | 0.263132999 |
| N | -3.674169065 | -0.35546906 | 0.108948682 |

| | | | |
|---|---|---|---|
| H | -2.476093069 | 2.930681005 | 2.5010196 |
| C | -2.705592502 | 4.415670054 | 3.964854992 |
| N | -3.177832951 | 3.584166547 | 2.999112131 |
| C | -4.479203271 | 3.532603998 | 2.613456065 |
| C | -5.390261165 | 4.382279874 | 3.23950865 |
| C | -4.949872125 | 5.251525131 | 4.237551175 |
| C | -3.601817926 | 5.269457214 | 4.602281117 |
| H | -3.238711272 | 5.940291276 | 5.37548072 |
| H | -5.655416479 | 5.917121625 | 4.73021045 |
| H | -6.433708958 | 4.354191196 | 2.939170582 |
| C | -1.241606197 | 4.353442165 | 4.288662917 |
| H | -0.977877208 | 5.127606984 | 5.014925917 |
| H | -0.982480552 | 3.375735429 | 4.715794165 |
| H | -0.630546711 | 4.491597568 | 3.388334988 |
| C | -4.858101837 | 2.548649338 | 1.547371855 |
| H | -5.849092379 | 2.780866456 | 1.146364631 |
| H | -4.130890535 | 2.547328725 | 0.728072846 |
| H | -4.888488262 | 1.529048058 | 1.955198224 |

**Supplementary Table 73 | Cartesian coordinate of the transition state for protonation of XXIV by LutH$^+$. Units are presented in Å.**

SCF energy (in toluene) = -3160.33093009 hartree

ZPE = 0.815146 hartree

Imaginary frequency: 1103*i*

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.39555315 | 0.497911238 | 0.447894075 |
| P | 0.403464816 | -0.981896572 | 2.49648311 |
| N | 1.737689151 | 1.074122439 | 0.762270434 |
| P | 0.09055375 | 2.017205525 | -1.609439228 |
| N | -1.139805493 | 1.66902953 | 1.452502621 |
| H | -1.071890718 | -2.056730301 | 5.914846763 |
| H | 0.467957967 | -1.240473923 | 5.615037601 |
| C | -0.267753024 | -1.927104168 | 5.176514348 |
| H | -1.019858604 | 0.659271222 | 4.713680998 |
| H | 0.204875224 | -2.904393855 | 5.042314344 |
| H | -2.451538511 | -0.350086582 | 4.934756119 |
| C | -1.654822526 | -0.090585074 | 4.223673967 |
| H | -2.682520092 | -2.569160916 | 4.0353839 |
| C | -0.88203168 | -1.378454408 | 3.873067863 |
| H | 0.623427591 | 1.262367939 | 3.383834088 |
| H | -2.123422442 | 0.363898786 | 3.34553403 |
| H | 1.969605247 | 0.302720553 | 4.025513461 |
| C | -1.889505802 | -2.397518841 | 3.293478343 |
| H | 2.22996746 | -2.363161048 | 4.598453787 |
| H | -2.353221777 | -2.034105046 | 2.370715143 |
| C | 1.376354197 | 0.507416238 | 3.128337152 |
| H | 3.941053612 | 1.446142968 | 3.297833429 |
| H | -1.431756417 | -3.363502613 | 3.066095491 |
| H | 3.346667699 | -1.378772483 | 3.626422925 |
| H | 0.111169841 | 3.576166935 | 0.936587895 |
| C | 2.733072414 | -2.288110773 | 3.631049062 |
| H | -1.377952181 | 5.487225326 | -1.058751872 |
| C | 3.557562831 | 1.474144806 | 2.281410195 |
| H | 3.428055646 | -3.136366578 | 3.559010737 |
| C | 2.25396373 | 1.040917961 | 2.026295802 |
| H | 0.498806138 | 5.234196919 | 0.419149487 |
| H | -1.987459114 | 3.894457326 | -0.57320895 |

| | | | |
|---|---|---|---|
| C | 0.639992092 | 4.168789609 | 0.185826292 |
| C | -1.354233499 | 4.415707494 | -1.302588445 |
| H | 5.375335312 | 2.248423742 | 1.40957366 |
| C | 1.776472093 | -2.35723435 | 2.418156646 |
| H | 1.712966125 | 3.961074308 | 0.267370832 |
| C | 4.354280387 | 1.919534936 | 1.228179935 |
| H | -1.803329841 | 4.297164143 | -2.294175589 |
| H | 0.659061974 | -4.043693222 | 3.299353122 |
| H | 3.178200099 | -1.200192015 | 1.162639919 |
| C | 0.103473445 | 3.913773352 | -1.24022459 |
| C | 1.132236857 | -3.758639039 | 2.353226431 |
| C | 2.634948648 | -2.150968775 | 1.149178222 |
| H | 3.38919087 | -2.950050715 | 1.122926558 |
| H | 1.02029964 | 5.771229759 | -1.846800371 |
| C | 3.826913782 | 1.931393568 | -0.061415524 |
| H | 0.396137266 | -3.845473074 | 1.549269338 |
| C | 2.510377095 | 1.512332493 | -0.271095092 |
| C | 0.997492274 | 4.730289701 | -2.199536935 |
| H | 2.035382383 | 4.373569497 | -2.199512385 |
| H | 1.927157796 | -4.491149813 | 2.15652451 |
| H | 4.423712253 | 2.263852567 | -0.906455063 |
| H | 2.061999661 | -2.227369783 | 0.223941273 |
| H | -2.640492965 | 2.153570933 | -2.784245445 |
| C | 1.903496871 | 1.515190999 | -1.64851569 |
| H | 0.638324041 | 4.745934265 | -3.228595419 |
| H | 2.507766944 | 2.116092331 | -2.337514345 |
| H | -2.227633223 | 0.426702297 | -2.652252077 |
| C | -2.073659299 | 1.333227342 | -3.243617438 |
| H | 1.897870596 | 0.484541427 | -2.027936537 |
| C | -0.571919907 | 1.662366115 | -3.393941797 |
| H | 0.172391196 | -0.412947322 | -3.264234755 |
| H | -2.501766871 | 1.157902187 | -4.240454034 |
| C | 0.164611715 | 0.428928679 | -3.957757579 |
| H | -0.97381301 | 3.7020031 | -4.169289338 |
| H | 0.647158092 | 3.076757349 | -4.570635858 |
| C | -0.402815078 | 2.801569391 | -4.418489898 |
| H | -0.354050978 | 0.103292819 | -4.869756635 |
| H | 1.197434845 | 0.668209403 | -4.241655658 |
| H | -0.782891194 | 2.439883237 | -5.384325839 |
| S | -0.338390531 | -2.682309849 | -1.081870301 |
| O | 0.855803144 | -3.494067959 | -1.340557149 |
| O | -1.225073402 | -3.052412803 | 0.036859388 |
| O | -0.018939304 | -1.171633651 | -1.085715226 |
| C | -1.400062641 | -2.884067394 | -2.607543921 |
| F | -2.440217534 | -2.027668786 | -2.574656767 |
| F | -0.683872169 | -2.643096452 | -3.713909173 |
| F | -1.867722217 | -4.130042125 | -2.648812952 |

| | | | |
|---|---|---|---|
| N | -2.356778843 | -0.256458044 | 0.043369104 |
| N | -3.394955573 | -0.634540776 | -0.12411686 |
| H | -1.96574477 | 2.467333742 | 2.061218232 |
| C | -2.3244737 | 4.115889753 | 3.613262969 |
| N | -2.785232731 | 3.295538319 | 2.637860809 |
| C | -4.075331656 | 3.338789538 | 2.225685058 |
| C | -4.964490154 | 4.246659847 | 2.805472153 |
| C | -4.514348329 | 5.1015441 | 3.80997272 |
| C | -3.182240605 | 5.036003338 | 4.217957958 |
| H | -2.802201463 | 5.689789834 | 4.99832478 |
| H | -5.195163486 | 5.814297228 | 4.270655718 |
| H | -5.996423067 | 4.274323231 | 2.466192292 |
| C | -0.881111446 | 3.985999667 | 4.020038608 |
| H | -0.606546944 | 4.775805709 | 4.725979021 |
| H | -0.702488872 | 3.018553112 | 4.508009311 |
| H | -0.213345689 | 4.048768373 | 3.152584852 |
| C | -4.504363822 | 2.377416896 | 1.15173871 |
| H | -5.511552689 | 2.617463866 | 0.797671404 |
| H | -3.819397648 | 2.40043758 | 0.296041383 |
| H | -4.517753684 | 1.347702792 | 1.53233633 |

**Supplementary Table 74 | Cartesian coordinate of the product complex for protonation of XXIV by LutH$^+$. Units are presented in Å.**

SCF energy (in toluene) = -3160.33535581 hartree

ZPE = 0.818313 hartree

| Atom | Coordinates (Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| Mo | -0.712471133 | 0.726910071 | 0.704379023 |
| P | 0.136302394 | -0.767925682 | 2.726204525 |
| N | 1.395012816 | 1.358607307 | 0.996830048 |
| P | -0.3316328 | 2.340549388 | -1.299352492 |
| N | -1.460614769 | 1.867570067 | 1.763745194 |
| H | -1.275841956 | -1.897973745 | 6.147024136 |
| H | 0.246726151 | -1.056936705 | 5.831867792 |
| C | -0.484700319 | -1.751058453 | 5.398267828 |
| H | -1.295941503 | 0.837146158 | 4.951588735 |
| H | -0.000942734 | -2.721027733 | 5.249953083 |
| H | -2.68865594 | -0.212652477 | 5.218485557 |
| C | -1.922183166 | 0.067397961 | 4.482773294 |
| H | -2.905839982 | -2.4233774 | 4.280330281 |
| C | -1.128747199 | -1.20145637 | 4.109158937 |
| H | 0.331513564 | 1.467055299 | 3.650879107 |
| H | -2.436318615 | 0.508234262 | 3.623830765 |
| H | 1.707704663 | 0.519487508 | 4.237992045 |
| C | -2.12264792 | -2.235170469 | 3.532397679 |
| H | 2.008709715 | -2.161030535 | 4.777725407 |
| H | -2.601851806 | -1.873885337 | 2.616743759 |
| C | 1.090354386 | 0.730600417 | 3.359035006 |
| H | 3.628051179 | 1.732713941 | 3.505489883 |
| H | -1.65080354 | -3.192613905 | 3.296769487 |
| H | 3.096655877 | -1.133251909 | 3.818158337 |
| H | -0.298283381 | 3.827846758 | 1.32517576 |
| C | 2.50060767 | -2.05402189 | 3.807814866 |
| H | -1.916405661 | 5.721828347 | -0.561645598 |
| C | 3.226625383 | 1.775540498 | 2.49663966 |
| H | 3.210843201 | -2.886802678 | 3.709027143 |
| C | 1.932979576 | 1.308296101 | 2.252050726 |
| H | 0.035086201 | 5.500138487 | 0.833835499 |
| H | -2.451058726 | 4.092464307 | -0.118271288 |
| C | 0.193317553 | 4.444946484 | 0.569205723 |
| C | -1.859712803 | 4.662037044 | -0.846500166 |

| | | | |
|---|---|---|---|
| H | 5.002553018 | 2.6338134 | 1.618014642 |
| C | 1.532224009 | -2.114952249 | 2.604191081 |
| H | 1.273069251 | 4.261493046 | 0.612270272 |
| C | 3.989384298 | 2.277747388 | 1.444112445 |
| H | -2.333476407 | 4.563531405 | -1.828964705 |
| H | 0.453722654 | -3.834462881 | 3.465438941 |
| H | 2.909430574 | -0.908543407 | 1.37044587 |
| C | -0.381717292 | 4.218371717 | -0.846774273 |
| C | 0.911242285 | -3.525421681 | 2.519277614 |
| C | 2.370476602 | -1.861214095 | 1.330559341 |
| H | 3.127996172 | -2.654646616 | 1.263142391 |
| H | 0.444668277 | 6.128582818 | -1.41347849 |
| C | 3.436899873 | 2.316207705 | 0.16564169 |
| H | 0.16649566 | -3.610393779 | 1.723430621 |
| C | 2.131257241 | 1.861669332 | -0.03466851 |
| C | 0.449371825 | 5.10144203 | -1.804483374 |
| H | 1.499577673 | 4.78605915 | -1.852262485 |
| H | 1.715712675 | -4.24098628 | 2.300621186 |
| H | 4.005158714 | 2.699309926 | -0.677563949 |
| H | 1.783858175 | -1.90506788 | 0.41186117 |
| H | -3.09740858 | 2.435084863 | -2.388534622 |
| C | 1.495895683 | 1.902286557 | -1.398851579 |
| H | 0.054261275 | 5.140959586 | -2.81939898 |
| H | 2.062937081 | 2.557023118 | -2.070141304 |
| H | -2.632060458 | 0.718660793 | -2.328588436 |
| C | -2.521239568 | 1.648597295 | -2.892087054 |
| H | 1.521609261 | 0.891243566 | -1.826687233 |
| C | -1.034388132 | 2.025941963 | -3.072358161 |
| H | -0.223867735 | -0.030610564 | -3.035440584 |
| H | -2.972403583 | 1.4943822 | -3.882090166 |
| C | -0.277757118 | 0.834717632 | -3.69764228 |
| H | -1.524312684 | 4.073655804 | -3.766236519 |
| H | 0.108600068 | 3.52279217 | -4.225090747 |
| C | -0.927113245 | 3.204381171 | -4.060229262 |
| H | -0.812797913 | 0.523791011 | -4.605191273 |
| H | 0.738758433 | 1.114383164 | -4.0023739 |
| H | -1.316587497 | 2.862559664 | -5.029452942 |
| S | -0.644165442 | -2.373549204 | -0.856088629 |
| O | 0.566301481 | -3.137741987 | -1.16671514 |
| O | -1.498991397 | -2.789867187 | 0.267993402 |
| O | -0.349699199 | -0.84660264 | -0.814071458 |
| C | -1.733414913 | -2.541763254 | -2.367811463 |
| F | -2.788395488 | -1.710335934 | -2.280077089 |
| F | -1.044792338 | -2.24960292 | -3.477288481 |
| F | -2.171801148 | -3.795872506 | -2.435838195 |
| N | -2.700566833 | -0.014167814 | 0.350099092 |
| N | -3.748042469 | -0.373383867 | 0.212443574 |

| | | | |
|---|---|---|---|
| H | -2.163983092 | 2.456974761 | 2.311854839 |
| C | -2.875667843 | 4.320048424 | 4.205668809 |
| N | -3.322644017 | 3.504767083 | 3.226067788 |
| C | -4.639894306 | 3.47717678 | 2.929571053 |
| C | -5.560853669 | 4.278492672 | 3.614257361 |
| C | -5.106741349 | 5.121965471 | 4.626184114 |
| C | -3.745653181 | 5.144413554 | 4.92711536 |
| H | -3.355931585 | 5.790319347 | 5.710072257 |
| H | -5.803707153 | 5.754211328 | 5.172797025 |
| H | -6.615149369 | 4.235133498 | 3.352437527 |
| C | -1.394664518 | 4.304128303 | 4.494096477 |
| H | -1.136518795 | 5.011920552 | 5.288722336 |
| H | -1.070965586 | 3.303892986 | 4.813547584 |
| H | -0.815776599 | 4.569042776 | 3.599420628 |
| C | -5.081355914 | 2.537457977 | 1.836022074 |
| H | -6.142283676 | 2.670656085 | 1.600381498 |
| H | -4.502971028 | 2.701416185 | 0.917485895 |
| H | -4.933444537 | 1.491039406 | 2.135775692 |

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**Supplementary Methods**

**X-ray Crystallography.** Crystallographic data of **2**·7/3$C_4H_8O$, **3**·1/6$C_6H_{14}$, **4,** and **5**·$C_4H_8O$ are summarized in Supplementary Tables 1 and 2. Selected bond lengths and angles are summarized in Supplementary Tables 3–6, and their ORTEP drawings are shown in Supplementary Figures 1–4. A preliminary X-ray analysis of **2**·7/3$C_4H_8O$ has shown that the chroride (Cl(2) and Cl (3)) and nitride (N(2) and N(3)) atoms bonded to molybdenum atom trans to each other are disordered between two positions in a ratio of 0.75:0.25. A preliminary X-ray analysis of **3**·1/6$C_6H_{14}$ has shown that there is a two-fold screw axis running through the Cl(1), N(1) and C(1) atoms and that the molybdenum nitride group (Mo(1)-N(2)) is crystallographically disordered between two symmetrical positions with one-half atomic occupancies. Thus, superficial but false elongation of the Mo≡N bonds are unavoidable for the crystallographic data of **2**·7/3$C_4H_8O$ and **3**·1/6$C_6H_{14}$, and their metric features around the molybdenum atoms are indiscussible. Diffraction data were collected at –75 °C (**2**·7/3$C_4H_8O$, **3**·1/6$C_6H_{14}$, and **5**·$C_4H_8O$) or –90 °C (**4**) on a Rigaku RAXIS RAPID imaging plate area detector with graphite-monochromated Mo Kα radiation (λ = 0.71075 Å). Reflections were collected for the 2$\theta$ range of 5° to 55°. Intensity data were corrected for Lorenz-polarization effects and for empirical absorption (ABSCOR for **2**·7/3$C_4H_8O$, **4**, and **5**·$C_4H_8O$) or numerical absorption (NUMABS for **3**·1/6$C_6H_{14}$). The structure solution and refinements were carried out by using the *CrystalStructure* crystallographic software package.[1] The positions of the non-hydrogen atoms were determined by direct methods (SHELX-97[2]) and subsequent Fourier syntheses (DIRDIF-99[3]), and were refined $F_o^2$ using all unique reflections by full-matrix least-squares with anisotropic thermal parameters except for all the THF molecules in **2**·7/3$C_4H_8O$, and one methyl carbon atom (C(4)) and hexane carbon atoms (C(13) and C(14)) in **3**·1/6$C_6H_{14}$. Location of the imide hydrogen atom (H49) of **5**·$C_4H_8O$ was found in a difference Fourier map and was refined isotropically, while all the other hydrogen atoms except for those in THF and hexane molecules in **2**·7/3$C_4H_8O$ and **3**·1/6$C_6H_{14}$ were placed at the calculated positions with fixed isotropic parameters.

For the crystallographic data of **2**·7/3$C_4H_8O$, one THF molecule is disordered between two positions (O(2)-C(28)-C(29)-C(30)-C(31) and O(3)-C(32)-C(33)-C(34)-C(35)) and were refined

with one-half occupancies. Other two THF molecules containing O(4) and O(5) atoms are disordered around two three-fold rotoinversion axes, where one-sixth moiety of five non-hydrogen atoms were solved with one oxygen atom, where its atomic occupancy is given as two thirds (32 electrons for non-hydrogen atoms in THF, divided by 6 asymmetric units, divided by 8 electrons for one oxygen atom). The total number of THF molecules per complex **2** is calculated as seven thirds (one for O(1), two halves for those containing O(2) and O(3) , and two sixths for those containing O(4) and O(5)). Consequently, the total void space is filled with the THF molecules.

For the crystallographic data of **3**·1/6$C_6H_{14}$, one methyl carbon atom (C(4)) was disordered and solved with isotropic thermal parameters. Thus, the alert level B errors (PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ……. 1) is not avoidable. A hexane molecule consisting of C(13) and C(14) atoms appears as a disorder to form a linearly extended carbon chains along the *c*-axis in **3**·1/6$C_6H_{14}$, where their atomic occupancies were given as one third, corresponding to one-sixth hexane molecule per complex **3**.

For the crystallographic data of **4**, the maximum residual peak exists very near to the molybdenum atom (0.910 Å), thus the alert level B errors (DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00_refine_diff_density_max given = 4.700 and PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 4.70 e$Å^{-3}$) are not avoidable.

## Computational details

### Three possible reaction pathways for formation of the six-coordinate imide complex XIII.

Because the formation of the six-coordinate imide complex **XIII** involves three elementary steps, protonation, reduction, and $N_2$ coordination, there are three reaction pathways, Paths E, F, and G, to be considered (Supplementary Figure 5). Details in Path E are discussed in the main text. In Path F, protonation of the nitride complex **XI** gives a cationic five-coordinate imide complex **XXII**. Dinitrogen attacks the vacant coordination site in **XXII** to give a cationic six-coordinate imide complex **XXIII**, and then the generated **XXIII** is reduced to give **XIII**. In Path G, dinitrogen first coordinates to **XI** to afford a six-coordinate nitride complex **XXIV** and then protonated. In all the pathways, the protonation step is found to be slightly endothermic, followed by a highly exothermic reduction step. The coordination of dinitrogen is also possible at room temperature.

**Supplementary References**

(1) *CrystalStructure 3.80: Single Crystal Structure Analysis Software*; Rigaku Corp: Tokyo, Japan, and MSC: The Woodlands, TX, pp 2000–2007.

(2) Sheldrick, G. M. *SHELX-97: Program for the Refinement of Crystal Structure*; University of Göttingen: Göttingen, Germany, 1997.

(3) Beurskens, P. T., Beurskens, G., de Gelder, R., García-Granda, S., Gould, R. O., Israël, R. & Smits, J. M. M. *The DIRDIF-99 Program System*; Crystallography Laboratory, University of Nijmegen: Nijmegen, The Netherlands, 1999.