Supplementary Information (SI) for Inorganic Chemistry Frontiers.

Three-Component Diazaphospholium Synthesis Enables P(V)-to-P(III) Conversion and Ylide-Mediated CO_2 and CS_2 Activation

Linwei Huang,[a] Jannis Fidelius,[a] Kai Schwedtmann,[a] Philipp Royla,[a] Rosa M. Gomila,[b] Antonio Frontera,[b] and Jan J. Weigand[a,*]

[a] *Chair of Inorganic Molecular Chemistry, Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01069 Dresden, Germany.*
[b] *Department of Chemistry, Universitat de Illes Balears, 07122 Palma de Mallorca, Spain.*

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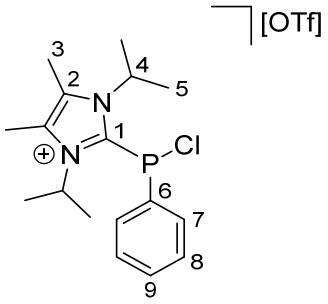
S1 General Remarks

Manipulations were performed in a Glovebox MB Unilab or using Schlenk techniques under an atmosphere of purified nitrogen or argon, respectively. All glassware was dried in oven at 160 °C prior to use. Dry, oxygen-free solvents: CH_2Cl_2, C_6H_5F, $CHCl_3$, CH_3CN were distilled from CaH_2; *n*-hexane, *n*-pentane, THF, Et_2O, toluene, benzene were distilled from potassium. Deuterated solvents, CD_2Cl_2, C_6D_6 and $CDCl_3$ were stored over 4 Å molecular sieves. CD_3CN was stored over 3 Å molecular sieves. AgOTf was purchased from BLD Pharm and used as received. Paraformaldehyde and potassium bis(trimethylsilyl)amide (KHMDS) were purchased from Sigma Aldrich and used as received. 4-(Dimethylamino)benzonitrile, 4-dimethylaminopyridine (DMAP), 4-nitrobenzaldehyde and sulfur were purchased from Sigma Aldrich and purified by sublimation prior to use. 4-Methoxybenzonitrile, benzonitrile, 4-methylbenzaldehyde, 4-methoxybenzaldehyde, DBU (1, 8-Diazabicyclo[5.4.0]undec-7-ene) and *E*-cinnamaldehyde were purchased from Sigma Aldrich and distilled in an inert atmosphere and stored over 4 Å molecular sieves prior to use. CS_2 was distilled in an inert atmosphere prior to use. [**L**$_{\mathbf{C}}$–TMS][OTf] was synthesized according to literature procedures.[1] NMR spectra were measured on a Bruker AVANCE III HD Nanobay 400 MHz UltraSield (^{1}H: 400.13 MHz, ^{13}C: 100.61 MHz, ^{31}P: 161.98 MHz) or on a Bruker AVANCE III HDX, 500 MHz Ascend (1H: 500.13 MHz, ^{13}C: 125.75 MHz, ^{31}P: 202.45 MHz). All ^{13}C NMR spectra were exclusively recorded with composite pulse decoupling. Reported numbers assigning atoms in the ^{13}C spectra were indirectly deduced from the cross-peaks in 2D correlation experiments (HMBC, HSQC). Chemical shifts were referenced to δ TMS = 0.00 ppm (^{1}H, ^{13}C), δ (H_3PO_4, 85%) = 0.00 ppm (^{31}P). Chemical shifts (δ) are reported in ppm. Coupling constants (J) are reported in Hz.

Melting points were recorded on an electrothermal melting point apparatus (Büchi Switzerland, Melting point M-560) in sealed capillaries under Nitrogen atmosphere and are uncorrected. Infrared (IR) and Raman spectra were recorded at ambient temperature using a Bruker Vertex 70 instrument equipped with a RAM II module (Nd-YAG laser, 1064 nm). The Raman intensities are reported in percent relative to the most intense peak and are given in parenthesis. An ATR unit (diamond) was used for recording IR spectra. The intensities are reported relative to the most intense peak and are given in parenthesis using the following abbreviations: vw = very weak, w = weak, m = medium, s = strong, vs = very strong. Elemental analysis was performed on a Vario MICRO cube Elemental Analyzer by Elementary Analysatorsysteme GmbH in CHNS modus.

S2 Synthetic procedures, spectroscopic data and additional remarks

S2.1 Preparation of [L$_C$PClPh][OTf]



A mixture of [**L$_C$**–TMS][OTf] (10.00 g, 24.84 mmol, 1.0 eq.) and $PPhCl_2$ (11.12 g, 8.43 mL, 62.1 mmol, 2.5 eq.) in PhF (60 mL) was heated at 80 ˚C in a pressure-sealed tube for 12 h. Removal of all volatiles afforded a sticky oil, which was treated with 10 mL Et_2O to give a white suspension. The mixture was filtered, and the solid was dried *in vacuo* to afford an analytically pure air- and moisture-sensitive off-white solid.

Yield: 15.30 g, 99%; **m.p.**: 67 °C. **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.62 (12H, m, H5), 2.48 (6H, s, H3), 5.02 (2H, m, H4), 7.51 (1H, m, H9), 7.58 (2H, m, H8), 7.62 (2H, m, H7). **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 10.9 (2C, s, C3), 22.4 (4C, s, C5), 53.2 (2C, d, $^3J_{CP}$ = 9 Hz, C4), 120.8 (1C, q, $^1J_{CF}$ = 321 Hz, OTf), 129.3 (2C, d, $^2J_{CP}$ = 20 Hz, C7), 130.0 (2C, d, $^3J_{CP}$ = 4 Hz, C8), 130.9 (1C, d, $^1J_{CP}$ = 27 Hz, C6), 131.3 (1C, d, $^4J_{CP}$ = 2 Hz, C9), 133.3 (2C, brs, C2), 138.7 (1C, d, $^1J_{CP}$ = 88 Hz, C1). **^{19}F{^{1}H} NMR** (470.59 MHz, $CDCl_3$, 300 K, [ppm]): δ = -78.3 (s, OTf). **^{31}P{^{1}H} NMR** ($CDCl_3$, 300 K, in ppm): δ = 46.6 (s).

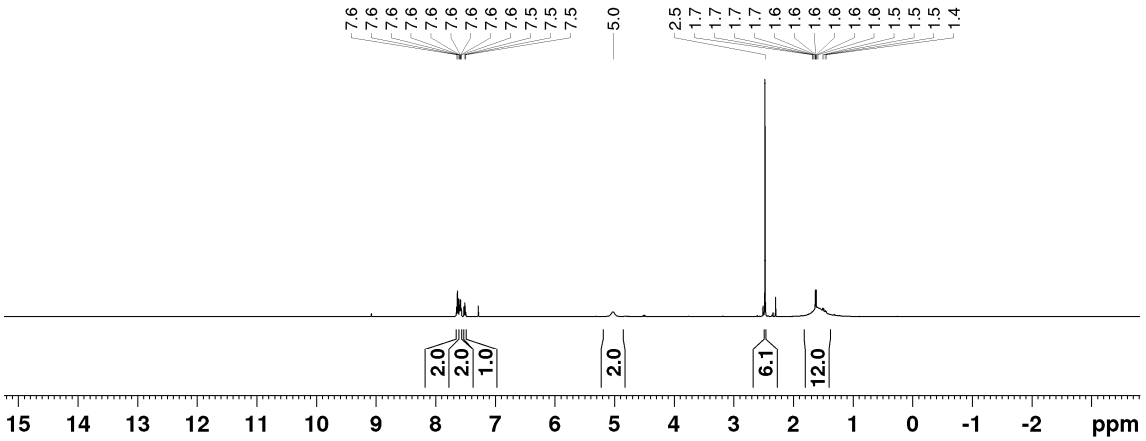


Figure S1. ^{1}H NMR spectrum of [**L$_C$**PClPh][OTf] (300 K, $CDCl_3$).

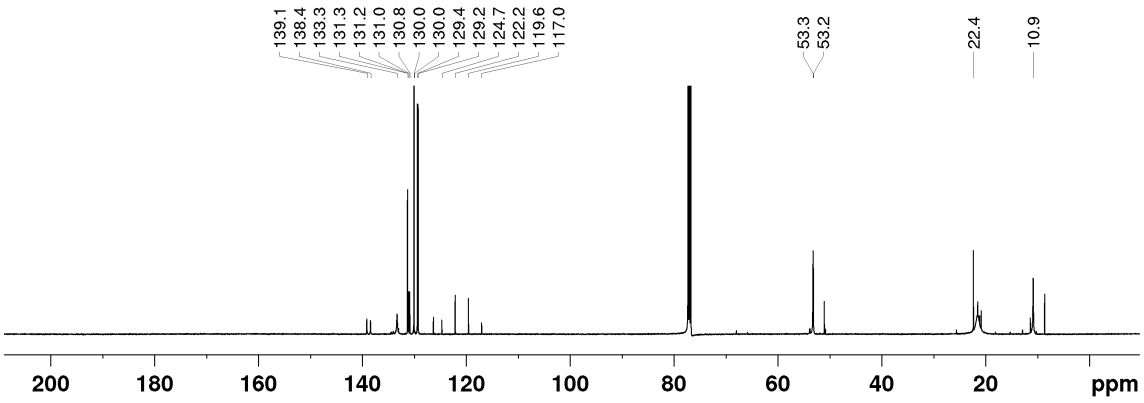


Figure S2. ^{13}C {^{1}H} NMR spectrum of [**Lc**PClPh][OTf] (300 K, $CDCl_3$).

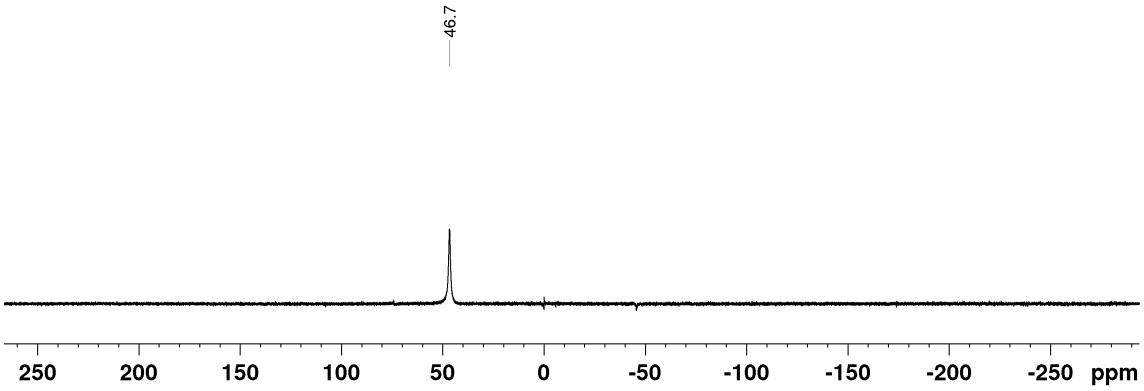


Figure S3. ^{31}P {^{1}H} NMR spectrum of [**Lc**PClPh][OTf] (300 K, $CDCl_3$).

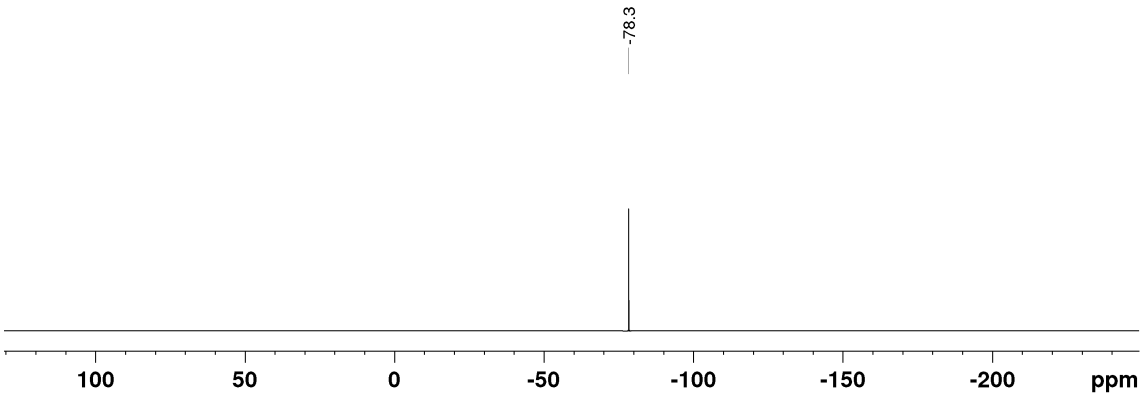
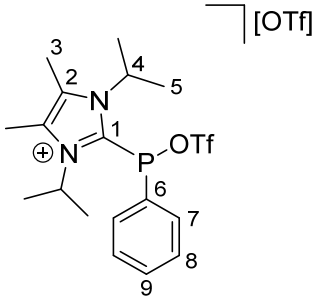


Figure S4. ^{19}F {^{1}H} NMR spectrum of [**Lc**PClPh][OTf] (300 K, $CDCl_3$).

S2.2 Preparation of 1[OTf]



A mixture of [**L$_C$**PClPh][OTf] (200 mg, 0.32 mmol, 1 eq.) and AgOTf (114 mg, 0.44 mmol, 1.05 eq.) in DCM (3 mL) were stirred for 4 h at room temperature. The suspension was filtered to remove AgCl. Removal of all volatiles gave a white, air and moisture sensitive solid.
Note: This compound is stable upon storage in glovebox. For the synthesis of azaphospholium salts, isolation of this compound is not necessary; after filtration to remove AgCl, the resulting filtrate was used directly in the cycloaddition reactions.

Yield: 240 mg, 97%; **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.63 (12H, m, H5), 2.54 (6H, s, H3), 4.95 (2H, m, H4), 7.61 (1H, m, H9), 7.66 (4H, m, H8, H7). **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 11.4 (2C, s, C3), 21.5 (4C, s, C5), 53.8 (2C, d, $^3J_{CP}$ = 9 Hz, C4), 119.7 (1C, q, $^1J_{CF}$ = 320 Hz, OTf), 128.7 (1C, d, $^2J_{CP}$ = 14 Hz, C6), 129.3 (2C, d, $^2J_{CP}$ = 19 Hz, C7), 130.5 (2C, d, $^2J_{CP}$ = 5 Hz, C8), 132.6 (1C, s, C9), 135.0 (2C, brs, C2), 136.3 (1C, d, $^1J_{CP}$ = 71 Hz, C1). **^{31}P{^{1}H} NMR** ($CDCl_3$, 300 K, in ppm): δ = 113.5 (s). **^{19}F{^{1}H} NMR** (470.59 MHz, $CDCl_3$, 300 K, [ppm]): δ = -76.3 (brs, OTf).

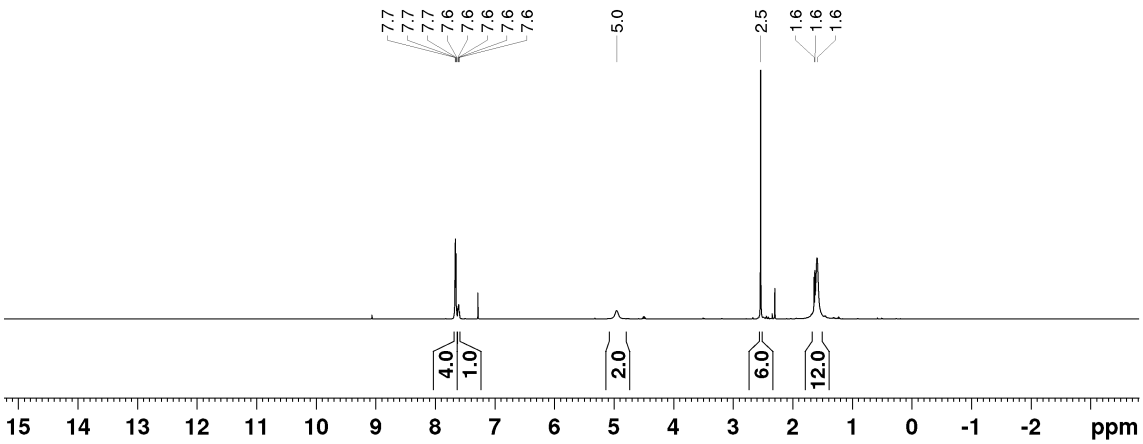


Figure S5. ^{1}H NMR spectrum of 1[OTf] (300 K, $CDCl_3$).

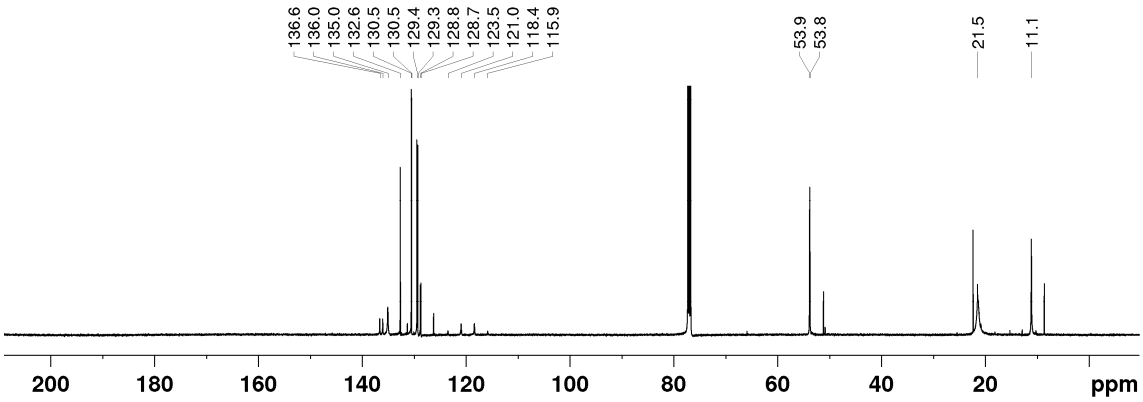


Figure S6. ^{13}C {^{1}H} NMR spectrum of **1**[OTf] (300 K, $CDCl_3$).

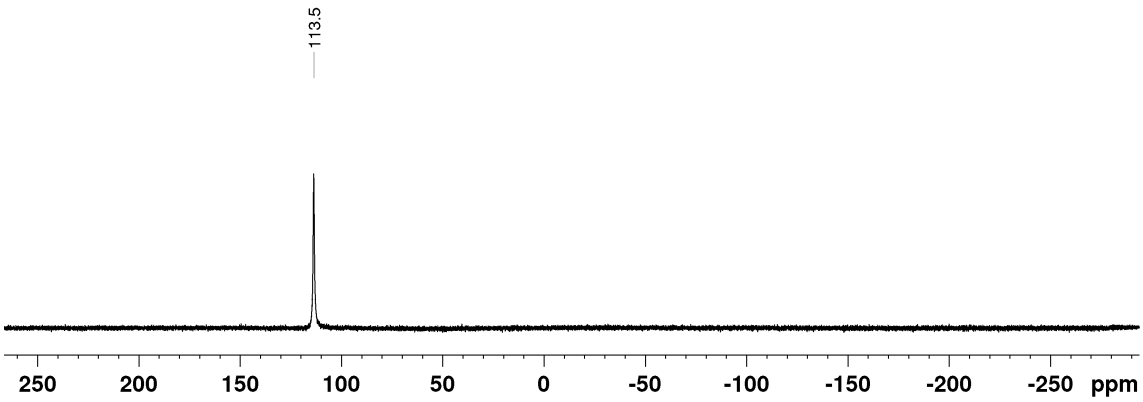


Figure S7. ^{31}P {^{1}H} NMR spectrum of **1**[OTf] (300 K, $CDCl_3$).

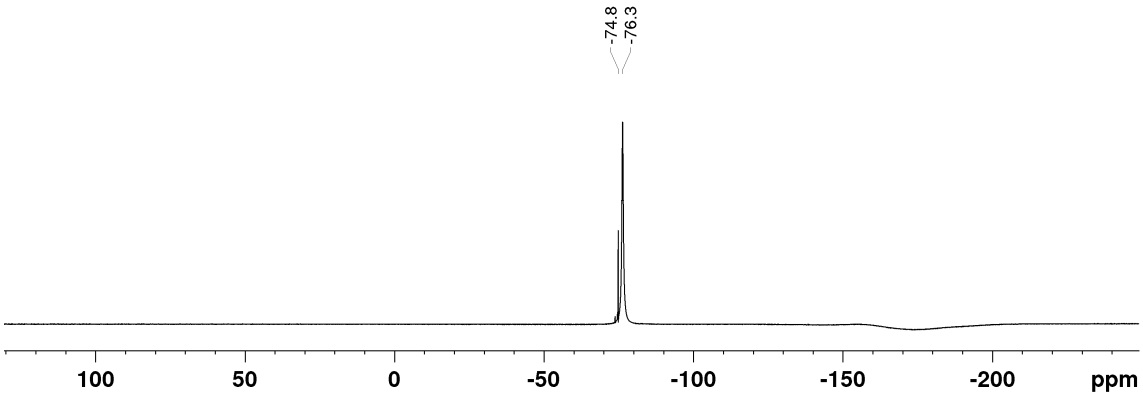
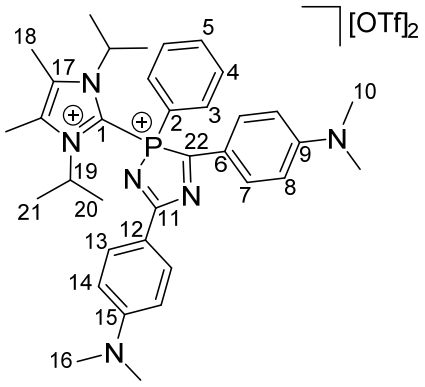


Figure S8. ^{19}F {^{1}H} NMR spectrum of **1**[OTf] (300 K, $CDCl_3$). (δ = - 74.8 ppm, AgOTf).

S2.3 Preparation of 2[OTf]$_2$



A mixture of [**L$_C$**PClPh][OTf] (640 mg, 1.35 mmol, 1eq.) and AgOTf (350 mg, 1.35 mmol, 1eq.) in DCM (10 mL) were stirred for 4 h at room temperature. The suspension was filtered to remove AgCl. 4-(Dimethylamino)benzonitrile (396 mg, 2.71 mmol) was added to the solution resulting in a deep blue solution and the reaction was allowed to stir for 16 h. Removal of all volatiles results in a blue solid, which was washed with 5 mL Et_2O three times to obtain the product as a blue solid. Suitable crystals for X-ray diffraction analysis can be obtained by layering a DCM solution with Et_2O at –30 °C.

Yield: 1.14 g, 96%; **m.p.**: 151 °C. **Raman** (100 mW, 500 scans, 298 K, [cm^{-1}]): 1612 (24), 1459 (8), 1393 (13), 1348 (8), 1313 (11), 1275 (53), 1232 (100), 1180 (16), 1151 (14), 1065 (20), 1033 (6), 992 (7), 957 (18), 912 (53), 843 (11), 759 (8), 739 (7), 701 (5), 618 (10), 429 (5), 346

(6), 169 (5), 75 (8). **IR** (ATR, 298 K, [cm^{-1}]): 2958 (vw), 2934 (vw), 1730 (vw), 1598 (m), 1460 (vw), 1414 (w), 1377 (m), 1346 (vw), 1318 (vw), 1260 (s), 1234 (m), 1221 (m), 1145 (vs), 1066 (m), 1027 (s), 953 (w), 937 (w), 907 (w), 878 (vw), 827 (w), 752 (w), 736 (w), 694 (vw), 635 (vs), 563 (m), 515 (m), 469 (w). **^{1}H NMR** (400.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 1.37 (6H, d, $^{3}J_{HH}$ = 6.9 Hz, H21), 1.66 (6H, d, $^{3}J_{HH}$ = 6.8 Hz, H20), 2.57 (6H, m, H18), 3.29 (6H, m, H16), 3.34 (6H, m, H10), 5.03 (2H, m, H19), 6.95 (4H, m, Ar-H), 7.77 (2H, m, Ar-H), 7.86 (1H, m, Ar-H), 8.21 (4H, m, Ar-H), 8.66 (2H, m, Ar-H), **^{13}C{^{1}H} NMR** (100.61 MHz, CD_2Cl_2, 300 K, in ppm): δ = 11.6 (2C, s, C18), 20.6 (2C, s, C21), 20.9 (2C, s, C20), 40.6 (2C, s, C16), 40.7 (2C, s, C10), 55.8 (2C, s, C19), 114.0 (1C, s, C5), 116.8 (1C, d, $^{1}J_{CP}$ = 30 Hz, C2), 118.5 (1C, d, $^{2}J_{CP}$ = 18 Hz, C6), 119.8 (2C, s, C13), 120.8 (2C, s, C4), 122.4 (2C, q, $^{3}J_{CF}$ = 320 Hz, OTf), 125.0 (2C, s, C14), 126.1 (2C, s, C8), 129.1 (1C, d, $^{1}J_{CP}$ = 20 Hz, C1), 130.4 (1C, d, $^{3}J_{CP}$ = 5 Hz, C12), 131.2 (2C, d, $^{3}J_{CP}$ = 15 Hz, C4), 131.8 (2C, d, $^{3}J_{CP}$ = 13 Hz, C7), 136.5 (2C, d, $^{2}J_{CP}$ = 3 Hz, C3), 136.8 (2C, d, $^{3}J_{CP}$ = 4 Hz, C17), 156.7 (1C, s, C15), 157.2 (1C, s, C9), 170.4 (1C, d, $^{2}J_{CP}$ = 9 Hz, C11), 183.3 (1C, d, $^{1}J_{CP}$ = 12 Hz, C22). **^{19}F NMR** (376.5 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.6 (s, OTf). **^{31}P{^{1}H} NMR** (100.61 MHz, CD_2Cl_2, 300 K, in ppm): δ = 46.8 (s). **Elemental analysis**: calculated for $C_{37}H_{45}F_6N_6O_6PS_2$: C, 50.56; H, 5.16; N, 9.56; S, 7.30; found: C, 50.03; H, 5.132; N, 9.29; S, 7.724.

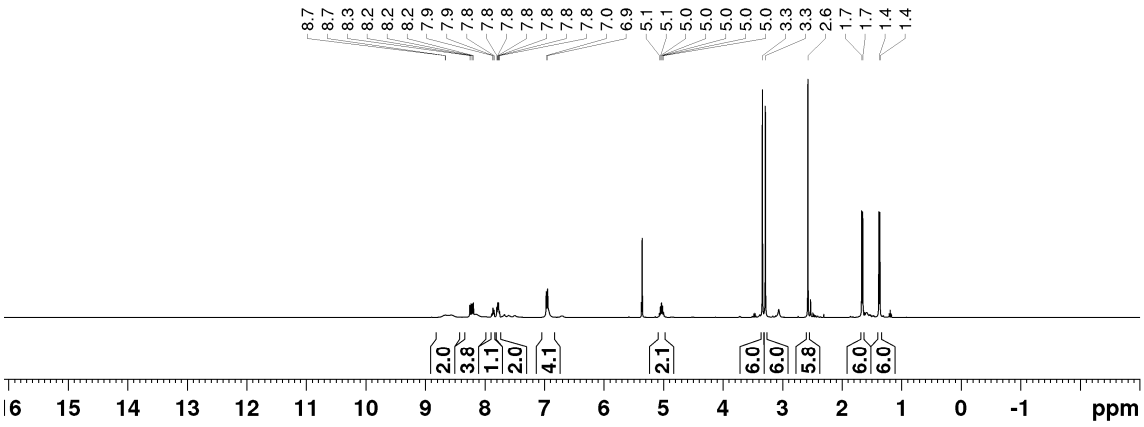


Figure S9. ^{1}H NMR spectrum of **2**[OTf]$_2$ (300 K, CD_2Cl_2).

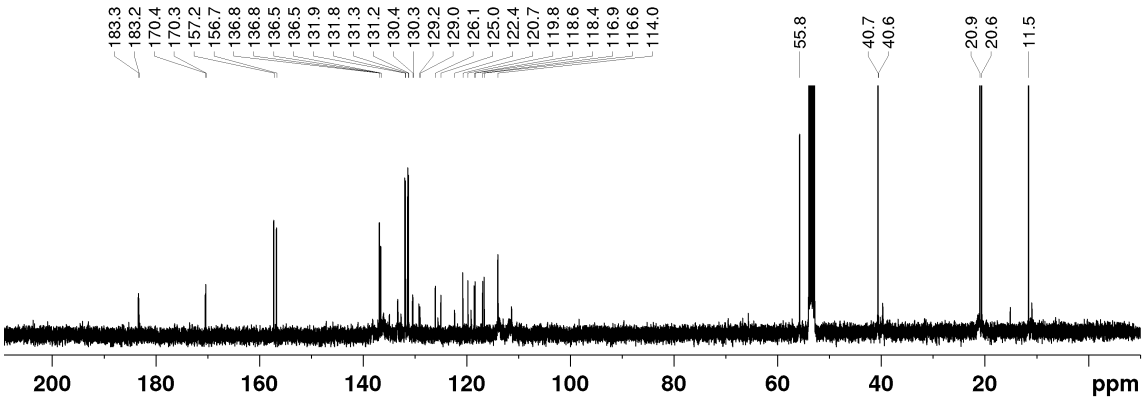


Figure S10. ^{13}C{^{1}H} NMR spectrum of **2**[OTf]$_2$ (300 K, CD_2Cl_2).

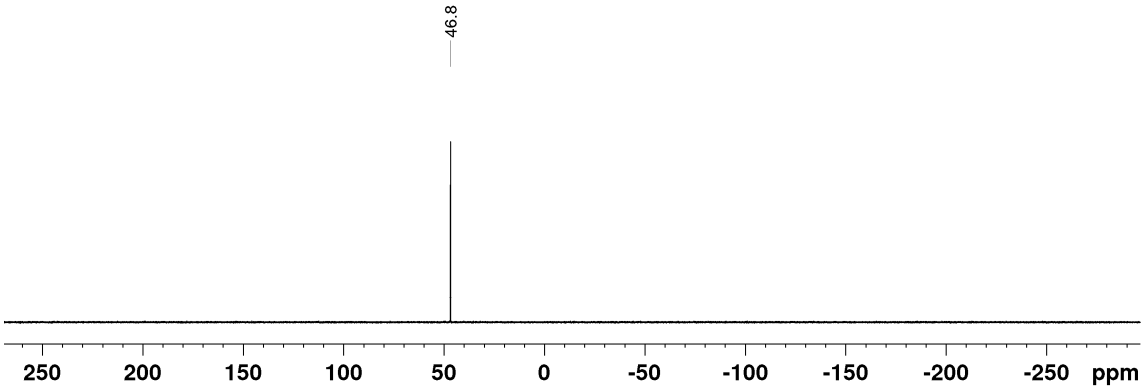


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of **2**$[OTf]_2$ (300 K, CD_2Cl_2).

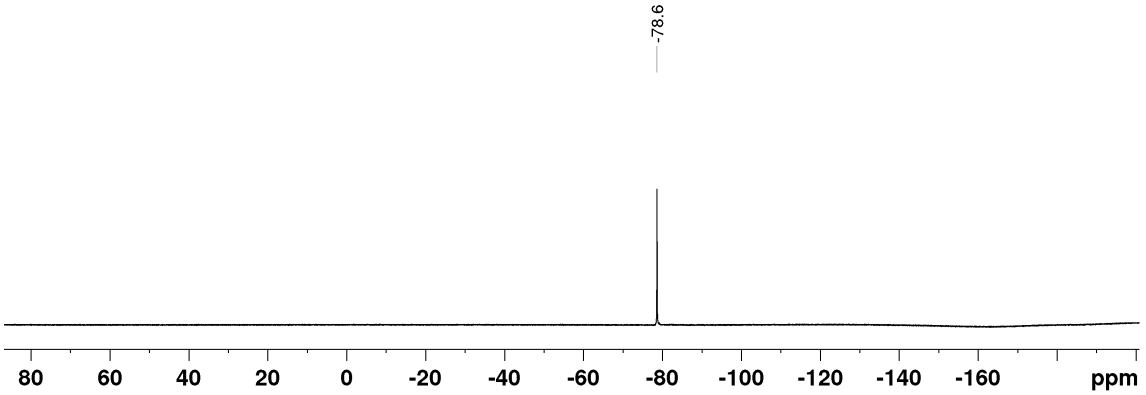
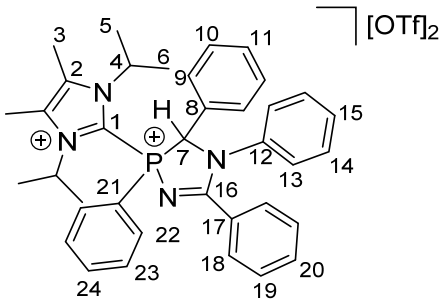


Figure S12. $^{19}F\{\}$ NMR spectrum of **2**$[OTf]_2$ (300 K, CD_2Cl_2).

S2.4 Preparation of 3a[OTf]$_2$



A mixture of [**L$_C$**PClPh][OTf] (6.00 g, 12.69 mmol, 1 eq.) and AgOTf (3.26 g, 12.69 mmol, 1eq.) in DCM (80 mL) was stirred at room temperature for 16 h to afford a suspension. The suspension was filtered to remove AgCl and obtain the solution of **1**[OTf]. Benzonitrile (1.31 g, 1.3 mL, 12.69 mmol, 1 eq.) and *N*-benzylideneaniline (2.3 g, 12.69 mmol, 1eq.) were added to the filtrate. The resulting yellow solution was heated at 80 ˚C in a pressure-sealed tube for 12 h. Removal of all volatiles gave a yellow viscous oil. Addition of *n*-pentane (20 mL) to the residue afforded a yellow suspension, which was filtrated, washed with Et_2O (20 mL), and dried *in vacuo* to obtain a white, air and moisture sensitive solid. Suitable crystals for X-ray diffraction analysis can be obtained by layering a DCM solution with Et_2O at –30°C. See **S3** for details of the diastereomeric configuration analysis.

Yield: 9.32 g, 84%. **m.p.** 208 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): No Raman spectrum could be obtained due to fluorescence of the compound. **IR** (ATR, 298 K, [cm^{-1}]):

3062 (vw), 3001 (vw), 2988 (vw), 2947 (vw), 2942 (vw), 2900 (vw), 1601 (vw), 1583 (vw), 1494 (w), 1473 (w), 1460 (w), 1419 (w), 1375 (w), 1276 (s), 1254 (vs), 1224 (m), 1189 (w), 1142 (s), 1110 (m), 1092 (w), 1083 (w), 1028 (vs), 996 (w), 947 (vw), 931 (vw), 900 (m), 850 (vw), 834 (vw), 800 (w), 794 (w), 782 (w), 763 (w), 754 (w), 732 (w), 722 (vw),709 (m), 698 (m), 665 (vw), 635 (vs), 590 (w), 572 (m), 539 (vw), 516 (s), 490 (s), 468 (w), 449 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 1.75 (H6, d, $^{3}J_{HH}$ = 6.8 Hz, 6H), 1.83 (H5, d, $^{3}J_{HH}$ = 7.0 Hz, 6H), 2.59 (H3, s, 6H), 5.19 (H4, m, 2H), 6.87 (H7, d, $^{2}J_{HP}$ = 11.0 Hz, 1H), 7.25 (Ar-H, m, 5H), 7.35 (Ar-H, m, 5H), 7.42 (Ar-H, m, 2H), 7.56 (Ar-H, m, 1H), 7.78 (Ar-H, m, 5H), 7.83 (Ar-H, m, 1H), 7.90 (Ar-H, m, 1H). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm) : δ = 11.5 (2C, s, C3), 20.9 (2C, s, C5), 20.9 (2C, s, C6), 56.1 (2C, s, C4), 71.5 (1C, d, $^{1}J_{CP}$ = 48.5 Hz, C7), 116.9 (1C, d, $^{1}J_{CP}$ = 108.4 Hz, C21), 120.8 (2C, q, $^{1}J_{CF}$ = 322 Hz, OTf), 128.0 (2C, s, C13), 128.4 (1C, s, C15), 129.1 (1C, d, $^{3}J_{CP}$ = 5.8 Hz, C17), 129.6 (2C, s, C9), 129.7 (1C, d, $^{1}J_{CP}$ = 99.5 Hz, C1), 130.1 (2C, s, C10), 130.1 (1C, s, C11), 130.5 (1C, s, C14), 130.9 (2C, s, C18), 131.3 (2C, s, C19), 131.3 (1C, s, C24), 133.3 (1C, s, C20), 133.3 (1C, s, C24), 133.4 (2C, s, C22), 136.5 (1C, d, $^{3}J_{CP}$ = 4.9 Hz, C8), 136.5 (2C, s, C23), 136.6 (2C, s, C2), 137.6 (1C, d, $^{3}J_{CP}$ = 3.3 Hz, C12), 178.6 (1C, d, $^{3}J_{CP}$ = 6.0 Hz, C16). Only the resonance of the major diastereomer are given. **^{19}F{^{1}H} NMR** (470.59 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.8 (s, OTf). **^{31}P{} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 55.0 (s) (93%), 60.2 (s) (7%). **Elemental analysis**: calculated for $C_{39}H_{41}F_6N_4O_6PS_2$: C, 53.79; H, 4.75; N, 6.43; S, 7.36; found: C, 53.53; H, 4.538; N, 6.42; S, 7.321.

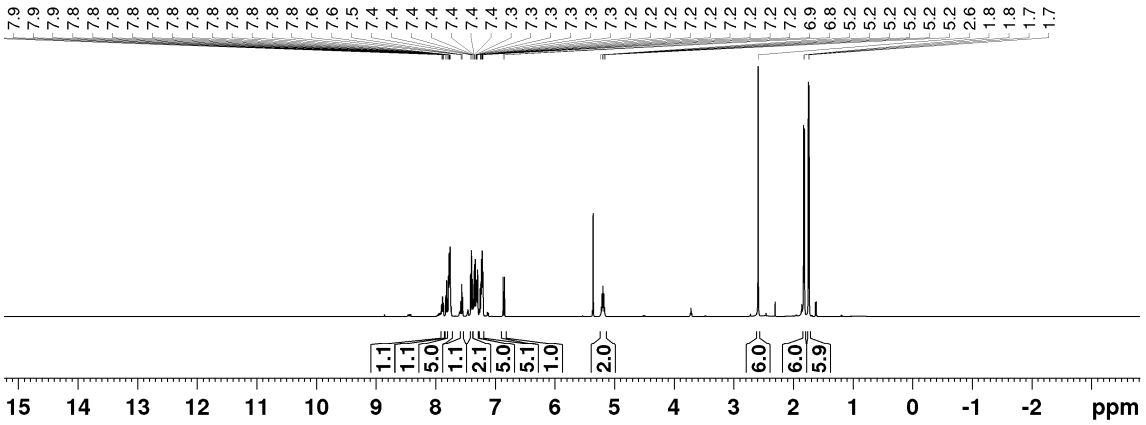


Figure S13. ^{1}H NMR spectrum of **3a**[OTf]$_2$ (300 K, CD_2Cl_2).

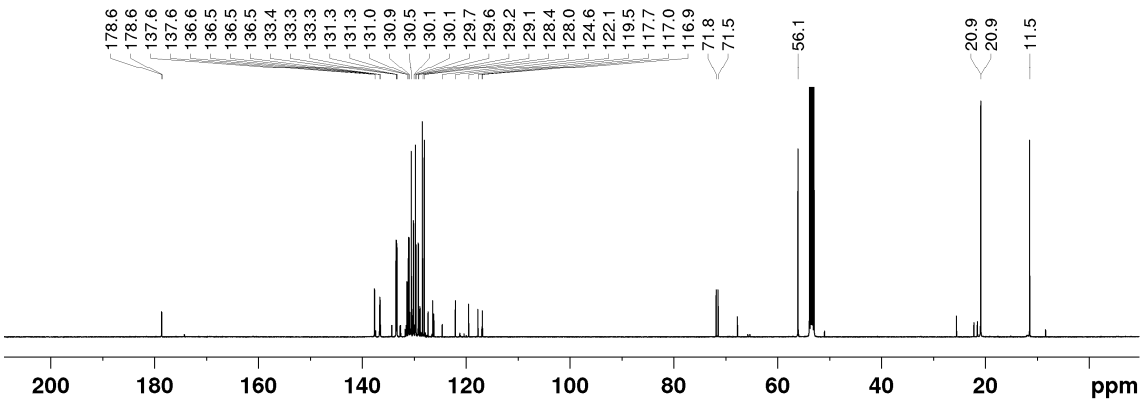


Figure S14. ^{13}C{^{1}H} NMR spectrum of **3a**[OTf]$_2$ (300 K, CD_2Cl_2).

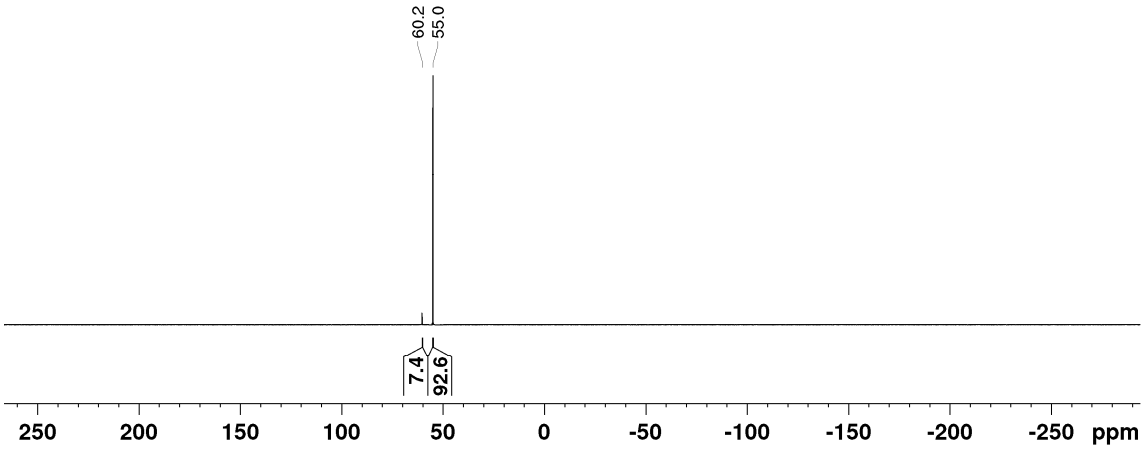


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of **3a**$[OTf]_2$ (300 K, CD_2Cl_2).

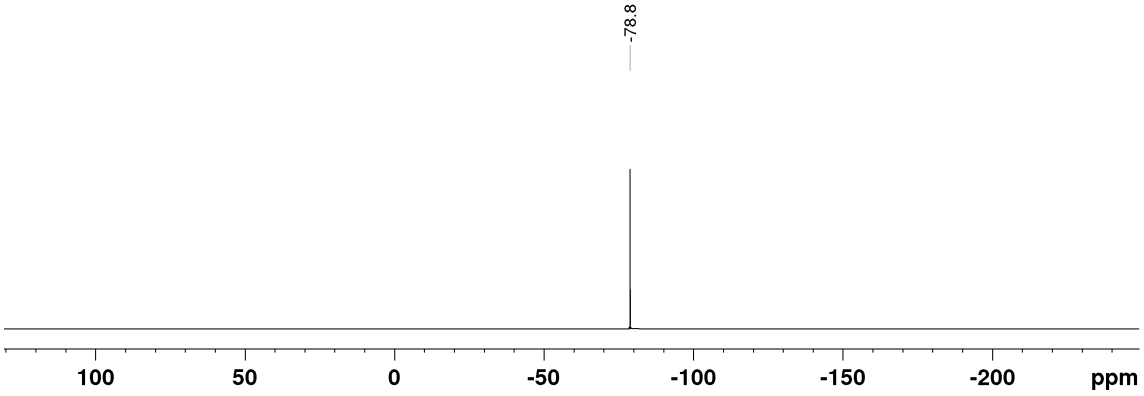
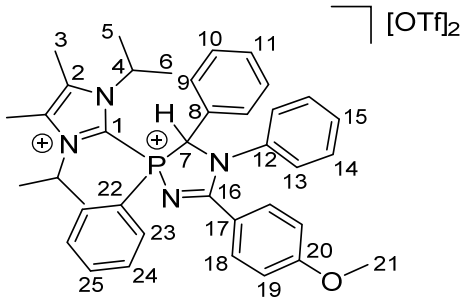


Figure S16. $^{19}F\{\}$ NMR spectrum of **3a**$[OTf]_2$ (300 K, CD_2Cl_2).

S2.5 Preparation of 3b[OTf]$_2$



A mixture of [$\mathbf{L_C}$PClPh][OTf] (500 mg, 1.06 mmol, 1 eq.) and AgOTf (272 mg, 1.06 mmol, 1 eq.) in DCM (10 mL) was stirred at room temperature for 16 h to afford a suspension. The mixture was filtered to remove AgCl and obtain the solution of **1**[OTf]. 4-Methoxybenzonitrile (141 mg, 128 mL, 1.06 mmol, 1 eq.) and *N*-benzylideneaniline (192 mg, 1.06 mmol, 1 eq.) were added to the filtrate. The resulting yellow solution was heated at 80˚C in a pressure-sealed tube for 12 h. Removal of all volatiles gave a pale-yellow solid, which was washed with Et_2O (4 mL) to afford a white solid. The product was collected by filtration and dried *in vacuo* to yield a white, air and moisture sensitive solid. Suitable crystals for X-ray diffraction analysis can be obtained by layering a DCM solution with Et_2O at room temperature.

Yield: 746 mg, 78%. **m.p.** 192 °C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3068 (29), 2990 (10), 2946 (24), 1608 (100), 1582 (25), 1525 (34), 1464 (16), 1445 (20), 1428 (62),

1410 (39), 1313 (13), 1278 (19), 1265 (24), 1207 (16), 1185 (30), 1160 (13), 1150 (11), 1032 (36), 1002 (34), 803 (15), 754 (9), 573 (9), 348 (10), 313 (9), 261 (10), 213 (10), 153 (19), 81 (99). **IR** (ATR, 298 K, [cm^{-1}]): 2361 (w), 2342 (vw), 1607 (w), 1581 (vw), 1495 (vw), 1452 (w), 1428 (m), 1407 (m), 1256 (vs), 1222 (m), 1180 (w), 1142 (s), 1109 (m), 1029 (vs), 996 (w), 947 (w), 912 (m), 850 (vw), 800 (w), 787 (w), 762 (w), 747 (w), 721 (vw), 708 (w), 691 (w), 652 (vw), 635 (vs), 585 (w), 571 (w), 516 (s), 497 (w), 484 (m), 445 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 1.73 (6H, d, $^{3}J_{HH}$ = 6.7 Hz, H6), 1.81 (6H, d, $^{3}J_{HH}$ = 6.9 Hz, H5), 2.58 (6H, s, H3), 3.86 (3H, s, H21), 5.21 (2H, br, H4), 6.79 (1H, d, $^{2}J_{HP}$ = 11.0 Hz, H7), 6.88 (2H, m, H19), 7.20 (2H, m, Ar-H), 7.27 (3H, m, Ar-H), 7.33 (5H, m, Ar-H), 7.73 (5H, m, Ar-H), 7.85 (2H, m, Ar-H). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm): δ = 11.5 (2C, s, C3), 20.9 (4C, m, C5, C6), 55.6 (1C, s, C21), 56.0 (2C, s, C4), 71.7 (1C, d, $^{2}J_{CP}$ = 48 Hz, C7), 113.8 (2C, s, C19), 118.0 (1C, d, $^{1}J_{CP}$ = 110 Hz, C22), 120.4 (1C, d, $^{3}J_{CP}$ = 20 Hz, C17), 120.8 (2C, q, $^{1}J_{CF}$ = 321 Hz, OTf), 126.8 (1C, s, C11), 127.5 (1C, s, $^{1}J_{CP}$ = 64 Hz, C1), 128.0 (2C, s, C13), 129.1 (2C, s, C9), 129.1 (1C, s, C12), 129.5 (1C, s, C15), 129.8 (2C, s, C14), 130.0 (2C, s, C24), 130.9 (2C, d, $^{2}J_{CP}$ = 14 Hz, C23), 131.2 (2C, s, C10), 133.3 (1C, d, $^{2}J_{CP}$ = 12 Hz, C8), 133.5 (2C, s, C18), 136.2 (2C, d, $^{3}J_{CP}$ = 4 Hz, C2), 137.4 (1C, s, C25), 164.0 (1C, s, C20), 177.5 (1C, d, $^{1}J_{CP}$ = 5 Hz, C16). Only the resonances of the major diastereomer are given. **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 59.2 (s) (15%), 53.3 (s) (85%). **^{19}F{^{1}H} NMR** (470.59 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.8 (s, OTf). **Elemental analysis**: calculated for $C_{40}H_{43}F_6N_4O_7PS_2$: C, 53.33; H, 4.81; N, 6.22; S, 7.12; found: C, 53.23; H, 4.982; N, 6.08; S, 7.265.

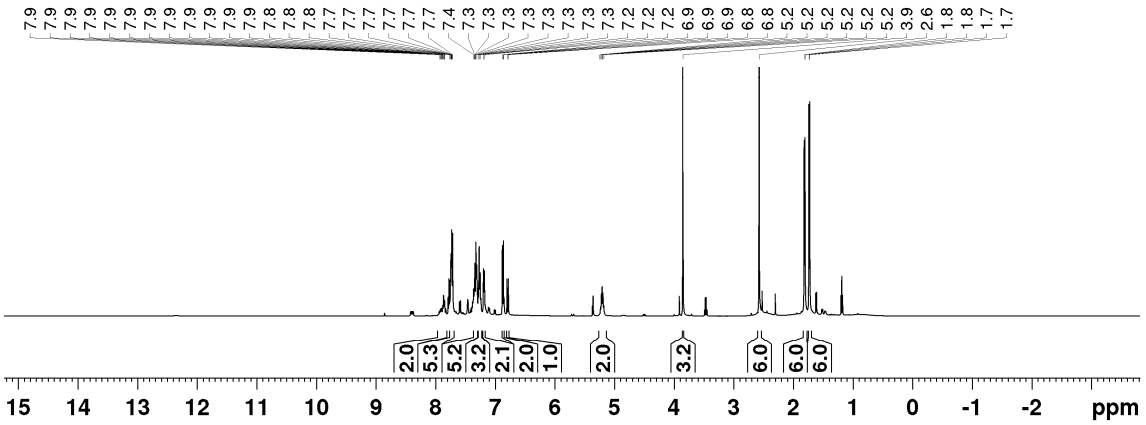


Figure S17. ^{1}H NMR spectrum of **3b**[OTf]$_2$ (300 K, CD_2Cl_2).

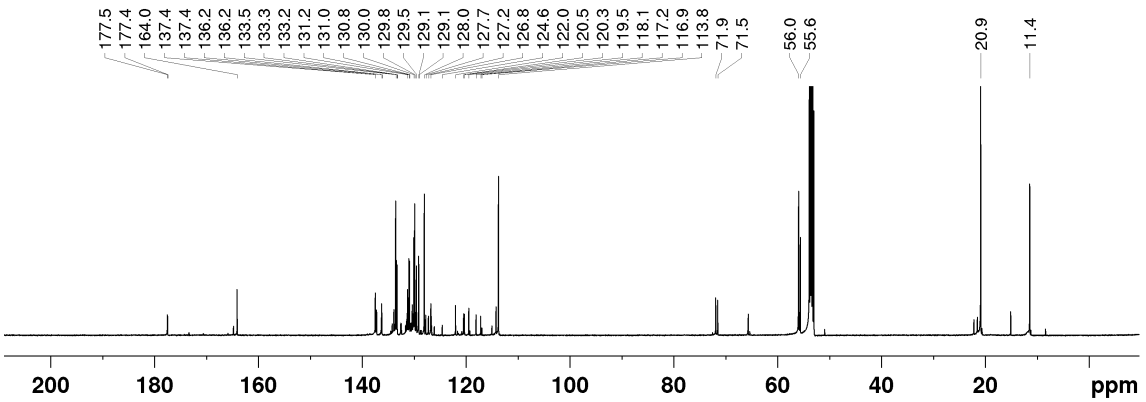


Figure S18. ^{13}C{^{1}H} NMR spectrum of **3b**[OTf]$_2$ (300 K, CD_2Cl_2).

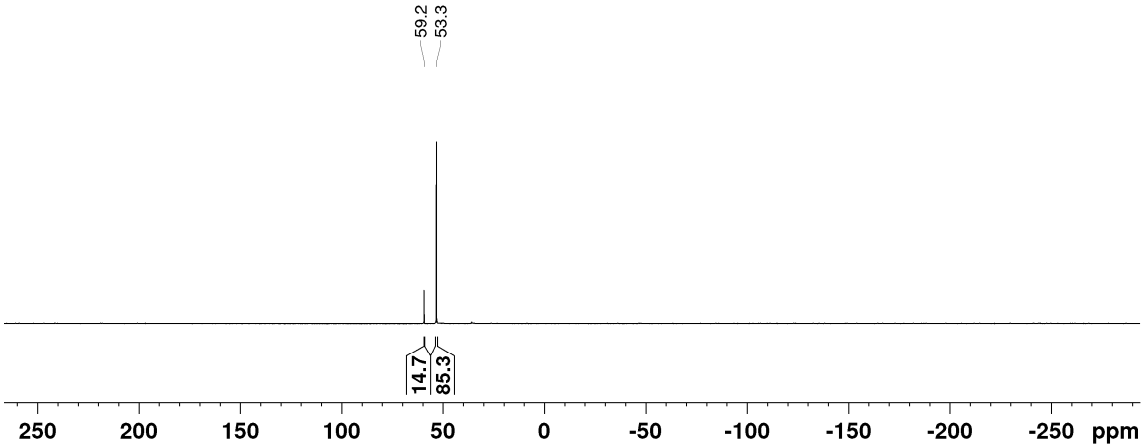


Figure S19. $^{31}P\{\}$ NMR spectrum of **3b**$[OTf]_2$ (300 K, CD_2Cl_2).

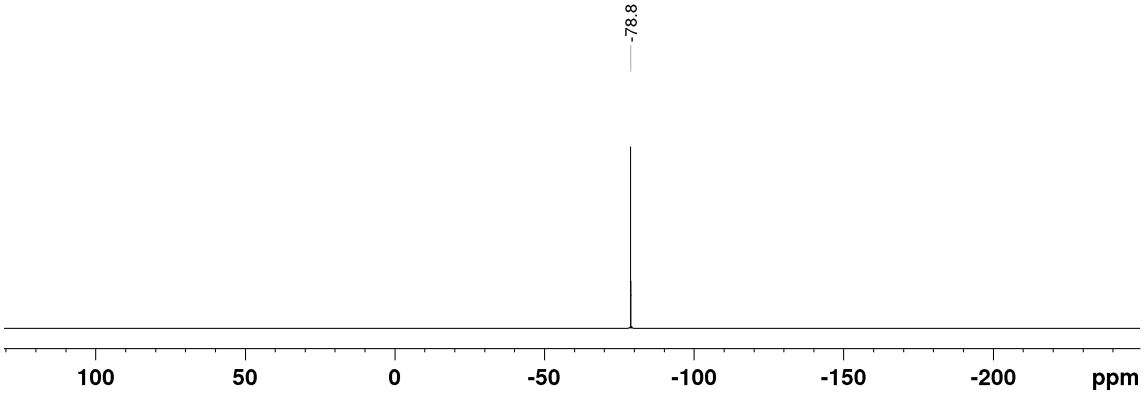


Figure S20. $^{19}F\{^1H\}$ NMR spectrum of **3b**$[OTf]_2$ (300 K, CD_2Cl_2).

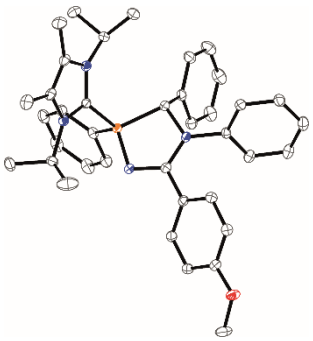
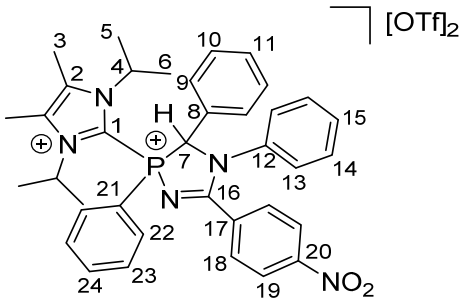


Figure S21. Molecular structure of *anti*-**3b**$^{2+}$ in *anti*-**3b**$[OTf]_2$; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.6 Preparation of 3c[OTf]$_2$



A mixture of [**L$_C$**PClPh][OTf] (500 mg, 1.06 mmol, 1 eq.) and AgOTf (272 mg, 1.06 mmol, 1 eq.) in DCM (10 mL) was stirred at room temperature for 16 h to afford a suspension. The mixture was filtered to remove AgCl and obtain the solution of **1**[OTf]. 4-Nitrobenzonitrile (157 mg, 1.06 mmol, 1 eq.) and *N*-benzylideneaniline (192 mg, 1.06 mmol, 1 eq.) were added to the filtrate. The resulting yellow solution was heated at 80˚C in a pressure-sealed tube for 12 h. Removal of all volatiles gave a yellow solid, which was washed with Et_2O (4 mL) and PhF (1 mL) to afford a white solid. The product was collected by filtration and dried *in vacuo* to yield a white, air and moisture sensitive solid.

Yield: 767 mg, 73%. **m.p.** 197.9 °C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3071 (30), 2958 (28), 1603 (100), 1584 (66), 1433 (70), 1350 (80), 1278 (71), 1108 (74), 1034 (77), 1002 (82). **IR** (ATR, 298 K, [cm^{-1}]): 2361 (w), 2341 (w), 1526 (w), 1495 (vw), 1474 (w), 1434 (w), 1402 (vw), 1348 (w), 1278 (m), 1257 (vs), 1224 (w), 1150 (m), 1109 (w), 1031 (s), 1016 (vw), 906 (w), 861 (vw), 792 (vw), 757 (w), 741 (vw), 734 (vw), 709 (w), 697 (w), 691 (w), 636 (vs), 573 (w), 517 (m), 491 (w). **^{1}H NMR** (400.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 1.73 (6H, d, $^3J_{HH}$ = 6.7 Hz, H5), 1.84 (6H, d, $^3J_{HH}$ = 6.9 Hz, H6), 2.61 (6H, s, H3), 5.17 (2H, sept, $^3J_{HH}$ = 6.7 Hz, H4), 6.92 (1H, d, $^2J_{HP}$ = 11.2 Hz, H7), 7.23 (3H, m, H9, H11), 7.32 (5H, m, H15, H22, H13), 7.42 (2H, m, H14), 7.79 (2H, m, H10), 7.89 (1H, m, H24), 7.92 (2H, m, H23), 8.07 (2H, d, $^3J_{HH}$ = 8.9 Hz, H18), 8.18 (2H, d, $^3J_{HH}$ = 8.9 Hz, H19). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm): δ = 11.5 (2C, s, C3), 20.9 (2C, s, C6), 20.9 (2C, s, C5), 56.3 (2C, s, C4), 71.7 (1C, d, $^1J_{CP}$ = 49 Hz, C7), 116.7 (1C, d, $^1J_{CP}$ = 107 Hz, C21), 120.8 (2C, q, $^1J_{CF}$ = 321 Hz, OTf), 123.2 (2C, s, C19), 125.7 (1C, d, $^3J_{CP}$ = 2 Hz, C17), 126.8 (1C, d, $^1J_{CP}$ = 131 Hz, C1), 128.0 (2C, s, C14), 129.4 (2C, d, $^3J_{CP}$ = 5 Hz, C9), 129.9 (2C, s, C13), 129.9 (2C, s, C10), 130.1 (1C, s, C11), 131.1 (2C, d, $^2J_{CP}$ = 15 Hz, C22), 131.3 (2C, s, C15), 131.7 (2C, s, C18), 133.8 (2C, d, $^3J_{CP}$ = 13 Hz, C23), 135.0 (1C, d, $^2J_{CP}$ = 20 Hz, C8), 135.6 (1C, d, $^3J_{CP}$ = 10 Hz, C12), 136.6 (2C, d, $^3J_{CP}$ = 5 Hz, C2), 137.9 (1C, d, $^4J_{CP}$ = 3 Hz, C24), 149.8 (1C, s, C20), 176.9 (1C, d, $^2J_{CP}$ = 6 Hz, C16). **^{31}P{^{1}H} NMR** (161.98 MHz, CD_2Cl_2, 300 K, in ppm): δ = 56.9 (s). **^{19}F{^{1}H} NMR** (376.5 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.7 (s, OTf). **Elemental analysis**: calculated for $C_{39}H_{40}F_6N_5O_8PS_2$ 0.35 CH_2Cl_2: C, 49.98; H, 4.34; N, 7.41; S, 6.78; found: C, 49.61; H, 4.577; N, 7.37; S, 7.308.

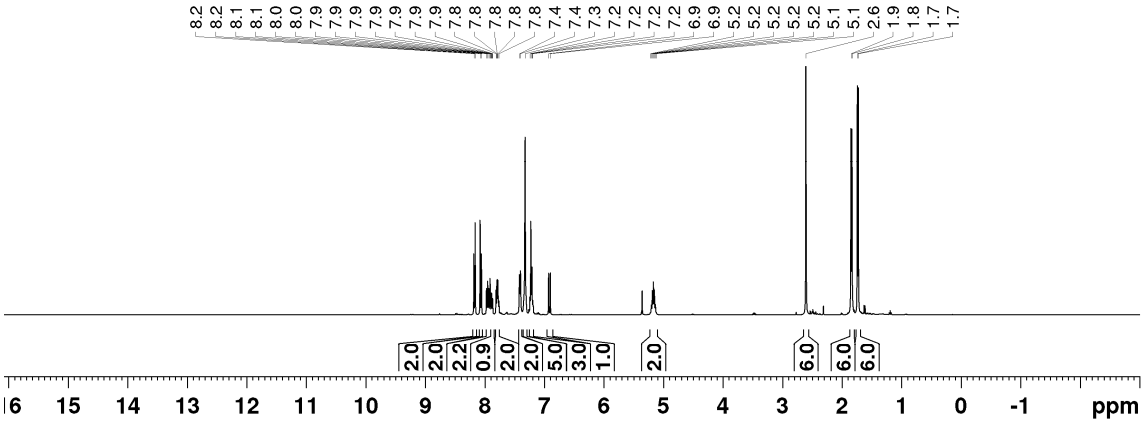


Figure S22. ^{1}H NMR spectrum of **3c**[OTf]$_2$ (300 K, CD_2Cl_2).

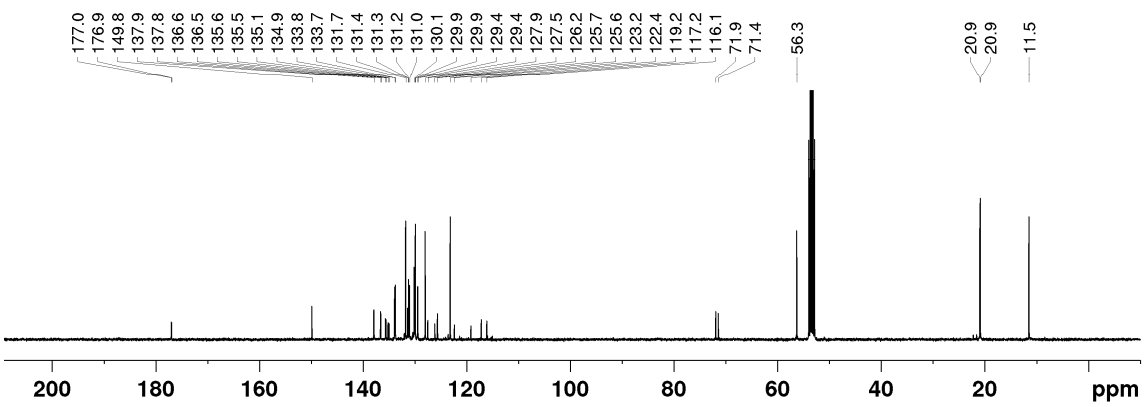


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of **3c**$[OTf]_2$ (300 K, CD_2Cl_2).

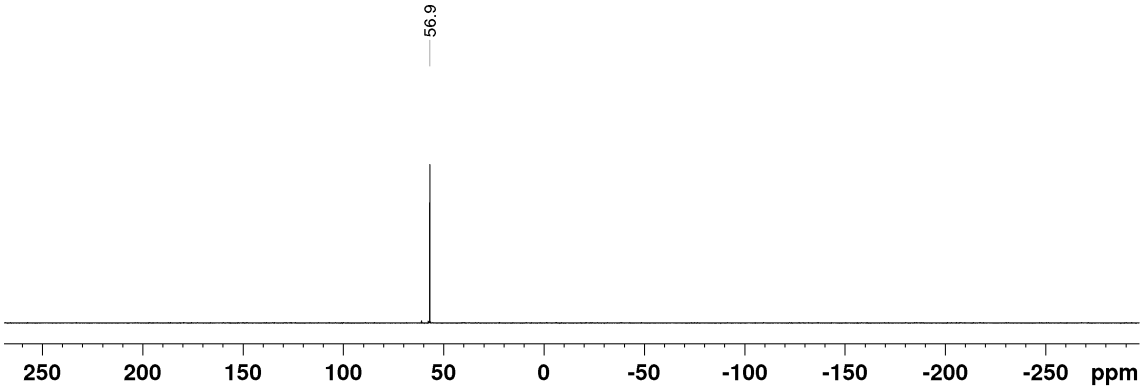


Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum of **3c**$[OTf]_2$ (300 K, CD_2Cl_2).

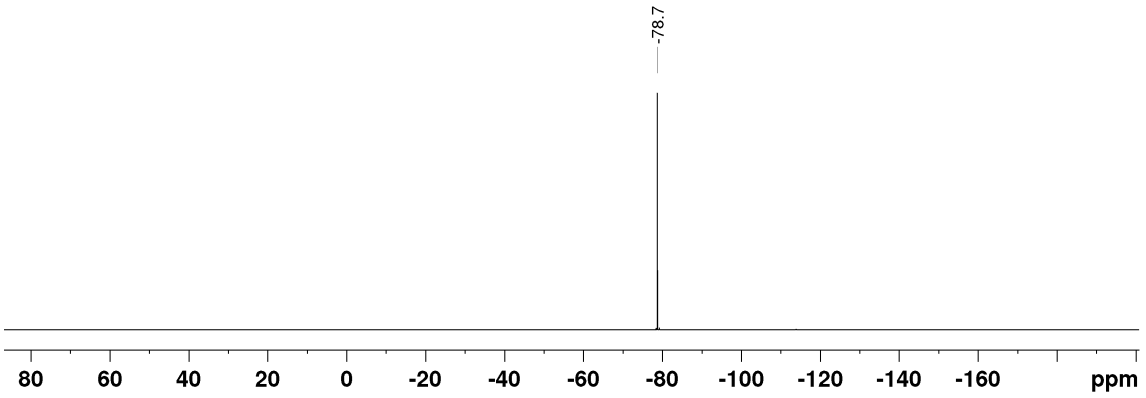
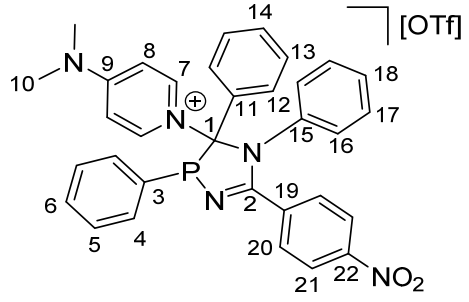


Figure S25. $^{19}F\{^{1}H\}$ NMR spectrum of **3c**$[OTf]_2$ (300 K, CD_2Cl_2).

S2.7 Preparation of 4[OTf]



A mixture of **3c**[OTf]$_2$ (300 mg, 0.33 mmol, 1 eq.) and DMAP (40.0 mg, 0.33 mmol, 1 eq.) in PhF (8 mL) were stirred at room temperature for 16 h, resulting in a white suspension. The solid was collected by filtrations to obtain a yellow, air and moisture sensitive solid. Suitable crystals for X-ray diffraction analysis can be obtained by layering a DCM solution with Et_2O at room temperature.

Yield: 206 mg, 89%. **m.p.** 220 °C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3070 (33), 2936 (10), 1601 (100), 1585 (43), 1562 (30), 1529 (10), 1354 (67), 1224 (17), 1107 (25), 1095 (13), 1075 (27), 1032 (43), 1001 (54), 949 (22), 856 (13), 817 (14), 746 (38), 620 (10). **IR** (ATR, 298 K, [cm^{-1}]): 1638 (m), 1558 (w), 1524 (w), 1492 (w), 1435 (vw), 1407 (vw), 1354 (w), 1320 (vw), 1307 (vw), 1264 (vs), 1222 (m), 1148 (m), 1133 (w), 1114 (vw), 1074 (m), 1054 (vw), 1029 (s), 1008 (vw), 999 (vw), 855 (w), 833 (w), 811 (w), 793 (vw), 762 (vw), 746 (w), 733 (m), 694 (m), 634 (vs), 572 (vw), 516 (w), 507 (w), 482 (w), 450 (vw), 470 (vs). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 3.23 (6H, m, H10), 6.65 (1H, m, Ar-H), 6.76 (2H, m, H16), 6.90 (1H, m, Ar-H), 7.03 (2H, m, Ar-H), 7.13 (5H, m, Ar-H), 7.23 (2H, m, Ar-H), 7.29 (2H, m, Ar-H), 7.40 (3H, m, Ar-H), 7.92 (1H, m, Ar-H), 8.01 (1H, m, Ar-H), 8.12 (2H, m, Ar-H), 8.22 (1H, m, Ar-H). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm) : δ = 40.7 (2C, s, C10), 40.8 (2C, s, C10), 84.7 (1C, d, $^1J_{CP}$ = 46 Hz, C1), 96.3 (1C, d, $^1J_{CP}$ = 51 Hz, C3), 100.5 (1C, d, $^1J_{CP}$ = 38 Hz, C3), 107.7 (2C, s, C16), 108.8 (2C, s, C16), 115.5 (1C, d, $^3J_{CP}$ = 21 Hz, C11), 121.5 (1C, q, $^1J_{CF}$ = 321 Hz, OTf), 123.7 (2C, s, C8), 123.8 (2C, s, C8), 128.0 (2C, s, Ar-C), 128.2 (1C, s, Ar-C), 128.6 (2C, s, Ar-C), 128.7 (2C, s, Ar-C), 128.9 (1C, s, Ar-C), 129.0 (1C, s, Ar-C), 129.1 (2C, s, Ar-C), 129.2 (2C, s, Ar-C), 129.3 (2C, s, Ar-C), 129.8 (1C, s, Ar-C), 131.0 (2C, s, Ar-C), 131.4 (1C, s, Ar-C), 131.5 (1C, s, Ar-C), 131.7 (2C, s, Ar-C), 132.1 (1C, s, Ar-C), 132.4 (1C, s, Ar-C), 132.6 (1C, s, Ar-C), 134.3 (1C, s, Ar-C), 138.8 (2C, d, $^3J_{CP}$ = 17 Hz, C7), 141.5 (2C, d, $^3J_{CP}$ = 15 Hz, C7), 149.2 (2C, s, C21), 149.5 (2C, s, C21), 156.4 (1C, s, C22), 157.0 (1C, s, C9), 157.9 (1C, s, C9), 164.2 (1C, s, C22), 167.8 (1C, d, $^2J_{CP}$ = 7 Hz, C2), 174.1 (1C, d, $^2J_{CP}$ = 10 Hz, C2). Because of overlapping, it is impossible to distinguish signals between two isomers. **^{19}F{^{1}H} NMR** (470.59 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.7 (s, OTf). **^{31}P{} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 109.8 (s) (43%), 100.5 (s) (57%). **Elemental analysis**: calculated for $C_{34}H_{29}F_3N_5O_5PS$ 0.45 CH_2Cl_2: C, 55.48; H, 4.04; N, 9.39; S, 4.30; found: C, 55.61; H, 3.719; N, 9.36; S, 3.996.

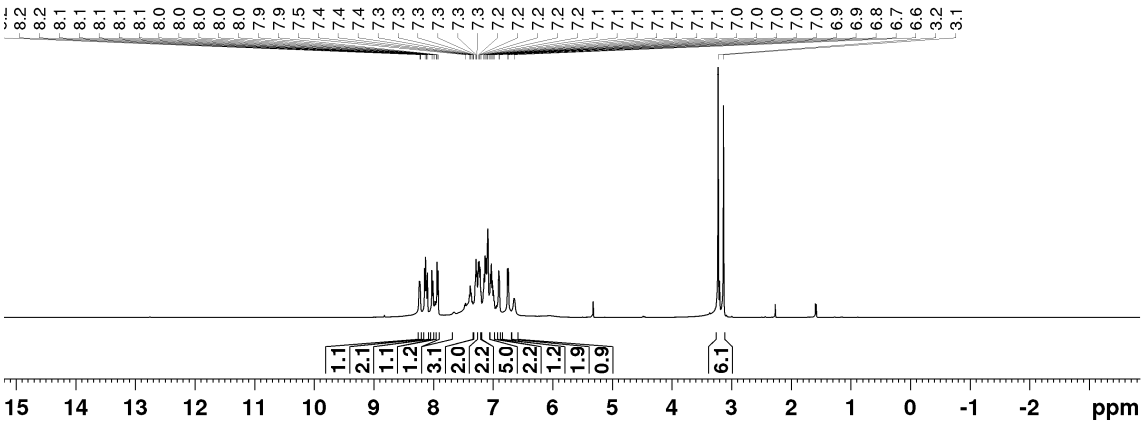


Figure S26. ^{1}H NMR spectrum of **4**[OTf] (300 K, CD_2Cl_2).

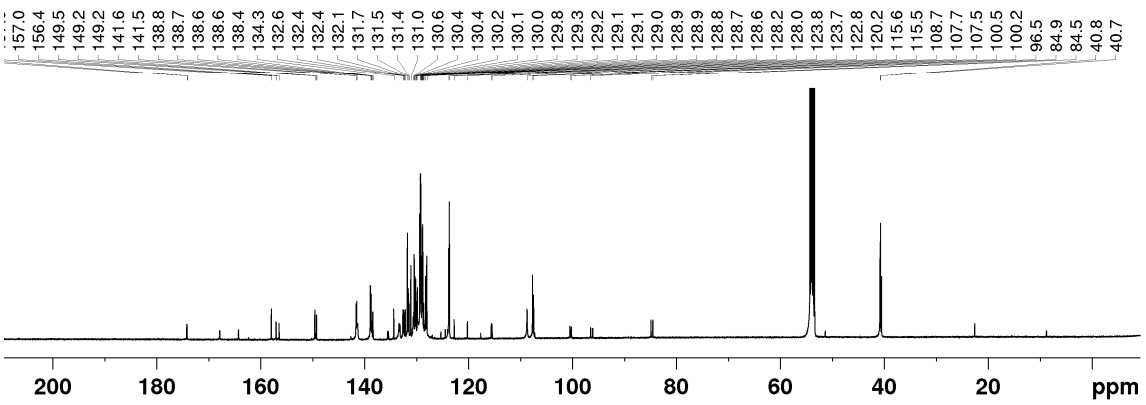


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of **4**[OTf] (300 K, CD_2Cl_2).

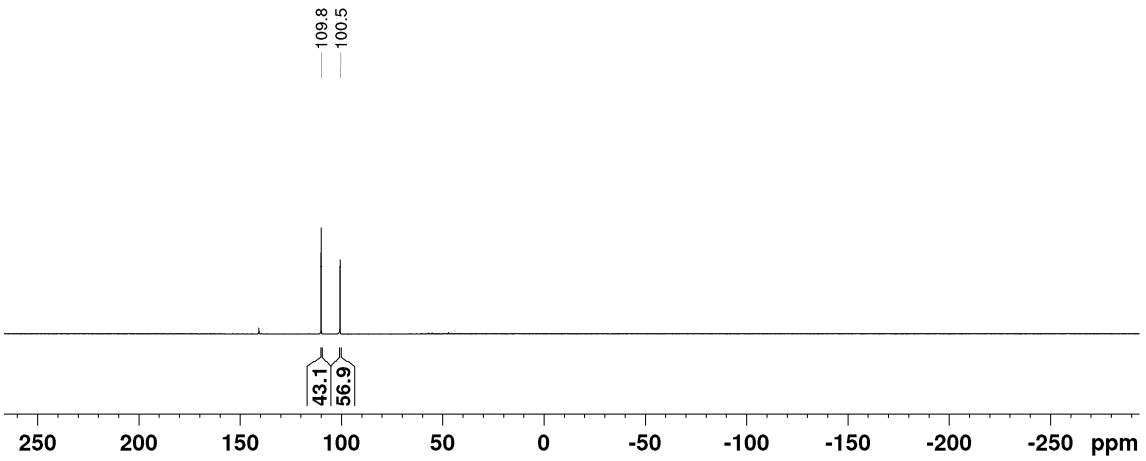


Figure S28. $^{31}P\{^{1}H\}$ NMR spectrum of **4**[OTf] (300 K, CD_2Cl_2).

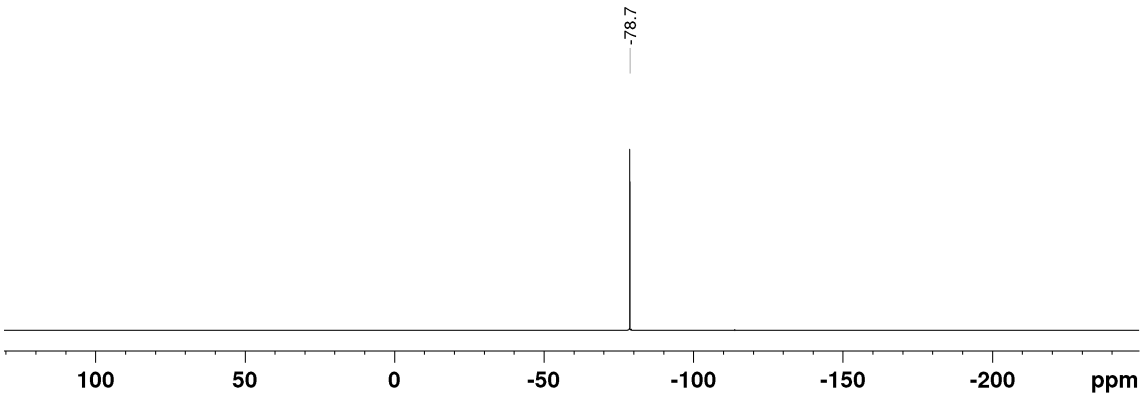


Figure S29. $^{19}F\{^{1}H\}$ NMR spectrum of **4**[OTf] (300 K, CD_2Cl_2).

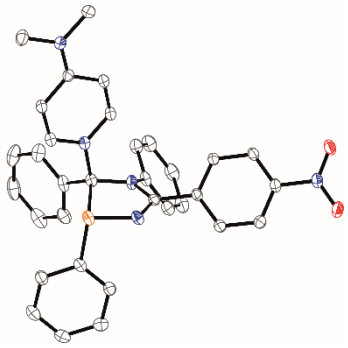
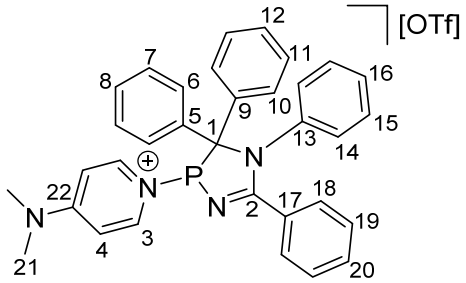


Figure S30. Molecular structure of **4**$^{+}$ in **4**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.8 Preparation of 5a[OTf]



To a suspension of **3a**[OTf]$_2$ (1.0 g, 1.15 mmol, 1 eq.) in PhF (10 mL) DMAP (140.3 mg, 1.15 mmol, 1 eq.) was added and the mixture was stirred at room temperature for 7 days, affording a yellow suspension. The solid was collected by filtration and evaporated *in vacuo* to obtain a white, air and moisture sensitive solid. Suitable crystals for X-ray diffraction analysis were obtained by layering a DCM solution with Et_2O at room temperature. For small-scale reaction (100 mg), the reaction can be completed within 16 h.

Yield: 721 mg, 95%. **m.p.** 210 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3067 (20), 1600 (51), 1580 (22), 1516 (16), 1444 (7), 1351 (11), 1268 (8), 1169 (12), 1034 (25), 999 (57), 949 (9), 826 (10), 773 (15), 677 (12), 626 (8), 616 (7), 494 (9), 313 (7), 267 (15), 250 (10), 229 (10), 92 (100). **IR** (ATR, 298 K, [cm^{-1}]): 2361 (m), 2341 (w), 1630 (s), 1572 (w), 1510 (w), 1481 (m), 1442 (w), 1402 (w), 1348 (m), 1262 (vs), 1219 (s), 1138 (m), 1043 (s), 1029 (vs), 1011 (m), 970 (w), 956 (w), 922 (w), 895 (w), 831 (s), 822 (s), 803 (m), 766 (w), 752 (s), 723 (m), 697 (s), 661 (w), 654 (w), 634 (vs), 590 (m), 573 (w), 514 (m), 492 (m), 476 (m). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 7.81-7.79 (m, H3, 2H), 7.65 (m, H4, 2H), 7.84-7.53 (m, Ar-H, 2H), 7.50-7.47 (m, Ar-H, 1H), 7.40-7.37 (m, Ar-H, 5H), 7.20-7.17 (m, Ar-H, 3H), 7.14-7.10 (m, Ar-H, 2H), 7.01-7.0 (m, Ar-H, 1H), 6.98-6.95 (m, Ar-H, 2H), 6.75-6.71 (m, Ar-H, 4H), 3.24 (s, H21, 6H). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm): δ = 40.4 (2C, s, C21), 84.6 (1C, s, $^{1}J_{CP}$ = 46.0 Hz, C1), 108.1 (2C, s, C14), 115.2 (1C, d, $^{2}J_{CP}$ = 20.9 Hz, C9), 122.4 (1C, q, $^{1}J_{CF}$ = 321.4 Hz, OTf), 124.1 (1C, s, C16), 127.2 (1C, s, C12), 127.5 (1C, s, C20), 128.0 (1C, s, C22), 128.3 (1C, s, C13), 128.7 (2C, s, C19), 129.2 (1C, s, C8), 129.9 (1C, d, $^{2}J_{CP}$ = 14.6 Hz, C5), 130.1 (1C, d, $^{3}J_{CP}$ = 7.8 Hz, C17), 130.2 (2C, s, C7),131.8 (2C, s, C11), 132.0 (2C, d, $^{3}J_{CP}$ = 6.1 Hz, C4), 134.4 (2C, s, C6),138.0 (2C, d, $^{2}J_{CP}$ = 29.8 Hz, C3), 139.4 (2C, s, C15), 140.7 (2C, s, C18), 157.4 (2C, s, C10), 175.8 (1C, d, $^{2}J_{CP}$ = 10.1 Hz, C2). **^{19}F{^{1}H} NMR** (470.59 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.8 (s, OTf). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 141.5 (s). **Elemental analysis**: calculated for $C_{34}H_{30}F_3N_4O_3PS$: C, 61.63; H, 4.56; N, 8.45; S, 4.84; found: C, 61.25; H, 4.470; N, 7.97; S, 4.533.

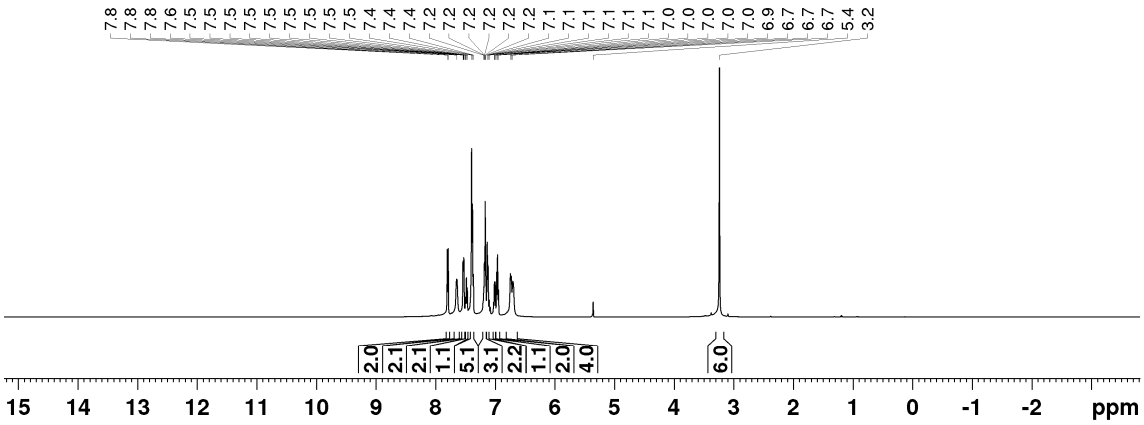


Figure S31. ^{1}H NMR spectrum of **5a**[OTf] (300 K, CD_2Cl_2).

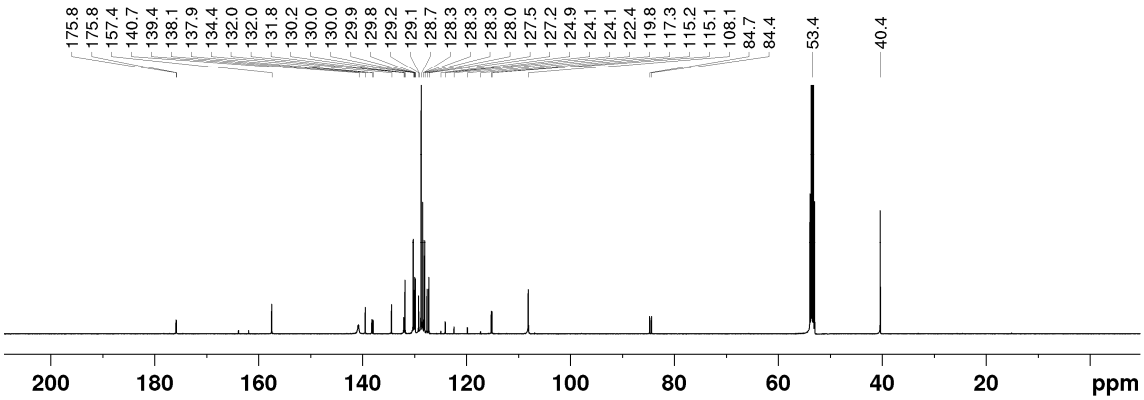


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of **5a**[OTf] (300 K, CD_2Cl_2).

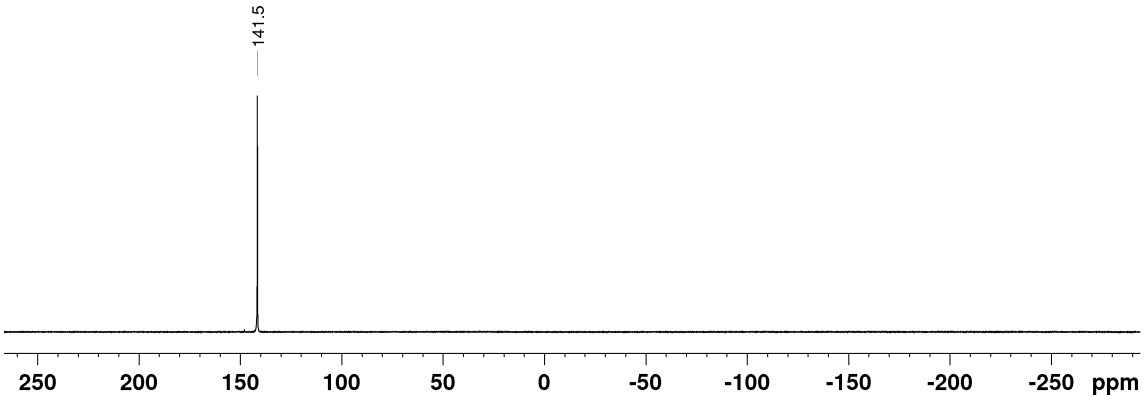


Figure S33. $^{31}P\{^{1}H\}$ NMR spectrum of **5a**[OTf] (300 K, CD_2Cl_2).

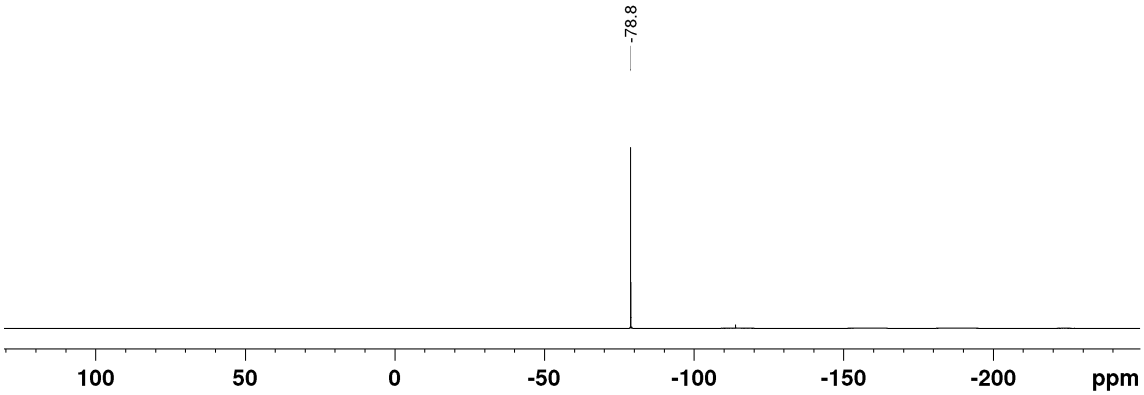


Figure S34. $^{19}F\{^{1}H\}$ NMR spectrum of **5a**[OTf] (300 K, CD_2Cl_2).

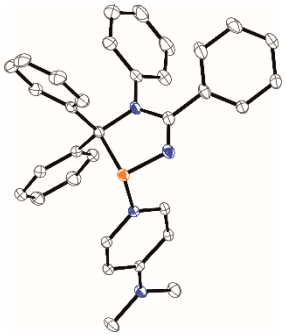
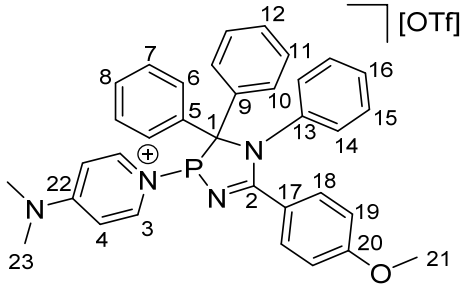


Figure S35. Molecular structure of **5a**$^{+}$ in **5a**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.9 Preparation of 5b[OTf]



A mixture of **3b**[OTf]$_2$ (150 mg, 0.17 mmol, 1 eq.) and DMAP (21.0 mg, 0.17mmol, 1 eq.) in PhF (4 mL) was stirred at room temperature for 2 days, affording a white suspension. The filtrates were collected and concentrated by evaporation. The crude solid was dissolved in DCM and then recrystallized by slowly diffused of Et_2O into the DCM solution at room temperature to give an air and moisture sensitive white solid as **5b**[OTf].

Yield: 30 mg, 52%. **m.p.** 203 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3061 (93), 2940 (38), 1613 (91), 1596 (73), 1579 (81), 1534 (34), 1182 (31), 1167 (31), 1041 (71), 1034 (66), 1001 (100), 945 (26), 834 (33), 769 (35), 676 (24). **IR** (ATR, 298 K, [cm^{-1}]): 1631 (m), 1611 (w), 1576 (w), 1488 (m), 1441 (w), 1401 (vw), 1348 (w), 1263 (vs), 1250 (s), 1220 (s), 1180 (w), 1145 (s), 1116 (vw), 1031 (vs), 1011 (m), 958 (w), 847 (w), 823 (m), 805 (m), 773 (m), 764 (m), 753 (m), 726 (m), 699 (s), 636 (vs), 587 (m), 572 (w), 528 (vw), 515 (m), 496 (w), 474 (w), 428 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 3.20 (6H, s, H23), 3.81 (3H, s, H21), 6.65 (2H, m, H4), 6.71 (2H, m, H14), 6.84 (2H, m, H19), 6.97 (3H, m, Ar-H), 7.03 (2H, m, H10), 7.11 (3H, m, Ar-H), 7.35 (3H, m, Ar-H), 7.49 (2H, m, H6), 7.59 (2H, m, H3), 7.74 (2H,

m, H18). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm) : δ = 40.8 (1C, s, C23), 55.9 (1C, s, C21), 85.2 (1C, d, $^{1}J_{CP}$ = 40 Hz, C1), 108.5 (2C, s, C4), 114.1 (2C, s, C19), 121.5 (1C, q, $^{1}J_{CF}$ = 321 Hz, OTf), 124.1 (1C, d, $^{3}J_{CP}$ = 6 Hz, C17), 127.4 (2C, s, C14), 127.9 (1C, s, C12), 128.2 (2C, s, C10), 128.7 (2C, d, $^{3}J_{CP}$ = 2 Hz, C6), 129.0 (2C, s, C11), 129.1 (2C, s, C7), 129.5 (1C, s, C8), 130.2 (2C, s, C15), 130.4 (2C, s, C16), 133.0 (2C, s, C18), 134.9 (1C, s, C9), 138.2 (1C, d, $^{2}J_{CP}$ = 30 Hz, C5), 140.3 (1C, s, C13), 141.1 (2C, br, C3), 157.8 (1C, s, C22), 163.0 (1C, s, C20), 175.7 (1C, d, $^{2}J_{CP}$ = 10 Hz, C2). **^{19}F{^{1}H} NMR** (470.59 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.8 (s, OTf). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 140.1 (s). **Elemental analysis**: calculated for $C_{35}H_{32}F_3N_4O_4PS$ 0.35 CH_2Cl_2: C, 58.77; H, 4.56; N, 7.76; S, 4.44; found: C, 58.52; H, 4.825; N, 8.17; S, 4.474.

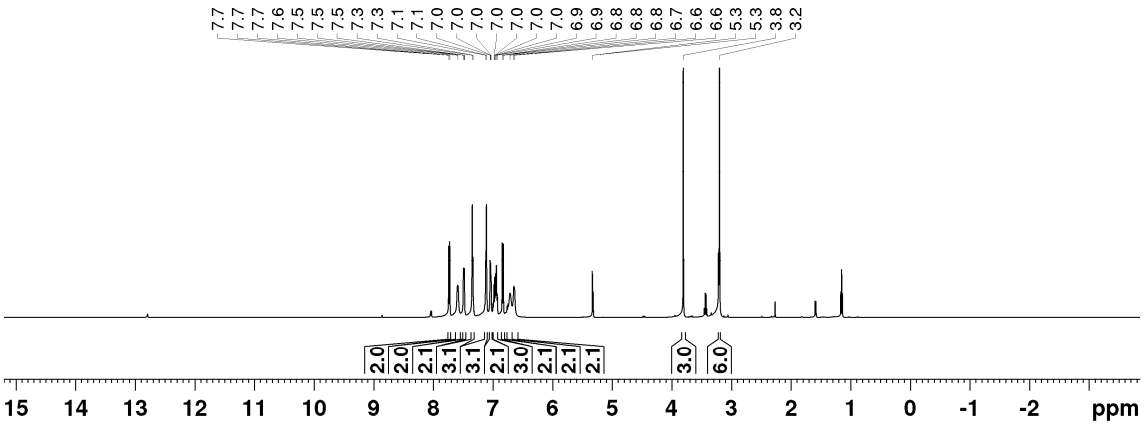


Figure S36. ^{1}H NMR spectrum of **5b**[OTf] (300 K, CD_2Cl_2).

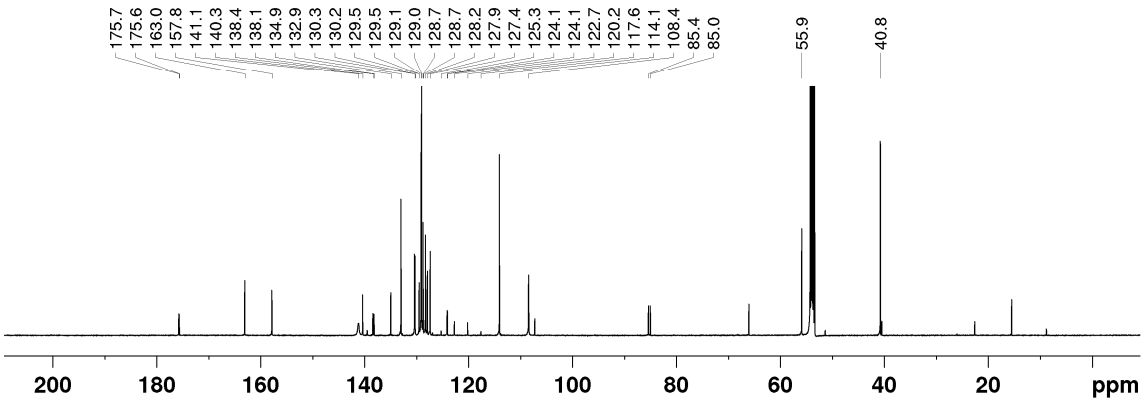


Figure S37. ^{13}C{^{1}H} NMR spectrum of **5b**[OTf] (300 K, CD_2Cl_2).

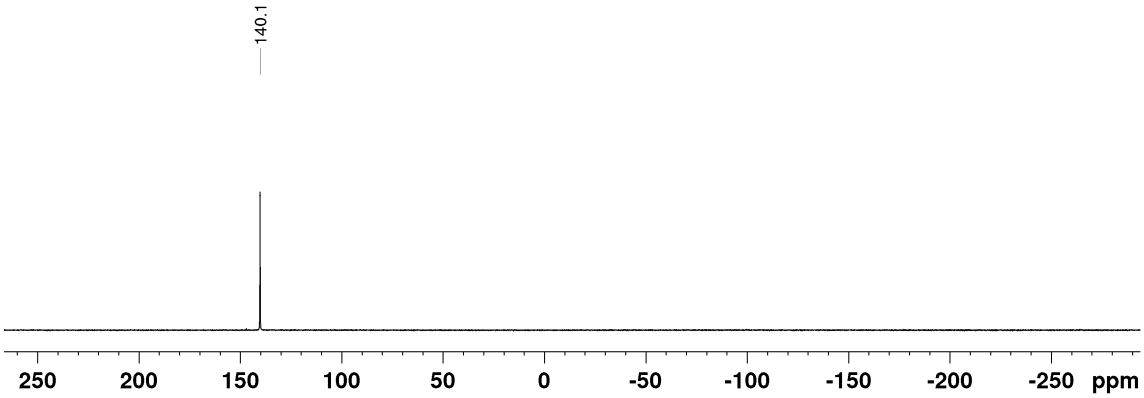


Figure S38. ^{31}P{^{1}H} NMR spectrum of **5b**[OTf] (300 K, CD_2Cl_2).

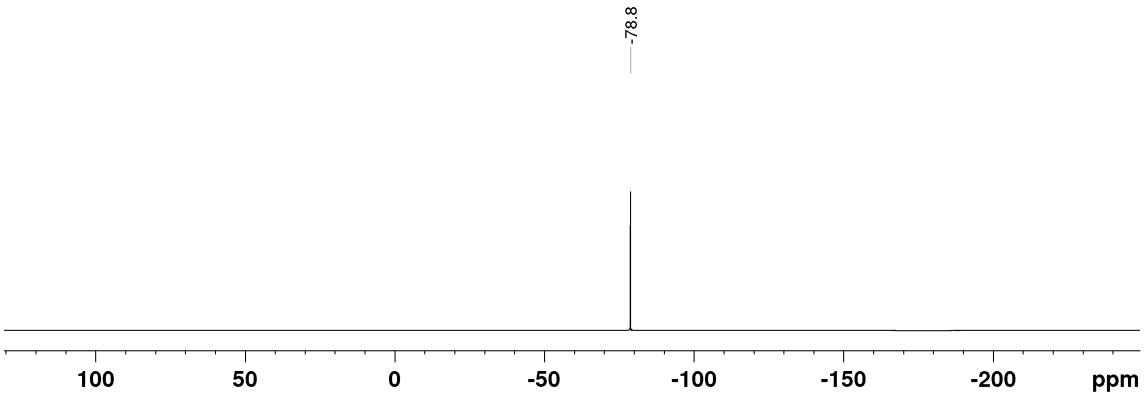


Figure S39. $^{19}F\{^{1}H\}$ NMR spectrum of **5b**[OTf] (300 K, CD_2Cl_2).

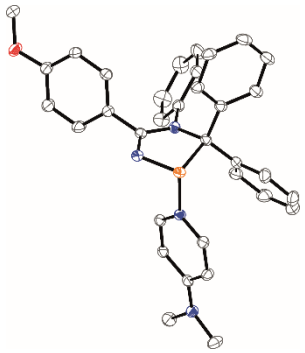
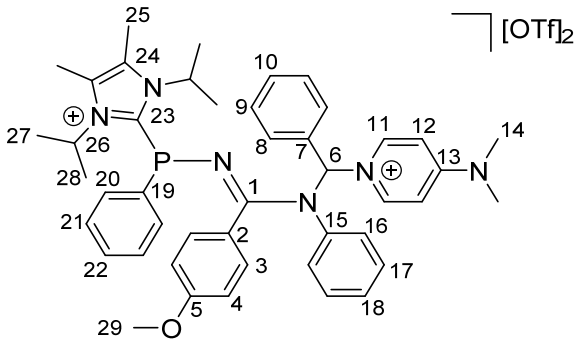


Figure S40. Molecular structure of **5b**$^{+}$ in **5b**[OTf] · 0.5 CH_2Cl_2; hydrogen atoms, the anion, and solvent molecules are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.10 Preparation of 6[OTf]$_2$



A mixture of **3b**[OTf]$_2$ (150 mg, 0.17mmol, 1 eq.) and DMAP (21.0 mg, 0.17mmol, 1 eq.) in PhF (4 mL) was stirred at room temperature for 2 days, resulting in a white suspension. The suspension was filtered and washed with PhF (3 x 1 mL) to obtain a white, air and moisture sensitive powder. Suitable crystals for X-ray diffraction analysis can be obtained by layering a DCM solution with Et_2O at room temperature.

Yield: 32 mg, 38%. **m.p.** 152 °C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3063 (100), 2945 (90), 1606 (90), 1586 (61), 1577 (64), 1562 (47), 1285 (54), 1033 (94), 1000 (87), 755 (49), 349 (74), 313 (73), 267 (89). **IR** (ATR, 298 K, [cm^{-1}]): 1644 (w), 1607 (vw), 1576 (w), 1560 (w), 1508 (w), 1496 (w), 1457 (vw), 1440 (vw), 1410 (vw), 1344 (vw), 1326 (vw), 1314 (vw), 1262 (vs), 1251 (s), 1221 (m), 1149 (m), 1115 (m), 1066 (vw), 1028 (s), 842 (w), 827 (vw), 806 (vw), 792 (vw), 778 (vw), 750 (w), 716 (vw), 703 (w), 689 (vw), 665 (vw), 649 (vw), 636 (vs), 573 (w), 544 (vw), 517 (m), 459 (vw), 448 (vw). **^{1}H NMR** (500.13 MHz, CD_3CN, 300

K, in ppm): δ = 1.00 (6H, d, $^{3}J_{HH}$ = 6.8 Hz, H28), 1.45 (6H, d, $^{3}J_{HH}$ = 7.0 Hz, H27), 2.30 (6H, s, H25), 3.24 (6H, s, H14), 3.68 (3H, s, H29), 5.08 (2H, sept, $^{3}J_{HH}$ = 6.9 Hz, H26), 6.75 (2H, m, H3), 6.97 (4H, m, Ar-H), 7.00 (3H, m, Ar-H), 7.14 (3H, m, Ar-H), 7.21 (2H, m, Ar-H), 7.32 (3H, m, Ar-H), 7.38 (4H, m, Ar-H), 8.22 (1H, s, H6), 8.24 (2H, d, $^{3}J_{HH}$ = 7.5 Hz, H11). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_3CN, 300 K, [ppm]): δ = 10.0 (2C, s, C25), 19.8 (2C, s, C28), 20.9 (2C, s, C27), 40.0 (2C, s, C14), 52.4 (2C, d, $^{3}J_{CP}$ = 14 Hz, C26), 55.1 (1C, s, C29), 79.7 (1C, s, C6), 107.9 (2C, s, C12), 113.9 (2C, s, C4), 115.1 (2C, d, $^{2}J_{CP}$ = 22 Hz, C20), 122.4 (2C, q, $^{1}J_{CF}$ = 321 Hz, OTf), 127.2 (1C, d, $^{3}J_{CP}$ = 9 Hz, C2), 128.3 (1C, s, Ar-C), 128.8 (2C, s, Ar-C), 129.0 (1C, s, Ar-C), 129.1 (2C, s, Ar-C), 129.2 (2C, s, Ar-C), 129.4 (2C, s, Ar-C), 129.9 (1C, s, Ar-C), 130.3 (2C, d, $^{3}J_{CP}$ = 8 Hz, C21), 130.8 (1C, s, C24), 131.4 (2C, s, Ar-C), 133.4 (1C, s, C15), 138.6 (1C, s, C7), 139.9 (2C, s, C11), 144.3 (1C, d, $^{1}J_{CP}$ = 70 Hz, C23), 157.1 (1C, s, C13), 160.3 (1C, s, C5), 162.8 (1C, d, $^{1}J_{CP}$ = 248 Hz, C19), 171.1 (1C, d, $^{2}J_{CP}$ = 32 Hz, C1). **^{19}F{^{1}H} NMR** (470.59 MHz, CD_3CN, 300 K, in ppm): δ = -79.3 (s, OTf). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_3CN, 300 K, in ppm): δ = 12.9 (s). **Elemental analysis**: calculated for $C_{47}H_{53}F_6N_6O_7PS_2$ 0.65 $C_4H_{10}O$: C, 55.61; H, 5.60; N, 7.85; S, 5.99; found: C, 55.29; H, 5.424; N, 7.53; S, 5.695.

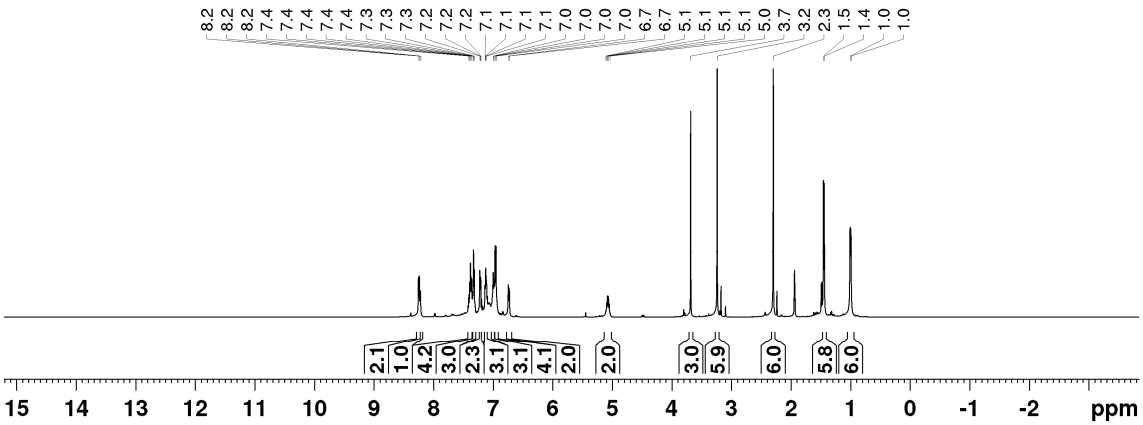


Figure S41. ^{1}H NMR spectrum of ring-opening product **6**[OTf]$_2$ (300 K, CD_3CN).

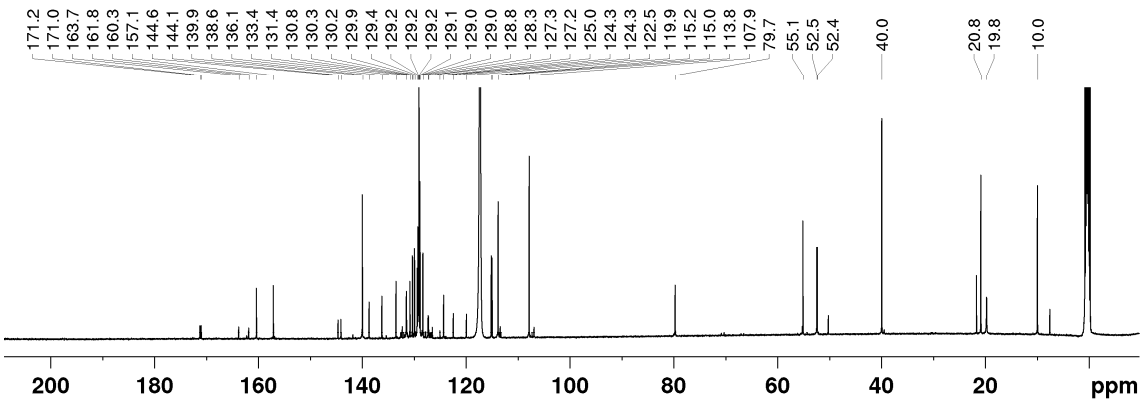


Figure S42. ^{13}C{^{1}H} NMR spectrum of ring-opening product **6**[OTf]$_2$ (300 K, CD_3CN).

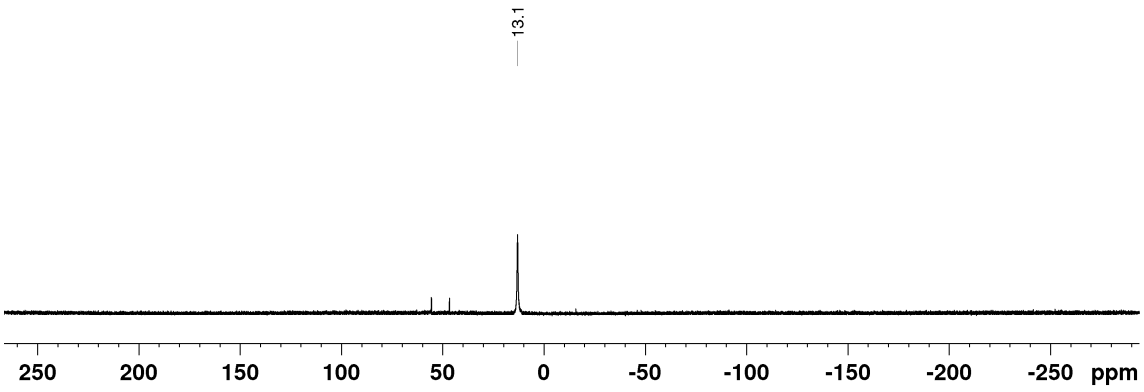


Figure S43. $^{31}P\{^{1}H\}$ NMR spectrum of ring-opening product **6[OTf]$_2$** (300 K, CD_3CN).

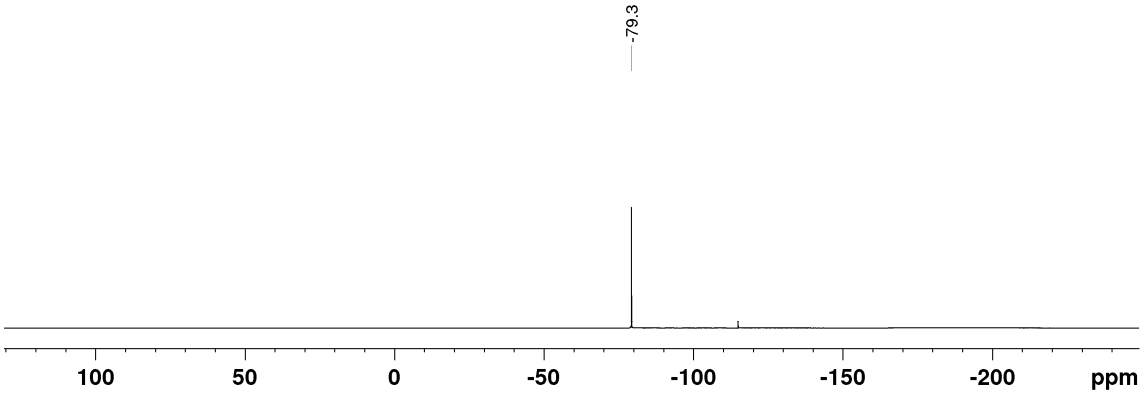


Figure S44. $^{19}F\{^{1}H\}$ NMR spectrum of ring-opening product **6**[OTf]$_2$ (300 K, CD_3CN).

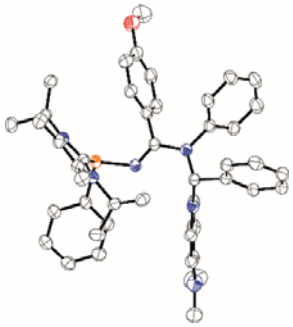
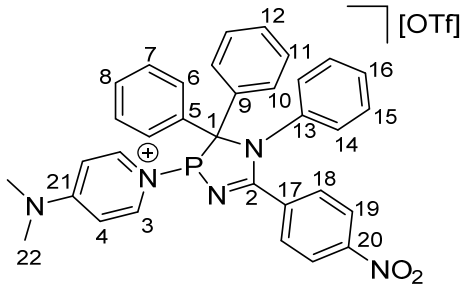


Figure S45. Molecular structure of ring-opening product **6**$^{2+}$ in **6**[OTf]$_2$ · 0.666 CH_2Cl_2; hydrogen atoms, the anions, and solvent molecules are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.11 Preparation of 5c[OTf]



The isolated **4**[OTf] (72 mg) was dissolved in DCM (2 mL) and stirred for 16 h. Subsequent removal of the solvent *in vacuo* afforded a pale yellow, air and moisture sensitive solid. Suitable crystals for X-ray diffraction analysis were obtained by layering a DCM solution with Et_2O at room temperature. Prolonging the reaction time (>1 week) for **3c**$[OTf]_2$ with DMAP can afford **5c**[OTf].

Yield: 72 mg, 99%. **m.p.** 215 °C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): No Raman spectrum could be obtained due to fluorescence of the compound. **IR** (ATR, 298 K, [cm^{-1}]): 1631 (m), 1567 (vw), 1524 (m), 1510 (w), 1487 (w), 1444 (vw), 1402 (vw), 1343 (m), 1315 (w), 1273 (m), 1257 (vs), 1221 (m), 1147 (m), 1041 (s), 1029 (vs), 1005 (vw), 868 (w), 859 (w), 826 (m), 803 (vw), 766 (w), 755 (m), 733 (m), 713 (w), 695 (m), 674 (vw), 636 (vs), 627 (m), 588 (w), 571 (vw), 516 (m), 503 (w), 493 (vw), 470 (w). **^{1}H NMR** (500.13 MHz, CD_3CN, 300 K, in ppm): δ = 3.15 (6H, s, H22), 6.61 (2H, m, Ar-H), 6.76 (2H, m, Ar-H), 6.95 (2H, m, Ar-H), 7.05 (6H, m, Ar-H), 7.39 (3H, m, Ar-H), 7.58 (2H, m, Ar-H), 7.66 (2H, m, H4), 7.99 (2H, m, H3), 8.16 (2H, m, H19). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_3CN, 300 K, in ppm) : δ = 39.6 (1C, s, C22), 39.9 (1C, s, C22), 84.6 (1C, d, $^{1}J_{CP}$ = 47 Hz, C1), 122.5 (1C, 1, $^{1}J_{CF}$ = 321 Hz, OTf), 123.3 (2C, s, C19), 128.6 (2C, s, Ar-C), 128.8 (2C, s, Ar-C), 129.2 (1C, d, $^{4}J_{CP}$ = 2 Hz, Ar-C), 130.4 (2C, d, $^{3}J_{CP}$ = 15 Hz, Ar-C), 131.6 (2C, s, C3), 131.6 (2C, s, Ar-C), 134.0 (2C, s, Ar-C), 137.8 (1C, d, $^{3}J_{CP}$ = 31 Hz, C13), 138.2 (1C, d, $^{3}J_{CP}$ = 6 Hz, C17), 138.5 (1C, s, C5), 138.8 (1C, s, C9), 141.0 (2C, br, C4), 149.4 (1C, s, C20), 157.5 (1C, s, C21), 172.5 (1C, d, $^{2}J_{CP}$ = 10 Hz, C2). **^{19}F{^{1}H} NMR** (470.59 MHz, CD_3CN, 300 K, in ppm): δ = -79.3 (s, OTf). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_3CN, 300 K, in ppm): δ = 139.8 (s). **Elemental analysis**: calculated for $C_{34}H_{29}F_3N_5O_5PS$ 0.25 CH_2Cl_2: C, 56.44; H, 4.08; N, 9.61; S, 4.40; found: C, 56.83; H, 3.473; N, 9.55; S, 4.181.

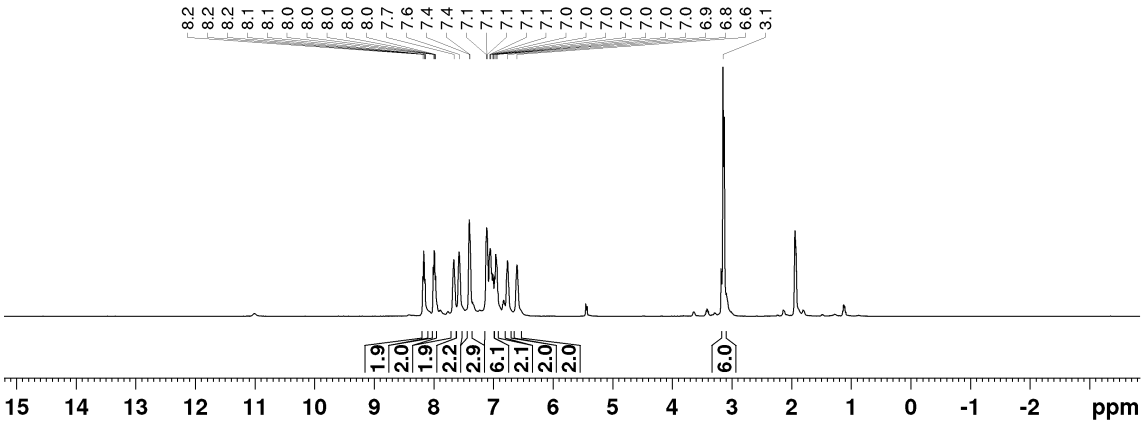


Figure S46. ^{1}H NMR spectrum of **5c**[OTf] (300 K, CD_3CN).

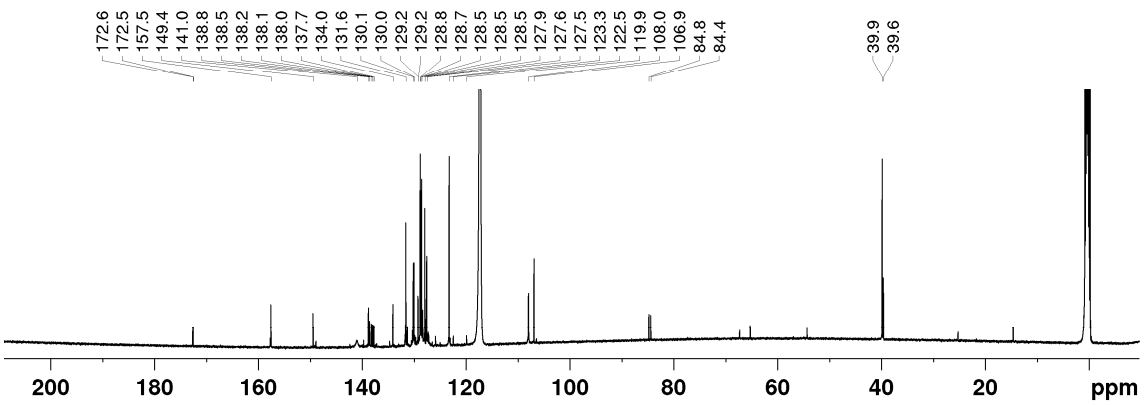


Figure S47. ^{13}C{^{1}H} NMR spectrum of **5c**[OTf] (300 K, CD_3CN).

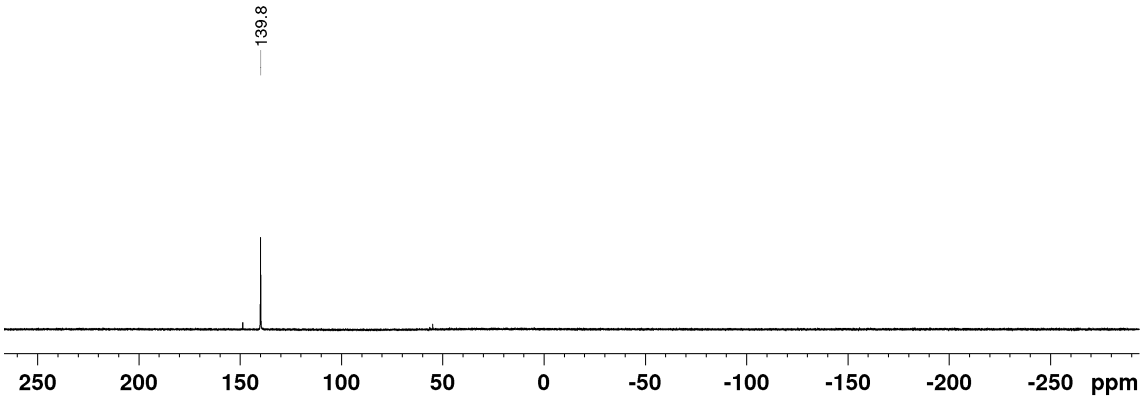


Figure S48. $^{31}P\{^{1}H\}$ NMR spectrum of **5c**[OTf] (300 K, CD_3CN).

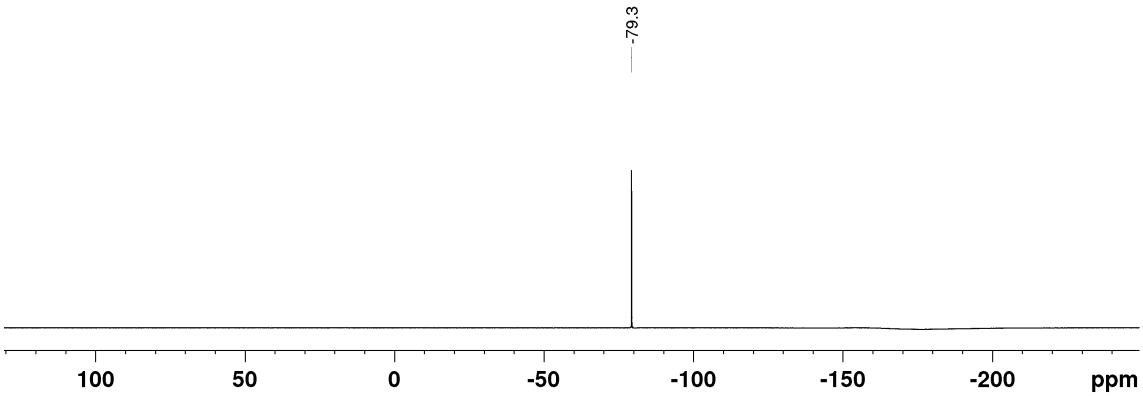


Figure S49. $^{19}F\{\}$ NMR spectrum of **5c**[OTf] (300 K, CD_3CN).

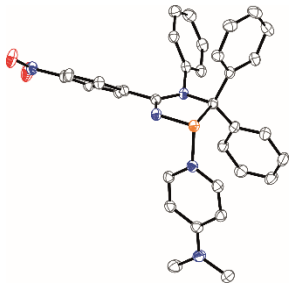
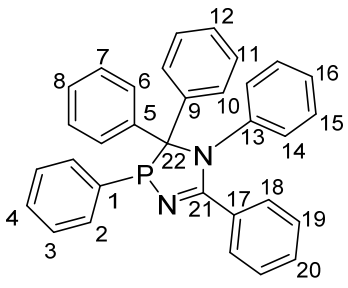


Figure S50. Molecular structure of **5c**$^{+}$ in **5c**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.12 Preparation of 7



PhMgBr (0.2 M in THF, 2.26 mL, 0.45 mmol, 1 eq.) was added dropwise to a suspension of **5a**[OTf] (300 mg, 0.45 mmol, 1 eq.) in THF (5 mL). The mixture was stirred at room temperature

for 2 h, affording a yellow solution. The solvent was removed *in vacuo*, and the residue was filtered over silica using Et_2O as eluent. Subsequent removal of the solvent *in vacuo* led to the isolation of a pale-yellow crystalline, air sensitive solid. Suitable crystals for X-ray diffraction analysis formed from an Et_2O solution at room temperature.

Yield: 156 mg, 74%. **m.p.** 178 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3060 (21), 1600 (38), 1543 (15), 1334 (6), 1177 (12), 1164 (15), 1126 (6), 1089 (6), 1033 (15), 1004 (50), 677 (9), 619 (6), 334 (6), 263 (12), 238 (15), 222 (9), 205 (6), 140 (35), 93 (100). **IR** (ATR, 298 K, [cm^{-1}]): 1586 (w), 1542 (w), 1488 (m), 1442 (w), 1434 (vw), 1331 (m), 1306 (w), 1290 (vw), 1250 (vw), 1125 (w), 1088 (vw), 1080 (vw), 1027 (vw), 1002 (vw), 984 (vw), 813 (w), 793 (m), 771 (w), 752 (s), 745 (m), 729 (s), 691 (vs), 660 (w), 619 (vw), 612 (w), 551 (vw), 525 (vw), 513 (vw), 501 (m), 453 (m). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 6.60 (2H, m, H14), 6.82 (3H, m, Ar-H), 6.84 (5H, m, Ar-H), 7.14 (4H, m, Ar-H), 7.23 (1H, m, H12), 7.26 (1H, m, H10), 7.31 (4H, m, H3, H4), 7.36 (1H, m, H20), 7.75 (4H, m, H18, H6). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm): δ = 82.7 (1C, d, $^1J_{CP}$ = 36 Hz, C22), 125.5 (1C, s, C16), 126.0 (2C, s, C19), 127.3 (2C, s, C15), 127.8 (1C, s, C20), 127.9 (2C, s, C14), 128.0 (1C, s, C4), 128.1 (2C, d, $^3J_{CP}$ = 7 Hz, C10), 128.3 (2C, d, $^3J_{CP}$ = 15 Hz, C3), 129.2 (2C, s, C7), 129.2 (2C, s, C11), 129.8 (1C, s, C8), 130.1 (2C, s, C18), 130.3 (1C, s, C12), 130.9 (2C, d, $^3J_{CP}$ = 14 Hz, C6), 132.7 (2C, d, $^2J_{CP}$ = 22 Hz, C2), 134.9 (1C, d, $^3J_{CP}$ = 6 Hz, C13), 137.6 (1C, s, C9), 138.5 (1C, d, $^1J_{CP}$ = 34 Hz, C1), 142.0 (1C, s, C5), 142.7 (1C, d, $^3J_{CP}$ = 25 Hz, C17), 167.5 (1C, d, $^2J_{CP}$ = 8 Hz, C21). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 98.1 (s). **Elemental analysis**: calculated for $C_{32}H_{25}N_2P$ 0.1 CH_2Cl_2: C, 80.82; H, 5.32; N, 5.87; found: C, 81.10; H, 5.272; N, 5.87.

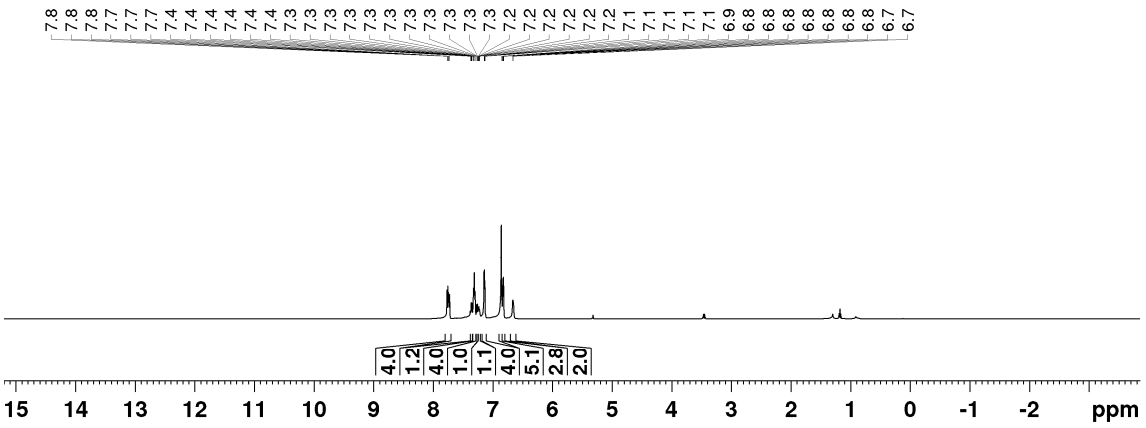


Figure S51. ^{1}H NMR spectrum of **7** (300 K, CD_2Cl_2).

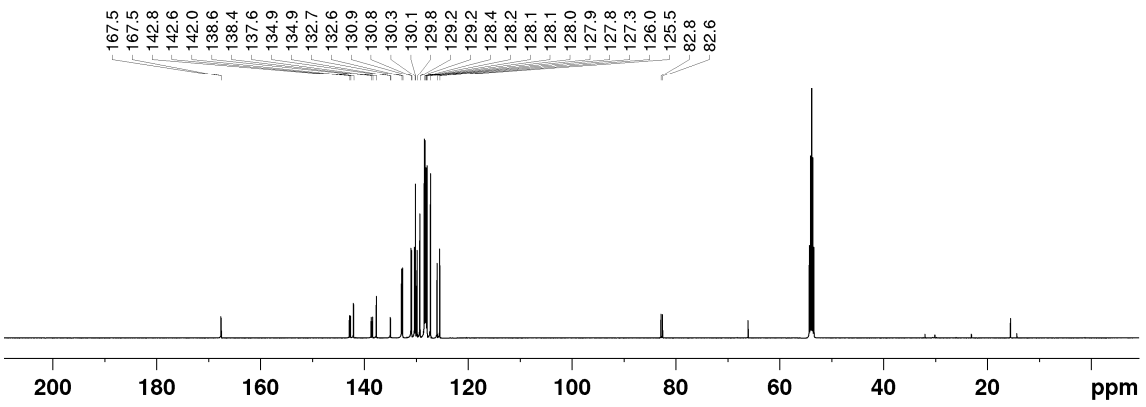


Figure S52. ^{13}C{H} NMR spectrum of **7** (300 K, CD_2Cl_2).

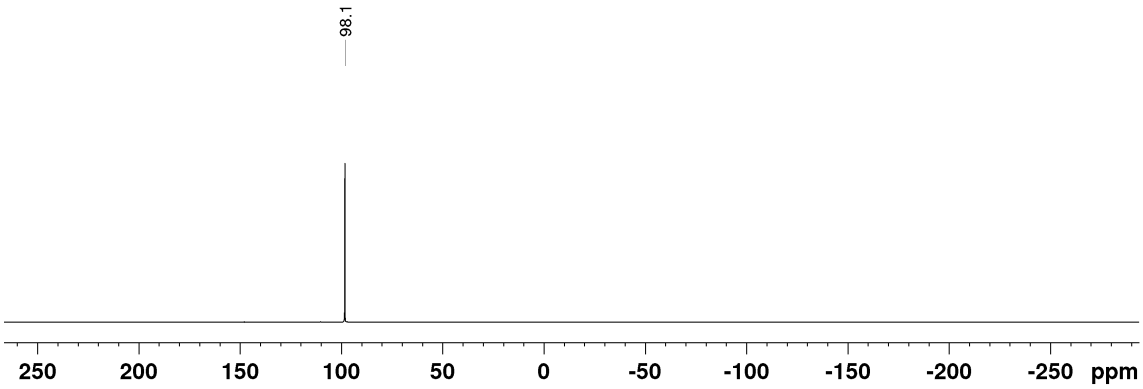


Figure S53. $^{31}P\{^{1}H\}$ NMR spectrum of **7** (300 K, CD_2Cl_2).

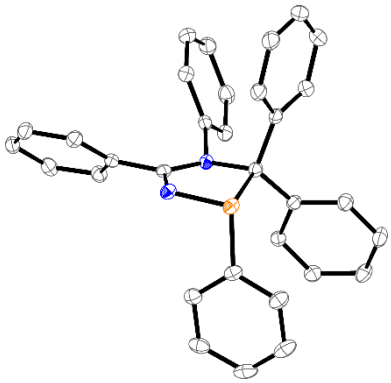
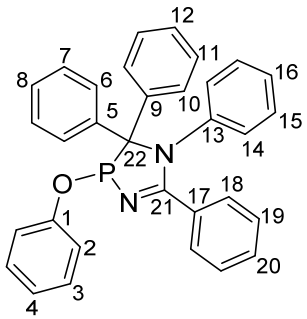


Figure S54. Molecular structure of **7**; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.13 Preparation of 8



A suspension of PhOH (43 mg, 0.45 mmol, 1 eq.), Et_3N (92 mg, 127 µL, 0.45 mmol, 1 eq.) and **5a**[OTf] (300 mg, 0.45 mmol, 1 eq.) in THF (4 mL) was heated at 60 °C for 2 hours. The solvent was removed *in vacuo* and the residue was filtered over silica using Et_2O/toluene (1:1) as eluent. Subsequent removal of the solvent *in vacuo* to obtain a white crystalline, air sensitive solid. Suitable crystals for X-ray diffraction analysis were obtained by layering a DCM solution with Et_2O at room temperature. KOPh can also be used under this condition to obtain **8**.

Yield: 152 mg, 69%. **m.p.** 189 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3064 (43), 1600 (66), 1521 (42), 1445 (10), 1352 (20), 1312 (5), 1279 (9), 1221 (7), 1206 (12), 1168 (18), 1031 (11), 1003 (75), 816 (8), 725 (10), 678 (11), 619 (7), 500 (5), 329 (7), 279 (7), 256 (11), 242 (9), 218 (6), 144 (19), 114 (66), 101 (90), 83 (100). **IR** (ATR, 298 K, [cm^{-1}]): 1587 (vw), 1520 (vw), 1485 (m), 1454 (vw), 1444 (vw), 1349 (w), 1277 (vw), 1206 (m), 1163 (vw), 1140 (vw), 1025 (vw), 963 (vw), 899 (vw), 855 (w), 826 (m), 815 (w), 800 (w), 766 (w), 749 (s), 721 (w),

711 (w), 693 (vs), 662 (vw), 626 (vw), 612 (vw), 500 (w), 495 (w), 479 (w), 410 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, [ppm]): δ = 6.77 (2H, m, H2), 6.85 (2H, m, H6), 6.93 (3H, m, H7, H8), 6.97 (1H, m, H4), 7.03 (3H, m, H15, H16), 7.12 (2H, m, H3), 7.38 (4H, m, H14, H19), 7.42 (2H, m, H12, H20), 7.52 (2H, m, H11), 7.79 (2H, m, H10), 7.82 (2H, m, H18). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, [ppm]): δ = 83.6 (1C, d, $^{1}J_{CP}$ = 47 Hz, C22), 119.8 (2C, d, $^{3}J_{CP}$ = 9 Hz, C2), 123.0 (1C, s, C4), 125.1 (1C, s, C8), 126.8 (1C, s, C16), 127.1 (2C, s, C6), 127.4 (2C, s, C15), 127.9 (2C, s, C7), 128.0 (1C, s, C12), 128.1 (2C, s, C19), 128.3 (2C, s, C11), 129.3 (2C, s, C3), 129.9 (2C, d, $^{3}J_{CP}$ = 12 Hz, C10), 130.2 (2C, d, $^{4}J_{CP}$ = 1 Hz, C14), 130.4 (2C, s, C18), 130.6 (1C, s, C20), 133.8 (1C, d, $^{3}J_{CP}$ = 4 Hz, C17), 135.0 (1C, d, $^{3}J_{CP}$ = 1 Hz, C13), 138.0 (1C, d, $^{2}J_{CP}$ = 32 Hz, C9), 140.6 (1C, s, C5), 155.9 (1C, d, $^{2}J_{CP}$ = 9 Hz, C1), 169.7 (1C, d, $^{2}J_{CP}$ = 11 Hz, C21). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 147.5 (s). **Elemental analysis**: calculated for $C_{32}H_{25}N_2OP$: C, 79.32; H, 5.20; N, 5.78; found: C, 79.13; H, 5.330; N, 5.66.

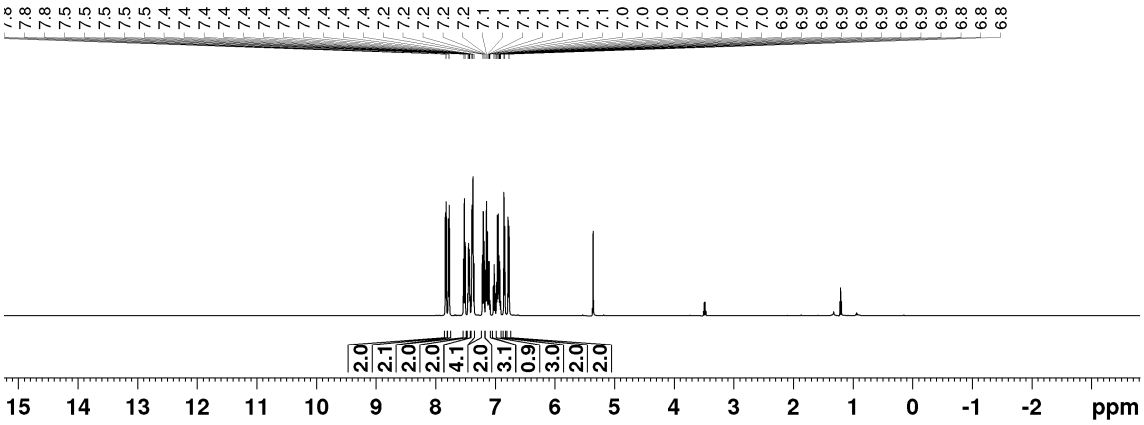


Figure S55. ^{1}H NMR spectrum of **8** (300 K, CD_2Cl_2).

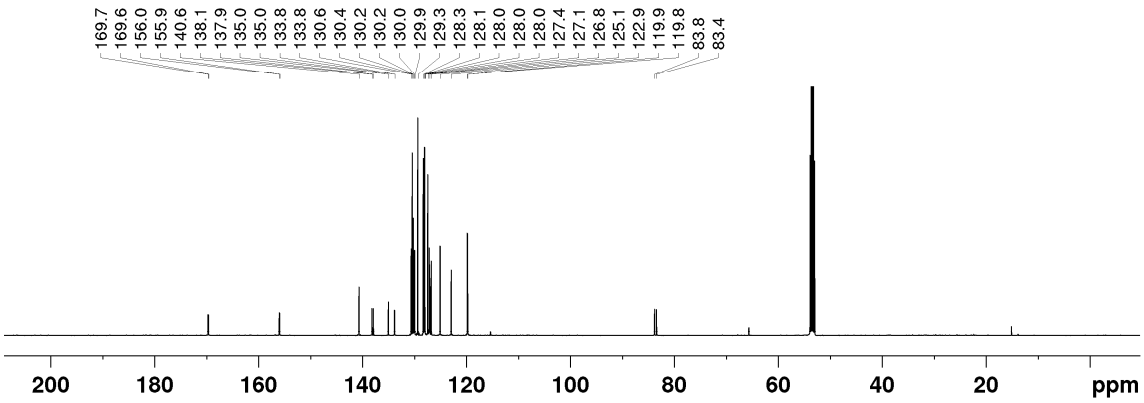


Figure S56. ^{13}C{^{1}H} NMR spectrum of **8** (300 K, CD_2Cl_2).

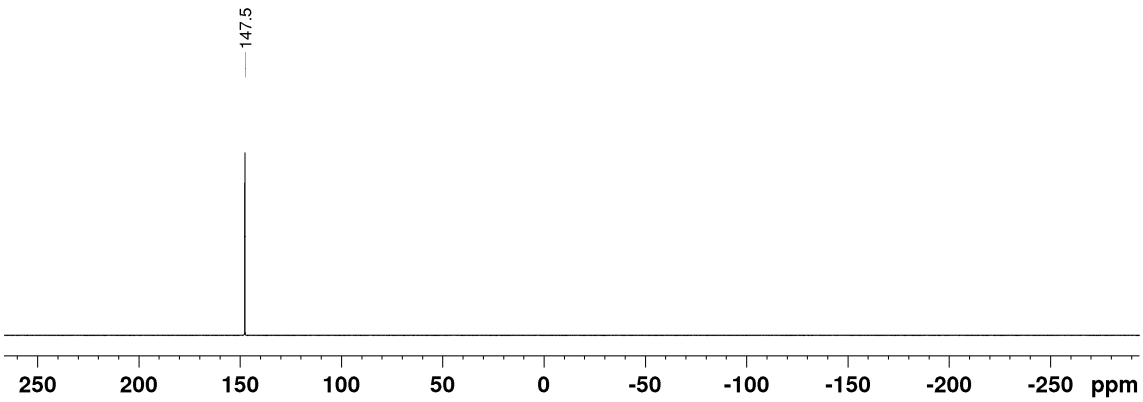


Figure S57. $^{31}P\{^{1}H\}$ NMR spectrum of **8** (300 K, CD_2Cl_2).

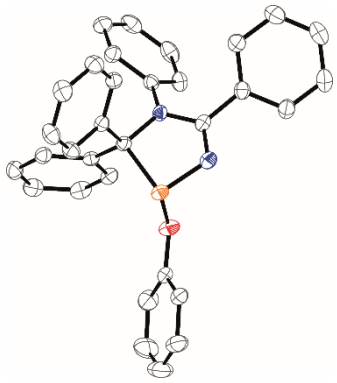
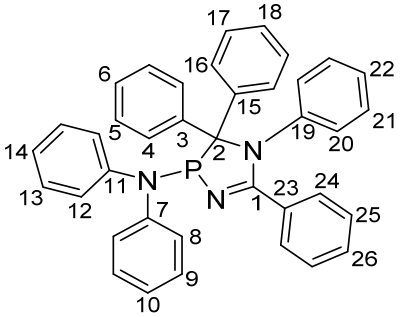


Figure S58. Molecular structure of **8**; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.14 Preparation of 9



THF (3 mL) was added to a mixture of **5a**[OTf] (150 mg, 0.23 mmol, 1 eq.) and $KNPh_2$ (47 mg, 0.23 mmol, 1 eq.). The mixture was stirred at room temperature for 2 h to afford a yellow solution. The solvent was removed *in vacuo* and the residue dissolved in Et_2O and filtered over silica using Et_2O as eluent. Subsequent removal of the solvent *in vacuo* obtained a pale yellow crystalline, air sensitive solid. Suitable crystals for X-ray diffraction analysis obtained by layering a DCM solution with Et_2O at room temperature.

Yield: 81 mg, 64%. **m.p.** 240 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3065 (57), 1598 (75), 1526 (31), 1445 (9), 1343 (14), 1284 (12), 1226 (9), 1192 (21), 1174 (18), 1160 (17), 1031 (23), 1003 (100), 802 (11), 674 (20), 619 (13), 326 (9), 242 (11), 88 (88). **IR** (ATR, 298 K, [cm^{-1}]): 3061 (vw), 3031 (vw), 2361 (vw), 2342 (vw), 1585 (w), 1533 (w), 1484 (s), 1443 (w), 1343 (m), 1309 (vw), 1276 (vw), 1255 (m), 1191 (w), 1176 (w), 1158 (vw), 1136 (vw), 1074

(vw), 1027 (w), 1018 (vw), 1002 (vw), 989 (vw), 949 (m), 923 (vw), 909 (vw), 890 (w), 880 (vw), 832 (m), 808 (w), 798 (w), 758 (s), 745 (m), 720 (vw), 692 (vs), 660 (w), 625 (w), 619 (vw), 598 (w), 552 (vw), 529 (s), 515 (w), 502 (w), 494 (w), 467 (vw), 448 (vw), 428 (vw), 405 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 6.39 (2H, m, Ar-H), 6.71 (2H, m, Ar-H), 6.89 (3H, m, Ar-H), 6.97 (1H, m, Ar-H), 7.10 (4H, m, Ar-H), 7.12 (3H, m, Ar-H), 7.28 (4H, m, Ar-H), 7.34 (3H, m, Ar-H), 7.42 (2H, m, Ar-H), 7.50 (2H, m, Ar-H), 7.55 (2H, m, Ar-H), 7.81 (2H, m, Ar-H). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm): δ = 81.7 (1C, d, $^{1}J_{CP}$ = 57 Hz, C2), 122.7 (2C, br, Ar-C), 123.3 (2C, br, Ar-C), 124.9 (1C, s, Ar-C), 125.1 (1C, s, Ar-C), 126.3 (1C, s, Ar-C), 126.7 (2C, s, Ar-C), 127.3 (2C, s, Ar-C), 127.6 (2C, s, Ar-C), 127.8 (2C, s, Ar-C), 128.0 (2C, s, Ar-C), 128.2 (2C, s, Ar-C), 128.3 (2C, s, Ar-C), 129.1 (2C, br, Ar-C), 129.2 (1C, s, Ar-C), 129.7 (1C, s, Ar-C), 129.9 (1C, s, Ar-C), 130.2 (2C, s, Ar-C), 130.4 (2C, s, Ar-C), 134.0 (1C, d, $^{3}J_{CP}$ = 4 Hz, Ar-C), 136.7 (1C, d, $^{3}J_{CP}$ = 2 Hz, Ar-C), 140.9 (1C, s, Ar-C), 141.9 (1C, d, $^{1}J_{CP}$ = 35 Hz, Ar-C), 144.5 (1C, s, Ar-C), 150.3 (1C, s, Ar-C), 165.8 (1C, d, $^{2}J_{CP}$ = 10 Hz, C1). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 108.4 (s). **Elemental analysis**: calculated for $C_{38}H_{30}N_3P$: C, 81.55; H, 5.40; N, 7.51; found: C, 81.07; H, 5.314; N, 7.70.

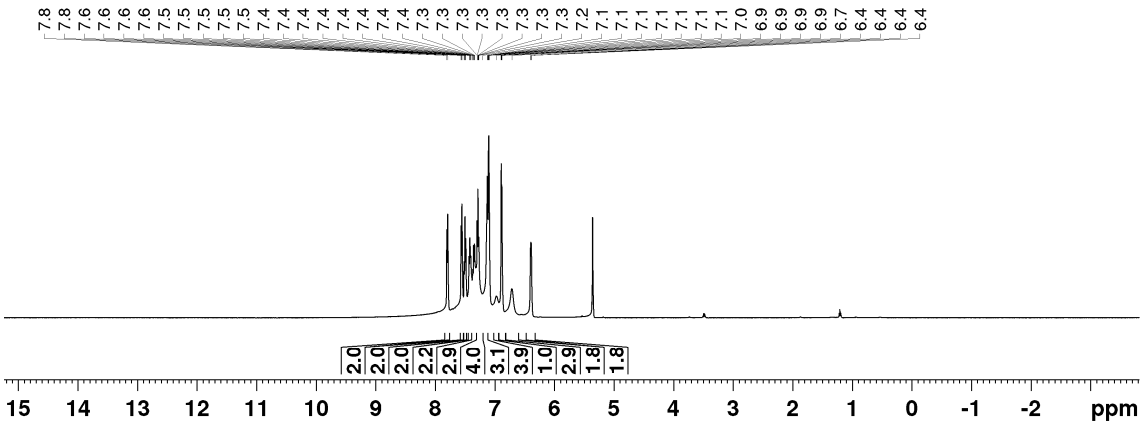


Figure S59. ^{1}H NMR spectrum of **9** (300 K, CD_2Cl_2).

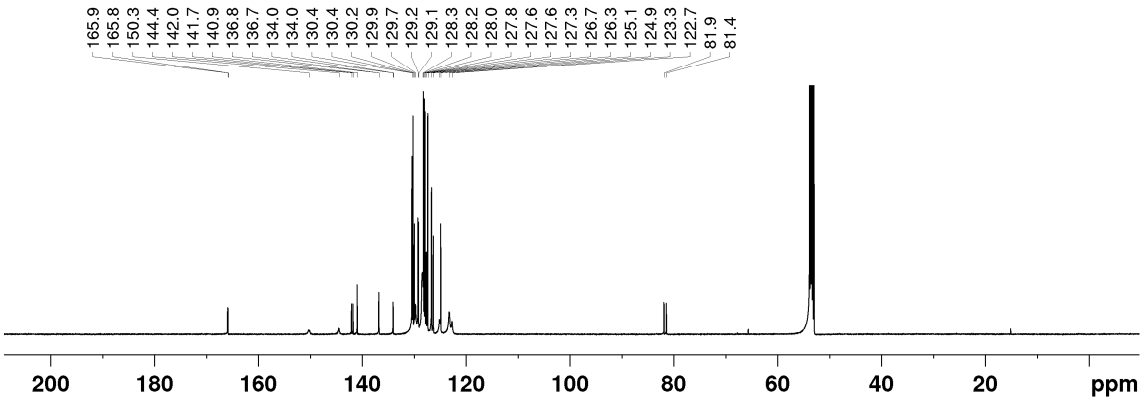


Figure S60. ^{13}C{^{1}H} NMR spectrum of **9** (300 K, CD_2Cl_2).

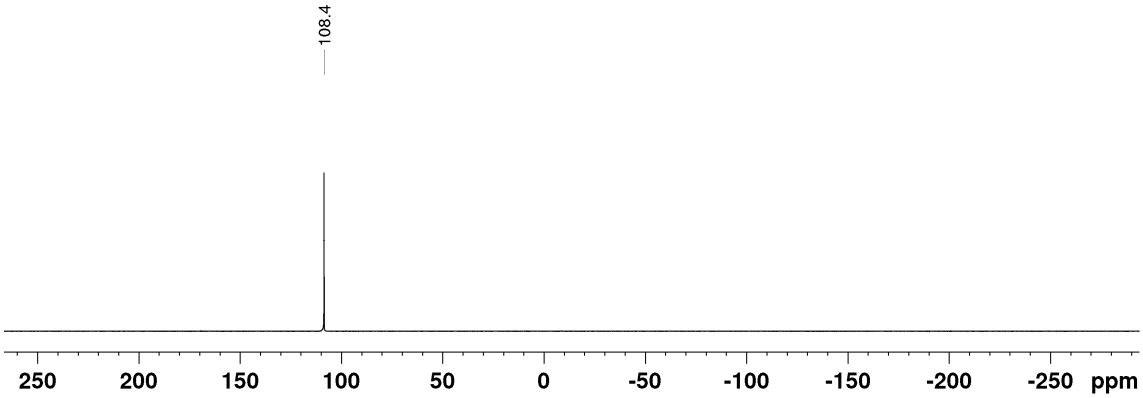


Figure S61. $^{31}P\{^{1}H\}$ NMR spectrum of **9** (300 K, CD_2Cl_2).

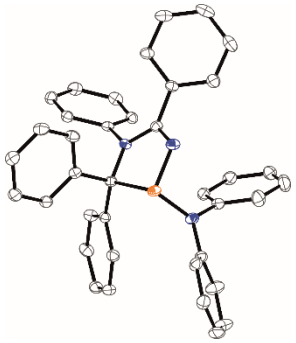
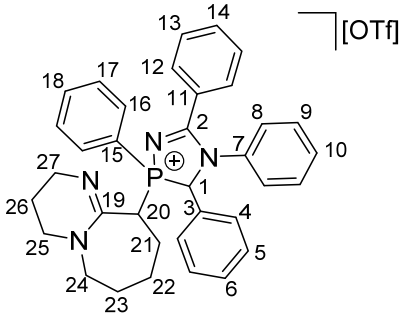


Figure S62. Molecular structure of **9**; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.15 Preparation of 10[OTf]



DBU (175 mg, 1.15 mmol, 1 eq.) in THF (5 mL) was added to a suspension of **3a**$[OTf]_2$ (1.0 g, 1.15 mmol, 1 eq.) in THF (15 mL). The suspension turned into yellow solution after 30 min from which a colorless solid precipitated for 16 h. The suspension was filtered and washed with THF and Et_2O (3 × 2 mL) to afford a white, air and moisture sensitive solid. Suitable crystals for X-ray diffraction analysis were obtained by layering a DCM solution with Et_2O at –30°C.

Yield: 648 mg, 78%. **m.p**.: 245 °C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3065 (18), 3050 (16), 2972 (9), 2938 (9), 2903 (7), 2858 (10), 1603 (47), 1553 (7), 1447 (9), 1384 (6), 1291 (7), 1223 (17), 1033 (26), 1002 (62), 755 (6), 731 (11), 618 (7), 312 (5), 267 (7), 221 (8), 184 (6), 98 (100). **IR** (ATR, 298 K, [cm^{-1}]): 3059 (vw), 3049 (vw), 2971 (vw), 2933 (vw), 2909 (vw), 2893 (vw), 2860 (vw), 1632 (w), 1604 (vw), 1585 (vw), 1551 (w), 1489 (w), 1459 (vw), 1445 (vw), 1439 (vw), 1377 (w), 1351 (vw), 1342 (vw), 1311 (vw), 1262 (vs), 1220 (w), 1186 (vw), 1151 (s), 1136 (m), 1111 (w), 1099 (vw), 1082 (vw), 1076 (vw), 1065 (vw), 1028

(s), 993 (vw), 949 (vw), 923 (vw), 870 (vw), 846 (vw), 828 (m), 777 (m), 763 (m), 747 (vw), 729 (m), 709 (m), 699 (s), 688 (m), 661 (vw), 635 (vs), 616 (w). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 8.09 (m, Ar-H, 2H), 7.75 (m, Ar-H, 3H), 7.60 (m, Ar-H, 4H), 7.53 (m, Ar-H, 3H), 7.47 (m, Ar-H, 1H), 7.35 (m, Ar-H, 2H), 7.12 (m, Ar-H, 3H), 6.68 (m, Ar-H, 2H), 5.53 (d, H1, $^{2}J_{HP}$ = 14 Hz, 1H), 4.14 (dd, H20, $^{2}J_{HP}$ = $^{3}J_{HH}$ = 12 Hz, 1H), 3.29 (m, DBU-H, 4H), 3.00 (m, DBU-H, 2H), 2.79 (m, 1H), 2.17 (m, DBU-H, 1H), 1.91 (m, DBU-H, 2H), 1.78 (m, DBU-H, 1H), 1.60 (m, DBU-H, 1H), 1.45 (m, DBU-H, 2H). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm) : δ = 20.8 (1C, s, C26), 26.5 (1C, d, $^{2}J_{CP}$ = 6 Hz, C21), 29.0 (1C, s, C27), 29.5 (1C, s, C25), 29.7 (1C, s, C24), 44.0 (1C, s, C22), 47.9 (1C, s, C23), 59.6 (1C, d, $^{1}J_{CP}$ = 104 Hz, C20), 67.7 (1C, d, $^{1}J_{CP}$ = 76 Hz, C1), 122.7 (1C, 1, $^{1}J_{CF}$ = 321 Hz, OTf), 127.5 (1C, s, C18), 128.2 (2C, s, C10), 128.6 (2C, s, C9), 129.7 (2C, d, $^{3}J_{CP}$ = 3 Hz, C4), 129.8 (1C, s, C6), 130.0 (2C, s, C8), 130.1 (1C, s, C18), 130.2 (2C, s, C12), 131.4 (1C, d, $^{2}J_{CP}$ = 12 Hz, C3), 132.0 (1C, s, C14), 132.9 (1C, s, C11), 133.5 (2C, d, $^{2}J_{CP}$ = 10 Hz, C16), 133.6 (2C, d, $^{3}J_{CP}$ = 3 Hz, C17), 134.4 (1C, d, $^{3}J_{CP}$ = 3 Hz, C7), 140.9 (1C, d, $^{1}J_{CP}$ = 11 Hz, C15), 159.5 (1C, d, $^{2}J_{CP}$ = 3 Hz, C19), 169.0 (1C, d, $^{2}J_{CP}$ = 5 Hz, C2). **^{19}F{^{1}H} NMR** (470.59 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.8 (s, OTf). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 23.4 (s) (86%), 18.0 (s) (14%). **Elemental analysis**: calculated for $C_{36}H_{36}F_3N_4O_3PS$ 0.1 CH_2Cl_2: C, 61.83; H, 5.20; N, 7.99; S, 4.57; found: C, 61.86; H, 4.971; N, 7.92; S, 4.670.

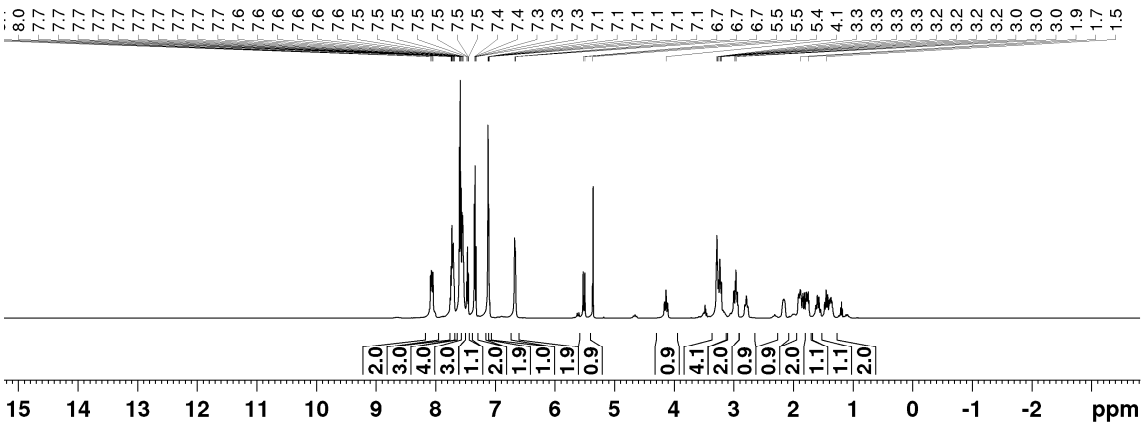


Figure S63. ^{1}H NMR spectrum of **10**[OTf] (300 K, CD_2Cl_2).

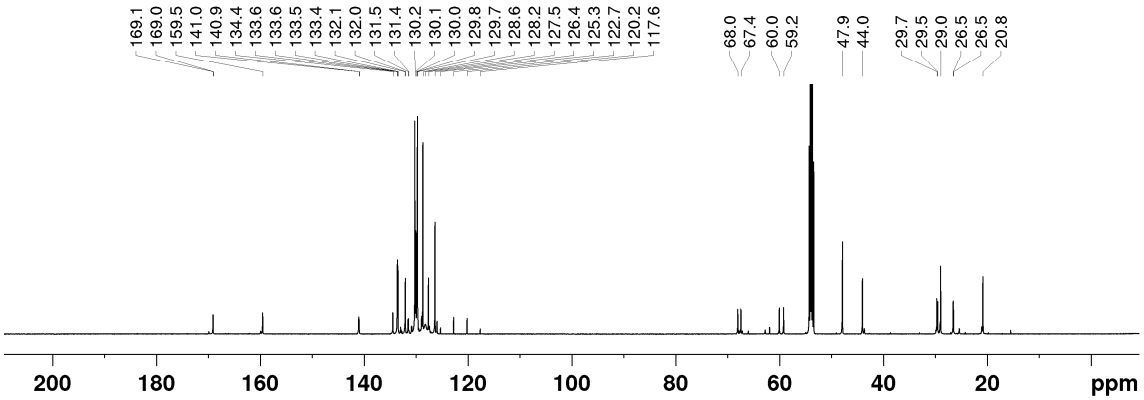


Figure S64. ^{13}C{^{1}H} NMR spectrum of **10**[OTf] (300 K, CD_2Cl_2).

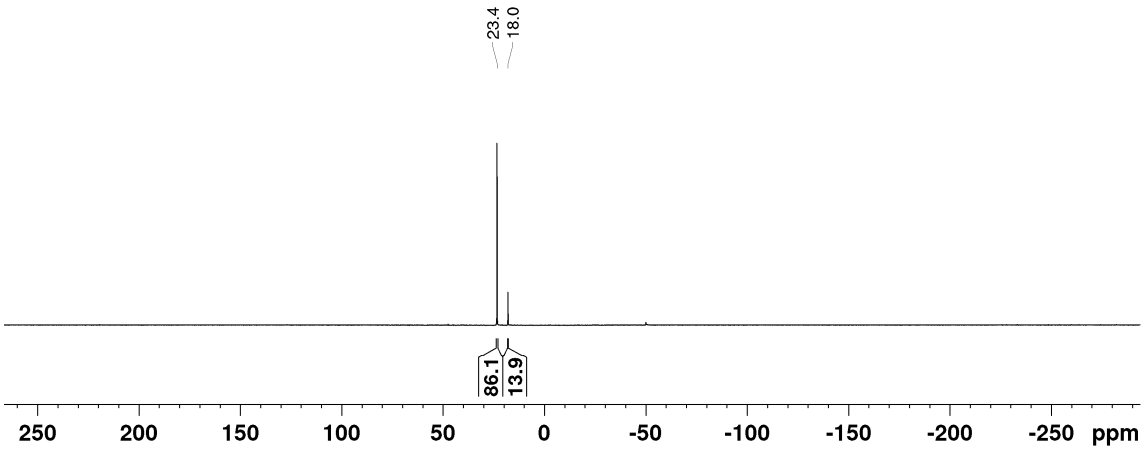


Figure S65. $^{31}P\{^{1}H\}$ NMR spectrum of **10**[OTf] (300 K, CD_2Cl_2).

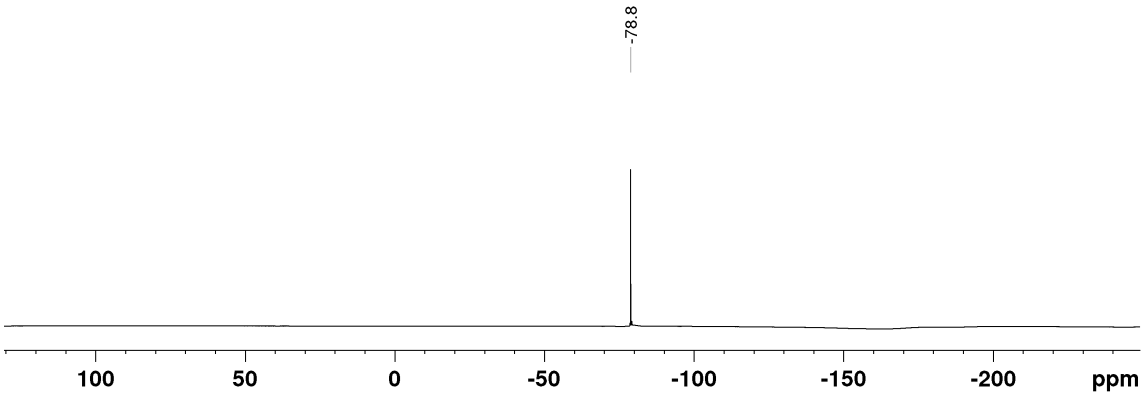


Figure S66. $^{19}F\{^{1}H\}$ NMR spectrum of **10**[OTf] (300 K, CD_2Cl_2).

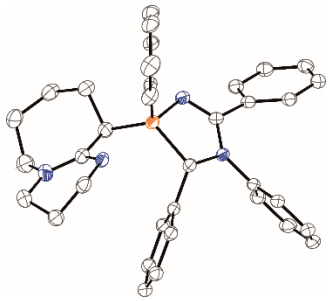
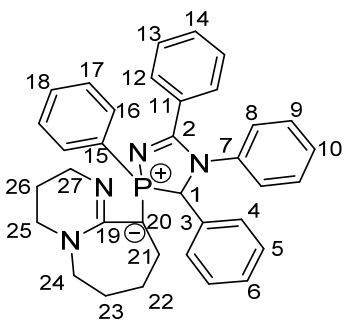


Figure S67. Molecular structure of *syn*-**10**$^{+}$ in *syn*-**10**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.16 Preparation of 11



Solid KHMDS (95%) (157 mg, 0.75 mmol, 1 eq.) was added to a suspension of **10**[OTf] (520 mg, 0.75 mmol, 1eq.) in THF (10 mL) at room temperature. The suspension turned to red immediately and gradually changed to orange in 30 minutes. After stirring for 2 h, all volatiles were removed *in vacuo*. The residue was extracted with Et_2O (2 × 5 mL), and the combined filtrates were concentrated *in vacuo* to dryness to afford the product as an orange powder. Suitable crystals for X-ray diffraction analysis can obtain by layering an Et_2O solution with *n*-hexane at room temperature. The solid decomposed slowly in the glovebox under N_2 atmosphere.

Yield: 203 mg, 86%. **m.p**.: 140°C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3071 (37), 3056 (63), 2951 (20), 2921 (25), 2817 (24), 1611 (100), 1575 (29), 1196 (16), 1001 (65), 92 (85), 73 (86). **IR** (ATR, 298 K, [cm^{-1}]): 2921 (vw), 2813 (vw), 2360 (w), 2341 (w), 1610 (vw), 1557 (m), 1491 (w), 1433 (w), 1348 (w), 1304 (w), 1264 (w), 1231 (m), 1189 (w), 1096 (m), 1026 (w), 912 (w), 789 (s), 760 (m), 732 (s), 717 (m), 690 (vs), 631 (s), 594 (m), 535 (m), 516 (m), 490 (m). **^{1}H NMR** (500.13 MHz, C_6D_6, 300 K, in ppm): δ = 1.24 (2H, m, H26), 1.44 (3H, m, H22), 1.58 (1H, m, DBU-H), 1.76 (1H, m, DBU-H), 2.26 (2H, m, DBU-H), 2.32 (3H, m, H24, DBU-H), 2.37 (1H, m, DBU-H), 3.05 (1H, m, DBU-H), 5.09 (1H, d, $^2J_{HP}$ = 12.7 Hz, H1), 6.70 (1H, m, H10), 6.80 (2H, m, H9), 6.90 (5H, m, Ar-H), 7.15 (3H, m, Ar-H), 7.24 (4H, m, Ar-H), 7.54 (2H, m, Ar-H), 7.77 (2H, m, H13), 7.89 (2H, m, H12). **^{13}C{^{1}H} NMR** (125.76 MHz, C_6D_6, 300 K, in ppm) : δ = 23.0 (1C, s, C26), 26.7 (1C, d, $^3J_{CP}$ = 6 Hz, C22), 30.5 (1C, s, C3), 30.7 (1C, d, $^2J_{CP}$ = 19 Hz, C21), 41.0 (1C, d, $^4J_{CP}$ = 6 Hz, C27), 48.8 (1C, s, C24), 55.4 (1C, s, C25), 61.1 (1C, d, $^1J_{CP}$ = 165 Hz, C20), 66.1 (1C, d, $^1J_{CP}$ = 79 Hz, C1), 123.8 (1C, s, C10), 124.1 (2C, s, C9), 126.7 (2C, s, Ar-C), 127.0 (2C, s, Ar-C), 127.6 (2C, s, Ar-C), 127.8 (2C, s, C13), 128.0 (2C, s, Ar-C), 128.1 (1C, s, Ar-C), 128.2 (1C, s, Ar-C), 128.6 (2C, s, Ar-C), 129.4 (1C, s, Ar-C), 129.8 (2C, s, C12), 134.7 (1C, d, $^2J_{CP}$ = 11 Hz, C3), 140.2 (1C, s, C11), 141.3 (1C, d, $^1J_{CP}$ = 141 Hz, C15), 145.3 (1C, d, $^3J_{CP}$ = 10 Hz, C7), 160.3 (1C, d, $^3J_{CP}$ = 5 Hz, C2), 161.6 (1C, d, $^2J_{CP}$ = 13 Hz, C19). **^{31}P{^{1}H} NMR** (202.46 MHz, C_6D_6, 300 K, in ppm): δ = -23.5 (s). **Elemental analysis**: calculated for $C_{35}H_{35}N_4P$ 0.1 KOTf: C, 75.08; H, 6.28; N, 9.98; S, 0.57; found: C, 74.92; H, 6.073; N, 9.73; S, 0.057.

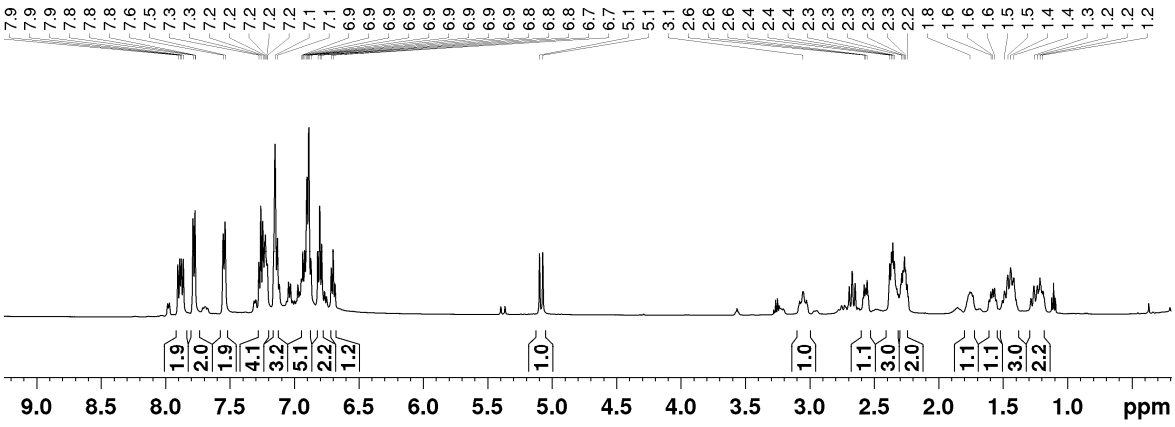


Figure S68. ^{1}H NMR spectrum of **11** (300 K, C_6D_6).

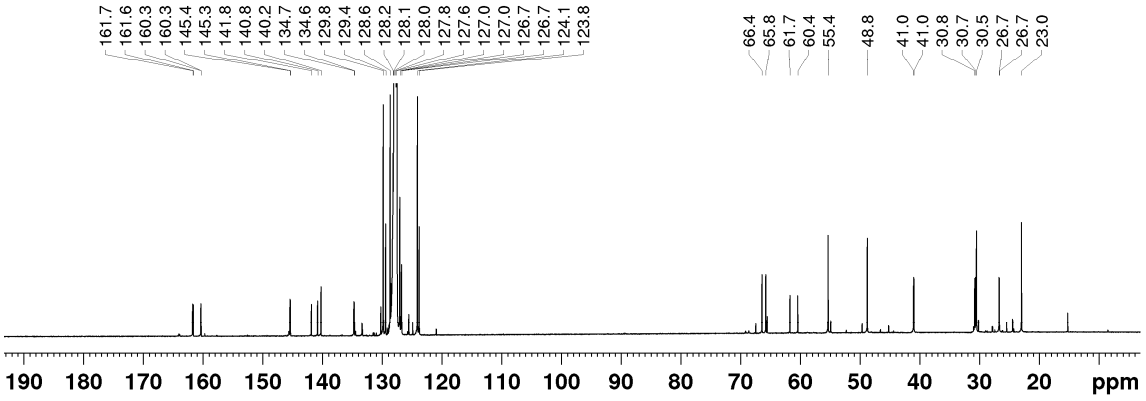


Figure S69. ^{13}C {H} NMR spectrum of **11** (300 K, C_6D_6).

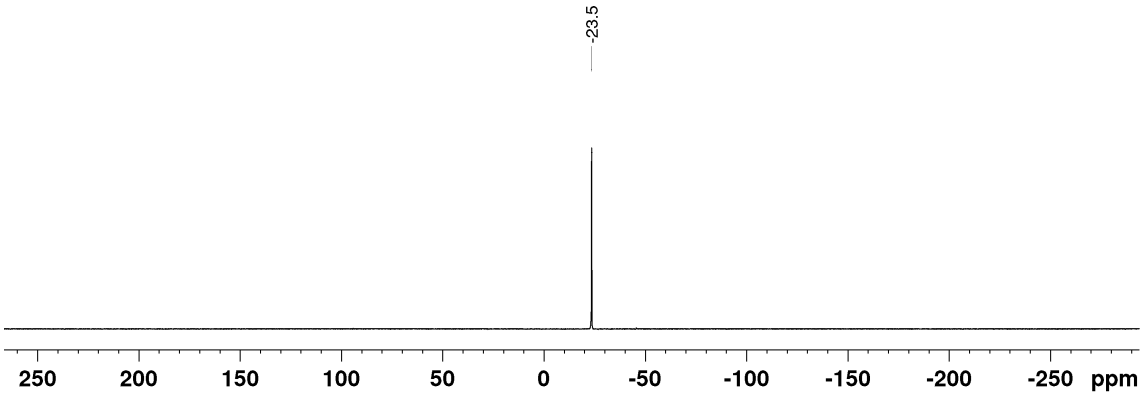


Figure S70. ^{31}P NMR spectrum of **11** (300 K, C_6D_6).

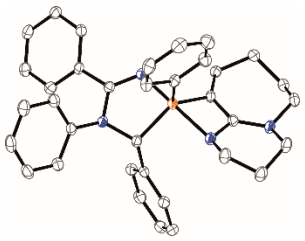
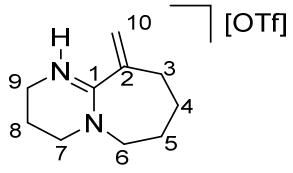


Figure S71. Molecular structure of **11**; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.17 Preparation of 13[OTf]



A mixture of **10**[OTf] (500 mg, 0.72 mmol, 1 eq.) and KHMDS (95%) (152 mg, 0.72 mmol, 1 eq.) in THF (10 mL) was allowed to stir at room temperature for 2 h. Paraformaldehyde (22 mg, 0.72 mmol, 1 eq.) was then added to the resulting orange solution, and the mixture was stirred for 16 h at room temperature. Silica (100 mg) was added to the solution and the mixture was stirred for 10 min. All volatiles were removed *in vacuo* and the crude mixture was purified

by column chromatography: Et_2O elution phase, phosphole oxide **12**, 154 mg, yield: 52%; DCM elution phase, **13**[OTf] 169 mg.

Yield: 74%. **m.p.** 63 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3098 (9), 2993 (36), 2959 (70), 2931 (36), 2896 (26), 2864 (27), 2210 (8), 1653 (27), 1628 (20), 1458 (33), 1449 (32), 1415 (17), 1336 (12), 1285 (18), 1276 (23), 1247 (12), 1224 (20), 1091 (14), 1080 (11), 1059 (15), 1029 (100), 999 (14), 904 (9), 891 (12), 814 (14), 756 (38), 712 (27), 605 (20), 574 (18), 492 (12), 410 (12), 350 (52), 334 (11), 313 (41), 278 (20), 252 (24), 232 (11), 149 (41), 77 (91). **IR** (ATR, 298 K, [cm^{-1}]): 3258 (vw), 3133 (vw), 2954 (vw), 2864 (vw), 1731 (vw), 1651 (w), 1626 (m), 1579 (w), 1447 (vw), 1414 (vw), 1378 (vw), 1366 (vw), 1323 (w), 1285 (s), 1271 (m), 1246 (vs), 1223 (s), 1209 (s), 1158 (s), 1138 (s), 1056 (vw), 1026 (vs), 996 (w), 959 (vw), 931 (m), 905 (vw), 892 (vw), 834 (vw), 813 (vw), 756 (w), 709 (vw), 678 (vw), 633 (vs), 573 (m), 516 (s), 492 (vw), 463 (vw), 407 (vw). **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.76 (4H, m, H5, H6), 2.08 (2H, quint, $^{3}J_{HH}$ = 5.8 Hz, H8), 2.40 (2H, m, H3), 3.45 (2H, m, H4), 3.50 (2H, m, H7), 3.55 (2H, t, $^{3}J_{HH}$ = 5.9 Hz, H9), 5.66 (2H, d, $^{2}J_{HH}$ = 28.0 Hz, H10), 8.98 (1H, s, NH). **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): (125,76 MHz, CD_2Cl_2, 300 K, in ppm): δ = 19.6 (1C, s, C8), 26.0 (1C, s, C6), 28.5 (1C, s, C5), 32.7 (1C, s, C3), 38.6 (1C, s, C9), 48.4 (1C, s, C7), 54.7 (1C, s, C4), 121.9 (1C, q, $^{1}J_{CF}$ = 121 Hz, OTf), 125.6 (1C, s, C10), 139.4 (1C, s, C2), 164.2 (1C, s, C1). **^{19}F{^{1}H} NMR** (470.59 MHz, $CDCl_3$, 300 K, [ppm]): δ = -78.4 (s, OTf). **Elemental analysis**: calculated for $C_{11}H_{17}F_3N_2O_3S$: C, 42.03; H, 5.45; N, 8.91; S, 10.20; found: C, 42.20; H, 5.362; N, 8.69; S, 10.118.

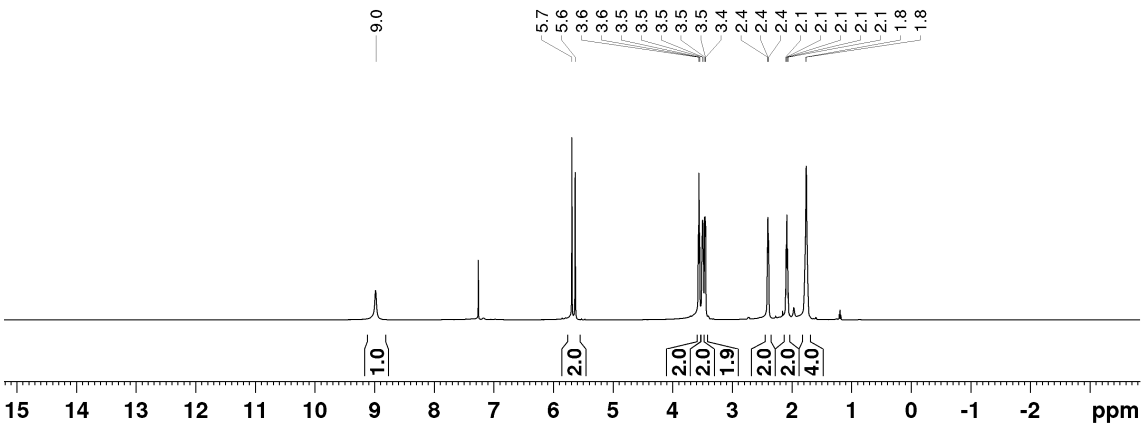


Figure S72. ^{1}H NMR spectrum of **13**[OTf] (300 K, $CDCl_3$).

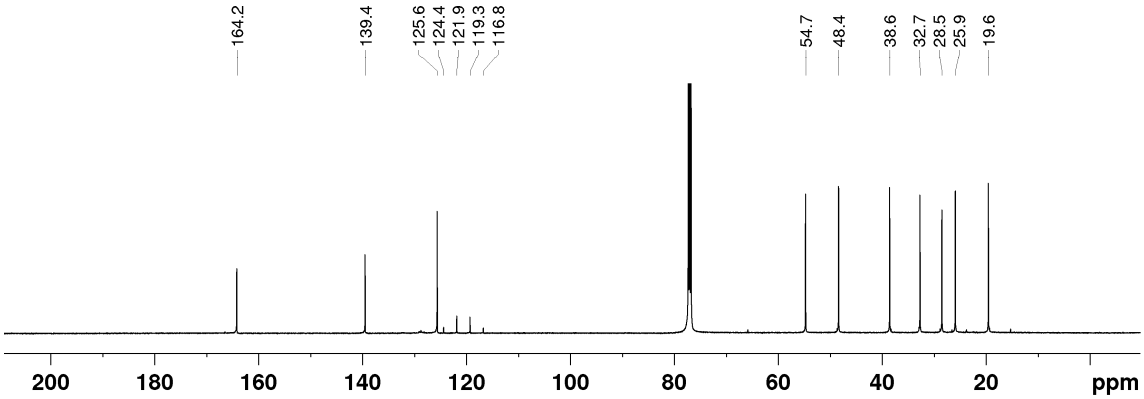


Figure S73. ^{13}C{^{1}H} NMR spectrum of **13**[OTf] (300 K, $CDCl_3$).

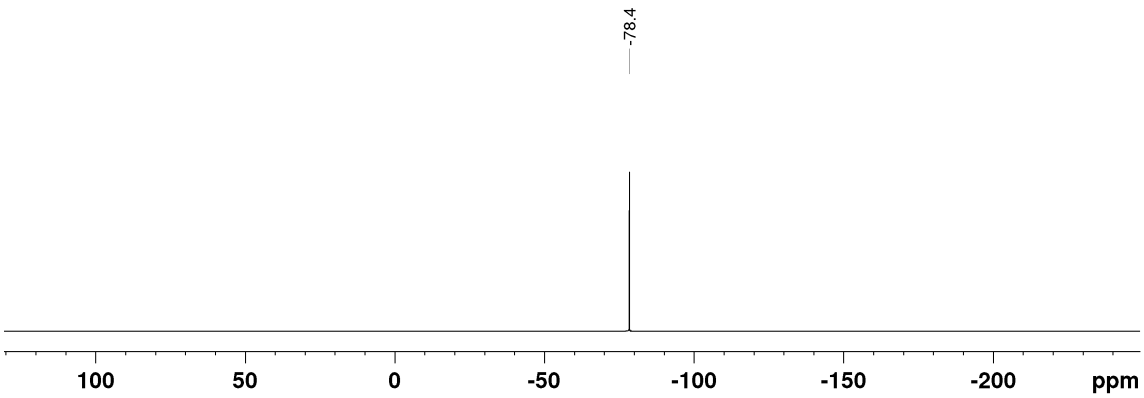
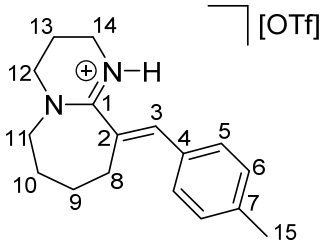


Figure S74. $^{19}F\{^{1}H\}$ NMR spectrum of **13**[OTf] (300 K, $CDCl_3$).

S2.18 Preparation of 14[OTf]



A mixture of KHMDS (95%) (152 mg, 0.72 mmol, 1 eq.) and **10**[OTf] (500 mg, 0.72 mmol, 1 eq.) were combined in THF (10 mL) in a 50 mL pressured flask and stirred at room temperature for 2 h. 4-Methylbenzaldehyde (87 mg, 0.72 mmol, 1 eq.) was then added, and the mixture was heated at 60 °C for 2 h. Silica (100 mg) was added to the solution and the mixture was stirred for 10 min. All volatiles were removed *in vacuo* and the crude mixture was purified by column chromatography: Et_2O elution phase, phosphole oxide **12**, 223 mg, yield: 75%; DCM elution phase, **14**[OTf] 188 mg. Suitable crystals for X-ray diffraction analysis can obtain by layering a DCM solution with Et_2O at room temperature. It was identified as *E*-**14**[OTf].

Yield: 64%. **m.p.** 148 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 2954 (15), 2926 (14), 1638 (48), 1609 (100), 1566 (34), 1385 (32), 1288 (28), 1274 (31), 1245 (26), 1226 (27), 1206 (39), 1189 (38), 1034 (33), 756 (23), 76 (31), 77 (8). **IR** (ATR, 298 K, [cm^{-1}]): 3261 (vw), 3113 (vw), 2952 (vw), 1635 (w), 1608 (w), 1562 (w), 1512 (vw), 1446 (vw), 1385 (vw), 1352 (vw), 1342 (vw), 1322 (w), 1277 (s), 1247 (vs), 1221 (m), 1205 (m), 1160 (s), 1090 (vw), 1070 (vw), 1027 (vs), 999 (vw), 958 (vw), 919 (vw), 896 (vw), 867 (vw), 846 (vw), 821 (w), 755 (w), 697 (vw), 631 (vs), 571 (w), 555 (vw), 516 (m), 483 (vw), 469 (vw), 454 (vw), 437 (vw), 409 (vw). **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]):: δ = 1.80 (2H, m, H9), 1.83 (2H, m, H10), 2.06 (2H, quint, $^{3}J_{HH}$ = 5.8 Hz, H13), 2.34 (3H, s, H15), 2.53 (2H, t, $^{3}J_{HH}$ = 5.0 Hz, H8), 3.50 (4H, m, H11,H4), 3.54 (2H, t, $^{3}J_{HH}$ = 6.2 Hz, H12), 7.03 (1H, s, H3), 7.16 (2H, d, $^{3}J_{HH}$ = 8.0 Hz, H5), 7.31 (2H, d, $^{3}J_{HH}$ = 8.0 Hz, H6), 9.08 (1H, s, NH). **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]):: δ = 19.7 (1C, s, C13), 21.3 (1C, s, C15), 25.5 (1C, s, C9), 26.3 (1C, s, C10), 27.9 (1C, s, C8), 38.8 (1C, s, C14), 48.1 (1C, s, C12), 53.7 (1C, s, C11), 120.6 (1C, q, $^{1}J_{CF}$ = 320 Hz, OTf), 129.3 (2C, s, C5), 129.4 (2C, s, C6), 130.0 (1C, s, C4), 131.2 (1C, s, C2), 138.8 (1C, s, C3), 139.2 (1C, s, C7), 164.8 (1C, s, C1). **^{19}F{^{1}H} NMR** (470.59 MHz, $CDCl_3$, 300 K, [ppm]): δ = -78.3 (s, OTf). **Elemental analysis**: calculated for $C_{18}H_{23}F_3N_2O_3S$: C, 53.46; H, 5.73; N, 6.93; S, 7.93; found: C, 53.21; H, 5.332; N, 6.57; S, 7.462.

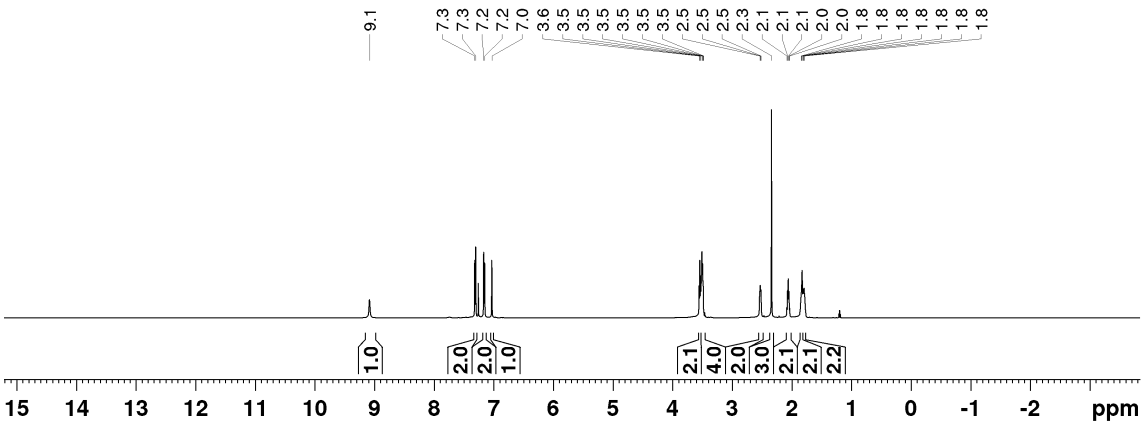


Figure S75. ^{1}H NMR spectrum of **14**[OTf] (300 K, $CDCl_3$).

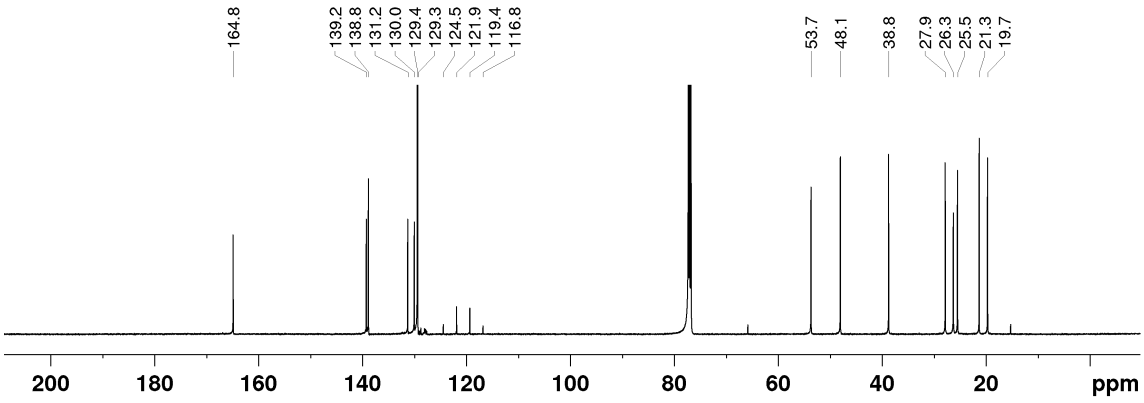


Figure S76. $^{13}C\{^{1}H\}$ NMR spectrum of **14**[OTf] (300 K, $CDCl_3$).

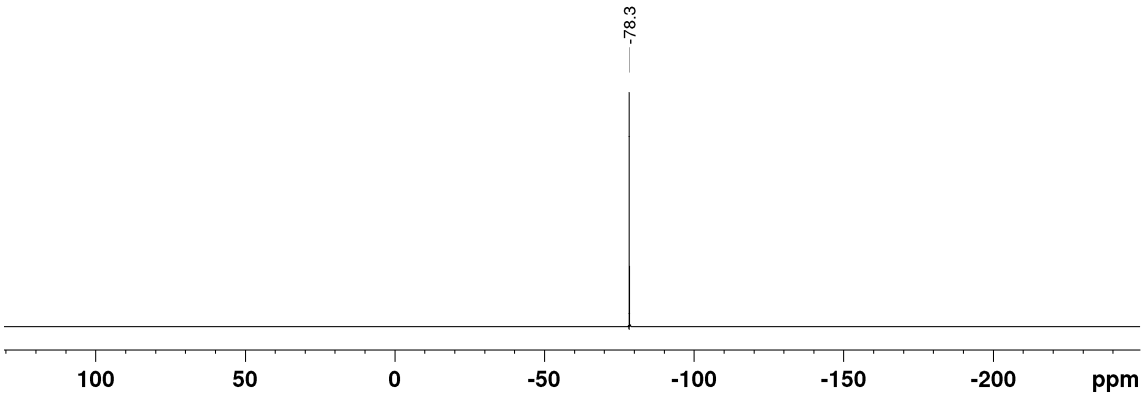


Figure S77. $^{19}F\{^{1}H\}$ NMR spectrum of **14**[OTf] (300 K, $CDCl_3$).

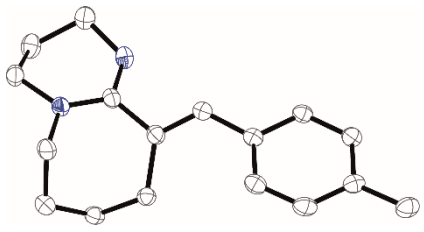
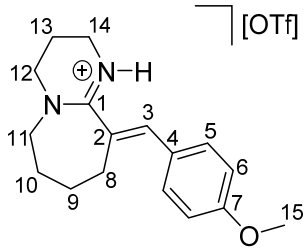


Figure S78. Molecular structure of *E*-**14**$^{+}$ in *E*-**14**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.19 Preparation of 15[OTf]



KHMDS (95%) (152 mg, 0.72 mmol, 1 eq.) and **10**[OTf] (500 mg, 0.72 mmol, 1 eq.) were combined in THF (10 mL) in a 50 mL pressured flask and stirred at room temperature for 2 h. 4-Methoxybenzaldehyde (98 mg, 1 equiv.) was then added, and the mixture was heated at 60 °C for 2 h. Silica (100 mg) was added to the solution and the mixture was stirred for 10 min. All volatiles were removed *in vacuo* and the crude mixture was purified by column chromatography: Et_2O elution phase, phosphole oxide **12**, 210 mg, yield: 71%; DCM elution phase, **15**[OTf] 223 mg. Suitable crystals for X-ray diffraction analysis can obtain by layering a DCM solution with Et_2O at room temperature. It was identified as *E*-**15**[OTf].

Yield: 76%. **m.p.** 130 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3006 (6), 2982 (11), 2953 (14), 2919 (17), 2881 (9), 2845 (6), 1644 (81), 1621 (100), 1608 (84), 1574 (43), 1449 (10), 1423 (8), 1380 (10), 1279 (20), 1248 (25), 1215 (46), 1184 (40), 1168 (6), 1034 (26), 922 (14), 823 (6), 810 (14), 758 (14), 716 (14), 633 (7), 617 (6), 459 (9), 428 (9), 349 (9), 316 (7), 259 (8), 186 (6), 165 (12), 148 (14), 87 (54), 252 (6), 149 (10), 77 (23). **IR** (ATR, 298 K, [cm^{-1}]): 3266 (vw), 2917 (vw), 1640 (w), 1617 (w), 1607 (w), 1573 (w), 1513 (w), 1461 (vw), 1448 (vw), 1378 (vw), 1325 (vw), 1281 (s), 1246 (vs), 1217 (m), 1182 (w), 1157 (s), 1085 (vw), 1029 (vs), 948 (vw), 914 (vw), 896 (vw), 868 (vw), 840 (w), 821 (vw), 808 (vw), 756 (vw), 720677 (vw), 637 (s), 573 (w), 535 (w), 517 (m), 455 (vw). **^{1}H NMR** (400.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 1.82 (2H, m, H13), 1.89 (2H, m, H11), 2.08 (2H, m, H10), 2.59 (2H, t, H9), 3.53 (6H, m, H15,H14,H12), 3.82 (3H, s, H8), 6.94 (2H, d, $^3J_{HH}$ = 8.4 Hz, H6), 7.00 (1H, s, H3), 7.44 (2H, d, $^3J_{HH}$ = 8.5 Hz, H5), 8.96 (1H, s, NH). **^{13}C{^{1}H} NMR** (100.61 MHz, CD_2Cl_2, 300 K, in ppm) : δ = 19.8 (1C, s, C9), 25.4 (1C, s, C12), 25.8 (1C, s, C10), 27.9 (1C, s, C8), 38.8 (1C, s, C11), 48.0 (1C, s, C14), 55.3 (1C, s, C15), 114.0 (1C, s, C5), 122.3 (1C, q, $^1J_{CF}$ = 320 Hz, OTf), 126.7 (1C, s, C4), 128.6 (1C, s, C2), 131.3 (1C, s, C6), 138.1 (1C, s, C3), 160.4 (1C, s, C7), 164.9 (1C, s, C1). **^{19}F{^{1}H} NMR** (376.5 MHz, CD_2Cl_2, 300 K, in ppm): δ = -78.9 (s, OTf). **Elemental analysis**: calculated for $C_{18}H_{23}F_3N_2O_4S$: C, 51.42; H, 5.51; N, 6.66; S, 7.63; found: C, 51.57; H, 5.126; N, 6.65; S, 8.052.

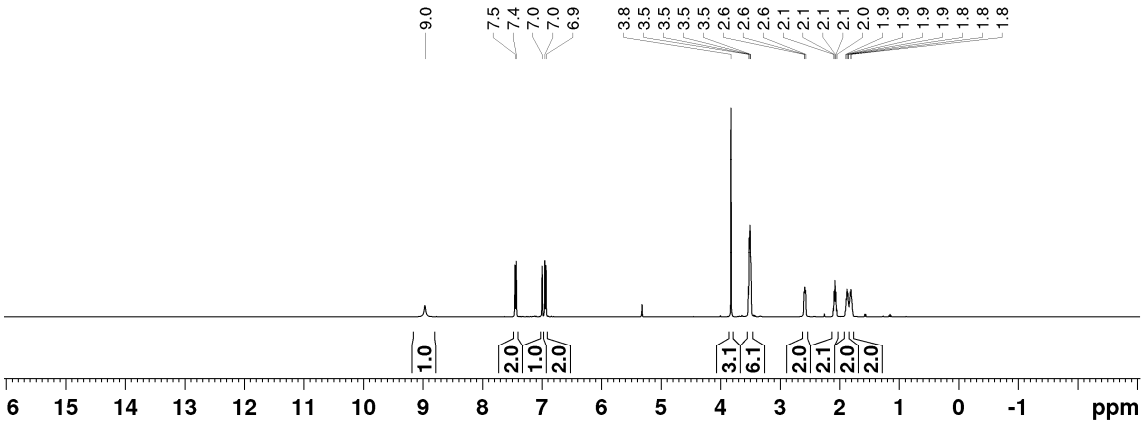


Figure S79. ^{1}H NMR spectrum of **15**[OTf] (300 K, $CDCl_3$).

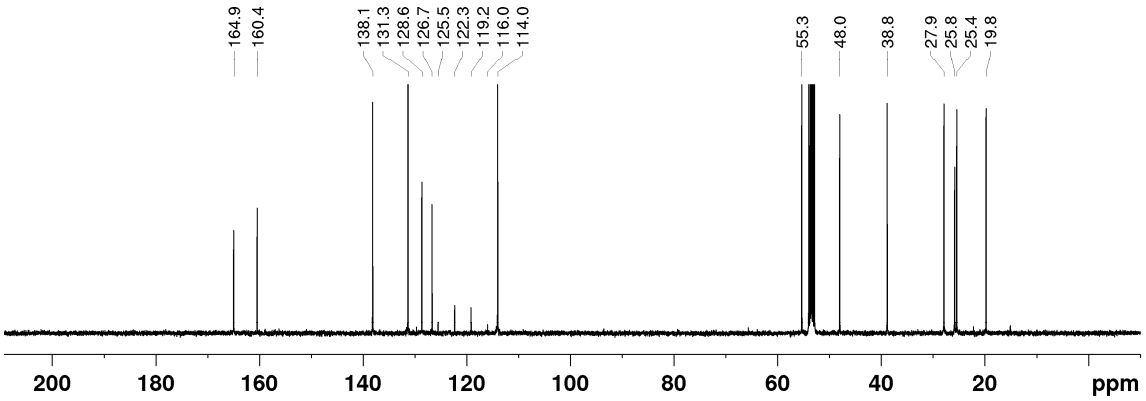


Figure S80. $^{13}C\{^{1}H\}$ NMR spectrum of **15**[OTf] (300 K, $CDCl_3$).

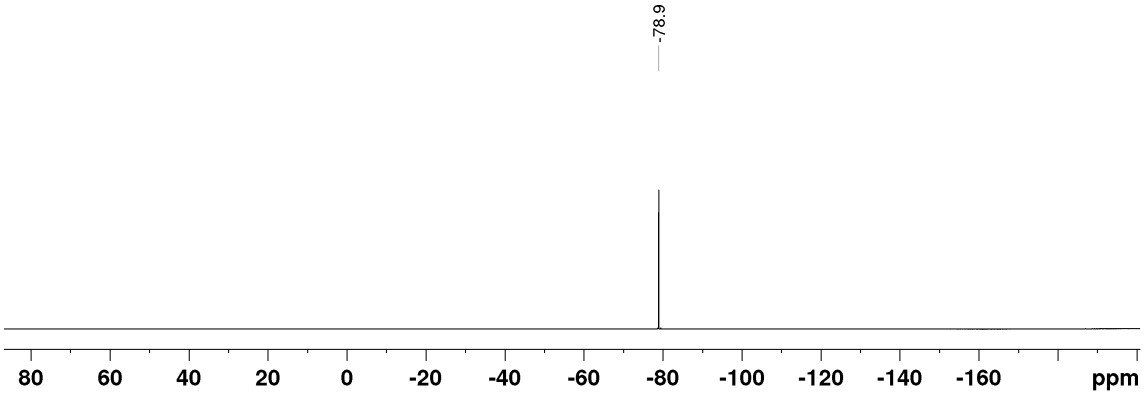


Figure S81. $^{19}F\{^{1}H\}$ NMR spectrum of **15**[OTf] (300 K, $CDCl_3$).

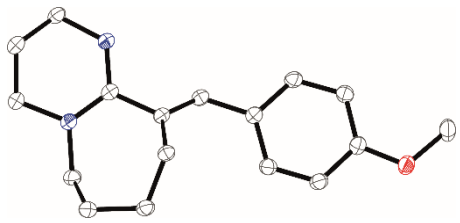
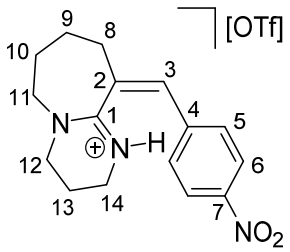


Figure S82. Molecular structure of *E*-**15**$^{+}$ in *E*-**15**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.20 Preparation of 16[OTf]



KHMDS (95%) (152 mg, 0.72 mmol, 1 eq.) and **10**[OTf] (500 mg, 0.72 mmol, 1 eq.) were combined in THF (10 mL) in a 50 mL pressured flask and stirred at room temperature for 2 h. 4-Nitrobenzaldehyde (109 mg, 0.72 mmol, 1 eq.) was then added, and the mixture was heated at 60°C for 2 h. Silica (100 mg) was added to the solution and the mixture was stirred for 10

min. All volatiles were removed *in vacuo* and the crude mixture was purified by column chromatography: Et_2O elution phase, phosphole oxide **12**, 243 mg, yield: 83%; DCM elution phase, **16**[OTf] 189 mg. Suitable crystals for X-ray diffraction analysis can obtain by layering a DCM solution with Et_2O at room temperature. It was identified as *Z*-**16**[OTf].

Yield: 60%. **m.p.** 148 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3077 (8), 2966 (8), 2925 (10), 1655 (30), 1633 (34), 1595 (61), 1461 (6), 1344 (100), 1211 (13), 1108 (25), 1039 (16), 999 (6), 911 (6), 870 (7), 758 (9), 719 (9), 349 (8), 315 (9), 174 (8), 135 (22), 83 (66). **IR** (ATR, 298 K, [cm^{-1}]): 3251 (vw), 3139 (vw), 2927 (vw), 1653 (w), 1631 (w), 1588 (w), 1519 (w), 1509 (w), 1492 (vw), 1448 (vw), 1401 (vw), 1384 (vw), 1349 (w), 1322 (w), 1282 (m), 1247 (vs), 1223 (m), 1143 (s), 1106 (vw), 1087 (vw), 1030 (s), 995 (vw), 950 (vw), 910 (vw), 897 (vw), 869 (vw), 852 (w), 822 (vw), 788 (vw), 754 (w), 700 (w), 670 (vw), 637 (vs), 572 (w), 555 (w), 515 (m), 494 (w), 467 (vw), 433 (vw), 415 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 1.87 (2H, m, H11), 1.94 (2H, m, H8), 2.17 (2H, m, H13), 2.58 (2H, m, H9), 3.62 (6H, m, H10, H14, H12), 7.20 (1H, s, H3), 7.69 (2H, d, $^3J_{HH}$ = 8.6 Hz, H5), 8.28 (2H, d, $^3J_{HH}$ = 8.6 Hz, H6), 9.40 (1H, s, NH). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm) : δ = 19.5 (1C, s, C13), 25.5 (1C, s, C11), 26.8 (1C, s, C8), 28.9 (1C, s, C9), 38.8 (1C, s, C12), 48.2 (1C, s, C10), 53.0 (1C, s, C14), 121.9 (1C, q, $^1J_{CF}$ = 320 Hz, OTf), 123.6 (1C, s, C6), 130.1 (1C, s, C5), 134.5 (1C, s, C2), 136.5 (1C, s, C3), 140.6 (1C, s, C4), 147.6 (1C, s, C7), 164.1 (1C, s, C1). **^{19}F{^{1}H} NMR** (470.59 MHz, CD_2Cl_2, 300 K, in ppm): δ = -79.0 (s, OTf). **Elemental analysis**: calculated for $C_{17}H_{20}F_3N_3O_5S$·0.1 KOTf: C, 45.22; H, 4.44; N, 9.25; S, 7.36; found: C, 45.25; H, 4.261; N, 8.88; S, 7.418.

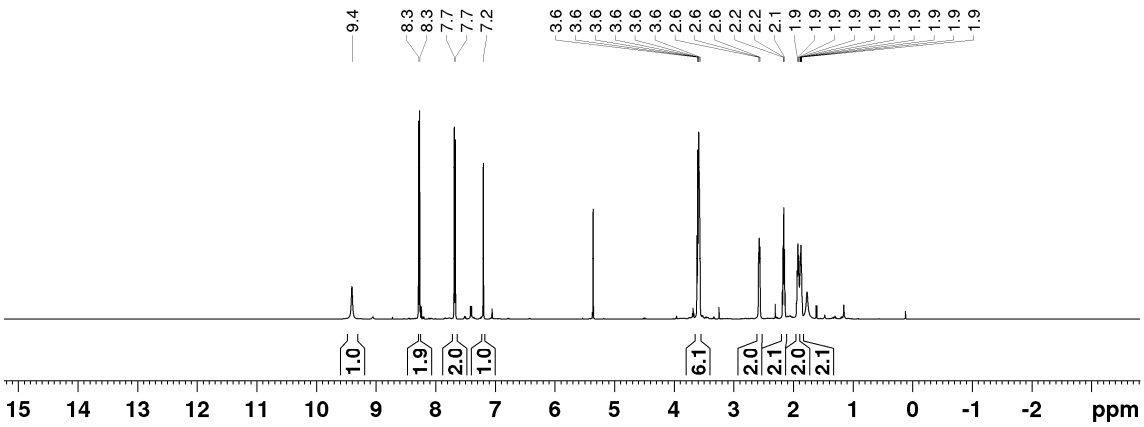


Figure S83. ^{1}H NMR spectrum of **16**[OTf] (300 K, CD_2Cl_2).

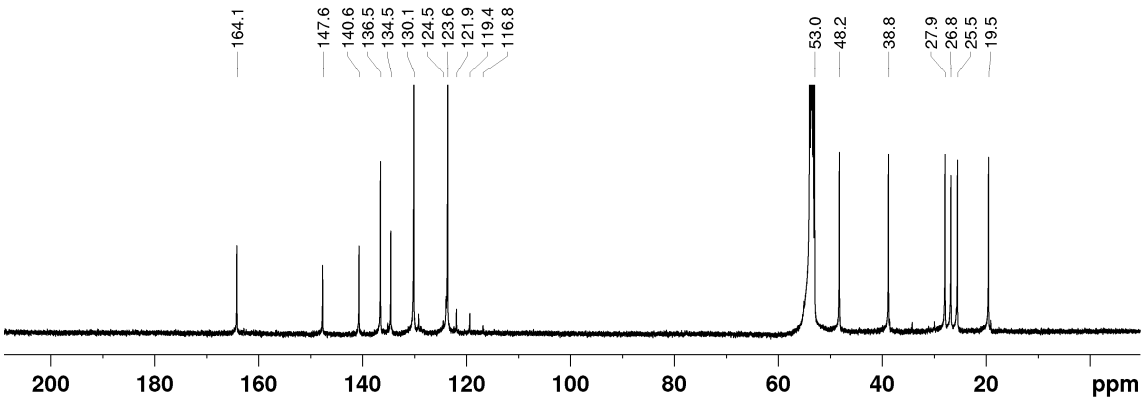


Figure S84. ^{13}C{^{1}H} NMR spectrum of **16**[OTf] (300 K, CD_2Cl_2).

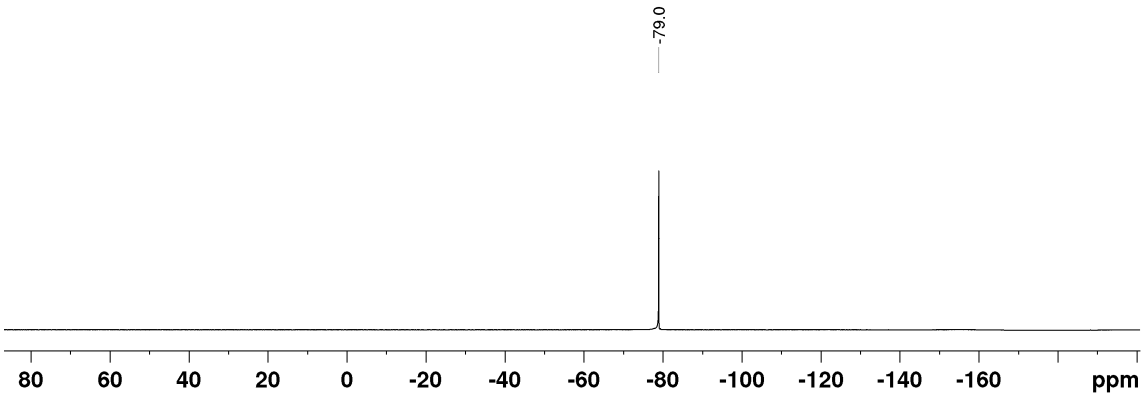


Figure S85. $^{19}F\{^{1}H\}$ NMR spectrum of **16**[OTf] (300 K, CD_2Cl_2).

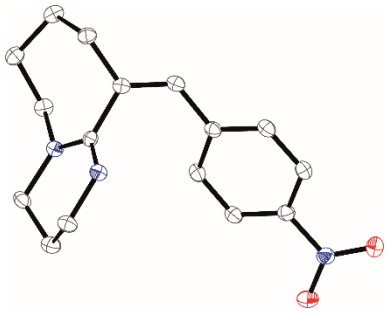
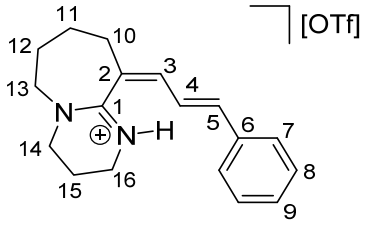


Figure S86. Molecular structure of *Z*-**16**$^{+}$ in *Z*-**16**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.21 Preparation of 17[OTf]



KHMDS (95%) (152 mg, 0.72 mmol, 1 eq.) and **10**[OTf] (500 mg, 0.72 mmol, 1 eq.) were combined in THF (10 mL) in a 50 mL pressured flask and stirred at room temperature for 2 h. *E*-cinnamaldehyde (95 mg, 0.72 mmol, 1 eq.) was then added, and the mixture was heated at 60°C for 2 h. Silica (100 mg) was added to the solution and the mixture was stirred for 10 min. All volatiles were removed *in vacuo* and the crude mixture was purified by column chromatography: Et_2O elution phase, phosphole oxide **12**, 231 mg, yield: 78%; DCM elution phase, **17**[OTf] 189 mg. Suitable crystals for X-ray diffraction analysis can obtain by layering a DCM solution with Et_2O at room temperature. It was identified as *Z, E*-**17**[OTf].

Yield: 63%. **m.p.** 127 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 2939 (5), 1624 (100), 1596 (78), 1570 (11), 1492 (7), 1449 (6), 1381 (7), 1365 (7), 1318 (15), 1289 (14), 1259 (9), 1206 (6), 1161 (32), 1131 (7), 1032 (8), 1000 (23), 233 (6), 74 (16). **IR** (ATR, 298 K, [cm^{-1}]): 3279 (vw), 3120 (vw), 2936 (vw), 2866 (vw), 1634 (m), 1606 (w), 1563 (w), 1491 (vw), 1448 (vw), 1379 (vw), 1345 (vw), 1320 (w), 1280 (m), 1252 (vs), 1221 (m), 1204 (m), 1152 (vs), 1079 (vw), 1030 (vs), 990 (vw), 965 (m), 947 (vw), 893 (vw), 843 (vw), 761 (m), 720 (vw), 693 (m), 634 (vs), 590 (vw), 571 (w), 542 (vw), 515 (m), 474 (vw), 455 (vw), 416 (vw), 492 (vw), 463 (vw), 407 (vw). **^{1}H NMR** (400.13 MHz, CD_2Cl_2, 300 K, [ppm]): δ = 1.82 (4H, m, H11,H14),

2.09 (2H, m, H15), 2.62 (2H, m, H10), 3.48 (2H, m, H16), 3.52 (4H, m, H13), 6.85 (1H, m, H3), 7.05 (2H, m, H7), 7.43 (3H, m, H9,H4,H5), 7.56 (2H, m, H8), 8.84 (1H, s, NH). **$^{13}C\{^{1}H\}$ NMR** (100.61 MHz, CD_2Cl_2, 300 K, [ppm]): δ = 19.8 (1C, s, C15), 25.1 (1C, s, C13), 25.2 (1C, s, C11), 26.9 (1C, s, C10), 38.9 (1C, s, C14), 48.0 (1C, s, C12), 53.4 (1C, s, C16), 121.4 (2C, s, C7), 122.3 (1C, q, $^{1}J_{CF}$ = 321 Hz, OTf), 127.3 (2C, s, C8), 128.8 (1C, s, C9), 129.1 (1C, s, C4), 129.2 (1C, s, C2), 136.2 (1C, s, C6), 137.9 (1C, s, C3), 141.0 (1C, s, C5), 164.3 (1C, s, C1). **$^{19}F\{^{1}H\}$ NMR** (376.5 MHz, CD_2Cl_2, 300 K, [ppm]): δ = -78.9 (s, OTf). **Elemental analysis**: calculated for $C_{19}H_{23}F_3N_2O_3S$: C, 54.80; H, 5.57; N, 6.73; S, 7.70; found: C, 54.56; H, 5.131; N, 6.51; S, 8.181.

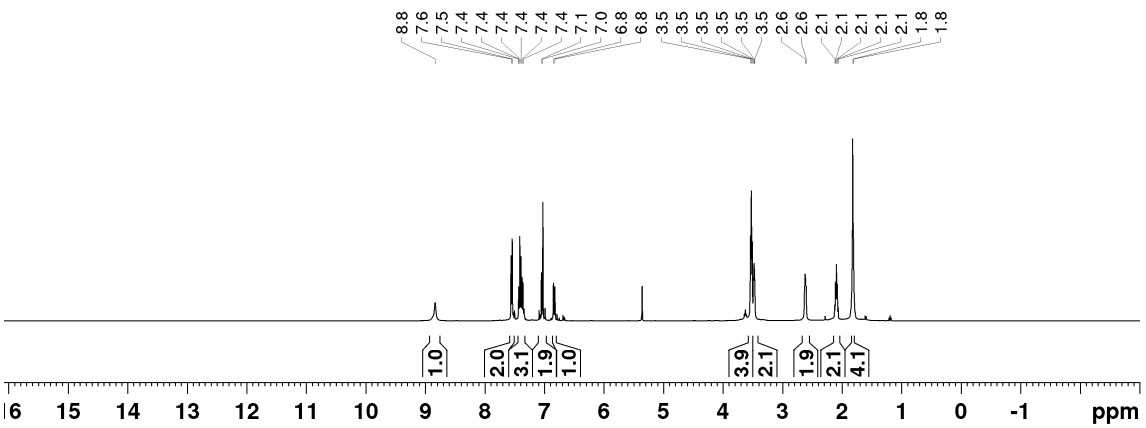


Figure S87. ^{1}H NMR spectrum of **17**[OTf] (300 K, CD_2Cl_2).

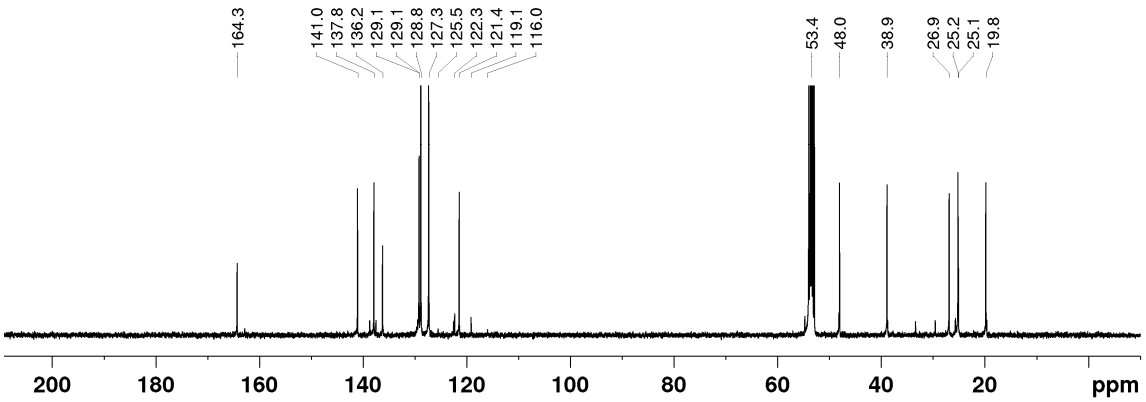


Figure S88. $^{13}C\{^{1}H\}$ NMR spectrum of **17**[OTf] (300 K, CD_2Cl_2).

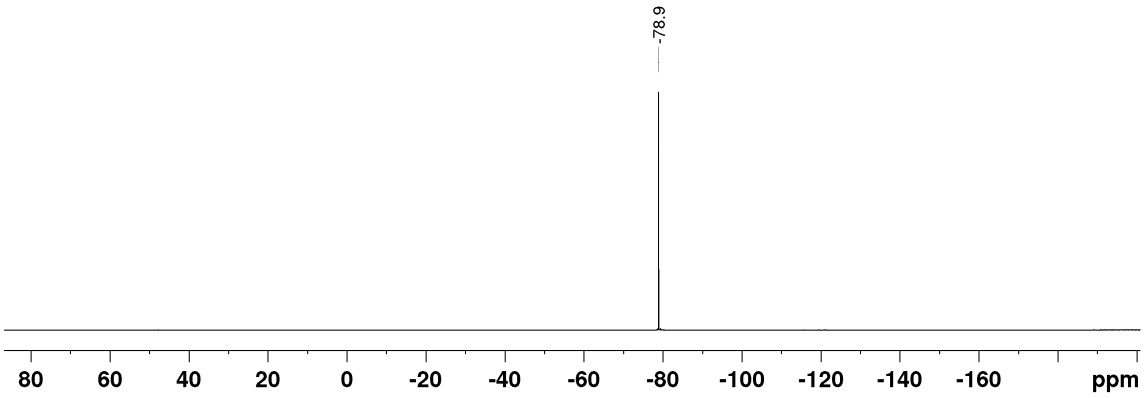


Figure S89. $^{19}F\{\}$ NMR spectrum of **17**[OTf] (300 K, CD_2Cl_2).

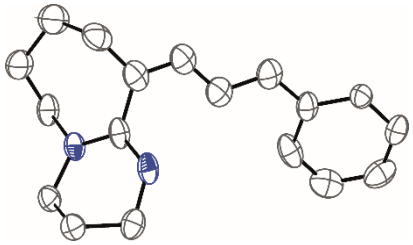
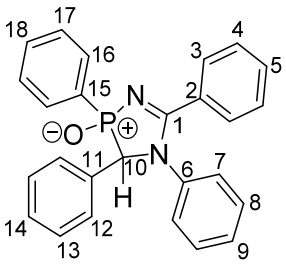


Figure S90. Molecular structure of *Z,E*-**17**$^+$ in *Z,E*-**17**[OTf]; hydrogen atoms and the anion are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.22 Preparation of 12



The phosphole oxide **12** was obtained from reactions of **13**[OTf]-**17**[OTf] and was collected in the Et_2O elution phrase. The yield was determined for each reaction independently: **13**[OTf], 52%; **14**[OTf], 75%; **15**[OTf], 71%; **16**[OTf], 83%; **17**[OTf], 78%.

m.p. 201 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3067 (20), 1600 (51), 1580 (22), 1516 (16), 1444 (7), 1351 (11), 1268 (8), 1169 (12), 1034 (25), 999 (57), 949 (9), 826 (10), 773 (15), 677 (12), 626 (8), 616 (7), 494 (9), 313 (7), 267 (15), 250 (10), 229 (10), 92 (100). **IR** (ATR, 298 K, [cm^{-1}]): 3052 (vw), 1601 (vw), 1585 (vw), 1519 (w), 1486 (w), 1458 (vw), 1436 (vw), 1382 (w), 1338 (vw), 1287 (vw), 1262 (vw), 1214 (w), 1180 (vw), 1134 (vw), 1118 (w), 1077 (vw), 1027 (vw), 1018 (vw), 1000 (vw), 947 (vw), 930 (vw), 856 (w), 785 (vw), 775 (vw), 767 (vw), 748 (vw), 734 (w), 714 (w), 691 (s), 662 (vw), 635 (vw), 618 (vw), 590 (vw), 578 (w), 515 (w), 480 (w), 467 (w), 449 (vw), 635 (vs), 590 (w), 572 (m), 539 (vw), 516 (s), 490 (s), 468 (w), 449 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 5.17 (1H, d, $^2J_{HP}$ = 17.0 Hz, H10), 6.97 (2H, m, Ar-H), 7.11 (4H, m, Ar-H), 7.14 (3H, m, Ar-H), 7.19 (2H, m, Ar-H), 7.32 (2H, m, Ar-H), 7.38 (2H, m, Ar-H), 7.49 (4H, m, Ar-H), 7.78 (2H, d, $^3J_{HH}$ = 7.4 Hz, H3). **^{13}C{^{1}H} NMR** (125,76 MHz, CD_2Cl_2, 300 K, in ppm) : **major** : δ = 70.8 (1C, d, $^1J_{CP}$ = 63 Hz, C10), 126.0 (2C, s, C13), 126.5 (1C, d, $^3J_{CP}$ = 4 Hz, C12), 127.1 (2C, s, C4), 127.3 (1C, d, $^3J_{CP}$ = 3 Hz, C17), 127.7 (1C, d, $^1J_{CP}$ = 13 Hz, C15), 127.9 (1C, s, C14), 128.6 (2C, d, $^3J_{CP}$ = 2 Hz, C6), 129.0 (2C,

s, C8), 129.2 (2C, s, C3), 130.3 (1C, s, C5), 131.6 (1C, s, C18), 131.9 (1C, d, $^{3}J_{CP}$ = 3 Hz, C6), 132.5 (2C, d, $^{2}J_{CP}$ = 9 Hz, C16), 135.6 (2C, s, C7), 142.4 (1C, d, $^{2}J_{CP}$ = 9 Hz, C11), 173.0 (1C, d, $^{2}J_{CP}$ = 3 Hz, C1). **minor** : δ = 67.5 (1C, d, $^{1}J_{CP}$ = 64 Hz, C10), 126.8 (2C, d, $^{3}J_{CP}$ = 6 Hz, C12), 128.1 (2C, s, C13), 128.5 (2C, s, C4), 128.8 (1C, d, $^{2}J_{CP}$ = 13 Hz, C11), 128.9 (2C, d, $^{3}J_{CP}$ = 2 Hz, C17), 129.0 (2C, s, C14), 130.0 (2C, s, C8), 131.3 (1C, d, $^{1}J_{CP}$ = 24 Hz, C15), 131.5 (2C, s, C3), 131.8 (1C, s, C5), 131.9 (1C, s, C18), 132.4 (1C, d, $^{3}J_{CP}$ = 3 Hz, C6), 132.6 (1C, s, C9), 132.7 (1C, d, $^{3}J_{CP}$ = 4 Hz, C2), 133.7 (2C, s, C7), 140.3 (2C, d, $^{2}J_{CP}$ = 10 Hz, C11), 171.3 (1C, d, $^{2}J_{CP}$ = 4 Hz, C1). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 56.5 (s) (79%), 47.2 (s) (21%).

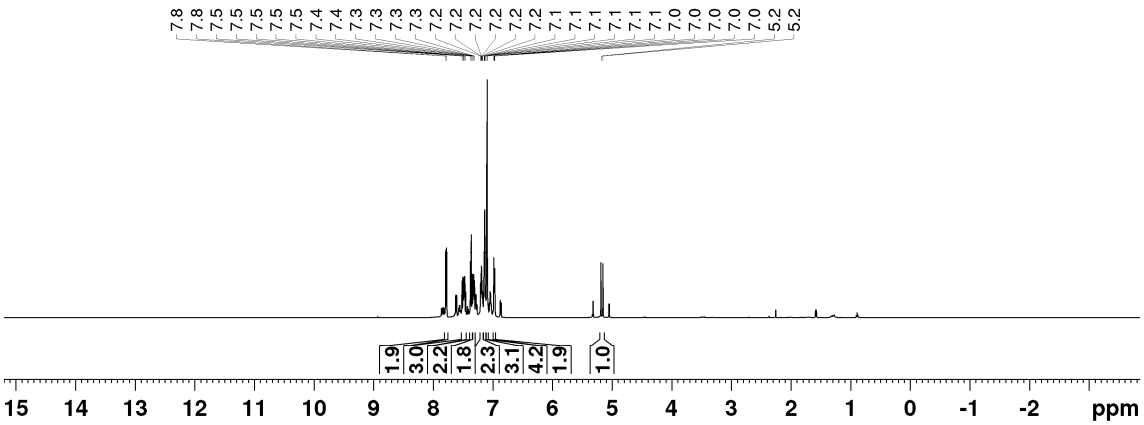


Figure S91. ^{1}H NMR spectrum of **12** (300 K, CD_2Cl_2).

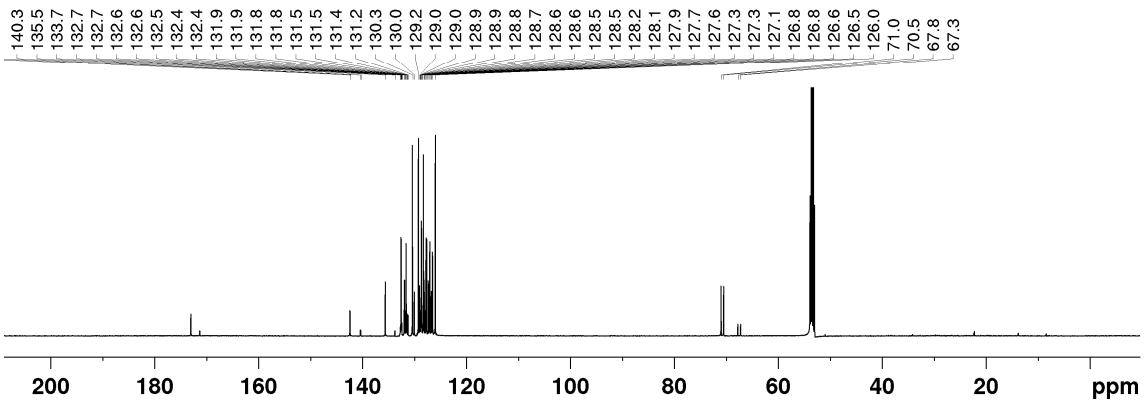


Figure S92. ^{13}C{^{1}H} NMR spectrum of **12** (300 K, CD_2Cl_2).

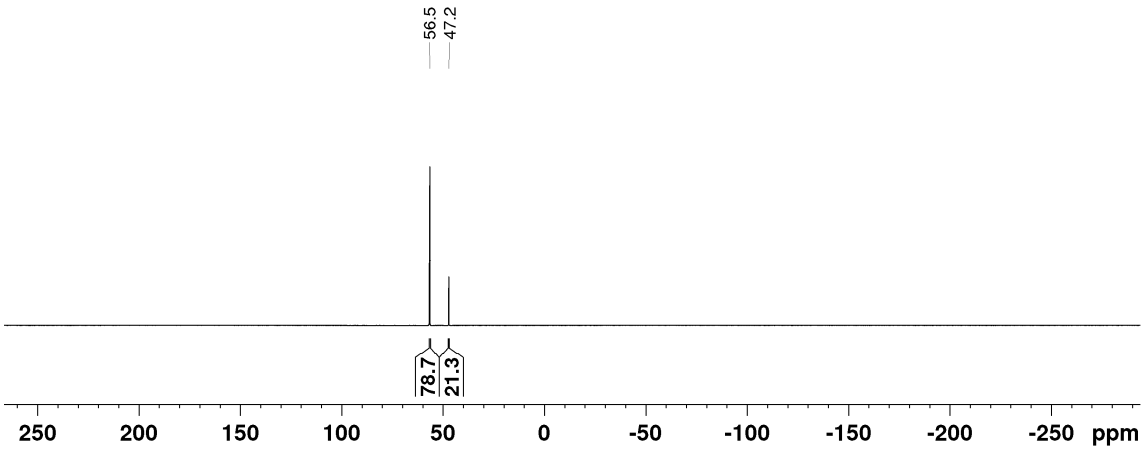


Figure S93. $^{31}P\{^{1}H\}$ NMR spectrum of **12** (300 K, CD_2Cl_2).

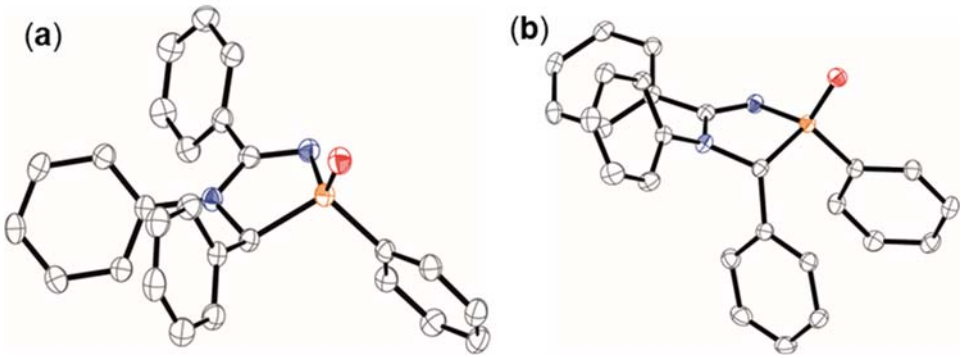
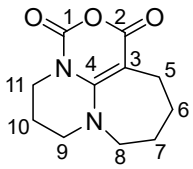


Figure S94. Molecular structure of **12**, (**a**) *syn*-, (**b**) *anti*-; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.23 Preparation of 18



A 10 mL Schlenk tube charged with **11** (200 mg) in THF (5 mL) was connected with a CO_2 cylinder. After replacing the atmosphere to CO_2 (1 bar), the deep orange solution was exposed to CO_2 and then rapidly turned yellow within seconds. The reaction mixture was kept under a CO_2 atmosphere for 10-30 min until no further color change was observed. Removal of all volatiles resulted in a yellow solid. The crude solid was washed with toluene to isolate **12**, and the residue was recrystallized by slow diffusion of Et_2O to a DCM solution at room temperature to give the white, air and moisture stable solid.

Yield: 58 mg, 71%. **m.p**. 163 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 2989 (63), 2967 (50), 2942 (88), 2924 (100), 2873 (61), 1740 (84), 1681 (64), 1569 (31), 1502 (19), 1479 (31), 1452 (36), 1442 (34), 1327 (22), 1287 (28), 1241 (17), 1200 (19), 1028 (17), 937 (22), 833 (25), 594 (45), 567 (31), 532 (25), 491 (17), 450 (17), 389 (20), 375 (17), 339 (17), 124 (23), 75 (97). **IR** (ATR, 298 K, [cm^{-1}]): 3357 (vw), 2921 (w), 2853 (vw), 1740 (s), 1683 (vs), 1575 (vs), 1502 (s), 1474 (m), 1440 (m), 1404 (m), 1373 (w), 1362 (w), 1324 (m), 1295 (w), 1287 (w), 1274 (w), 1237 (m), 1199 (w), 1187 (vw), 1172 (vw), 1147 (w), 1130 (vw), 1110 (vw), 1094 (vw), 1048 (w), 1024 (w), 999 (vw), 964 (m), 954 (m), 914 (vw), 902 (vw), 886 (vw), 830 (vw),

774 (vw), 753 (m), 740 (vs), 719 (w), 688 (vw), 660 (w), 591 (vw), 566 (vw), 528 (vw), 491 (vw), 475 (s), 448 (vw). **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, in ppm): δ =1.90 (m, 2H, H6), 1.94 (m, 2H, H7), 2.12 (m, 2H, H10), 2.64 (m, 2H, H5), 3.37 (m, 2H, H9), 3.57 (m, 2H, H8), 3.90 (m, 2H, H11). **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, in ppm): δ =21.7 (1C, s, C10), 22.7 (1C, s, C5), 23.8 (1C, s, C6), 24.6 (1C, s, C7), 41.6 (1C, s, C11), 48.4 (1C, s, C9), 52.1 (1C, s, C8), 82.9 (1C, s, C3), 148.5 (1C, s, C1), 154.2 (1C, s, C4), 160.3 (1C, s, C2). **Elemental analysis**: calculated for $C_{11}H_{14}N_2O_3$ 0.1 $C_4H_{10}O$ 0.05 C_7H_8: C, 60.24; H, 6.63; N, 11.96; found: C, 60.26; H, 6.43; N, 11.64.

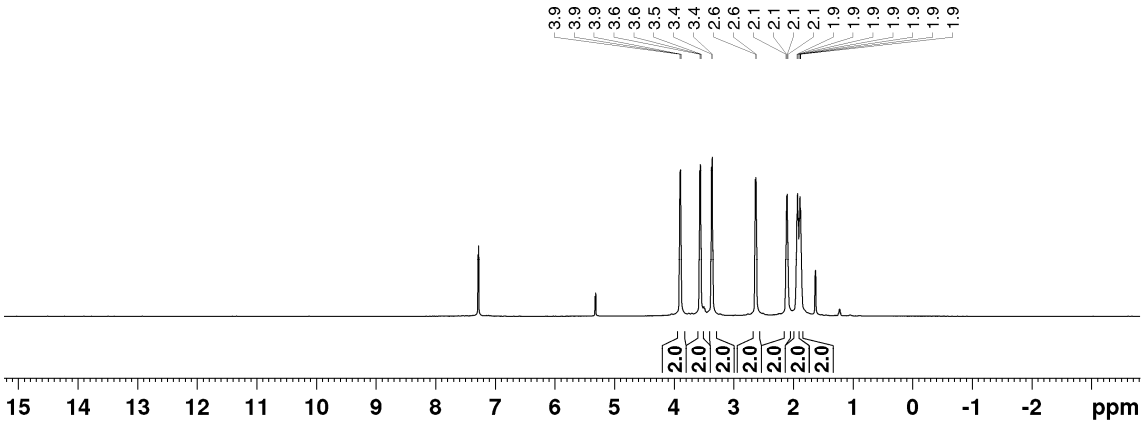


Figure S95. ^{1}H NMR spectrum of **18** (300 K, $CDCl_3$).

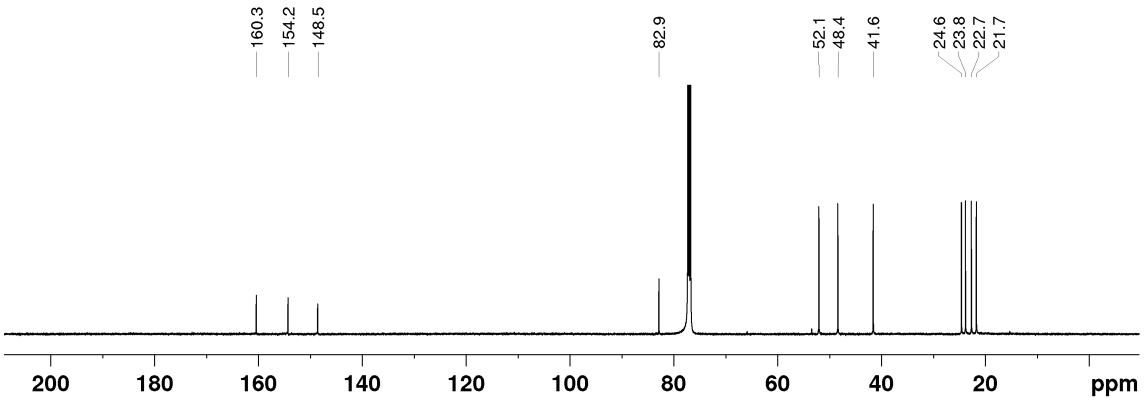


Figure S96. ^{13}C{^{1}H} NMR spectrum of **18** (300 K, CD_2Cl_2).

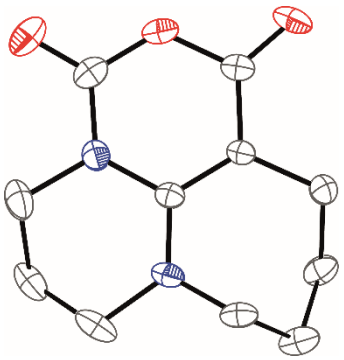
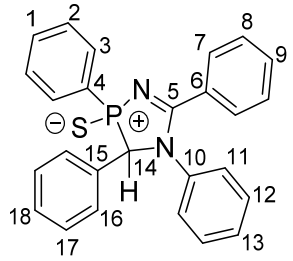


Figure S97. Molecular structure of **18**; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.24 Preparation of 19



A THF solution of CS_2 (20 mg/mL, 1.4 mL; 28 mg, 0.37 mmol, 2 eq.) was added to a solution of **11** (200 mg, 0.18 mmol, 1 eq.) in THF (4 mL) at room temperature. The mixture was stirred at room temperature for 10 min. Removal of all volatiles resulted in a yellow solid, which was washed with Et_2O (5 mL) and toluene (5 mL) to remove phosphole sulfide. Combination of filtrates and drying for recrystallization with Et_2O to obtain **19** as air and moisture stable yellow powder. Suitable crystals for X-ray diffraction analysis were obtained by layering a THF solution with *n*-pentane at room temperature.

Yield: 93 mg, 60%. **m.p.** 193 °C. **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): 3065 (72), 2974 (10), 2873 (16), 1600 (89), 1587 (37), 1515 (43), 1485 (10), 1446 (13), 1380 (16), 1296 (12), 1259 (11), 1221 (24), 1181 (14), 1158 (16), 1108 (14), 1028 (16), 1001 (100), 647 (11), 631 (11), 616 (14), 572 (13), 288 (9), 266 (10), 254 (11), 241 (17), 212 (13), 183 (11), 145 (23), 107 (79), 86 (86). **IR** (ATR, 298 K, [cm^{-1}]): 2361 (m), 2341 (w), 1584 (vw), 1512 (s), 1484 (s), 1455 (w), 1446 (w), 1436 (w), 1376 (s), 1338 (w), 1307 (w), 1256 (vw), 1220 (vw), 1127 (vw), 1108 (m), 1077 (w), 1027 (w), 1015 (vw), 998 (vw), 944 (w), 917 (vw), 855 (s), 837 (w), 790 (s), 770 (m), 754 (m), 738 (s), 724 (s), 704 (vs), 692 (vs), 660 (m), 645 (s), 631 (m), 611 (w), 571 (m), 560 (vw), 518 (w), 498 (m), 474 (w), 429 (w). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 6.94 (1H, m, H14), 8.49 (2H, m, H12), 8.74 (3H, m, H13, H17), 8.88 (2H, m, H3), 8.96 (3H, m, Ar-H), 9.01 (2H, m, Ar-H), 9.08 (1H, m, Ar-H), 9.20 (3H, m, Ar-H), 9.27 (2H, m, H7), 9.62 (2H, m, H16). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm) : δ = 73.6 (1C, d, $^1J_{CP}$ = 45 Hz, C14), 128.2 (2C, s, C12), 128.7 (1C, s, C13), 130.0 (2C, d, $^4J_{CP}$ = 2 Hz, C11), 130.0 (1C, s, C18), 130.1 (1C, s, C9), 130.6 (2C, s, C7), 130.7 (2C, s, C17), 130.8 (2C, d, $^2J_{CP}$ = 28 Hz, C3), 131.8 (1C, s, C1), 132.6 (2C, d, $^3J_{CP}$ = 11 Hz, C16), 133.1 (2C, s, C8), 133.4 (1C, d, $^2J_{CP}$ = 19 Hz, C15), 134.0 (2C, d, $^3J_{CP}$ = 3 Hz, C2), 136.2 (1C, d, $^3J_{CP}$ = 4 Hz, C6), 137.5 (1C, d, $^1J_{CP}$ = 96 Hz, C4), 142.8 (1C, d, $^3J_{CP}$ = 10 Hz, C10), 172.2 (1C, d, $^2J_{CP}$ = 8 Hz, C5). **^{31}P{^{1}H} NMR** (202.46 MHz, CD_2Cl_2, 300 K, in ppm): δ = 87.1 (s). **Elemental analysis**: calculated for $C_{26}H_{21}N_2PS$: C, 73.57; H, 4.99; N, 6.60; S, 7.55; found: C, 73.13; H, 5.283; N, 6.41; S, 7.081.

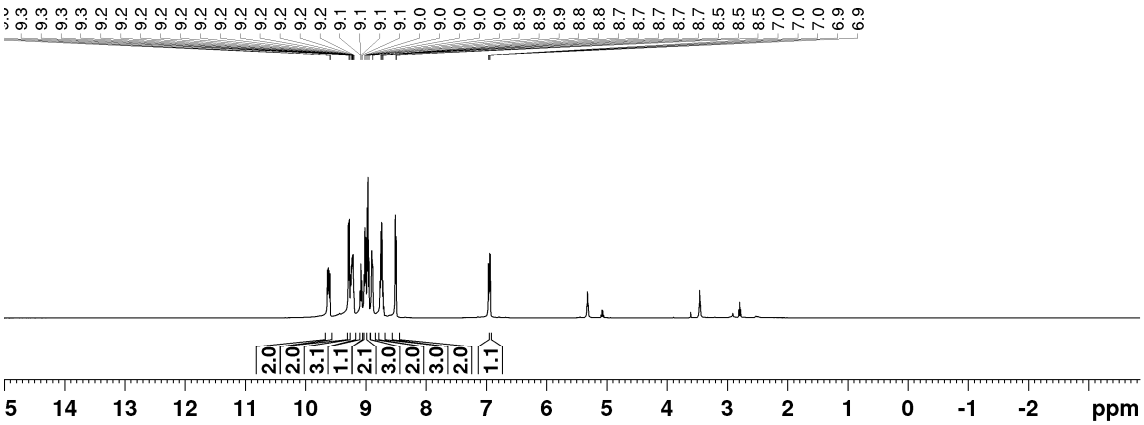


Figure S98. ^{1}H NMR spectrum of **19** (300 K, CD_2Cl_2).

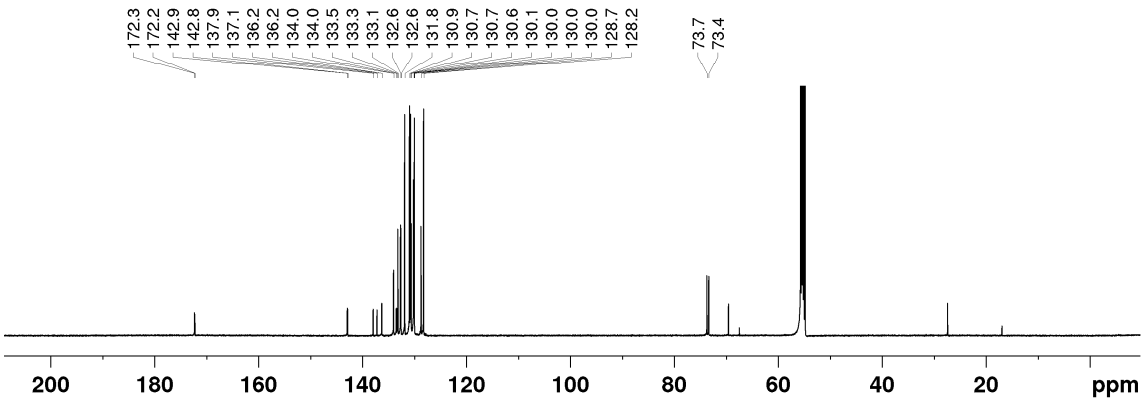


Figure S99. $^{13}C\{^{1}H\}$ NMR spectrum of **19** (300 K, CD_2Cl_2).

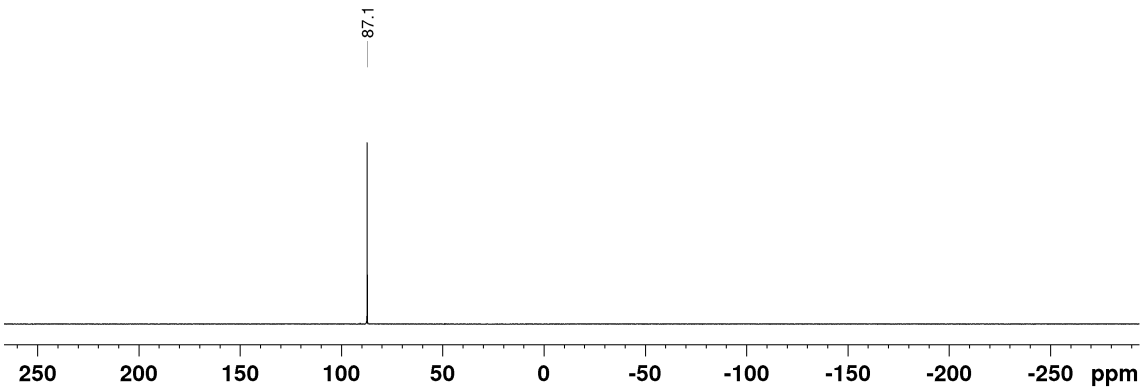


Figure S100. $^{31}P\{^{1}H\}$ NMR spectrum of **19** (300 K, CD_2Cl_2).

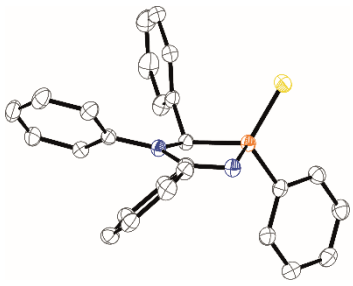
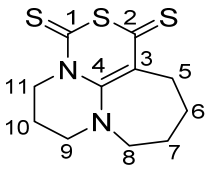


Figure S101. Molecular structure of *syn*-**19** in *syn*-**19** · THF; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S2.25 Preparation of 20



A THF solution of CS_2 (20 mg/mL, 1.4 mL; 28 mg, 0.37 mmol, 2 eq.) was added to a solution of **11** (200 mg, 0.18 mmol, 1 eq.) in THF (4 mL) at room temperature. The mixture was stirred at room temperature for 10 min. Removal of all volatiles resulted in a yellow solid, which was washed with Et_2O (5 mL) and toluene (5 mL) to remove phosphole sulfide **19**. The remaining powder was obtained as a yellow, air and moisture stable solid. Suitable crystals for X-ray diffraction analysis were obtained by layering a DCM solution with pentane at room temperature.

Yield: 52 mg, 52%. **m.p**. 197 °C (decomp.). **Raman** (100 mW, 50 scans, 298 K, [cm^{-1}]): No Raman spectrum could be obtained due to fluorescence of the compound. **IR** (ATR, 298 K, [cm^{-1}]): 2929 (vw), 2862 (vw), 2002 (vw), 1638 (vw), 1550 (vs), 1447 (m), 1425 (s), 1406 (w), 1375 (vw), 1362 (w), 1337 (vw), 1312 (w), 1289 (vs), 1278 (m), 1252 (s), 1213 (w), 1202 (m), 1171 (w), 1140 (w), 1111 (vw), 1095 (vw), 1082 (w), 1068 (w), 1051 (w), 1017 (m), 991 (m), 978 (w), 956 (vw), 940 (vs), 914 (vw), 900 (w), 823 (w), 804 (vw), 762 (vw), 730 (vw), 694 (s), 638 (vw), 590 (vw), 576 (vw), 556 (vw), 533 (vw), 522 (vw), 464 (vw), 427 (w), 406 (vw). **^{1}H NMR** (500.13 MHz, CD_2Cl_2, 300 K, in ppm): δ = 4.49 (m, 2H, H11), 3.63 (m, 2H, H8), 3.49 (m, 2H, H9), 3.07 (m, 2H, H5), 2.21 (m, 2H, H10), 1.96 (m, 2H, H7), 1.88 (m, 2H, H6). **^{13}C{^{1}H} NMR** (125.76 MHz, CD_2Cl_2, 300 K, in ppm): δ = 194.1 (1C, s, C2), 193.4 (1C, s, C4), 151.6 (1C, s, C1), 118.7 (1C, s, C3), 53.8 (1C, s, C8), 49.6 (1C, s, C9), 48.9 (1C, s, C11), 29.6 (1C, s, C7), 22.4 (1C, s, C6), 21.6 (1C, s, C5), 21.3 (1C, s, C10). **Elemental analysis**: calculated for $C_{11}H_{14}N_2S_3$ 0.05 KOTf 0.1 C_7H_8: C, 48.83; H, 4.88; N, 9.69; S, 33.83; found: C, 48.47; H, 4.88; N, 9.90; S, 33.399.

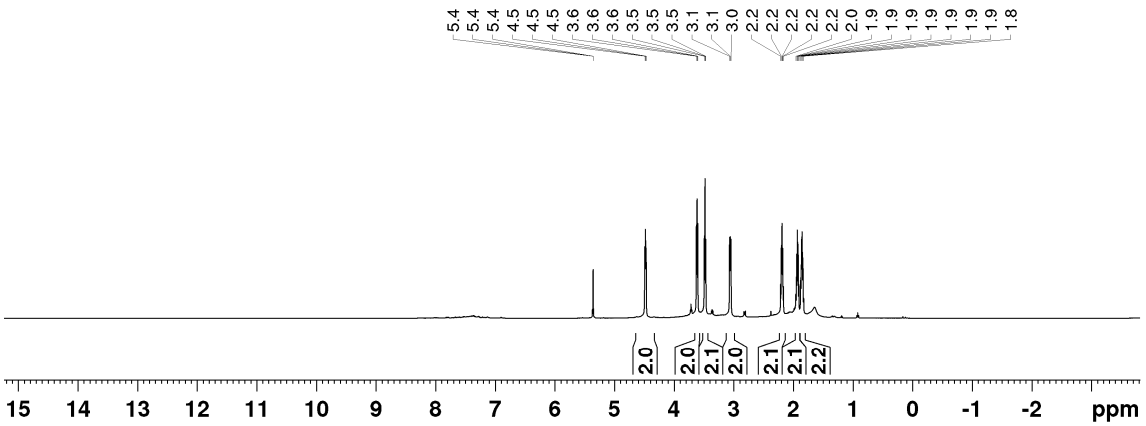


Figure S102. ^{1}H NMR spectrum of **20** (300 K, CD_2Cl_2).

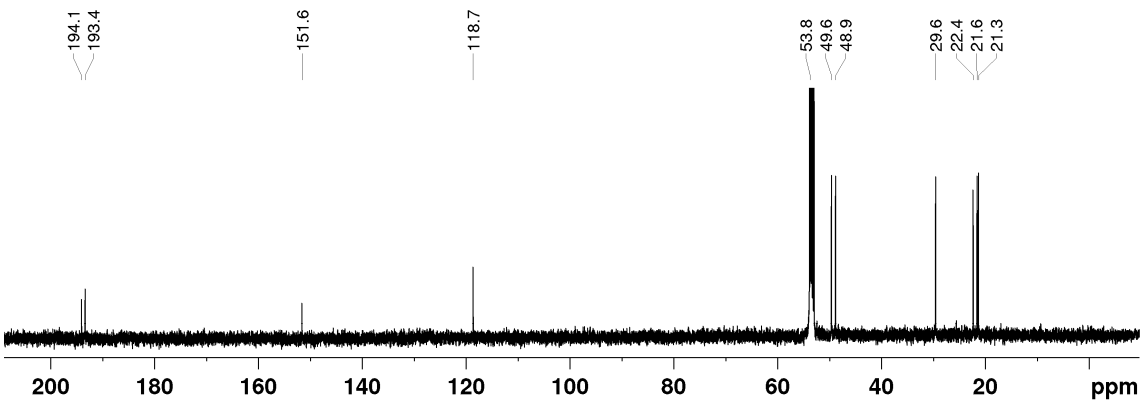


Figure S103. ^{13}C{^{1}H} NMR spectrum of **20** (300 K, CD_2Cl_2).

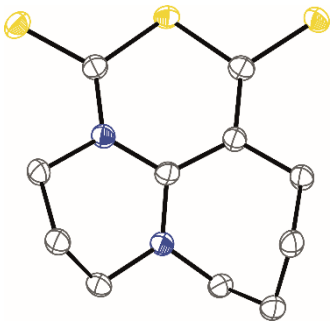


Figure S104. Molecular structure of **20**; hydrogen atoms are omitted for clarity and thermal ellipsoids are displayed at 50% probability (100 K).

S3 The diastereomeric configurations analysis for 3a[OTf]$_2$

The ^{31}P NMR spectroscopy of **3a**[OTf]$_2$ revealed two diastereomers with chemical shifts observed at 55.0 ppm (major) and 60.2 ppm (minor). According to literature, *syn*-structure shows larger $^2J_{HP}$ coupling constant between diastereomers.[2] Thus, the resonance with a chemical shift of 55.0 ppm and $^2J_{HP}$ (11.1 Hz) is recognized as *syn*-(S_P, R_C)-**3a**[OTf]$_2$ (**Figure S106a**). The minor diastereomer is recognized as *anti*-(S_P, S_C) (**Figure S106b**).

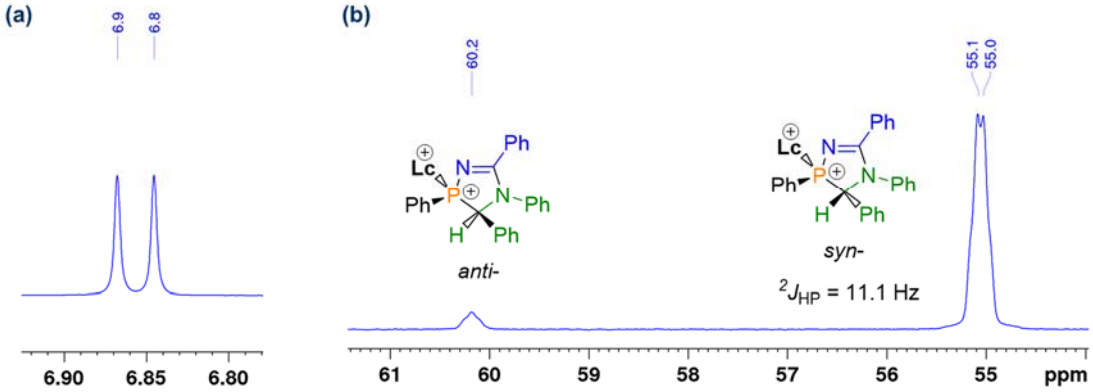


Figure S105. (**a**) The ^{1}H NMR spectrum of 3° H (C2-H, *syn*-) (6.8-6.9 ppm). (**b**) The ^{31}P NMR spectrum of the isolated diastereomeric mixture of **3a**[OTf]$_2$.

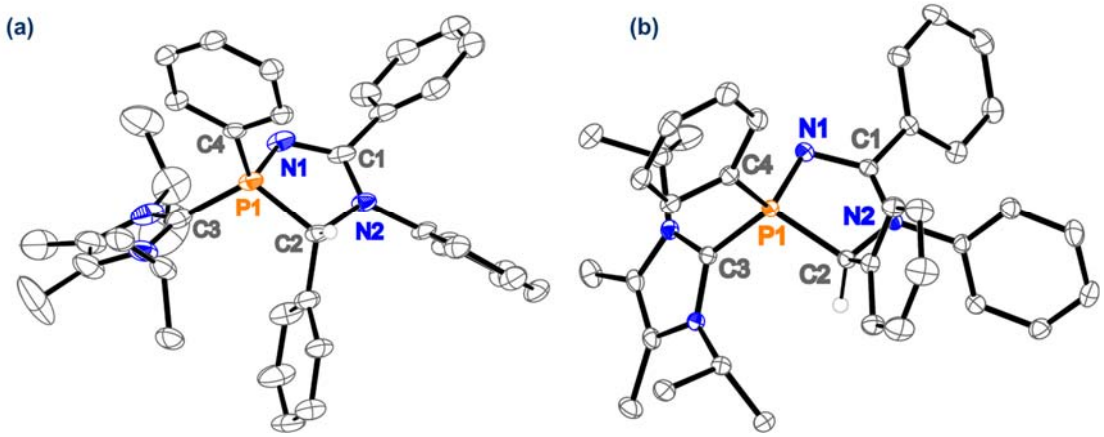
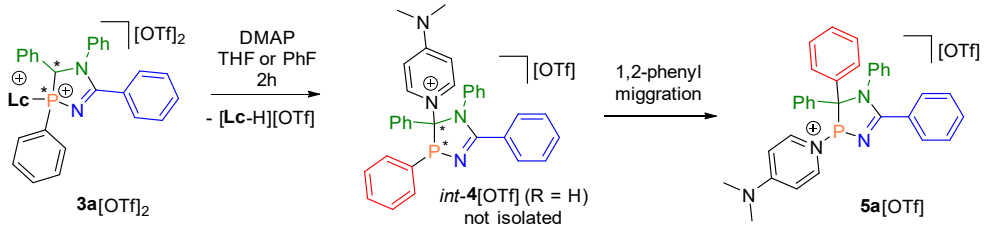


Figure S106. Molecular structures of **3a**$^{2+}$ in **3a**[OTf]$_2$, (**a**) *syn*-(S_P, R_C)-**3a**[OTf]$_2$; (**b**) *anti*-(S_P, S_C)-**3a**[OTf]$_2$.; hydrogen atoms and anions are omitted for clarity, thermal ellipsoids are displayed at 50% probability (100 K); selected bond lengths (in Å) and angles (in °). (a) P1-N1 1.633(4), P1-C2 1.851(4), P1-C3 1.813(4), P1-C4 1.769(4), C1-N1 1.336(6), C1-N2 1.348(5), N2-C2 1.486(5), N1-P1-C2 97.90(17). (b) P1-N1 1.6312(12), P1-C2 1.8705(14), P1-C3 1.8160(14), P1-C4 1.7682(15), C1-N1 1.3377(19), C1-N2 1.3384(18), N2-C2 1.4845(17), N1-P1-C2 97.28(6).

S4 Reaction of 3a-c[OTf]$_2$ with N-bases

S4.1 Reaction of 3a[OTf]$_2$ with DMAP

DMAP (4.2 mg, 0.034 mmol, 1 eq.) was added to the suspension of **3a**[OTf]$_2$ (30 mg, 0.034 mmol, 1 eq.) in PhF (1 mL) and stirred for 2 h, resulting in a clear yellow solution. Subsequent ^{31}P{H} NMR analysis of an aliquot removed from the reaction mixture revealed resonances at 112.3 ppm and 98.0 ppm, attributable to intermediate species. However, upon solvent removal only the 1,2-phenyl migration product **5a**[OTf] and [**L$_C$**-H][OTf] were obtained. Continued stirring the mixture in THF or PhF for 16 h, leading to **5a**[OTf] precipitated from the solution.



Scheme S1. Reaction of **3a**[OTf]$_2$ with DMAP.

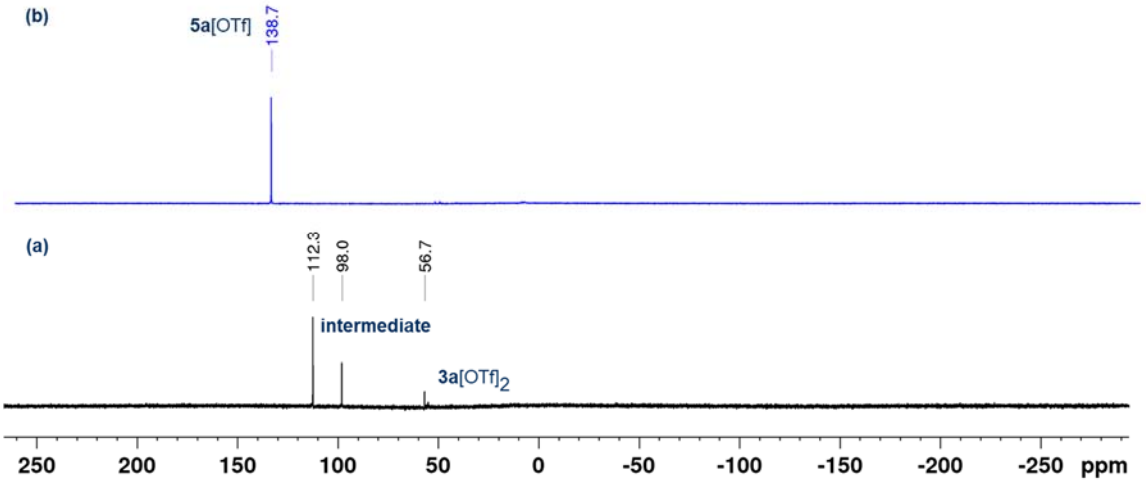


Figure S107. ^{31}P{} NMR spectrum of the reaction mixture of **3a**[OTf]$_2$ with 1 eq. DMAP in PhF, (C_6D_6 cap., 300 K). (**a**) 2 h, PhF, **3a**[OTf]$_2$ and intermediates were observed. (**b**) For 16 h, the suspension dissolved in DCM, only **5a**[OTf] was observed.

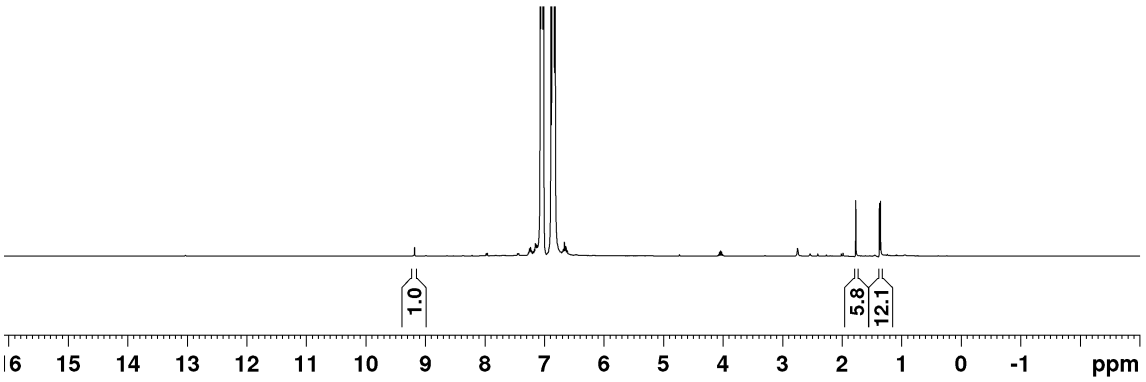


Figure S108. ^{1}H NMR spectrum of filtered PhF phase from the reaction of **3a**[OTf]$_2$ with 1 eq. DMAP in PhF for 16 h (C_6D_6 cap., 300 K). Integrated resonances correspond to the side product [**Lc**–H][OTf].

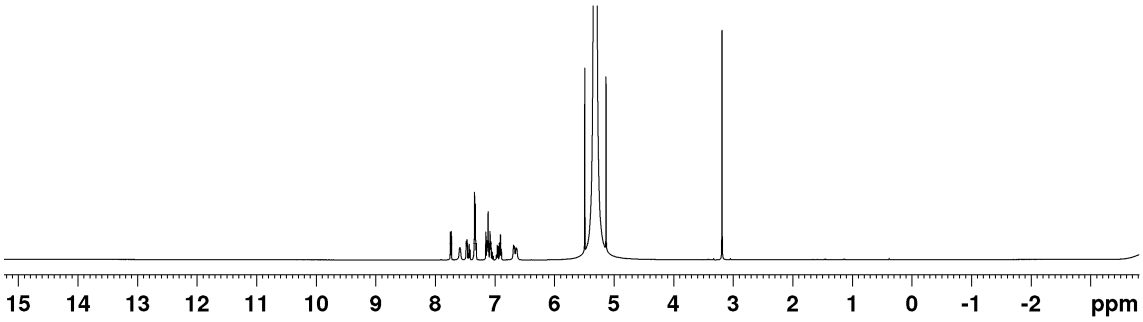
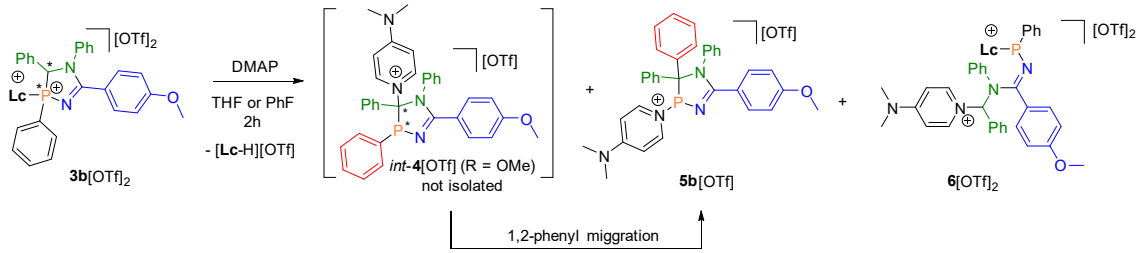


Figure S109. ^{1}H NMR spectrum of the suspension from the reaction of **3a**[OTf]$_2$ with 1 eq. DMAP in PhF for 16 h (C_6D_6 cap., DCM as solvent, 300 K).

S4.2 Reaction of 3b[OTf]$_2$ with DMAP

DMAP (21 mg, 0.17 mmol, 1 eq.) was added to a suspension of **3b**[OTf]$_2$ (150 mg, 0.17 mmol, 1 eq.) in PhF (5 mL) and stirred for 2 h, resulting in a clear yellow solution. ^{31}P{} NMR spectroscopy revealed resonances at 112.8 and 96.3 ppm, assignable to intermediates. Upon extending the reaction 2 days, the solution turned to a yellow suspension. Filtration and collection of the insoluble solid afforded the C-P bond cleavage compound **6**[OTf]$_2$, while the filtrate was dried and recrystallized by slow diffusion of Et_2O to a DCM solution at room temperature to give **5b**[OTf].



Scheme S2. Reaction of **3b**[OTf]$_2$ with DMAP.

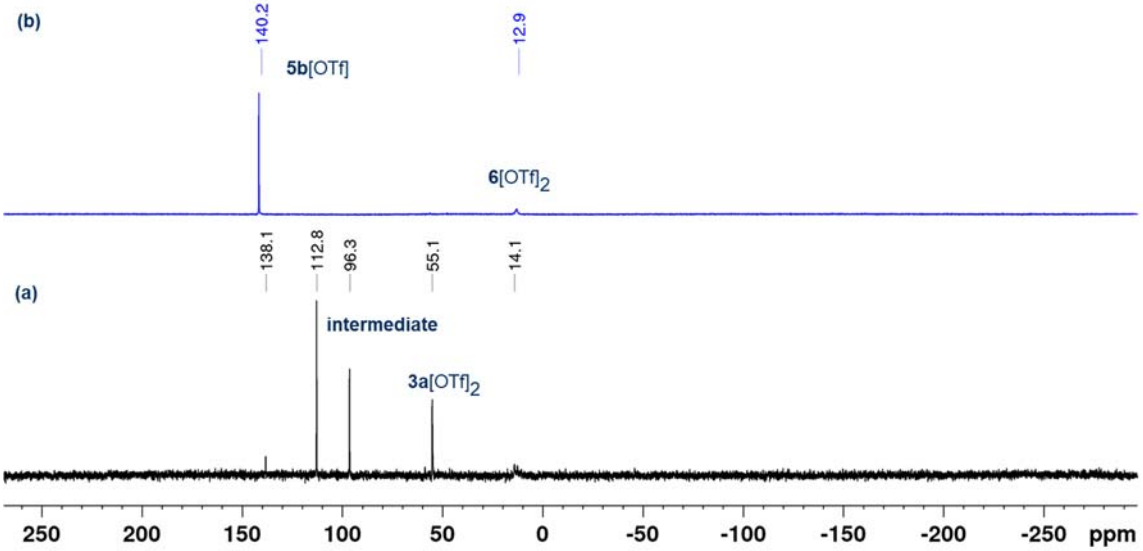
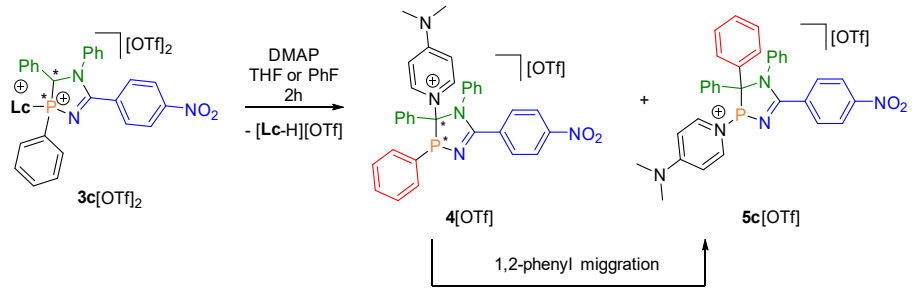


Figure S110. ^{31}P{} NMR spectrum of reaction of **3b**[OTf]$_2$ with 1 eq. DMAP in PhF, (C_6D_6 cap., 300 K). (**a**) 2 h, **3b**[OTf]$_2$, **6**[OTf]$_2$ and intermediates were observed. (**b**) For 16 h, the suspension was dissolved in DCM, **5b**[OTf] and **6**[OTf]$_2$ were observed.

S4.3 Reaction of 3c[OTf]$_2$ with DMAP

DMAP (40 mg, 0.33 mmol, 1 eq.) was added to a suspension of **3c**[OTf]$_2$ (300 mg, 0.33 mmol, 1 eq.) in PhF (5 mL) and stirred for 16 h, yielding a yellow suspension. The suspension was filtered and the solid was characterized as **4**[OTf]. Dissolving **4**[OTf] in DCM and stirring for 16 h afforded **5c**[OTf], which was isolated in quantitative yield after removal of all volatiles *in vacuo*. Prolonging the reaction in PhF for one week also led to a chemoselective formation of **5c**[OTf].



Scheme S3. Reaction of **3c**[OTf]$_2$ with DMAP.

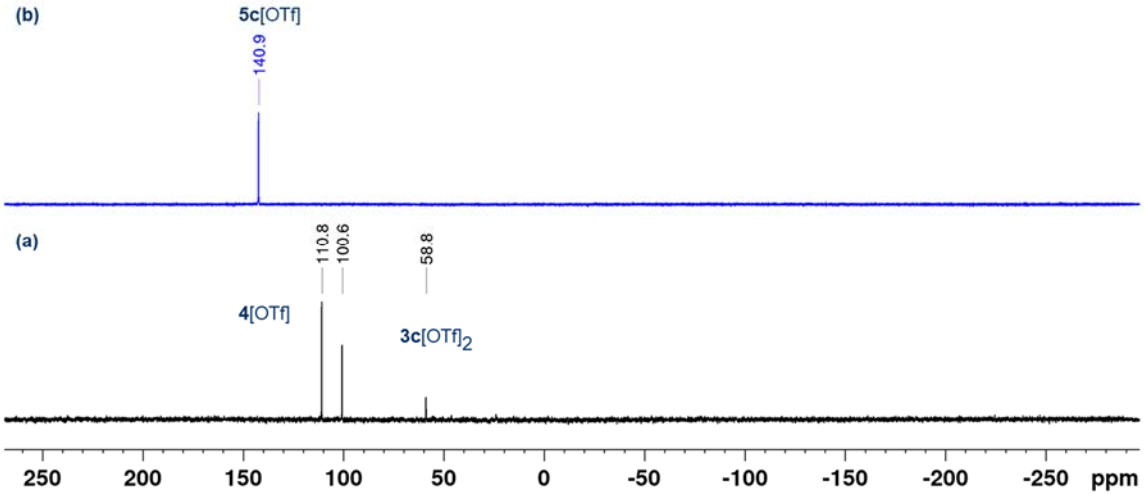


Figure S111. ^{31}P{} NMR spectrum of reaction of **3c**[OTf]$_2$ with 1 eq. DMAP in PhF, (C_6D_6 cap., 300 K). (**a**) 2 h, **3c**[OTf]$_2$ and **4**[OTf] were observed. (**b**) The suspension was dissolved in DCM and stirred for 16 h, and only **5c**[OTf] was observed.

S4.4 Reaction of 3a[OTf]$_2$ with other N-bases

Other neutral nitrogen-based bases, such as DIPEA, Et_3N, DBN were as screened. No reaction was observed for DIPEA or Et_3N, whereas DBN leads to a product mixture which were not able to separate or identify. The ^{31}P NMR spectra recorded for the reactions of **3a**[OTf]$_2$ with DBN in PhF or THF reveal the formation of non-separable mixtures (**FigureS112-113**).

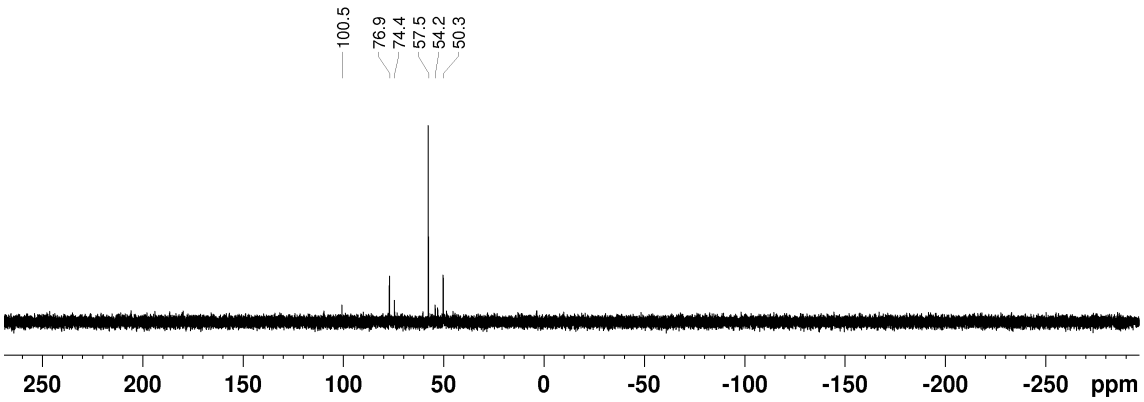


Figure S112. $^{31}P\{\}$ NMR spectrum of reaction of **3a**$[OTf]_2$ with 1 eq. DBN in THF, (C_6D_6 cap., 300 K).

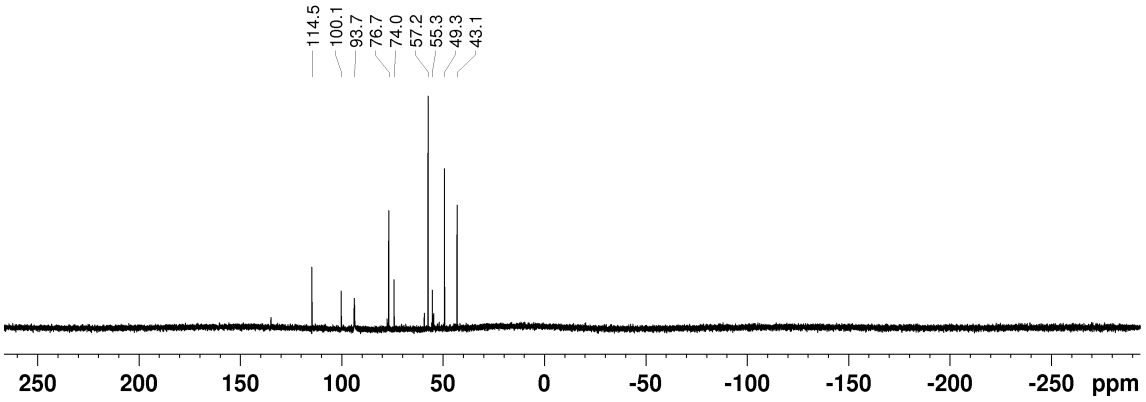


Figure S113. $^{31}P\{\}$ NMR spectrum of reaction of **3a**$[OTf]_2$ with 1 eq. DBN in PhF, (C_6D_6 cap., 300 K).

S5 CO_2 activation

A 10 mL Schlenk tube charged with **11** (200 mg) in THF (5 mL) was connected with a CO_2 cylinder (**Fig. S112**, blue). After replacing the atmosphere to CO_2 (1 bar), the deep orange solution was exposed to CO_2 and then rapidly turned yellow within seconds. The reaction mixture was kept under a CO_2 atmosphere for 10-30 min until no further visibly color change was observed (**Fig. S112**, red).

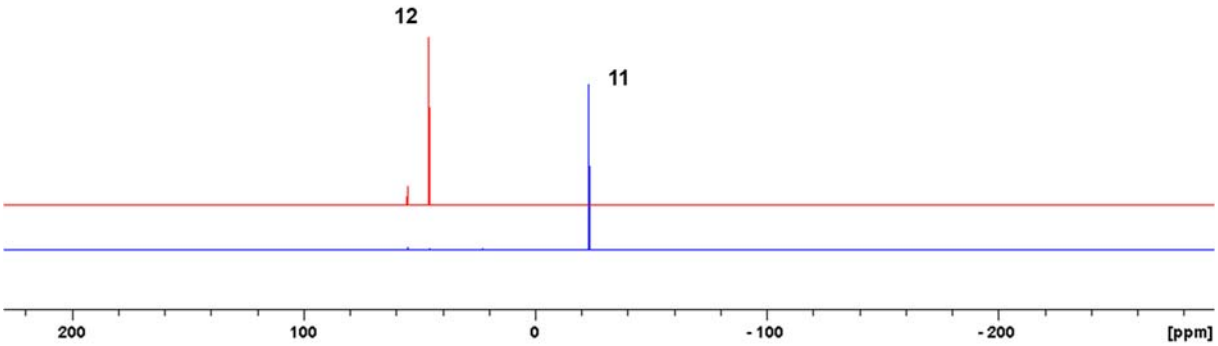


Figure S114. $^{31}P\{^1H\}$ NMR spectrum of CO_2 activation before (blue) and after 20 min (red) (C_6D_6 cap., 300 K).

Figure S115. The colour change of the solution of **11** in THF under a CO_2 atmosphere (1 atm) within 20 min.

S6 CS_2 activation

To a solution of **11** (50 mg, 0.09 mmol, 1 eq.) in THF (3 mL), CS_2 (14 mg, 0.18 mmol, 2 eq.) was added at room temperature, and the color change was monitored. The ^{31}P NMR spectrum of the starting materials is shown in Fig. S116d (blue), and then the spectrum was recorded after 10 min is shown in **Fig. S114d** (red).

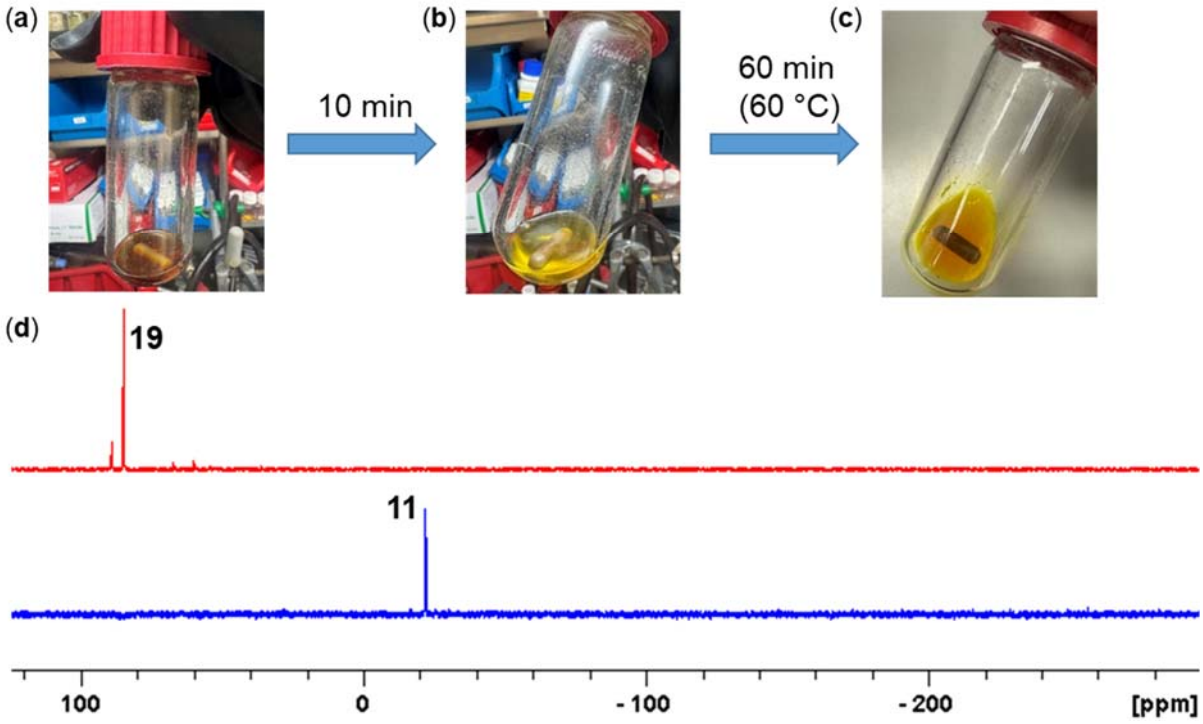


Figure S116. Color change during the reaction of **11** with CS_2, r.t. (**a**) Starting materials; (**b**) 10 min; (**c**) 20 min. (**d**) The ^{31}P NMR spectrum of **11** (blue). 2 eq. CS_2, r.t., C_6D_6, 10 min (red).

S7 X-ray Diffraction Refinements

Suitable single crystals were coated with Paratone-N oil, mounted using a nylon loop and frozen in the cold nitrogen stream. X-ray diffraction data were collected at 100 K unless otherwise mentioned on a Rigaku Oxford Diffraction SuperNova diffractometer using either Cu K_α radiation (λ = 1.54184 Å) or Mo K_α (λ = 0.71073 Å) generated by Nova micro-focus sources. Reflections were collected with an Atlas S2 detector. The data reduction and absorption correction was performed using CrysAlisPro[3] software. Using Olex2[4], the structures were solved with SHELXT[5] by direct methods and refined with SHELXL[6] by least-square minimization against F^2 using first isotropic and later anisotropic thermal parameters for all non-hydrogen atoms. Hydrogen atoms were added to the structure models on calculated positions using the riding model. All other hydrogen atoms were localized in the difference Fourier map. Images of the structures were produced with the Olex2 software. All structures have been deposited with the Cambridge Crystallographic Data Centre (CCDC) and can be accessed free of charge under the numbers 2543129–2543151.

Occuring disorders in the structure refinements of *syn*-**3a**[OTf]$_2$ · CH_2Cl_2, *E*-**15**[OTf], and **22**[OTf]$_2$ · 1.25 CH_2Cl_2 could be modelled and refined without the use of constraints or restraints. In the structure refinements of **2**[OTf]$_2$, **5a**[OTf] · 0.5 CH_2Cl_2, **6**[OTf]$_2$ · 0.666 CH_2Cl_2, and **10**[OTf] SADI, SIMU, and RIGU restraints were applied to solve occurring disorders of the triflate anions or the cations. The crystal of *syn*-**3a**[OTf]$_2$ · CH_2Cl_2 was obtained and measured as a non-merohedral twin, but only the reflections of the major component were used for structure solution and refinement. The crystal of **18** was obtained, measured, and refined as a non-merohedral twin (BASF = 0.5379). In the refinement of **5b**[OTf] · 0.5 CH_2Cl_2 one triflate anion was found to be disordered over three positions, which was modelled using RIGU, SIMU, SADI and EADP commands and the occupancies have been set to 0.7, 0.2 and 0.1, respectively. Due to low occupancy, the minor part was refined isotropically. The PLATON/SQUEEZE[7] extension in Olex2 was used for a solvent mask in the refinement of **5a**[OTf]$_2$ · 0.5 CH_2Cl_2 (solvent mask for 0.5 CH_2Cl_2 per asymmetric unit), **6**[OTf]$_2$ · 0.666 CH_2Cl_2 (solvent mask for 0.666 CH_2Cl_2 per asymmetric unit) and **22**[OTf]$_2$ · 1.25 CH_2Cl_2 (solvent mask for 1.25 CH_2Cl_2 per asymmetric unit).

compound	**2**[OTf]$_2$	*anti*-**3a**[OTf]$_2$	*syn*-**3a**[OTf]$_2$ · CH_2Cl_2	*anti*-**3b**[OTf]$_2$
Empirical formula	$C_{37}H_{45}F_6N_6O_6PS_2$	$C_{39}H_{41}F_6N_4O_6PS_2$	$C_{40}H_{43}Cl_2F_6N_4O_6PS_2$	$C_{40}H_{43}F_6N_4O_7PS_2$
Formula weight	878.88	870.85	955.77	900.87
Temperature/K	100.00(10)	99.98(10)	100.01(10)	100.00(10)
Crystal system	monoclinic	orthorhombic	monoclinic	orthorhombic
Space group	$P2_1/c$	Pbca	$P2_1/c$	Pbca
a/Å	9.1704(2)	17.74070(10)	9.43440(10)	17.84400(10)
b/Å	23.2550(3)	15.85540(10)	42.3893(6)	16.05310(10)
c/Å	19.6069(3)	28.0985(2)	11.1640(2)	28.8792(2)
α/°	90	90	90	90
β/°	101.091(2)	90	100.123(2)	90
γ/°	90	90	90	90
Volume/Å^3	4103.23(12)	7903.71(9)	4395.18(11)	8272.49(9)
Z	4	8	4	8
ρ_{calc}g/cm^3	1.423	1.464	1.444	1.447
μ/mm^{-1}	2.245	2.314	3.224	2.249
F(000)	1832.0	3616.0	1976.0	3744.0
Crystal size/mm^3	0.184 × 0.104 × 0.086	0.22 × 0.17 × 0.11	0.343 × 0.213 × 0.116	0.206 × 0.126 × 0.097
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.962 to 136.5	6.292 to 153.488	4.168 to 136.46	6.12 to 153.306
Index ranges	-11 ≤ h ≤ 11, -20 ≤ k ≤ 28, -23 ≤ l ≤ 23	-20 ≤ h ≤ 22, -20 ≤ k ≤ 16, -35 ≤ l ≤ 31	-11 ≤ h ≤ 11, -50 ≤ k ≤ 50, -13 ≤ l ≤ 13	-22 ≤ h ≤ 19, -19 ≤ k ≤ 16, -36 ≤ l ≤ 36
Reflections collected	35409	93192	16085	89140
Independent reflections	7484 [R_{int} = 0.0638, R_{sigma} = 0.0456]	8298 [R_{int} = 0.0410, R_{sigma} = 0.0170]	7896 [R_{int} = 0.0031, R_{sigma} = 0.0154]	8679 [R_{int} = 0.0434, R_{sigma} = 0.0196]
Data/restraints/parameters	7484/222/606	8298/0/529	7896/0/657	8679/0/548
Goodness-of-fit on F^2	1.050	1.065	1.110	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0646, wR_2 = 0.1639	R_1 = 0.0358, wR_2 = 0.0951	R_1 = 0.0771, wR_2 = 0.2068	R_1 = 0.0355, wR_2 = 0.0927
Final R indexes [all data]	R_1 = 0.0803, wR_2 = 0.1794	R_1 = 0.0392, wR_2 = 0.0975	R_1 = 0.0808, wR_2 = 0.2090	R_1 = 0.0397, wR_2 = 0.0962
Largest diff. peak/hole / e Å^{-3}	0.80/-0.34	0.63/-0.45	0.99/-0.38	0.90/-0.60
CCDC	2543129	2543138	2543136	2543144

compound	**5a**[OTf] · 0.5 CH_2Cl_2	**5b**[OTf] · 0.5 CH_2Cl_2	**5c**[OTf]	**4**
Empirical formula	$C_{34.5}ClF_3H_{31}N_4O_3PS$	$C_{35.5}H_{33}ClF_3N_4O_4PS$	$C_{34}H_{29}N_5O_5F_3PS$	$C_{34}H_{29}N_5O_5F_3PS$
Formula weight	705.11	735.14	707.65	707.65
Temperature/K	100.00(10)	100.01(10)	100.01(10)	100.01(10)
Crystal system	triclinic	triclinic	monoclinic	monoclinic
Space group	P-1	P-1	P21/n	P21/c
a/Å	10.4342(3)	13.2969(3)	9.17460(10)	15.66520(10)
b/Å	10.5465(2)	15.9518(4)	10.54190(10)	10.46510(10)
c/Å	16.4251(3)	17.2318(3)	33.3887(5)	20.0155(2)
α/°	86.891(2)	98.847(2)	90	90
β/°	84.174(2)	98.504(2)	96.8680(10)	90.5890(10)
γ/°	69.862(2)	105.389(2)	90	90
Volume/$Å^3$	1687.86(7)	3413.07(14)	3206.11(7)	3281.13(5)
Z	2	4	4	4
$\rho_{calc}g/cm^3$	1.387	1.431	1.466	1.433
μ/mm^{-1}	2.525	2.544	1.972	1.927
F(000)	730.0	1524.0	1464.0	1464.0
Crystal size/mm^3	0.2 × 0.18 × 0.13	0.243 × 0.181 × 0.041	0.2 × 0.13 × 0.01	0.18 × 0.13 × 0.08
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.41 to 153.24	5.296 to 153.532	5.332 to 153.676	5.642 to 153.374
Index ranges	-13 ≤ h ≤ 9, -13 ≤ k ≤ 13, -20 ≤ l ≤ 18	-13 ≤ h ≤ 16, -19 ≤ k ≤ 20, -21 ≤ l ≤ 21	-10 ≤ h ≤ 11, -13 ≤ k ≤ 12, -41 ≤ l ≤ 41	-19 ≤ h ≤ 19, -13 ≤ k ≤ 10, -24 ≤ l ≤ 25
Reflections collected	18674	40277	37891	38707
Independent reflections	7009 [R_{int} = 0.0154, R_{sigma} = 0.0155]	14201 [R_{int} = 0.0315, R_{sigma} = 0.0340]	6717 [R_{int} = 0.0453, R_{sigma} = 0.0314]	6869 [R_{int} = 0.0356, R_{sigma} = 0.0231]
Data/restraints/parameters	7009/6/490	14201/639/984	6717/0/444	6869/0/444
Goodness-of-fit on F^2	1.023	1.041	1.055	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0321, wR_2 = 0.0807	R_1 = 0.0540, wR_2 = 0.1493	R_1 = 0.0483, wR_2 = 0.1247	R_1 = 0.0586, wR_2 = 0.1580
Final R indexes [all data]	R_1 = 0.0328, wR_2 = 0.0812	R_1 = 0.0608, wR_2 = 0.1575	R_1 = 0.0555, wR_2 = 0.1293	R_1 = 0.0633, wR_2 = 0.1620
Largest diff. peak/hole / e $Å^{-3}$	0.33/-0.36	0.88/-1.08	0.99/-0.55	0.91/-0.50
CCDC	2543134	2543145	2543142	2543140

compound	**6** · 0.666 CH_2Cl_2	**7**	**8**	**9**
Empirical formula	$C_{47.67}H_{54.33}Cl_{1.33}F_6N_6O_7PS_2$	$C_{32}H_{25}N_2P$	$C_{32}H_{25}N_2OP$	$C_{38}H_{30}N_3P$
Formula weight	1079.58	468.51	484.51	559.62
Temperature/K	100.01(10)	100.00(10)	150.00(10)	100.00(10)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	P21/n	$P2_1/n$	$P2_1/c$	P-1
a/Å	17.3414(7)	13.50722(5)	9.01480(10)	9.5529(2)
b/Å	18.3069(6)	18.70307(8)	33.8472(4)	9.55480(10)
c/Å	17.6341(9)	19.49900(9)	9.00450(10)	15.9643(2)
α/°	90	90	90	85.1780(10)
β/°	108.228(5)	93.7865(4)	111.609(2)	82.7180(10)
γ/°	90	90	90	86.5190(10)
Volume/$Å^3$	5317.3(4)	4915.21(4)	2554.41(6)	1438.44(4)
Z	4	8	4	2
$\rho_{calc}g/cm^3$	1.349	1.266	1.260	1.292
μ/mm^{-1}	2.452	1.159	1.162	1.089
F(000)	2248.0	1968.0	1016.0	588.0
Crystal size/mm^3	0.328 × 0.256 × 0.01	0.393 × 0.231 × 0.191	0.252 × 0.194 × 0.064	0.37 × 0.274 × 0.197
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.24 to 136.496	6.556 to 153.544	5.222 to 153.072	5.598 to 153.478
Index ranges	-20 ≤ h ≤ 20, -11 ≤ k ≤ 22, -21 ≤ l ≤ 21	-15 ≤ h ≤ 17, -23 ≤ k ≤ 23, -23 ≤ l ≤ 24	-11 ≤ h ≤ 9, -42 ≤ k ≤ 41, -10 ≤ l ≤ 11	-12 ≤ h ≤ 11, -11 ≤ k ≤ 9, -20 ≤ l ≤ 20
Reflections collected	43868	58615	23421	16353
Independent reflections	9707 [R_{int} = 0.0989, R_{sigma} = 0.0606]	10295 [R_{int} = 0.0241, R_{sigma} = 0.0157]	5295 [R_{int} = 0.0299, R_{sigma} = 0.0219]	5969 [R_{int} = 0.0183, R_{sigma} = 0.0191]
Data/restraints/parameters	9707/334/704	10295/0/631	5295/0/325	5969/0/379
Goodness-of-fit on F^2	1.031	1.012	1.040	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0749, wR_2 = 0.2038	R_1 = 0.0314, wR_2 = 0.0782	R_1 = 0.0331, wR_2 = 0.0827	R_1 = 0.0351, wR_2 = 0.0890
Final R indexes [all data]	R_1 = 0.0913, wR_2 = 0.2189	R_1 = 0.0328, wR_2 = 0.0794	R_1 = 0.0375, wR_2 = 0.0861	R_1 = 0.0360, wR_2 = 0.0896
Largest diff. peak/hole / e $Å^{-3}$	0.67/-0.43	0.26/-0.40	0.22/-0.29	0.27/-0.38
CCDC	2543147	2543139	2543135	2543133

compound	**10**[OTf]	**11**	*syn*-**12**	*anti*-**12**
Empirical formula	$C_{36}H_{36}N_4O_3F_3PS$	$C_{35}H_{35}N_4P$	$C_{26}H_{21}N_2OP$	$C_{26}H_{21}N_2OP$
Formula weight	692.72	542.64	408.42	408.42
Temperature/K	100.00(10)	100.00(10)	100.01(10)	99.97(10)
Crystal system	monoclinic	triclinic	orthorhombic	triclinic
Space group	$P2_1/c$	P-1	$P2_12_12_1$	P-1
a/Å	10.0429(3)	10.5011(2)	5.74170(10)	10.6649(3)
b/Å	19.3727(4)	12.0748(2)	17.5861(3)	11.0616(4)
c/Å	17.4908(4)	12.6952(2)	20.7540(2)	11.2084(3)
α/°	90	93.1740(10)	90	105.269(3)
β/°	101.484(2)	109.5810(10)	90	103.598(3)
γ/°	90	110.2380(10)	90	112.485(3)
Volume/Å^3	3334.85(14)	1396.04(4)	2095.62(5)	1091.77(7)
Z	4	2	4	2
ρ_{calc}g/cm^3	1.380	1.291	1.294	1.242
μ/mm^{-1}	1.824	1.109	1.313	1.261
F(000)	1448.0	576.0	856.0	428.0
Crystal size/mm^3	0.27 × 0.07 × 0.04	0.18 × 0.15 × 0.07	0.42 × 0.07 × 0.04	0.377 × 0.267 × 0.174
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.886 to 144.248	7.534 to 153.376	6.588 to 153.668	8.828 to 153.148
Index ranges	-11 ≤ h ≤ 12, -23 ≤ k ≤ 20, -21 ≤ l ≤ 21	-13 ≤ h ≤ 13, -14 ≤ k ≤ 15, -16 ≤ l ≤ 15	-7 ≤ h ≤ 7, -22 ≤ k ≤ 22, -26 ≤ l ≤ 18	-10 ≤ h ≤ 13, -13 ≤ k ≤ 13, -13 ≤ l ≤ 14
Reflections collected	19978	20058	22305	10030
Independent reflections	6561 [R_{int} = 0.0568, R_{sigma} = 0.0591]	5853 [R_{int} = 0.0328, R_{sigma} = 0.0336]	4386 [R_{int} = 0.0662, R_{sigma} = 0.0439]	4470 [R_{int} = 0.0235, R_{sigma} = 0.0295]
Data/restraints/parameters	6561/6/488	5853/0/361	4386/0/271	4470/0/271
Goodness-of-fit on F^2	1.026	1.035	1.038	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0610, wR_2 = 0.1579	R_1 = 0.0358, wR_2 = 0.0849	R_1 = 0.0391, wR_2 = 0.0969	R_1 = 0.0342, wR_2 = 0.0836
Final R indexes [all data]	R_1 = 0.0854, wR_2 = 0.1735	R_1 = 0.0428, wR_2 = 0.0891	R_1 = 0.0424, wR_2 = 0.0996	R_1 = 0.0384, wR_2 = 0.0870
Largest diff. peak/hole / e Å^{-3}	0.78/-0.31	0.37/-0.33	0.50/-0.45	0.28/-0.39
CCDC	2543149	2543151	2543148	2543130

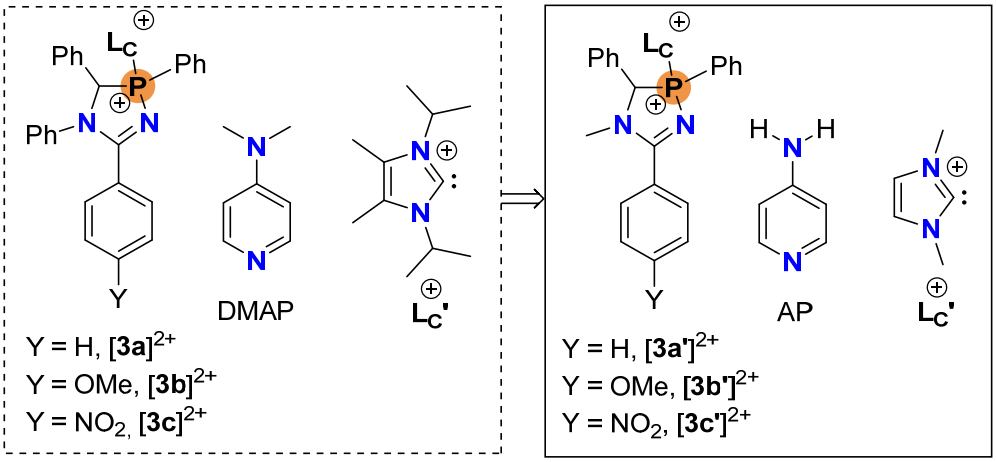
compound	**14**[OTf]	**15**[OTf]	**16**[OTf]	**17**[OTf]
Empirical formula	$C_{18}H_{23}N_2O_3F_3S$	$C_{18}H_{23}N_2O_4F_3S$	$C_{17}H_{20}F_3N_3O_5S$	$C_{19}H_{23}F_3N_2O_3S$
Formula weight	404.44	420.44	435.42	416.45
Temperature/K	100.00(10)	100.01(10)	100.01(10)	100.00(10)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P21/n	P21/n	P21/n	$P2_1/n$
a/Å	10.2066(2)	10.82670(10)	10.84420(10)	9.9108(2)
b/Å	10.9132(2)	9.20870(10)	12.17370(10)	11.9804(2)
c/Å	17.0530(3)	19.7763(2)	15.17710(10)	16.9047(4)
α/°	90	90	90	90
β/°	99.618(2)	99.7160(10)	109.7600(10)	101.724(2)
γ/°	90	90	90	90
Volume/Å^3	1872.78(6)	1943.41(3)	1885.61(3)	1965.31(7)
Z	4	4	4	4
ρ_{calc}g/cm^3	1.434	1.437	1.534	1.407
μ/mm^{-1}	1.998	1.988	2.131	1.922
F(000)	848.0	880.0	904.0	872.0
Crystal size/mm^3	0.35 × 0.27 × 0.07	0.24 × 0.17 × 0.09	0.34 × 0.13 × 0.04	0.148 × 0.109 × 0.062
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.458 to 153.026	8.75 to 153.276	8.782 to 153.404	9.112 to 136.476
Index ranges	-11 ≤ h ≤ 12, -13 ≤ k ≤ 8, -21 ≤ l ≤ 18	-13 ≤ h ≤ 11, -11 ≤ k ≤ 9, -24 ≤ l ≤ 24	-13 ≤ h ≤ 12, -15 ≤ k ≤ 15, -19 ≤ l ≤ 18	-11 ≤ h ≤ 9, -14 ≤ k ≤ 14, -20 ≤ l ≤ 19
Reflections collected	11711	12319	20646	20835
Independent reflections	3891 [R_{int} = 0.0281, R_{sigma} = 0.0273]	4048 [R_{int} = 0.0315, R_{sigma} = 0.0278]	3950 [R_{int} = 0.0331, R_{sigma} = 0.0221]	3596 [R_{int} = 0.0326, R_{sigma} = 0.0198]
Data/restraints/parameters	3891/0/264	4048/0/254	3950/0/262	3596/18/253
Goodness-of-fit on F^2	1.057	1.039	1.025	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0348, wR_2 = 0.0914	R_1 = 0.0369, wR_2 = 0.0982	R_1 = 0.0312, wR_2 = 0.0799	R_1 = 0.0660, wR_2 = 0.1705
Final R indexes [all data]	R_1 = 0.0369, wR_2 = 0.0932	R_1 = 0.0408, wR_2 = 0.1021	R_1 = 0.0352, wR_2 = 0.0832	R_1 = 0.0710, wR_2 = 0.1752
Largest diff. peak/hole / e Å^{-3}	0.36/-0.40	0.40/-0.53	0.31/-0.41	1.50/-0.55
CCDC	2543132	2543150	2543141	2543137

compound	**18**	*syn*-**19** · THF	**20**
Empirical formula	$C_{11}H_{14}N_2O_3$	$C_{30}H_{29}N_2OPS$	C11H14N2S3
Formula weight	222.24	496.58	270.42
Temperature/K	100.00(10)	99.96(17)	100.0(3)
Crystal system	triclinic	orthorhombic	triclinic
Space group	P-1	Pbca	P-1
a/Å	8.3201(4)	18.9446(4)	8.7162(7)
b/Å	9.4397(4)	10.6707(2)	9.4346(7)
c/Å	13.2132(6)	24.9740(4)	15.1842(9)
α/°	85.276(4)	90	83.523(6)
β/°	86.892(4)	90	78.698(6)
γ/°	87.524(4)	90	78.006(6)
Volume/Å^3	1031.93(8)	5048.55(16)	1194.32(15)
Z	4	8	4
ρ_{calc}g/cm^3	1.430	1.307	1.504
μ/mm^{-1}	0.875	1.936	5.444
F(000)	472.0	2096.0	568.0
Crystal size/mm^3	0.398 × 0.265 × 0.057	0.12 × 0.1 × 0.05	0.29 × 0.11 × 0.02
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.722 to 153.432	8.48 to 153.894	5.952 to 153.482
Index ranges	-10 ≤ h ≤ 9, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16	-22 ≤ h ≤ 18, -12 ≤ k ≤ 10, -31 ≤ l ≤ 28	-9 ≤ h ≤ 10, -10 ≤ k ≤ 11, -19 ≤ l ≤ 19
Reflections collected	8152	16462	11671
Independent reflections	8152 [R_{int} = ?, R_{sigma} = 0.0288]	5008 [R_{int} = 0.0354, R_{sigma} = 0.0343]	4945 [Rint = 0.0407, Rsigma = 0.0498]
Data/restraints/parameters	8152/0/290	5008/0/316	4945/0/289
Goodness-of-fit on F^2	1.031	1.045	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0397, wR_2 = 0.1027	R_1 = 0.0407, wR_2 = 0.1047	R1 = 0.0415, wR2 = 0.1042
Final R indexes [all data]	R_1 = 0.0533, wR_2 = 0.1074	R_1 = 0.0496, wR_2 = 0.1115	R1 = 0.0504, wR2 = 0.1118
Largest diff. peak/hole / e Å^{-3}	0.26/-0.24	0.57/-0.42	0.61/-0.38
CCDC	2543131	2543146	2543143

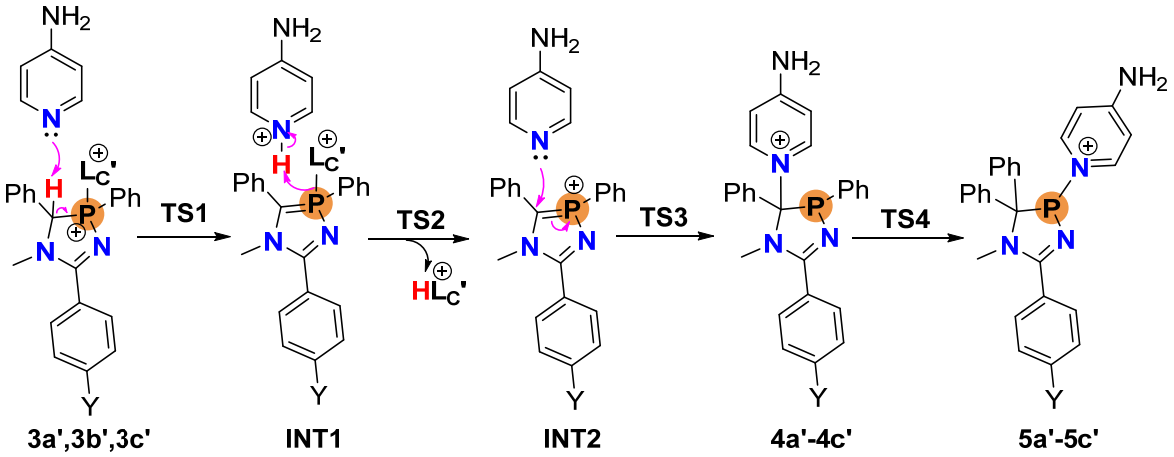
S8 Computational Details of P(V)-to-P(III) Conversion

S8.1 Computational Methodology and Simplifications

The geometries and energies of all systems included in this study were fully optimized without symmetry constrains at the RI-BP86-D4/def2-TZVP level of theory.[8-11] The calculations have been performed by using the program ORCA22 version 6.0 For the calculations we have used the BP86 functional[8,9] with the D4 correction for dispersion and the triple-ζ def2- TZVP basis set.[11] In order to reproduce solvent effects, we have used the conductor-like continuum model CPCM (for fluorobenzene),[13] which is a variant of the dielectric continuum solvation models. The minimum nature of the complexes and compounds have been confirmed by doing frequency calculations. The transition states were initially located using the NEB tool[14] of ORCA 6.0. They only present one negative frequency that corresponds to the movement of atoms connecting the intermediates. The ΔG° energies were computed at normal conditions. For computational efficiency, the reactants were simplified as depicted in **Scheme S4**. Specifically, the phenyl group bonded to one of the nitrogen atoms of the phosphadiazole ring was replaced with a methyl group, as this group is not involved in the mechanistic steps. DMAP was replaced by *p*-aminopyridine (AP), and the N-heterocyclic carbene (**Lc**) was simplified by replacing methyl groups with hydrogen atoms and isopropyl groups with methyl atoms (denoted as **Lc'**). To differentiate theoretical models from experimental compounds, a prime symbol (*e.g.,* **3a'**) is used for the theoretical species.



Scheme S4 Experimental reactants (left) and the simplified models (right) used in the DFT study.



Scheme S5 Proposed mechanism for the transformation of **3a-c'** to **5a-c'** *via* **4a-c'**, respectively.

S8.2 Transition State Geometries

The geometries of the transition states for Y = H described in the main text (**Fig. 3**) are provided in **Fig. S115**. The other TS geometries (for Y = NO_2 and OMe) are very similar and provided as cartesian coordinates.

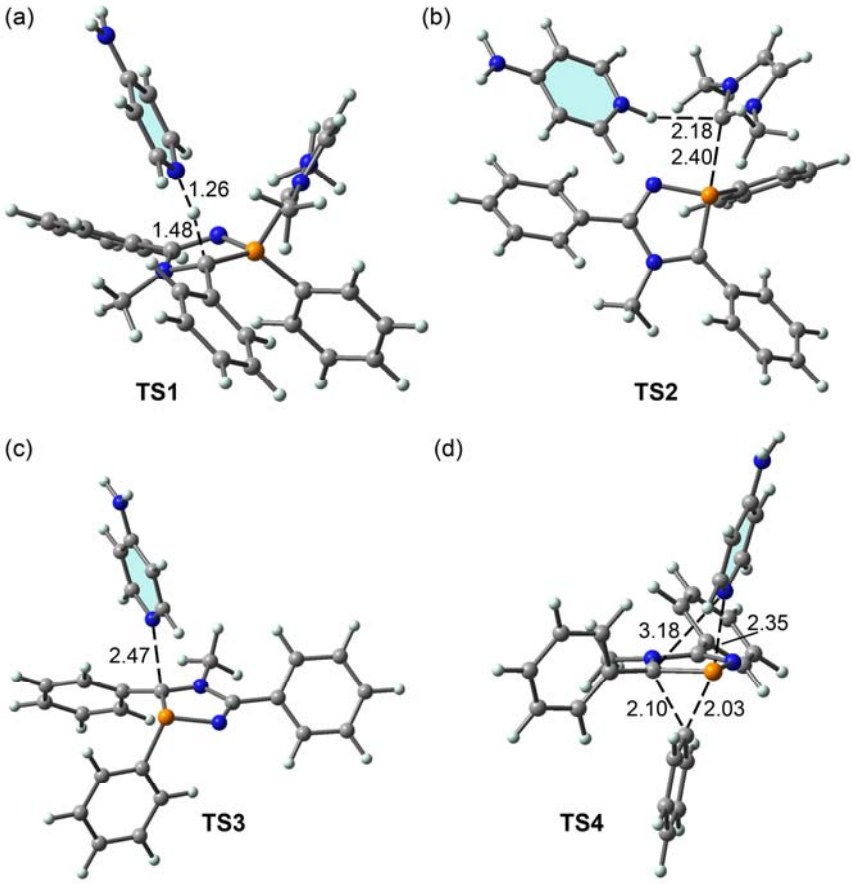


Figure S117. BP86-D4/def2-TZVP optimized geometries of TS1-TS4 for Y = H. Distances in Å.

S9 Computational Details of CO_2 and CS_2 activation

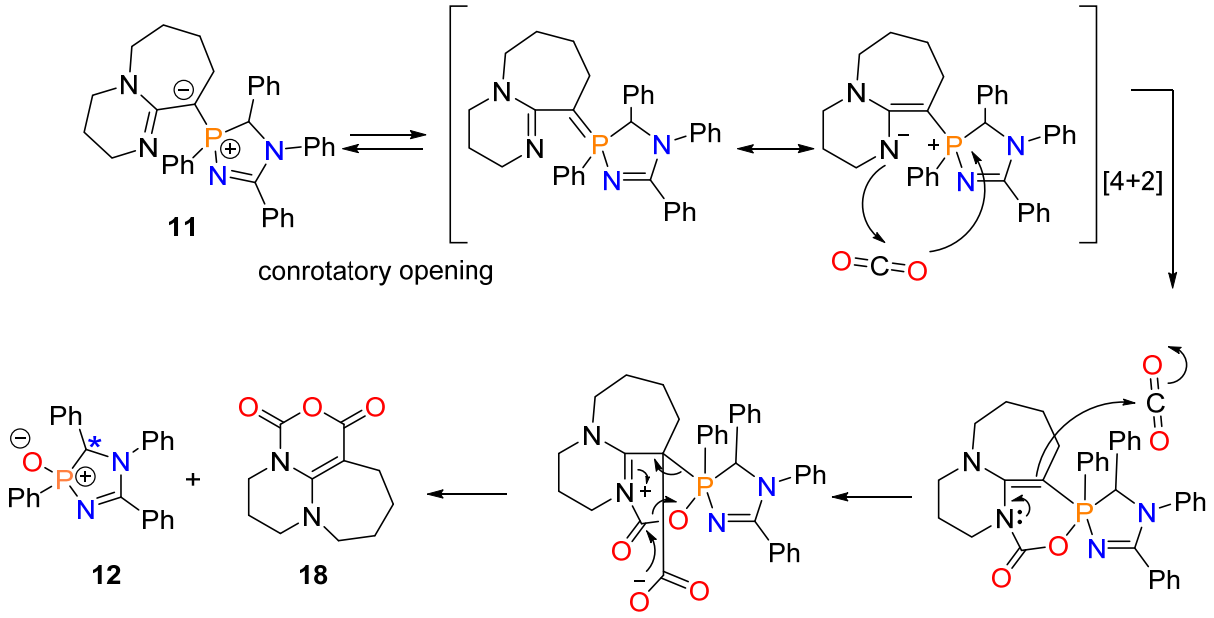


Figure S118 Proposed mechanism for the reaction of 11 with CO_2 to yield 12 and tricyclic product **18**.

The geometric features of the transition states and intermediates of the CO_2 and CS_2 activation are given in **Figure S117**.

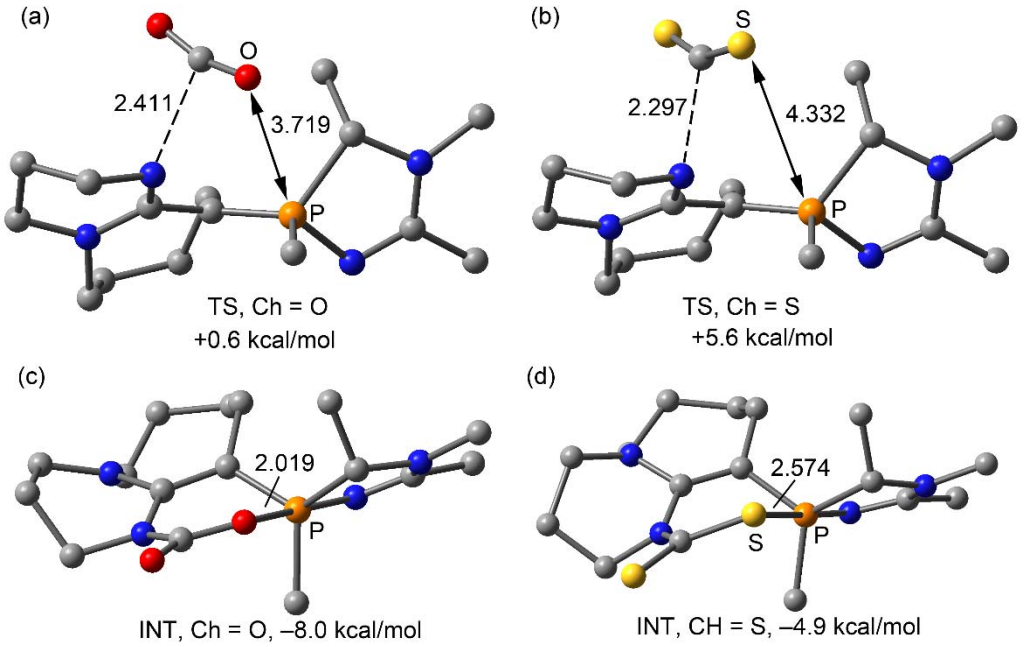


Figure S 119 BP86-D4/def2-TZVP geometries of the transition states for the (4+2) cycloaddition of **11'** with CO_2 (a) and CS_2 (b) and the resulting intermediates (**INT**) for CO_2 (c) and CS_2 (d). Distances in Å.

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Cartesian Coordinates

3a′+AP

P	7.28117461870939	11.24418131840493	18.09130024605708
N	6.53182583083307	10.86298492024926	20.86810239679977
N	6.64155122953553	9.03721833319409	19.67628573200752
N	8.49388949039663	10.45461411048940	17.34236424253130
N	9.42218441321597	12.56203235463598	17.66614355505942
C	6.82951720843652	10.38164059763305	19.63812682901279
C	6.67833129465939	12.24420445584587	21.32176944908959
H	6.26343156692890	12.93259548460125	20.57722576130478
C	6.18991847669575	9.81564833825997	21.69264349382133
C	6.25461418619500	8.67278148884680	20.94566616542788
C	6.73298067600977	8.10810373714138	18.53914571478355
H	7.58912264258358	8.38225244696851	17.91298108330528
C	5.76718482833420	11.30508566810150	17.16836217362228
C	5.78974535296948	10.94882258552137	15.80995082756519
H	6.70591656424371	10.55995406470315	15.36477240655973
C	4.63074072222852	11.09647977268184	15.05025686053999
H	4.63305489045538	10.81266582561276	13.99776035248570
C	3.47023122955323	11.61064053223540	15.63650681442310
H	2.56843084694860	11.73138521741016	15.03544082667208
C	3.45204397024480	11.96593800357809	16.99037989451020
H	2.54205803510494	12.36309551977742	17.43988217947566
C	4.59768040316324	11.80752244848422	17.76476158178075
H	4.57760075190798	12.08474801113272	18.82034617841974
C	8.13353792866924	12.90204348812773	18.30427912899826
H	8.31046926533595	13.10113952912678	19.36920539816506
C	7.36835788412474	14.01727360676573	17.65083484918280
C	7.22634876428498	14.07063949190591	16.25692697429836
H	7.73956447751837	13.34371932643809	15.62459117682293
C	6.44120033470640	15.06314590391431	15.67323305061740
H	6.34120517667139	15.10744498971825	14.58860986632063
C	5.78949632384792	16.00468977452916	16.47597163974802
H	5.17814832294031	16.78179495663464	16.01682103400200
C	5.93911308114510	15.96375140798215	17.86400652617628
H	5.45365284460714	16.71313693940266	18.48949247635612
C	6.72956027285817	14.97329349543412	18.44985098712339
H	6.87042809038615	14.96389362454775	19.53321379421215

C	10.40530623232042	13.63728286886914	17.53595425039682
C	9.56381694818862	11.27581297231217	17.27415192045757
C	10.83388189915273	10.73659581924807	16.78315572733334
C	10.81507112968550	9.81693584128724	15.71948491601666
H	9.86625028619279	9.56111733873358	15.24885710065408
C	12.00528099308407	9.25700557971518	15.26531063185588
H	11.99331837077358	8.56441577405401	14.42368300591363
C	13.21442324991641	9.57954781566444	15.89098099115629
H	14.14495757927907	9.13527055453445	15.53632542971329
C	13.23252048861302	10.46441411747291	16.97323751057463
H	14.17229278073989	10.69784211066461	17.47372537717975
C	12.05009188265752	11.05183933062999	17.41558930928279
H	12.06601415693273	11.71373524423550	18.28051412952281
H	11.13503580776455	13.37193054618991	16.76592807264634
H	9.88330466587329	14.55437265490970	17.23583111292672
H	10.92359932269254	13.81367634109380	18.48968028343799
H	6.86448725659486	7.09677220835386	18.93551256314820
H	5.80632641778947	8.15547435973514	17.95281097425836
H	6.05201542662869	7.64167063365788	21.21084278501249
H	5.93066396027919	9.96593476878784	22.73413163098483
H	6.12359083121757	12.36228431074143	22.25751269444191
H	7.74417344770524	12.44552821755804	21.48766786602786
C	11.43467643906269	9.44935056105530	20.59567835425664
C	12.31644614472069	10.41916007054039	21.12693557831865
C	11.80267846274799	11.73169474071820	21.25617183059450
C	10.49716612268456	11.98774842080086	20.87216454471395
C	10.14989740461369	9.82186651909926	20.24192132824597
H	11.76021660210002	8.41747850969486	20.45915317950601
H	12.41818867036862	12.53393623488798	21.66561372613021
H	10.10754134218731	13.00531187042136	20.98572223002998
H	9.48012997497880	9.07021657704127	19.81698169699161
N	13.59364888426082	10.11581035437587	21.46656159292707
N	9.64723200388246	11.06913171887649	20.36346948520524
H	14.17360158938820	10.78957309537170	21.95241757859446
H	13.91127422847069	9.15393041862813	21.47373923426098

TS1 Y=H

P	-1.08486747660871	-0.41443548249715	-0.56976756382491
N	-1.96507103889241	-0.44712372875108	2.19328307417978
N	-1.70250802327932	-2.42387162226143	1.30480488905666
N	0.15101890522537	-1.31808788662112	-1.18036055145394
N	1.03261996216568	0.81077211892141	-1.18574774920005
C	-1.61247588626864	-1.09238051078634	1.05296482818370
C	-2.06940005206995	1.00144713121120	2.39339909276691
H	-2.25164103288864	1.50343846141565	1.43808082318272
C	-2.25820966291707	-1.37635727730366	3.16790220753534
C	-2.09534836322410	-2.61323500419027	2.61012594346550
C	-1.51799473615815	-3.50871906243516	0.32728385583540
H	-0.69306639022518	-3.25023506475248	-0.34612562545118
C	-2.57141594295400	-0.61567140292517	-1.54889253213078
C	-2.41697028235846	-0.81039437138839	-2.93276305754065
H	-1.41976838260760	-0.91547117273366	-3.36137689458534
C	-3.54765503019698	-0.88932331332035	-3.74402713084905
H	-3.43547656259458	-1.04996782188634	-4.81644684833052
C	-4.82305688749212	-0.76665699139222	-3.18291357237764
H	-5.70430960025622	-0.82801620564490	-3.82213379721504
C	-4.97712796848126	-0.56998696453352	-1.80589983038282
H	-5.97424926633592	-0.48037560117462	-1.37447907391116
C	-3.85372148695611	-0.49278249697032	-0.98577793354989
H	-3.98182003788773	-0.33551219115347	0.08710367630701
C	-0.11544690351501	1.06468299221254	-0.29457175295350
H	0.56000374224340	0.70667904565826	0.98081147640589
C	-0.67988619753093	2.44119909143167	-0.24701972107058
C	-1.89690196659390	2.76352818326773	-0.87329409877996
H	-2.41598539230568	2.01347303048328	-1.47036489567478
C	-2.44359381596875	4.04429180576210	-0.76019502976197
H	-3.38915961950909	4.27322622671741	-1.25269455255548
C	-1.77174939467611	5.03301390706923	-0.04011585055166
H	-2.19319822023520	6.03507217326142	0.04077893145675
C	-0.54656885453328	4.73573118549757	0.56569175026418
H	-0.00855300060612	5.50831909404709	1.11604543752084
C	-0.01300225255328	3.45152257910960	0.47095000202491
H	0.94698395015959	3.23538958988029	0.94322595696512
C	1.80206819940093	1.91990459813321	-1.74653887782119
C	1.17756153059882	-0.49462234700776	-1.49993543642394
C	2.37725288614043	-1.04831724304910	-2.13216909383920
C	2.23540656863992	-2.10997044465030	-3.04404944196816
H	1.23751323210713	-2.47701488455737	-3.28237092309895

C	3.36011624682313	-2.67208197546018	-3.64113425000022
H	3.24457346617386	-3.48150192368524	-4.36217570556255
C	4.63621547619358	-2.19859204415164	-3.31838490449110
H	5.51581616397399	-2.64086258505496	-3.78694958715236
C	4.78659051858786	-1.16284728306815	-2.39122525634993
H	5.78228863517159	-0.80617914716892	-2.12689695988201
C	3.66452620795411	-0.58539866178714	-1.80132980808260
H	3.79072557195932	0.20545889289823	-1.06165763203866
H	2.40953497601909	1.54768093303679	-2.57613328088698
H	1.10770130722039	2.68391102427460	-2.11839398170884
H	2.45606025917051	2.38092160370944	-0.99359160333222
H	-1.29078863026471	-4.42802686837287	0.87560731194817
H	-2.44342256665076	-3.63975331109706	-0.24790244413752
H	-2.23498164576731	-3.60246931861464	3.03038423022059
H	-2.56644756747392	-1.08463770203279	4.16509680794887
H	-2.90768694961036	1.19607151100234	3.07061375555397
H	-1.14321298467128	1.38703806587999	2.83377833868539
C	2.79094734092311	-1.33501411854500	2.78001240389255
C	3.23074310294397	-0.46816820040961	3.81653087616629
C	2.65997182691203	0.83230888773615	3.85246772570844
C	1.73589120960358	1.19563083939938	2.89938238252765
C	1.85647372446753	-0.89156360204302	1.87243397824651
H	3.19557744597221	-2.34314132680355	2.68946893473012
H	2.95350723396426	1.54840034398529	4.62008861896899
H	1.29577735250943	2.19353766546953	2.89459742211363
H	1.50623848629493	-1.52813884492169	1.05793627487019
N	4.14588380557666	-0.85957942704513	4.72283703254730
N	1.32676154695507	0.35380021855654	1.92243318286256
H	4.47397858702852	-0.23093568894063	5.44723327263436
H	4.57041060403890	-1.77903007883954	4.68245275415103

INT1 Y=H

P	7.73004795152998	11.38803664608723	17.82446245342653
N	7.02659439548042	11.72269426351638	20.65644184491384
N	6.94344323646966	9.65633559997917	19.95521450435027
N	9.24789669898560	10.84489937757616	17.41206872539490
N	9.47511557754787	13.12043675720549	17.30210865222360
C	7.08175555699084	10.95361556471625	19.52767419571356
C	7.14131297223607	13.17826361937702	20.74886357689292
H	6.32575141508217	13.66220630745713	20.19936438377972
C	6.81313555215269	10.92271317898576	21.75536247528578
C	6.76776515520412	9.63074880217990	21.32000794170798
C	6.93894291413620	8.44403061381024	19.13500824448099
H	7.73415173453106	8.49473625825867	18.38557957025589
C	6.53613975084075	10.49881345241172	16.80714207097750
C	6.94484894703357	10.01516705370588	15.55343015875392
H	7.98369350257578	10.13150768599612	15.24226527558420
C	6.01640285676708	9.40726580900312	14.70839958429867
H	6.33203026100530	9.03132507587578	13.73465753107702
C	4.67746504836690	9.29798667562604	15.09856856875095
H	3.95173628726574	8.83309196082008	14.43062838145022
C	4.26243780678409	9.80101649567037	16.33598621847048
H	3.21511737271289	9.73147687094755	16.63146205592930
C	5.18738548732156	10.40235444730027	17.18842037038048
H	4.85549634523590	10.80888295145242	18.14659748143480
C	8.12302522764043	13.07062370574090	17.71489067730160
H	9.93161829585829	9.34945481132962	17.38613838999709
C	7.20430794089538	14.18756573494052	17.82979884851603
C	5.83310494604085	13.96426964529226	17.56542023752774
H	5.51725166845756	13.01777710699703	17.12634089879365
C	4.87899089780628	14.95509501472690	17.79748193110477
H	3.82954309679758	14.75365641651571	17.57911629138120
C	5.26827591969999	16.20862877878067	18.27174182202324
H	4.52734163669992	16.99005847004240	18.43950637100238
C	6.62358135908054	16.45520496387398	18.52043899324584
H	6.93838699762865	17.43019775950895	18.89415641227093
C	7.57745786430533	15.46142202290079	18.31695994052183
H	8.61523062974185	15.67108467443576	18.57353512764281
C	10.10006734991239	14.35440753894889	16.81066943342169
C	10.06696341619272	11.90904194303997	17.21122051727027
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C	13.22326106930194	10.66473727912186	15.58043928166078
H	13.51294384089048	10.03288786912404	14.74035849960509
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H	15.25919855587927	11.10453607677218	16.15660899402594
C	13.83144289940054	12.10824602012235	17.42861624709364

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H	10.92307260433759	14.08920645243921	16.14122144411193
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H	7.09432591577743	13.45226678669151	21.80675018017843
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H	10.03506152077541	5.33865514963347	16.00419456915741
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N	12.38725695636635	4.75931745335632	17.16727806262902
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C	-1.61428815805349	-1.08898078319237	1.53497294868711
C	-1.79948021352671	0.58307154896388	3.38047314245223
H	-2.68685021860622	1.12260932717629	3.73215783459049
C	-3.20184003962989	-1.48628550907852	3.11497493624789
C	-3.25107252750718	-2.51369674352468	2.21730168884414
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C	-2.43500401040463	-0.07278350193388	-1.09599893807287
C	-2.21362614800804	-0.55223854309905	-2.39568728642930
H	-1.20596509213325	-0.56455233987172	-2.81334033941130
C	-3.29013072150452	-1.01881194500173	-3.15126657866529
H	-3.12079433454306	-1.39832247827774	-4.15945272239757
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C	-4.80380754464048	-0.50325637873250	-1.32718130500686
H	-5.81403885490877	-0.47319412562425	-0.91816592708500
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C	1.65938352262810	2.82187348936460	-2.05134699024474
C	1.31573737751655	0.60622467192391	-0.85687575248424
C	2.73880038893212	0.23328934658551	-0.89900155600597
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C	5.39708302874857	-0.64877595371941	-0.78479582749361
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C	5.08187055442242	0.66828920077270	-0.43952041128149
H	5.86853021331576	1.35684189409686	-0.12961040996967
C	3.76081314802173	1.11179343024551	-0.49908729776527
H	3.52854189633431	2.13570794285049	-0.20628333788659
H	2.42803616768829	2.27019182713490	-2.60204641307054
H	1.01363805695773	3.35924589239995	-2.75311359730560

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H	-1.92824570558500	-4.13921431551992	0.40250788501235
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H	-3.88604462454558	-3.39185882891979	2.18571344664162
H	-3.77852463046460	-1.30796221400262	4.01554994429418
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H	-1.24497315867362	1.21900889023350	2.68126078191333
C	2.88407538522091	-3.68058049332721	2.22401922538976
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C	3.68451562611730	-1.40412975859190	2.50835134746768
C	2.43750777755220	-0.96075546780846	2.15265702332215
C	1.65873014726505	-3.16804675497838	1.88065107130349
H	3.02561799979270	-4.76047820468644	2.24373889990320
H	4.46130333692220	-0.67987469895457	2.74808603977863
H	2.18586802886378	0.09460673951025	2.09187096778862
H	0.81303219988230	-3.80034328427157	1.61885925643721
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C	5.58086585175974	11.31772813846618	16.37413386577775
H	6.38325410926270	10.90271981565463	15.76376073574778
C	4.26366935835485	11.28288019501376	15.92202735081669
H	4.03604851992790	10.84042620447641	14.95165910930170
C	3.23533390378008	11.81424787483238	16.70962126232288
H	2.20681791877314	11.78518816871267	16.34831959043681
C	3.51826465213144	12.37132199370923	17.95828707896558
H	2.71418748444697	12.77382881625613	18.57484720946087
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H	5.06167281736551	12.82065873566125	19.40682146431493
C	8.51386175858325	13.02924460048702	17.15866647641095
C	8.33126317101406	14.44646447194709	16.89895235286624
C	7.04064653496051	14.91497528878862	16.57695698508384
H	6.21554666412025	14.20936526249567	16.49072816643306
C	6.83130818191317	16.26912760144178	16.33292283299876
H	5.83594759651835	16.62167068968316	16.06206152359236
C	7.89264079896873	17.17319200732240	16.43652923942406
H	7.72289326841589	18.23486850439949	16.25410612516673
C	9.16994572303441	16.72021108078682	16.78425116820170
H	9.99184708019766	17.42877303072933	16.88975651841382
C	9.39579369964028	15.36604189514399	17.00789089823280
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C	11.08408724383368	7.68920386127025	16.10920771534552
H	10.77529005116397	6.69572977189617	15.78323146798376
C	12.44205481223931	7.98969148686262	16.25357388116023
H	13.19450547587701	7.22995512094838	16.04018678982111
C	12.83581093317304	9.26056825763696	16.68062104980048
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H	11.43696883743171	13.17133790600583	16.39911731920911
C	9.74305683358958	11.74849701761137	21.11851570677628
C	8.84047236878537	12.60841472065883	21.77903637557452
C	8.73449686600148	13.92264187665147	21.27535865598282
C	9.49373757755377	14.28875647942837	20.17390251119565
C	10.45795466781139	12.22715390635302	20.02999006122257
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H	8.06944815390887	14.64795132022936	21.74731110476294
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H	3.35627216390418	-1.85789299438448	-0.08419272625919
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H	12.23663628682910	3.17796456923345	16.73093701321378
C	12.21259898876917	2.37022317499344	17.46346737413838
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C	13.57484599561324	-0.04520429730617	25.14406055414866
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H	10.44051935969246	1.89513316525371	23.24230062692257
H	10.53542152619769	0.79895218021289	24.63893455101584
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C	9.80029325649528	-3.34770596551221	24.15102329528622
C	10.25986486568791	-2.13511281884504	23.69833733055647
C	9.58664649848736	-2.62885072870432	21.51010209711995
H	8.64692517038013	-4.49954022828700	21.14442628790865
H	9.91990816464413	-3.59828384689300	25.20430002553057
H	10.74876351642089	-1.41972168737883	24.35245618518653
H	9.55123717969004	-2.29115770219096	20.47755477247451
N	8.72669676955867	-5.45448331349200	23.65931279948839
N	10.15108177714844	-1.76780035827875	22.39976493790918
H	8.81411688612949	-5.75224184127504	24.62356263735564
H	8.31065906877379	-6.10780905146787	23.00637201427604

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P	0.28003367330037	-0.94544753636308	-1.24142295304942
N	1.59352332951863	-0.87775632920422	-0.15162415229984
N	0.35221104114558	0.95724488236862	0.50697305853947
C	0.75719707413601	0.70410595663161	-2.31514940491670
C	1.87704613158031	1.52204662345978	-2.14232580194010
H	2.45543503216208	1.48995882280162	-1.21815054302278
C	2.26853785212128	2.38410650801751	-3.16833106983133
H	3.15237317053530	3.00986695987858	-3.03965662391130
H	1.83642789273126	3.12526496909810	-5.15096963235128
C	1.52968282669578	2.44782826412345	-4.35350309603615
C	0.39766221869731	1.64272395462980	-4.51695633538324
H	-0.17860066528675	1.68475957974175	-5.44193792679567
C	0.00572718579703	0.77706979595139	-3.49866324641047
H	-0.87263796567077	0.14254743365359	-3.63197454729455
C	-0.40238897529658	0.57600148190584	-0.56730283764918
C	-1.69013543809849	1.22463698755292	-0.87668314912089
C	-1.77461453473761	2.48345405095912	-1.49218962262883
H	-0.86395626692884	3.00311722836746	-1.79113477735986
C	-3.02098515747375	3.04229640671491	-1.76622488291827
H	-3.08057658870184	4.01288002027437	-2.25937797924177
C	-4.19044743648436	2.35741023495343	-1.42215632251509
H	-5.16398917361664	2.79692060979622	-1.64121606236180
C	-4.11069208243945	1.10665624949303	-0.80714807360134
H	-5.02019817289308	0.56677388984717	-0.54203091299155
C	-2.86569695992878	0.53501400946888	-0.54022731195322
H	-2.79872443526905	-0.44201700723714	-0.06113680329979
C	0.16552680092150	2.24071353535236	1.19760790511456
C	1.46247936546154	0.09304824341955	0.69908939051522
C	2.42758842163306	0.30356158990767	1.78859090841442
C	3.78652661831588	0.08069804399111	1.51001041085014
H	4.07921291945125	-0.19914566153033	0.49801392819277
C	4.73560440576494	0.20996521232500	2.52004287830348
H	5.79026794851486	0.04881567827586	2.29567841267123
C	4.33550804753431	0.53839596813860	3.81908445149544
H	5.07950888041427	0.63441474581514	4.61035900068059
C	2.98222262310666	0.73441137592136	4.10729431722358
H	2.66745428325632	0.96869146650771	5.12438170114923
C	2.02837581465464	0.62438417510317	3.09642545093382
H	0.97250365425087	0.75246251193380	3.33619573035725
H	1.12131422159506	2.55895608742376	1.62325446950214

H	-0.18127567829818	2.99063122740210	0.48129969450041
H	-0.57942990781026	2.14541972087792	1.99819960848689
C	-2.46899526402399	-4.15405787365564	0.23036393966216
C	-1.97139675179825	-4.70593943976780	1.43433253985090
C	-0.81847984872710	-4.10193953056519	1.98891252208390
C	-0.24206083728323	-3.02010631271062	1.34816389355389
C	-1.81698572557439	-3.07501813191314	-0.33437164527708
H	-3.34534530517034	-4.58039520354406	-0.25933845242862
H	-0.37592399228649	-4.48810601757790	2.90783946721684
H	0.66178591931202	-2.55296231121453	1.74400369774085
H	-2.16420491964419	-2.65068777038437	-1.28139826104936
N	-2.58026672134142	-5.76144223723872	2.03382936242154
N	-0.72932179134917	-2.49482731539799	0.20742629588479
H	-2.15717264414644	-6.21702963295530	2.83248245148718
H	-3.33723411232870	-6.25037619082422	1.57274694080677

5a’

P	0.71548755382213	-1.19519457946167	-1.25750105941891
N	1.83459597366339	-1.06730445302522	-0.02226890224927
N	0.75843776038920	0.96170149832981	0.28100212798326
C	0.64372362116322	1.28843496027715	-2.17953898968534
C	1.68072049342199	2.22452226954485	-2.07880615418374
H	2.07326719896939	2.51135189404826	-1.10498653874648
C	2.24510583809327	2.78843205436868	-3.22537696108340
H	3.05056174857051	3.51624204982261	-3.12370763231188
H	2.23565303864316	2.85820627391391	-5.38491492944514
C	1.79176206148397	2.41889340507341	-4.49131026588504
C	0.78221667691575	1.46029769277736	-4.60668923498449
H	0.43951598435840	1.13822406004365	-5.59053123327291
C	0.22594104066361	0.89227190048326	-3.46323102179106
H	-0.52780946636272	0.11146216464770	-3.57464342625466
C	0.04013504025058	0.60242540863805	-0.95202836090768
C	-1.45898898110551	0.72599911559947	-0.75117265603917
C	-2.32687335189615	1.23028527824260	-1.72845262658685
H	-1.92876084239179	1.61597275521955	-2.66512033638645
C	-3.70636511980877	1.26589061231450	-1.50832259096735
H	-4.36098329184528	1.66651952635862	-2.28326643980132
C	-4.24422783543885	0.81123368434074	-0.30420474837417
H	-5.32066314840621	0.84661563445658	-0.13369763367040
C	-3.38613627897625	0.33660832099240	0.69185562915702
H	-3.78850472222197	0.00570213805717	1.65031074308048
C	-2.01228765125977	0.29701199682488	0.46982135956156
H	-1.35595326963308	-0.07009840298865	1.25963338454194
C	0.49534565237649	2.26399542135895	0.89243449703031
C	1.69885275984008	0.05812882091105	0.66845721381868
C	2.57731423526769	0.27811872405934	1.83271816098764
C	3.92396097959579	-0.10440907485756	1.71222013838695
H	4.27403016925934	-0.50817540000996	0.76272988136094
C	4.78773201977148	0.03182322011403	2.79563921804245
H	5.83521779803283	-0.25220651592634	2.69115718652899
C	4.31104570305825	0.52127512605866	4.01557871644360
H	4.98698386307233	0.61923597653409	4.86561113741607
C	2.96615754023256	0.87533097452248	4.14939791428834
H	2.58782402954035	1.23765870422425	5.10557370726860
C	2.10089153902859	0.76334617975464	3.06135787525682
H	1.04894292034377	1.02040153560865	3.18454020734374
H	1.40096464806535	2.63259345723448	1.38587889311815
H	0.19980185380873	2.97116560109212	0.10868561089410
H	-0.32186005784067	2.20980928869901	1.62594097046535
C	-2.73836129533701	-3.23163324366090	-0.46210135303142
C	-2.59910397640400	-3.72447922983439	0.86049589713911
C	-1.38486561943607	-3.43661441574117	1.53553663366983
C	-0.41094959971556	-2.69548396342326	0.91018599232537
C	-1.71771060659316	-2.50996471108812	-1.02677444861719
H	-3.64285634443898	-3.42167238075506	-1.03886227548238
H	-1.21025321224677	-3.80084791261045	2.54783255853442
H	0.54308543072207	-2.44701198733218	1.37642197323541
H	-1.78099244560083	-2.12206593853031	-2.04384920331149
N	-3.58075477223235	-4.43766432036862	1.45021574242727
N	-0.57264993274846	-2.23230104337038	-0.35330438010831
H	-3.46254540205471	-4.82779300538083	2.37738894615463
H	-4.43066794842932	-4.67231714618190	0.95173108613544

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P	7.24687805839241	11.27458073713417	18.05461384883264
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N	6.67437940962351	9.03277595679579	19.61616566080223
N	8.44408169900306	10.52103760005596	17.26204335406396

N	9.35317558332435	12.63390650226694	17.60610906593210
C	6.84647180567293	10.37976602356452	19.60088229988547
C	6.72975372345194	12.20261406296322	21.32987872256456
H	6.28580635618498	12.90154870553611	20.61240621768913
C	6.28446672152586	9.76094154570486	21.66347398576729
C	6.33533882163941	8.63563688415298	20.88944438465419
C	6.73737025949096	8.13243992199394	18.45462635657389
H	7.58029869670866	8.42162037631084	17.81710886907972
C	5.70057710347761	11.32630261275649	17.18422010739325
C	5.69023849883433	11.01340030377595	15.81513151215818
H	6.60362506566146	10.66768422086125	15.33013085932880
C	4.50395006951530	11.14921701501000	15.09643008321554
H	4.48143562465819	10.89893775686903	14.03568682922305
C	3.34783165323569	11.60908453115270	15.73422510307791
H	2.42430976908422	11.72105313449542	15.16529589283403
C	3.36226070873746	11.92139685279928	17.09861672208576
H	2.45567032579296	12.27657848113444	17.58832997381205
C	4.53632587315606	11.77381534307574	17.83168651548082
H	4.54159375891170	12.01606685301592	18.89603944029519
C	8.08019835915656	12.93542020714392	18.29026511236549
H	8.28125945242051	13.10872535695998	19.35584848263625
C	7.27776697738742	14.05720561333397	17.69242265361012
C	7.08321346393199	14.14074845322442	16.30632948874947
H	7.58028567056077	13.43354546183931	15.63975462509513
C	6.26741121259863	15.13767839362664	15.77472311567670
H	6.12629202032948	15.20485509723112	14.69584430533958
C	5.63696855363997	16.05425359398608	16.62219589712814
H	5.00119582822742	16.83484760069031	16.20393708219798
C	5.83877440700729	15.98375884220684	18.00225069099215
H	5.36961644349429	16.71362668096492	18.66232228987133
C	6.66029711014434	14.98872675364741	18.53563153487740
H	6.84231270004281	14.95665407987341	19.61241913893984
C	10.29537787077027	13.73976376050322	17.44730206750869
C	9.51735001325711	11.35014235804301	17.19279288335552
C	10.76897611013250	10.82600009038047	16.68106601831839
C	10.72690757115323	9.76347670386565	15.74662049816760
H	9.76044312052841	9.40875129976583	15.39087013365184
C	11.88808095781181	9.19588543384138	15.26775015148739
H	11.86617423424692	8.39847097599292	14.52522823776794
C	13.14342139736399	9.64797116034322	15.73365437491617
C	13.19948783114607	10.67144141601556	16.70132805689251
H	14.15351588982659	11.00695996429736	17.10239529818910
C	12.02481324852181	11.25471621594808	17.15439811417399
H	12.09066179544517	12.01083568636806	17.93385083701370
H	10.95479359090090	13.54006888060893	16.59730650916013
H	9.72567514515996	14.65560463975389	17.24719715880782
H	10.89705422861227	13.88598559677260	18.35667047523748
H	6.87308658517960	7.11087531014816	18.82211834256142
H	5.79878142823161	8.19890047522185	17.88960020132174
H	6.15266807569005	7.59672905720882	21.13785021170862
H	6.06031289913582	9.88548261727744	22.71637716000965
H	6.20035428749077	12.29392128658646	22.28318899538732
H	7.79762281337154	12.41299531494768	21.47001633635402
C	11.52378509269792	9.49722353838998	20.26971216786699
C	12.43336641205561	10.47332911039050	20.73458850657300
C	11.90920930150379	11.76772931863193	20.95676408709212
C	10.56486306603269	12.00239417526151	20.71846453960570
C	10.20094451937904	9.84744928655604	20.06245293044299
H	11.85551391686062	8.47721710737375	20.07212147979566
H	12.54662524505602	12.57202548954761	21.32694571130003
H	10.16557895776167	13.00503747263056	20.90611079979225
H	9.50715397273868	9.09058142078185	19.68877302052127
N	13.75091187865034	10.19354969606499	20.92289154827856
N	9.68774869745775	11.07783892608793	20.27297325083729
H	14.34273643747035	10.85396965113345	21.41383571814749
H	14.06691698840025	9.23061865253473	20.92082379034510
O	14.21318316931220	9.03614570496871	15.20556460217773
C	15.53059207532423	9.46324396247642	15.60304403246131
H	15.68867759783253	9.28965379502776	16.67783603475959
H	16.22265763885311	8.84602256906392	15.02338979463872
H	15.68488869858861	10.52471640240447	15.36061058288594

TS1 Y=OMe

P	-1.13370269495072	-0.38316700287179	-0.58771084476997
N	-1.92666574409578	-0.44184147115866	2.20703163402228
N	-1.71623518126001	-2.40562071032480	1.27721082144659
N	0.09486538594194	-1.27266880579927	-1.22742254574771
N	0.94430899919329	0.87137171695321	-1.27081928820745

C	-1.61535108487299	-1.07091366444508	1.04507214667800
C	-2.00542065906794	1.00377030332044	2.43553881571082
H	-2.35368455445895	1.51107850881786	1.52969758143282
C	-2.20586907281766	-1.38483872098368	3.17243277776189
C	-2.07516209760477	-2.61367534621825	2.58909813093596
C	-1.56916199167686	-3.47500343448062	0.27706569192335
H	-0.77328945559843	-3.20225705176165	-0.42529449901961
C	-2.64155089430361	-0.60899381142138	-1.53206433096582
C	-2.51741539490432	-0.79491177543791	-2.92001115024591
H	-1.52882276621683	-0.87685071259378	-3.37307215057279
C	-3.66552595839638	-0.89667953296754	-3.70406872719907
H	-3.57569718069234	-1.04948255473801	-4.77975538371633
C	-4.92936169227191	-0.80776589060709	-3.11166984904900
H	-5.82442835782020	-0.88807888537917	-3.72921059740876
C	-5.05383812600789	-0.62032075183877	-1.73036673575785
H	-6.04187065937872	-0.55676884655484	-1.27402260178918
C	-3.91253323132152	-0.51831455302834	-0.93801131974437
H	-4.01813250846198	-0.36710346567095	0.13845101245874
C	-0.16644551580771	1.09877860239714	-0.32918251901904
H	0.56827396660138	0.70801095507095	0.90834049687421
C	-0.73030746012838	2.46904544429070	-0.21734851489733
C	-2.00922529434517	2.78568501199555	-0.70864062619288
H	-2.57961731142305	2.03704872974390	-1.25954101516480
C	-2.55446776987346	4.05910135393579	-0.52330831612688
H	-3.54876825735009	4.28258770306999	-0.91146833692547
C	-1.82079113919153	5.04779735476603	0.13339580820830
H	-2.24049449575541	6.04459768862471	0.26929149176440
C	-0.53605724549012	4.75630230787258	0.60427590413969
H	0.04899533672996	5.52830644703786	1.10535339075197
C	-0.00260821542154	3.47929936639508	0.43976062718743
H	1.00196456870673	3.26723586744604	0.81099014500783
C	1.61402706735860	1.99406901841412	-1.92595340406040
C	1.10216312050721	-0.43781239758159	-1.59105254268190
C	2.26964256656867	-0.97067801105736	-2.27255779571309
C	2.12391396404746	-2.11813066565937	-3.08629685947559
H	1.13477480361383	-2.55912749892990	-3.20519324307935
C	3.20903611723226	-2.66594991477605	-3.73930358378692
H	3.10183617796002	-3.53649393284003	-4.38621713553643
C	4.49196154252001	-2.09533879544666	-3.58755134931640
C	4.65954351867112	-0.97353614566282	-2.75113309765541
H	5.64379395791225	-0.53586999449449	-2.59723059718074
C	3.55669166412893	-0.42360288993781	-2.10949475435849
H	3.71026107370184	0.42625869273483	-1.44450420516168
H	2.14823459622559	1.62251313645503	-2.80504521924033
H	0.85887520619028	2.72581648661599	-2.23976595641283
H	2.32331564300703	2.49545833161500	-1.25301111470244
H	-1.31487044161072	-4.40133706172776	0.80133216114754
H	-2.51723719640704	-3.60132934949066	-0.26104742068086
H	-2.21550622808062	-3.60830142881248	2.99598446830801
H	-2.48115953473103	-1.10698479158037	4.18303012697054
H	-2.71549006775134	1.18310821913252	3.24897882798894
H	-1.02136772676976	1.39743126151286	2.71145597772148
C	2.84951079514230	-1.36650599424927	2.60655514987446
C	3.32701041334634	-0.50869218963158	3.63337444832024
C	2.77105501206314	0.79709022097240	3.69188561746165
C	1.82109605527513	1.17242947194199	2.76933465789590
C	1.89150224091795	-0.91164960518918	1.72927531972490
H	3.24276302297011	-2.37754416863374	2.49958529934472
H	3.09509397943368	1.50700942603673	4.45295976882814
H	1.38956587493045	2.17410592052416	2.77995969936085
H	1.50990008464519	-1.53906102696235	0.92170831544952
N	4.26463317746231	-0.91329562372797	4.51134011125554
N	1.37458530528012	0.33749440013993	1.80314395818391
H	4.61751799692913	-0.29237130247278	5.23055743739305
H	4.67514416692293	-1.83823218936187	4.45726324758598
O	5.48035091580568	-2.69502331632995	-4.27098077860964
C	6.81165804369033	-2.15318089039183	-4.18954461246529
H	7.19155354961688	-2.20244601098695	-3.15812278741109
H	7.42310941496117	-2.78675298082276	-4.83829954286319
H	6.83361879010543	-1.11591170279419	-4.55512415620725

INT1 Y=OMe

P	7.61540414334997	11.35917945365330	17.77856646153634
N	7.12019252906172	11.70199554709953	20.64322773620633
N	6.92118711709807	9.64380826458421	19.93615070587020
N	9.09721039884519	10.76282386982101	17.29704679839281
N	9.38341041953077	13.03025916798038	17.13326850593094
C	7.06436766589355	10.94109891895769	19.50873279961634

C	7.29208356679408	13.15151031748385	20.73162405421761
H	6.46626431424912	13.66747868166005	20.22811542121387
C	6.96986688448184	10.89795330082171	21.74976488882724
C	6.85241307690982	9.61157117284936	21.31044198806616
C	6.82667309056947	8.44131910000989	19.10602675461906
H	7.58148016055992	8.47261586597061	18.31415840570013
C	6.34666597977017	10.51363783148618	16.81944505147625
C	6.68282847357912	10.00999614074808	15.55226208601192
H	7.71381055884783	10.07374467601860	15.20237090256547
C	5.69433678142178	9.44274321301710	14.74872401218616
H	5.95301476701616	9.04925487069650	13.76515586286779
C	4.36947057244293	9.39247843466500	15.19501757422918
H	3.59752584433409	8.95831308113705	14.55904533302431
C	4.02858823910594	9.91164815247380	16.44836085229034
H	2.99303107813947	9.88500259026953	16.78853137419612
C	5.01338915427374	10.47371344592715	17.25961258291606
H	4.74243200022731	10.89173135180601	18.23206872045060
C	8.06233773101564	13.02788104747071	17.64515845631744
H	9.87102123867794	9.31127056828498	17.42618148387581
C	7.20571709747939	14.18407578477675	17.81594012411021
C	5.81050329095707	14.02900718292666	17.64724118441640
H	5.41895446147199	13.09521634585139	17.24258157090055
C	4.92741022347340	15.07259818500146	17.92526801030325
H	3.85683455844117	14.92509755573925	17.77856223424964
C	5.41208647458641	16.30993099609666	18.35207389375511
H	4.72580127167266	17.13223661996615	18.55314058411097
C	6.79176275882737	16.48710853821352	18.50985630467952
H	7.18128889031448	17.44838547081953	18.84709771313264
C	7.67625549227289	15.44164664461843	18.26016677911097
H	8.73860111607171	15.59837649723321	18.44396694625633
C	9.99364584480730	14.23073330226869	16.54882741533687
C	9.93409404522744	11.79893735535379	17.02075163699836
C	11.32188750320733	11.56729825421278	16.61826562152733
C	11.61103193298200	10.64589879628669	15.58934965300469
H	10.79081716165524	10.16999673895440	15.05070647495335
C	12.91737126781349	10.36800005403511	15.22798708293997
H	13.14627841098364	9.67983104024094	14.41423020288816
C	13.98724685141224	11.00788123912672	15.88780583050745
C	13.71471558844658	11.93404781690486	16.91181614612856
H	14.52300095512874	12.44358879230213	17.43272611709958
C	12.39435421960819	12.20463791384114	17.26402785167774
H	12.19803787163000	12.91260046271814	18.07085827135773
H	10.75065326054008	13.91983242328600	15.82302369368829
H	9.21302193093327	14.81216937162290	16.04503718166355
H	10.46606453011845	14.85712292818217	17.31556522307791
H	7.01041576424648	7.57386794584576	19.74790107118593
H	5.83336779808007	8.36401350895841	18.64793568053306
H	6.72837880625740	8.68619651991996	21.86031192702641
H	6.95702848563746	11.30420054321453	22.75417183739383
H	7.31331933653490	13.42344552468932	21.79095965826878
H	8.23257925099516	13.43542477503332	20.24719305106063
C	10.84851519906307	6.20892330952662	16.60474725759502
C	12.09913762058935	6.15610710451740	17.28106198403585
C	12.48282869092498	7.30119380454465	18.03255895651734
C	11.65317687955504	8.39294632344152	18.08200151090393
C	10.07141819538600	7.33647176372555	16.70193087711611
H	10.50413744217617	5.36787389293702	16.00395467659003
H	13.43498354129292	7.32603396180122	18.56112390380079
H	11.91519546637526	9.30257714940084	18.61998065534775
H	9.11589580589141	7.43046915376017	16.18670451237209
N	12.88841126930450	5.07096319446532	17.20616913679908
N	10.46116693874125	8.40333535022857	17.43858609522292
H	13.78237055288451	5.03318751263038	17.68298495262035
H	12.61991006247239	4.25756095080622	16.66366704231359
O	15.22158014061407	10.67090370252159	15.46412151163331
C	16.35473686526354	11.34947885400642	16.03570118775121
H	16.43331568162820	11.14670811466182	17.11469123555051
H	17.22908225073462	10.94252312587797	15.51963779172160
H	16.29137919909217	12.43325385801258	15.85828247615853

TS2 Y=OMe

P	-1.08951662820108	0.57355922510478	-0.08694389104215
N	-2.27774746449771	-0.66605445342868	2.66118780704804
N	-2.27860568585519	-2.27716283536572	1.23760365380411
N	0.40826392120437	-0.19094881709335	-0.29153743217540
N	0.81187502983999	1.86382209639863	-1.27197468144809
C	-1.64873469947016	-1.09948440164873	1.52837665619157
C	-1.91727576996502	0.55229878582353	3.38058074220069

H	-2.82449823339600	1.05889568199255	3.73046210605998
C	-3.26684752146987	-1.54541067738622	3.06391476016047
C	-3.27101933568752	-2.56522264485896	2.15643461028125
C	-1.98983652430000	-3.09394632828271	0.06333824382498
H	-1.07617777243784	-2.71654602617406	-0.40609848948712
C	-2.45254362531593	-0.06677751173144	-1.09811671984686
C	-2.21558198446350	-0.53970344868716	-2.39741721694490
H	-1.20281278415051	-0.54790249757862	-2.80286396379177
C	-3.28200769285919	-1.00522195836299	-3.16774508737025
H	-3.10027778070936	-1.37868943278065	-4.17606116134965
C	-4.58145907995494	-0.98368685477636	-2.65058062649961
H	-5.41383425445905	-1.33965704576648	-3.25841979260038
C	-4.81732895240840	-0.50464675611293	-1.35790594138909
H	-5.83199789206526	-0.48080194656846	-0.95959339451305
C	-3.75377088512077	-0.05216547836772	-0.57640602402975
H	-3.93720761026449	0.31737314522883	0.43351483567685
C	-0.53215706479407	1.97817563729881	-1.09995316760139
H	0.55200824951198	-1.38048930045733	1.52579204017643
C	-1.27006786226036	3.19284828929013	-1.42294168702998
C	-2.49334164513559	3.10204709608769	-2.11902445601503
H	-2.84914125796732	2.13179179520954	-2.45984681687625
C	-3.22129366740417	4.25315769113548	-2.40928407321839
H	-4.15272564718719	4.17497648938085	-2.97024224880925
C	-2.76050635296963	5.50327363177036	-1.98715367920968
H	-3.33738636172602	6.40130399786728	-2.20987809632486
C	-1.55914224780664	5.60370536656910	-1.27703463199000
H	-1.20618643658952	6.57639687710679	-0.93378113049498
C	-0.81339261534851	4.46156288276598	-1.00455389036326
H	0.10758195775162	4.54679110587195	-0.42678665874599
C	1.63169694744052	2.83091020071948	-2.02051058921104
C	1.29887157167022	0.61051640122559	-0.82032627959177
C	2.71435984102772	0.23791585832055	-0.85267038452533
C	3.03662471984701	-1.11953806141020	-1.07653422797556
H	2.23745426634573	-1.81509038100373	-1.33180026672559
C	4.34211595684699	-1.56430256264996	-0.99914494236742
H	4.59885358930793	-2.60322229415763	-1.20631277803654
C	5.38130329677015	-0.66350455714323	-0.68393981711721
C	5.07613193746081	0.68921379360807	-0.44914169418562
H	5.85838232798514	1.40347078016013	-0.19955346994523
C	3.75655369934853	1.12550082354984	-0.53653297477633
H	3.54587687151041	2.17156142027112	-0.31656088760100
H	2.39978249622841	2.28202053663641	-2.57478761903045
H	0.98035612812885	3.36530973354458	-2.71938281271474
H	2.11190374908769	3.55992891009053	-1.35677487891780
H	-1.85457933250345	-4.14169036014168	0.36106432896928
H	-2.81428598206692	-3.03031824832078	-0.65873825563236
H	-3.88595503777845	-3.45626193211723	2.10035622614459
H	-3.86952497878017	-1.38756085104708	3.95113740511200
H	-1.28202244080460	0.31747190386980	4.24489926257665
H	-1.37693854078527	1.21428602268019	2.69428472516339
C	2.96362428604097	-3.55237752801829	2.17331791226430
C	4.00213061611891	-2.65243032389537	2.53920695362719
C	3.68792517432560	-1.26610431022966	2.56111064617944
C	2.42728234496024	-0.84800525178549	2.22234404878253
C	1.72267341432530	-3.06540243128228	1.85039546841203
H	3.14127045847747	-4.62667650426180	2.14462015096332
H	4.43981419880533	-0.52802598764237	2.83550644954081
H	2.14211512016001	0.20067628067089	2.20490419017444
H	0.89853466135496	-3.71173929814068	1.56638188277227
N	5.23227308700877	-3.09622209088300	2.84693010623329
N	1.46341399570677	-1.73717410140826	1.88168983740547
H	5.96698697222509	-2.46003423814297	3.13407893839996
H	5.45136628246907	-4.08614847076655	2.85179877451196
O	6.62071779133015	-1.19186993352233	-0.63097452297622
C	7.74085144760985	-0.30282344248703	-0.45973744009943
H	8.62976351287299	-0.93714441945684	-0.52300391207642
H	7.76540491517121	0.45061319049560	-1.26037083080018
H	7.70767854268286	0.19269203459794	0.52280017081606

INT2 Y=OMe

P	7.53362455129389	11.99521254508272	18.28644692674988
N	8.39406838948571	10.61797634335597	17.82310409866012
N	9.52183776806883	12.33388909584504	16.73717257325751
C	5.85436069299534	11.89141498660596	17.59815018880875
C	5.60232215018716	11.30113085002189	16.34961143975735
H	6.41933328490881	10.86940678632286	15.77094442102152
C	4.29735925474671	11.26174715318190	15.86313088246716
H	4.09387743853371	10.79954679936486	14.89654132915290

C	3.25077575144941	11.81380130601662	16.61126601851050
H	2.23210761874559	11.78133490802573	16.22331079277175
C	3.50312341191792	12.39509392625717	17.85554967191899
H	2.68468490598874	12.81298307787078	18.44230797180679
C	4.80556013934351	12.42779185259281	18.35809689925464
H	5.00945604215440	12.86749996237488	19.33545271793477
C	8.48699631933492	13.05942154958218	17.17800929728296
C	8.28994456877204	14.47588704588454	16.91862548551037
C	7.00114051307433	14.93022972427537	16.57134769167123
H	6.18680403960567	14.21529324445801	16.46361679603843
C	6.78052764817139	16.28337030590599	16.33045102836156
H	5.78683930845398	16.62502638237082	16.04019035517692
C	7.82776361400793	17.19991456073129	16.46249840068110
H	7.64886274776585	18.26059440253402	16.28293767346067
C	9.10285815397570	16.76016034067797	16.83400249016818
H	9.91394710349768	17.47788940225733	16.95992366639046
C	9.34071430173037	15.40724763477818	17.05413381596714
H	10.31440199636061	15.06486176169043	17.40414842033601
C	10.54752623455106	12.85522739707618	15.82687740969505
C	9.45720262783563	10.94648611747451	17.15026158346625
C	10.51414855712523	9.99607429195227	16.81502718716147
C	10.13714153327978	8.66157454518565	16.54542994110223
H	9.07839474689280	8.40350882020487	16.54004373121810
C	11.08917039258038	7.69437105748213	16.29014354564005
H	10.80454310988699	6.66703228190832	16.06349727294009
C	12.46009297029833	8.02241399427240	16.32275559079111
C	12.85200160441034	9.33883661172734	16.62342023430984
H	13.90405723605436	9.60916031942411	16.68545061376321
C	11.88268221976924	10.30928966521416	16.86089955736416
H	12.21376433437547	11.31217327943961	17.12822846783235
H	10.87585028164990	12.04451892365102	15.17001554844474
H	10.10930796573241	13.66788434423623	15.23847502756329
H	11.40241334741820	13.24222626468396	16.39470821215239
C	9.79095258344575	11.74423174124718	21.09579120508782
C	8.89021847049230	12.57957436308444	21.78932258730905
C	8.76392236477339	13.90367985943102	21.31803355916258
C	9.50239033518167	14.30244090233765	20.21375093188264
C	10.48397024316574	12.25445827407209	20.00753705480472
H	9.94610047464228	10.71012675703835	21.40712918916188
H	8.09779924909681	14.61076132186334	21.81545686943369
H	9.40145437360258	15.32706219628245	19.84556540089929
H	11.19179958071417	11.60818606157251	19.48045862448821
N	8.14645587040881	12.11660669101709	22.83946921055099
N	10.35423369556813	13.50942316841224	19.53367344957395
H	7.67985950695995	12.78286381958106	23.44366016127535
H	8.40232040956812	11.23686351455200	23.27224804793496
O	13.31222883492982	7.00916758225701	16.06098468985119
C	14.72227245415712	7.27780231526757	16.08445483670596
H	15.04373627756375	7.60945013615661	17.08362702217881
H	15.20506824856695	6.32703301755243	15.83951052839295
H	14.99146705073208	8.03476763627658	15.33203678474358

TS3 Y=OMe

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N	-0.71535455404085	-2.09757450632239	-0.03400015134859
N	0.52920869828648	-0.18966425333560	-0.52222368679158
C	-2.95117501144552	-0.63699293565412	-0.94038106756850
C	-2.68459300458780	-1.11940358275970	-2.22856656525034
H	-1.78400538324944	-1.70322339981989	-2.42082693348504
C	-3.58846878910790	-0.86071744402481	-3.25860316536825
H	-3.39092657646564	-1.24369284256693	-4.26059626845689
H	-5.44645811132216	0.08742367554249	-3.81814220662119
C	-4.74385117452504	-0.11329788015638	-3.00863789502564
C	-5.00754389809934	0.36413906436938	-1.72309476685928
H	-5.91562787357396	0.93429158365718	-1.52485803597792
C	-4.11738812953057	0.09462129163067	-0.68193153810573
H	-4.33060904136520	0.45050077997031	0.32731124612853
C	-0.56685871925001	0.42660499432844	-0.06961263256946
C	-0.96462429861283	1.80279596394744	-0.32251420027908
C	-0.85116069707902	2.34264067348265	-1.61880925543395
H	-0.38617256017588	1.76187539439082	-2.41584740811426
C	-1.40455688208560	3.58814006182254	-1.90616829509918
H	-1.32572408243399	3.99120406225388	-2.91611002733885
C	-2.06965394388138	4.30951196637477	-0.91159495473870
H	-2.49502593717772	5.28711859649117	-1.14000084545314
C	-2.19944133001878	3.77121171866823	0.37235654170138
H	-2.72472925524779	4.32837315066642	1.14852654479053
C	-1.66305595294734	2.52094723125223	0.66532555827355

H	-1.74442416903268	2.09353801648636	1.66443644085239
C	1.74520513743412	0.51833845857970	-0.93237678880487
C	0.43651118241858	-1.63575432615005	-0.40408578979402
C	1.56828949529234	-2.50163652131836	-0.73444928746472
C	1.29113523799843	-3.70023816183452	-1.42812420300149
H	0.26507998069100	-3.90967751847326	-1.72967581678265
C	2.29878480046088	-4.59747075032165	-1.72403121908166
H	2.09479039506397	-5.51560184492820	-2.27467089274863
C	3.62034653929681	-4.34039272555793	-1.30734347116791
C	3.90487705921656	-3.17016341548541	-0.58218270339741
H	4.91067942713564	-2.96779823227167	-0.21977513584282
C	2.88443679413022	-2.26319646886443	-0.30816189862176
H	3.12200645000360	-1.38676832287746	0.29323532026300
H	2.22894599120540	-0.02288359711307	-1.75145172364503
H	1.48077414644933	1.52817284156162	-1.25436152979216
H	2.43380949027674	0.59308582213570	-0.08064379470222
C	1.64612103284930	-0.38999811516330	3.87150949291099
C	2.49158902931334	0.72491120320248	4.07190331049457
C	2.24460237946218	1.86596493388154	3.27487748556416
C	1.20513168877061	1.83887781042684	2.35872925609099
C	0.63284994508434	-0.31123501029433	2.93022909272032
H	1.77623726119650	-1.30108101587455	4.45712193911802
H	2.85636865630632	2.76302409273452	3.38080423498839
H	0.99576057689767	2.71564158389106	1.73890701851459
H	-0.03943218222409	-1.16058062026012	2.77798579321104
N	3.51643884159911	0.68977135889183	4.96891252112624
N	0.39819120660228	0.77877603037307	2.17747005660234
H	4.00712188130984	1.54224597072724	5.20981222380958
H	3.57699910344373	-0.06906807885711	5.63675712841335
O	4.53351318752626	-5.27706899918515	-1.64293960655253
C	5.89552702476997	-5.07890142031176	-1.23821496227377
H	5.97944156027754	-5.04096869622246	-0.14109171792398
H	6.44345508295825	-5.94630336994120	-1.61853853260463
H	6.30826305084897	-4.15824282324117	-1.67887981550423

4b’ Y=OMe

P	11.99256990880781	-1.10440445866047	20.48646257538785
N	13.27279839495874	-0.88561383201993	21.58851522151659
N	11.57837729590617	0.15184383188107	22.81273566984854
C	12.21338976501968	0.29893141090245	19.34928059843434
C	13.15289844066183	1.31969277909024	19.55838876579331
H	13.82133044979972	1.27076812995171	20.41824204545835
C	13.22874128401023	2.38828093405645	18.66531066675276
H	13.96304634013645	3.17902370287991	18.82510464543532
H	12.42918715652418	3.28401416614486	16.86892270002937
C	12.36657175251476	2.44652451066379	17.56493865731191
C	11.44002407371175	1.42399870889635	17.34401589730349
H	10.77947561942429	1.46068054071975	16.47705956653072
C	11.37234632495286	0.34632412758994	18.22659887637085
H	10.65915639164976	-0.46118570729426	18.04567392371707
C	10.70070158593938	-0.43109459274426	21.83371419604448
C	9.56568694018632	0.44513659216141	21.37355232207610
C	9.85727519606051	1.68623276378569	20.78534622926547
H	10.89219700685990	2.00447904341215	20.67322780990232
C	8.85192345991232	2.54133170444237	20.34195329573583
H	9.12877856395508	3.49311903910210	19.89325963006544
C	7.50566979813133	2.16661726480855	20.47533465100752
C	7.19680351891918	0.94014506722228	21.08542220595014
H	6.14927614798436	0.66579014943239	21.20941986926712
C	8.21048235925460	0.10252442258771	21.53057397437830
H	7.91867739285792	-0.82705708915371	22.01804677216384
C	11.13914768955141	1.23392456588978	23.69781895026321
C	12.91635640117259	-0.26002024030728	22.67011724472668
C	13.89792971292924	-0.00511924201762	23.74469288132424
C	15.23740525987672	0.21135108991123	23.38021857106868
H	15.49983579706981	0.20869003705166	22.32258692339684
C	16.20939223824173	0.40881350602782	24.35706221021279
H	17.24427995059151	0.58634125730380	24.06314856276270
C	15.86186789350160	0.37321912415636	25.71114816749873
H	16.62454950886202	0.52459258845254	26.47571761811228
C	14.53665587028708	0.13589125812339	26.08401181453623
H	14.26453378142959	0.09050218499384	27.13896172010715
C	13.55885084187216	-0.04681501881007	25.10707215859471
H	12.53096870660639	-0.23859140256883	25.41641207402075
H	12.01530679913530	1.77717331661723	24.06275988127081
H	10.49933748975303	1.92813142944037	23.14056662231602
H	10.56541842154793	0.86365591743698	24.56277999382404
C	9.08385502319469	-3.84853773471340	21.94027429592695

C	9.20661722880573	-4.23298916772962	23.29994937544843
C	9.83024428880356	-3.30661170137442	24.17312218320460
C	10.28202988968465	-2.10312488413970	23.68980442957768
C	9.56862712345422	-2.63499915971885	21.52352713774659
H	8.62142801208830	-4.51155426700622	21.20998831087215
H	9.96713897258528	-3.53685516035782	25.22899326364011
H	10.78077076320517	-1.37548126953604	24.32268013290111
H	9.51163178350894	-2.31299423215558	20.48693633474999
N	8.75407905009807	-5.42402295337128	23.73896612142640
N	10.15242601675126	-1.76034303400400	22.38646714236111
H	8.86120327402167	-5.70377710796789	24.70656998217602
H	8.32922459699136	-6.09082417584336	23.10580190189466
O	6.44998654848628	2.91038201122891	20.06453640316894
C	6.71900811754578	4.17107615860628	19.43797670397412
H	7.24021975715407	4.85354094145047	20.12751214941151
H	7.31619598776068	4.03852383850821	18.52224899494268
H	5.73996751529274	4.58726202656457	19.18105499679347

TS4 Y=OMe

P	0.32940423615509	-0.94531741642584	-1.37242506999739
N	1.61982661655885	-0.87543069918723	-0.25919348462285
N	0.32342891916530	0.90826654344565	0.43115258525771
C	0.77620177402255	0.77721737371421	-2.37562874206977
C	1.88495819987149	1.59715488806751	-2.14426289653355
H	2.43542825021847	1.53969625820614	-1.20438844962099
C	2.30289047505059	2.49063806118995	-3.13142169817525
H	3.17756405970153	3.11819002179375	-2.95658452205350
H	1.92936625695945	3.28321150792172	-5.10601994607424
C	1.60171706553117	2.58216217552984	-4.33782871437759
C	0.48096262656720	1.77552064766014	-4.55997205028695
H	-0.06556616562431	1.84071157991217	-5.50142184117155
C	0.06120941329140	0.87930910427779	-3.57865733709096
H	-0.80913623177053	0.24484038081553	-3.75669447399737
C	-0.40212090336315	0.54188124905684	-0.67103815687645
C	-1.71510544708430	1.15928138981106	-0.94745251548713
C	-1.85694425007192	2.40745805404373	-1.57224086381320
H	-0.97364726067208	2.94414541349858	-1.91840048933079
C	-3.12737693659796	2.94087379449567	-1.78282928660988
H	-3.23107640144109	3.90531416525787	-2.28073714856535
C	-4.26297364583849	2.24121050270701	-1.36496917068992
H	-5.25501913153212	2.66122715310481	-1.53320144245769
C	-4.12569253065264	1.00105218134814	-0.73823422755175
H	-5.00863932963198	0.44944286059170	-0.41390931813669
C	-2.85768925797017	0.45589754749421	-0.53317178506902
H	-2.74558709322812	-0.51152931536122	-0.04318930340831
C	0.11696622411127	2.19474495713938	1.11068463959216
C	1.44994898038400	0.06258091802174	0.62714157291426
C	2.36613702028791	0.24768493114043	1.75320387580465
C	3.73142672452988	-0.05170852989651	1.55677295807708
H	4.06379695119053	-0.36442850083326	0.56704095740863
C	4.63431157796272	0.04823539659473	2.59792048301990
H	5.69322479882569	-0.16354626588656	2.45059285047449
C	4.19526333385083	0.42742992626094	3.88268844167712
C	2.83211997429409	0.69384930059216	4.10144502955780
H	2.46547100103319	0.95856718742104	5.09108700191615
C	1.93515558501846	0.60866529485903	3.03986914161756
H	0.87843552392701	0.78864892871291	3.23762184053617
H	1.05799867063048	2.50854429505848	1.57116842776160
H	-0.19519722451783	2.94515609034637	0.37810863868063
H	-0.66012924804514	2.11015271683282	1.88174254228511
C	-2.44030929591470	-4.11228583857566	0.26647454089933
C	-1.94250669598621	-4.57285471337294	1.50805116603204
C	-0.76706805077666	-3.95595955430567	1.99688307552632
C	-0.17011483294769	-2.94967218650845	1.25924295238990
C	-1.76894084581175	-3.10100358725082	-0.39483973715097
H	-3.33420644269862	-4.55454313048755	-0.17497791602988
H	-0.32335854082069	-4.27413703541689	2.94108378066605
H	0.75100988056057	-2.47473405307937	1.60224243142255
H	-2.12249078934912	-2.74169247205245	-1.36575359315168
N	-2.57187571412794	-5.55457924598556	2.20514312991523
N	-0.65865998046238	-2.50965963824679	0.08382821507735
H	-2.14764595449846	-5.95087429548178	3.03421000331477
H	-3.34492376813886	-6.06369765467317	1.79564736115276
O	5.15310113953776	0.49958061571024	4.83218605861641
C	4.77037655544647	0.88690730588140	6.15968106768689
H	5.69692982790017	0.89324548404313	6.74168368421825
H	4.32392467710313	1.89321310516657	6.16349539193151
H	4.06576965988761	0.16157649530233	6.59515947497016

5b' Y=OMe

P	0.68914062170777	-1.21035424374522	-1.30323124190557
N	1.82764739400721	-1.06061137497926	-0.09097442632545
N	0.68403503244596	0.91964061713480	0.27353335836083
C	0.63848357631295	1.29177133608945	-2.17854362170163
C	1.65667265420511	2.24206225419660	-2.02393989497256
H	2.01506230323896	2.51231373443317	-1.03254120398410
C	2.24591471783434	2.84431680235742	-3.13743804081113
H	3.03423073529496	3.58353807784257	-2.99194640682137
H	2.30054134926838	2.96949633479295	-5.29380183116601
C	1.83816354480178	2.49901384311536	-4.42577349514138
C	0.85066259952521	1.52592940530674	-4.59544532973063
H	0.54419391860791	1.22285468167059	-5.59704711082428
C	0.26802921697243	0.92053494482646	-3.48380893668082
H	-0.46963357535655	0.13149327966143	-3.63711961269771
C	-0.00032479809578	0.57835517639455	-0.98346435063939
C	-1.50324384563128	0.70664962141554	-0.82149876261456
C	-2.34206987109214	1.22436577620569	-1.81730683751565
H	-1.91740054305375	1.60690044561291	-2.74357776789952
C	-3.72532024235294	1.28103728270807	-1.62805288277742
H	-4.35603273125506	1.69330654229709	-2.41658022802109
C	-4.29710604355527	0.83374567480243	-0.43666963612152
H	-5.37626714591209	0.88675645495816	-0.28961651499969
C	-3.46875352963329	0.34314905833569	0.57634941692137
H	-3.89714034626748	0.01737756252416	1.52535672955947
C	-2.09089464058150	0.28273658721784	0.38519369583347
H	-1.45723042415007	-0.09186018068191	1.18973744929059
C	0.40175993912408	2.21684087255250	0.88715162912105
C	1.65892640230616	0.03924809216672	0.64032614030798
C	2.52459814828254	0.25579332506223	1.80589338528866
C	3.86354401899515	-0.18339806128536	1.72246246167989
H	4.21125939632512	-0.62996578099601	0.79162253464077
C	4.72339736994033	-0.04340055319489	2.79552565664460
H	5.76428985170447	-0.36005730847504	2.73038529030457
C	4.26273011814808	0.51334866918110	4.00500894765584
C	2.92157657139154	0.91825010782196	4.11655353090653
H	2.53498905915285	1.32361841924036	5.04944767053002
C	2.07110051505459	0.79557401811469	3.01992582530929
H	1.02933268120406	1.09053812274098	3.14037907151539
H	1.30851468703091	2.61173619669189	1.35891272415283
H	0.07003007064277	2.91338608686691	0.10834099292678
H	-0.39762532188003	2.14700660385527	1.63936869263356
C	-2.72908531173406	-3.27217070047352	-0.39344720172817
C	-2.56138201865472	-3.72228752114699	0.94063668352425
C	-1.33999378316779	-3.39951233074392	1.58595263321220
C	-0.38499576622857	-2.66846998430930	0.92062862686948
C	-1.72731823552158	-2.55442880267557	-0.99673347753290
H	-3.64127199098345	-3.48948482443636	-0.94796399123533
H	-1.14466740287540	-3.72967194950513	2.60615344126051
H	0.57515248526101	-2.39643811890169	1.36050518086766
H	-1.81320288816352	-2.19412120711420	-2.02244625743553
N	-3.52457895892138	-4.42792493487880	1.56983671175057
N	-0.57410950826707	-2.24593505712471	-0.35281028954424
H	-3.38354584673627	-4.79000421418032	2.50506351215992
H	-4.37783972633554	-4.69183817119867	1.09238450231065
O	5.17842227955314	0.60784815931055	4.99527503717426
C	4.76938211711331	1.17083620238336	6.24908171952976
H	4.42304748327084	2.20831904392641	6.12250037911146
H	3.97650007897907	0.56517168009231	6.71497263440868
H	5.66171157870361	1.15632756613995	6.88237235506476

3c'+AP

P	7.32845147777220	11.26237130573752	18.03613673992255
N	6.57798623487643	10.87745793785895	20.81461036136568
N	6.66611284623308	9.05694538002534	19.61362497784105
N	8.53732299804308	10.48624102114348	17.26526801451478
N	9.44074629193587	12.60813213680944	17.58181678956276
C	6.88245690059364	10.39729698676124	19.58536330732350
C	6.72909124586746	12.25509390890419	21.27760616074239
H	6.32110101809425	12.95071006455942	20.53600100467373
C	6.20446245285786	9.83225385331789	21.62839516481660
C	6.25671169749337	8.69255989608183	20.87612785008394
C	6.73995539618623	8.13439422048748	18.47005546242433
H	7.59704899171272	8.39832664601742	17.84145861729234
C	5.79234409147926	11.30741795363756	17.14691407113433
C	5.77450302576339	10.96369531154277	15.78528893525616
H	6.68247188765395	10.60195500410281	15.30223372089588

C	4.58436406760824	11.08496148423128	15.06991908815907
H	4.55536604223037	10.80899947503075	14.01578527842796
C	3.43160597865040	11.56070533369281	15.70232042020334
H	2.50491614084997	11.65909618729089	15.13595231396037
C	3.45315507946921	11.90470738775573	17.05894261415642
H	2.54935941244902	12.27131443468506	17.54558795895552
C	4.63031651799253	11.77147896645271	17.78916280097770
H	4.63854758454795	12.03669229948764	18.84784809605245
C	8.16188039002192	12.92566086709762	18.25116349319078
H	8.36433259219351	13.10326651813106	19.31541686849898
C	7.36367742495171	14.04566651067513	17.64786039134733
C	7.14948378518282	14.11557609925882	16.26393311233800
H	7.63772675156396	13.40406093289495	15.59538179211043
C	6.31936410802279	15.10273092210101	15.73572031571027
H	6.16112056425936	15.15925642276081	14.65868665674217
C	5.69417647554798	16.02194904921197	16.58431605204228
H	5.04492432601273	16.79283490036715	16.16869952139503
C	5.91784833177521	15.96689710303371	17.96175808257512
H	5.45343454908387	16.69968831946534	18.62199871688772
C	6.75375438535672	14.98246876699772	18.49180959137624
H	6.95171477361230	14.96223082222882	19.56599449873128
C	10.41831137864516	13.68820419387862	17.45687820564691
C	9.58956712189105	11.32453334928566	17.19436346257468
C	10.87053183152805	10.78563603020268	16.72151254935084
C	10.87482036709340	9.89041237888566	15.63925212102894
H	9.94484075006671	9.67039615077488	15.11656237225411
C	12.06431560709119	9.29312911099922	15.23682205846426
H	12.10998175230591	8.60854726457106	14.39129999607609
C	13.22483965376393	9.57469629498957	15.95423608803502
C	13.24337045540243	10.44056536908923	17.04394034550666
H	14.17737446357418	10.60983641688698	17.57672437099093
C	12.05674887255040	11.05912752667732	17.42313947103710
H	12.04491699642743	11.71110443006959	18.29552952027139
H	11.16504830263118	13.42047593543036	16.70439790370028
H	9.89545477964258	14.59774242715694	17.13567257573007
H	10.91467494690212	13.88011082958058	18.41922141527514
H	6.85872647379860	7.11843827741269	18.85847761236868
H	5.81137340963231	8.19959412614346	17.88863916148682
H	6.03134207662849	7.66405596136336	21.13321099919003
H	5.93382924838311	9.98209175355582	22.66716577622572
H	6.16920130200032	12.36959964616655	22.21073038329276
H	7.79368287158846	12.45341155132907	21.45299002834935
C	11.41217909602734	9.40995666076773	20.60809904193445
C	12.28004695219920	10.36686461204930	21.18662747518140
C	11.78467751283333	11.69094449652503	21.27567601939487
C	10.51043653225272	11.96869725489019	20.81149101678670
C	10.15916002655294	9.80444731192340	20.17492555589755
H	11.72353158211167	8.37029247291414	20.50071115398484
H	12.38956217989759	12.48426913542846	21.71683535548413
H	10.13466555561058	12.99458476667616	20.89389307620942
H	9.50104504484779	9.06323475189295	19.71461233882044
N	13.52282875369967	10.04005379571538	21.61146886226769
N	9.67488553023152	11.06241470777072	20.25789604507134
H	14.10220075144826	10.71311312742418	22.09874697278578
H	13.83634572030233	9.07683744865980	21.61573318686877
N	14.49957437534671	8.90223073119148	15.55318729493380
O	15.48639912119726	9.12639260790113	16.25206865326279
O	14.45607594594639	8.17598275397929	14.56405978256739

TS1 Y=NO_2

P	-1.2076240	-0.3528814	-0.5044892
N	-2.1400666	-0.3656613	2.2364199
N	-1.7482445	-2.3510142	1.4175702
N	0.0354217	-1.2523851	-1.1089609
N	0.9235743	0.8739937	-1.0996569
C	-1.7312457	-1.0254313	1.1236154
C	-2.3386164	1.0789031	2.3902463
H	-3.2555541	1.2425253	2.9664804
C	-2.3937675	-1.2780806	3.2369481
C	-2.1501269	-2.5201587	2.7229335
C	-1.4981624	-3.4612115	0.4833477
H	-0.7154932	-3.1694658	-0.2249160
C	-2.6914445	-0.5412449	-1.4848048
C	-2.5378008	-0.6165007	-2.8810505
H	-1.5411272	-0.6385564	-3.3231788
C	-3.6681975	-0.6824913	-3.6924092
H	-3.5560068	-0.7512776	-4.7743386
C	-4.9441420	-0.6658567	-3.1190951

H	-5.8255749	-0.7175548	-3.7583613
C	-5.0977649	-0.5892785	-1.7309551
H	-6.0948878	-0.5840088	-1.2908367
C	-3.9739643	-0.5254917	-0.9101718
H	-4.1033653	-0.4664386	0.1717483
C	-0.2433639	1.1352405	-0.2337735
H	0.3681220	0.8249543	1.0568341
C	-0.8107603	2.5122942	-0.2130741
C	-2.0167415	2.8303737	-0.8615767
H	-2.5315469	2.0760292	-1.4563449
C	-2.5598241	4.1142037	-0.7710127
H	-3.4969227	4.3413029	-1.2797985
C	-1.8954602	5.1086457	-0.0520952
H	-2.3146288	6.1127385	0.0108939
C	-0.6814480	4.8143401	0.5764781
H	-0.1494863	5.5911056	1.1262423
C	-0.1515156	3.5276261	0.5043574
H	0.7996087	3.3127572	0.9946338
C	1.7181170	1.9788901	-1.6353243
C	1.0628577	-0.4288354	-1.4156129
C	2.2650818	-0.9884988	-2.0464462
C	2.1140416	-2.0272149	-2.9824873
H	1.1143969	-2.3720869	-3.2422332
C	3.2312782	-2.6024458	-3.5776954
H	3.1460586	-3.3955805	-4.3186624
C	4.4936608	-2.1453346	-3.2074078
C	4.6766330	-1.1359222	-2.2663399
H	5.6872642	-0.8292581	-2.0026255
C	3.5538772	-0.5533530	-1.6871609
H	3.6852097	0.2215249	-0.9324530
H	2.3376755	1.6082231	-2.4564338
H	1.0406774	2.7539889	-2.0137868
H	2.3608623	2.4238725	-0.8638479
H	-1.1822854	-4.3324136	1.0652276
H	-2.4244936	-3.6950311	-0.0565306
H	-2.2408077	-3.5019310	3.1727146
H	-2.7347911	-0.9732380	4.2192290
H	-1.4873856	1.5179015	2.9216384
H	-2.4381805	1.5542539	1.4099533
C	2.4233917	-1.1779661	3.1301601
C	2.7219350	-0.3046873	4.2109530
C	2.1416509	0.9912816	4.1686143
C	1.3418090	1.3438376	3.1052424
C	1.6075384	-0.7430982	2.1103971
H	2.8441136	-2.1827343	3.0961668
H	2.3329268	1.7124159	4.9628932
H	0.8995263	2.3384102	3.0416390
H	1.3664137	-1.3866706	1.2624832
N	3.5154445	-0.6865462	5.2285981
N	1.0652591	0.4968467	2.0867349
H	3.7495125	-0.0503551	5.9823329
H	3.9566627	-1.5989794	5.2421390
N	5.6989402	-2.7690628	-3.8328280
O	6.7944029	-2.3554602	-3.4580701
O	5.4988735	-3.6467865	-4.6690196

INT1 Y=NO_2

P	7.55752638944025	11.37339221903174	17.75696087180255
N	6.95770742326850	11.64998962663642	20.62154199997122
N	6.78225841218054	9.61052977186925	19.86269123652506
N	9.02082986880478	10.73263853659977	17.30638536265348
N	9.39452795591136	12.99876697186019	17.21781030315378
C	6.96756197861480	10.91111268849753	19.47476190047986
C	7.12109931459652	13.10016345026479	20.74343683503284
H	6.32176277866343	13.62073096452656	20.20363691425196
C	6.73086164476739	10.82711119767109	21.70123170354992
C	6.62768639377413	9.55044173417034	21.22892167409346
C	6.69752339192777	8.43128668175370	18.99624700216679
H	7.45266545593849	8.48973573262432	18.20686102568944
C	6.24442818731611	10.61947205220448	16.78365378907095
C	6.54534813787560	10.14306325092596	15.49794666310772
H	7.57344770429621	10.17477327656201	15.13559853633216
C	5.52552728090577	9.63478173461394	14.69366007360599
H	5.75562277991319	9.25911020245892	13.69630665535669
C	4.20648720996965	9.61816957196595	15.15877326165225
H	3.41074239897874	9.22882368583041	14.52298229855700
C	3.90132254740449	10.11011993858268	16.43235559241184
H	2.87051036539893	10.10797060568583	16.78777420177481

C	4.91709320395126	10.61058855290540	17.24509301474005
H	4.67317443543783	11.00625768481011	18.23373218626579
C	8.05315092411807	13.03056746445926	17.66351342241235
H	9.82945629339501	9.19038863670402	17.60613707768750
C	7.22103422685866	14.20932657276420	17.83025921142797
C	5.83518732447458	14.10386671802212	17.57154730979233
H	5.44097694087223	13.19915184525711	17.10865451265834
C	4.96576171440875	15.16003544068864	17.84373877675128
H	3.90215403321359	15.05095924729593	17.62835761720534
C	5.45729469564971	16.36189704879253	18.35645343809486
H	4.78190855744420	17.19336138282281	18.55727267707524
C	6.82886866794909	16.49124325736313	18.60214297545065
H	7.22304958424246	17.42459424854179	19.00563504868675
C	7.69828450143242	15.43098532735862	18.35710466577312
H	8.75140069676138	15.54839311101521	18.61084451080175
C	10.08298837824063	14.19980877182454	16.72828518344972
C	9.89626285052634	11.75282332098406	17.08036856072052
C	11.28641722059636	11.45412777419539	16.72762275434318
C	11.53709162931088	10.50444604071723	15.71866457436738
H	10.70850822385204	10.14037275905289	15.11168904556557
C	12.81872423969984	10.01383348765433	15.51315968920853
H	13.03068457205614	9.25595196852888	14.76126988589111
C	13.85284365057204	10.50312087777139	16.31004987222530
C	13.65778563324127	11.51753697165007	17.24493941767700
H	14.50475682955827	11.89092949275170	17.81900252788542
C	12.36381310717933	11.98608995834152	17.45885404109674
H	12.18375549472834	12.72825734078768	18.23711357247614
H	10.87019481080764	13.89778831618271	16.03168577929320
H	9.35639646823619	14.83313506115974	16.20662211753354
H	10.52568106397148	14.77107432175763	17.55333889729537
H	6.88192458720375	7.54506760914573	19.61173031649279
H	5.70465325414236	8.36608175334928	18.53520922547589
H	6.45885664284936	8.61567058674567	21.75070616214178
H	6.65916609487837	11.21361479999353	22.71112692479427
H	7.08149613602286	13.35514760625043	21.80636556473580
H	8.08611482572280	13.39477095844400	20.31924118501246
C	11.54638584582242	6.56472758055842	16.50659195068542
C	12.71761905720827	6.69082674814417	17.30748322264729
C	12.71586740954411	7.70654276826399	18.30578387832488
C	11.63264761000345	8.53543078751480	18.43273475029867
C	10.50232544327852	7.43444312718918	16.68563696534367
H	11.47867871587207	5.79624709467321	15.73748612535868
H	13.57511791462537	7.84155393234736	18.96140598075484
H	11.60314093674021	9.34832156179931	19.15570963054686
H	9.60590109356644	7.40068445747767	16.06839042229229
N	13.77382093677475	5.88698153768492	17.13187799947396
N	10.54246968931745	8.40311981959903	17.63503142250299
H	14.63666765811196	6.03058601022332	17.64586698690393
H	13.79612678025595	5.19984362354596	16.38604545846303
N	15.18569785694900	9.86562163035191	16.21616071898874
O	15.21634727933469	8.72710499835580	15.73028295919131
O	16.14810699904234	10.48458931184489	16.65999665447684

TS2 Y=NO_2

P	-1.06527892233249	0.50812771882398	-0.15688686206198
N	-2.23892046084104	-0.61071072759802	2.62613851227283
N	-2.25084744260930	-2.26040649031187	1.24319245325516
N	0.41229439238583	-0.28218934139403	-0.39347492101167
N	0.84405052049950	1.78920080371251	-1.32640135582676
C	-1.62160632330947	-1.07399457739264	1.49846429481549
C	-1.87752499384833	0.62954650269583	3.30874048380625
H	-2.78504666541825	1.15554253142079	3.62778329209246
C	-3.21958123975989	-1.48220558636308	3.06140633636487
C	-3.23065950372045	-2.52590995448043	2.18019681792565
C	-1.97341640985883	-3.10353215993550	0.08376732582136
H	-1.05096663768204	-2.75146189086979	-0.38853956403200
C	-2.48424398757199	-0.08849469260191	-1.10894455360601
C	-2.31093044014835	-0.54945157128720	-2.42311985643952
H	-1.31553646107658	-0.58021787029743	-2.86809496122898
C	-3.41982901507560	-0.97165687849501	-3.15741021215000
H	-3.28783255878997	-1.33763255750725	-4.17609177483202
C	-4.69741451913457	-0.91646429570987	-2.59077979093964
H	-5.56293124597363	-1.23798239663005	-3.17087476952904
C	-4.86946388629481	-0.44801774705049	-1.28412841785148
H	-5.86742630086101	-0.39627104162207	-0.84814496948830
C	-3.76389105985561	-0.04088926524250	-0.53729168173893
H	-3.89971361405021	0.32209451181586	0.48230772242763
C	-0.50374974682190	1.92206791519823	-1.14800680415394

H	0.50335366792021	-1.49772556832145	1.64837135035292
C	-1.22325531486205	3.15378190268303	-1.44209852380839
C	-2.45573169403370	3.09098415342680	-2.12611022046909
H	-2.83098362326373	2.13051769325056	-2.47387561839420
C	-3.16691403698205	4.25684805605451	-2.39722964501499
H	-4.10522633742854	4.20049304071013	-2.94923659372735
C	-2.67931381273786	5.49487253304182	-1.96905399181915
H	-3.24232991105584	6.40492867495517	-2.17804599016224
C	-1.46877521460448	5.56808186603818	-1.27099938400843
H	-1.09517851077015	6.53144547847825	-0.92339921777860
C	-0.74067769931634	4.41069973598897	-1.01609963059423
H	0.18669757137627	4.47590975676198	-0.44614278526183
C	1.69494200032614	2.76247766799767	-2.03102911024220
C	1.30089892646275	0.52430291672795	-0.91503283968447
C	2.71862383601360	0.12323469663142	-0.90667239230623
C	3.01596719879502	-1.21506212070172	-1.22220982941204
H	2.23039188386639	-1.85418973434976	-1.62282792935587
C	4.28773692440731	-1.72563539279891	-0.99896678360522
H	4.54356803003894	-2.75697560852816	-1.23713715859954
C	5.24005643455136	-0.89650106938193	-0.40884622428975
C	4.99567538957119	0.44714524988778	-0.13671658445845
H	5.77574576326545	1.06036276909985	0.31210758114703
C	3.73224910598318	0.96251869355408	-0.40995688215814
H	3.52402357380755	2.00345683000983	-0.16574990825369
H	2.46969789377402	2.21740131955006	-2.58041194317507
H	1.07133642653819	3.32260478128409	-2.73519959692776
H	2.16698925313389	3.46867115579901	-1.33718737683597
H	-1.85906609530857	-4.14754311340254	0.40149466340296
H	-2.79503773890828	-3.03672581418025	-0.64105656185428
H	-3.84280453640798	-3.42044849068672	2.15589769589713
H	-3.81220405667176	-1.30454413372315	3.95180097219643
H	-1.25741273037545	0.41852961229045	4.18985076975973
H	-1.32145366608752	1.26283553255499	2.60827293984937
C	3.03681256317463	-3.56928768433328	2.16033739225217
C	4.05670545588290	-2.62727323401580	2.47800589705110
C	3.67711957495751	-1.25622427513329	2.54155132638398
C	2.38702477410572	-0.89148730704950	2.26063618873584
C	1.76309454969934	-3.13541377277907	1.89545011391585
H	3.25782166032818	-4.63499766147762	2.11520250656721
H	4.40827403286010	-0.49223191637808	2.80046538029215
H	2.05461186593081	0.14354740921028	2.27525643924841
H	0.95682935992431	-3.81746773086089	1.63435614016078
N	5.32232132944497	-3.00872983614829	2.69992758747125
N	1.44774578245920	-1.81755421093617	1.94254081697618
H	6.06061560059710	-2.32897477269760	2.86206489754441
H	5.59916311038085	-3.98345031139835	2.64945624208372
N	6.50819807712156	-1.50505304887847	0.04972491158555
O	7.06754440829981	-0.94939177935244	1.00563631910019
O	6.87788075830237	-2.54083733064075	-0.49382797007178

INT2 Y=NO_2

P	7.68970834471257	11.72687719641231	18.20474796190694
N	8.65698578195721	10.45357137233306	17.64802423061402
N	9.61377558079900	12.32797099920057	16.66427078654563
C	5.99726200409988	11.47829785825660	17.60568209225088
C	5.73191978368981	11.05541062403965	16.29254859144569
H	6.55090128850897	10.85691628665042	15.60079939518226
C	4.41142301188612	10.88380660005804	15.88463184341856
H	4.19743552336891	10.55109802613429	14.86845059607185
C	3.36179161511175	11.13606870068266	16.77640480883153
H	2.33030039522526	11.00041470115970	16.44939187014572
C	3.62798512909372	11.55131104793229	18.08264827197330
H	2.80881110743637	11.73661046378326	18.77766386680072
C	4.94832942242461	11.71883100740862	18.50510363743239
H	5.16553453915049	12.03284943162259	19.52693712444329
C	8.51748640872269	12.93471000998790	17.13938515364499
C	8.18671305804955	14.33994214890711	16.98935687722848
C	6.82756086243070	14.69634997254771	16.84844190240958
H	6.06769382849395	13.91707071016739	16.81042631690708
C	6.46071284210086	16.03190693542073	16.72318753620623
H	5.41055712084834	16.29338353229916	16.59271216682244
C	7.43469316094023	17.03453739368423	16.76613693530936
H	7.14399716205214	18.08163841108908	16.67633801842229
C	8.78173518243232	16.69611349670035	16.93087421051118
H	9.53991727492920	17.47756983298041	16.98331177959759
C	9.15993145024248	15.36160573709249	17.03330380639277
H	10.20739071020411	15.11466955246597	17.19264911678722
C	10.62695130141616	12.95442038627135	15.80910718134607

C	9.67241571606453	10.92713776496017	17.00124483875508
C	10.84138827014245	10.11434565839335	16.62402021894866
C	10.62933795087757	8.89614228360592	15.95881736668234
H	9.61569240933770	8.59392126456641	15.69671337730728
C	11.71090995740659	8.08146801068783	15.63863490546659
H	11.58386179358819	7.13629347057936	15.11378754059415
C	12.98883211920834	8.49392076521682	16.00898949834265
C	13.22140382691645	9.68315396253697	16.69597728248048
H	14.23750017735814	9.94402093492530	16.98674249029761
C	12.13834004609597	10.50176779358276	17.00285329771904
H	12.27833376120995	11.41354179222076	17.58674103918342
H	11.01557939112390	12.19732243809126	15.12113383716432
H	10.16296718071758	13.77090744993299	15.24659695729727
H	11.45252297939361	13.34039850856192	16.41973623649733
C	9.86130252383033	11.26831869351915	21.30673082602685
C	9.36996937100162	12.47311970462594	21.85101302184319
C	9.67052331879237	13.65590942247141	21.14272038702419
C	10.40840894306791	13.57289754555739	19.97116831912652
C	10.58724693695633	11.30436702055374	20.12513673275958
H	9.67827585907768	10.31535289241016	21.80558150926453
H	9.33716228002647	14.62692867446498	21.51236243440630
H	10.65698334845717	14.49289070737360	19.43546322097819
H	10.96628123950349	10.36943047128092	19.70336203812921
N	8.60702948092997	12.49031833313472	22.98678764630485
N	10.86486595463558	12.42551323216414	19.43019335623263
H	8.46386917567791	13.37166320301339	23.46639663780125
H	8.59435581635861	11.66765492222061	23.57885718779931
N	14.15013919538637	7.62358214477703	15.66826794048115
O	13.90831828684764	6.57239196829626	15.07560559779571
O	15.26581547967775	8.02125569098095	16.00374125863332

TS3 Y=NO_2

P	-1.61483513121416	-0.83096952029369	0.55576979654866
N	-0.41873733772649	-1.89806039644146	-0.05850606589546
N	0.40674563101250	0.16211044032639	-0.75558419728082
C	-2.93743437891210	-1.01333740783026	-0.70853165566355
C	-2.67939576864556	-1.13733031656467	-2.08180497823610
H	-1.65342473804660	-1.15410005608419	-2.45208826472158
C	-3.73970518070073	-1.25282388279826	-2.97809685331526
H	-3.54051489850673	-1.35183507126072	-4.04580466364899
H	-5.88535365392360	-1.33963921102735	-3.21378415311051
C	-5.05859441484825	-1.24683034010095	-2.50872969924315
C	-5.31827204827198	-1.13459107760674	-1.14155210156511
H	-6.34514097447807	-1.14575713522038	-0.77493927107649
C	-4.25883581147678	-1.02051995008785	-0.23816608897439
H	-4.45509568130735	-0.94194946006528	0.83273087648117
C	-0.66672068599903	0.62568384913901	-0.09552855447308
C	-1.10591929088128	2.01525242336278	-0.11059346653995
C	-2.47522597844816	2.30082832732576	-0.27880332762349
H	-3.18290494203803	1.48881653076742	-0.43719846673688
C	-2.92042562972901	3.62095030233764	-0.28678801853746
H	-3.97929931790023	3.83140794559947	-0.43767182105776
C	-2.01616397195001	4.66843353853716	-0.09760672286377
H	-2.36926895897235	5.70014468456072	-0.09444279618574
C	-0.65842157445843	4.39381968021002	0.10262925326979
H	0.04458686536101	5.20850911938802	0.27749667613664
C	-0.20407074894684	3.08019058242261	0.09285976860699
H	0.84097320709246	2.86463867130277	0.30991691200023
C	1.27107882538632	0.97817908649959	-1.61675836411982
C	0.54870684867618	-1.27106325502756	-0.62852658398991
C	1.74518684092376	-1.96368317379526	-1.14227543795587
C	1.56118539541953	-3.21899689822887	-1.74808107393733
H	0.55150048605255	-3.61511037250722	-1.85033025477542
C	2.65503849305678	-3.94702159592583	-2.20279548423070
H	2.54007968149570	-4.91621642309208	-2.68496503273696
C	3.93081307267419	-3.41505486828571	-2.02800244895051
C	4.14706592989189	-2.18592013872532	-1.41112835353385
H	5.16547313948758	-1.82429483783965	-1.28102680970625
C	3.04552890470835	-1.45774713025619	-0.97204115740315
H	3.21027890829396	-0.50469948298915	-0.47055057005025
H	1.63179711861759	0.35704576157193	-2.44284962702882
H	0.68285887532549	1.81312806818660	-2.01116527451021
H	2.13156806029150	1.37479839874141	-1.06404889276589
C	0.18707651845529	1.59254802250550	4.30672614425959
C	1.44819448775140	1.05313234013266	4.65631855056657
C	2.14255807019044	0.33936010030997	3.65224101031675
C	1.56553287318304	0.20953030924795	2.40052271036584
C	-0.30274120797991	1.39887624588981	3.02771680165964

H	-0.40029537215610	2.15006091453566	5.03728038509578
H	3.11544891686304	-0.10899439363013	3.85639485816213
H	2.08001202782997	-0.34728915507545	1.61349881242535
H	-1.27813786604913	1.80036973867511	2.73947414252847
N	1.97527944096832	1.23059752167833	5.89543694516585
N	0.37112965649323	0.72667543148195	2.07896468552976
H	2.82903998817154	0.75986475104621	6.16729950297582
H	1.42820704554259	1.65565297858064	6.63328549923508
N	5.10851668053464	-4.19118209169691	-2.50879980023860
O	6.21956504003390	-3.69091271004380	-2.33058642499193
O	4.88390853378217	-5.27467541186215	-3.04641057365505

4c′

P	11.97426706867623	-1.09402069795770	20.49172418589573
N	13.25721272354981	-0.84718560348265	21.58613798317315
N	11.55320820323638	0.15776869403876	22.82562211440796
C	12.17680068479908	0.29858515891464	19.34161961443412
C	13.11029639709717	1.32849082880446	19.53416104867441
H	13.78380225252347	1.29585632653203	20.39067958938691
C	13.17575979295295	2.38514511706231	18.62668215148335
H	13.90585332185607	3.18236718139886	18.77226660974605
H	12.36129612051727	3.25227057493477	16.82311311800825
C	12.30812372183962	2.42322917892941	17.52976242301672
C	11.38647145352576	1.39270653344670	17.32648043210315
H	10.72059896493380	1.41512424573509	16.46329020135212
C	11.32984839834610	0.32551769493346	18.22232562617363
H	10.62171807619487	-0.48908231922285	18.05370994771427
C	10.67896768937162	-0.43465096613041	21.84925551384870
C	9.54495863766335	0.44204576889131	21.38010828742883
C	9.85209606227958	1.69420240541505	20.81732054673732
H	10.88928470445982	2.01419896680430	20.73593924906855
C	8.84179146287977	2.53800568792116	20.36297762383120
H	9.10599623399188	3.50300752167496	19.92996663589067
C	7.50273537661547	2.15210703378322	20.45881450237888
H	6.71268740261295	2.81099739045858	20.09797064789996
C	7.18471559539467	0.92178815661979	21.03282754164727
H	6.14293061838975	0.61575081183901	21.13275937185573
C	8.19567329490283	0.07617834523441	21.49529069721323
H	7.90620179274082	-0.86619557962292	21.95864283628605
C	11.10969737996255	1.23364670924884	23.71815142887977
C	12.89446059608923	-0.23452524742311	22.67051286859862
C	13.88375270665693	0.02137089021052	23.74142751878856
C	15.21800377092577	0.25296151896390	23.36547980995110
H	15.47291784424502	0.26253770079649	22.30655886610893
C	16.20004549243093	0.44977863540155	24.32958860197998
H	17.23787156002347	0.64029398164741	24.06211718104540
C	15.83720645939969	0.39386567305860	25.67397776282789
C	14.52923511086552	0.14454598072174	26.08033923350928
H	14.29972137148678	0.09416006381395	27.14311253053601
C	13.55264371728692	-0.03628214836570	25.10558044414703
H	12.52969333371187	-0.23928900100797	25.42076813334540
H	11.98030214532509	1.79774560759981	24.06487793137991
H	10.44733624932060	1.91543463881040	23.17242557685371
H	10.55930491200399	0.85495779360806	24.59435027074699
C	9.09622686640884	-3.86695022525574	21.96015979676752
C	9.19367511833974	-4.23486067850561	23.32687022482502
C	9.78983654682696	-3.29111652996371	24.20190321053759
C	10.24094584625840	-2.09008447509382	23.71377836299504
C	9.57861123244953	-2.65434195162357	21.53895058117820
H	8.65482182702296	-4.54221587697068	21.22810999725392
H	9.90422554402183	-3.50619680922583	25.26362994690662
H	10.71559481452874	-1.35038006716274	24.35065319449369
H	9.53963523094311	-2.34727412687217	20.49701310852966
N	8.74400779895571	-5.42373365950170	23.77052034704591
N	10.13863840761414	-1.76361455279573	22.40259330314075
H	8.83052829879957	-5.69002993405401	24.74419481644889
H	8.33607137160756	-6.10161727152578	23.13766278015773
N	16.88271264740620	0.59941176834072	26.71362524245848
O	16.52548724974542	0.53075358478525	27.89068235183605
O	18.02787460798504	0.82282608138486	26.32213608706884

TS4 Y=NO_2

P	0.04038027409177	-0.99434830909691	-1.51048002830343
N	1.38429088361770	-0.92656236728847	-0.44192600747832
N	0.14640378555825	0.89810175309453	0.26055466935925
C	0.51722034448471	0.69233069507487	-2.55486363907749
C	1.65562899839744	1.48438025892072	-2.37785618121710
H	2.25440646502321	1.41095184933791	-1.46959993964452

C	2.04605423587202	2.36944868049163	-3.38494586765946
H	2.94404899132940	2.97422496019898	-3.25369697060760
H	1.59471635920085	3.17356960540564	-5.33758516864249
C	1.28894799700742	2.47919382085285	-4.55453659745775
C	0.13902521530021	1.69972089801751	-4.72107426763136
H	-0.45192940822576	1.77994796500546	-5.63402213376478
C	-0.25438093792642	0.81475324073463	-3.72025234343801
H	-1.15095643321955	0.20601005392193	-3.85314504859981
C	-0.63182852916378	0.52160072004896	-0.80483746299624
C	-1.92102262628318	1.16537992018634	-1.09569150229669
C	-2.02032950952213	2.50403766359785	-1.51070448165044
H	-1.11667220792521	3.09512240849458	-1.66016075315082
C	-3.26789862053403	3.05784147293172	-1.78372348937326
H	-3.33760205129736	4.09203726095759	-2.12160009772949
C	-4.42696775193154	2.28816473724617	-1.63581199363730
H	-5.40222595439417	2.72641267692997	-1.84960437490724
C	-4.33419790950176	0.95753720620822	-1.22394956127466
H	-5.23527722152783	0.35424278150123	-1.11091892401652
C	-3.08571007195374	0.39127681603064	-0.96470350609091
H	-3.00814561888368	-0.64553929952038	-0.63764721387377
C	0.03477576634475	2.21833854526733	0.89389775230015
C	1.26097821043822	0.03688850244935	0.41370244053780
C	2.22495794498517	0.21788367202775	1.51854608356500
C	3.59645663902681	0.15359658381828	1.22865719108694
H	3.91896458962400	0.01399939653292	0.19719139331931
C	4.53383817926976	0.25607087597092	2.25212195849387
H	5.60429060096145	0.22102281511836	2.05728255090687
C	4.07932876447101	0.39923926154517	3.56081480846713
C	2.72440299630459	0.43568914961964	3.88080716918186
H	2.42242197038834	0.52544073247884	4.92280251532502
C	1.79344576597772	0.34877422900549	2.84951547868101
H	0.72890788160644	0.34771379931398	3.08754563282871
H	0.57938344886796	2.21788114171103	1.84008912596310
H	0.46527392820049	2.98819039970248	0.23764885783138
H	-1.02094528563284	2.44591923080360	1.07529458799860
C	-2.59396888749947	-4.20482935203681	0.19247354942515
C	-2.12253346545644	-4.58267992992604	1.47245073362714
C	-0.98950922939506	-3.89337921447538	1.96691229596156
C	-0.41029912157412	-2.90000807681451	1.19998755715381
C	-1.94361672755458	-3.19823279852940	-0.49514378727731
H	-3.45151607832565	-4.70729230409777	-0.25630418394901
H	-0.56412375867227	-4.14796523557089	2.93833962360219
H	0.48145434108767	-2.37711439193197	1.54974874991098
H	-2.27465777858152	-2.90524799026536	-1.49590636945610
N	-2.72992290677960	-5.55791017726290	2.19329318498340
N	-0.87637545123409	-2.53530474550895	-0.01058211784549
H	-2.33602187051704	-5.87846176081071	3.06875467226788
H	-3.48500664698067	-6.10324818683329	1.79729021024769
N	5.07802104682829	0.50508642600697	4.66231027609210
O	4.63911078075105	0.62023571589965	5.80684574983551
O	6.26650565547685	0.46986621750807	4.34639519409395

5c′

P	0.67569344852194	-1.22335015820291	-1.29259014946890
N	1.83203539682205	-1.08748375493333	-0.07980707517856
N	0.71628280306265	0.91222841452526	0.28319304898583
C	0.64969644369478	1.28126016349853	-2.16660812657578
C	1.67138021410350	2.22919849016885	-2.02153838117637
H	2.03570807925510	2.50513457041602	-1.03372401486783
C	2.25403743759164	2.82640746828174	-3.14131795670794
H	3.04496194214850	3.56437156291142	-3.00433261018744
H	2.29184791742939	2.94514637197248	-5.29807912945250
C	1.83464027831478	2.47869261572276	-4.42521954267269
C	0.84060834550733	1.51034928482355	-4.58491785181686
H	0.52331589776826	1.20810295413619	-5.58331016605461
C	0.26472151575201	0.90968340109570	-3.46736918937927
H	-0.48177176691328	0.12724936993253	-3.61270340466458
C	0.01266400288395	0.57550101572092	-0.96631979375880
C	-1.48638050769807	0.72427522538780	-0.78956465540653
C	-2.31959332414621	1.28320788488023	-1.76724204421727
H	-1.89262059851358	1.67650073329085	-2.68805454006618
C	-3.69970728351441	1.36578412390035	-1.56540842028587
H	-4.32736629854351	1.81010355547587	-2.33869127692704
C	-4.27165613522740	0.90356850247131	-0.37975892864048
H	-5.34808527375096	0.97760065136748	-0.22252065936645
C	-3.44778052997067	0.36943491029296	0.61480356794115
H	-3.87687655484570	0.03098055996154	1.55892599090510
C	-2.07314689766852	0.28218220707780	0.41085248949019

H	-1.44258509976572	-0.12635109636025	1.20154841530025
C	0.43993650919369	2.19830421296976	0.92557956574183
C	1.68060130402084	0.02066588814333	0.63033674562105
C	2.56780353893133	0.24286539255334	1.79347318311022
C	3.93627571489714	-0.03362165871630	1.64046244794478
H	4.30572430900976	-0.36849475082956	0.67204834683635
C	4.80558784722964	0.11749884162430	2.71622232225009
H	5.87288598366225	-0.07557483595330	2.62350999009488
C	4.28504406502099	0.51937528239276	3.94439148108383
C	2.92901595046800	0.77337764383763	4.13209064975677
H	2.57050319435782	1.06792584557229	5.11673453669533
C	2.06930259900635	0.63988963921151	3.04522426027326
H	1.00384537379147	0.81999874832617	3.18525210094068
H	1.34089177767811	2.56765400549087	1.42723509706543
H	0.13683486237983	2.92061543433295	0.15878955668464
H	-0.37681222827381	2.11812161793104	1.65711221227524
C	-2.72907056747071	-3.27889764708310	-0.38378834388511
C	-2.54961344632150	-3.75899465355013	0.93897192597136
C	-1.32037721672574	-3.45218479362252	1.57892644164939
C	-0.37039791166751	-2.70968637352757	0.92077814679404
C	-1.73224418851083	-2.55136853711986	-0.98189190804398
H	-3.64653096227218	-3.48272094550190	-0.93465740138516
H	-1.11461166906579	-3.80588811389527	2.58910113650522
H	0.59465983590114	-2.45338816365343	1.35805760722922
H	-1.82765524121545	-2.17094261323113	-1.99937024202850
N	-3.50588519883102	-4.47723516227587	1.56099199097345
N	-0.57019783479659	-2.25845415356440	-0.34292477705640
H	-3.35858185798704	-4.85632226966254	2.48881349395170
H	-4.36670350611364	-4.72612909382417	1.08849841155775
N	5.20875006299448	0.67369366408590	5.10324603231159
O	6.40034583150930	0.43827830456031	4.90636123945803
O	4.71166873690182	1.02504531716325	6.17390158387240

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P	-0.17654108832808	-0.53293832036996	0.89321475924637
N	-1.07890444985458	-0.25126508717020	2.35122382296477
C	0.75875485196879	-2.03583237534946	1.36019938125695
C	-1.72785301902202	-1.01833542236136	-0.05899732230103
C	0.70201135062976	0.95224946229382	0.64156561898176
C	-2.29709069453553	-0.67373318547264	2.21738777247513
H	1.82917793882072	-1.83577605990798	1.23635522103753
H	0.54603414309920	-2.28586806975890	2.40743207441820
H	0.47743332730347	-2.87455485109674	0.70961567673817
N	-2.71008556736517	-1.21680150463216	1.01071202351166
H	-1.52750274996026	-1.97229884004221	-0.57088989903213
C	-2.13989046839920	0.05937780571142	-1.06185175155116
C	1.38733676628036	0.61384553322598	-0.54335563907364
C	0.43436483132205	2.27075149214995	1.29799466553779
C	-3.27845469680888	-0.61677853133598	3.35462219020167
C	-4.09439596902219	-1.49998639858844	0.67611993071203
H	-1.30961906426025	0.23184776219198	-1.75763515089807
H	-3.02976364863426	-0.23948940298633	-1.63586010557501
H	-2.36231029958600	1.00456999666446	-0.54600189062069
N	0.91746285477644	-0.56837452005028	-1.00078735831644
N	2.39665339548318	1.32709868499161	-1.16107404966619
H	-0.07997087537874	2.07878616550765	2.25141960216852
H	-0.26263849668569	2.88866042602624	0.69279760940447
C	1.69206498847819	3.10792574617304	1.54533242155293
H	-2.77302175423652	-0.18877577579024	4.22541400560164
H	-4.15194895745767	0.00423253571166	3.10448785471114
H	-3.65050985389028	-1.61953967850356	3.61415446234915
H	-4.12729464381694	-2.22364696808393	-0.14971057494575
H	-4.60962787376029	-1.94586790652953	1.53564830894947
H	-4.65683345439766	-0.60235287045878	0.36051697360145
C	1.73933921802678	-1.36119006326782	-1.89242529161328
C	3.19653940346318	2.28571771430356	-0.39540415125454
C	3.17691787731900	0.64911925582050	-2.20579019201516
H	2.36586558330369	2.56475929191758	2.23053752078612
H	1.40712094081299	4.04564978365771	2.05107187659567
C	2.45035322503629	3.45105618600942	0.26069904195009
C	2.37721317296627	-0.43056159514232	-2.92577243977950
H	1.11034978932401	-2.11705764812858	-2.38716603540882
H	2.53971931616918	-1.92129086652854	-1.35753696728782
H	3.92028220063289	2.70323940337654	-1.11234089483679
H	3.78702228153315	1.75303472494157	0.37943923893070
H	4.08165188030357	0.18936073234476	-1.75561066744268
H	3.52959937841217	1.41402556801457	-2.91689295905645

H	1.76438667687666	3.90200353565104	-0.47736197777413
H	3.21100474703091	4.21611839962889	0.48866276649425
H	3.04639522862791	-0.97745690503437	-3.60798629682908
H	1.58119969200591	0.03163631511966	-3.53054162678232
O	-3.23937111705550	-3.21012733956871	-2.62676311846665
C	-2.12633788892420	-3.57658296590048	-2.61515754868689
O	-1.01628842862683	-3.94858336937415	-2.60371091096340

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P	-0.18833072168695	-0.51244592977054	0.90118258985964
N	-1.08915568106545	-0.22776700301455	2.35620869101841
C	0.74042800411295	-2.02382197871380	1.35365141114146
C	-1.73273644943172	-0.99602819101002	-0.05603143093750
C	0.71017243510870	0.95817028494125	0.64294165841168
C	-2.30533518390678	-0.66094150502720	2.22227566723086
H	1.80845161573396	-1.85166758492935	1.18023582664881
H	0.56543698812103	-2.25267861888588	2.41280429617721
H	0.40899206800510	-2.86623930117571	0.73102315709768
N	-2.71362048607024	-1.19890707061280	1.01496834007789
H	-1.52196892514980	-1.94721226757076	-0.56482341375584
C	-2.14869371685575	0.08315362754369	-1.05382765098989
C	1.38895540063130	0.62066794197528	-0.54766553059165
C	0.45095021631772	2.27907560395390	1.29942297896181
C	-3.28221639069848	-0.61502081801494	3.36407064180928
C	-4.07882074183083	-1.55663110039891	0.68440752401011
H	-1.32409394284065	0.25163639075735	-1.75706505011395
H	-3.04235670784893	-0.21426427925682	-1.62297197781122
H	-2.36610787320908	1.02917823889749	-0.53693206238793
N	0.91316558781694	-0.55235726185100	-1.01578491961258
N	2.40003207530431	1.33778951059685	-1.16109703094329
H	-0.07166714569409	2.09048350365482	2.24901942640956
H	-0.23614788228605	2.90436097660077	0.69043578135810
C	1.71399155796725	3.10477911692384	1.55745090101707
H	-2.77844003605565	-0.17680060790010	4.23069592456048
H	-4.16635505895100	-0.00829889624286	3.11662852646629
H	-3.63654961668346	-1.62252971837655	3.63008291209522
H	-4.07481355510463	-2.36522279604737	-0.06096776270769
H	-4.60180162981500	-1.92421905942437	1.57510855674103
H	-4.65766598048147	-0.71318253388483	0.26590761306963
C	1.71329151995241	-1.33092871948333	-1.93588933995629
C	3.21192695415716	2.27838922862275	-0.38559208848893
C	3.17009700859740	0.66835500006079	-2.21834370395332
H	2.38020371833622	2.55242516308658	2.24275584284828
H	1.43399539334833	4.04197993485066	2.06700661366095
C	2.48035381405295	3.44860327016240	0.27808295955114
C	2.35487238089918	-0.38763253211408	-2.95528418299282
H	1.06569689998217	-2.06431967527237	-2.44276822345891
H	2.51008996603349	-1.91851792067936	-1.42488124258899
H	3.94243971876946	2.69213461886482	-1.09779688422910
H	3.79393332482718	1.73177526427338	0.38594771770273
H	4.07028276420277	0.18970718525782	-1.77859937722270
H	3.53074376246788	1.44107670353680	-2.91690743142301
H	1.80173062794627	3.91365244447137	-0.45800019193601
H	3.25017460905745	4.20212674975967	0.51374699284540
H	3.01341039424712	-0.92833929051679	-3.65270445636681
H	1.56036640350226	0.09495535158939	-3.54587099191106
C	-2.12342512532316	-3.67035936834531	-2.59320934251234
S	-0.82543017565713	-4.36218624898959	-2.06994652249506
S	-3.41808140285265	-2.96828353287247	-3.11314109138382

TS Fig.6 (Ch=O)

P	-0.44941735455773	-0.71678792622076	0.84689428109761
N	-0.93853723773119	-0.23248425751349	2.40267967938329
C	0.38051412064620	-2.32082471724074	1.00377660722597
C	-2.21805620127708	-1.14376891515556	0.29766703514442
C	0.44469214396180	0.47882071988545	0.04654616008636
C	-2.19862749374388	-0.53307448316795	2.59201117774047
H	1.41241381272820	-2.16234809194670	1.33819658768559
H	-0.16411920886381	-2.90885393790769	1.75552453928651
H	0.38029869906086	-2.82881002898141	0.03474240116606
N	-2.93143300470808	-1.10215594683173	1.58142623682666
H	-2.23330169100243	-2.16533493369379	-0.10988070055744
C	-2.77423967576338	-0.14963909635068	-0.72155212577873
C	1.44932669600909	0.06519037171105	-0.90349515225911
C	-0.00334474663422	1.92517437592621	0.18459364941146
C	-2.84783973968451	-0.27148290321919	3.92020820626927
C	-4.36249407628759	-1.34852681750788	1.62161284890767
H	-2.08294831668354	-0.04763712042342	-1.56773588025956

H	-3.75093878835467	-0.46799906656470	-1.11393457831101
H	-2.88626170427269	0.84755576468871	-0.27299528767650
N	1.32061580530891	-1.04781450559233	-1.60131507042808
N	2.55576816936663	0.89899595961280	-1.03209758814214
H	-0.98410729730898	1.94939594954776	0.68617411233752
H	-0.16926952771285	2.35947303266432	-0.81937694191761
C	0.93571664469662	2.84840765651438	0.97686383977782
H	-2.10615125697018	0.18133979971167	4.58429013201011
H	-3.70661271991336	0.40842722257553	3.82009940163721
H	-3.21271909833962	-1.20387833781673	4.37645258674274
H	-4.69239151534164	-1.50733904387894	2.65427182664866
H	-4.94533945786355	-0.51564965464066	1.19244123609431
H	-4.59179223045271	-2.25860547878431	1.04858300030724
C	2.48388893214239	-1.43315249054942	-2.38939088687224
C	3.03276946995054	1.70504587279965	0.08880432283605
C	3.44505853418838	0.82750289899928	-2.19274114615043
H	1.07190103608988	2.42095105789526	1.98445927727971
H	0.45406818585102	3.83274937389155	1.10578821775123
C	2.30071155791015	3.03295166982773	0.31661628273493
C	2.98156871840906	-0.22701199396952	-3.19095768577117
H	2.20482059891078	-2.26396258062447	-3.05513909737249
H	3.30720960589871	-1.80852567234886	-1.74497352319048
H	4.09895538927306	1.90477426237699	-0.10211031675262
H	2.97330514358237	1.10222656338719	1.01153951852484
H	4.46416834821880	0.57780681476575	-1.84097402411770
H	3.51024373175931	1.82185809726908	-2.67234165581779
H	2.19351081315875	3.55457068048654	-0.65018041237198
H	2.93334263264079	3.67397135794141	0.95350534234349
H	3.81024756048702	-0.48023267678426	-3.87040434944741
H	2.14756863680731	0.14932837644136	-3.80193139773680
O	-0.57817494162284	-0.90498060967350	-3.66272510864986
C	-0.60102092137159	-1.77281285975948	-2.86522241402471
O	-0.86354678059463	-2.74282373177162	-2.24429316365130

TS Fig.6 (Ch=S)

P	-0.48252854412797	-0.62348275196573	0.81394958087885
N	-1.01960212034699	-0.08879209625829	2.33994153109617
C	0.37487342318085	-2.19895317640729	1.11014317981665
C	-2.21400603884938	-1.14260699977318	0.26544071690014
C	0.42487445143454	0.58977095839203	0.02617394518215
C	-2.21845184020417	-0.56472421476982	2.56498797017861
H	1.40808785762836	-1.99377589024176	1.41320489148199
H	-0.15160088283647	-2.71109062755610	1.92814427525628
H	0.37437718947395	-2.80919682808825	0.20286827770002
N	-2.87219438370167	-1.26364300312004	1.57997190646088
H	-2.16512350303263	-2.12376552784945	-0.22968197075783
C	-2.90926669188626	-0.11487038708536	-0.62461216575817
C	1.43146588494812	0.11738906271020	-0.87540192144330
C	-0.02401430109905	2.03239723483337	0.15334653285045
C	-2.87987330272398	-0.37367116780936	3.89790744013280
C	-4.25864870110951	-1.69596261172771	1.65671474817402
H	-2.34531153404483	0.03294057031712	-1.55226561983091
H	-3.92344059671525	-0.44429812187012	-0.89320457254556
H	-2.98261686982340	0.85702200479609	-0.11560377332815
N	1.25196595372420	-1.05917417471864	-1.46340071829632
N	2.54990771113709	0.90333819859805	-1.09631450790795
H	-0.96848413671818	2.05855821420480	0.71855039211919
H	-0.25731533896354	2.43273149866140	-0.85044338406402
C	0.96115545358543	2.98257415744076	0.84764789219742
H	-2.21169747786326	0.20947318448105	4.53806083718694
H	-3.84027283822727	0.15318980290409	3.79839435562489
H	-3.08186637100872	-1.34104818040092	4.38197508918983
H	-4.49655449619401	-2.02693004896473	2.67451260734467
H	-4.97049584330604	-0.90314991115239	1.36942392226061
H	-4.40337665573451	-2.54933295828981	0.98069748209258
C	2.37295486316050	-1.63111746813849	-2.18659598602528
C	3.04109692659801	1.81222345730131	-0.05948855664588
C	3.53949942244716	0.54744847374062	-2.11937000053072
H	1.16276873250084	2.60404528228834	1.86389239630768
H	0.48807653452040	3.97251936203887	0.95948244792386
C	2.27944837338849	3.13353104757858	0.09264799882934
C	3.05157922194864	-0.55988618650125	-3.04270403761684
H	1.99155646592658	-2.45823195145912	-2.80613334302140
H	3.11044885507053	-2.07648713032849	-1.48672054024220
H	4.08961700100751	2.02977794285558	-0.31047982540587
H	3.03960649640991	1.28431210048012	0.91220979282409
H	4.46738167997683	0.21919954278927	-1.61191900559800
H	3.79492058091297	1.45395621572926	-2.69491168913024

H	2.10184239067924	3.55973972001888	-0.90925434235087
H	2.93137374088217	3.84099188466882	0.63143294272638
H	3.90513517005968	-0.95864690327926	-3.61218473915920
H	2.32175172042516	-0.16693018893861	-3.76497809339456
C	-0.45201572889974	-0.99515370477627	-3.00354179869806
S	-0.89442040736257	-2.52446297197756	-3.05755361299302
S	-0.52066861624774	0.54131119661940	-3.41470516799208

INT Fig.6 (Ch=O)

P	2.32984264	7.83807868	3.38809588
N	2.21228690	8.57446844	4.97224678
C	3.14692801	6.29614485	3.93162416
C	0.45345490	7.81074290	3.20382862
C	3.34805398	9.05069991	2.60335838
C	0.97979480	8.62595002	5.36980883
H	3.53630770	6.44504933	4.94452535
H	2.41026790	5.48220380	3.92384512
H	3.95449044	6.03084259	3.23927323
N	-0.02247231	8.17663086	4.53446047
H	0.16468021	6.77548126	2.96598908
C	-0.04929579	8.75346869	2.10724301
C	4.29948479	8.66564743	1.67839099
C	3.11878224	10.50880196	2.95431214
C	0.61329189	9.14959117	6.73010360
C	-1.44473214	8.25681111	4.79439148
H	0.37255284	8.45170545	1.14310857
H	-1.14611353	8.71237281	2.03081275
H	0.24207951	9.79321645	2.31277068
N	4.29483367	7.45753378	0.98070054
N	5.38862326	9.48879841	1.43417198
H	2.15036673	10.58606499	3.46693130
H	3.01717207	11.07755730	2.01152942
C	4.16842277	11.20756975	3.83075680
H	1.53017729	9.46647262	7.23544312
H	-0.07586551	10.00439576	6.66145788
H	0.12200732	8.37591517	7.33955582
H	-1.63302302	8.25431786	5.87385935
H	-1.91148962	9.16074774	4.36397534
H	-1.94854976	7.37791195	4.36391305
C	5.41596989	7.20731403	0.07193440
C	6.07440236	10.11575829	2.56587965
C	6.04260571	9.58450743	0.12626058
H	4.33464076	10.59674589	4.73246251
H	3.76824650	12.17817070	4.16647747
C	5.48301830	11.42742175	3.08936508
C	5.61756778	8.44379802	-0.79520601
H	5.14113975	6.32557181	-0.51475612
H	6.32556570	6.98822634	0.65661527
H	7.11429696	10.28328212	2.24415793
H	6.09724809	9.38579667	3.39348651
H	7.13213856	9.52501870	0.29432358
H	5.84384656	10.56821682	-0.33690734
H	5.33508947	12.12231795	2.24472219
H	6.22406744	11.89403309	3.75912398
H	6.38262019	8.28427184	-1.56888167
H	4.67082658	8.66781711	-1.30923497
O	2.14130261	6.90721554	1.60609435
C	3.09372947	6.69414920	0.75298930
O	3.05118030	5.90553023	-0.18885752

INT Fig.6 (Ch=S)

P	2.16628038991809	7.85933832198408	3.24491915725072
N	2.25688368754827	8.41211567325027	4.90289263061032
N	-0.03279717151812	8.18734187052226	4.66412295370802
N	4.30966989956606	7.51162322404200	0.93881627483424
N	5.12537966868119	9.68441891175797	1.17898302333783
C	2.87205019554885	6.19806953254090	3.53482297298552
C	1.07542178745678	8.47657185956057	5.43417720945885
C	0.88329172658287	8.83716900772281	6.87971909880913
C	-1.41445457871004	8.34296468756815	5.07469555506690
C	0.28036898279814	8.00203797496066	3.24824711533765
H	-0.10973613392390	7.03119717226266	2.90146252375492
C	-0.25740145685116	9.13362243300890	2.36846072334508
C	4.15550965216400	8.76113984798788	1.57195740236201
C	3.19694757078329	9.09617149448600	2.48793136593050
C	2.98246420792515	10.53194069935425	2.91602208787354
H	2.06356071336013	10.59014565255010	3.51374618603074

H	2.81300405368488	11.14006745683831	2.00918657106266
C	4.11748597385368	11.16921312761358	3.73667416561620
H	4.38822534060041	10.48176515244967	4.55400454903804
H	3.73752819385098	12.09073365901078	4.20668852807824
C	5.34480622970704	11.51580418345390	2.89608936174652
H	5.07254529678526	12.26016922355866	2.12844384568949
H	6.11392777099589	11.98019516942772	3.53502156428736
C	5.97431181893458	10.30640196001900	2.20195809587440
H	6.90375845536523	10.61604943901996	1.70248662960565
H	6.24906620322483	9.55501760999765	2.96576085172365
C	5.68835923458999	9.45575355541981	-0.15642508967636
H	6.34060596567864	10.30321846933075	-0.40401281098133
H	4.85433282760368	9.46788183402246	-0.87301072649965
C	6.41821337342043	8.10329290446400	-0.25386108159425
H	7.48211810358125	8.19501512105756	0.01219804788489
H	6.35698130280665	7.71917426490471	-1.28203436519093
C	5.72522818066630	7.14687365819027	0.72351135906218
H	5.73873847678380	6.11407986118394	0.35975162388888
H	6.20843675683321	7.19353317572222	1.71204921728862
C	3.29107135911850	6.79656067106322	0.28557586667541
H	0.15832361503303	9.05359158078847	1.35626316739492
H	-1.35281806500851	9.07909532014575	2.29162375251021
H	0.01165642784727	10.11475948141799	2.78283762896930
H	-1.50324033460307	8.20713438791154	6.15818780362430
H	-1.83013206851871	9.33119290876034	4.81073548841336
H	-2.03150146377040	7.57279099775402	4.58818660173559
H	1.86541543763355	9.03424511511890	7.31904907205226
H	0.25033535808005	9.72966315110692	6.99329228973658
H	0.40392570311952	8.01726698303284	7.43566089072809
H	3.41673651655306	6.22517780541422	4.48654025376535
H	2.03703384195922	5.48807687407014	3.60054747365919
H	3.52221416909094	5.88764287100611	2.71245781943173
S	3.65544697523077	5.75825960539311	-0.97595276495358
S	1.68689184793819	7.03159000777104	0.85457541865682

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P	9.89003973144595	6.73752356282169	19.74971269344028
O	10.67741482880614	7.81970303739321	20.40794207564287
N	9.09324513112549	7.09655986795324	18.30778151923514
N	10.63688530018954	5.51288234670121	17.59045077023139
C	8.65309792627064	5.98797323498552	20.84656262885917
C	9.63867466220471	6.42178795392565	17.32853738275853
C	9.18509564284533	6.64062889873705	15.91420597167686
C	11.28912551778143	4.65790379261434	16.61998623897053
C	10.93006143408124	5.35028055854975	19.02091060518697
H	10.53743250205910	4.37256847133448	19.35743360308715
C	12.40807591999178	5.47503383380493	19.37777224334487
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H	8.79804883076541	5.71494576060060	15.46362846699431
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H	11.05521741989726	3.59543967187322	16.80828235858221
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19’

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18

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20

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H	8.32225994680258	-0.61925102455971	9.82564103180881
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3a’ + DBU

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C	6.63503575482191	9.88305886231621	19.25888301615113

C	6.81223609438377	11.40861763007211	21.26273424863955
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C	5.93827722455568	8.03096110851742	20.27734046598311
C	6.18548203133619	7.88484580560724	17.77675040854928
H	7.08144728773893	8.09865591228071	17.18452118460297
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C	5.45205315429465	11.54980022998254	15.78647571791581
H	6.25344296396885	11.14602438207638	15.16696384296058
C	4.29324007108689	12.06709617700588	15.21022769760646
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H	2.61078218031718	12.98223851998977	18.04025309131853
C	4.55349114932749	12.05303845766864	18.00494306603024
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C	8.31995243683480	12.30117894583931	18.42241250279340
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C	7.45277173120482	14.23435346670311	17.03899724519231
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H	-6.40931968097045	2.09287992213016	-3.35482415789819
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C	1.85600383094148	-0.22829340350214	1.69366720617761
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C	1.32226199230779	-1.42858924863441	0.95668067556196
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H	0.48676798228586	-1.08880983926666	0.33589708886528
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H	0.30626468317913	-2.12602290917197	2.74444053602492

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H	3.90233235825031	0.25822153507179	4.16912744706165
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H	2.70026419593769	-2.35375507090538	4.13189227035605
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INT1

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N	6.78426083034724	9.76564374481037	20.00312623950684
N	8.97489817292785	10.76963074509273	17.42098034774759
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C	7.12506640042278	13.27846358290651	20.78162811723269
H	6.33300508380696	13.78531010834972	20.21822561890437
C	6.78578288374149	11.02760226626185	21.81168164453578
C	6.68319848002550	9.73826409799542	21.37596159266433
C	6.71437073621716	8.56772983182757	19.16425300801940
H	7.49031283737310	8.60904535370469	18.39276313355839
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C	5.52867081948987	9.68008867954268	14.78921627431098
H	5.77055736472428	9.30806188078254	13.79309844426565
C	4.20659218343081	9.64617642416114	15.24580203550467
H	3.42062636058598	9.24393215903761	14.60593685517605
C	3.88575823182200	10.14356253128767	16.51307679020518
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C	11.26624983009460	11.43921382891827	16.81813549390520
C	11.52299011645478	10.50737219281812	15.79710896303295
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C	12.83257948731624	10.15112408963419	15.48133700219644
H	13.02526173943864	9.44846832843963	14.66966940663921
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H	14.92778797148155	10.45120077501572	15.92508085344253
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H	14.48906836654429	12.10442253564920	17.73387503656064
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H	9.39126298558412	14.81021670521491	16.17944603896296
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H	5.73203990548628	8.49039848853645	18.68292813548372
H	6.54740798302153	8.81516361196838	21.92690605870757
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C	11.56939422134334	8.53410603073870	18.78765102482167

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H	11.19186163383484	9.06255345459043	19.67276324780554
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H	12.21134481611317	4.79358375006137	16.00764091467153
H	11.21980127074188	5.75524361261644	14.91546503268347
H	13.33911370457818	6.79072600517494	17.37679163159997
H	12.64745915545717	5.33086266604662	18.11088330337297
H	10.03032697645201	4.09642413574124	17.21709321058945
H	10.33132058297013	3.41687009117106	15.62025660257337
H	13.02687080870245	7.25887730918068	19.75673194068537
H	11.38068501208616	6.60527202577201	19.74376003213296
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C	-0.53327617280807	2.97029744242613	-0.38846200983640
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C	-2.65647880499614	1.21433936613467	-2.38575260275443
C	-3.67566940532725	0.76621923242832	-0.21679524719603
N	0.65217969299230	3.01600211799295	-1.03268530225611
C	-1.20938531668834	4.12966112488952	0.15670656329912
C	2.41258646683448	1.52584588527212	-2.08943971458911
H	-1.77257995543437	1.41705861736778	-2.99151259483395
C	-3.91234073205829	1.12738586800330	-2.98632666939257
C	-4.93000584226138	0.69407999241111	-0.82558053920375
H	-3.57789867094451	0.62052358195002	0.85995849221313
C	1.27715501635789	4.26300567896518	-1.51235973684015
C	-2.61437028219936	4.23275544645094	0.04274450514712
C	-0.49979896309928	5.13996551052817	0.84672273360067
C	2.50532111277671	0.52820007995899	-3.07851670070965
C	3.57275685745715	2.21577965443457	-1.69129250625079
H	-4.00823221562290	1.26458441206875	-4.06387721633410
C	-5.04768773118118	0.87549734553338	-2.20710492083762
H	-5.81598223231012	0.49764515195612	-0.22111855390814
H	1.75472252349339	4.06088067206116	-2.47600453485582
H	0.49402650616248	5.01883108556279	-1.63074722984358
H	2.03037457576144	4.63372017023542	-0.80815151587408
H	-3.17027312052824	3.47180952185324	-0.50120451430045
C	-3.27908382959277	5.33184531554661	0.57497126400421
C	-1.17810124566958	6.21846725814679	1.40191010333856
H	0.57644413125549	5.05133386686533	0.99265016165742
H	1.60494741847850	-0.00651872452253	-3.38037405355191
C	3.73032991284669	0.24801808886923	-3.67573204477891
C	4.79840657975961	1.91924969483505	-2.28297388393432
H	3.53305101244713	2.95899259474275	-0.89531982620025
H	-6.02840714883838	0.82009725891343	-2.68063261051142
H	-4.35899388225666	5.41978405794439	0.45597580331483
C	-2.56641225341426	6.32312863135986	1.25820339509329
H	-0.62587202114430	6.98052965067845	1.95189948480453
H	3.79166010319771	-0.50904468269890	-4.45768075225077
C	4.87841953846889	0.94271410315425	-3.28044266683745
H	5.69516296629357	2.45089343153917	-1.96442203187621
H	-3.09336180945165	7.17802913905206	1.68293352034056
H	5.83714525987661	0.72443716554490	-3.75167616516122
H	1.44234724527898	-0.75631819062636	-0.50548174467542
N	2.14305028779120	-1.33724548575967	-0.02996985248189
C	1.92403687499188	-2.67584573472560	-0.02398661996125
C	3.28917921485100	-0.69587141995394	0.59701179507851
C	0.76289495536211	-3.12335763894889	-0.74306771816449
N	2.73804523996697	-3.47057360081752	0.71710398335866
C	3.57315022071983	-1.42671531080369	1.90392854043385
H	3.03614014380723	0.35799827134320	0.77116186896525
H	4.17136047201173	-0.71683737178890	-0.06629503164677
C	0.08278135638803	-4.46249353501523	-0.54491881360446
H	0.72641943271639	-2.71029560784409	-1.75838698644962
C	3.06916092997927	-4.85379017301683	0.28673807754222
C	3.78108779552331	-2.90116891345577	1.59905739342754
H	4.47075596706371	-1.03069713850027	2.39722755069670
H	2.72735815740403	-1.28649297661080	2.59374350982107

H	-0.77700627004933	-4.49119573022071	-1.23194816791091
H	-0.35055509599717	-4.49851267919050	0.47298635850006
C	0.90297130798877	-5.74155280440735	-0.73546733822417
C	1.96502423066737	-5.90250264360115	0.34496716779898
H	3.88653609209192	-5.16919017733444	0.94740511124604
H	3.48321126066515	-4.80579276875304	-0.73532063631394
H	4.76129618554381	-3.04197649628473	1.11182451128499
H	3.79395678320861	-3.49556191454129	2.52500425231109
H	1.37639895035923	-5.74575094220115	-1.73149109183770
H	0.22241655952209	-6.60615945668482	-0.70722727536593
H	1.50016695154387	-5.89728737240126	1.34523684377506
H	2.45840136590681	-6.88075171343679	0.23697148232158
H	-0.26985372287261	-2.19744928801002	-0.18452604011617
C	-1.38083954990290	-1.78333073692522	0.37966305547202
N	-2.54794967033190	-2.23723673400541	-0.15503131475366
N	-1.57021814915761	-1.84453125883262	1.72747086381062
C	-3.46449375287500	-2.53484266426659	0.83576344221190
C	-2.79540160819932	-2.35517393913973	-1.58740046005958
C	-0.54919729021161	-1.48989761663127	2.70563397646195
C	-2.84630210645033	-2.28890371140461	2.02816970520888
H	-4.46202500284953	-2.90004332761627	0.62103919918818
H	-1.84823327430267	-2.21404223043173	-2.11666992658945
H	-3.19853118425056	-3.34922675681502	-1.81545587164693
H	-3.50848442545955	-1.58804966617251	-1.91449134188290
H	-0.93666423522838	-0.73732620604445	3.40413636075791
H	-0.23451019982262	-2.37844608451059	3.26797466534839
H	0.30835154468867	-1.07746210752301	2.16375601994679
H	-3.20397314337470	-2.40366948231535	3.04495808998697

INT2 +HLc

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C	8.36166284201990	12.79636875830263	17.48715603937040
C	9.10755216874297	10.87968672223608	16.38497844141196
C	5.31469122231296	12.16519489529179	15.35906309818555
C	4.83784844561795	13.37775072545634	17.41563244457642
N	9.43752803560028	12.11895142355820	16.82874747397015
C	8.23388200893163	14.24231005710432	17.63780734350719
C	10.06225375533302	9.90883315878333	15.83548713459795
H	5.92101975361687	11.43267122490973	14.82231432878757
C	4.34940906705034	12.92045034005177	14.69316270648613
C	3.89877126579249	14.15423571620139	16.73049910160304
H	5.04172532368208	13.58626241068964	18.46632109451114
C	10.76703113185031	12.72568800534086	16.75853469688381
C	8.54567988731350	15.14076185662576	16.59480951085411
C	7.68710972550334	14.77781985891477	18.82164673118830
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C	3.64929845161341	13.92537767279359	15.37410027720820
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H	10.66600786236602	13.79865144954027	16.56738243125935
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C	8.34231311503885	16.51073616312129	16.74650716961175
C	7.45559464865486	16.14653000808475	18.96196102520410
H	7.46370807729230	14.10960976640021	19.65858162441199
H	8.65537082129527	9.24012511159421	14.34391286794128
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C	10.01417050309557	10.40880775157203	20.50921654696639
C	7.13129170033563	8.03157218922678	18.39284566161897
C	9.18183662496410	8.19270607838141	19.77245085754304
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C	5.64182204277871	7.87988385191694	18.67468563071497
C	9.88492546526337	8.94282740209187	20.89134215496732
H	10.38656970115015	11.01822737122517	21.34198528829932
H	10.70091724089832	10.53722806310129	19.65660151741224
H	7.60138781221093	7.04174770156023	18.41837562307208
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H	8.92408103350014	7.17481481493024	20.09453702957941
H	5.47538674477612	7.59992112399281	19.72779863048100
H	5.29680555757724	7.02752669722770	18.06981200528352
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C	1.97955262638601	11.19655318720990	16.41515102259364
C	0.69785218060194	12.69938154023100	17.94447980195652
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H	0.13499442702303	13.55830426510359	17.56077402922022
H	0.17516397740179	12.26999530981519	18.80751091145676
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H	3.68108483624219	9.84704990666228	14.99490071572195
H	2.54799988669563	8.46063845925184	14.88435208872397
H	2.54177872032420	9.73335639667470	13.62139393649891
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C	8.14201406126372	12.54863238735229	17.74245939785650
C	8.79355173144326	10.75551819359232	16.34398500400374
C	5.06426712291035	11.99530019906724	15.40717891589093
C	4.58573512880885	13.16697064979993	17.48584251341241
N	9.14142548800261	11.95890750583798	16.85724530503437
C	7.86625263979880	14.00659795197158	17.68144570559466
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